A COMPARATIVE STUDY BETWEEN MM3 AND X-RAY DIFFRACTION OF PHARMACEUTICAL COMPOUNDS.

by

STACY MARIE DEGUTIS

(Under the direction of J. Phillip Bowen)

ABSTRACT

MM3 is a widely used molecular mechanics computer program used to calculate the three dimensional structure of molecules. It has been parameterized for several individual classes of functional groups. This paper examines the accuracy of MM3 in calculating the structure of compounds that contain multiple functional groups. The calculated values from MM3 will be compared to data from x-ray diffraction, a commonly used method of determining molecular structure. The number and type of missing parameters will be examined. The accuracy of MM3's calculated values will be compared to the values measured by x-ray diffraction.

Based on the results of this study MM3 is fairly accurate at calculating complex molecular structure. Certain properties specific to the solid state such as molecular vibration and intermolecular forces must be accounted for in order to improve the accuracy of MM3 in calculating solid phase structure.

INDEX WORDS: Molecular mechanics, MM3, X-ray diffraction, Crystal, Parameters, Torsion angle, Bond length, Bond angle.

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CHAPTER 1

THEORY

Drug development is a long and involved process often taking find years to bring a single product to the market. Determining the three-dimensional structure of the drug molecule and lead candidates is very important in understanding how the drug binds to its receptor. Usually, the most important bonding forces between a drug and its receptor are hydrogen bonding and van der Waals forces. Small changes in the molecule's atomic parameters can have a large impact on the drug' s effectiveness The drug molecule will adopt a conformation in its receptor that maximizes favorable interactions and minimizes unfavorable interactions.[1]

X-ray diffraction traditionally has been used to determine the three-dimensional structure of drugs. The conformational preference and receptor-ligand binding is measured in the solid phase; x-rays have a wavelength comparable to the interatomic distance of covalent bonds found in crystals .[2] The crystal functions as a diffraction grating. The diffraction pattern generated is limited by the amount of long-range repetition between molecules in the crystal. If there is more than one conformation present in the crystal the diffraction pattern may indicate that the overall structure is disordered. The diffraction data arises from Couric interference between all the molecules in the crystal. Variation in intensities of the diffraction maximum contains information on the three-dimensional arrangement of atoms in the molecule. This information is used to calculate an electron density map of the molecule. The map acts as a guide to fit an atomic model of the molecule to the data. The atomic coordinates from the model are used to calculate the diffraction pattern. The calculated and experimental diffraction patterns are compared, and the atomic model is adjusted so that the difference between the two patterns is then minimized.

There are a number of problems associated with x-ray diffraction. One difficulty inherent in the method is that the bond length is determined from the electron density of the bond. Lone pairs or very electronegative groups can distort this length which can result in the calculated bond length deviating from the actual bond length by a small amount. The interaction between a drug molecule and its receptor may rely a great deal on non-bonded interactions and these can vary

greatly with small changes in distance. The electron density map from the x-ray diffraction data represents the averaged atomic distance between electron clouds and not the actual interatomic distance between atomic nuclei. The electron density map from the x-ray diffraction data represents an "averaged" electron density map of all of the molecules in the crystal. Variation from this average may result in a part of the molecule falling below the cutoff limit for noise in the analysis .[3] X-ray diffraction (XRD) cannot accurately determine the position of hydrogen atoms clearly because the electron associated with the hydrogen is usually found closer to the other atom.

Since the molecules of the drug are in the solid state during the XRD their amount of free movement is greatly reduced when compared to the gaseous state. In a gas a molecule normally has 3n-6 degrees of freedom to move (rotation and translation). In the solid state the molecule does not have this freedom and instead the energy is converted to vibrational modes. These vibrational states will further distort the bond length. One way of compensating for this distortion is to remove thermal energy from the system by running the analysis at liquid nitrogen or liquid helium temperatures. This will cause the number of vibrational states to collapse at the bottom of each bond's potential energy well.

The phenomenon of piezoelectricity will also affect the displacement of electrons in a bond. When the electrons are placed in an electric field (like the kind generated by x-rays) the electron cloud will be displaced relative to the positive nuclei. The electron density will then increase between the two nuclei involved in the bond. The nuclei will then be attracted closer to each other and the bond will shorten as a result.[4]

For financial reasons, pharmaceutical companies often try to shorten the amount of time it takes to bring a new drug to market. The problems associated with x-ray crystallography can lengthen the amount of time a compound spends in the development phase. Pharmaceutical companies have been trying to find ways to shorten the development time. One possible method is to use computer programs to model potential compounds to determine their structure. The use of molecular mechanics is one computer-based approach. Molecular mechanics is a mathematical treatment of chemical structures. It differs from quantum mechanics in that it focuses on the motion of the nucleus, ignoring the motions of the electrons. This assumption is possible due to the Born-Oppenheimer approximation.[5] The molecule is viewed as

being similar to a series of masses connected by springs. The energy of the system would be equal to the sum of various physical, chemical, and electronic effects.[6] These effects could be mathematically represented by a series of equations with adjustable parameters. Because of the ball-and-spring assumption these equations would be describe the effects of nearly harmonic forces on the system.[7] Deviations in bond lengths, angles, and/or torsional angles would lead to an increase in the molecule's overall energy. The energies of a system's electrons can be accounted for by careful parameterization and careful formulation of the starting potential energy functions used in the calculation.

The set of equations and related parameters used to describe a molecule's potential energy surface is termed a force field. There has always been a trade-off between the accuracy of the equations versus the computer time needed to process them. Initially force fields used for small molecules have utilized more mathematically rigorous functions as compared to force fields used with large molecules.[8] As computers have increased in computational power and speed the complexity of the mathematical functions used has also been able to increase. Early force fields were more limited in the type of data (chemical, thermodynamic, or vibrational) that they could generate without *ad hoc* adjustments. The more recent force fields are now capable of providing this information without making major adjustments.

Molecular mechanics is a rational extension of earlier concepts of the bonding between atoms in a molecule. It builds upon some of the basic ideas used to describe vibrational spectroscopy.[9] Some of the fundamental concepts behind molecular mechanics were outlined in a paper by D. H. Andrews in 1930. More significant attempts to apply the method to chemical problems did not occur until 1946. In that year papers were published by three independent research teams. The first paper was written by T. L. Hill and its topic was how steric effects such as van der Waals interactions, stretching, and bending deformations would affect congested systems. Hill proposed how these interactions could be used to determine information about the molecule's structure[10]. At the same time the team of Dostrovsky, Hughes, and Ingold used a similar line of reasoning to examine the rates at which different halides underwent the S_N2 reaction.[11] The third paper, by Westheimer and Mayer, was the most conclusive of the three. Westheimer and Mayer examined how some of the structural features of a series of optically active halogenated biphenyl compounds affected the rate of racemization.[12] This topic was not as

complex as Ingold's group and was therefore more convincing to other chemists. Because of the complexity of the calculations molecular mechanics was not more widely applied to chemical problems until the introduction of commercially available computers in the 1950s. The early programs were written with specific compounds in mind and were not meant to be applied to a variety of structures.[13]

The molecular mechanics program MM3 was used in this study. It was developed by Allinger and coworkers and was an outgrowth of the MM1 and MM2 series.[14] In this program the total energy of a molecule is assumed to arise from the sum of several components that represent the mechanical, chemical, and structural elements of the molecule (equation 1).

Equation 1

$$E_{Tot} = E_{Bend} + E_{Stretch} + E_{Torsion} + E_{vdW} + E_{Ele} + E_{Cross\text{-}terms}$$

The energy of each respective component is summed over all of the relevant parts of the molecule. The cross-terms component allows more accurate results to be generated by coupling one or more of the basic terms together. Cross-terms are the result of expanding the program's mathematical potential functions into a power series. In the physical structure the two (or more) coupled terms interact with each other to a certain degree.[15]

The first term in equation 1 is the energy needed to stretch or compress a bond (equation 2).

Equation 2

Bond stretching: $143.88\ (K_s/2)\ (\Delta l)^2\ [1 - C_s \Delta l + 7/12\ C_s^2\ (\Delta l)^2\ ]$

K_s: force constant for stretching

Δl: difference between measured and equilibrium bond lengths

Chemical bonds do not vibrate like mechanical springs. Therefore Hooke's law, which mathematically describes this kind of behavior, cannot be used to describe the vibrational behavior of molecules. Bond stretching is better described by a Morse curve;[16] however, this type of mathematical function does not easily translate into a practical use. The majority of chemical bonds lie at or near the bottom of their potential energy well. Quadratic functions overlap the bottom of this well and can be used to describe the vibrational behavior of molecules. In MM2, the power series was expanded out to the cubic term but serious problems arose when the bond length was significantly stretched. At longer bond lengths, the cubic term will dominate, and the

energy of the bond will increase to negative infinity.[17] Visually the molecule will appear to fly apart in this situation. In MM3, this condition was avoided by adding higher-powered terms like a quartic term. The quartic term also gives more accurate values when compared to experimental bond lengths.

In MM3 the function used for angle bending is again in a Hooke's law-type format.[18] It uses up to a quadratic term to reproduce values within 10° of the actual value (equation 3).

Equation 3

$$\text{Angle bending} = 0.043828\ (K_b/2)\ (\Delta\theta)^2[1 - 0.014(\Delta\theta) + 5.6(10^{-5})\ (\Delta\theta)^2 - 7.0(10^{-7})\ (\Delta\theta)^3 + 9.0(10^{-10})\ (\Delta\theta)^4]$$

K_b: force constant for bending

$\Delta\theta$: difference between measured and equilibrium bond angles

For planar trigonal systems like those in a carbonyl carbon a modification was made to the computation. These centers remain flat and the π bonds do not distort out-of-plane to relieve strain. A programming workaround was used to accurately represent this situation: a force constant is introduced between the $C_{sp}2$ center and an imaginary point lying in a plane defined by the 3 attached atoms in the angle.[19]

Torsional strain plays an important part in determining the molecule's energy. The strain is not the result of the van der Waals radii of the respective vicinal hydrogens interacting with each other. Instead it arises from repulsion between the electron density of the carbon-hydrogen bonds. A staggered conformation puts the hydrogens further from each other and therefore minimizes repulsion.[20] This repulsive effect is reproduced in MM3 by using a three-term Fourier series (equation 4).

Equation 4

$$\text{Torsion angles} = V_1/2\ (1 + \cos\omega) + V_2/2\ (1 - \cos 2\omega) + V_3/2\ (1 + \cos 3\omega)$$

ω: torsion angle

The three terms (V_1, V_2, V_3) can be selected to reproduce the energy curve of the respective torsion angle. V_1 is interpreted to be a dipole-dipole term. V_2 is important in molecules with 2-fold barriers found in ethylene. It is a result of either conjugation or hyperconjugation.[21] V_3 is important in molecules with 3-fold barriers. It results from steric factors.

MM3 calculates the energies of non-bonded potentials by using a variant of a Lennard-Jones potential.[22] This function is both simple and fast to calculate (equation 5).

Equation 5

$$\text{Van der Waals} = \varepsilon \left\{ -2.25\,(r_v/r)^6 + 2.90(10^{-5})\exp[-12.00(r/r_v)] \right\}$$

ε: energy parameter which determines the depth of the potential well

r_v: sum of the van der Waals radii of the interacting atoms

Originally a 6-12 potential was used but it was determined that the repulsive part of the function was too steep for organic molecules (Lennard-Jones). Lifson and Warshel determined that using a power of 9 or 10 instead would "soften" the curve and give more reasonable results. In MM3 the repulsive part of the 6-12 potential has been replaced with an exponential. This gives more accurate values.

MM3 must also be able to validly define electrostatic potentials as well. The difficulty lies in assigning a localized point charge to an atom when there is no way to accurately determine the charge. Instead MM3 uses a dipole-dipole formula (equation 6) for calculating electrostatic interactions[23].

Equation 6

$$\text{Dipole} - \text{dipole} = \frac{F\mu_i\mu_j(\cos\chi - 3\cos\alpha\cos\beta)}{R^3 D}$$

χ is the angle between the dipoles.
α and β are the angles between the dipole axes and the lines along which the R is measured.
R is the distance between the midpoints of the bonds.
D is the dielectric constant.

An overall net dipole was determined from the interactions of the individual bond dipoles. This approach works well if the structure does not have any net charges. In this case both charge-charge and charge-dipole interactions must be calculated as well. This can be very time consuming, particularly when attempting to dock a small molecule into a receptor site. These difficulties coupled with lack of parameters have resulted in the MMFF force field becoming the industrial standard.

It is also necessary to add cross terms to the potential energy equation to accurately reproduce vibrational frequencies.[24] A cross term couples one or more of the basic energy

functions together. In theory every motion in a given molecular structure is coupled to every other motion. Realistically two motions that are far apart from each other will have a cross term whose value is very close to zero. When developing a force field for a given molecule usually only those cross terms which are deemed necessary are added. Some examples of cross terms used in MM3 are: stretch-bend, torsion-stretch, and Urey-Bradley terms.

In molecular mechanics it is assumed that the parameters used for one molecule can be transferred to other molecules. This does not mean that parameters can be transferred from one molecular mechanics program to a different program. This is due to the fact that each program tends to use different forms of each equation for each type of potential energy function. The parameters must be determined for each unique combination of atoms. Each atom may be of a different type depending on whether it is singly, doubly, or triply bonded. Add to this the number of elements that can have multiple bonded states and the number of overall atom types increases dramatically. It is possible to have a combination of atoms that do not have every parameter determined. The calculated values in this situation may not be as accurate as if all of the parameters were determined. MM3 uses a subroutine that calculates a "best guess parameter" in these cases.

There are 2 widely used approaches to determining parameters. They are (1) inspection on a trial-and-error basis; or (2) using least-squares methods to optimize parameters to the best fit between calculated and experimental data.[25] Each method has its benefits and drawbacks. Trial-and-error methods are very time intensive but generally lead to better concurrence between target and calculated properties. This method determines parameters by functional group. Least-squares methods have trouble in evaluating the overall performance of a set of force field parameters. Deviations between calculated and experimental values are not equally important for each type of parameter (bond lengths, angles, dipole moments, etc.). Also, the quality of the experimental data is important as well. Different experimental methods will produce data with varying degrees of accuracy.[26]

MM3 must also account for certain types of chemical phenomena that are more accurately defined by molecular orbital theory. Some examples are the electronegativity, anomeric, and Bohlmann effects. These phenomena are collectively referred to as chemical effects.

The electronegativity effect is an effect where the length of a chemical bond is dependent on the electronegativity of the attached substituents.[27] An attached electronegative atom will shorten the bond while an attached electropositive atom will lengthen the bond. The bond distortion can be explained in molecular orbital terms. There is more p character on the carbon in the C – X bond pair when X is more electronegative than hydrogen. This is due to X having a greater tendency to shift electron density closer to it relative to the carbon. The s and p orbitals must be conserved in the hybrid orbital on this carbon. As a result the hybrid orbital involved in the bond will have greater s character and therefore be shorter. MM3 reproduces the electronegativity effect by examining the connectivity of all the bonds in a molecule. When an electronegative atom is present, MM3 shortens the default bond length by a given amount. The amount of shortening depends on both the electronegativity of the substituent and the total number of electronegative atoms attached to a given atom.[28] This effect also affects bonds not directly attached to the electronegative substituent and rapidly diminishes with increasing distance from the substituent.

The anomeric effect occurs in cyclic systems of the type $CH_3O\text{-}CH_2\text{-}X$. In these systems the more stable conformation is the one where the methoxy group is in the axial position.. The axial C-O bond lengthens while the internal C-O bond shortens.[29] One interpretation is that some type of dipole-dipole interaction is taking place between the polar bonds in this system. This interaction can be reduced when the substituent is in an axial position. Another interpretation involves the molecular orbitals. In this case the anomeric effect arises from an interaction between a lone pair of electrons on the ring oxygen and a σ^* orbital associated with the bond to the C-2 substituent. Delocalization of the lone pair electrons becomes possible when the lone pair of electrons on the ring oxygen is antiperiplanar to the axial bond.

The third chemical effect measured by MM3 is the Bohlmann effect. This effect involves the C-H bond adjacent to an atom bearing a lone pair of electrons (ex. alcohols and amines). If the C-H bond is *anti* to the lone pair it lengthens by a small amount and its corresponding stretching frequency is lower than expected. A resonance effect similar to the anomeric effect is thought to be taking place.[31]

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CHAPTER 2
EXPERIMENTAL PROCEDURE

The first step in our study was to select a variety of molecules representing different drug classes and structures. This was accomplished by referring to the most recent edition of the Physician's Desk Reference and to the text Human Pharmacology (3rd ed.). The pharmacology text classified drugs according to what bodily system they acted upon – heart, nervous system, lungs, endocrine system, etc. There are several ways to classify drugs: pharmacology, structure, mechanism of action, diseases, etc. In some cases (such as the nervous system or the drug class antibiotics) the drug groups were further subdivided by specific structural category. For example:

1) nervous system:
    a) antidepressants – tricyclics, monoamine oxidase inhibitors, selective serotonin reuptake inhibitors
    b) pain control – opioid analgesics, non-steroidal antiinflammatory agents, anaesthetics

Another form of classification was by specific drug action on a particular bodily system. Examples are:

a) Antibiotics – bacterial cell wall inhibitors, those that inhibit bacterial ribosomal action, bacterial folate antagonists.
b) Antimycobacterial (tuberculosis) agents.
c) Antifungal agents.
d) Antiviral agents.
e) Antihelmintic (nematodes and protozoa) agents

Once a representative sample of molecular structures was chosen the next step was to locate their respective x-ray crystal structure data. This was done by searching the Cambridge Crystallographic Database. Not all of the drugs that were initially chosen have had their x-ray

crystal structure determined. Of those that were determined, many were discovered at or near room temperature. Even in the solid state there will still be movement of nuclei within the respective electron clouds. The bond lengths in the solid state are labeled r_α and must have a correction factor applied to them to account for thermal motion. These correction factors are often not very accurate because they are describing the average bond length.

The Cambridge data files must be converted to a format readable by MM3. This was done by using the program MEDIT. After the file is converted to an MM3 input file it was checked to make sure its format is correct. The connectivity of atoms in the molecule can also be checked using MEDIT.

Once an adequate MM3 input file has been generated for each structure the molecular mechanics calculations were begun. The default option for energy minimization in MM3 – block diagonal Newton-Raphson – was used. It was faster than the full Newton-Raphson method and more likely to converge to a minimum if the beginning structure is far from an energy minimum. The calculation results were printed and the vibrational frequencies were reviewed to find negative values. The presence of a negative value would indicate that the structure is in a transition state. Molecules whose calculations fell into this category were discarded. Although the torsion driver routine could have been used to "drive" the structure over the energy barrier and then minimized using the full Newton-Raphson method, this approach was not followed due to time constraints.

One class of molecules – the phenothiazene antipsychotics – diverged in the VESCF calculation. This was compensated for by converting the calculation to SCF format where the structure is approximate. The original MM3 input file was energy minimized and the structure output file (*.PUN) was saved as a new input file (*1.MM3). The structure in the new input file was minimized, and the output file (*1.PUN) was saved as *2.MM3. An F-matrix is generated as part of the output file. In the molecular structure data file a change was made on line 68 of the name card. This change was to specify the optimization option as by energy change. Once this was done the file was optimized, and the numbers generated were taken as final values.

CHAPTER 3
DATA

Only relevant calculated structural features of the drug molecule were compared. The salient molecular features selected were the ones thought to be pharmacologically significant – including heteroatoms, or were regions that were either strained or in a sterically crowded area. Hydrogen atoms that were not attached to a heteroatom or in a sterically crowded area were not examined due to the aforementioned problems with x-ray diffraction. Missing parameters that involved non-selected atoms were identified and are listed. The cutoff points for differences between MM3 and crystal values were: 0.02 Å for bond lengths, 5 degrees for bond angles, and 10 degrees for torsion angles. These values were chosen because the amount of energy needed to deform the molecule past these limits becomes prohibitive.

I. Antianxiety drugs

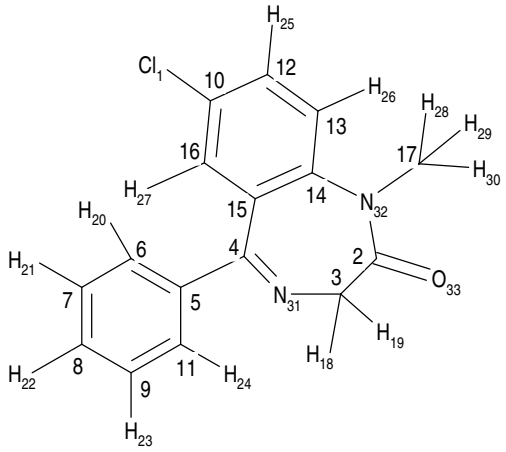
Anxiety is a mental disorder associated with stress. Some of its forms are: 1) panic disorder, 2) simple phobias, 3) social phobias, and 4) obsessive-compulsive disorder. Originally barbiturates were used to treat these disorders but they have unpleasant side effects (sedation, motor incoordination). Benzodiazepines were introduced in the 1960s and are used for short-term treatment[1].

Drug: Diazepam

The missing parameters are for torsion angles involving the far side of the 7-member ring. Both nitrogen atoms and the keto oxygen were part of the torsion angles. A bending parameter for angle N(31)-C(3)-C(2) was also missing.

The carbon-hydrogen bond lengths between C(3)-H(18) and C(3)-H(19) were calculated by MM3 to be longer than the crystal values. The bond between C(3)-N(31) was longer in the crystal than in MM3.

Fig. 1 Diazepam



There were no significant differences in bond angle values between the crystal and MM3. Neither were there any large differences in torsion angle values between the crystal and MM3. The molecule's π-system was nonplanar in the crystal. In MM3 the π-system was determined to be planar.

II. Glucocorticoids

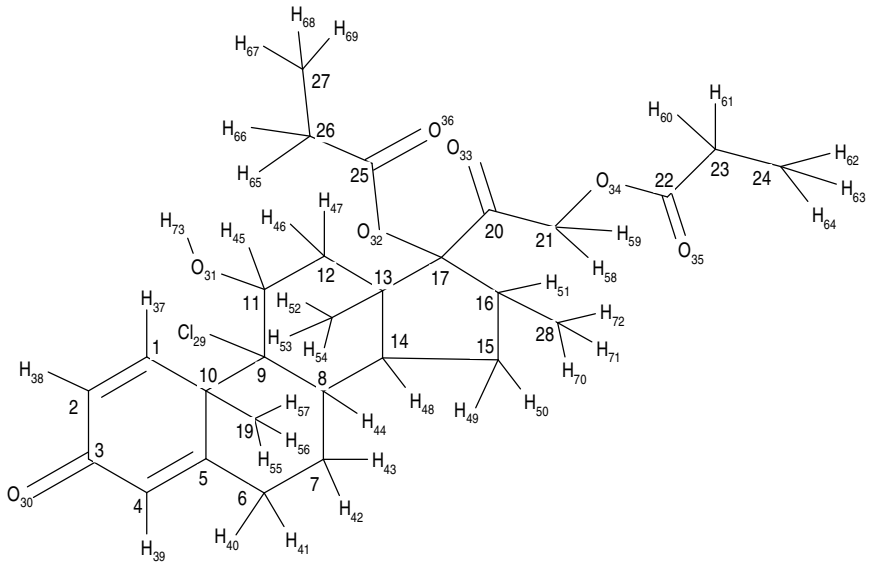
Cortisol, the body's endogenous glucocorticoid, is synthesized in the adrenal cortex. It is involved in the regulation of metabolism, the stress response, selected aspects of central nervous system functioning, and the immune response. Synthetic glucocorticoids are used as part of replacement therapy in adrenal insufficiencies, anti-inflammatory and immunosuppressive action, and the treatment of mycloproliferative diseases. Glucocorticoid receptors are found in many different types of body tissues[2].

Drug: Betamethasone dipropionate

The carbon-hydrogen bond lengths between atoms C(1), C(2), C(3), C(4), C(7), and C(8) are all longer in MM3 by more than 0.02 Å when compared to the crystal values. The carbon-hydrogen bond length between C(8)-H(44), C(11)-H(45), C(16)-H(51), C(21)-H(58), C(21)-H(59), C(23)-H(60), C(26)-H(65), and C(26)-H(66) are significantly longer in MM3 than in the crystal. Some of the carbon-carbon and carbon-oxygen bonds (C(17)-C(20), C(21)-O(34), C(23)-C(24), and C(26)-C(27)) located in the two side chains are longer in MM3.

Several carbon-carbon-hydrogen bond angles are greater in the crystal (C(7)-C(8)-H(44), C(28)-C(16)-H(51), and C(27)-C(26)-H(65)) and less for others (C(9)-C(8)-H(44), C(14)-C(8)-H(44), C(13)-C(14)-H(48), C(17)-C(16)-H(51), C(20)-C(21)-H(59), C(22)-C(23)-H(60), and H(65)-C(26)-H(66)).

Fig. 2 Betamethasone dipropionate



There is a difference of 129.9 degrees between MM3 and crystal values for the torsion angle value for the atoms C(6)-C(7)-C(8)-H(44). The carbons are all ring atoms and the hydrogen is a bridgehead atom. Several of the torsion angle values for atoms C(22), C(23), C(25), C(26), O(34), O(35), H(60), H(61), and H(65) are less in MM3 than in the crystal. These atoms are part of one of the two side chains. The torsion angle for atoms C(22)-O(34)-C(21)-H(59) is also greater in the crystal than MM3. The torsion angle for the chain atoms C(17)-O(32)-C(25)-O(36) is 76.5 degrees less in MM3 than the crystal.

III. Neoplastic drugs

These drugs are used in the treatment of cancer, and there are several mechanisms of action by which these drugs can kill cancer cells. Alkylating agents can form covalent cross links in a cell's DNA, which then prevent the strands from separating during the cell's growth cycle. Antimetabolites mimic the structures of normal metabolic constituents well enough to disrupt the enzymes involved in cellular metabolic processes. Some antibiotics are used in cancer treatment.

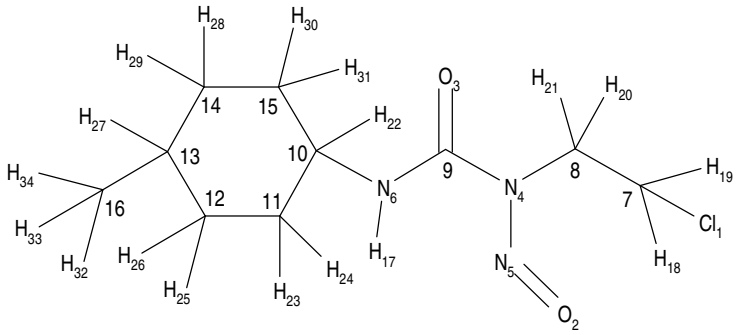
They are believed to function by DNA intercalation, free radical generation, and by disrupting the function of the cell membrane.

Many neoplastic drugs must undergo chemical or enzymatic modification in order to become actively cytotoxic. Neoplastic drugs may also attack healthy growing cells in the body which can result in unpleasant side effect[3].

Drug: Lomustine

The missing torsional parameters are found in the side chain that contains both amide and nitrosamide functional groups. Five of the torsion angles contain the nitrosamide group (O(2)-N(4)-N(5)) or part of it (N(4)-N(5)). One torsion angle contains the chloride atom (Cl(1)-C(7)-C(8)-N(4)). It is noted that only the torsion angle H(20)-C(8)-N(4)-N(5) is missing parameters and not the angle H(21)-C(8)-N(4)-N(5).

Fig. 3 Lomustine



There are stretching and dipole parameters missing for the bonds between the atoms N(4), N(5), and O(2). There are also bending parameters missing for the angles between O(2), N(4), N(5), C(8), and C(9).

Several carbon-hydrogen bonds and one nitrogen-hydrogen bond are much longer in MM3 than the crystal. They are the bonds between C(7), H(18), and H(9) and between C(8), H(20), and H(21). The carbon-hydrogen bond length for the two bonds C(10)-H(22) and C(13)-H(27) is also longer in MM3. The bond between N(6) and H(17) is more than 0.2 Å longer in MM3 than the crystal. The nitrosamide group O(2)-N(5) has a longer bond in the crystal than MM3. Only 4 carbon-carbon bonds have significant differences in their lengths; they are the bonds between C(7)-C(8), C(12)-C(13), C(13)-C(14), and C(10)-C(15). The carbon atoms C(10),

C(12), C(13), C(14) and C(15) are all part of the cyclohexane ring while C(7) and C(8) are in the side chain.

There are 4 bond angles which have values that differ significantly between the crystal and MM3. The bond angle for the group O(2)-N(5)-N(4) differs the most (greater by 10 degrees in MM3). The angle between Cl(1)-C(7)-H(19) is more than 5 degrees less in MM3 than in the crystal. The bond angle between N(4)-C(8)-H(20) decreases between crystal and MM3 values by almost 10 degrees. The corresponding angle H(20)-C(8)-H(21) increases between crystal and MM3 by more than 7.5 degrees.

Most of the torsion angles whose values differ much between crystal and MM3 involve the atoms on the amide/nitrosamide-containing side chain. The torsion angles between the chain atoms C(9), N(6), and H(17) and the ring atoms C(10), C(11), C(15), and H(22) differ by more than 30 degrees between the crystal and MM3. The torsion angles between atoms O(3), N(4), N(5), C(7), C(8), H(20) and H(21) vary by about 10 to 13 degrees between crystal and MM3.

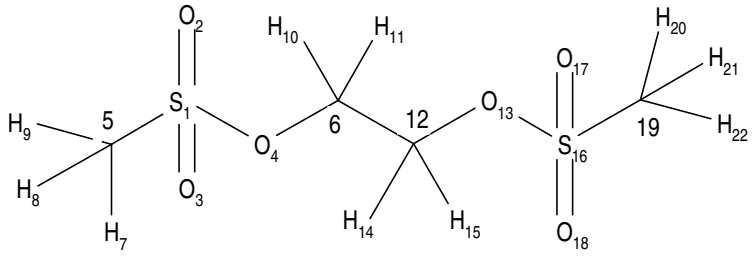
Drug: Busulfan

The missing torsion angle parameters are for the atoms in both sulfonate ester groups. Examples are the torsion angles C(12)-C(6)-O(4)-S(1) and C(6)-C(12)-O(13)-S(16) and the angles C(6)-O(4)-S(1)-C(5) and C(12)-O(13)-S(16)-C(19). Two torsion angles that include hydrogen are missing parameters; they are H(7)-C(5)-S(1)-O(4) and H(10)-C(6)-O(4)-S(1). One stretching parameter is missing. It is for the sulfur-oxygen bonds S(1)-O(4) and O(13)-S(16). Three bending parameters are missing. The angles O(4)-S(1)-O(3)/O(2) and O(13)-S(16)-O(17)/O(18) have the same estimated parameters read in. The same holds true for corresponding angles C(5)-S(1)-O(4) and C(19)-S(16)-O(13) and the angles C(6)-O(4)-S(1) and C(12)-O(13)-S(16).

Most of the bond lengths calculated by MM3 differ appreciably from the crystal values. In the sulfone functional groups two sulfur-oxygen bonds,S(1)-O(2) and S(16)-O(17), are 0.0202 Å greater in MM3 than the crystal. The ester bond between S(1)-O(4) and O(13)-S(16) is almost 0.2 Å longer in MM3. The oxygen-carbon bond between O(4)-C(6) and C(12)-O(13) is 0.035 Å longer in MM3. The carbon-carbon bond between C(6)-C(12) is 0.036 Å longer in MM3. The

carbon-hydrogen bonds between atoms C(12), H(14), and H(15) are much longer in MM3 than in the crystal (by 0.1555 and 0.2321 Å, respectively).

Fig. 4 Busulfan



There are only three bond angles that differ significantly between MM3 and the crystal. They are the two angles between the ester oxygen-sulfur-methyl carbon (O(4)-S(1)-C(5) and O(13)-S(16)-C(19)). The third angle is the one between atoms H(14)-C(12)-H(15).

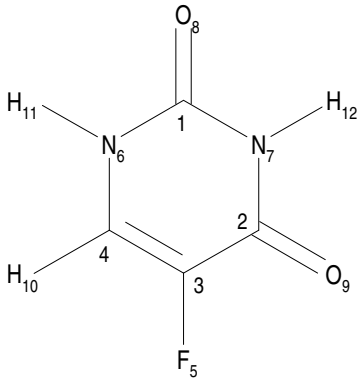
There are three torsion angles whose MM3 values are more than 20 degrees less than the crystal. The first angle is the one between atoms C(6)-C(12)-O(13)-S(16). The next two angles describe the position of the hydrogen atoms H(14) and H(15) in relation to the ester linkage C(12)-O(13)-S(16).

Drug: 5-fluorouracil

There are π-atom parameters missing for this molecule. MM3 substituted π-atom parameters for atom type 2 (Csp^2 alkene) for atom types 162 (Csp^2 in a nucleic acid), 151 (delocalized Nsp^2 in an amide), and 96 (carbonyl oxygen bonded to N then Csp^2). One set of torsional parameters is missing for the side of the ring defined by atoms C(1)-N(7)-C(2)-C(3). Parameters are missing for the angle C(2)-C(3)-C(4)-N(6) on the side of the ring.. There are parameters missing for the 3 angles that include the fluoride atom. They are angles F(5)-C(3)-C(2)-N(7), F(5)-C(3)-C(2)-O(9), and F(5)-C(3)-C(4)-N(6). There are 2 bonding parameters that are missing. They are for the bond angles C(3)-C(2)-N(7) and F(5)-C(3)-C(2).

The bond lengths of the two carbons , C(1) and C(2), linked to the amide nitrogen , N(7), are both shorter in MM3 than in the crystal. Only one of the carbonyl double bonds, C(2)-O(9), is longer in MM3 even though both are part of the π-system. The 2 hydrogens, H(11) and H(12), bonded to their respective amide nitrogens , N(6) and N(7), have bond lengths that are more than 0.07 Å shorter in MM3 than the crystal.

Fig. 5 5-Fluorouracil



The bond angles with the greatest differences between MM3 and crystal values include the ring atoms C(2), C(3), C(4), N(6), and N(7) and the substituent atoms F(5), O(9), and H(10). Two of the angles include an amide nitrogen; they are angles C(3)-C(2)-N(7) and N(6)-C(4)-H(10). Three of the bond angles include the ring carbons; they are angles C(3)-C(2)-O9, C(2)-C(3)-C(4), and C(2)-C(3)-F5.

In this molecule there are no torsion angles that differ by more than 10 degrees between the MM3 and crystal values.

IV. Antihelmintics

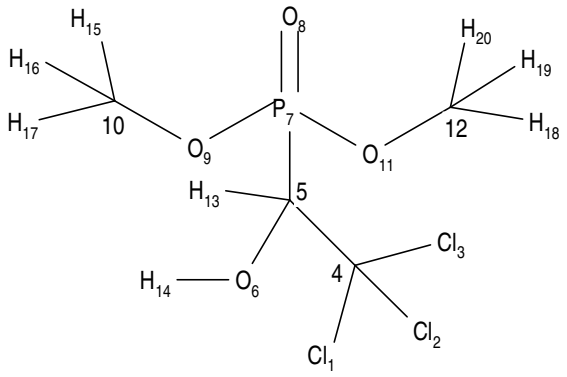
Helminths consist of nematodes and flatworms. These parasitic worms tend to be found in areas where sanitation and public health measures are poor. The life cycles of many helminths can be complex, often involving intermediate hosts. Many nematode species reside in the human gastrointestinal tract. Trematodes may live in a specific organ system depending on the species[4].

Drug Metrifonate

The missing parameters for this molecule are centered around the bonds between the phosphate group and its substituents. Three of the torsion angles include the hydroxy oxygen O(6) and one of the phosphorous oxygens (O(8), O(9), O(11)). There are two torsion angles between a substituent group and the phosphorous atom that are missing parameters. They are angles C(1)-C(4)-C(5)-P(7) and P(7)-C(5)-O(6)-H(14).

There is one bending parameter missing. It is for the bond angle O(6)-C(5)-P(7).

Fig. 6 Metrifonate



The bond lengths whose values differ the most all include an oxygen atom bonded to another atom. The bonds between the phosphorous atom P(7) and the oxygen atoms O(8), O(9), and O(11) are all longer in MM3 than the crystal. The bond between O(6)-H(14) is almost 0.15 Å shorter in MM3. The bond between O(9)-C(10) is shorter in MM3 but the length for the corresponding bond O(11)-C(12) is not shortened by the same amount.

There are only 3 bond angles whose MM3 values differ by much from the crystal. Two of the angles are between the hydrogen atom H(13) and atoms on the side chain. They are angles C(4)-C(5)-H(13) and O(6)-C(5)-H(13). The third bond angle is O(9)-P(7)-O(1).

Many of the measured torsion angle values for MM3 and the crystal vary by significant amounts. The torsion angles between carbon C(4) and the phosphate oxygens O(8), O(9), and O(11) are 12 – 18 degrees less in MM3 than in the crystal. The two torsion angles C(5)-P(7)-O(9)-C(10) and C(5)-P(7)-O(11)-C(12) do not vary by the same amount. The angle C(5)-P(7)-O(9)-C(10) is almost 59 degrees greater in MM3 than in the crystal while the angle C(5)-P(7)-O(11)-C(12) is more than 13 degrees less in MM3. The three torsion angles between the hydroxy oxygen O(6) and the phosphate oxygens O(8), O(9), and O(11) are 11 – 17 degrees less in MM3. The two torsion angles between O(8) and carbons C(10) and C(12) do not vary by the same amount. Angle O(8)-P(7)-O(9)-C(10) varies by more than 59 degrees in MM3 while angle O(8)-P(7)-O(11)-C(12) varies by only about 12 degrees in MM3. Angle C(10)-O(9)-P(7)-O(11) is nearly 60 degrees less in MM3 than the crystal. Three torsion angles vary by close to 100 degrees between MM3 and the crystal; they are angles C(4)-C(5)-O(6)-H(14), P(7)-C(5)-O(6)-H(14), and H(13)-C(5)-C(6)-H(14).

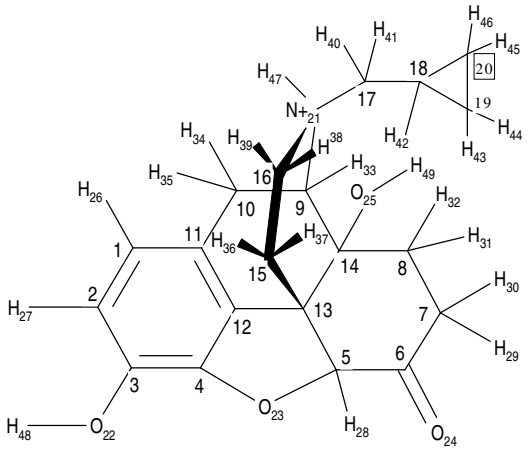
V. Opioid Analgesics

Opioids relieve moderate to severe pain by binding to a certain set of cell surface receptors. They can also be used to treat acute diarrhea, cough suppression, and maintenance therapy in opiate addiction. There are 3 types of opioid receptors that have been identified: μ, κ, and δ. Activation of one of these receptors changes the conductance of K^+ and Ca^{2+} ions. This in turn leads to inhibition of neuronal activity and a reduction in the transmission rate of painful stimuli[5].

Drug: Naltrexone

The missing torsion angle parameters are located in 2 areas: the N-alkylpiperidine region and the furan ring bonded to one of the cyclohexyl rings. The angles in the N-alkylpiperidine area are: C(18)-C(17)-N(21)-C(9), C(18)-C(17)-N(21)-C(16), C(18)-C(17)-N(21)-H(47), N(21)-C(17)-C(18)-C(19), N(21)-C(17)-C(18)-C(20), and N(21)-C(17)-C(18)-H(42). The angles in the furan/cyclohexyl ring area are: C(6)-C(5)-O(23)-C(4), O(23)-C(5)-C(6)-C(7), C(12)-C(13)-C(5)-O(23), and O(23)-C(5)-C(6)-O(24).

Fig. 7 Naltrexone



There are 2 bending parameters missing. They are for angle C(6)-C(5)-O(23) and angle C(18)-C(17)-N^+(21).

The bond lengths between some of the molecule's heteroatoms and their corresponding hydrogens are shorter in MM3 than in the crystal. They are bonds N^+(21)-H(47), O(22)-H(48), and O(25)-H(49). One bond in the cyclopropane ring (C(19)-C(20)) is longer in MM3. One of the carbon-carbon bonds (C(17)-C(18)) connecting the cyclopropane ring to the piperidine ring is

longer in MM3. Two carbon-oxygen bonds are shorter in MM3; they are bonds C(3)-O(22) and C(4)-O(23). One of the carbon-carbon bonds in the cyclohexanone ring is longer in MM3. The carbon-oxygen bond C(4)-O(23) in the furan ring is almost 0.16 Å shorter in MM3 than the crystal.

There are several bond angles between carbon and hydrogen that vary by near 20 degrees between the MM3 and crystal values. They are angles C(17)-C(18)-H(42), C(19)-C(18)-H(42), C(20)-C(18)-H(42), C(18)-C(19)-H(43), C(18)-C(19)-H(44), C(20)-C(19)-H(43), C(20)-C(19)-H(44), C(18)-C(20)-H(46), C(19)-C(20)-H(45), and C(19)-C(20)-H(46). All of these angles are in the cyclopropyl group. There are 3 bond angles that involve methylene groups. Angle H(40)-C(17)-H(41) is only 5 degrees greater in MM3 while angles H(43)-C(19)-H(44) and H(45)-C(20)-H(46) are more than 55 degrees greater in MM3. The bond angles between some of the ring carbons and the hydroxyl oxygens are a little more than 5 degrees less in MM3. The two angles are C(2)-C(3)-O(22) and C(9)-C(14)-O(25).

Many of the torsion angles whose values differ significantly between MM3 and the crystal contain ring atoms. The angles in the furan and cyclohexanone rings are: C(4)-O(23)-C(5)-C(6), C(5)-C(6)-C(7)-C(8), C(6)-C(5)-C(13)-C(14), C(7)-C(6)-C(5)-O(13), C(7)-C(6)-C(5)-O(23), C(7)-C(6)-C(5)-H(28), C(8)-C(7)-C(6)-O(24), C(8)-C(14)-O(25)-H(49), C(13)-C(5)-C(6)-O(24), O(23)-C(5)-C(6)-O(24), and C(13)-C(14)-O(25)-H(49). The angles in the N-alkylpiperidine ring are: C(9)-N^+(21)-C(17)-H(40), C(9)-N^+(21)-C(17)-H(41), C(16)-N^+(21)-C(17)-H(40), C(16)-N^+(21)-C(17)-H(41), and H(41)-C(17)-N^+(21)-H(47). Many of the cyclopropyl ring torsion angles vary by 20 – 46 degrees between MM3 and the crystal. The angles are: C(17)-C(18)-C(19)-H(43), C(17)-C(18)-C(19)-H(44), C(17)-C(18)-C(20)-H(45), C(17)-C(18)-C(20)-H(46), C(18)-C(19)-C(20)-H(45), C(18)-C(19)-C(20)-H(46), C(18)-C(20)-C(19)-H(43), C(18)-C(20)-C(19)-H(44), C(19)-C(18)-C(20)-H(45), C(19)-C(18)-C(20)-H(46) , C(19)-C(20)-C(18)-H(42), C(20)-C(18)-C(19)-H(43), C(20)-C(19)-C(18)-H(42), H(42)-C(18)-C(19)-H(43), H(42)-C(18)-C(20)-H(46), H(43)-C(19)-C(20)-H(45), and H(44)-C(19)-C(20)-H(46).

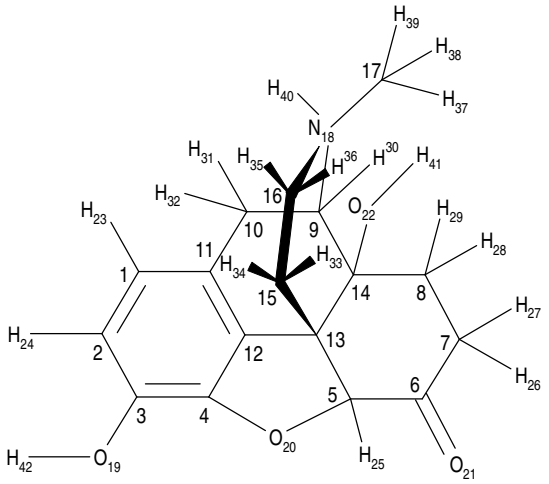
Drug: Oxymorphone

Even though oxymorphone and naltrexone share the same basic structure the number of missing parameters is not the same. Oxymorphone's missing parameters are concentrated around the furan-cyclohexanone region. The torsion angles are C(6)-C(5)-O(20)-C(4), O(20)-C(6)-C(5)-C(7), C(12)-C(13)-C(5)-O(20), and O(20)-C(5)-C(6)-O(21).

Only one bending parameter is missing. It is for angle C(6)-C(5)-O(20).

Many of the bond lengths calculated by MM3 for this molecule are longer than the crystal values. The bonds that involve hydrogen have the greatest difference. These bonds are: C(5)-C(13), C(5)-H(25), C(7)-H(26), C(7)-H(27), C(8)-H(28), C(8)-H(29), C(9)-H(30), C(10)-

Fig. 8 Oxymorphone



H(31), C(10)-H(32), C(15)-H(33), C(15)-H(34), C(16)-H(35), C(16)-H(36), N^{+}(18)-H(40), O(19)-H(42), and O(22)-H(41). All of the bond lengths calculated for the phenyl ring vary by 0.0202-0.0526 Å. Those bond lengths are: C(1)-C(2), C(2)-C(3), C(3)-C(4), C(4)-C(12), and C(11)-C(12). Five of the bonds in the cyclohexanone ring are longer in MM3 than in the crystal. They are: C(5)-C(6), C(5)-C(13), C(6)-C(7), C(7)-C(8), and C(8)-H(14). Only one of the carbon-oxygen bonds in the furan ring is shorter in MM3; it is bond C(4)-O(20). One carbon-hydroxy oxygen bond , C(3)-O(19), is almost 0.1 Å shorter in MM3 but the other carbon-hydroxy oxygen bond , C(14)-O(22), is more than 0.03 Å longer in MM3. The carbon-carbonyl oxygen bond C(6)-O(21) is more than 0.03 Å longer in MM3. Three of the bonds in the piperidine ring are longer in MM3 than in the crystal. They are: C(9)-C(14), C(13)-C(15), and C(15)-C(16). The nitrogen-methyl carbon bond is almost 0.04 Å longer in MM3.

There are only 4 bond angles that differ by more than 5 degrees between MM3 and the crystal values. They are angles C(6)-C(7)-C(8), C(10)-C(9)-H(30), N^{+}(18)-C(9)-H(30), and H(31)-C(10)-H(32).

The torsion angles that vary by more than 10 degrees between MM3 and crystal tend to bridge the ring system in this molecule. The angles located in the benzyl ring are: C(2)-C(3)-O(19)-H(42) and C(4)-C(3)-O(19)-H(42). The angles that bridge the benzyl and furan rings are: C(3)-C(4)-O(20)-C(5) and C(5)-O(20)-C(4)-C(12). The angles that are located in the cyclohexanone ring are: C(5)-C(6)-C(7)-C(8), C(5)-C(6)-C(7)-H(26), C(5)-C(6)-C(7)-H(27), C(6)-C(7)-C(8)-C(14), C(6)-C(7)-C(8)-H(29), C(8)-C(7)-C(6)-O(21), C(13)-C(5)-C(6)-O(21), C(13)-C(14)-O(22)-H(41), C(14)-C(8)-C(7)-H(26), C(14)-C(8)-C(7)-H(27), C(14)-C(13)-C(5)-H(25), O(21)-C(6)-C(5)-H(25), O(21)-C(6)-C(7)-H(26), O(21)-C(6)-C(7)-H(27), H(26)-C(7)-C(8)-H(28), and H(27)-C(7)-C(8)-H(29). The angles that bridge the cyclohexanone and furan rings are: C(4)-O(20)-C(5)-C(6), C(4)-O(20)-C(5)-C(13), C(4)-O(20)-C(5)-H(25), C(6)-C(5)-C(13)-C(12), C(6)-C(5)-C(13)-C(14), C(7)-C(6)-C(5)-C(13), C(7)-C(6)-C(5)-O(20), C(14)-C(13)-C(5)-O(20), and O(20)-C(5)-C(6)-O(21). The angles that bridge the cyclohexanone and piperidine rings are: C(6)-C(5)-C(13)-C(15) and C(13)-C(14)-C(9)-H(30). The angles that bridge the cyclohexanone and cyclohexyl rings are: C(8)-C(14)-C(9)-H(30) and C(9)-C(14)-O(22)-H(41). The angles located in the cyclohexyl ring are: C(10)-C(9)-C(14)-O(22), H(30)-C(9)-C(10)-H(31), and H(30)-C(9)-C(10)-H(32). The angles that bridge the furan and piperidine rings are: C(15)-C(13)-C(5)-O(20) and C(15)-C(13)-C(5)-H(25).

VI. Non-steroidal Anti-inflammatory Drugs (NSAID)

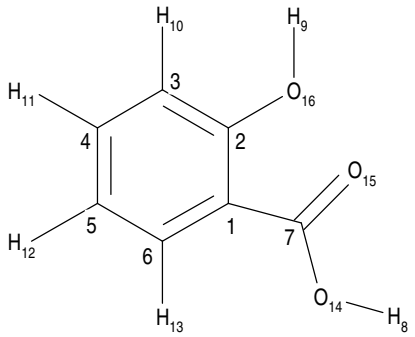
These drugs are used to treat mild pain, elevated body temperature, arthritis, and gout. NSAIDs exert their effects by inhibiting prostaglandin synthesis. They act locally to block pain rather than by preventing its recognition by the brain. NSAIDs also have an anti-inflammatory effect on the body[6].

Drug: Salicylic acid

There is only one torsional angle that is missing parameters. It is angle C(1)-C(7)-O(14)-H(8) and it is located in the carboxylic acid side chain.

The bond between the ring and the side chain, C(1)-C(7), is longer in MM3 than in the crystal. One carbon-oxygen bond, C(2)-O(16), is more than 0.11 Å longer in the crystal. Another carbon-oxygen bond on the side chain, C(7)-H(14), is 0.06 Å longer in MM3. Two ring carbon-hydrogen bonds, C(6)-H(13) and C(7)-H(14), are more than 0.11 Å longer in MM3. There are two oxygen-hydrogen bonds that are shorter in MM3 than the crystal but not by the same amount. Bond H(8)-O(14) is approximately 0.025 Å shorter while bond H(9)-O(16) is 0.065 Å shorter.

Fig. 9 Salicylic acid



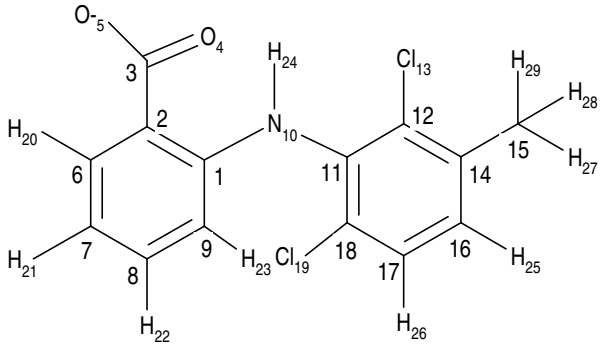
There are no bond angles that vary by more than 5 degrees between crystal and MM3 values. Neither are there any torsion angles that vary by more than 10 degrees between crystal and MM3.

Drug: Meclofenamate

Four of the torsion angles that are missing parameters link one of the phenyl rings with the arylamine bridge. They are angles C(12)-C(11)-N(10)-C(1), C(18)-C(11)-N(10)-C(1), C(2)-C(1)-N(10)-C(11), and C(9)-C(1)-N(10)-C(11). Two torsion angles are between the amine nitrogen and a ring chloride. They are angles N(10)-C(11)-C(12)-Cl(13) and N(10)-C(11)-C(18)-Cl(19).

There are three bond angles that are missing parameters. Two of them are located on the carboxylate side chain. They are angles C(2)-C(3)-O(4) and C(2)-C(3)-O(5). The third angle is located on the arylamine bridge. It is angle C(1)-N(10)-C(11)

Fig. 10 Meclofenamate



There are three carbon-carbon bond lengths in the phenyl rings that are longer in MM3 than in the crystal. They are bonds C(1)-C(9), C(2)-C(6), and C(11)-C(18). One bond length in one of the phenyl rings is longer in the crystal. It is bond C(11)-C(12). Three bonds that include a hydrogen atom are longer in MM3 than in the crystal. They are the bond lengths C(6)-H(20), C(9)-H(23), and N(10)-H(24). One carbon-nitrogen bond length is longer in MM3. It is bond C(1)-N(10). The bond that connects the carboxylate side chain , C(2)-C(3), with a phenyl ring is longer in the crystal. The bond that connects the methyl group , C(14)-C(15), with a phenyl ring is also longer in the crystal.

There are four bond angles that vary by more than 5 degrees. The angle C(3)-C(2)-C(6) connects the carboxylate group with a phenyl ring. Two of the angles are located on the arylamine bridge. They are angles C(1)-N(10)-C(11) and C(1)-N(10)-H(24). The fourth angle is located on a phenyl ring. It is angle C(2)-C(6)-H(20).

Several of the torsion angles have values that by more than 10 degrees connect the phenyl rings through the arylamine bridge. They are the angles C(1)-N(10)-C(11)-C(12), C(1)-N(10)-C(11)-C(18), C(2)-C(1)-N(10)-C(11), C(2)-C(1)-N(10)-H(24), C(9)-C(1)-N(10)-C(11), N(10)-C(1)-C(9)-H(23), C(12)-C(11)-N(10)-H(24), and C(18)-C(11)-N(10)-H(24). Two torsion angles are between the carboxylate group and the phenyl ring. They are angles C(3)-C(2)-C(1)-C(9) and C(3)-C(2)-C(1)-N(10).

VII. Anesthetics

Anesthesia is a controlled loss of bodily sensation. It can be either local or general. General anesthesia also involves loss of consciousness. General anesthesia can be administered

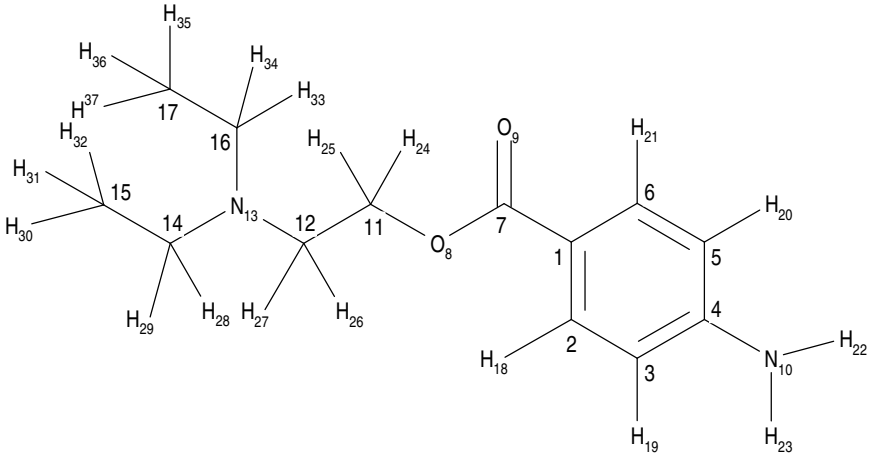
by either inhalation or injection. IV anesthetic drugs act at specific cell surface receptors depending on the drug[7].

Drug: Procaine

There are no missing parameters for this molecule.

Several of the bond lengths for this molecule vary by more than 0.02 Å between crystal and MM3. The bond length connecting the phenyl ring with the ester side chain , C(1)-C(7), is longer in MM3. Two bond lengths in the phenyl ring are longer in MM3. They are bonds C(2)-C(3) and C(5)-C(6). Two carbon-nitrogen bonds are longer in MM3. They are C(4)-N(10) and N(13)-C(14). The bond length between the carbonyl carbon and the ester oxygen , C(7)-O(8), is longer in MM3. There are 7 bonds that include hydrogen atoms whose lengths vary significantly between MM3 and crystal. Three of the bond lengths are longer in MM3; they are for bonds N(10)-H(23), C(12)-H(26), and C(12)-H(27). Four of the bond lengths are shorter in MM3; they are for bonds C(14)-H(28), C(14)-H(29), C(16)-H(33), and C(16)-H(34). One carbon-carbon bond length ,C(11)-C(12), in the ester side chain is longer in MM3. Two carbon-carbon bond lengths ,C(14)-C(15) and C(16)-C(17), in the diethylamine group are longer in MM3.

Fig. 11 Procaine



The bond angles that vary more than 5 degrees between crystal and MM3 are located in two general areas: the phenyl ring and the alkylamine portion of the side chain. The bond angles on the phenyl ring are C(1)-C(7)-O(8), C(1)-C(7)-O(9), and H(22)-N(10)-H(23). One bond angle is located between the ester oxygen and the diethylamine group; it is angle C(11)-C(12)-H(27).

The bond angles located in the diethylamine group are: C(15)-C(14)-H(28), C(15)-C(14)-H(29), H(28)-C(14)-H(29), N(13)-C(16)-H(33), C(17)-C(16)-H(33), and H(33)-C(16)-H(34).

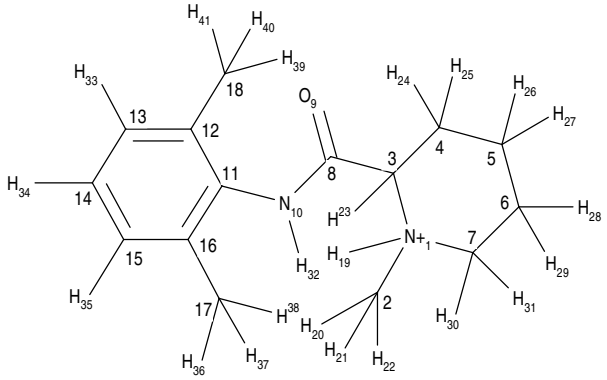
Some of the torsion angles whose variance is greater than 10 degrees are located on the phenyl ring. The torsion angle C(1)-C(7)-O(8)-C(11) links the phenyl ring with the ester group. The torsion angles C(3)-C(4)-N(10)-H(22), C(3)-C(4)-N(10)-H(23), C(5)-C(4)-N(10)-H(22), and C(5)-C(4)-N(10)-H(23)link the phenyl ring with the amine group. One torsion angle is in the region of the ester group on the side chain; it is angle C(7)-O(8)-C(11)-C(12). Several torsion angles are located in the diethylamine portion of the side chain. They are angles C(11)-C(12)-N(13)-C(14), C(11)-C(12)-N(13)-C(16), C(12)-N(13)-C(14)-H(29), C(14)-N(13)-C(12)-H(26), C(14)-N(13)-C(12)-H(27), C(16)-N(13)-C(12)-H(27), and C(16)-N(13)-C(14)-H(29).

Drug: Mepivicaine

This molecule is missing parameters for 4 torsion angles. Two of the torsion angles link the amide side chain with the piperidine ring. They are angles C(8)-C(3)-N^+(1)-C(2) and C(8)-C(3)-N^+(1)-C(7). Two of the torsion angles link the amide side chain with the phenyl ring. They are angles N(10)-C(11)-C(12)-C(18) and N(10)-C(11)-C(16)-C(17).

Five of the carbon-hydrogen bond lengths on the piperidine ring are longer in MM3 than in the crystal. They are bonds C(3)-H(23), C(4)-H(24), C(4)-H(25), C(5)-H(26), and C(5)-H(27). One of the carbon-carbon bond lengths on the piperidine ring is longer in MM3. It is bond C(6)-C(7). There are 3 bond lengths that include the amide nitrogen. They are bonds C(8)-N(10), N(10)-C(11), and N(10)-H(32).

Fig. 12 Mepivicaine



There are 2 bond angles linking the phenyl ring with the methyl substituent that vary by more than 5 degrees. They are angles C(12)-C(18)-H(39) and C(12)-C(18)-H(41). Two bond angles are located on the methyl substituent; they are angles H(39)-C(18)-H(41) and H(40)-C(18)-H(41). There are two bond angles that include the amide nitrogen. They are angles C(8)-N10-H(32) and C(11)-N10-H(32). One bond angle is located on the piperidine ring. It is angle C(3)-N^+1-H(19).

The torsion angles that vary by more than 10 degrees link one of the rings with the amide bridge. The angles located on the N-methylpiperidine ring are: N^+(1)-C(3)-C(8)-O(9), C(3)-C(8)-N(10)-H(32), C(4)-C(3)-C(8)-O(9), O(9)-C(8)-C(3)-H(23), and N(10)-C(8)-C(3)-H(23). The angles located on the phenyl ring are: C(11)-C(12)-C(18)-H(40), C(11)-C(12)-C(18)-H(41), C(12)-C(11)-N(10)-H(32), C(13)-C(12)-C(18)-H(39), C(13)-C(12)-C(18)-H(40), C(13)-C(12)-C(18)-H(41), and C(16)-C(11)-N(10)-H(32).

VIII. Antibiotics

Antibiotic drugs exert their effects on invading organisms in one of five major ways:

1) Inhibiting synthesis of and damaging the cell wall.
2) Inhibiting synthesis of or damaging the cytoplasmic membrane.
3) Altering the synthesis or metabolism of nucleic acids.
4) Inhibiting or modifying protein synthesis.
5) Modifying energy metabolism.

The best way to determine which antibiotic to use is by identifying the invading microbe. The susceptibility of the organism to the antibiotic must also be considered. Many microorganisms today are becoming resistant to the most commonly used antibiotics[8].

Drug: Demeclocycline

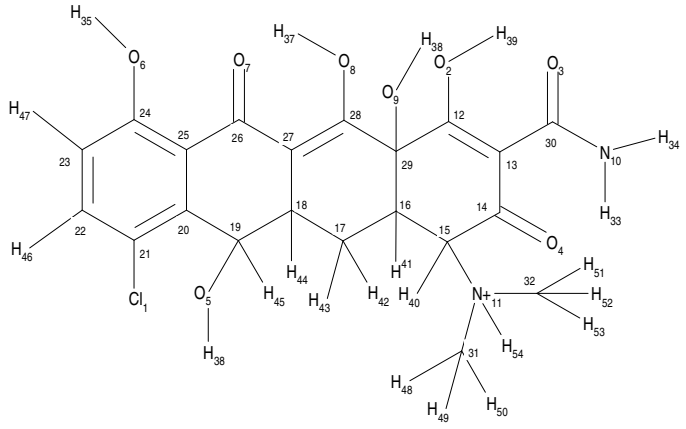
The bulk of the missing parameters are for torsion angles located on the third and fourth rings. The angles are: O(9)-C(29)-C(12)-O(2), C(16)-C(29)-C(12)-O(2), C(28)-C(29)-C(12)-O(2), C(14)-C(13)-C(30)-O(3), O(9)-C(29)-C(28)-O(8), C(12)-C(29)-C(28)-C(8), C(16)-C(29)-C(28)-O(8), N^+(11)-C(15)-C(14)-C(13), C(14)-C(15)-N^+(11)-C(31), C(14)-C(15)-N^+(11)-C(32),

C(30)-C(13)-C(14)-C(15), and C(29)-C(12)-O(2)-H(39). Two angles are located on the amide side chain. They are: C(14)-C(13)-C(30)-N(10), and C(13)-C(30)-N(10).

There are π-atom parameters missing for this molecule. The missing parameters are for atom types 96-151, 81-151, 101-151, 151-3, and 151-162. MM3 substituted more than one atom type for some of the missing parameters. Atom types 2 and 7 were substituted for atom type 96. Atom type 7 was substituted for atom type 81. Atom types 2 and 7 were substituted for atom type 101. Atom types 2 and 40 were substituted for atom type 151. Atom types 2 and 3 were substituted for atom type 162.

Several bond lengths that included heteroatoms differed by more than 0.02 Å between MM3 and the crystal values. These bonds were Cl(1)-C(21), O(2)-H(39), O(3)-C(30), O(5)-H(38), O(6)-C(24), O(7)-C(26), O(8)-C(28), O(8)-H(37), O(9)-H(36), N(10)-C(30), N(10)-H(33), N(10)-H(34), N^{+}(11)-C(15), N^{+}(11)-C(31), and N^{+}(11)-H(54). There were 3 carbon-hydrogen bond lengths that were more than 0.1 angstrom longer in MM3. They are C(17)-H(43), C(18)-H(44), and C(19)-H(45). There is one carbon-carbon bond that is shorter in MM3 and 8 that are longer. The shorter bond length is C(12)-C(13). The longer bond lengths are C(13)-C(14), C(13)-C(30), C(18)-C(19), C(20)-C(21), C(22)-C(23), C(25)-C(26), and C(26)-C(27).

Fig. 13 Demeclocycline



There are 5 bond angles that vary by more than 5 degrees between MM3 and the crystal. They are angles C(19)-O(5)-H(38), C(24)-O(6)-H(35), H(33)-N(10)-H(34), C(20)-C(19)-H(45), and C(12)-C(29)-C(28).

The torsion angles that vary by more than 10 degrees are scattered across all 4 rings. The angles located on the amide side chain are: O(3)-C(30)-N(10)-H(33), O(3)-C(30)-C(13)-C(12),

O(3)-C(30)-C(13)-C(14), O(4)-C(14)-C(13)-C(30), N(10)-C(30)-C(13)-C(12), and N(10)-C(30)-C(13)-C(14). The angles located on the fourth ring are: O(4)-C(14)-C(13)-C(12), C(12)-C(29)-O(9)-H(38), C(16)-C(29)-O(9)-H(38), C(28)-C(29)-O(9)-H(38), and C(29)-C(28)-O(8)-H(37). The angles located on the second and third ring are: O(8)-C(28)-C(27)-C(18), C(18)-C(19)-O(5)-H(38), C(19)-C(18)-C(27)-C(26), C(19)-C(18)-C(27)-C(28), C(19)-C(20)-C(25)-C(26), H(36)-O(5)-C(19)-H(45) and C(20)-C(19)-O(5)-H(36). The angles located on the first and second rings are: C(19)-C(20)-C(21)-C(22), C(19)-C(20)-C(25)-C(24), C(25)-C(20)-C(19)-H(45), and C(25)-C(24)-O(6)-H(35).

Drug: Streptomycin

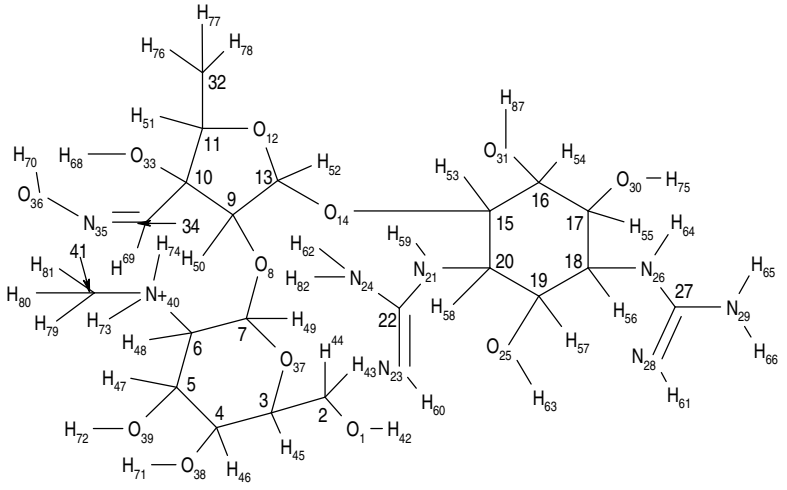
The missing parameters are located primarily around the guanidium side chains and their connection to the remainder of the molecule. The angles located on the ether bridge and linked to the amine side chain are: O(14)-C(15)-C(20)-N(21), C(15)-C(20)-N(21)-C(22), C(15)-C(20)-N(21)-H(59), and C(16)-C(15)-C(20)-N(21). The angles located on the cyclohexyl ring and linked to one of the amine side chains are: C(16)-C(17)-C(18)-N(26), C(17)-C(18)-N(26)-C(27), C(18)-C(19)-C(20)-N(21), C(19)-C(18)-N(26)-C(27), C(19)-C(20)-N(21)-C(22), and C(20)-C(19)-C(18)-N(26). The angles located on one of the guanidium side chains are: N(28)-C(27)-N(26)-C(18), N(29)-C(27)-N(26)-C(18), N(23)-C(22)-N(21)-C(20), N(24)-C(22)-N(21)-C(20), N(21)-C(22)-N(23)-H(60), N(21)-C(22)-N(24)-H(62), N(21)-C(22)-N(24)-H(82), N(24)-C(22)-N(21)-H(59), N(24)-C(22)-N(23)-H(60), N(26)-C(27)-N(28)-H(61), N(26)-C(27)-N(29)-H(65), N(26)-C(27)-N(29)-H(66), N(26)-C(27)-N(29)-H(65), N(29)-C(27)-N(28)-H(61), and H(56)-C(18)-N(26)-H(64). Some of the missing parameters are for torsion angles that link a hydroxyl group with one of the guanidium side chains. The angles are: N(21)-C(20)-C(19)-O(25), O(25)-C(19)-C(18)-N(26), N(26)-C(18)-C(17)-O(30), O(33)-C(10)-C(34)-N(35), and H(70)-O(36)-N(35)-C(34). There is one bond that is missing parameters. It is the oxygen-nitrogen bond O(35)-N(36).

The bond angles that are missing parameters are located primarily around the cyclohexyl ring and guanidium side chains. The angles are: C(17)-C(18)-N(26), C(19)-C(18)-N(26), C(15)-C(20)-N(21), C(19)-C(20)-N(21), C(20)-N(21)-H(59), N(21)-C(22)-N(24), H(62)-N(24)-H(82),

C(18)-N(26)-H(64), N(26)-C(27)-N(29), and H(65)-N(29)-H(66). Two bond angles are located on the oxime side chain. They are: C(34)-N(35)-O(36) and H(70)-O(36)-N(35).

The bond lengths that vary by more than 0.02 Å between MM3 and the crystal can be grouped into 5 general categories: carbon-heteroatom bonds, carbon-hydrogen bonds, carbon-carbon bonds, oxygen-hydrogen bonds, and nitrogen-hydrogen bonds. Most of the carbon-heteroatom bond lengths are longer in MM3 than in the crystal. Those bonds are: O(1)-C(2), C(6)-N^+(40), C(7)-O(8), O(8)-C(9), C(10)-O(34), C(11)-O(12), O(12)-C(13), C(13)-O(14), C(16)-O(31), C(17)-O(30), C(20)-N(21), N(21)-C(22), N(26)-C(27), C(27)-N(28), N^+(40)-C(41), and C(27)-N(29). The carbon-hydrogen bond lengths are longer in MM3 than in the crystal. Those bonds are: C(9)-H(50), C(13)-H(52), C(15)-H(53), C(16)-H(54), C(17)-H(55), C(18)-H(56), and C(19)-H(57). The majority of the carbon-carbon bond lengths are longer in MM3. Those bonds are: C(3)-C(4), C(5)-C(6), C(9)-C(10), C(9)-C(13), C(10)-C(11), C(15)-C(20), and C(16)-C(17). The oxygen-hydrogen bond lengths are all shorter in MM3. Those bonds are: O(25)-H(63), O(31)-H(67), O(33)-H(68), O(36)-H(70), O(38)-H(71), and O(39)-H(72). Most of the nitrogen-hydrogen bond lengths are longer in MM3. Those bonds are: N(21)-H(59), N(23)-

Fig. 14 Streptomycin



H(60), N(24)-H(62), N(24)-H(82), N(26)-H(64), N(28)-H(61), N(29)-H(65), N(29)-H(66), N^+(40)-H(73), and N^+(40)-H(74). There is one oxygen-nitrogen bond length that is longer in MM3 than in the crystal. It is bond length N(35)-O(36).

The bond angles that vary by more than 5 degrees are scattered across the molecule. Three angles ,C(3)-C(4)-C(5), C(3)-O(37)-C(7), and C(5)-C(4)-O(38), are located on the

tetrahydropyran ring. One angle, C(11)-O(12)-C(13), is located on the tetrahydrofuran ring. Three angles ,C(4)-O(38)-H(71), C(5)-O(39)-H(72), and H(73)-N^+(40)-H(74), are located on side chains off of the tetrahydropyran ring. Four angles, C(22)-N(23)-H(60), C(27)-N(28)-H(61), C(27)-N(29)-H(66), and H(65)-N(29)-H(66), are located on the guanidium side chains. Two angles, C(16)-O(31)-H(67) and C(10)-O(33)-H(68), are located on hydroxyl side chains. One angle, C(34)-N(35)-O(36), is located on the oxime side chain.

The torsion angles that vary by more than 10 degrees link the various rings with one of their side chains. The angles that link a hydroxyl group with the tetrahydropyran ring are: O(1)-C(2)-C(3)-C(4), O(1)-C(2)-C(3)-O(37), C(3)-C(4)-O(38)-H(71), C(4)-C(5)-O(39)-H(72), C(5)-C(4)-O(38)-H(71), C(6)-C(5)-C(4)-O(38), C(6)-C(5)-O(39)-H(72), O(39)-C(5)-C(6)-N^+(40), and C(7)-C(6)-C(5)-O(39). One angle links a hydroxyl group with the tetrahydrofuran ring; it is angle O(33)-C(10)-C(9)-H(50). The angles located on the tetrahydropyran ring are: C(2)-C(3)-O(37)-C(7), C(3)-C(4)-C(5)-C(6), O(39)-C(5)-C(6)-N^+(40), and C(4)-C(5)-C(6)-C(7). The angles that link an guanidium side chain with the tetrahydropyran ring are: C(4)-C(5)-C(6)-N^+(40), C(5)-C(6)-N^+(40)-C(41), C(5)-C(6)-N^+(40)-H(73), C(5)-C(6)-N^+(40)-H(74), C(7)-C(6)-N^+(40)-H(73), and C(7)-C(6)-N^+(40)-H(74). The angles that are located on the ether bridge are: C(6)-C(7)-O(8)-C(9), O(8)-C(9)-C(13)-O(12), O(8)-C(9)-C(13)-O(14), O(8)-C(9)-C(13)-H(52), C(9)-C(13)-O(14)-C(15), C(10)-C(9)-C(13)-O(14), C(11)-O(12)-C(13)-O(14), O(12)-C(13)-O(14)-C(15), C(13)-O(14)-C(15)-H(53), C(15)-O(14)-C(13)-H(52), and O(14)-C(13)-C(9)-H(50). The angles that link a substituent group with the tetrahydrofuran ring are: C(9)-C(10)-O(33)-H(68), C(9)-C(10)-C(34)-N(35), C(9)-C(10)-C(34)-H(69), C(11)-C(10)-O(33)-H(68), C(11)-C(10)-C(34)-N(35), C(11)-C(10)-C(34)-H(69), C(13)-C(9)-C(10)-O(33), and C(13)-C(9)-C(10)-C(34). The angles that link a substituent group with the cyclohexyl ring are: C(15)-C(16)-O(31)-H(67), C(15)-C(20)-N(21)-C(22), C(15)-C(20)-N(21)-H(59), C(17)-C(16)-O(31)-H(67), C(17)-C(18)-N(26)-H(64), C(18)-C(19)-O(25)-H(63), C(19)-C(18)-N(26)-H(64), C(19)-C(20)-N(21)-C(22), C(19)-C(20)-N(21)-H(59), C(20)-C(19)-O(25)-H(63), C(22)-N(21)-C(20)-H(58), H(54)-C(16)-O(31)-H(67), H(56)-C(18)-N(26)-H(64), and H(57)-C(19)-O(25)-H(63). The angles located on an guanidium substituent are: N(21)-C(22)-N(23)-H(60), N(21)-C(22)-N(24)-H(62), N(21)-C(22)-N(24)-H(82), N(23)-C(22)-N(24)-H(62), N(23)-C(22)-N(24)-H(82), N(24)-C(22)-N(23)-H(60), N(26)-C(27)-N(29)-H(65), N(28)-C(27)-N(29)-H(65), and H(57)-C(29)-

O(25)-H(63). The angles located on the oxime substituent are: O(33)-C(10)-C(34)-N(35), O(33)-C(10)-C(34)-H(69), C(34)-C(10)-C(9)-H(50), and C(34)-C(10)-O(33)-H(68).

For this molecule energy minimization in MM3 was not accomplished under 11 iterations in 3 VESCF cycles. The minimization was stopped at this point. The results for this molecule are not at their lowest values.

Drug: Clavulanate

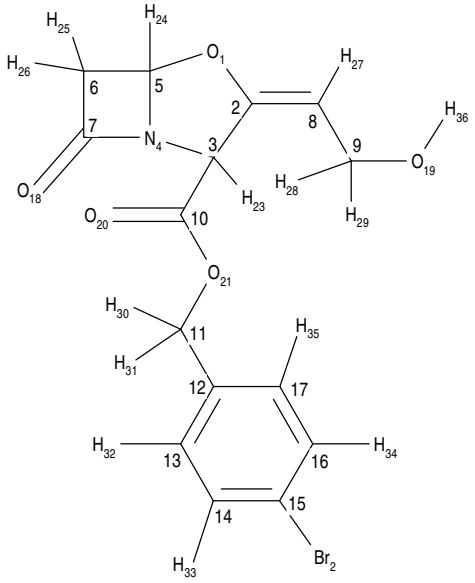
The missing parameters are primarily for torsion angles located in the fused ring system. The angles located on the furan portion of the system are: N(4)-C(3)-C(2)-O(1), C(3)-N(4)-C(5)-O(1), and C(2)-O(1)-C(5)-N(4). The angles located on the 4-membered ring are: C(5)-C(6)-C(7)-N(4), H(25)-C(6)-C(7)-N(4), C(5)-N(4)-C(7)-C(6), C(5)-N(4)-C(7)-O(18), C(7)-N(4)-C(5)-C(6), and C(7)-N(4)-C(5)-H(24). The angles that link both rings are: C(7)-N(4)-C(5)-O(1), O(1)-C(5)-C(6)-C(7), C(2)-C(3)-N(4)-C(7), C(3)-N(4)-C(7)-C(6), and C(3)-N(4)-C(7)-O(18). The angles that link the furan ring with the ester side chain are: C(10)-C(3)-C(2)-O(1), N(4)-C(3)-C(10)-O(21), and C(10)-C(3)-N(4)-C(7).

There are some bond lengths and angles that are missing parameters. The bond length is N(4)-C(7). The bond angles are: C(3)-N(4)-C(7), C(5)-N(4)-C(7), N(4)-C(5)-O(1), N(4)-C(5)-O(1), N(4)-C(7)-C(6), and N(4)-C(7)-O(18).

The bond lengths that vary by more than 0.02 Å are scattered across the molecule. The bond lengths located on the fused ring system are: O(1)-C(2), C(2)-C(3), C(3)-N(4), C(7)-O(18), and C(3)-C(10). The bond lengths located on the alkyl substituent on the ring are: C(8)-C(9) and C(9)-O(19). The bond lengths located on the ester bridge are: C(10)-O(20) and C(11)-O(21). The bond lengths located on the benzyl ring are: C(11)-C(12), C(12)-C(13), C(12)-C(17), C(13)-C(14), C(14)-C(15), and C(14)-H(33).

Five bond angles that vary by more than 5 degrees are located on the fused ring system. Those bonds are: C(2)-C(3)-N(4), C(3)-N(4)-C(5), C(3)-N(4)-C(7), O(1)-C(5)-N(4), and N(4)-C(5)-H(24). Two bond angles are located on the benzyl ring. Those bonds are: C(11)-C(12)-C(13) and C(12)-C(13)-C(14).

Fig. 15 Clavulanate



Several of the torsion angles that vary by more than 10 degrees are located on the fused ring system. The angles are: O(1)-C(5)-N4-C(3), O(1)-C(5)-C(6)-C(7), O(1)-C(5)-C(6)-H(25), O(1)-C(5)-C(6)-H(26), C(2)-C(3)-N(4)-C(5), C(3)-N(4)-C(5)-C(6), C(3)-N(4)-C(5)-H(24), C(3)-N(4)-C(7)-C(6), C(3)-N(4)-C(7)-O(18), C(5)-N(4)-C(3)-H(23), H(24)-C(5)-C(6)-H(26), and C(7)-C(6)-C(5)-H(24). Some of the torsion angles link the ring system with either substituent group. The angles are: C(2)-C(8)-C(9)-O(19), C(5)-N(4)-C(3)-C(10), C(8)-C(2)-C(3)-C(10), C(8)-C(9)-O(19)-H(36), and O(19)-C(9)-C(8)-H(27). Two of the torsion angles link the benzyl ring with the ester bridge. The angles are: C(13)-C(12)-C(11)-O(21) and C(17)-C(12)-C(11)-O(21).

Drug: Cephalosporin

The majority of missing parameters are for torsion angles located on the fused ring system. Those angles are: C(6)-S(40)-C(14)-C(15), C(6)-S(40)-C(14)-H(31), C(6)-S(40)-C(14)-N(34), C(12)-C(6)-S(40)-C(14), C(12)-C(13)-N(34)-C(16), C(13)-C(12)-C(6)-S(40), C(13)-N(34)-C(14)-S(40), C(13)-N(34)-C(16)-C(15), C(13)-N(34)-C(16)-O(29), C(14)-C(15)-C(16)-N(34), C(14)-N(34)-C(16)-C(15), C(14)-N(34)-C(16)-O(29), H(25)-C(6)-S(40)-C(14), C(16)-N(34)-C(14)-C(15), H(30)-C(13)-N(34)-C(16), C(16)-N(34)-C(14)-H(31), C(16)-N(34)-C(14)-S(40), and H(32)-C(15)-C(16)-N(34). Some of the torsion angles link the ester substituent with the ring system. Those angles are: C(1)-C(13)-N(34)-C(16), C(3)-C(4)-O(38)-C(5), O(38)-C(4)-

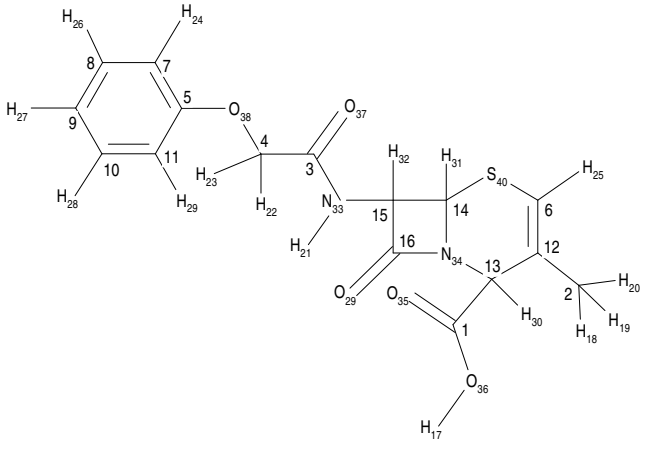
C(3)-N(33), N(34)-C(13)-C(1)-O(36), and O(38)-C(4)-C(3)-O(37). One torsion angle links the ring system with the amide substituent. It is angle N(33)-C(15)-C(16)-N(34).

Two bond lengths are missing parameters. They are bonds C(6)-S(40) and C(16)-N(34). Several bond angles that are missing parameters are located on the fused ring system. One bond angle is located on the ester portion of the side chain. It is angle C(3)-C(4)-O(38). The other angles are: C(12)-C(6)-S(40), H(25)-C(6)-S(40), N(34)-C(14)-S(40), N(34)-C(16)-C(15), N(34)-C(16)-O(39), C(13)-N(34)-C(16), C(14)-N(34)-C(16), and C(6)-S(40)-C(14).

The bond lengths that vary by more than 0.02 Å are spread across the whole molecule. The majority of them are longer in MM3 than in the crystal. The bond lengths located on the carboxylic acid substituent are: C(1)-O(35), C(1)-O(36), and H(17)-O(36). The bond lengths located on the amide portion of the side chain are: C(3)-N(33) and H(21)-N(33). The bond lengths located on the ester portion of the side chain are: C(4)-H(22), C(4)-H(23), C(4)- O(38), and C(5)-O(38). The bond lengths located on the phenyl ring are: C(5)-C(7), C(5)-C(11), C(7)-C(8), and C(7)-H(24). The bond lengths located on the fused ring system are: C(6)-H(25), C(6)-S(40), C(12)-C(13), C(13)-H(30), C(14)-C(15), C(14)-H(31), C(14)-N(34), and C(16)-N(34).

The bond angles that vary by more than 5 degrees are scattered across the molecule. One bond angle, H(22)-C(4)-O(38), is located on the ester portion of the side chain. Five bond angles

Fig. 16 Cephalosporin



link the amide portion of the side chain with the fused ring system. The angles are: C(14)-C(15)-N(33), C(16)-C(15)-N(33), H(32)-C(15)-N(33), C(3)-N(33)-H(21), and C(15)-N(33)-H(21). Seven bond angles are located on the fused ring system. The angles are: C(15)-C(14)-H(31), C(15)-C(14)-S(40), H(31)-C(14)-S(40), N(34)-C(14)-S(40), C(12)-C(6)-H(25), C(12)-C(6)-

S(40), and C(13)-N(34)-C(14). Two bond angles,C(1)-C(13)-H(30) and C(1)-O(36)-H(17), are located on the carboxylic acid substituent. Four bond angles are located on the phenyl ring. The angles are: C(5)-C(7)-H(24), C(8)-C(7)-H(24), C(5)-C(11)-H(29), and C(10)-C(11)-H(29).

Most of the torsion angles that vary by more than 10 degrees are located on the fused ring system. The torsion angles that link the carboxylic acid substituent with the ring are: C(1)-C(13)-N(34)-C(14), C(1)-C(13)-N(34)-C(16), C(12)-C(13)-C(1)-O(35), C(12)-C(13)-C(1)-O(36), H(30)-C(13)-C(1)-O(35), H(30)-C(13)-C(1)-O(36), N(34)-C(13)-C(1)-O(35), and N(34)-C(13)-C(1)-O(36). The angles that link the amide part of the side chain with the ring system are: C(3)-N(33)-C(15)-C(14), C(3)-N(33)-C(15)-C(16), C(3)-N(33)-C(15)-H(32), C(14)-C(15)-N(33)-H(21), C(16)-C(15)-N(33)-H(21), H(21)-N(33)-C(15)-H(32), H(31)-C(14)-C(15)-N(33), N(33)-C(15)-C(14)-N(34), N(33)-C(15)-C(14)-S(40), N(33)-C(15)-C(16)-N(34), and N(33)-C(15)-C(16)-O(39). One torsion angle (C(2)-C(12)-C(13)-H(30)) links the methyl substituent with the fused ring system. The angles located on the fused ring system are: C(6)-C(12)-C(13)-H(30), C(6)-C(12)-C(13)-N(34), C(12)-C(13)-N(34)-C(14), C(12)-C(13)-N(34)-C(16), C(13)-N(34)-C(14)-C(15), C(13)-N(34)-C(14)-H(31), C(13)-N(34)-C(14)-S(40), C(13)-N(34)-C(16)-C(15), C(13)-N(34)-C(16)-O(39), C(14)-C(15)-C(16)-N(34), C(14)-C(15)-C(16)-O(39), C(14)-N(34)-C(13)-H(30), C(14)-N(34)-C(16)-C(15), C(14)-N(34)-C(16)-O(39), C(15)-C(14)-N(34)-C(16), C(16)-C(15)-C(14)-H(31), C(16)-C(15)-C(14)-N(34), C(16)-N(34)-C(13)-H(30), C(16)-N(34)-C(14)-H(31), C(16)-N(34)-C(14)-S(40), H(31)-C(14)-C(15)-N(33), H(32)-C(15)-C(14)-N(34), H(32)-C(15)-C(14)-S(40), H(32)-C(15)-C(16)-N(34), and H(32)-C(15)-C(16)-O(39). The angles that link the phenyl ring with the ester are: C(5)-O(38)-C(4)-H(23), C(7)-C(5)-C(11)-H(29), and H(29)-C(11)-C(5)-O(38).

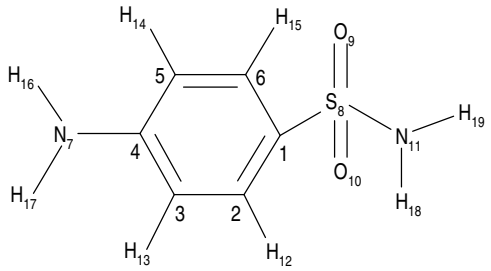
Drug: Sulfanilamide

Three torsion angles and one bond angle are missing parameters. All of the angles link the phenyl ring with the sulfonamide substituent. The torsion angles are: C(1)-S(8)-N(11)-H(18), C(2)-C(1)-S(8)-N(11), and C(6)-C(1)-S(8)-N(11). The bond angle is C(1)-S(8)-N(11). Most of the bond lengths varying by more than 0.02 Å are located on the sulfonamide substituent. Those bond lengths are: C(1)-S(8), S(8)-O(10), S(8)-N(11), and N(11)-H(18). Two bond

lengths, C(4)-N(7) and N(7)-H(16), are located on the amino substituent. There is only one bond angle that varies by more than 5 degrees. It is angle H(16)-N(7)-H(17).

There are four torsion angles that vary by more than 10 degrees. Three are located on the sulfonamide substituent. The angles are: C(1)-S(8)-N(11)-H(19), O(9)-S(8)-N(11)-H(19), and O(10)-S(8)-N(11)-H(19). One torsion angle, C(3)-C(4)-N(7)-H(16), links the phenyl ring with the amino substituent.

Fig. 17 Sulfanilamide

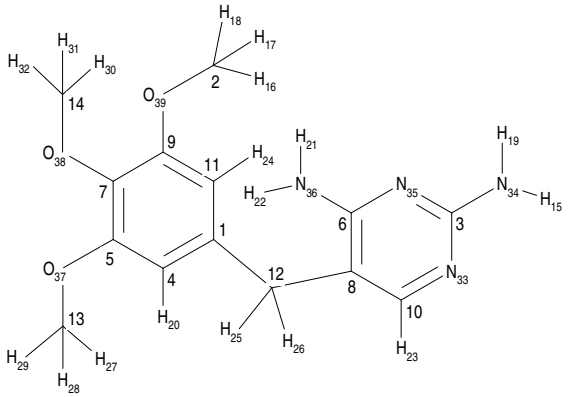


Drug: Trimethoprim

The two bond angles that are missing parameters are both located on one of the amino substituents. The two angles are: H(15)-N(34)-H(19) and H(21)-N(36)-H(22).

The bond lengths that vary by more than 0.02 Å are either carbon-heteroatom bonds, carbon-hydrogen bonds, or nitrogen-hydrogen bonds. The carbon-heteroatom bond lengths are: C(5)-O(37), C(6)-N(36), C(7)-O(38), and C(9)-O(39). The carbon-hydrogen bond lengths are located on one of the methoxy substituents. The bond lengths are: C(14)-H(30), C(14)-H(31), and C(14)-H(32). The nitrogen-hydrogen bond lengths are: H(19)-N(34) and H(22)-N(36).

Fig. 18 Trimethoprim



There is only one bond angle that varies by more than 5 degrees. It is located on one of the methoxy substituents. It is angle C(7)-O(38)-C(14).

The torsion angles that vary by more than 10 degrees are located either on the diazine ring or the benzyl ring. The angles on the diazine ring are: C(1)-C(12)-C(8)-C(6), C(1)-C(12)-C(8)-C(10), C(6)-N(35)-C(3)-N(34), C(8)-C(6)-N(36)-H(22), C(12)-C(8)-C(6)-N(35), H(15)-N(34)-C(3)-N(33), and H(15)-N(34)-C(3)-N(35). The angles located on the benzyl ring are: C(5)-C(7)-O(38)-C(14) and C(9)-C(7)-O(38)-C(14).

IX. Antifungals

Most fungal infections are superficial but there are some strains that can produce life-threatening infections. Fungal infections usually need one or more of the host's defense mechanisms to be disabled by a predisposing condition in order to successfully infect the organism. Many antifungal drugs are toxic and are therefore limited in their use. The principal antifungal drugs and their mechanisms of action are:

1) Polyenes- the drug binds to sterols in the cell membrane thus affecting its integrity. Potassium and magnesium ions can then leak from the cell.
2) Flucytosine- an antimetabolite that after being converted to an active form inhibits the synthesis of DNA.
3) Imidazoles- in actively growing fungi the drug inhibits the synthesis of membrane sterols.
4) Griseofulvin- the drug inhibits fungal mitosis.
5) Allylamines- by interfering with the synthesis of ergosterol by blocking an enzyme[9].

Drug: Griseofulvin

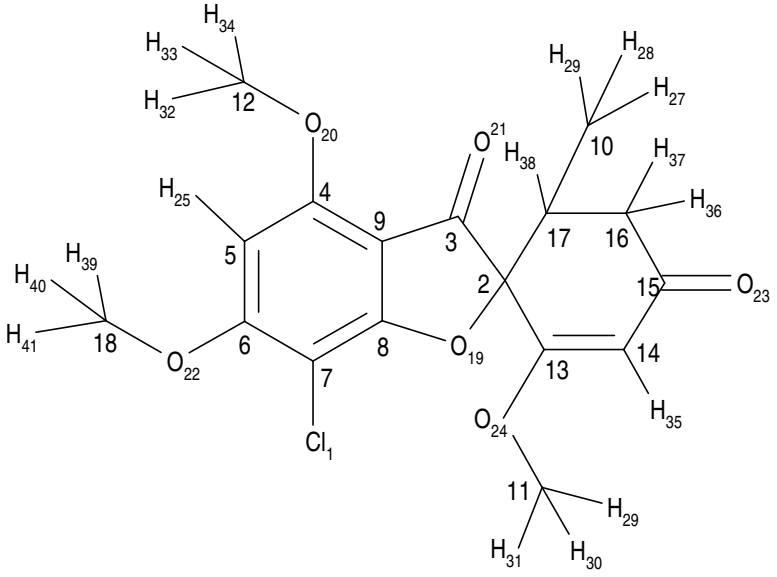
The missing parameters are for torsion angles located in the ring system of this molecule. Two torsion angles, C(3)-C(2)-O(19)-C(8) and O(19)-C(2)-C(3)-C(9), are located in the five-membered ring. The remaining torsion angles are: Cl(1)-C(7)-C(6)-O(22), Cl(1)-C(7)-C(8)-O(19), C(3)-C(2)-C(13)-O(24), O(19)-C(2)-C(13)-C(14), C(17)-C(2)-C(13)-O(24), O(19)-C(2)-C(3)-O(21), and O(19)-C(2)-C(13)-O(24). There are parameters missing for two bond angles. The angles are C(3)-C(2)-O(19) and C(13)-C(2)-O(19).

There are π-atom parameters missing for this molecule. Parameters of atom types (2-81) and (81-81) are missing. MM3 substitutes atom type 7 for atom type 81.

The bond lengths that vary by more than 0.02 Å between the crystal and MM3 values are located in one of the molecule's rings. The bond lengths located in the phenyl ring are: C(4)-O(20), C(5)-C(6), C(5)-H(25), and C(6)-O(22). The bond lengths located in the five-membered ring are: C(2)-C(3) and C(8)-O(19). The bond lengths located in the six-membered ring are: C(10)-C(17), C(13)-O(24), C(14)-C(15), C(15)-C(16), C(16)-H(36), C(16)-H(37), and C(17)-H(38).

There are no bond angles in this molecule that vary by more than 5 degrees between crystal and MM3 values. Most of the torsion angles that vary by more than 10 degrees are located in the six-membered ring. The angles are: C(13)-C(14)-C(15)-C(16), C(13)-C(14)-C(15)-O(23), C(14)-C(13)-C(2)-C(17), C(14)-C(15)-C(16)-C(17), C(14)-C(15)-C(16)- H(36), C(14)-C(15)-C(16)-H(37), C(17)-C(16)-C(15)-O(23), O(23)-C(15)-C(16)-H(36), and O(23)-C(15)-C(16)-H(37). There are two torsion angles located in the five-membered ring. The angles are: C(3)-C(2)-C(13)-C(14) and C(8)-O(19)-C(2)-C(13).

Fig. 19 Griseofulvin

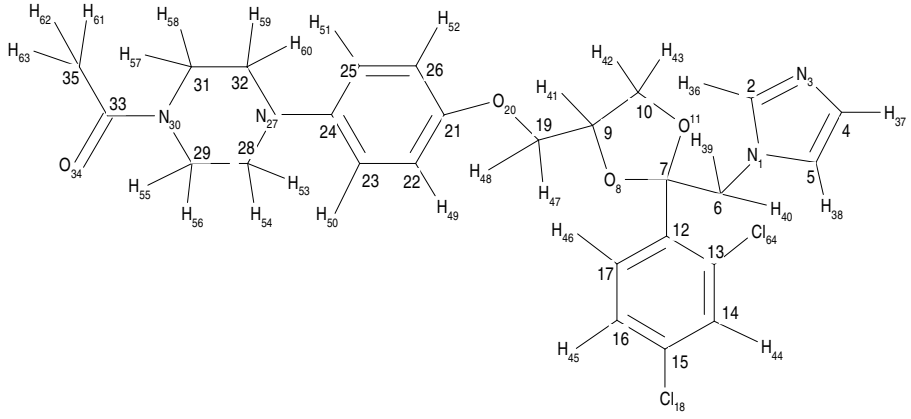


Drug: Ketoconazole

The missing parameters for this molecule are for torsion angles located in one of the rings in this molecule. The angles that bridge the imidazoles and 1,3-dioxolane rings are: N(1)-C(6)-C(7)-O(8), N(1)-C(6)-C(7)-O(11), C(7)-C(6)-N(1)-C(2), and C(7)-C(6)-N(1)-C(5). The angle that bridges the imidazole and phenyl rings is N(1)-C(6)-C(7)-C(12). There is one angle located in the imidazole ring; it is N(3)-C(2)-N(1)-C(6). There are two angles located in the dioxolane ring, one of which is a bond angle. The angles are O(8)-C(9)-C(19)-O(20) and C(7)-C(6)-N(1)

Many of the bond lengths calculated by MM3 for this molecule vary by more than 0.02 Å from the crystal values. The bond lengths located in the imidazole ring are: N(1)-C(6), N(3)-C(4), C(4)-H(37), and C(4)-H(38). The bond lengths located in the dioxolane ring are: C(6)-C(7), C(7)-C(12), O(8)-C(9), and C(10)-O(11). The bond lengths located in the phenyl ring are: C(12)-C(13), C(16)-C(17), O(20)-C(21), C(21)-C(22), C(21)-C(26), C(23)-C(24), and C(24)-C(25). The bond lengths located in the piperazine ring are: C(24)-N(27), C(28)-H(53), C(28)-H(54), C(29)-H(55), N(30)-C(33), C(31)-H(57), C(31)-H(58), C(32)-H(59), and C(32)-H(60). There is one bond length located on the keto side chain. It is carbon-carbon bond C(33)-C(35).

Fig. 20 Ketoconazole



There are five bond angles that vary by more than 5 degrees between crystal and MM3 values. One angle, C(7)-O(11)-C(10), is located in the dioxolane ring. Two angles, C(22)-C(21)-C(26) and C(21)-C(26)-C(25), are located in the phenyl ring. Two angles, N(30)-C(31)-H(57) and H(59)-C(32)-H(60), are located in the piperazine ring.

The torsion angles that vary by more than 10 degrees between crystal and MM3 values are located in one of 3 rings: the dioxolane, phenyl, or piperazine ring. The torsion angles located in the dioxolane ring are: O(8)-C(7)-O(11)-C(10), O(8)-C(9)-C(19)-O(20), C(9)-O(8)-C(7)-C(12), and C(10)-O(11)-C(7)-C(12). The torsion angles located in the phenyl ring are: C(19)-O(20)-C(21)-C(22), O(20)-C(21)-C(26)-H(52), C(21)-C(26)-C(25)-C(24), C(22)-C(21)-C(26)-H(52),C(22)-C(23)-C(24)-C(25), and C(23)-C(24)-C(25)-C(26). The torsion angles that link the phenyl ring with the piperazine ring are: C(23)-C(24)-N(27)-C(28), C(23)-C(24)-N(27)-C(32), C(25)-C(24)-N(27)-C(28), and C(25)-C(24)-N(27)-C(32). The torsion angles located in the piperazine ring are: C(29)-N(30)-C(33)-O(34), C(29)-N(30)-C(33)-C(35), and H(57)-C(31)-C(32)-H(60).

X. Antimycobacterials

Mycobacteria cause the illnesses tuberculosis and leprosy. Both are chronic diseases that require long-term treatment. The drugs used to treat tuberculosis have 3 mechanisms of action:

1. Inhibiting the synthesis of protein.
2. Inhibiting synthesis of the cell wall.
3. Other mechanisms.

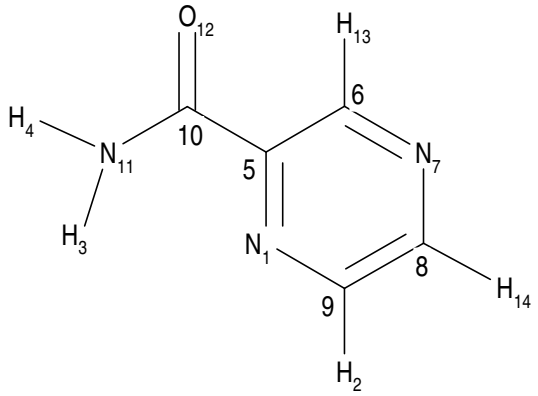
One of the major drugs used to treat leprosy, dapsone, functions by inhibiting dihydropteroate synthetase in the folate pathway[10].

Drug: Pyrazinamide

The missing parameters for this molecule are for angles that link the diazine ring with the amide substituent. The torsion angles that are missing parameters are: N(1)-C(5)-C(10)-N(11), N(1)-C(5)-C(10)-O(12), N(7)-C(6)-C(5)-C(10), and C(10)-C(5)-N(1)-C(9). The bond angles that are missing parameters are: N(1)-C(5)-C(10) and C(5)-C(10)-N(11).

There are π-atom parameters missing for this molecule. Parameters for atom types (37-162), (37-151), (2-162), (2-151), (162-151), (162-96), and (151-96) are missing. MM3 substitutes π-atom parameters of atom type 2 for atom type 37, atom type 2 for atom type 96, atom types 2 and 40 for atom type 151, and atom types 2 and 3 for atom type 162.

Fig. 21 Pyrazinamide



The bond lengths that vary by more than 0.02 Å between crystal and MM3 values are located either in the diazine ring or the amide substituent. The bond lengths located in the diazine ring are: H(2)-C(9), C(5)-C(6), C(6)-H(13), C(8)-C(9), and C(8)-H(14). The bond lengths located in the amide substituent are: H(3)-N(11), H(4)-N(11), and C(10)-N(11). There are no bond angles in this molecule that vary by more than 5 degrees between crystal and MM3 values.

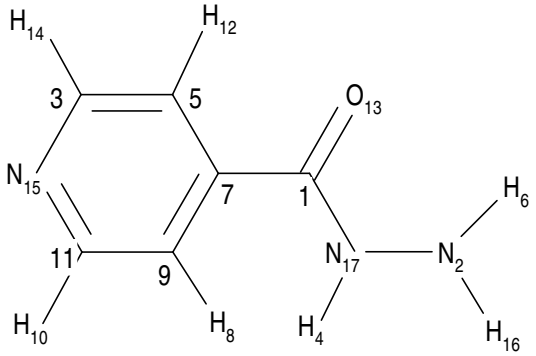
The torsion angles that vary by more than 10 degrees between crystal and MM3 values are located primarily in the diazine ring. The angles are: N(1)-C(5)-C(6)-H(13), N(1)-C(9)-C(8)-H(14), C(6)-N(7)-C(8)-H(14), and C(8)-N(7)-C(6)-H(13). Two angles, H(3)-N(11)-C(10)-C(5) and H(3)-N(11)-C(10)-O(12), are located on the amide substituent.

Drug: Isoniazid

Most of the missing parameters for this molecule are for angles located on the hydrazide substituent. The torsion angles are: C(1)-N(17)-N(2)-H(6), O(13)-C(1)-N(17)-N(2), C(7)-C(1)-N(17)-H(4), and O(13)-C(1)-N(17)-H(4). The torsion angles that link the pyridine ring with the hydrazide substituent are: C(7)-C(1)-N(17)-N(2), C(5)-C(7)-C(1)-N(17), and C(9)-C(7)-C(1)-N(17). The bond angles located in the hydrazide substituent are: O(13)-C(1)-N(17), C(1)-N(17)-N(2), and C(1)-N(17)-H(4). One bond angle, C(7)-C(1)-N(17), links the pyridine ring with the hydrazide substituent. One bond length, C(1)-N(17), is missing parameters.

Pi-atom parameters of atom types (3-37) are missing for this molecule. MM3 substitutes π-atom parameters of atom types (2-2) in their place.

Fig. 22 Isoniazid



Several of the bond lengths that vary by more than 0.02 Å between crystal and MM3 values are located on the hydrazide substituent. The bond lengths are: C(1)-N(17), N(2)-H(6), N(2)-N(17), and H(4)-N(17). There are 3 bond lengths located on the pyridine ring. The bond lengths are C(3)-H(14), H(10)-C(11), and C(11)-N(15).

There are only 2 bond angles in this molecule that vary by more than 5 degrees between crystal and MM3 values. The angles are H(16)-N(2)-N(17) and C(1)-N(17)-H(4).

The torsion angles that vary by more than 10 degrees between crystal and MM3 values are either located on the hydrazide substituent or link the hydrazide substituent with the pyridine ring. The angles located on the hydrazide substituent are: C(1)-N(17)-N(2)-H(6), N(2)-N(17)-C(1)-O(13), H(4)-N(17)-C(1)-O(13), H(4)-N(17)-N(2)-H(6), and H(4)-N(17)-N(2)-H(16). The angles that link the hydrazide substituent with the pyridine ring are: N(2)-N(17)-C(1)-C(7), H(4)-N(17)-C(1)-C(7), C(5)-C(7)-C(1)-O(13), C(5)-C(7)-C(1)-N(17), and C(9)-C(7)-C(1)-N(17).

XI. Antivirals

A virus consists of a core genome of nucleic acid which is contained in a protein shell and sometimes is surrounded by a lipoprotein membrane. Viruses cannot reproduce on their own and must use the DNA/RNA replicating mechanism of a host cell. The mechanisms of action for antiviral drugs are:

1) Interfering with viral nucleic acid synthesis or regulation.

2) Interfering with the binding of the virus cell.

3) Interrupting the uncoating of a viral cell.

4) Stimulating the host's immune system.

Antiviral drugs must often penetrate infected cells in order to effect a therapeutic response. This can result in toxic effects to healthy cells which will limit a drug's usefulness [11].

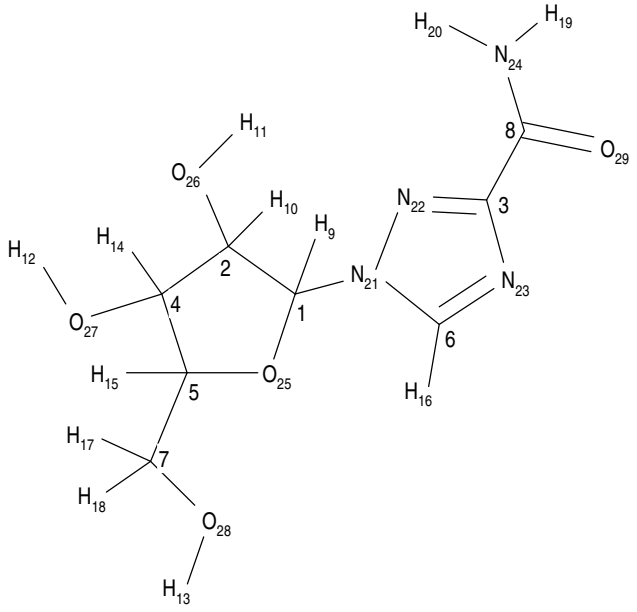
Drug: Ribavarin

Many of the missing parameters for this molecule are for torsion or bond angles located on the imidazole ring. The torsion angles that link the tetrahydrofuran ring with the imidazole ring are: N(23)-C(6)-N(21)-C(1), C(3)-N(22)-N(21)-C(1), C(2)-C(1)-N(21)-C(6), C(2)-C(1)-N(21)-N(22), C(4)-C(2)-C(1)-N(21), N(21)-C(1)-O(25)-C(5), O(25)-C(1)-N(21)-C(6), H(9)-C(1)-N(21)-N(22), H(10)-C(2)-C(1)-N(21), N(21)-C(1)-C(2)-O(26), and O(25)-C(1)-N(21)-N(22). The torsion angles that link the amide substituent with the imidazole ring are: C(8)-C(3)-N(23)-C(6), C(8)-C(3)-N(22)-N(21), N(22)-C(3)-C(8)-N(24), N(22)-C(3)-C(8)-O(29), N(23)-C(3)-C(8)-N(24), and N(23)-C(3)-C(8)-O(29). The bond angles that link the tetrahydrofuran ring with the imidazole ring are: C(2)-C(1)-N(21), O(25)-C(1)-N(21), and C(1)-N(21)-N(22). The bond angles that link the amide substituent with the imidazole ring are: N(22)-C(3)-C(8), N(23)-C(3)-C(8), and C(3)-C(8)-N(24).

There are π-atom parameters missing for this molecule. The missing parameters are for atom types (2-162), (2-151), (2-79), (162-40), (162-37), (162-151), (162-79), (40-151), (40-79), (37-151), (37-79), and (151-79). MM3 substituted π-atom parameters of atom types 2 and 37 for atom type 37, atom types 2 and 40 for atom type 40, atom types 2 and 7 for atom type 79, atom types 2 and 40 for atom type 151, and atom types 2 and 3 for atom type 162

. Several of the bond lengths that vary by more than 0.02 Å are located on the tetrahydrofuran ring. The bond lengths are: C(1)-H(9), C(1)-O(25),C(2)-H(10), C(4)-H(14), C(5)-H(15), and C(5)-O(25). The carbon-hydrogen bond lengths vary by more than 0.13 Å. The bond length C(1)-N(21) varies by more than 0.02 Å. There are two bond lengths, C(6)-H(16) and C(6)-N(21), located in the imidazole ring that are longer in MM3 than in the crystal. The carbon-hydrogen bond is longer in MM3 by more than 0.2 Å. There are three oxygen-hydrogen bond lengths that vary by more than 0.2 Å. The bond lengths are H(11)-O(26), H(12)-O(27), and H(13)-O(28). There are three bond lengths on the amide substituent- C(8)-N(24), H(19)-N(24), and H(20)-N(24), that are longer in MM3 than in the crystal. The two hydrogen-nitrogen bonds vary by more than 0.1 angstrom.

Fig. 23 Ribavarin



Most of the bond angles that vary by more than 5 degrees between crystal and MM3 are located on the tetrahydrofuran ring or link it with one of the substituents. The angles are: H(9)-C(1)-N(21), H(9)-C(1)-O(25), C(4)-C(2)-H(10), C(2)-C(4)-H(14), H(14)-C(4)-O(27), C(4)-C(5)-H(15), C(7)-C(5)-H(15), H(15)-C(5)-O(25), C(2)-O(26)-H(11), and C(4)-O(27)-H(12). There are 3 bond angles located on the amide substituent; the angles are: C(8)-N(24)-H(19), C(8)-N(24)-H(20), and H(19)-N(24)-H(20). There is one bond angle located on the side chain attached to the tetrahydrofuran ring. The angle is C(7)-O(28)-H(13).

Many of the torsion angles that vary by more than 10 degrees between crystal and MM3 are located on the tetrahydrofuran ring. The angles are: C(1)-O(25)-C(5)-H(15), C(4)-C(2)-C(1)-H(9), C(5)-O(25)-C(1)-H(9), and H(10)-C(2)-C(1)-O(25). Some of the torsion angles link the tetrahydrofuran ring with one of its substituents. The angles are: C(1)-C(2)-O(26)-H(11), C(2)-C(4)-O(27)-H(12), C(4)-C(2)-O(26)-H(11), C(5)-C(4)-O(27)-H(12), C(5)-C(7)-O(28)-H(13), H(9)-C(1)-C(2)-O(26), H(10)-C(2)-O(26)-H(11), H(12)-O(27)-C(4)-H(14), and H(15)-C(5)-C(7)-O(28). There are two torsion angles, H(9)-C(1)-N(21)-N(22) and C(6)-N(21)-C(1)-H(9), that link the imidazole ring with the tetrahydrofuran ring. There are two torsion angles, C(3)-C(8)-N(24)-H(19) and C(3)-C(8)-N(24)-H(20), that link the imidazole ring with its amide substituent. There are two torsion angles, H(19)-N(24)-C(8)-O(29) and H(20)-N(24)-C(8)-O(29), that are located on the amide substituent.

XII. Antiarhythmic drugs

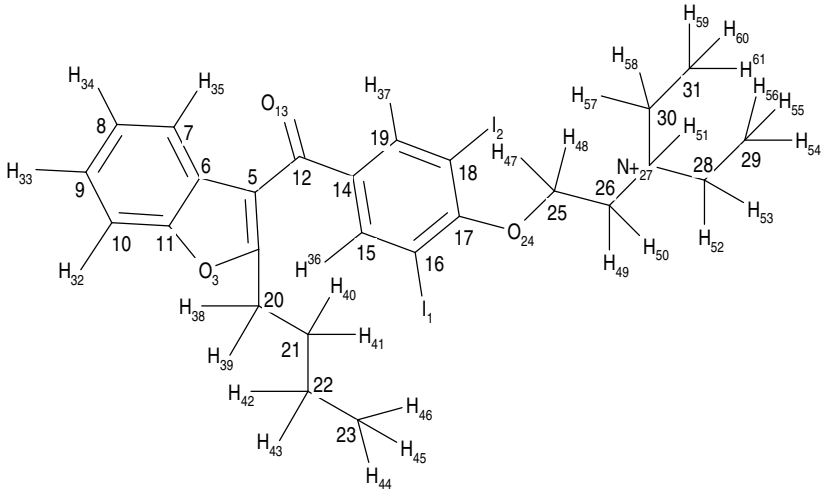
Arrhythmia is a term used to describe any abnormality in the normal rhythmic function of the heart. Major classes of arrythmias are atrial and ventricular fibrillation. Fibrillation is an irregular or disorganized wave of contraction (usually multiple) that spreads randomly through cardiac tissue. It can lead to heart failure. Some mechanisms of action of antiarhythmic drugs are: sodium or calcium channel blockade, β-receptor blockade, or prolonging repolarization of cardiac muscle[12].

Drug: Amiodarone

There are parameters missing for two torsion angles. One angle, C(21)-C(20)-C(4)-O(3), links the furan ring with the butyl substituent. The second angle, O(24)-C(25)-C(26)-N(27), is located on the side chain that contains both ether and amine functional groups.

Most of the bond lengths that vary between crystal and MM3 values do not vary by more 0.03 Å. There are two bond lengths, O(3)-C(4) and C(5)-C(12), located on the furan ring. There are several bond lengths located on one of the two phenyl rings. The bond lengths are: C(8)-C(9), C(9)-C(10), C(10)-C(11), C(15)-H(36), C(16)-C(17), C(17)-C(18), C(17)-O(24), and C(19)-H(37). One bond length, C(12)-O(13), is located on the carbonyl functional group. There are two bond lengths, C(20)-C(21) and C(22)-C(23), located on the butyl side chain. There are four bond lengths located on the amine section of the side chain. The bond lengths are: C(26)-N^+(27), N^+(27)-H(51), C(28)-C(29), and C(30)-C(31).

Fig. 24 Amiodarone



There are 4 bond angles located in one of the phenyl rings that vary by more than 5 degrees between crystal and MM3 values. The angles are: I(1)-C(16)-C(15), I(1)-C(16)-C(17), C(14)-C(19)-H(37), and C(18)-C(19)-H(37). There are 3 bond angles that connect one of the phenyl rings with the ether side chain. The angles are: C(16)-C(17)-O(24), C(18)-C(17)-O(24), and C(17)-O(24)-C(25). There are 2 bond angles, C(26)-N^+(27)-H(51) and C(30)-N^+(27)-H(51), that are located on the amine segment of the side chain.

There is one torsion angle that links the furan ring with the butyl substituent, C(5)-C(4)-C(20)-C(21), that varies by more than 10 degrees between crystal and MM3 values. There are 3 torsion angles varying by more than 10 degrees that link the phenyl ring with the ether side chain. The angles are: C(16)-C(17)-O(24)-C(25), C(17)-O(24)-C(25)-C(26), and C(18)-C(17)-O(24)-C(25). There are 4 torsion angles located on the amine segment of the side chain that vary by more than 10 degrees. The angles are: C(26)-N^+(27)-C(30)-C(31), C(28)-N^+(27)-C(30)-C(31), C(29)-C(28)-N^+(27)-H(51), and C(31)-C(30)-N^+(27)-H(51).

XIII. Antihypertensive drugs

The definition of hypertension is an elevation of arterial blood pressure above a defined normal value. Hypertension can lead to or exacerbate several other diseases such as atherosclerosis, coronary artery disease, aortic aneurysm, congestive heart failure, stroke, diabetes, and renal and retinal disease. There are several classes of antihypertensive drugs with different mechanisms of action. The major mechanisms of action are: decreasing the force and rate of cardiac contraction, decreasing the blood volume, relaxing vascular smooth muscle, and decreasing sympathetic nervous system output[13].

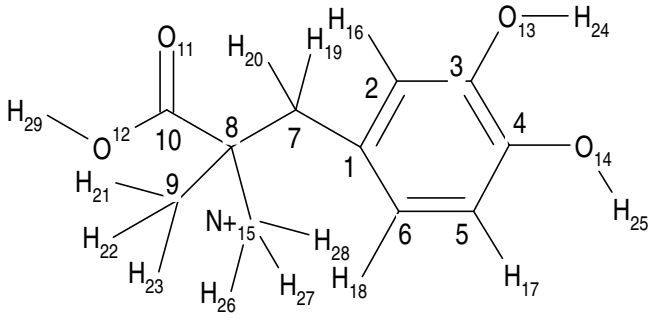
Drug: Methyl-dopa

There are parameters missing for one torsion angle that links the amine functional group with the carboxylic acid functional group. It is angle N(15)-C(8)-C(10)-O(12).

The bond lengths that vary the most (more than 0.1 Å) are located either in a hydroxyl group or the amine group. The bond lengths are: C(3)-O(13), C(4)-O(14), O(13)-H(24), O(14)-H(25), N^+(15)-H(26), N^+(15)-H(27), and N^+(28). There are bond lengths that vary by more than 0.02 Å in the side chain and carboxylic acid group. The bond lengths in the side chain are: C(7)-

C(8), C(7)-H(19), and C(7)-H(20). The bond lengths in the carboxylic acid group are: C(8)-C(10), C(10)-O(12), and O(12)-H(29).

Fig. 25 Methyl-dopa



There is one bond angle that varies by more than 5 degrees between crystal and MM3 values for this molecule. The angle is C(10)-O(12)-H(29) and it is located on the carboxylic acid functional group.

There are 5 torsion angles linking the benzyl ring with the side chain that vary by more than 10 degrees between crystal and MM3 values. The angles are: C(2)-C(1)-C(7)-C(8), C(2)-C(1)-C(7)-H(19), C(2)-C(1)-C(7)-H(20), C(6)-C(1)-C(7)-H(19), and C(6)-C(1)-C(7)-H(20).

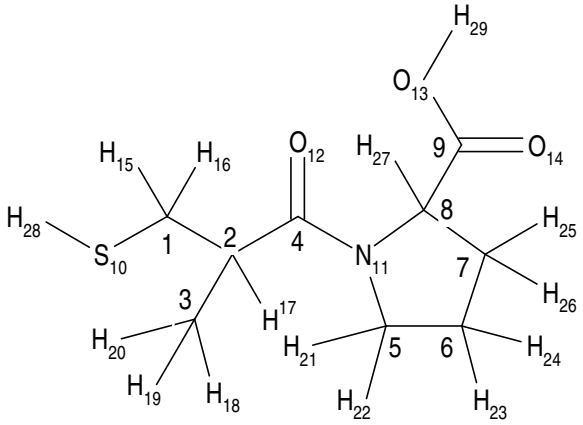
Drug: captopril

There are no missing parameters for this molecule.

There are 4 bond lengths located on the pyrrolidine ring that vary by more than 0.02 Å between crystal and MM3 values. The bond lengths are: C(4)-N(11), C(5)-C(6), C(6)-C(7), and C(7)-C(8). There are 3 bond lengths located on the substituent attached to the ring nitrogen that vary by more than 0.02 Å. The bond lengths are: C(2)-C(3), C(4)-O(12), and S(10)-H(28). There is one bond length, O(13)-H(29), located on the carboxylic acid substituent that varies by more than 0.1 Å between crystal and MM3 values.

Several bond angles that vary by more than 5 degrees between crystal and MM3 values are located on the pyrrolidine ring. The angles are: C(6)-C(5)-H(21), H(23)-C(6)-H(24), C(6)-C(7)-H(25), C(8)-C(7)-H(25), H(25)-C(7)-H(26), and C(9)-C(8)-H(27). There is one bond angle, C(1)-S(10)-H(28), located on the thiol segment of the side chain. There is one bond angle, C(9)-O(13)-H(29), located on the carboxylic acid substituent.

Fig. 26 Captopril



Most of the torsion angles that vary by more than 10 degrees between crystal and MM3 values are located on the pyrrolidine ring or link the ring with one of the substituent groups. The torsion angles located on the pyrrolidine ring are: C(5)-C(6)-C(7)-H(25), C(5)-C(6)-C(7)-H(26), C(6)-C(7)-C(8)-H(27), C(7)-C(6)-C(5)-H(22), C(8)-C(7)-C(6)-H(24), C(8)-N(11)-C(5)-H(21), N(11)-C(8)-C(7)-H(25), N(11)-C(8)-C(7)-H(26), H(21)-C(5)-C(6)-H(23), H(22)-C(5)-C(6)-H(24), H(23)-C(6)-C(7)-H(25), H(24)-C(6)-C(7)-H(25), H(24)-C(6)-C(7)-H(26), H(25)-C(7)-C(8)-H(27), and H(26)-C(7)-C(8)-H(27). The torsion angles that link the side chain with the pyrrolidine ring are: C(1)-C(2)-C(4)-N(11), C(3)-C(2)-C(4)-N(11), and N(11)-C(4)-C(2)-H(17). The torsion angles that link the carboxylic acid substituent with the pyrrolidine ring are: C(7)-C(8)-C(9)-O(13), C(7)-C(8)-C(9)-O(14), N(11)-C(8)-C(9)-O(13), and N(11)-C(8)-C(7)-H(26). There are two torsion angles, O(13)-C(9)-C(8)-H(27) and O(14)-C(9)-C(8)-H(27), located on the carboxylic acid substituent. There are 3 torsion angles located on the side chain. The angles are: C(1)-C(2)-C(4)-O(12), C(3)-C(2)-C(4)-O(12), and O(12)-C(4)-C(2)-H(17).

Drug: Fosinopril

The missing parameters for this molecule are for torsion angles that include the phosphate functional group. The angles are: O(7)-C(27)-O(6)-P(1), P(1)-C(16)-C(15)-O(4), P(1)-C(16)-C(15)-N(9), C(15)-C(16)-P(1)-O(5), C(15)-C(16)-P(1)-O(6), O(6)-C(27)-O(7)-C(31), and C(15)-C(16)-P(1)-C(17).

The bond lengths that vary by more than 0.02 Å are located in several areas. There is one bond length, P(1)-C(17), located in the phosphate group. There is one bond length, O(3)-C(14),

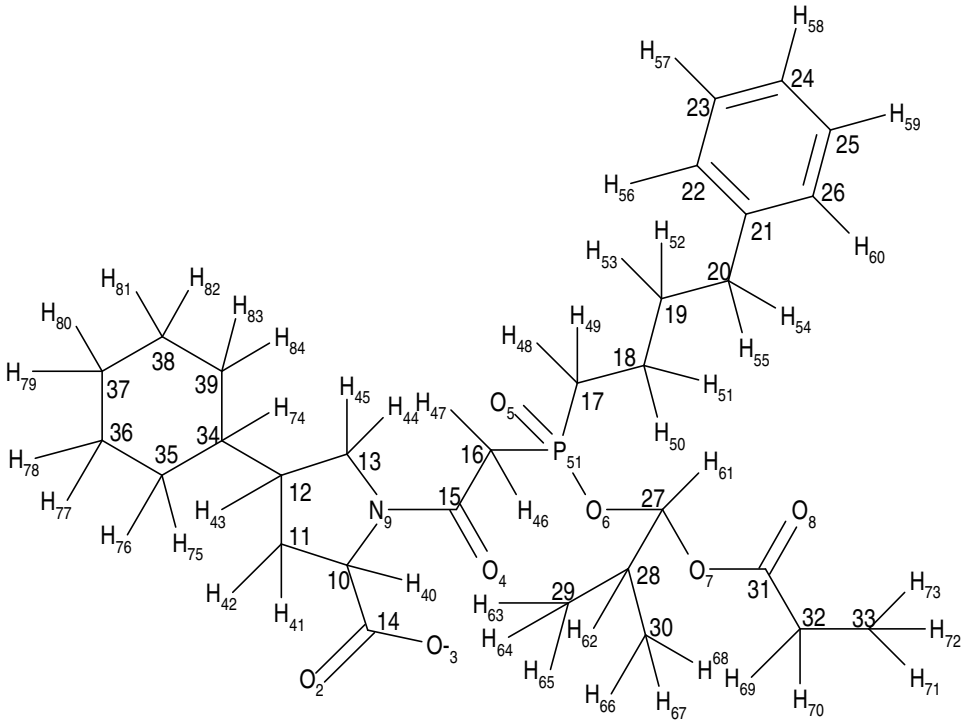
located in the carboxylate group. There is one bond length, O(4)-C(15), located in the carbonyl group attached to the phosphate group. There are 6 bond lengths located in the ester segment of the substituent attached to the phosphate group. The bond lengths are: O(7)-C(27), O(7)-C(31), C(27)-C(28), C(27)-H(61), C(32)-C(33), and C(32)-H(70). There are several bond lengths located in the pyrrolidine ring. The bond lengths are: N(9)-C(15), C(10)-H(40), C(11)-H(41), C(11)-H(42), C(12)-H(43), C(13)-H(44), and C(13)-H(45). There are 4 bond lengths located in the carbonyl group attached to the phosphate group. The bond lengths are: C(15)-C(16), C(16)-H(46), C(16)-H(47), and C(17)-C(18). There are two bond lengths, C(19)-C(20) and C(20)-C(21), located in the butyl side chain. There are 3 bond lengths located in the benzyl ring. The bond lengths are: C(21)-C(26), C(22)-H(56), and C(26)-H(60). There are 4 bond lengths located in the cyclohexyl ring. The bond lengths are: C(34)-C(35), C(37)-C(38), C(38)-C(39), and C(39)-H(84).

There are 3 bond angles in this molecule that vary by more than 5 degrees between crystal and MM3 values. The angles are: C(14)-C(10)-H(40, C(34)-C(12)-H(43), and N(9)-C(15)-C(16).

Many of the torsion angles that vary by more than 10 degrees between crystal and MM3 values are located either in the phosphate functional group or the pyrrolidine ring. The angles in the phosphate group are: P(1)-C(16)-C(15)-O(4), P(1)-C(16)-C(15)-N(9), O(5)-P(1)-O(6)-C(27), O(5)-P(1)-C(16)-C(15), O(5)-P(1)-C(16)-H(46), O(5)-P(1)-C(16)-H(47), O(5)-P(1)-C(17)-C(18), O(6)-P(1)-C(16)-C(15), O(6)-P(1)-C(16)-H(46), O(6)-P(1)-C(16)-H(47), C(16)-P(1)-O(6)-C(27), and C(17)-P(1)-O(6)-C(27). The angles located in the pyrrolidine ring are: N(9)-C(15)-C(16)-H(46), N(9)-C(15)-C(16)-H(47), C(10)-N(9)-C(13)-H(44), C(10)-N(9)-C(15)-C(16), C(12)-C(11)-C(10)-H(40), C(13)-N(9)-C(10)-C(14), C(13)-N(9)-C(10)-H(40), and C(13)-C(12)-C(34)-C(39). There are several torsion angles that link the carboxylate group with the pyrrolidine ring. The angles are: O(2)-C(14)-C(10)-N(9), O(2)-C(14)-C(10)-C(11), O(2)-C(14)-C(10)-H(40), O(3)-C(14)-C(10)-N(9), O(3)-C(14)-C(10)-C(11), and O(3)-C(14)-C(10)-H(40). One torsion angle, O(4)-C(15)-N(9)-C(10), links the ketone group with the pyrrolidine ring. There are 3 torsion angles that link the ester group with the phosphate group. The angles are: O(6)-C(27)-O(7)-C(31), C(28)-C(27)-O(7)-C(31), and C(31)-O(7)-C(27)-H(61). One torsion angle, C(17)-

C(18)-C(19)-C(20), is located on the butyl chain. Three torsion angles link the butyl chain with the benzyl ring. The angles are: C(19)-C(20)-C(21)-C(22), C(19)-C(20)-C(21)-C(26), and C(20)-C(21)-C(26)-H(60). One torsion angle, C(39)-C(34)-C(12)-H(43), is located on the cyclohexyl ring.

Fig. 27 Fosinopril



XIV. Drugs That Affect the Sympathetic Nervous System

The sympathetic nervous system controls the action of smooth muscle, cardiac muscle, and glandular cells. Sympathetic neurons use norepinephrine to transmit information. Drugs in this category can either mimic or block the actions of the sympathetic system. Some of their mechanisms of action are: modulation of noradrenergic transmission in neurons, catecholamine activation of adrenergic receptors, direct-acting receptor agonists, and indirect action (facilitating release of norepinephrine or blocking its reuptake)[14].

Drug: Timolol

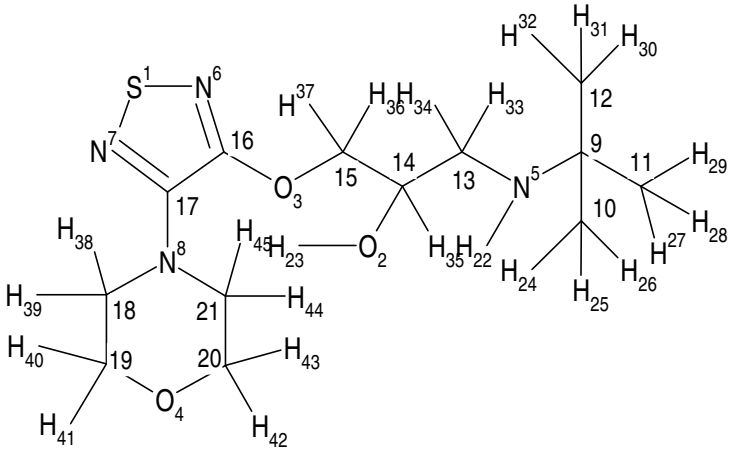
The missing parameters for this molecule are primarily for angles located in either the thioimine or 6-membered rings. The torsion angles located in the 1,2,5-thiadiazole ring are:

S(1)-N(6)-C(16)-O(3), N(7)-C(17)-C(16)-O(3), and C(15)-O(3)-C(16)-N(6). The torsion angles located in the 6-membered ring are: O(4)-C(19)-C(18)-N(8), O(4)-C(20)-C(21)-N(8), C(20)-C(21)-N(8)-C(17), C(20)-C(21)-N(8)-C(18), C(19)-C(18)-N(8)-C(21), and H(44)-C(21)-N(8)-C(18). There are several torsion angles that link the two rings. The angles are: N(8)-C(17)-N(7)-S(1), N(8)-C(17)-C(16)-O(3), N(7)-C(17)-N(8)-C(18), N(7)-C(17)-N(8)-C(21), and C(19)-C(18)-N(8)-C(17). There is one torsion angle, O(2)-C(14)-C(15)-O(3), that links the hydroxyl group with the ether group. There are 3 bond angles located on the 6-membered ring. The angles are: C(18)-N(8)-C(21), C(19)-C(18)-N(8), and C(20)-C(21)-N(8). There is one bond angle, N(6)-C(16)-O(3), that links the 1,2,5-thiadiazole ring with the ether group.

There are π-atom parameters of atom types (42-40) missing for this molecule. MM3 substituted π-atom parameters of atom types 2 and 40 for atom type 40, atom types 2 and 42 for atom type 42, and atom type 2 for atom type 161.

The bond lengths that vary by more than 0.02 Å between crystal and MM3 values are spread across the molecule. There are 3 bond lengths, S(1)-N(6), C(16)-C(17), and N(7)-C(17), located on the 1,2,5-thiadiazole ring. There are 3 bond lengths, N(8)-C(18), N(8)-C(21), and C(20)-C(21), located on the 6-membered ring. One bond length, N(8)-C(17), links both rings. One bond length, O(2)-H(23), is located on the hydroxyl group. One bond length, O(3)-C(16), is located in the ether group. One bond length, N(5)-H(22), is located in the amine group. One bond length, C(9)-C(11), is located in the tert-butyl group. One bond length, C(14)-H(35), is located on the propyl segment of the side chain.

Fig. 28 Timolol



Several of the bond angles that vary by more than 5 degrees between crystal and MM3 values are located on the 6-membered ring. The angles are: C(19)-C(18)-H(38), H(38)-C(18)-H(39), O(4)-C(19)-H(40), C(18)-C(19)-H(41), N(8)-C(21)-H(44), N(8)-C(21)-H(45), and C(20)-C(21)-H(44). One bond angle, C(17)-N(8)-C(21), links the two rings. One bond angle, O(3)-C(15)-H(36), is located in the ether group. Two bond angles, C(14)-C(15)-H(36) and H(36)-C(15)-H(37), are located on the propyl segment of the side chain.

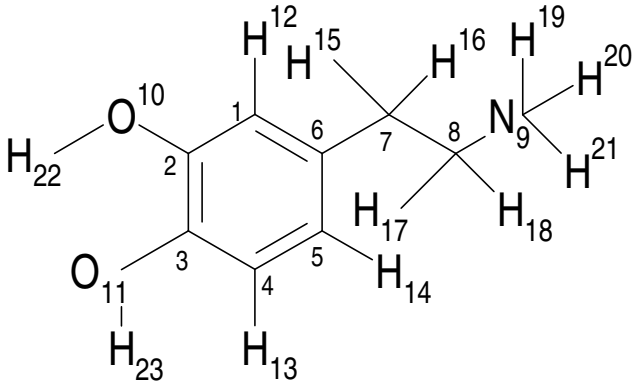
The torsion angles that vary by more than 10 degrees are located in various areas in the molecule. One angle, O(2)-C(14)-C(13)-N(5), links a hydroxyl group with the amine group. Three torsion angles, O(2)-C(14)-C(15)-O(3), O(2)-C(14)-C(15)-H(36), and O(2)-C(14)-C(15)-H(37), link a hydroxyl group with the ether group. Two angles, O(3)-C(15)-C(14)-C(13) and O(3)-C(15)-C(14)-H(35), link the ether group with the propyl chain. Three angles, C(13)-C(14)-O(2)-H(23), C(15)-C(14)-O(2)-H(23), and H(23)-O(2)-C(14)-H(35), link a hydroxyl group with the propyl chain. Two angles, N(5)-C(13)-C(14)-C(15) and N(5)-C(13)-C(14)-H(35), link the amine group with the propyl chain. Five angles are located on the propyl chain. The angles are: C(13)-C(14)-C(15)-H(36), C(13)-C(14)-C(15)-H(37), H(34)-C(13)-C(14)-H(35), H(35)-C(14)-C(15)-H(36), and H(35)-C(14)-C(15)-H(37). Three angles, N(6)-C(16)-O(3)-C(15), C(15)-O(3)-C(16)-C(17), and C(16)-O(3)-C(15)-H(36), link an imine group with the ether group. One angle, C(9)-N(5)-C(13)-C(14), is located on the tert-butyl amine group. Eight angles link the 5-membered ring with the 6-membered ring. The angles are: N(7)-C(17)-N(8)-C(21), C(16)-C(17)-N(8)-C(21), C(17)-N(8)-C(18)-C(19), C(17)-N(8)-C(18)-H(38), C(17)-N(8)-C(18)-H(39), C(17)-N(8)-C(21)-C(20), C(17)-N(8)-C(21)-H(44), and C(17)-N(8)-C(21)-H(45). Thirteen angles are located on the 6-membered ring. O(4)-C(19)-C(18)-H(38), N(8)-C(18)-C(19)-H(40), C(19)-O(4)-C(20)-H(42), C(19)-O(4)-C(20)-H(43), C(21)-N(8)-C(18)-H(38), C(21)-N(8)-C(18)-H(39), H(38)-C(18)-C(19)-H(40), H(38)-C(18)-C(19)-H(41), H(39)-C(18)-C(19)-H(40), H(39)-C(18)-C(19)-H(41), H(42)-C(20)-C(21)-H(44), H(42)-C(20)-C(21)-H(45), and H(43)-C(20)-C(21)-H(44).

Drug: Dopamine

There are no missing parameters for this molecule.

The bond lengths that vary by more than 0.02 Å are located either in the benzyl ring or are heteroatom-hydrogen bonds. Three bond lengths are located in the benzyl ring. One, C(1)-C(2), is a carbon-carbon bond. The other two bond lengths, C(2)-O(10) and C(3)-O(11), link the benzyl ring with a hydroxyl group. One bond length, C(7)-C(8), is located on the ethyl chain. There are three nitrogen-hydrogen bond lengths that vary by more than 0.07 Å. The bond lengths are: N^+(9)-H(19), N^+(9)-H(20), and N^+(9)-H(21). There are two oxygen-hydrogen bond lengths that vary by more than 0.1 Å. The bond lengths are: O(10)-H(22) and O(11)-H(23). There are four bond angles that vary by more than 5 degrees between crystal and MM3 values. The angles are: H(19)-N^+(9)-H(20), H(20)-N^+(9)-H(21), C(2)-O(10)-H(22), and C(3)-O(11)-H(23). There are no torsion angles in this molecule that vary by more than 10 degrees.

Fig. 29 Dopamine



Drug: Atenolol

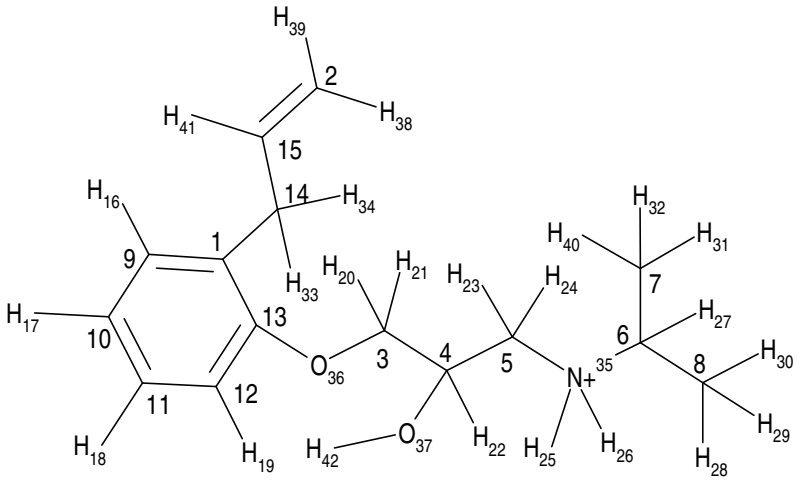
There is one torsion angle that is missing parameters. The angle is O(36)-C(3)-C(4)-O(37).

There are 6 bond lengths located on the benzyl ring that vary by more than 0.02 Å between crystal and MM3 values. The bond lengths are: C(1)-C(9), C(1)-C(13), C(9)-H(16), C(12)-C(13), C(12)-H(19), and C(13)-O(36). There are 4 bond lengths located on the alkene side chain. The bond lengths are: C(2)-C(15), C(14)-C(15), C(14)-H(33), and C(14)-H(34). There are 3 bond lengths located on the propyl chain. The bond lengths are: C(3)-C(4), C(4)-C(5), and C(4)-H(22). One bond length, C(5)-N^+(35), links the propyl chain with the amine group. Two bond lengths, C(6)-C(8) and C(6)-H(27), are located on the tert-butyl group. Three bond lengths

are located on the amine group. The bond lengths are: C(6)-N^+(35), H(25)-N^+(35), and H(26)-N^+(35). One bond length, O(37)-H(42), is located on a hydroxyl group.

There are 9 bond angles located on the alkene side chain that vary by more than 5 degrees between crystal and MM3 values. The angles are: C(15)-C(2)-H(38), C(15)-C(2)-H(39), H(38)-C(2)-H(39), C(15)-C(14)-H(33), C(15)-C(14)-H(34), H(33)-C(14)-H(34), C(2)-C(15)-C(14), C(2)-C(15)-H(41), and C(14)-C(15)-H(41). There are 4 bond angles located on the propyl chain. The angles are: C(3)-C(4)-C(5), C(3)-C(4)-H(22), C(5)-C(4)-H(22), and H(22)-C(4)-O(37).There are 5 bond angles located on the tert-butyl amine group. The angles are: C(7)-C(6)-H(27), H(27)-C(6)-N^+(35), C(5)-N^+(35)-C(6), C(5)-N^+(35)-H(26), and H(25)-N^+(35)-H(26). One bond angle, C(1)-C(9)-H(16), is located on the benzyl ring. Three bond angles link the aromatic ring with the alkene side chain. The angles are: C(1)-C(14)-C(15), C(1)-C(14)-H(33), and C(1)-C(14)-H(34).

Fig. 30 Atenolol



There are 5 torsion angles linking the benzyl ring with the alkene side chain that vary by more than 10 degrees between crystal and MM3 values. The angles are: C(1)-C(14)-C(15)-C(2), C(1)-C(14)-C(15)-H(41), C(9)-C(1)-C(14)-C(15), C(9)-C(1)-C(14)-H(33), and C(9)-C(1)-C(14)-H(34). Two torsion angles, C(2)-C(15)-C(14)-H(33) and H(33)-C(14)-C(15)-H(41), are located on the alkene side chain. Five torsion angles are located on the benzyl ring. The angles are: C(13)-C(1)-C(9)-H(16), C(13)-C(1)-C(14)-C(15), C(13)-C(1)-C(14)-H(33), C(13)-C(1)-C(14)-H(34), and C(14)-C(1)-C(9)-H(16). Six torsion angles link the propyl chain with the amine group. The angles are: C(3)-C(4)-C(5)-N^+(35), C(4)-C(5)-N^+(35)-C(6), C(4)-C(5)-

N^+(35)-H(25), C(4)-C(5)-N^+(35)-H(26), H(22)-C(4)-C(5)-N^+(35), and N^+(35)-C(5)-C(4)-O(37). Two torsion angles, C(5)-C(4)-C(3)-O(36) and H(22)-C(4)-C(3)-O(36), link the ether group with the propyl chain. Three torsion angles link the hydroxyl group with the propyl chain. The angles are: C(3)-C(4)-O(37)-H(42), C(5)-C(4)-O(37)-H(42), and H(22)-C(4)-O(37)-H(42). Seven torsion angles are located on the tert-butyl amine group. The angles are: C(5)-N^+(35)-C(6)-C(7), C(5)-N^+(35)-C(6)-C(8), C(5)-N^+(35)-C(6)-H(27), C(7)-C(6)-N^+(35)-H(25), C(8)-C(6)-N^+(35)-H(25), H(25)-N^+(35)-C(6)-H(27), and H(26)-N^+(35)-C(6)-H(27).

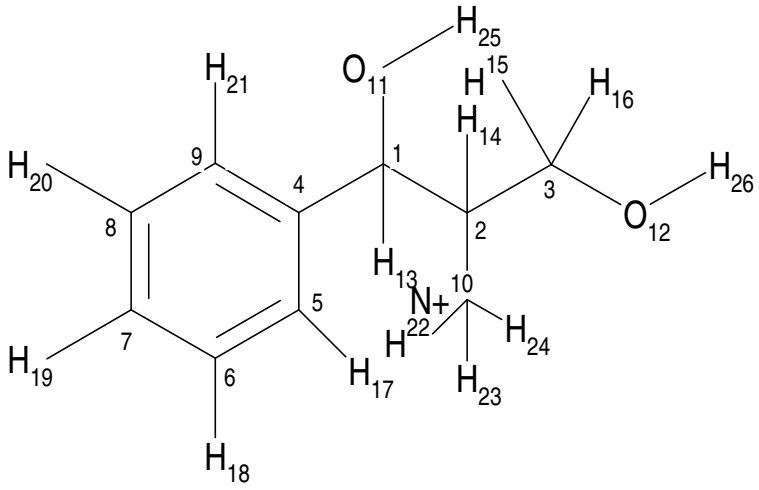
Drug: Phenyl-propanolamine

There are no missing parameters for this molecule.

There are three bond lengths that vary by more than 0.02 Å located on the hydroxyl group. They are bond lengths C(1)-O(11), O(11)-H(25), and O(12)-H(26). There are three bond lengths located on the ammonium group. They are bond lengths N^+(10)-H(22), N^+(10)-H(23), and N^+(10)-H(24). There is one bond length located on the phenyl ring. It is bond length C(4)-C(5).

There are five bond angles that vary by more than 5 degrees that include the ammonium group. The angles are: N^+(10)-C(2)-H(14), C(2)-N^+(10)-H(22), C(2)-N^+(10)-H(23), H(22)-N^+(10)-H(23), and H(23)-N^+(10)-H(24). There are two bond angles located on the hydroxyl group. The angles are: C(2)-C(3)-O(12) and C(3)-O(12)-H(26). There is one bond angle, C(3)-C(2)-H(14), located on the propyl chain.

Fig. 31 Phenyl-propanolamine



There are nine torsion angles linking the propyl chain with the hydroxyl group that vary by more than 10 degrees between crystal and MM3 values. The angles are: C(1)-C(2)-C(3)-O(12), C(2)-C(1)-O(11)-H(25), C(2)-C(3)-O(12)-H(26), C(3)-C(2)-C(1)-O(11), C(4)-C(1)-O(11)-H(25), C(9)-C(4)-C(1)-O(11), O(11)-C(1)-C(2)-H(14), O(12)-C(3)-C(2)-H(14), and H(13)-C(1)-O(11)-H(25). There are 13 torsion angles that include the ammonium group. The angles are: C(1)-C(2)-N^+(10)-H(22), C(1)-C(2)-N^+(10)-H(23), C(1)-C(2)-N^+(10)-H(24), C(3)-C(2)-N^+(10)-H(22), C(3)-C(2)-N^+(10)-H(23), C(3)-C(2)-N^+(10)-H(24), C(4)-C(1)-C(2)-N^+(10), N^+(10)-C(2)-C(1)-O(11), N^+(10)-C(2)-C(1)-H(13), N^+(10)-C(2)-C(3)-O(12), H(14)-C(2)-N^+(10)-H(22), H(14)-C(2)-N^+(10)-H(23), and H(14)-C(2)-N^+(10)-H(24). There are five torsion angles that include part of the phenyl ring and the propyl chain. The angles are: C(2)-C(1)-C(4)-C(9), C(3)-C(2)-C(1)-C(4), C(3)-C(2)-C(1)-H(13), C(4)-C(1)-C(2)-H(14), and C(9)-C(4)-C(1)-H(13).

XV. Antidepressants

Depression is a disorder of mood. It has cognitive, affective, motor, and somatic symptoms. Some of its symptoms are: loss of interest or pleasure in activities, decreased appetite, insomnia, fatigue, feelings of guilt, and thoughts about death and suicide. In its most severe form depression can lead to death by suicide. There are 4 major classes of antidepressant drugs:

1. Tricyclics.
2. Monoamine oxidase inhibitors.
3. Selective serotonin reuptake inhibitors.
4. Atypical antidepressants.

Many antidepressants work by modulating the release and/or reuptake several neurotransmitters in the brain[15].

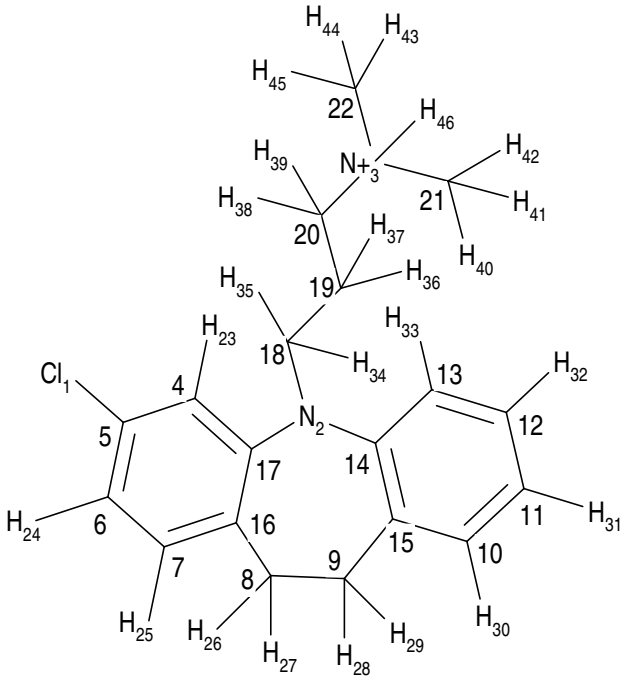
Drug: Chlorimipramine

There are 4 torsion angles in the arylamine group that are missing parameters. The angles are: C(4)-C(17)-N(2)-C(14), C(13)-C(14)-N(2)-C(17), C(16)-C(17)-N(2)-C(14), and C(15)-C(14)-N(2)-C(17). The bond angle C(14)-N(2)-C(17), located in the arylamine group is missing parameters.

There are two bond lengths located in the arylamine group, N(2)-C(14) and N(2)-C(17), that vary by more than 0.02 Å between MM3 and crystal values. There are 4 bond lengths located on the ammonium group. The bonds are: N^{+}(3)-C(20), N^{+}(3)-C(21), N^{+}(3)-C(22), and N^{+}(3)-H(46). There are 4 bond lengths located on one of the aryl rings. The bonds are: C(5)-C(6), C(7)-H(25), C(11)-C(12), and C(12)-C(13). Five bond lengths are located on the 7-membered ring. The bonds are: C(8)-H(26), C(8)-H(27), C(9)-C(15), C(9)-H(28), and C(9)-H(29). There is one bond length, C(18)-C(19), located on the alkyl bridge. Six bond lengths are located on one of the methyl groups. The bonds are: C(21)-H(40), C(21)-H(41), C(21)-H(42), C(22)-H(43), C(22)-H(44), and C(22)-H(45).

There are 5 bond angles that vary by more than 5 degrees between MM3 and crystal values. One bond angle, C(14)-N(2)-C(17), is located in the arylamine group. Two bond angles, C(21)-N^{+}(3)-H(46) and N^{+}(3)-C(21)-H(42), are located in the ammonium group. One bond angle, H(26)-C(8)-H(27), is located in the 7-membered ring. One bond angle, H(40)-C(21)-H(42), is located in a methyl group.

Fig. 32 Chlorimipramine



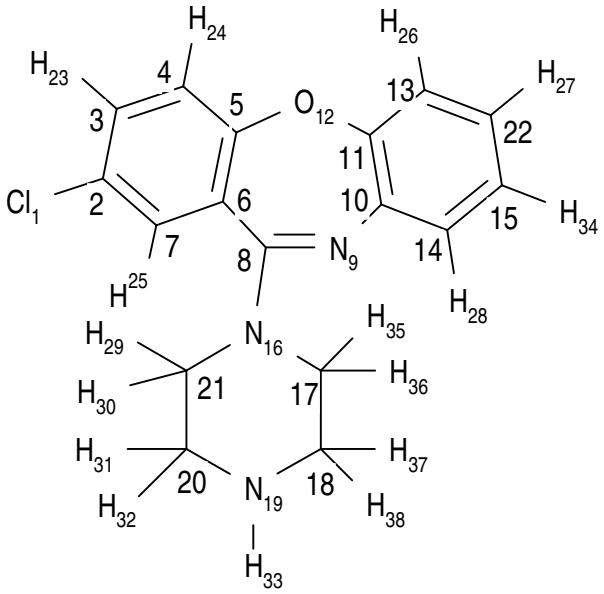
There are 7 torsion angles located in the arylamine group that vary by more than 10 degrees between MM3 and crystal values. The angles are: N(2)-C(18)-C(19)-C(20), C(4)-C(17)-

N(2)-C(14), C(4)-C(17)-N(2)-C(18), C(14)-N(2)-C(17)-C(16), C(14)-N(2)-C(18)-C(19), C(16)-C(17)-N(2)-C(18), and C(17)-N(2)-C(18)-C(19). Two torsion angles, N^{+}(3)-C(20)-C(19)-C(18) and H(44)-C(22)-N^{+}(3)-H(46), are located in the ammonium group. Two torsion angles, C(16)-C(8)-C(9)-H(28) and C(16)-C(8)-C(9)-H(29), are located in the 7-membered ring.

Drug: Amoxapine

There are 8 torsion angles located in the piperazine ring that are missing parameters. The angles are: C(18)-C(17)-N(16)-C(8), C(20)-C(21)-N(16)-C(8), N(16)-C(17)-C(18)-N(19), N(16)-C(17)-C(18)-H(37), N(16)-C(21)-C(20)-N(19), C(20)-C(21)-N(16)-C(17), H(29)-C(21)-N(16)-C(17), and C(18)-C(17)-N(16)-C(21). There are two torsion angles, N(9)-C(8)-N(16)-C(17) and N(9)-C(8)-N(16)-C(21), that link the pyridine-type nitrogen atom with the piperazine ring. One torsion angle, N(9)-C(10)-C(11)-O(12), links the furan-type oxygen atom with the pyridine-type nitrogen atom.

Fig. 33 Amoxapine



Three bond angles located on the piperazine ring are missing parameters. The angles are: C(17)-N(16)-C(21), C(18)-C(17)-N(16), and C(20)-C(21)-N(16).

There are two bond lengths located on the phenyl ring that vary by more than 0.02 Å between MM3 and crystal values. The bonds are: C(4)-C(5) and C(5)-C(6). Six bond lengths are located on the piperazine ring. The bond lengths are: N(16)-C(17), N(16)-C(21), C(17)-

C(18), C(18)-H(38), N(19)-H(33), and C(21)-H(30). Two bond lengths, C(5)-O(12) and C(11)-O(12), are located on the 7-membered ring.

Two bond angles that vary by more than 5 degrees between MM3 and crystal values are located on the 7-membered ring. The angles are: C(10)-C(11)-O(12) and C(5)-O(12)-C(11). Eight bond angles are located on the piperazine ring. The angles are: C(8)-N(16)-C(17), N(16)-C(17)-H(35), N(16)-C(17)-H(36), C(18)-C(17)-H(35), H(35)-C(17)-H(36), C(17)-C(18)-H(37), N(19)-C(18)-H(37), and H(37)-C(18)-H(38).

Ten torsion angles located on the piperazine ring vary by more than 10 degrees between MM3 and crystal values. The angles are: C(8)-N(16)-C(17)-C(18), C(8)-N(16)-C(17)-H(35), C(8)-N(16)-C(17)-H(36), C(8)-N(16)-C(21)-C(20), C(8)-N(16)-C(21)-H(29), C(8)-N(16)-C(21)-H(30), N(16)-C(17)-C(18)-H(37), N(19)-C(18)-C(17)-H(35), C(20)-N(19)-C(18)-H(37), and H(33)-N(19)-C(18)-H(37). Five torsion angles link one of the phenyl rings with the furan-type oxygen atom. The angles are: C(4)-C(5)-O(12)-C(11), C(5)-O(12)-C(11)-C(10), C(5)-O(12)-C(11)-C(13), C(8)-C(6)-C(5)-O(12), and C(6)-C(5)-O(12)-C(11). One torsion angle, C(6)-C(8)-N(16)-C(17), links the phenyl ring with the piperazine ring. Two torsion angles, C(8)-N(9)-C(10)-C(14) and N(9)-C(8)-N(16)-C(17), link the 7-membered ring with the piperazine ring. One torsion angle, N(9)-C(10)-C(11)-O(12), links the pyridine-type nitrogen atom with the furan-type oxygen atom. One torsion angle, C(10)-N(9)-C(8)-N(16), links the pyridine-type nitrogen atom with the piperazine ring.

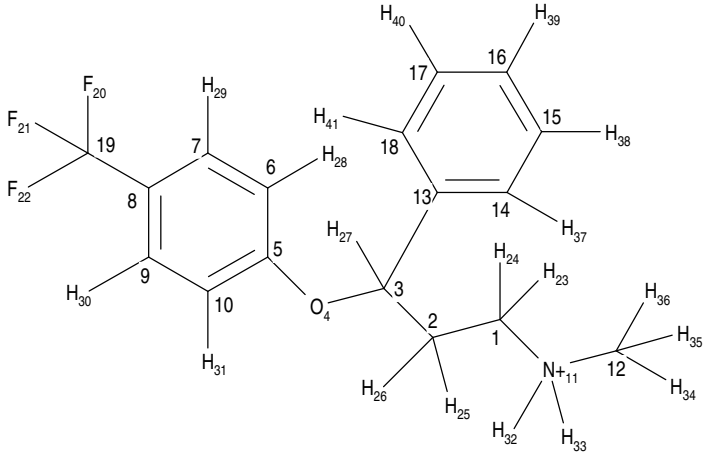
Drug: Fluoxetine

The 3 torsion angles that are missing parameters link the benzyl ring with the phenoxy group. The angles are: O(4)-C(3)-C(13)-C(14), O(4)-C(3)-C(13)-C(18), and C(13)-C(3)-O(4)-C(5). One bond angle, C(13)-C(3)-O(4), is missing parameters.

Two bond lengths that vary by more than 0.02 Å are located on the alkyl chain between the phenoxy group and the ammonium group. The bond lengths are: C(2)-C(3) and C(3)-H(27). Three bond lengths are located in the phenoxy group. The bonds are: O(4)-C(5), C(5)-C(10), and C(7)-C(8). Four bond lengths are located in the trifluoromethyl group. The bonds are: C(8)-C(19), C(19)-F(20), C(19)-F(21), and C(19)-F(22). Three bond lengths are located in the benzyl

group. The bonds are: C(13)-C(18), C(16)-C(17), and C(17)-C(18). Three bond lengths are located in the ammonium group. The bonds are: N^{+}(11)-C(12), N^{+}(11)-H(32), and N^{+}(11)-H(33).

Fig. 34 Fluoxetine



Two bond angles located in the trifluoromethyl group vary by more than 5 degrees between MM3 and crystal values. The angles are: F(20)-C(19)-F(21) and F(21)-C(19)-F(22).

Four torsion angles that vary by more than 10 degrees between MM3 and crystal values are located in the phenoxy group. The angles are: C(3)-O(4)-C(5)-C(6), C(3)-O(4)-C(5)-C(10), O(4)-C(3)-C(13)-C(14), and C(5)-O(4)-C(3)-H(27). One torsion angle, C(2)-C(1)-N^{+}(11)-H(33), is located in the ammonium group. One torsion angle, C(9)-C(8)-C(19)-F(20), links the trifluoromethyl group with the phenoxy group.

XVI. Antipsychotics

Psychosis is a thought disorder. Some of its symptoms are: disturbances in perception of reality, impaired cognitive functioning, and reduced or inappropriate mood. Schizophrenia is the illness most often linked with psychosis. Antipsychotics function by interacting with several neurotransmitters. Antipsychotic efficacy is primarily dependent on how well the drug can disrupt dopaminergic neurotransmission[16].

Drug: Thioridazine

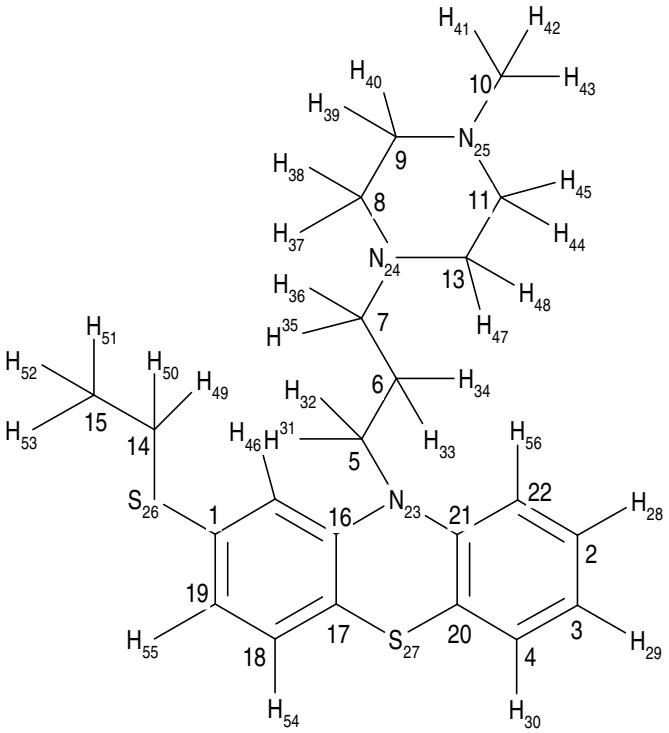
Eight torsion angles located in the arylsulfide group are missing parameters. The angles are: C(15)-C(14)-S(26)-C(1), H(49)-C(14)-S(26)-C(1), C(12)-C(1)-S(26)-C(14), C(19)-C(1)-S(26)-C(14), C(16)-C(12)-C(1)-S(26), C(18)-C(19)-C(1)-S(26), S(26)-C(1)-C(12)-H(46), and

S(26)-C(1)-C(19)-H(55). Four torsion angles are located in the arylamine group. The angles are: C(6)-C(5)-N(23)-C(16), C(6)-C(5)-N(23)-C(21), C(7)-C(6)-C(5)-N(23), and N(23)-C(5)-C(6)-H(33). Two torsion angles link the arylamine group with the thiophene-type sulfur atom. The angles are: N(23)-C(16)-C(17)-S(27) and N(23)-C(21)-C(20)-S(27).

One bond length, C(1)-S(26), located in the arylsulfide group is missing parameters. Three bond angles, C(12)-C(1)-S(26), C(14)-S(26)-C(1), and C(19)-C(1)-S(26), are located in the arylsulfide group. One bond angle, C(6)-C(5)-N(23), is located in the arylamine group.

No bond lengths for this molecule vary by more than 0.02 Å between MM3 and crystal values. No bond angles for this molecule vary by more than 5 degrees between MM3 and crystal values. No torsion angles for this molecule vary by more than 10 degrees between MM3 and crystal values.

Fig. 35 Thioridazine



Drug: Chlorprothixene

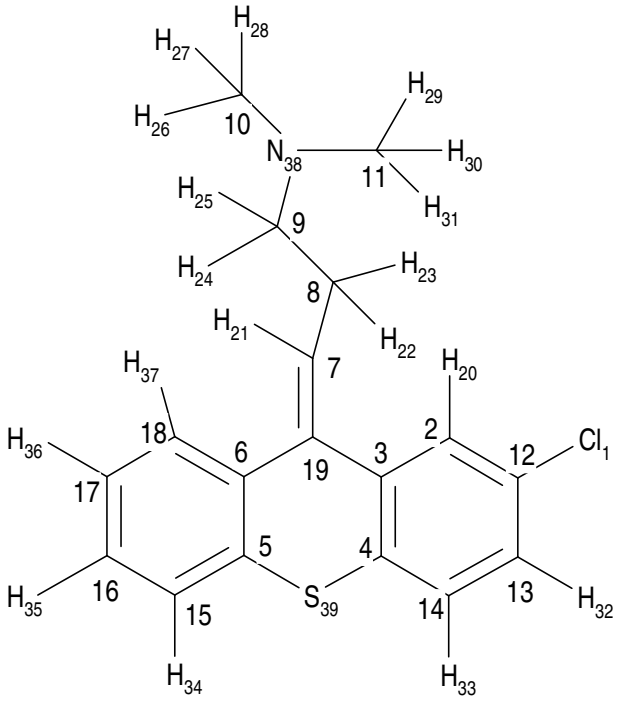
There are no missing parameters for this molecule.

One bond length, C(7)-C(8), located in the propyl chain varies by more than 0.02 Å between MM3 and crystal values. Seven bond lengths are located in one of the N-methyl groups.

The bonds are: C(10)-H(26), C(10)-H(27), C(10)-H(28), C(11)-H(29), C(11)-H(30), C(11)-H(31), and C(11)-N(38). Two bond lengths, C(12)-C(13) and C(16)-C(17), are located in one of the phenyl rings.

One bond angle, H(30)-C(11)-N(38), that varies by more than 5 degrees between MM3 and crystal values is located in one of the N-methyl groups. One torsion angle, C(9)-C(8)-C(7)-C(19), located in the propyl chain varies by more than 10 degrees between MM3 and crystal values.

Fig. 36 Chlorprothixene



Drug: Molindone

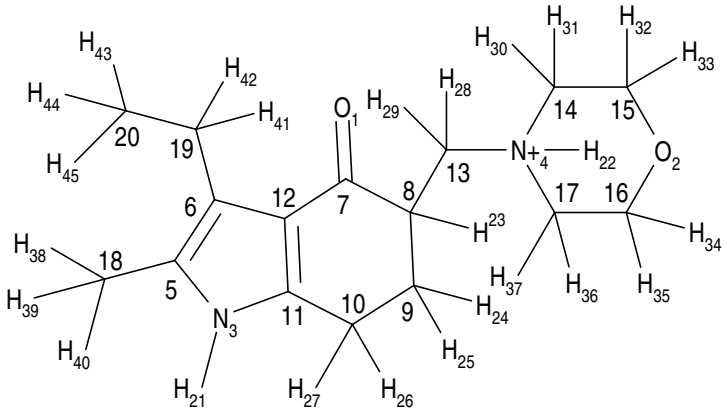
Pi-atom parameters of atom types (81-40) and (40-3) are missing for this molecule. MM3 substitutes π-atom parameters of atom types (2-2) in their place. MM3 also substitutes π-atom parameters of atom types (7-2) for (81-2), (7-2) for (81-160), (40-2) for (40-160), (2-2) for (2-160), (3-2) for (3-160), and (2-2) for (160-2).

Two torsion angles, C(9)-C(10)-C(11)-N(3) and C(7)-C(12)-C(11)-N(3), located on the cyclohexanone ring are missing parameters.

Four bond lengths that vary by more than 0.02 Å between MM3 and crystal values are located in the pyrrole-type ring. The bond lengths are: N(3)-C(11), N(3)-H(21), C(5)-C(6), and C(6)-C(12). Seven bond lengths are located in the cylcohexenone ring. The bond lengths are: C(7)-C(12), C(8)-C(13), C(8)-H(23), C(9)-H(24), C(9)-H(25), C(10)-H(26), and C(10)-H(27). Eleven bond lengths are located in the six-membered ring. The bonds are: N^+(4)-C(14), N^+(4)-H(22), C(14)-H(30), C(14)-H(31), C(15)-H(32), C(15)-H(33), C(16)-H(34), C(16)-H(35), C(17)-H(36), C(17)-H(37), and C(19)-H(20).

No bond angles in this molecule vary by more than 5 degrees between MM3 and crystal values. Four torsion angles, N^+(4)-C(13)-C(8)-C(7), N^+(4)-C(13)-C(8)-C(9),C(8)-C(13)-N^+(4)-C(17) and N^+(4)-C(13)-C(8)-H(23), that vary by more than 10 degrees between MM3 and crystal values link the ammonium nitrogen atom with the cyclohexanone ring. Four torsion angles are located in the six-membered ring. The angles are: C(13)-N^+(4)-C(17)-H(37), H(31)-C(14)-C(15)-H(33), H(34)-C(16)-C(17)-H(37), and H(35)-C(16)-C(17)-H(37). Four torsion angles are located in the cyclohexanone ring. The angles are: C(11)-C(10)-C(9)-H(25), C(12)-C(7)-C(8)-C(13), H(25)-C(9)-C(10)-H(26), and H(25)-C(9)-C(10)-H(27). One torsion angle, C(12)-C(6)-C(19)-C(20), is located in the pyrrole-type ring.

Fig. 37 Molindone



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CHAPTER 4
CONCLUSIONS

MM3 begins its analysis of a molecule by determining what types of atoms are present in the molecule. The program also determines what atom type each atom is. The combination of bond angle type and atom type help to determine the specific nature of the local electronic environment. The molecules in this study often included several combinations of different functional groups in a single compound. These arrangements led to combinations of atom types not previously parameterized.

The majority of missing parameters are for torsion angles. Almost all of these angles include either part of a π-system and/or a heteroatom. The V_2 parameter is connected to the bond order of the central bond B-C in an A-B-C-D system;[1] if B-C is part of a π-system this can affect its stability. Some of the torsion angles that were missing parameters varied from the crystal values by a sizeable amount (20º-40º). The majority of torsion angles that were missing parameters varied between 10º-20º from the crystal values. Torsion angles varied more as a group when compared to bond lengths and bond angles. Torsion angles can take less energy to deform than a bond length or bond angle. Losing stability from disrupting part of a π-system or by having a locally unfavorable torsion angle in the crystal may be compensated for by crystal packing forces or intermolecular forces.

Bond lengths in MM3 that are missing parameters were generally heteroatom – heteroatom bonds; however, there were some carbon-heteroatom bonds that were also missing parameters. Bond lengths that include hydrogen showed the largest degree of variance between crystal and MM3 values. Bonds to hydrogen are difficult to locate accurately in x-ray diffraction because it is the center of electron density which is being measured; the single hydrogen electron is often pulled toward the atom it is bonded to. Bond lengths in x-ray diffraction also depend on the vibrational motion of the entire crystal which can vary with the temperature of the crystal. Several carbon-hydrogen bond lengths were longer in MM3 than in the crystal. These changes

can possibly be explained by a combination of electronegativity effects, the *trans* lone pair effect, and steric effects.[2] Carbon-carbon bond length changes most often took place in rings (saturated or unsaturated). Several carbon-nitrogen and carbon-oxygen bond lengths were longer in the crystal than the MM3 values. This effect could be due to distortion of the bond's electron density by the heteroatom lone pair.

The total number of bond angles that varied by more than 5º between crystal and MM3 values was smaller than the number of bond lengths or torsion angles. MM3 estimates the parameters for angle bending from the geometry of the center atom and the types of atoms (non-hydrogen or hydrogen) attached to the center atom.[3] The bond angle is also affected by the length of the attached bonds and 1,3 nonbonded interactions. In this data set MM3 predicted the bond angles of the ring atoms in 3-,4-, and 5-membered rings usually within 5º-10º of the crystal value. Bond angles between ring atoms and hydrogen atoms varied more (10º-20º) between crystal and MM3 values; this could be due to greater nonbonded interactions in these types of rings.

Overall, MM3 can calculate fairly accurately the molecular structure when compared to x-ray diffraction. Crystal packing forces, intermolecular forces, and vibrational motion must be accounted for if a more accurate calculation of structure is desired.

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APPENDIX

SUPPLEMENTARY MATERIAL FOR CHAPTER 3

Table 1. Diazepam

I. Missing Parameters

A. Missing for atoms 2- 3- 31- 4 (type 162- 1- 37- 2)
Missing for atoms 31- 3- 2- 32 (type 37- 1- 162- 151)
Missing for atoms 31- 3- 2- 33 (type 37- 1- 162- 79)
Missing for atoms 31- 3- 2 (type 37- 1- 162) angle type 2

B. Estimated Parameters

4 torsional parameters are read in

Atom type numbers	V1	V2	V3
162 1 37 2	0.000	0.160	0.090
37 1 162 151	0.000	0.160	0.090
37 1 162 79	0.000	0.160	0.090

1 bending parameter is read in

Atom type numbers	Kb	Theta
37 1 162	0.695	109.500

II. Bond Lengths

Bond	Length Crystal	Length MM3	Difference (in Å)
Cl(1) - C(10)	1.7367	1.7317	0.0050
C(2) - C(3)	1.5052	1.5238	-0.0186
C(2) - N(32)	1.3660	1.3863	-0.0203
C(2) - O(33)	1.2179	1.2206	-0.0027
C(3) - H(18)	1.0588	1.1162	-0.0574
C(3) - H(19)	1.0230	1.1167	-0.0937
C(3) - N(31)	1.4607	1.4349	0.0258
C(4) - C(5)	1.4927	1.4834	0.0093
C(4) - C(15)	1.4803	1.4888	-0.0085
C(4) - N(31)	1.2864	1.2878	-0.0014
C(5) - C(6)	1.3926	1.4047	-0.0121
C(5) - C(11)	1.3922	1.4051	-0.0129
C(6) -C(7)	1.3893	1.3963	-0.0070
C(7) - C(8)	1.3847	1.3948	-0.0101
C(8) - C(9)	1.3838	1.3963	-0.0125
C(9) - C(11)	1.3829	1.3947	-0.0118
C(10) - C(12)	1.3807	1.3946	-0.0139
C(10) - C(16)	1.3719	1.3906	-0.0187
C(12) - C(13)	1.3796	1.3910	-0.0114
C(13) - C(14)	1.3939	1.4075	-0.0136
C(14) - C(15)	1.4072	1.4131	-0.0059
C(14) - N(32)	1.4219	1.4283	-0.0064
C(15) - C(16)	1.3955	1.4057	-0.0102
C(17) - N(32)	1.4694	1.4596	0.0098
		RMS value:	0.0255

Bond angles begin on next page.

III. Bond Angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(1) - C(2) - N(32)	115.287	117.041	-1.754
C(3) - C(2) - O(33)	122.975	120.154	2.821
N(32) - C(2) - O(33)	121.715	122.805	-1.090
C(2) - C(3) - H(18)	108.770	112.604	-3.834
C(2) - C(3) - H(19)	106.863	110.666	-3.803
C(2) - C(3) - N(31)	110.492	109.732	0.760
H(18) - C(3) - H(19)	109.171	106.016	3.155
H(18) - C(3) - N(31)	111.964	110.562	1.402
H(19) - C(3) - N(31)	109.439	107.099	2.340
C(5) - C(4) - C(15)	119.535	120.396	-0.861
C(5) - C(4) - N(31)	116.710	118.214	-1.504
C(15) - C(4) - N(31)	123.691	121.355	2.336
C(4) - C(5) - C(6)	122.603	121.062	1.541
C(4) - C(5) - C(11)	118.545	120.388	-1.843
C(6) - C(5) - C(11)	118.850	118.548	0.302
C(5) - C(6) - C(7)	120.391	120.672	-0.281
C(6) - C(7) - C(8)	120.327	120.150	0.177
C(7) - C(8) - C(9)	119.360	119.769	-0.409
C(8) - C(9) - C(11)	120.629	120.119	0.510
C(1) - C(10) - C(12)	119.688	119.840	-0.152
C(1) - C(10) - C(16)	119.230	119.865	-0.635
C(12) - C(10) - C(16)	121.052	120.295	0.757
C(5) - C(11) - C(9)	120.430	120.735	-0.305
C(10) - C(12) - C(13)	118.749	119.652	-0.903
C(12) - C(13) - C(14)	121.414	120.784	0.630
C(13) - C(14) - C(15)	119.467	119.552	-0.085
C(13) - C(14) - N(32)	118.481	117.869	0.612
C(15) - C(14) - N(32)	122.021	122.572	-0.551
C(4) - C(15) - C(14)	122.211	122.595	-0.384
C(4) - C(15) - C(16)	119.584	118.588	0.996
C(14) - C(15) - C(16)	118.186	118.788	-0.602
C(10) - C(16) - C(15)	121.131	120.927	0.204
C(3) - N(31) - C(4)	118.065	117.585	0.480
C(2) - N(32) - C(14)	123.068	119.794	3.274
C(2) - N(32) - C(17)	116.619	119.848	-3.229
C(14) - N(32) - C(17)	119.032	119.584	-0.552

RMS value: 1.670

IV. Dihedral Angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
Cl(1)-C(10)-C(12)-C(13)	177.5	179.9	-2.4
Cl(1)-C(10)-C(16)-C(15)	-177.6	0.2	-2.6
C(2)-C(3)-N(31)-C(4)	-74.7	-73.6	-1.1
C(2)-N(32)-C(14)-C(13)	130.2	133.5	-3.3
C(2)-N(32)-C(14)-C(15)	-51.9	-47.5	-4.4
C(3)-C(2)-N(32)-C(14)	13.5	9.9	3.6
C(3)-C(2)-N(32)-C(17)	-179.6	179.8	-0.6
C(3)-N(31)-C(4)-C(5)	-174.1	-179.8	5.7
C(3)-N(31)-C(4)-C(15)	2.9	-1.9	4.8

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(4)-C(5)-C(6)-C(7)	-178.8	-179.6	0.8
C(4)-C(5)-C(11)-C(9)	178.5	179.7	-1.2
C(4)-C(15)-C(14)-C(13)	-178.7	177.6	-3.7
C(4)-C(15)-C(14)-N(32)	3.3	-1.4	4.7
C(4)-C(15)-C(16)-C(10)	178.5	-177.8	3.7
C(4)-N(31)-C(3)-H(18)	46.7	51.2	-4.5
C(4)-N(31)-C(3)-H(19)	167.9	166.3	1.6
C(5)-C(4)-C(15)-C(14)	-142.8	-133.8	-9
C(5)-C(4)-C(15)-C(16)	38.8	44.3	-5.5
C(5)-C(6)-C(7)-C(8)	0.4	-0.3	0.7
C(5)-C(11)-C(9)-C(8)	0.3	0.3	0
C(6)-C(5)-C(4)-C(15)	25.5	27.6	-2.1
C(6)-C(5)-C(4)-N(31)	-157.3	-154.6	-2.7
C(6)-C(5)-C(11)-C(9)	-1.0	-0.9	-0.1
C(6)-C(7)-C(8)-C(9)	-1.1	-0.3	-0.8
C(7)-C(6)-C(5)-C(11)	0.6	0.9	-0.3
C(7)-C(8)-C(9)-C(11)	0.8	0.3	0.5
C(10)-C(12)-C(13)-C(14)	0.1	-0.1	0.2
C(10)-C(16)-C(15)-C(14)	0.0	0.3	-0.3
C(11)-C(5)-C(4)-C(15)	-154	-153.0	-1
C(11)-C(5)-C(4)-N(31)	23.2	24.8	-1.6
C(12)-C(10)-C(16)-C(15)	0.4	0.0	0.4
C(12)-C(13)-C(14)-C(15)	0.3	0.4	-0.1
C(12)-C(13)-C(14)-N(32)	178.3	179.4	-1.1
C(13)-C(12)-C(10)-C(16)	-0.4	-0.1	-0.3
C(13)-C(14)-C(15)-C(16)	-0.4	-0.5	0.1
C(13)-C(14)-N(32)-C(17)	-36.5	-36.4	-0.1
C(14)-C(15)-C(4)-N(31)	40.2	48.4	-8.2
C(14)-N(32)-C(2)-O(33)	-168.2	-170.2	2
C(15)-C(14)-N(32)-C(17)	141.5	142.6	-1.1
C(16)-C(15)-C(4)-N(31)	-138.1	-133.5	-4.6
C(16)-C(15)-C(14)-N(32)	-178.3	-179.4	1.1
C(17)-N(32)-C(2)-O(33)	-1.3	-0.3	-1
H(18)-C(3)-C(2)-N(32)	-58.3	-54.8	-3.5
H(18)-C(3)-C(2)-O(33)	123.4	125.3	-1.9
H(19)-C(3)-C(2)-N(32)	-176	-173.2	-2.8
H(19)-C(3)-C(2)-O(33)	5.7	6.8	-1.1
N(31)-C(3)-C(2)-N(32)	65.0	68.8	-3.8
N(31)-C(3)-C(2)-O(33)	-113.3	-111.1	-2.2
		RMS value:	3.1

Table 2. Beclamethasone dipropionate

I. Missing parameters

A. Missing for atoms 1-10-9-29 (type 2-1-1-12)
Missing for atoms 20-17-32-25 (type 3-1-75-3)
Missing for atoms 20-21-34-22 (type 3-1-75-3)

B. Estimated Parameters
2 torsional parameters are read in

Atom type numbers				V1	V2	V3
2	1	1	12	0.000	0.000	0.270
3	1	75	3	0.000	0.000	0.200

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(2)	1.3109	1.3375	-0.0266
C(1)-C(10)	1.5030	1.5137	-0.0107
C(2)-C(3)	1.4580	1.4842	-0.0262
C(3)-C(4)	1.4593	1.4852	-0.0259
C(3)-O(30)	1.2376	1.2280	0.0096
C(4)-C(5)	1.3405	1.3424	-0.0019
C(5)-C(6)	1.5045	1.5088	-0.0043
C(5)-C(10)	1.5112	1.5195	-0.0083
C(6)-C(7)	1.5145	1.5369	-0.0224
C(7)-C(8)	1.5170	1.5396	-0.0226
C(8)-C(9)	1.5625	1.5558	0.0067
C(8)-C(14)	1.5264	1.5377	-0.0113
C(8)-H(44)	0.9257	1.1094	-0.1837
C(9)-C(10)	1.5913	1.5820	0.0093
C(9)-C(11)	1.5456	1.5546	-0.0090
C(9)-Cl(29)	1.8354	1.8468	-0.0114
C(10)-C(19)	1.5447	1.5583	-0.0136
C(11)-C(12)	1.5338	1.5417	-0.0079
C(11)-O(31)	1.4170	1.4318	-0.0148
C(11)-H(45)	0.8985	1.1174	-0.2189
C(12)-C(13)	1.5401	1.5406	-0.0005
C(13)-C(14)	1.5339	1.5379	-0.0040
C(13)-C(17)	1.5898	1.5793	0.0105

Bond	Length Crystal	MM3	Difference (in Å)
C(13)-C(18)	1.5369	1.5490	-0.0121
C(14)-C(15)	1.5197	1.5309	-0.0112
C(14)-H(48)	1.0107	1.1156	-0.1049
C(15)-C(16)	1.5387	1.5541	-0.0154
C(16)-C(17)	1.5719	1.5884	-0.0165
C(16)-C(28)	1.5421	1.5313	0.0108
C(16)-H(51)	0.9561	1.1136	-0.1575
C(17)-C(20)	1.5186	1.5392	-0.0206
C(17)-O(32)	1.4661	1.4533	0.0128
C(20)-C(21)	1.5205	1.5245	-0.0040
C(20)-O(33)	1.2046	1.2123	-0.0077
C(21)-O(34)	1.4121	1.4455	-0.0334
C(21)-H(58)	0.9920	1.1046	-0.1126
C(21)-H(59)	0.9291	1.1078	-0.1787
C(22)-C(23)	1.4994	1.4962	0.0032
C(22)-O(34)	1.3417	1.3591	-0.0174
C(22)-O(35)	1.1962	1.2139	-0.0177
C(23)-C(24)	1.4723	1.5252	-0.0529
C(23)-H(60)	0.9322	1.1119	-0.1797
C(23)-H(61)	0.9331	1.1118	-0.1787
C(25)-C(26)	1.4875	1.4960	-0.0085
C(25)-O(32)	1.3435	1.3606	-0.0171
C(25)-O(36)	1.2107	1.2144	-0.0037
C(26)-C(27)	1.4379	1.5250	-0.0871
C(26)-H(65)	1.0652	1.1119	-0.0467
C(26)-H(66)	0.9596	1.1118	-0.1522
		RMS value:	0.0750

III. Bond Angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(2)-C(1)-C(10)	125.356	125.020	0.336
C(1)-C(2)-C(3)	120.766	120.874	-0.108
C(2)-C(3)-C(4)	117.543	116.638	0.905
C(2)-C(3)-O(30)	121.557	121.673	-0.116
C(4)-C(3)-O(30)	120.891	121.689	-0.798
C(3)-C(4)-C(5)	121.558	121.942	-0.384
C(4)-C(5)-C(6)	121.709	120.733	0.976
C(4)-C(5)-C(10)	122.992	123.548	-0.556
C(6)-C(5)-C(10)	115.298	115.697	-0.399

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(5)-C(6)-C(7)	110.965	110.144	0.821
C(6)-C(7)-C(8)	112.608	111.582	1.026
C(7)-C(8)-C(9)	111.744	111.828	-0.084
C(7)-C(8)-C(14)	111.738	110.931	0.807
C(7)-C(8)-H(44)	113.998	106.676	7.322
C(9)-C(8)-C(14)	109.715	110.745	-1.030
C(9)-C(8)-H(44)	105.193	108.484	-3.291
C(14)-C(8)-H(44)	103.979	107.986	-4.007
C(8)-C(9)-C(10)	110.307	111.204	-0.897
C(8)-C(9)-C(11)	113.288	111.240	2.048
C(8)-C(9)-Cl(29)	107.982	108.115	-0.133
C(10)-C(9)-C(11)	115.412	115.139	0.273
C(10)-C(9)-Cl(29)	105.357	106.100	-0.743
C(11)-C(9)-Cl(29)	103.699	104.455	-0.756
C(1)-C(10)-C(5)	111.669	111.975	-0.306
C(1)-C(10)-C(9)	110.040	110.584	-0.544
C(1)-C(10)-C(19)	106.464	105.627	0.837
C(5)-C(10)-C(9)	107.129	107.467	-0.338
C(5)-C(10)-C(19)	107.787	106.949	0.838
C(9)-C(10)-C(19)	113.805	114.268	-0.463
C(9)-C(11)-C(12)	113.620	113.753	-0.133
C(9)-C(11)-O(31)	107.310	109.145	-1.835
C(9)-C(11)-H(45)	106.087	109.235	-3.148
C(12)-C(11)-O(31)	113.299	108.130	5.169
C(12)-C(11)-H(45)	107.826	108.109	-0.283
O(31)-C(11)-H(45)	108.353	108.333	0.020
C(11)-C(12)-C(13)	112.829	114.060	-1.231
C(12)-C(13)-C(14)	108.854	107.141	1.713
C(12)-C(13)-C(17)	115.990	115.905	0.085
C(12)-C(13)-C(18)	111.336	110.152	1.184
C(14)-C(13)-C(17)	99.733	101.717	-1.984
C(14)-C(13)-C(18)	112.058	112.502	-0.444
C(17)-C(13)-C(18)	108.394	109.223	-0.829
C(8)-C(14)-C(13)	114.101	113.044	1.057
C(8)-C(14)-C(15)	119.149	119.341	-0.192
C(8)-C(14)-H(48)	110.076	107.624	2.452
C(13)-C(14)-C(15)	103.155	101.853	1.302
C(13)-C(14)-H(48)	101.905	108.333	-6.428
C(15)-C(14)-H(48)	106.823	106.032	0.791

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(14)-C(15)-C(16)	103.694	103.719	-0.025
C(15)-C(16)-C(17)	106.107	106.006	0.101
C(15)-C(16)-C(28)	112.558	110.927	1.631
C(15)-C(16)-H(51)	104.883	106.191	-1.308
C(17)-C(16)-C(28)	116.924	118.058	-1.134
C(17)-C(16)-H(51)	103.417	108.401	-4.984
C(28)-C(16)-H(51)	111.876	106.669	5.207
C(13)-C(17)-C(16)	103.748	102.953	0.795
C(13)-C(17)-C(20)	111.725	111.778	-0.053
C(13)-C(17)-O(32)	102.726	105.717	-2.991
C(16)-C(17)-C(20)	119.494	117.025	2.469
C(16)-C(17)-O(32)	108.649	108.431	0.218
C(20)-C(17)-O(32)	109.132	110.166	-1.034
C(17)-C(20)-C(21)	118.446	117.281	1.165
C(17)-C(20)-O(33)	121.610	122.348	-0.738
C(21)-C(20)-O(33)	119.877	120.299	-0.422
C(20)-C(21)-O(34)	112.393	111.837	0.556
C(20)-C(21)-H(58)	108.254	111.623	-3.369
C(20)-C(21)-H(59)	99.938	109.320	-9.382
O(34)-C(21)-H(58)	116.090	110.163	5.927
O(34)-C(21)-H(59)	109.856	107.326	2.530
H(58)-C(21)-H(59)	109.066	106.325	2.741
C(23)-C(22)-O(34)	112.393	111.260	1.133
C(23)-C(22)-O(35)	125.546	125.717	-0.171
O(34)-C(22)-O(35)	122.028	123.023	-0.995
C(22)-C(23)-C(24)	114.745	112.992	1.753
C(22)-C(23)-H(60)	104.105	109.268	-5.163
C(22)-C(23)-H(61)	109.207	109.257	-0.050
C(24)-C(23)-H(60)	110.045	109.319	0.726
C(24)-C(23)-H(61)	111.343	109.294	2.049
H(60)-C(23)-H(61)	106.888	106.503	0.385
C(26)-C(25)-O(32)	111.039	111.127	-0.088
C(26)-C(25)-O(36)	126.238	125.683	0.555
O(32)-C(25)-O(36)	122.721	123.185	-0.464
C(25)-C(26)-C(27)	117.889	113.027	4.862
C(25)-C(26)-H(65)	107.237	109.237	-2.000
C(25)-C(26)-H(66)	105.052	109.208	-4.156
C(27)-C(26)-H(65)	114.740	109.331	5.409
C(27)-C(26)-H(66)	111.752	109.342	2.410

H(65)-C(26)-H(66)	97.953	106.485		-8.532
C(11)-O(31)-H(73)	112.347	108.874		3.473
C(17)-O(32)-C(25)	120.659	118.946		1.713
C(21)-O(34)-C(22)	115.545	116.829		-1.284
			RMS value:	2.6293

IV. Dihedral Angles

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(1)-C(2)-C(3)-C(4)	3.6	0.0	3.6
C(1)-C(2)-C(3)-O(30)	-177.4	180.0	2.6
C(1)-C(10)-C(5)-C(4)	-1.4	0.4	-1.8
C(1)-C(10)-C(5)-C(6)	178.1	178.7	-0.6
C(1)-C(10)-C(9)-C(8)	-176.9	-176.7	-0.2
C(1)-C(10)-C(9)-C(11)	53.1	55.6	-2.5
C(1)-C(10)-C(9)-Cl(29)	-60.6	-59.4	-1.2
C(2)-C(1)-C(10)-C(5)	2.2	0.0	2.2
C(2)-C(1)-C(10)-C(9)	121.1	119.8	1.3
C(2)-C(1)-C(10)-C(19)	-115.2	-116.1	0.9
C(2)-C(3)-C(4)-C(5)	-3.0	0.4	-3.4
C(3)-C(2)-C(1)-C(10)	-3.5	-0.1	-3.4
C(3)-C(4)-C(5)-C(6)	-177.5	-178.8	1.3
C(3)-C(4)-C(5)-C(10)	2.0	-0.6	2.6
C(4)-C(5)-C(6)-C(7)	123.0	121.0	2.0
C(4)-C(5)-C(10)-C(9)	-122.0	-121.2	-0.8
C(4)-C(5)-C(10)-C(19)	115.2	115.6	-0.4
C(5)-C(4)-C(3)-O(30)	178.1	-179.6	2.3
C(5)-C(6)-C(7)-C(8)	52.2	53.3	-1.1
C(5)-C(10)-C(9)-C(8)	-55.3	-54.2	-1.1
C(5)-C(10)-C(9)-C(11)	174.7	178.1	-3.4
C(5)-C(10)-C(9)-Cl(29)	61.0	63.1	-2.1
C(6)-C(5)-C(10)-C(9)	57.5	57.1	0.4
C(6)-C(5)-C(10)-C(19)	-65.3	-66.0	0.7
C(6)-C(7)-C(8)-C(9)	-53.5	-54.1	0.6
C(6)-C(7)-C(8)-C(14)	-176.9	-178.3	1.4
C(6)-C(7)-C(8)-H(44)	65.6	-64.3	230.1
C(7)-C(6)-C(5)-C(10)	-56.6	-57.3	0.7
C(7)-C(8)-C(9)-C(10)	55.3	55.1	0.2
C(7)-C(8)-C(9)-C(11)	-173.6	-175.1	1.5
C(7)-C(8)-C(9)-Cl(29)	-59.3	-61.0	1.7
C(7)-C(8)-C(14)-C(13)	-179.2	-175.5	-3.7

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(7)-C(8)-C(14)-C(15)	-56.8	-55.8	-1.0
C(7)-C(8)-C(14)-H(48)	67.0	64.9	2.1
C(8)-C(9)-C(10)-C(19)	63.7	64.3	-0.6
C(8)-C(9)-C(11)-C(12)	47.4	47.1	0.3
C(8)-C(9)-C(11)-O(31)	-78.6	-73.7	-4.9
C(8)-C(9)-C(11)-H(45)	165.7	168.0	-2.3
C(8)-C(14)-C(13)-C(12)	-59.0	-59.9	0.9
C(8)-C(14)-C(13)-C(17)	179.1	178.0	1.1
C(8)-C(14)-C(13)-C(18)	64.6	61.3	3.3
C(8)-C(14)-C(15)-C(16)	-170.6	-168.5	-2.1
C(9)-C(8)-C(14)-C(13)	56.3	59.7	-3.4
C(9)-C(8)-C(14)-C(15)	178.7	179.4	-0.7
C(9)-C(8)-C(14)-H(48)	-57.5	-59.8	2.3
C(9)-C(11)-C(12)-C(13)	-50.4	-50.7	0.3
C(9)-C(11)-O(31)-H(73)	177.4	-170.1	12.5
C(10)-C(9)-C(8)-C(14)	179.8	179.4	0.4
C(10)-C(9)-C(8)-H(44)	-68.9	-62.3	-6.6
C(10)-C(9)-C(11)-C(12)	176.0	174.8	1.2
C(10)-C(9)-C(11)-O(31)	49.9	53.9	-4.0
C(10)-C(9)-C(11)-H(45)	-65.8	-64.4	-1.4
C(11)-C(9)-C(8)-C(14)	-49.1	-50.9	1.8
C(11)-C(9)-C(8)-H(44)	62.2	67.5	-5.3
C(11)-C(9)-C(10)-C(19)	-66.3	-63.4	-2.9
C(11)-C(12)-C(13)-C(14)	54.4	54.8	-0.4
C(11)-C(12)-C(13)-C(17)	165.8	167.5	-1.7
C(11)-C(12)-C(13)-C(18)	-69.7	-67.9	-1.8
C(12)-C(11)-C(9)-Cl(29)	-69.4	-69.3	-0.1
C(12)-C(11)-O(31)-H(73)	51.1	65.6	-14.5
C(12)-C(13)-C(14)-C(15)	170.3	170.8	-0.5
C(12)-C(13)-C(14)-H(48)	59.6	59.2	0.4
C(12)-C(13)-C(17)-C(16)	-151.8	-150.6	-1.2
C(12)-C(13)-C(17)-C(20)	78.1	83.0	-4.9
C(12)-C(13)-C(17)-O(32)	-38.7	-36.9	-1.8
C(13)-C(12)-C(11)-O(31)	72.5	70.7	1.8
C(13)-C(12)-C(11)-H(45)	-167.6	-172.2	4.6
C(13)-C(14)-C(8)-H(44)	-55.8	-58.9	3.1
C(13)-C(14)-C(15)-C(16)	-43.0	-43.2	0.2
C(13)-C(17)-C(16)-C(15)	10.1	8.7	1.4
C(13)-C(17)-C(16)-C(28)	-116.4	-116.3	-0.1

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(13)-C(17)-C(16)-H(51)	120.2	122.3	-2.1
C(13)-C(17)-C(20)-C(21)	-97.0	-95.9	-1.1
C(13)-C(17)-C(20)-O(33)	80.1	81.0	-0.9
C(13)-C(17)-O(32)-C(25)	-171.5	-171.5	0.0
C(14)-C(8)-C(9)-Cl(29)	65.2	63.3	1.9
C(14)-C(13)-C(17)-C(16)	-35.2	-34.8	-0.4
C(14)-C(13)-C(17)-C(20)	-165.2	-161.2	-4.0
C(14)-C(13)-C(17)-O(32)	77.9	78.9	-1.0
C(14)-C(15)-C(16)-C(17)	19.4	20.9	-1.5
C(14)-C(15)-C(16)-C(28)	148.5	150.2	-1.7
C(14)-C(15)-C(16)-H(51)	-89.7	-94.3	4.6
C(15)-C(14)-C(8)-H(44)	66.6	60.8	5.8
C(15)-C(14)-C(13)-C(17)	48.4	48.7	-0.3
C(15)-C(14)-C(13)-C(18)	-66.1	-68.0	1.9
C(15)-C(16)-C(17)-C(20)	135.3	131.7	3.6
C(15)-C(16)-C(17)-O(32)	-98.7	-103.0	4.3
C(16)-C(15)-C(14)-H(48)	64.0	70.0	-6.0
C(16)-C(17)-C(13)-C(18)	82.1	84.3	-2.2
C(16)-C(17)-C(20)-C(21)	141.7	145.8	-4.1
C(16)-C(17)-C(20)-O(33)	-41.2	-37.3	-3.9
C(16)-C(17)-O(32)-C(25)	-62.0	-61.7	-0.3
C(17)-C(13)-C(14)-H(48)	-62.3	-62.8	0.5
C(17)-C(20)-C(21)-O(34)	163.1	159.2	3.9
C(17)-C(20)-C(21)-H(58)	33.6	35.3	-1.7
C(17)-C(20)-C(21)-H(59)	-80.4	-82.1	1.7
C(17)-O(32)-C(25)-C(26)	171.6	176.7	-5.1
C(17)-O(32)-C(25)-O(36)	-80.6	-4.1	-76.5
C(18)-C(13)-C(14)-H(48)	-176.8	-179.6	2.8
C(18)-C(13)-C(17)-C(20)	-47.9	-42.1	-5.8
C(18)-C(13)-C(17)-O(32)	-164.8	-162.0	-2.8
C(19)-C(10)-C(9)-Cl(29)	-180.0	-178.4	-1.6
C(20)-C(17)-C(16)-C(28)	8.8	6.7	2.1
C(20)-C(17)-C(16)-H(51)	-114.6	-114.7	0.1
C(20)-C(17)-O(32)-C(25)	69.8	67.6	2.2
C(20)-C(21)-O(34)-C(22)	-78.0	-82.5	4.5
C(21)-C(20)-C(17)-O(32)	15.9	21.3	-5.4
C(21)-O(34)-C(22)-C(23)	-179.1	177.6	3.3
C(21)-O(34)-C(22)-O(35)	-1.1	-2.5	1.4
C(22)-O(34)-C(21)-H(58)	47.4	42.3	5.1

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(22)-O(34)-C(21)-H(59)	171.7	157.6	14.1
C(24)-C(23)-C(22)-O(34)	156.3	-179.2	24.5
C(24)-C(23)-C(22)-O(35)	-21.6	0.8	-22.4
C(27)-C(26)-C(25)-O(32)	177.1	179.4	-2.3
C(27)-C(26)-C(25)-O(36)	-3.3	0.3	-3.6
C(28)-C(16)-C(17)-O(32)	134.9	132.0	2.9
Cl(29)-C(9)-C(8)-H(44)	176.5	-178.4	5.1
Cl(29)-C(9)-C(11)-O(31)	164.6	169.8	-5.2
Cl(29)-C(9)-C(11)-H(45)	48.9	51.6	-2.7
O(32)-C(17)-C(16)-H(51)	11.4	10.6	0.8
O(32)-C(17)-C(20)-O(33)	-167.0	-161.7	-5.3
O(32)-C(25)-C(26)-H(65)	45.8	57.5	-11.7
O(32)-C(25)-C(26)-H(66)	-57.7	-58.6	0.9
O(33)-C(20)-C(21)-O(34)	-14.0	-17.8	3.8
O(33)-C(20)-C(21)-H(58)	-143.5	-141.7	-1.8
O(33)-C(20)-C(21)-H(59)	102.5	100.9	1.6
O(34)-C(22)-C(23)-H(60)	36.0	58.8	-22.8
O(34)-C(22)-C(23)-H(61)	-77.9	-57.3	-20.6
O(35)-C(22)-C(23)-H(60)	-141.9	-121.1	-20.8
O(35)-C(22)-C(23)-H(61)	104.2	122.7	-18.5
O(36)-C(25)-C(26)-H(65)	-134.6	-121.7	-12.9
O(36)-C(25)-C(26)-H(66)	121.9	122.2	-0.3
		RMS value:	22.3

Table 3. Lomustine

I. Missing parameters

A. Missing for atoms 1-7-8-4 (type 12-1-1-151)

Missing for atoms 2-5-4-8 (type 7-72-151-1)

Missing for atoms 2-5-4-9 (type 7-72-151-162)

Missing for atoms 5-4-9-3 (type 72-151-162-94)

Missing for atoms 7-8-4-5 (type 1-1-151-72)

Missing for atoms 20-8-4-5 (type 5-1-151-72)

Missing for atoms 5-4-9-6 (type 72-151-162-151)

Missing for bond 2-5 (type 7-72)

Missing for bond 4-5 (type 72-151)

Missing for 8-4-5 (type 1-151-72) angle type 1

Missing for 5-4-9 (type 72-151-162) angle type 1

Missing for 2-5-4 (type 7-72-151) angle type 1

B. Estimated Parameters

7 torsional parameters are read in

Atom type numbers				V1	V2	V3
12	1	1	151	0.000	0.000	0.270
7	72	151	1	0.000	11.600	0.000
7	72	151	162	0.000	11.600	0.000
72	151	162	94	0.000	11.600	0.000
1	1	151	72	0.000	0.160	0.090
5	1	151	72	0.000	0.160	0.090
72	151	162	151	0.000	11.600	0.000

2 stretching parameters are read in

Bond type		K(s)	L(0)
7	72	33.4731	1.0620
72	151	9.5632	1.2600

2 dipole parameters are read in

Bond type		Moment
7	72	-0.4500
72	151	0.0000

3 bending parameters are read in

Atom type numbers			Kb	Theta
1	151	72	0.695	120.000
72	151	162	0.695	120.000
7	72	151	0.695	120.000

II. Bond lengths

Bond	Length		Difference
	Crystal	MM3	(in angstroms)
Cl(1)-C(7)	1.8309	1.8011	0.0298
O(2)-N(5)	1.2172	1.0623	0.1549
O(3)-C(9)	1.2126	1.2289	-0.0163
N(4)-N(5)	1.3330	1.2679	0.0651
N(4)-C(8)	1.4813	1.4670	0.0143
N(4)-C(9)	1.4304	1.3927	0.0377
N(6)-C(9)	1.3234	1.3837	-0.0603
N(6)-C(10)	1.4619	1.4619	0.0000
N(6)-H(17)	0.7961	1.0305	-0.2344
C(7)-C(8)	1.4455	1.5198	-0.0743
C(7)-H(18)	1.0119	1.1057	-0.0938
C(7)-H(19)	0.9696	1.1060	-0.1364
C(8)-H(20)	0.9604	1.1125	-0.1521
C(8)-H(21)	1.0079	1.1129	-0.1050
C(10)-C(11)	1.5080	1.5251	-0.0171
C(10)-C(15)	1.5028	1.5249	-0.0221
C(10)-H(22)	0.9606	1.1150	-0.1544
C(11)-C(12)	1.5204	1.5305	-0.0101
C(12)-C(13)	1.4996	1.5389	-0.0393
C(13)-C(14)	1.5051	1.5389	-0.0338
C(13)-C(16)	1.5274	1.5374	-0.0100
C(13)-H(27)	0.9622	1.1171	-0.1549
C(14)-C(15)	1.5166	1.5306	-0.0140
		RMS value:	0.0973

III. Bond Angles

Bond	Theta (in degrees)		Difference
	Crystal	MM3	(in degrees)
N(5)-N(4)-C(8)	121.781	120.851	0.930
N(5)-N(4)-C(9)	118.269	119.097	-0.828
C(8)-N(4)-C(9)	119.934	120.024	-0.090
O(2)-N(5)-N(4)	114.648	124.731	-10.083
C(9)-N(6)-C(10)	122.884	121.761	1.123
C(9)-N(6)-H(17)	119.361	118.228	1.133
C(10)-N(6)-H(17)	117.649	119.889	-2.240
Cl(1)-C(7)-C(8)	106.528	111.123	-4.595
Cl(1)-C(7)-H(18)	108.793	107.053	1.740
Cl(1)-C(7)-H(19)	112.438	106.971	5.467
C(8)-C(7)-H(18)	115.320	111.863	3.457
C(8)-C(7)-H(19)	109.067	111.490	-2.423

Bond angles (cont.)

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
H(18)-C(7)-H(19)	104.843	108.098	-3.255
N(4)-C(8)-C(7)	108.841	111.893	-3.052
N(4)-C(8)-H(20)	120.937	111.285	9.652
N(4)-C(8)-H(21)	114.537	110.376	4.161
C(7)-C(8)-H(20)	105.490	109.131	-3.641
C(7)-C(8)-H(21)	108.559	108.899	-0.340
H(20)-C(8)-H(21)	97.426	105.004	-7.578
O(3)-C(9)-N(4)	118.855	122.589	-3.734
O(3)-C(9)-N(6)	126.607	122.947	3.660
N(4)-C(9)-N(6)	114.533	114.463	0.070
N(6)-C(10)-C(11)	109.871	110.902	-1.031
N(6)-C(10)-C(15)	111.738	110.981	0.757
N(6)-C(10)-H(22)	108.742	109.617	-0.875
C(11)-C(10)-C(15)	110.269	109.440	0.829
C(11)-C(10)-H(22)	108.755	107.516	1.239
C(15)-C(10)-H(22)	107.377	108.285	-0.908
C(10)-C(11)-C(12)	111.394	111.878	-0.484
C(11)-C(12)-C(13)	112.278	111.444	0.834
C(12)-C(13)-C(14)	109.902	109.478	0.424
C(12)-C(13)-C(16)	110.895	110.880	0.015
C(12)-C(13)-H(27)	105.193	108.588	-3.395
C(14)-C(13)-C(16)	112.741	110.880	1.861
C(14)-C(13)-H(27)	108.716	108.582	0.134
C(16)-C(13)-H(27)	109.090	108.366	0.724
C(13)-C(14)-C(15)	111.844	111.576	0.268
C(10)-C(15)-C(14)	111.763	111.899	-0.136
		RMS value:	3.333

IV. Dihedral Angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
Cl(1)-C(7)-C(8)-N(4)	175.9	178.8	-2.9
Cl(1)-C(7)-C(8)-H(20)	44.7	55.2	-10.5
Cl(1)-C(7)-C(8)-H(21)	-58.9	-58.9	0.0
O(2)-N(5)-N(4)-C(8)	4.3	-0.4	4.7
O(2)-N(5)-N(4)-C(9)	-177.2	-178.5	1.3
O(3)-C(9)-N(4)-N(5)	168.1	179.2	-11.1
O(3)-C(9)-N(4)-C(8)	-13.3	1.1	-14.4
O(3)-C(9)-N(6)-C(10)	-8.4	3.0	-11.4
O(3)-C(9)-N(6)-H(17)	175.5	179.0	-3.5

Dihedral angles (cont.)

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
N(4)-C(8)-C(7)-H(18)	-63.3	-61.6	-1.7
N(4)-C(8)-C(7)-H(19)	54.3	59.6	-5.3
N(4)-C(9)-N(6)-C(10)	172.4	-177.1	-10.5
N(4)-C(9)-N(6)-H(17)	-3.7	-1.2	-2.5
N(5)-N(4)-C(8)-C(7)	-85.8	-96.0	10.2
N(5)-N(4)-C(8)-H(20)	36.4	26.4	10.0
N(5)-N(4)-C(8)-H(21)	152.5	142.5	10.0
N(5)-N(4)-C(9)-N(6)	-12.6	-0.7	-11.9
N(6)-C(9)-N(4)-C(8)	166.0	-178.8	-25.2
N(6)-C(10)-C(11)-C(12)	-178.3	-179.2	0.9
N(6)-C(10)-C(15)-C(14)	177.7	179.0	-1.3
C(7)-C(8)-N(4)-C(9)	95.6	82.0	13.6
C(9)-N(4)-C(8)-H(20)	-142.1	-155.6	13.5
C(9)-N(4)-C(8)-H(21)	-26.1	-39.4	13.3
C(9)-N(6)-C(10)-C(11)	-120.0	-158.4	38.4
C(9)-N(6)-C(10)-C(15)	117.3	79.7	37.6
C(9)-N(6)-C(10)-H(22)	-1.1	-39.9	38.8
C(10)-C(11)-C(12)-C(13)	55.8	57.2	-1.4
C(10)-C(15)-C(14)-C(13)	-56.3	-56.9	0.6
C(11)-C(10)-N(6)-H(17)	56.2	25.7	30.5
C(11)-C(10)-C(15)-C(14)	55.2	56.3	-1.1
C(11)-C(12)-C(13)-C(14)	-55.1	-55.2	0.1
C(11)-C(12)-C(13)-C(16)	179.5	-177.9	-2.6
C(11)-C(12)-C(13)-H(27)	61.7	63.2	-1.5
C(12)-C(11)-C(10)-C(15)	-54.7	-56.5	1.8
C(12)-C(11)-C(10)-H(22)	62.8	60.9	1.9
C(12)-C(13)-C(14)-C(15)	55.2	55.1	0.1
C(14)-C(15)-C(10)-H(22)	-63.1	-60.6	-2.5
C(15)-C(10)-N(6)-H(17)	-66.5	-96.2	29.7
C(15)-C(14)-C(13)-C(16)	179.4	177.7	1.7
C(15)-C(14)-C(13)-H(27)	-59.5	-63.3	3.8
H(17)-N(6)-C(10)-H(22)	175.1	144.2	30.9
H(18)-C(7)-C(8)-H(20)	165.5	174.8	-9.3
H(18)-C(7)-C(8)-H(21)	61.9	60.7	1.2
H(19)-C(7)-C(8)-H(20)	-76.9	-64.0	-12.9
H(19)-C(7)-C(8)-H(21)	179.5	-178.1	-2.4
		RMS value:	14.8

Table 4. Busulfan

I. Missing parameters

A. Missing for atoms 10-6-4-1 (type 5-1-6-18)
Missing for atoms 12-6-4-1 (type 1-1-6-18)
Missing for atoms 6-4-1-2 (type 1-6-18-7)
Missing for atoms 7-5-1-4 (type 5-1-18-6)
Missing for atoms 6-4-1-5 (type 1-6-18-1)
Missing for atoms 6-12-13-16 (type 1-1-6-18)
Missing for atoms 12-13-16-19 (type 1-6-18-1)
Missing for bond 1-4 (type 6-18)
Missing for bond 13-16 (type 6-18)
Missing for 4-1-2 (type 6-18-7) angle type 1
Missing for 4-1-3 (type 6-18-7) angle type 1
Missing for 5-1-4 (type 1-18-6) angle type 1
Missing for 6-4-1 (type 1-6-18) angle type 1
Missing for 12-13-16 (type 1-6-18) angle type 1
Missing for 13-16-17 (type 6-18-7) angle type 1
Missing for 13-16-18 (type 6-18-7) angle type 1
Missing for 19-16-13 (type 1-18-6) angle type 1

B. Estimated Parameters

5 torsional parameters are read in

Atom type numbers				V1	V2	V3
5	1	6	18	0.000	0.000	0.200
1	1	6	18	0.000	0.000	0.200
1	6	18	7	0.000	0.000	0.300
5	1	18	6	0.000	0.000	0.270
1	6	18	1	0.000	0.000	0.300

1 stretching parameter is read in

Bond type		K(s)	L(0)
6	18	3.4836	1.7600

3 bending parameters are read in

Atom type numbers			Kb	Theta
6	18	7	0.695	109.500
1	18	6	0.695	109.500
1	6	18	0.695	110.000

II. Bond lengths

Bond	Length		Difference
	Crystal	MM3	(in Å)
S(1)-O(2)	1.4221	1.4423	-0.0202
S(1)-O(3)	1.4271	1.4425	-0.0154
S(1)-O(4)	1.5689	1.7596	-0.1907
S(1)-C(5)	1.7447	1.7759	-0.0312
O(4)-C(6)	1.4536	1.4186	0.0350
C(6)-C(12)	1.4892	1.5253	-0.0361
C(12)-O(13)	1.4536	1.4186	0.0350
C(12)-H(14)	0.9609	1.1164	-0.1555
C(12)-H(15)	0.8839	1.1160	-0.2321
O(13)-S(16)	1.5689	1.7596	-0.1907
S(16)-O(17)	1.4221	1.4423	-0.0202
S(16)-O(18)	1.4271	1.4425	-0.0154
S(16)-C(19)	1.7447	1.7759	-0.0312
		RMS value:	0.1102

III. Bond Angles

Bond	Theta (in degrees)		Difference
	Crystal	MM3	(in degrees)
O(2)-S(1)-O(3)	118.682	118.438	0.244
O(2)-S(1)-O(4)	104.510	107.710	-3.200
O(2)-S(1)-C(5)	110.309	106.158	4.151
O(3)-S(1)-O(4)	109.481	108.753	0.728
O(3)-S(1)-C(5)	109.421	106.418	3.003
O(4)-S(1)-C(5)	103.236	109.078	-5.842
S(1)-O(4)-C(6)	118.687	115.848	2.839
O(4)-C(6)-C(12)	105.096	108.415	-3.319
C(6)-C(12)-O(13)	105.096	108.415	-3.319
C(6)-C(12)-H(14)	110.475	109.938	0.537
C(6)-C(12)-H(15)	110.442	110.064	0.378
O(13)-C(12)-H(14)	105.146	110.063	-4.917
O(13)-C(12)-H(15)	108.166	110.142	-1.976
H(14)-C(12)-H(15)	116.714	108.218	8.496
C(12)-O(13)-S(16)	118.687	115.848	2.839
O(13)-S(16)-O(17)	104.510	107.710	-3.200
O(13)-S(16)-O(18)	109.480	108.753	0.727
O(13)-S(16)-C(19)	103.235	109.078	-5.843
O(17)-S(16)-O(18)	118.683	118.438	0.245
O(17)-S(16)-C(19)	110.309	106.158	4.151

Bond	Theta (in degrees) Crystal	MM3		Difference (in degrees)
O(18)-S(16)-C(19)	109.421	106.418		3.003
			RMS value:	3.601

V. Dihedral Angles

Bond	Omega (in degrees) Crystal	MM3		Difference (in degrees)
O(2)-S(1)-O(4)-C(6)	168.9	169.2		-0.3
O(3)-S(1)-O(4)-C(6)	40.8	39.7		1.1
O(4)-C(6)-C(12)-O(13)	-180.0	-180.0		0.0
O(4)-C(6)-C(12)-H(14)	-67.1	-59.6		-7.5
O(4)-C(6)-C(12)-H(15)	63.6	59.5		4.1
C(5)-S(1)-O(4)-C(6)	-75.7	-76.0		0.3
C(6)-C(12)-O(13)-S(16)	-152.4	-178.0		25.6
C(12)-O(13)-S(16)-O(17)	-168.9	-169.2		0.3
C(12)-O(13)-S(16)-O(18)	-40.8	-39.7		-1.1
C(12)-O(13)-S(16)-C(19)	75.7	76.0		-0.3
H(14)-C(12)-O(13)-S(16)	91.0	61.7		29.3
H(15)-C(12)-O(13)-S(16)	-34.4	-57.5		23.1
			RMS value:	13.3

Table 5. 5-Fluorouracil

I. Missing parameters

A. Pi-atom parameter of atom types (162-151) is missing.
Pi-atom parameter of atom types (151-96) is missing.
Missing for atoms 1-7-2-3 (type 162-151-162-2).
Missing for atoms 2-3-4-6 (type 162-2-2-151).
Missing for atoms 5-3-2-7 (type 11-2-162-151).
Missing for atoms 5-3-2-9 (type 11-2-162-96).
Missing for atoms 5-3-4-6 (type 11-2-2-151).
Missing for atoms 3-2-7 (type 2-162-151) angle type 1.
Missing for atoms 5-3-2 (type 11-2-162) angle type 1.

B. Estimated Parameters
Pi-atom parameters of type (2-2) are used for (162-151).
Pi-atom parameters of type (2-2) are used for (151-96).

5 torsional parameters are read in

Atom type numbers				V1	V2	V3
162	151	162	2	0.000	11.600	0.000
151	2	2	162	0.000	11.600	0.000
11	2	162	151	0.000	11.600	0.000
11	2	162	96	0.000	11.600	0.000
11	2	2	151	0.000	11.600	0.000

2 bending parameters are read in

Atom type numbers			Kb	Theta
2	162	151	0.695	120.000
11	2	162	0.695	120.000

III. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-N(6)	1.3678	1.3785	-0.0107
C(1)-N(7)	1.4151	1.3840	0.0311
C(1)-O(8)	1.2357	1.2271	0.0086
C(2)-C(3)	1.4858	1.4772	0.0086
C(2)-N(7)	1.4115	1.3819	0.0296
C(2)-O(9)	1.1860	1.2457	-0.0597
C(3)-C(4)	1.3365	1.3425	-0.0060
C(3)-F(5)	1.3490	1.3531	-0.0041
C(4)-N(6)	1.4303	1.4142	0.0161

Bond	Length Crystal	MM3	Difference (in Å)
C(4)-H(10)	1.1000	1.0974	0.0026
N(6)-H(11)	1.1000	1.0283	0.0717
N(7)-H(12)	1.1000	1.0291	0.0709
		RMS value:	0.0367

IV. Bond Angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
N(6)-C(1)-N(7)	118.727	114.858	3.869
N(6)-C(1)-O(8)	123.734	122.640	1.094
N(7)-C(1)-O(8)	117.493	122.502	-5.009
C(3)-C(2)-N(7)	109.703	116.974	-7.271
C(3)-C(2)-O(9)	129.587	120.488	9.099
N(7)-C(2)-O(9)	120.474	122.538	-2.064
C(2)-C(3)-C(4)	128.005	118.284	9.721
C(2)-C(3)-F(5)	112.306	123.642	-11.336
C(4)-C(3)-F(5)	119.603	118.074	1.529
C(3)-C(4)-N(6)	116.318	120.892	-4.574
C(3)-C(4)-H(10)	121.841	123.169	-1.328
N(6)-C(4)-H(10)	121.841	115.939	5.902
C(1)-N(6)-C(4)	121.737	123.436	-1.699
C(1)-N(6)-H(11)	119.131	121.337	-2.206
C(4)-N(6)-H(11)	119.131	115.227	3.904
C(1)-N(7)-C(2)	125.287	125.555	-0.268
C(1)-N(7)-H(12)	117.356	116.938	0.418
C(2)-N(7)-H(12)	117.357	117.507	-0.150
		RMS value:	6.122

V. Dihedral Angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-N(6)-C(4)-C(3)	-1.4	0.0	-1.4
C(1)-N(6)-C(4)-H(10)	178.6	-180.0	-1.4
C(1)-N(7)-C(2)-C(3)	4.7	0.0	4.7
C(1)-N(7)-C(2)-O(9)	179.7	-180.0	-0.3
C(2)-C(3)-C(4)-N(6)	4.0	0.0	4.0
C(2)-C(3)-C(4)-H(10)	-176.0	180.0	4.0
C(2)-N(7)-C(1)-N(6)	-3.0	0.0	-3.0

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(2)-N(7)-C(1)-O(8)	179.4	180.0	-0.6
C(3)-C(2)-N(7)-H(12)	-175.3	-180.0	4.7
C(3)-C(4)-N(6)-H(11)	178.6	-180.0	-1.4
C(4)-C(3)-C(2)-N(7)	-5.5	0.0	-5.5
C(4)-C(3)-C(2)-O(9)	-179.8	180.0	1.2
C(4)-N(6)-C(1)-N(7)	0.9	0.0	0.9
C(4)-N(6)-C(1)-O(8)	178.3	-180.0	-1.7
F(5)-C(3)-C(2)-N(7)	177.9	180.0	-2.1
F(5)-C(3)-C(2)-O(9)	3.6	0.0	3.6
F(5)-C(3)-C(4)-N(6)	-179.7	-180.0	0.3
F(5)-C(3)-C(4)-H(10)	0.3	0.0	0.3
N(6)-C(1)-N(7)-H(12)	177.0	180.0	-3.0
N(7)-C(1)-N(6)-H(11)	-179.1	180.0	0.9
O(8)-C(1)-N(6)-H(11)	-1.7	0.0	-1.7
O(8)-C(1)-N(7)-H(12)	-0.6	0.0	-0.6
O(9)-C(2)-N(7)-H(12)	-0.3	0.0	-0.3
H(10)-C(4)-N(6)-H(11)	-1.4	0.0	-1.4
		RMS value:	2.6

Table 6. Metrifonate

I. Missing parameters

A. Missing for atoms 1-4-5-7 (type 12-1-1-153).
Missing for atoms 6-5-7-8 (type 6-1-153-7).
Missing for atoms 6-5-7-9 (type 6-1-153-159).
Missing for atoms 6-5-7-11 (type 6-1-153-159).
Missing for atoms 7-5-6-14 (type 153-1-6-21).
Missing for atoms 6-5-7 (type 6-1-153) angle type 1.

B. Estimated parameters

4 torsional parameters are read in

Atom type numbers	V1	V2	V3
12 1 1 153	0.000	0.000	0.270
6 1 153 7	0.000	0.000	0.270
6 1 153 159	0.000	0.000	0.270
153 1 6 21	0.000	0.000	0.200

1 bending parameter is read in

Atom type numbers	Kb	Theta
6 1 153	0.695	109.500

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in angstroms)
Cl(1)-C(4)	1.7557	1.7714	-0.0157
Cl(2)-C(4)	1.7776	1.7722	0.0054
Cl(3)-C(4)	1.7727	1.7771	-0.0044
C(4)-C(5)	1.5356	1.5554	-0.0198
C(5)-O(6)	1.4376	1.4360	0.0016
C(5)-P(7)	1.8316	1.8408	-0.0092
C(5)-H(13)	1.1000	1.1075	-0.0075
O(6)-H(14)	1.1000	0.9512	0.1488
P(7)-O(8)	1.4506	1.4723	-0.0217
P(7)-O(9)	1.5309	1.5833	-0.0524
P(7)-O(11)	1.5534	1.5978	-0.0444
O(9)-C(10)	1.4514	1.4296	0.0218
O(11)-C(12)	1.4381	1.4308	0.0073

RMS value: 0.0470

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3		Difference (in degrees)
Cl(1)-C(4)-Cl(2)	110.129	110.282		-0.1530
Cl(1)-C(4)-Cl(3)	107.855	107.948		-0.0930
Cl(1)-C(4)-C(5)	110.128	109.262		0.8660
Cl(2)-C(4)-Cl(3)	107.766	109.855		-2.0890
Cl(2)-C(4)-C(5)	110.593	110.377		0.2160
Cl(3)-C(4)-C(5)	110.302	109.070		1.2320
C(4)-C(5)-O(6)	110.691	107.185		3.5060
C(4)-C(5)-P(7)	117.629	120.288		-2.6590
C(4)-C(5)-H(13)	101.022	108.178		-7.1560
O(6)-C(5)-P(7)	103.014	105.806		-2.7920
O(6)-C(5)-H(13)	116.136	108.173		7.9630
P(7)-C(5)-H(13)	108.972	106.717		2.2550
C(5)-O(6)-H(14)	110.691	110.205		0.4860
C(5)-P(7)-O(8)	111.682	114.091		-2.4090
C(5)-P(7)-O(9)	108.248	104.696		3.5520
C(5)-P(7)-O(11)	104.171	104.058		0.1130
O(8)-P(7)-O(9)	116.114	115.221		0.8930
O(8)-P(7)-O(11)	118.498	114.862		3.6360
O(9)-P(7)-O(11)	96.513	102.480		-5.9670
P(7)-O(9)-C(10)	122.613	121.349		1.2640
P(7)-O(11)-C(12)	123.839	121.851		1.9880
			RMS value:	3.2908

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
Cl(1)-C(4)-C(5)-O(6)	-172.4	-173.0	0.6
Cl(1)-C(4)-C(5)-P(7)	69.7	66.3	3.4
Cl(1)-C(4)-C(5)-H(13)	-48.8	-56.5	7.7
Cl(2)-C(4)-C(5)-O(6)	65.7	65.6	0.1
Cl(2)-C(4)-C(5)-P(7)	-52.3	-55.1	2.8
Cl(2)-C(4)-C(5)-H(13)	-170.7	-178.0	7.3
Cl(3)-C(4)-C(5)-O(6)	-53.4	-55.2	1.8
Cl(3)-C(4)-C(5)-P(7)	-171.4	-175.9	4.5
Cl(3)-C(4)-C(5)-H(13)	70.2	61.2	9.0
C(4)-C(5)-O(6)-H(14)	180.0	-79.6	100.4
C(4)-C(5)-P(7)-O(8)	90.7	76.2	14.5
C(4)-C(5)-P(7)-O(9)	-38.4	-50.7	12.3
C(4)-C(5)-P(7)-O(11)	-140.3	-157.9	17.6
C(5)-P(7)-O(9)-C(10)	118.4	177.3	-58.9

Dihedral angles (cont.)

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(5)-P(7)-O(11)-C(12)	-67.9	-81.1	13.2
O(6)-C(5)-P(7)-O(8)	-31.3	-45.2	13.9
O(6)-C(5)-P(7)-O(9)	-160.4	-172.1	11.7
O(6)-C(5)-P(7)-O(11)	97.7	80.7	17.0
P(7)-C(5)-O(6)-H(14)	-53.4	49.9	-103.3
O(8)-P(7)-C(5)-H(13)	-155.2	-160.3	5.1
O(8)-P(7)-O(9)-C(10)	-8.1	51.1	-59.2
O(8)-P(7)-O(11)-C(12)	56.9	44.4	12.5
O(9)-P(7)-C(5)-H(13)	75.7	72.9	2.8
O(9)-P(7)-O(11)-C(12)	-178.6	170.1	10.3
C(10)-O(9)-P(7)-O(11)	-134.3	-74.4	-59.9
O(11)-P(7)-C(5)-H(13)	-26.2	-34.4	8.2
H(13)-C(5)-O(6)-H(14)	65.6	163.9	-98.3
		RMS value:	39.9262

VI. Other

1. In MM3 calculation geometry optimization can not be accomplished and optimization switches to energy minimization.

Table 7. Naltrexone

I. Missing parameters

A. Missing for atoms 6-5-23-4 (type 3-1-41-2)
Missing for atoms 23-5-6-7 (type 41-1-3-1)
Missing for atoms 18-17-21-9 (type 22-1-39-1)
Missing for atoms 12-13-5-23 (type 2-1-1-41) 5-membe
Missing for atoms 18-17-21-16 (type 22-1-39-1)
Missing for atoms 18-17-21-47 (type 22-1-39-48)
Missing for atoms 21-17-18-19 (type 39-1-22-22)
Missing for atoms 21-17-18-20 (type 39-1-22-22)
Missing for atoms 21-17-18-42 (type 39-1-22-5)
Missing for atoms 23-5-6-24 (type 41-1-3-7)
Missing for atoms 6-5-23 (type 3-1-41) angle type 2
Missing for atoms 18-17-21 (type 22-1-39) angle type 1

B. Estimated Parameters

8 torsional parameters are read in

Atom type numbers	V1	V2	V3
3 1 42 2	0.000	0.160	0.090
41 1 3 1	0.000	0.160	0.090
22 1 39 1	0.000	0.000	0.270
2 1 1 41	0.000	0.000	0.270
22 1 39 48	0.000	0.000	0.270
39 1 22 22	0.000	0.000	0.270
39 1 22 5	0.000	0.000	0.270
41 1 3 7	0.000	0.160	0.090

2 bending parametersare read in

Atom type numbers	Kb	Theta
3 1 41	0.695	109.500
22 1 39	0.695	109.500

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in angstroms)
C(1)-C(2)	1.3906	1.4025	-0.0119
C(1)-C(11)	1.4096	1.4017	0.0079
C(2)-C(3)	1.3996	1.4044	-0.0048
C(3)-C(4)	1.3919	1.3974	-0.0055
C(3)-O(22)	1.3581	1.2437	0.1144
C(4)-C(12)	1.3776	1.3797	-0.0021
C(4)-O(23)	1.3900	1.2317	0.1583
C(5)-C(6)	1.5400	1.5379	0.0021
C(5)-C(13)	1.5385	1.5555	-0.0170
C(5)-O(23)	1.4650	1.4572	0.0078

Bond	Length Crystal	MM3	Difference (in angstroms)
C(6)-C(7)	1.4960	1.5239	-0.0279
C(6)-O(24)	1.2006	1.2131	-0.0125
C(7)-C(8)	1.5344	1.5291	0.0053
C(8)-C(14)	1.5192	1.5199	-0.0007
C(9)-C(10)	1.5526	1.5425	0.0101
C(9)-C(14)	1.5519	1.5399	0.0120
C(9)-N+(21)	1.5236	1.5232	0.0004
C(10)-C(11)	1.5181	1.5069	0.0112
C(11)-C(12)	1.3690	1.3825	-0.0135
C(12)-C(13)	1.5149	1.5008	0.0141
C(13)-C(14)	1.5307	1.5285	0.0022
C(13)-C(15)	1.5388	1.5494	-0.0106
C(14)-O(25)	1.4433	1.4476	-0.0043
C(15)-C(16)	1.5216	1.5279	-0.0063
C(16)-N+(21)	1.5125	1.5054	0.0071
C(17)-C(18)	1.4878	1.5224	-0.0346
C(17)-N+(21)	1.5016	1.5029	-0.0013
C(17)-H(40)	1.1000	1.0993	0.0007
C(17)-H(41)	1.1000	1.1007	-0.0007
C(18)-C(19)	1.5015	1.5154	-0.0139
C(18)-C(20)	1.4958	1.5152	-0.0194
C(18)-H(42)	1.1000	1.0900	0.0100
C(19)-C(20)	1.4839	1.5113	-0.0274
C(19)-H(43)	1.1000	1.0868	0.0132
C(19)-H(44)	1.1000	1.0871	0.0129
C(20)-H(45)	1.1000	1.0871	0.0129
C(20)-H(46)	1.1000	1.0869	0.0131
N+(21)-H(47)	1.1000	1.0340	0.0660
O(22)-H(48)	1.1000	0.9600	0.1400
O(25)-H(49)	1.1000	0.9422	0.1578
		RMS value:	0.0482

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(2)-C(1)-C(11)	119.429	120.220	-0.791
C(1)-C(2)-C(3)	123.319	121.095	2.224
C(2)-C(3)-C(4)	115.756	118.124	-2.368
C(2)-C(3)-O(22)	124.208	119.177	5.031
C(4)-C(3)-O(22)	120.037	122.679	-2.642
C(3)-C(4)-C(12)	120.911	119.508	1.403
C(3)-C(4)-O(23)	126.835	125.284	1.551
C(12)-C(4)-O(23)	112.195	115.132	-2.937

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(6)-C(5)-C(13)	113.358	115.309	-1.951
C(6)-C(5)-O(23)	107.939	107.601	0.338
C(6)-C(5)-H(28)	106.762	107.837	-1.075
C(13)-C(5)-O(23)	105.694	105.742	-0.048
C(13)-C(5)-H(28)	108.965	110.224	-1.259
O(23)-C(5)-H(28)	114.289	110.036	4.253
C(5)-C(6)-C(7)	116.135	119.035	-2.900
C(5)-C(6)-O(24)	120.722	120.590	0.132
C(7)-C(6)-O(24)	123.143	120.182	2.961
C(6)-C(7)-C(8)	111.199	114.233	-3.034
C(7)-C(8)-C(14)	108.847	112.526	-3.679
C(10)-C(9)-C(14)	115.807	115.399	0.408
C(10)-C(9)-N+(21)	112.770	117.468	-4.698
C(14)-C(9)-N+(21)	105.461	103.228	2.233
C(9)-C(10)-C(11)	113.546	113.952	-0.406
C(1)-C(11)-C(10)	124.753	125.007	-0.254
C(1)-C(11)-C(12)	116.743	117.206	-0.463
C(10)-C(11)-C(12)	118.394	117.546	0.848
C(4)-C(12)-C(11)	123.659	123.382	0.277
C(4)-C(12)-C(13)	108.581	108.451	0.130
C(11)-C(12)-C(13)	127.753	128.037	-0.284
C(5)-C(13)-C(12)	98.375	96.785	1.590
C(5)-C(13)-C(14)	118.208	120.002	-1.794
C(5)-C(13)-C(15)	112.347	112.340	0.007
C(12)-C(13)-C(14)	108.476	107.985	0.491
C(12)-C(13)-C(15)	109.579	108.152	1.427
C(14)-C(13)-C(15)	109.113	110.136	-1.023
C(8)-C(14)-C(9)	111.797	114.235	-2.438
C(8)-C(14)-C(13)	112.148	111.856	0.292
C(8)-C(14)-O(25)	110.327	113.178	-2.851
C(9)-C(14)-C(13)	106.973	107.082	-0.109
C(9)-C(14)-O(25)	107.363	101.392	5.971
C(13)-C(14)-O(25)	108.015	108.395	-0.380
C(13)-C(15)-C(16)	111.894	112.282	-0.388
C(15)-C(16)-N+(21)	110.558	110.089	0.469
C(18)-C(17)-N+(21)	111.643	115.068	-3.425
C(18)-C(17)-H(40)	114.812	110.882	3.930
C(18)-C(17)-H(41)	106.073	110.434	-4.361
N+(21)-C(17)-H(40)	114.812	106.773	8.039
N+(21)-C(17)-H(41)	106.074	106.092	-0.018
H(40)-C(17)-H(41)	102.142	107.178	-5.036
C(17)-C(18)-C(19)	118.655	118.558	0.097
C(17)-C(18)-C(20)	117.980	118.707	-0.727
C(17)-C(18)-H(42)	92.018	114.389	-22.371
C(19)-C(18)-C(20)	59.349	59.824	-0.475
C(19)-C(18)-H(42)	135.010	117.096	17.914

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(20)-C(18)-H(42)	135.590	117.668	17.922
C(18)-C(19)-C(20)	60.138	60.080	0.058
C(18)-C(19)-H(43)	138.534	117.759	20.775
C(18)-C(19)-H(44)	138.517	117.322	21.195
C(20)-C(19)-H(43)	138.534	117.469	21.065
C(20)-C(19)-H(44)	138.517	117.430	21.087
H(43)-C(19)-H(44)	60.061	115.541	-55.480
C(18)-C(20)-C(19)	60.514	60.095	0.419
C(18)-C(20)-H(45)	138.380	117.269	21.111
C(18)-C(20)-H(46)	138.317	117.679	20.638
C(19)-C(20)-H(45)	138.380	117.510	20.870
C(19)-C(20)-H(46)	138.316	117.415	20.901
H(45)-C(20)-H(46)	60.227	115.601	-55.374
C(9)-N+(21)-C(16)	113.214	111.953	1.261
C(9)-N+(21)-C(17)	114.424	115.383	-0.959
C(9)-N+(21)-H(47)	103.409	101.392	2.017
C(16)-N+(21)-C(17)	110.387	112.656	-2.269
C(16)-N+(21)-H(47)	108.084	105.665	2.419
C(17)-N+(21)-H(47)	106.686	108.645	-1.959
C(3)-O(22)-H(48)	124.208	110.140	14.068
C(4)-O(23)-C(5)	104.583	108.135	-3.552
C(14)-O(25)-H(49)	110.328	110.130	0.198

RMS value: 12.317

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(2)-C(3)-C(4)	2.7	2.2	0.5
C(1)-C(2)-C(3)-O(22)	-177.4	-176.2	-1.2
C(1)-C(11)-C(10)-C(9)	178.0	178.3	-0.3
C(1)-C(11)-C(12)-C(4)	4.0	7.2	-3.2
C(1)-C(11)-C(12)-C(13)	-177.1	-177.5	0.4
C(2)-C(1)-C(11)-C(10)	175.7	172.5	3.2
C(2)-C(1)-C(11)-C(12)	-0.4	-1.7	1.3
C(2)-C(3)-C(4)-C(12)	0.8	3	-2.2
C(2)-C(3)-C(4)-O(23)	-176.2	-173.7	-2.5
C(2)-C(3)-O(22)-H(48)	180.0	178.5	1.5
C(3)-C(2)-C(1)-C(11)	-2.9	-2.8	-0.1
C(3)-C(4)-C(12)-C(11)	-4.3	-7.9	3.6
C(3)-C(4)-C(12)-C(13)	176.6	175.9	0.7
C(3)-C(4)-O(23)-C(5)	162.1	167.4	-5.3
C(4)-C(3)-O(22)-H(48)	-0.1	0.2	-0.3
C(4)-C(12)-C(11)-C(10)	-172.4	-167.5	-4.9
C(4)-C(12)-C(13)-C(5)	22.9	18.2	4.7
C(4)-C(12)-C(13)-C(14)	146.5	142.8	3.7

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(4)-C(12)-C(13)-C(15)	-94.5	-98	3.5
C(4)-O(23)-C(5)-C(6)	-91.8	-102.4	10.6
C(4)-O(23)-C(5)-C(13)	29.8	21.3	8.5
C(4)-O(23)-C(5)-H(28)	149.6	140.4	9.2
C(5)-C(6)-C(7)-C(8)	-52.5	-34.6	-17.9
C(5)-C(13)-C(12)-C(11)	-156.1	-157.7	1.6
C(5)-C(13)-C(14)-C(8)	42.1	38.2	3.9
C(5)-C(13)-C(14)-C(9)	165.0	164	1.0
C(5)-C(13)-C(14)-O(25)	-79.7	-87	7.3
C(5)-C(13)-C(15)-C(16)	-169.9	-171.6	1.7
C(5)-O(23)-C(4)-C(12)	-15.1	-9.4	-5.7
C(6)-C(5)-C(13)-C(12)	86.5	95.9	-9.4
C(6)-C(5)-C(13)-C(14)	-29.7	-19.4	-10.3
C(6)-C(5)-C(13)-C(15)	-158.2	-151.2	-7.0
C(6)-C(7)-C(8)-C(14)	62.7	53.6	9.1
C(7)-C(6)-C(5)-C(13)	35.0	17.2	17.8
C(7)-C(6)-C(5)-O(23)	151.7	134.9	16.8
C(7)-C(6)-C(5)-H(28)	-85.0	-106.4	21.4
C(7)-C(8)-C(14)-C(9)	-176.9	-176.3	-0.6
C(7)-C(8)-C(14)-C(13)	-56.8	-54.5	-2.3
C(7)-C(8)-C(14)-O(25)	63.7	68.3	-4.6
C(8)-C(7)-C(6)-O(24)	127.8	150.4	-22.6
C(8)-C(14)-C(9)-C(10)	64.0	64.2	-0.2
C(8)-C(14)-C(9)-N+(21)	-170.6	-166.3	-4.3
C(8)-C(14)-C(13)-C(12)	-68.6	-71.2	2.6
C(8)-C(14)-C(13)-C(15)	172.0	170.9	1.1
C(8)-C(14)-O(25)-H(49)	180.0	-25.8	-154.2
C(9)-C(10)-C(11)-C(12)	-5.9	-7.6	1.7
C(9)-C(14)-C(13)-C(12)	54.3	54.7	-0.4
C(9)-C(14)-C(13)-C(15)	-65.1	-63.2	-1.9
C(9)-C(14)-O(25)-H(49)	57.9	-148.6	-153.5
C(9)-N+(21)-C(16)-C(15)	54.5	58.1	-3.6
C(9)-N+(21)-C(17)-C(18)	-52.7	-57.2	4.5
C(9)-N+(21)-C(17)-H(40)	80.2	66.4	13.8
C(9)-N+(21)-C(17)-H(41)	-167.8	-179.6	11.8
C(10)-C(9)-C(14)-C(13)	-59.1	-60.2	1.1
C(10)-C(9)-C(14)-O(25)	-174.9	-173.7	-1.2
C(10)-C(9)-N+(21)-C(16)	65.0	59.8	5.2
C(10)-C(9)-N+(21)-C(17)	-62.7	-70.8	8.1
C(10)-C(9)-N+(21)-H(47)	-178.3	172.1	9.6
C(10)-C(11)-C(12)-C(13)	6.5	7.9	-1.4
C(11)-C(10)-C(9)-C(14)	33.6	35.2	-1.6
C(11)-C(10)-C(9)-N+(21)	-88.0	-86.9	-1.1
C(11)-C(12)-C(4)-O(23)	173.1	169.1	4.0
C(11)-C(12)-C(13)-C(14)	-32.6	-33.1	0.5
C(11)-C(12)-C(13)-C(15)	86.5	86.1	0.4

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(12)-C(4)-C(3)-O(22)	-179.1	-178.7	-0.4
C(12)-C(13)-C(5)-O(23)	-31.5	-22.8	-8.7
C(12)-C(13)-C(14)-O(25)	169.6	163.4	6.2
C(12)-C(13)-C(15)-C(16)	-61.7	-65.9	4.2
C(13)-C(5)-C(6)-O(24)	-145.3	-167.8	22.5
C(13)-C(12)-C(4)-O(23)	-6.0	-7.1	1.1
C(13)-C(14)-C(9)-N+(21)	66.3	69.3	-3.0
C(13)-C(14)-O(25)-H(49)	-57.1	98.9	204.0
C(13)-C(15)-C(16)-N+(21)	-50.2	-47.9	-2.3
C(14)-C(9)-N+(21)-C(16)	-62.3	-68.4	6.1
C(14)-C(9)-N+(21)-C(17)	170.0	161.0	9.0
C(14)-C(9)-N+(21)-H(47)	54.4	43.8	10.6
C(14)-C(13)-C(5)-O(23)	-147.8	-138.1	-9.7
C(14)-C(13)-C(15)-C(16)	57.0	51.8	5.2
C(15)-C(13)-C(5)-O(23)	83.8	90.0	-6.2
C(15)-C(13)-C(14)-O(25)	50.2	45.5	4.7
C(15)-C(16)-N+(21)-C(17)	-175.7	-169.9	-5.8
C(15)-C(16)-N+(21)-H(47)	-59.4	-51.4	-8.0
C(16)-N+(21)-C(17)-C(18)	178.2	172.6	5.6
C(16)-N+(21)-C(17)-H(40)	-48.9	-63.9	15.0
C(16)-N+(21)-C(17)-H(41)	63.1	50.2	12.9
C(17)-C(18)-C(19)-C(20)	107.3	108.4	-1.1
C(17)-C(18)-C(19)-H(43)	-23.6	1.1	-24.7
C(17)-C(18)-C(19)-H(44)	-121.8	-144.1	22.3
C(17)-C(18)-C(20)-C(19)	-108.4	-108.2	-0.2
C(17)-C(18)-C(20)-H(45)	120.5	144.2	-23.7
C(17)-C(18)-C(20)-H(46)	22.5	-0.8	23.3
C(18)-C(17)-N+(21)-H(47)	61.0	55.9	5.1
C(18)-C(19)-C(20)-H(45)	131.0	107.2	23.8
C(18)-C(19)-C(20)-H(46)	-130.9	-107.8	-23.1
C(18)-C(20)-C(19)-H(43)	130.9	107.8	23.1
C(18)-C(20)-C(19)-H(44)	-130.0	-107.3	-22.7
C(19)-C(18)-C(17)-N+(21)	-140.2	-146.5	6.3
C(19)-C(18)-C(17)-H(40)	86.9	92.2	-5.3
C(19)-C(18)-C(17)-H(41)	-25.1	-26.5	1.4
C(19)-C(18)-C(20)-H(45)	-131.0	-107.6	-23.4
C(19)-C(18)-C(20)-H(46)	130.9	107.3	23.6
C(19)-C(20)-C(18)-H(42)	124.7	106.9	17.8
C(20)-C(18)-C(17)-N+(21)	-71.8	-77.3	5.5
C(20)-C(18)-C(17)-H(40)	155.3	161.4	-6.1
C(20)-C(18)-C(17)-H(41)	43.3	42.8	0.5
C(20)-C(18)-C(19)-H(43)	-130.9	-107.4	-23.5
C(20)-C(18)-C(19)-H(44)	130.9	107.5	23.4
C(20)-C(19)-C(18)-H(42)	-125.6	-107.8	-17.8
N+(21)-C(9)-C(14)-O(25)	-49.4	-44.2	-5.2
N+(21)-C(17)-C(18)-H(42)	74.1	68.8	5.3

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
O(22)-C(3)-C(4)-O(23)	3.9	4.6	-0.7
O(23)-C(5)-C(6)-O(24)	-28.6	-50.1	21.5
H(40)-C(17)-C(18)-H(42)	-58.8	-52.5	-6.3
H(40)-C(17)-N+(21)-H(47)	-166.1	179.4	14.5
H(41)-C(17)-C(18)-H(42)	-170.8	-171.2	0.4
H(41)-C(17)-N+(21)-H(47)	-54.1	-66.6	12.5
H(42)-C(18)-C(19)-H(43)	103.5	144.8	-41.3
H(42)-C(18)-C(19)-H(44)	5.3	-0.3	5.6
H(42)-C(18)-C(20)-H(45)	-6.3	-0.8	-5.5
H(42)-C(18)-C(20)-H(46)	-104.3	-145.8	41.5
H(43)-C(19)-C(20)-H(45)	-98.0	-144.9	46.9
H(43)-C(19)-C(20)-H(46)	0.0	0.1	-0.1
H(44)-C(19)-C(20)-H(45)	0.1	-0.1	0.2
H(44)-C(19)-C(20)-H(46)	98.2	144.9	-46.7
		RMS value:	29.9

Table 8. Oxymorphone

I. Missing parameters

A. Missing for atoms 6-5-20-4 (type 3-1-42-2)
Missing for atoms 20-6-5-7 (type 41-1-3-1)
Missing for atoms 12-13-5-20 (type2-1-1-41)
Missing for atoms 20-5-6-21 (type 41-1-3-7)
Missing for atoms 6-5-20 (type 3-1-41) angle type 2

B. Estimated Parameters

4 torsional parameters are read in

Atom type numbers	V1	V2	V3
3 1 42 2	0.000	0.160	0.090
41 1 3 1	0.000	0.160	0.090
2 1 1 41	0.000	0.000	0.270
41 1 3 7	0.000	0.160	0.090

1 bending parameter is read in

Atom type numbers	Kb	Theta
3 1 41	0.695	109.500

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in angstroms)
C(1)-C(2)	1.3521	1.4034	-0.0513
C(1)-C(11)	1.3812	1.4014	-0.0202
C(2)-C(3)	1.3566	1.4092	-0.0526
C(3)-C(4)	1.3703	1.3948	-0.0245
C(3)-O(19)	1.3433	1.2436	0.0997
C(4)-C(12)	1.3445	1.3788	-0.0343
C(4)-O(20)	1.3602	1.2316	0.1286
C(5)-C(6)	1.5172	1.5387	-0.0215
C(5)-C(13)	1.4980	1.5553	-0.0573
C(5)-O(20)	1.4383	1.4571	-0.0188
C(5)-H(25)	0.9498	1.1135	-0.1637
C(6)-C(7)	1.4760	1.5256	-0.0496
C(6)-O(21)	1.1817	1.2132	-0.0315
C(7)-C(8)	1.4847	1.5275	-0.0428
C(7)-H(26)	0.9415	1.1133	-0.1718

Bond	Length Crystal	MM3	Difference (in angstroms)
C(7)-H(27)	0.9609	1.1112	-0.1503
C(8)-C(14)	1.4912	1.5191	-0.0279
C(8)-H(28)	0.9371	1.1117	-0.1746
C(8)-H(29)	0.9571	1.1107	-0.1536
C(9)-C(10)	1.5244	1.5431	-0.0187
C(9)-C(14)	1.5023	1.5400	-0.0377
C(9)-N+(18)	1.5058	1.5213	-0.0155
C(9)-H(30)	1.0101	1.1040	-0.0939
C(10)-C(11)	1.4676	1.5071	-0.0395
C(10)-H(31)	0.9450	1.1071	-0.1621
C(10)-H(32)	0.9305	1.1095	-0.1790
C(11)-C(12)	1.3356	1.3828	-0.0472
C(12)-C(13)	1.5163	1.5009	0.0154
C(13)-C(14)	1.5222	1.5282	-0.0060
C(13)-C(15)	1.5192	1.5502	-0.0310
C(14)-O(22)	1.4143	1.4465	-0.0322
C(15)-C(16)	1.4822	1.5281	-0.0459
C(15)-H(33)	0.9474	1.1092	-0.1618
C(15)-H(34)	0.9452	1.1090	-0.1638
C(16)-N+(18)	1.4842	1.5030	-0.0188
C(16)-H(35)	0.9504	1.0990	-0.1486
C(16)-H(36)	0.9569	1.1007	-0.1438
C(17)-N+(18)	1.4597	1.4979	-0.0382
N+(18)-H(40)	0.9848	1.0348	-0.0500
O(19)-H(42)	0.7710	0.9598	-0.1888
O(22)-H(41)	0.8554	0.9423	-0.0869

RMS value: 0.1082

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(2)-C(1)-C(11)	121.170	120.357	0.813
C(1)-C(2)-C(3)	121.164	120.799	0.365
C(2)-C(3)-C(4)	117.587	118.158	-0.571
C(2)-C(3)-O(19)	122.461	122.252	0.209
C(4)-C(3)-O(19)	119.920	119.576	0.344
C(3)-C(4)-C(12)	120.249	119.675	0.574
C(3)-C(4)-C(20)	128.390	125.053	3.337
C(12)-C(4)-C(20)	111.274	115.189	-3.915

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(6)-C(5)-C(13)	111.899	115.733	-3.834
C(6)-C(5)-O(20)	108.596	107.949	0.647
C(6)-C(5)-H(25)	107.029	107.543	-0.514
C(13)-C(5)-O(20)	105.002	105.793	-0.791
C(13)-C(5)-H(25)	111.536	109.932	1.604
O(20)-C(5)-H(25)	112.829	109.795	3.034
C(5)-C(6)-C(7)	117.279	119.456	-2.177
C(5)-C(6)-O(21)	120.945	120.435	0.510
C(7)-C(6)-O(21)	121.676	119.895	1.781
C(6)-C(7)-C(8)	109.075	114.934	-5.859
C(6)-C(7)-H(26)	110.526	108.224	2.302
C(6)-C(7)-H(27)	110.279	109.034	1.245
C(8)-C(7)-H(26)	109.600	109.679	-0.079
C(8)-C(7)-H(27)	108.245	108.875	-0.630
H(26)-C(7)-H(27)	109.078	105.693	3.385
C(7)-C(8)-C(14)	109.998	112.688	-2.690
C(7)-C(8)-H(28)	110.072	109.654	0.418
C(7)-C(8)-H(29)	109.018	108.599	0.419
C(14)-C(8)-H(28)	108.464	109.772	-1.308
C(14)-C(8)-H(29)	108.450	109.783	-1.333
H(28)-C(8)-H(29)	110.817	106.126	4.691
C(10)-C(9)-C(14)	115.583	115.338	0.245
C(10)-C(9)-N+(18)	113.223	117.497	-4.274
C(10)-C(9)-H(30)	96.576	107.565	-10.989
C(14)-C(9)-N+(18)	106.152	103.000	3.152
C(14)-C(9)-H(30)	106.737	108.477	-1.740
N+(18)-C(9)-H(30)	118.691	104.170	14.521
C(9)-C(10)-C(11)	114.500	114.023	0.477
C(9)-C(10)-H(31)	106.299	110.358	-4.059
C(9)-C(10)-H(32)	108.019	108.632	-0.613
C(11)-C(10)-H(31)	107.529	109.862	-2.333
C(11)-C(10)-H(32)	109.195	107.524	1.671
H(31)-C(10)-H(32)	111.310	106.089	5.221
C(1)-C(11)-C(10)	125.832	124.988	0.844
C(1)-C(11)-C(12)	116.429	117.233	-0.804
C(10)-C(11)-C(12)	117.630	117.497	0.133
C(4)-C(12)-C(11)	123.277	123.285	-0.008
C(4)-C(12)-C(13)	108.640	108.470	0.170
C(11)-C(12)-C(13)	128.004	128.068	-0.064
C(5)-C(13)-C(12)	97.191	97.035	0.156
C(5)-C(13)-C(14)	117.914	119.764	-1.850

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(5)-C(13)-C(15)	112.126	112.238	-0.112
C(12)-C(13)-C(14)	107.408	107.757	-0.349
C(12)-C(13)-C(15)	109.774	108.282	1.492
C(14)-C(13)-C(15)	111.222	110.347	0.875
C(8)-C(14)-C(9)	112.404	114.138	-1.734
C(8)-C(14)-C(13)	112.565	111.740	0.825
C(8)-C(14)-O(22)	110.363	113.274	-2.911
C(9)-C(14)-C(13)	105.404	107.068	-1.664
C(9)-C(14)-O(22)	103.072	101.501	1.571
C(13)-C(14)-O(22)	112.575	108.435	4.140
C(13)-C(15)-C(16)	111.044	112.408	-1.364
C(13)-C(15)-H(33)	108.431	110.227	-1.796
C(13)-C(15)-H(34)	109.256	109.476	-0.220
C(16)-C(15)-H(33)	108.438	109.134	-0.696
C(16)-C(15)-H(34)	108.929	109.605	-0.676
H(33)-C(15)-H(34)	110.744	105.773	4.971
C(15)-C(16)-N+(18)	110.433	109.663	0.770
C(15)-C(16)-H(35)	109.369	112.887	-3.518
C(15)-C(16)-H(36)	108.454	111.584	-3.130
N+(18)-C(16)-H(35)	109.848	107.206	2.642
N+(18)-C(16)-H(36)	109.372	107.547	1.825
H(35)-C(16)-H(36)	109.339	107.719	1.620
C(9)-N+(18)-C(16)	114.594	112.359	2.235
C(9)-N+(18)-C(17)	112.569	114.100	-1.531
C(9)-N+(18)-H(40)	103.061	101.465	1.596
C(16)-N+(18)-C(17)	110.367	113.128	-2.761
C(16)-N+(18)-H(40)	103.850	105.983	-2.133
C(17)-N+(18)-H(40)	111.851	108.737	3.114
C(3)-O(19)-H(42)	110.588	110.268	0.320
C(4)-O(20)-C(5)	104.549	108.351	-3.802
C(14)-O(22)-H(41)	112.717	110.055	2.662

RMS value: 3.017

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(2)-C(3)-C(4)	-1.9	-2.0	0.1
C(1)-C(2)-C(3)-O(19)	176.0	176.6	-0.6
C(1)-C(11)-C(10)-C(9)	-179.3	-179.4	0.1

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(1)-C(11)-C(10)-H(31)	-61.4	-54.9	-6.5
C(1)-C(11)-C(10)-H(32)	59.5	60.1	-0.6
C(1)-C(11)-C(12)-C(4)	-4.1	-7.3	3.2
C(1)-C(11)-C(12)-C(13)	179.5	178.1	1.4
C(2)-C(1)-C(11)-C(10)	-173.7	-172.1	-1.6
C(2)-C(1)-C(11)-C(12)	2.4	1.6	0.8
C(2)-C(3)-C(4)-C(12)	0.3	-3.4	3.7
C(2)-C(3)-C(4)-O(20)	176.6	173.2	3.4
C(2)-C(3)-O(19)-H(42)	-17.4	0.5	-17.9
C(3)-C(2)-C(1)-C(11)	0.5	2.9	-2.4
C(3)-C(4)-C(12)-C(11)	2.9	8.3	-5.4
C(3)-C(4)-C(12)-C(13)	179.8	-176.2	-4.0
C(3)-C(4)-O(20)-C(5)	-156.5	-168.0	11.5
C(4)-C(3)-O(19)-H(42)	160.5	179.0	-18.5
C(4)-C(12)-C(11)-C(10)	172.3	166.9	5.4
C(4)-C(12)-C(13)-C(5)	-23.1	-17.4	-5.7
C(4)-C(12)-C(13)-C(14)	-145.4	-141.8	-3.6
C(4)-C(12)-C(13)-C(15)	93.5	98.8	-5.3
C(4)-O(20)-C(5)-C(6)	84.7	104.4	-19.7
C(4)-O(20)-C(5)-C(13)	-35.1	-20.1	-15.0
C(4)-O(20)-C(5)-H(25)	-156.8	-138.7	-18.1
C(5)-C(6)-C(7)-C(8)	55.6	29.5	26.1
C(5)-C(6)-C(7)-H(26)	-65.0	-93.5	28.5
C(5)-C(6)-C(7)-H(27)	174.3	152.0	22.3
C(5)-C(13)-C(12)-C(11)	153.7	157.8	-4.1
C(5)-C(13)-C(14)-C(8)	-40.8	-38.9	-1.9
C(5)-C(13)-C(14)-C(9)	-163.6	-164.5	0.9
C(5)-C(13)-C(14)-O(22)	84.7	86.7	-2.0
C(5)-C(13)-C(15)-C(16)	168.6	172.1	-3.5
C(5)-C(13)-C(15)-H(33)	49.6	50.1	-0.5
C(5)-C(13)-C(15)-H(34)	-71.2	-65.9	-5.3
C(5)-O(20)-C(4)-C(12)	20.0	8.7	11.3
C(6)-C(5)-C(13)-C(12)	-83.8	-97.8	14.0
C(6)-C(5)-C(13)-C(14)	30.8	17.3	13.5
C(6)-C(5)-C(13)-C(15)	161.9	149.1	12.8
C(6)-C(7)-C(8)-C(14)	-62.6	-51.5	-11.1
C(6)-C(7)-C(8)-H(28)	177.9	-174.1	-8.0
C(6)-C(7)-C(8)-H(29)	56.3	70.4	-14.1
C(7)-C(6)-C(5)-C(13)	-38.9	-12.1	-26.8
C(7)-C(6)-C(5)-O(20)	-154.4	-130.4	-24.0
C(7)-C(6)-C(5)-H(25)	83.5	111.2	-27.7
C(7)-C(8)-C(14)-C(9)	174.7	177	-2.3

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(7)-C(8)-C(14)-C(13)	55.8	55.3	0.5
C(7)-C(8)-C(14)-O(22)	-70.9	-67.5	-3.4
C(8)-C(7)-C(6)-O(21)	-120.8	-155.8	35.0
C(8)-C(14)-C(9)-C(10)	-61.1	-63.9	2.8
C(8)-C(14)-C(9)-N+(18)	172.5	166.8	5.7
C(8)-C(14)-C(9)-H(30)	45	56.8	-11.8
C(8)-C(14)-C(13)-C(12)	67.5	70.5	-3.0
C(8)-C(14)-C(13)-C(15)	-172.3	-171.5	-0.8
C(8)-C(14)-O(22)-H(41)	90.7	31.6	59.1
C(9)-C(10)-C(11)-C(12)	4.6	6.9	-2.3
C(9)-C(14)-C(8)-H(28)	-64.9	-60.5	-4.4
C(9)-C(14)-C(8)-H(29)	55.5	55.8	-0.3
C(9)-C(14)-C(13)-C(12)	-55.3	-55.2	-0.1
C(9)-C(14)-C(13)-C(15)	64.8	62.8	2.0
C(9)-C(14)-O(22)-H(41)	-149.1	154.4	56.5
C(9)-N+(18)-C(16)-C(15)	-53.8	-58.5	4.7
C(9)-N+(18)-C(16)-H(35)	66.9	64.4	2.5
C(9)-N+(18)-C(16)-H(36)	-173.1	180	6.9
C(10)-C(9)-C(14)-C(13)	61.9	60.3	1.6
C(10)-C(9)-C(14)-O(22)	-179.9	173.9	6.2
C(10)-C(9)-N+(18)-C(16)	-65.4	-59.1	-6.3
C(10)-C(9)-N+(18)-C(17)	61.8	71.4	-9.6
C(10)-C(9)-N+(18)-H(40)	-177.5	-171.9	-5.6
C(10)-C(11)-C(1)-H(23)	2.5	6.1	-3.6
C(10)-C(11)-C(12)-C(13)	-4.1	-7.7	3.6
C(11)-C(1)-C(2)-H(24)	-174.8	179.9	5.3
C(11)-C(10)-C(9)-C(14)	-35.6	-34.6	-1.0
C(11)-C(10)-C(9)-N+(18)	87.2	87.2	0.0
C(11)-C(10)-C(9)-H(30)	-147.7	-155.8	8.1
C(11)-C(12)-C(4)-O(20)	-174	-168.6	-5.4
C(11)-C(12)-C(13)-C(14)	31.4	33.4	-2.0
C(11)-C(12)-C(13)-C(15)	-89.7	-85.9	-3.8
C(12)-C(4)-C(3)-O(19)	-177.7	178	4.3
C(12)-C(11)-C(10)-H(31)	122.5	131.4	-8.9
C(12)-C(11)-C(10)-H(32)	-116.6	-113.6	-3.0
C(12)-C(13)-C(5)-O(20)	34.3	21.6	12.7
C(12)-C(13)-C(5)-H(25)	156.8	140.1	16.7
C(12)-C(13)-C(14)-O(22)	-166.9	-164	-2.9
C(12)-C(13)-C(15)-C(16)	61.8	66.1	-4.3
C(12)-C(13)-C(15)-H(33)	-57.3	-55.9	-1.4
C(12)-C(13)-C(15)-H(34)	-178.1	-171.8	-6.3
C(13)-C(5)-C(6)-O(21)	137.5	173.2	-35.7

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(13)-C(12)-C(4)-O(20)	3	6.9	-3.9
C(13)-C(14)-C(8)-H(28)	176.3	177.8	-1.5
C(13)-C(14)-C(8)-H(29)	-63.3	-65.9	2.6
C(13)-C(14)-C(9)-N+(18)	-64.5	-69	4.5
C(13)-C(14)-C(9)-H(30)	167.9	-179	-13.1
C(13)-C(14)-O(22)-H(41)	-36	-93	57.0
C(13)-C(15)-C(16)-N+(18)	48.8	47.7	1.1
C(13)-C(15)-C(16)-H(35)	-72.2	-71.8	-0.4
C(13)-C(15)-C(16)-H(36)	168.7	166.7	2.0
C(14)-C(8)-C(7)-H(26)	58.5	70.7	-12.2
C(14)-C(8)-C(7)-H(27)	177.4	-174.1	-8.5
C(14)-C(9)-C(10)-H(31)	-154.2	-158.9	4.7
C(14)-C(9)-C(10)-H(32)	86.3	85.2	1.1
C(14)-C(9)-N+(18)-C(16)	62.4	68.9	-6.5
C(14)-C(9)-N+(18)-C(17)	-170.4	-160.6	-9.8
C(14)-C(9)-N+(18)-H(40)	-49.7	-43.9	-5.8
C(14)-C(13)-C(5)-O(20)	148.4	136.8	11.6
C(14)-C(13)-C(5)-H(25)	-89.1	-104.8	15.7
C(14)-C(13)-C(15)-C(16)	-57	-51.6	-5.4
C(14)-C(13)-C(15)-H(33)	-176	-173.6	-2.4
C(14)-C(13)-C(15)-H(34)	63.2	70.5	-7.3
C(15)-C(13)-C(5)-O(20)	-80.5	-91.4	10.9
C(15)-C(13)-C(5)-H(25)	42	27.1	14.9
C(15)-C(13)-C(14)-O(22)	-46.8	-46	-0.8
C(15)-C(16)-N+(18)-C(17)	177.9	170.5	7.4
C(15)-C(16)-N+(18)-H(40)	57.8	51.5	6.3
C(16)-N+(18)-C(9)-H(30)	-177.5	-177.9	0.4
C(17)-N+(18)-C(9)-H(30)	-50.3	-47.5	-2.8
C(17)-N+(18)-C(16)-H(35)	-61.4	-66.6	5.2
C(17)-N+(18)-C(16)-H(36)	58.6	49	9.6
N+(18)-C(9)-C(10)-H(31)	-31.4	-37	5.6
N+(18)-C(9)-C(10)-H(32)	-151	-153	2.0
N+(18)-C(9)-C(14)-O(22)	53.7	44.5	9.2
N+(18)-C(16)-C(15)-H(33)	167.9	170.3	-2.4
N+(18)-C(16)-C(15)-H(34)	-71.5	-74.3	2.8
O(19)-C(3)-C(2)-H(24)	-8.7	-0.4	-8.3
O(19)-C(3)-C(4)-O(20)	-1.4	-5.5	4.1
O(20)-C(5)-C(6)-O(21)	22	54.9	-32.9
O(21)-C(6)-C(5)-H(25)	-100.1	-63.5	-36.6
O(21)-C(6)-C(7)-H(26)	118.6	81.2	37.4
O(21)-C(6)-C(7)-H(27)	-2.1	-33.3	31.2
O(22)-C(14)-C(8)-H(28)	49.6	55	-5.4

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
O(22)-C(14)-C(8)-H(29)	170	171.3	-1.3
O(22)-C(14)-C(9)-H(30)	-73.9	-65.5	-8.4
H(26)-C(7)-C(8)-H(28)	-60.9	-51.9	-9.0
H(26)-C(7)-C(8)-H(29)	177.3	-167.5	-15.2
H(27)-C(7)-C(8)-H(28)	57.9	63.3	-5.4
H(27)-C(7)-C(8)-H(29)	-63.8	-52.2	-11.6
H(30)-C(9)-C(10)-H(31)	93.7	80	13.7
H(30)-C(9)-C(10)-H(32)	-25.8	-35.9	10.1
H(30)-C(9)-N+(18)-H(40)	70.3	69.3	1.0
H(33)-C(15)-C(16)-H(35)	46.9	50.8	-3.9
H(33)-C(15)-C(16)-H(36)	-72.3	-70.7	-1.6
H(34)-C(15)-C(16)-H(35)	167.5	166.2	1.3
H(34)-C(15)-C(16)-H(36)	48.3	44.7	3.6
H(35)-C(16)-N+(18)-H(40)	178.6	174.3	4.3
H(36)-C(16)-N+(18)-H(40)	-61.4	-70.1	8.7
		RMS value:	13.9

Table 9. Salicylic acid

I. Missing parameters

A. Missing for atoms 1-7-14-8 (type 2-3-75-24)

B. Estimated Parameters

4 torsional parameters are read in

Atom type numbers	V1	V2	V3
2 3 75 24	0.000	2.470	-0.600

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in angstroms)
C(1)-C(2)	1.4040	1.4125	-0.0085
C(1)-C(6)	1.3963	1.4040	-0.0077
C(1)-C(7)	1.4581	1.5051	-0.0470
C(2)-C(3)	1.3829	1.3979	-0.0150
C(2)-O(16)	1.3574	1.2441	0.1133
C(3)-H(10)	0.9861	1.1012	-0.1151
C(6)-H(13)	0.9825	1.1024	-0.1199
C(7)-H(14)	1.3089	1.3704	-0.0615
C(7)-O(15)	1.2345	1.2172	0.0173
H(8)-O(14)	0.9994	0.9737	0.0257
H(9)-O(16)	1.0300	0.9646	0.0654
		RMS value:	0.0721

III. Bond angles

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(2)-C(1)-C(6)	118.567	119.513	-0.946
C(2)-C(1)-C(7)	120.378	124.392	-4.014
C(6)-C(1)-C(7)	121.055	116.096	4.959
C(1)-C(2)-C(3)	119.590	119.360	0.230
C(1)-C(2)-O(16)	122.791	123.183	-0.392
C(3)-C(2)-O(16)	117.617	117.457	0.160
C(1)-C(6)-H(13)	117.368	120.822	-3.454
C(1)-C(7)-O(14)	115.990	120.775	-4.785
C(1)-C(7)-O(15)	122.802	120.856	1.946
O(14)-C(7)-O(15)	121.204	118.369	2.835
C(7)-O(14)-H(8)	111.441	107.662	3.779
C(2)-O(16)-H(9)	106.201	109.282	-3.081

RMS value: 3.206

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(2)-O(16)-H(9)	2.2	0.0	2.2
C(1)-C(7)-O(14)-H(8)	-177.0	180.0	3.0
C(2)-C(1)-C(6)-H(13)	177.1	-180.0	-2.9
C(2)-C(1)-C(7)-O(14)	-179.6	-180.0	0.4
C(2)-C(1)-C(7)-O(15)	1.1	0.0	1.1
C(3)-C(2)-C(1)-C(6)	0.4	0.0	0.4
C(3)-C(2)-C(1)-C(7)	-179.6	180.0	0.4
C(3)-C(2)-O(16)-H(9)	-178.4	-180.0	1.6
C(6)-C(1)-C(2)-O(16)	179.8	-180.0	-0.2
C(6)-C(1)-C(7)-O(14)	0.5	0.0	0.5
C(6)-C(1)-C(7)-O(15)	-178.8	-180.0	1.2
C(7)-C(1)-C(2)-O(16)	-0.1	0.0	-0.1
C(7)-C(1)-C(6)-H(13)	-2.9	0.0	-2.9
H(8)-O(14)-C(7)-O(15)	2.3	0.0	2.3
H(10)-C(3)-C(2)-O(16)	-3.1	0.0	-3.1

RMS value: 1.9

Table 10. Meclofenamate

I. Missing parameters

A. Missing for atoms 1-2-3-4 (type 2-2-3-47)

Missing for atoms 12-11-10-1 (type 2-2-8-2)

Missing for atoms 18-11-10-1 (type 2-2-8-2)

Missing for atoms 2-1-10-11 (type 2-2-8-2)

Missing for atoms 9-1-10-11 (type 2-2-8-2)

Missing for atoms 10-11-12-13 (type 8-2-2-12)

Missing for atoms 10-11-18-19 (type 8-2-2-12)

Missing for atoms 2-3-4 (type 2-3-47) angle tpe 1

Missing for atoms 2-3-5 (type 2-3-47) angle type 1

Missing for atoms 1-10-11 (type 8-2-2-12) angle type 1

B. Estimated Parameters

3 torsional parameters are read in

Atom type numbers	V1	V2	V3
2 2 3 47	0.000	11.600	0.000
2 2 8 2	0.000	0.000	0.000
8 2 2 12	0.000	11.600	0.000

2 bending parameters are read in

Atom type numbers	Kb	Theta
2 3 47	0.695	120.000
2 8 2	0.695	110.000

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in angstroms)
C(1)-C(2)	1.4327	1.4244	0.0083
C(1)-C(9)	1.3873	1.4079	-0.0206
C(1)-N(10)	1.3568	1.4018	-0.0450
C(2)-C(3)	1.4845	1.3795	0.1050
C(2)-C(6)	1.3869	1.4078	-0.0209
C(3)-O(4)	1.2435	1.2541	-0.0106
C(3)-O(5)	1.2733	1.2579	0.0154
C(6)-H(20)	0.9902	1.1023	-0.1121
C(9)-H(23)	1.0040	1.1020	-0.0980
N(10)-C(11)	1.4070	1.3937	0.0133
N(10)-H(24)	0.9176	1.0122	-0.0946

	Length			Difference
Bond	Crystal	MM3		(in angstroms)
C(11)-C(12)	1.4409	1.4124		0.0285
C(11)-C(18)	1.3541	1.3992		-0.0451
C(14)-C(15)	1.5422	1.5105		0.0317
C(18)-C(19)	1.7472	1.7382		0.0090
			RMS value:	0.0575

III. Bond angles

	Theta (in degrees)			Difference
Bond	Crystal	MM3		(in degrees)
C(2)-C(1)-C(9)	118.892	118.287		0.605
C(2)-C(1)-N(10)	120.941	124.344		-3.403
C(9)-C(1)-N(10)	120.159	117.362		2.797
C(1)-C(2)-C(3)	122.088	126.670		-4.582
C(1)-C(2)-C(6)	116.816	118.619		-1.803
C(3)-C(2)-C(6)	121.059	114.710		6.349
C(2)-C(3)-O(4)	120.246	119.120		1.126
C(2)-C(3)-O(5)	117.409	116.542		0.867
O(4)-C(3)-O(5)	122.310	124.335		-2.025
C(2)-C(6)-H(20)	109.095	120.632		-11.537
C(1)-C(9)-H(23)	120.099	120.175		-0.076
C(1)-N(10)-C(11)	124.053	115.829		8.224
C(1)-N(10)-H(24)	119.406	111.373		8.033
C(11)-N(10)-H(24)	116.368	110.792		5.576
N(10)-C(11)-C(12)	119.567	122.567		-3.000
N(10)-C(11)-C(18)	123.994	118.973		5.021
C(12)-C(11)-C(18)	116.438	118.438		-2.000
C(11)-C(12)-Cl(13)	118.242	120.379		-2.137
C(11)-C(12)-C(14)	120.264	121.111		-0.847
Cl(13)-C(12)-C(14)	121.490	118.508		2.982
C(12)-C(14)-C(15)	119.964	121.887		-1.923
C(11)-C(18)-Cl(19)	119.337	121.238		-1.901
			RMS value:	4.505

IV. Dihedral angles

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(1)-C(2)-C(3)-O(4)	0.5	-1.1	1.6
C(1)-C(2)-C(3)-O(5)	178.4	179.6	-1.2
C(1)-C(2)-C(6)-H(20)	-176.2	-179.2	3.0

	Omega (in degrees)			Difference
Bond	Crystal	MM3		(in degrees)
C(1)-N(10)-C(11)-C(12)	98.7	75.8		22.9
C(1)-N(10)-C(11)-C(18)	-81.4	-105.9		24.5
C(2)-C(1)-C(9)-H(23)	-167.8	-178.3		10.5
C(2)-C(1)-N(10)-C(11)	-174.6	-134.9		-39.7
C(2)-C(1)-N(10)-H(24)	0.4	-7.1		7.5
C(3)-C(2)-C(1)-C(9)	-175.1	176.9		-8.0
C(3)-C(2)-C(1)-N(10)	3.9	-2.1		6.0
C(3)-C(2)-C(6)-H(20)	1.6	1.2		0.4
O(4)-C(3)-C(2)-C(6)	-177.2	178.5		-4.3
O(5)-C(3)-C(2)-C(6)	0.7	-0.9		1.6
C(6)-C(2)-C(1)-C(9)	2.7	-2.7		5.4
C(6)-C(2)-C(1)-N(10)	-178.3	178.3		-3.4
C(9)-C(1)-N(10)-C(11)	4.4	46.1		-41.7
C(9)-C(1)-N(10)-H(24)	179.4	173.9		5.5
N(10)-C(1)-C(9)-H(23)	13.1	0.8		12.3
N(10)-C(11)-C(12)-Cl(13)	-0.9	-0.7		-0.2
N(10)-C(11)-C(12)-C(14)	179.9	179.8		0.1
N(10)-C(11)-C(18)-Cl(19)	0.6	-0.6		1.2
C(11)-C(12)-C(14)-C(15)	179.3	179.4		-0.1
C(12)-C(11)-N(10)-H(24)	-76.5	-52.3		-24.2
C(12)-C(11)-C(18)-Cl(19)	-179.6	177.8		-2.6
Cl(13)-C(12)-C(11)-C(18)	179.2	-179.0		1.8
Cl(13)-C(12)-C(14)-C(15)	0.2	-0.1		0.3
C(18)-C(11)-N(10)-H(24)	103.4	126.0		-22.6
			RMS value:	4.6

Table 11. Procaine

I. Missing parameters

No missing parameters for this molecule.

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(2)	1.3851	1.3970	-0.0119
C(1)-C(6)	1.4050	1.3994	0.0056
C(1)-C(7)	1.4608	1.4959	-0.0351
C(2)-C(3)	1.3688	1.3967	-0.0279
C(3)-C(4)	1.4060	1.4025	0.0035
C(4)-C(5)	1.3991	1.4049	-0.0058
C(4)-N(10)	1.3677	1.3975	-0.0298
C(5)-C(6)	1.3596	1.3946	-0.0350
C(7)-O(8)	1.3318	1.3640	-0.0322
C(7)-O(9)	1.2198	1.2189	0.0009
O(8)-C(11)	1.4590	1.4455	0.0135
N(10)-H(22)	0.9984	1.0154	-0.0170
N(10)-H(23)	0.8736	1.0154	-0.1418
C(11)-C(12)	1.5037	1.5294	-0.0257
C(12)-N(13)	1.4769	1.4684	0.0085
C(12)-H(26)	1.0792	1.1234	-0.0442
C(12)-H(27)	0.9726	1.1109	-0.1383
N(13)-C(14)	1.4404	1.4682	-0.0278
N(13)-C(16)	1.4678	1.4667	0.0011
C(14)-C(15)	1.4858	1.5319	-0.0461
C(14)-H(28)	1.2409	1.1251	0.1158
C(14)-H(29)	1.2304	1.1146	0.1158
C(16)-C(17)	1.5076	1.5323	-0.0247
C(16)-H(33)	1.1715	1.1134	0.0581
C(16)-H(34)	1.1819	1.1106	0.0713
		RMS value:	0.0601

III. Bond angles

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(2)-C(1)-C(6)	117.744	120.038	-2.294
C(2)-C(1)-C(7)	123.238	119.725	3.513

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(6)-C(1)-C(7)	119.013	120.236	-1.223
C(1)-C(2)-C(3)	122.117	119.866	2.251
C(2)-C(3)-C(4)	119.895	120.750	-0.855
C(3)-C(4)-C(5)	118.113	118.744	-0.631
C(3)-C(4)-N(10)	120.209	120.632	-0.423
C(5)-C(4)-N(10)	121.648	120.617	1.031
C(4)-C(5)-C(6)	121.251	120.766	0.485
C(1)-C(6)-C(5)	120.866	119.831	1.035
C(1)-C(7)-O(8)	112.449	120.098	-7.649
C(1)-C(7)-O(9)	125.225	119.772	5.453
O(8)-C(7)-O(9)	122.325	120.098	2.227
C(7)-O(8)-C(11)	118.331	116.627	1.704
C(4)-N(10)-H(22)	118.403	113.746	4.657
C(4)-N(10)-H(23)	115.842	113.758	2.084
H(22)-N(10)-H(23)	122.583	109.387	13.196
O(8)-C(11)-C(12)	109.121	110.343	-1.222
C(11)-C(12)-N(13)	113.387	114.979	-1.592
C(11)-C(12)-H(26)	111.211	109.936	1.275
C(11)-C(12)-H(27)	112.619	106.679	5.940
N(13)-C(12)-H(26)	111.382	110.412	0.970
N(13)-C(12)-H(27)	106.264	108.610	-2.346
H(26)-C(12)-H(27)	101.246	105.743	-4.497
C(12)-N(13)-C(14)	113.172	112.801	0.371
C(12)-N(13)-C(16)	114.937	115.328	-0.391
C(14)-N(13)-C(16)	112.250	111.587	0.663
N(13)-C(14)-C(15)	115.526	113.727	1.799
N(13)-C(14)-H(28)	105.838	110.245	-4.407
N(13)-C(14)-H(29)	110.831	109.172	1.659
C(15)-C(14)-H(28)	114.760	109.588	5.172
C(15)-C(14)-H(29)	113.324	107.302	6.022
H(28)-C(14)-H(29)	94.459	106.515	-12.056
N(13)-C(16)-C(17)	116.105	115.665	0.440
N(13)-C(16)-H(33)	102.350	108.778	-6.428
N(13)-C(16)-H(34)	112.057	109.385	2.672
C(17)-C(16)-H(33)	119.090	108.561	10.529
C(17)-C(16)-H(34)	110.276	109.408	0.868
H(33)-C(16)-H(34)	94.981	104.448	-9.467

RMS value: 4.740

Dihedral angles begin on next page

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(2)-C(3)-C(4)	-0.3	-0.2	-0.1
C(1)-C(6)-C(5)-C(4)	0.8	0.3	0.5
C(1)-C(7)-O(8)-C(11)	178.5	-170.6	-10.9
C(2)-C(1)-C(6)-C(5)	0.1	0.3	-0.2
C(2)-C(1)-C(7)-O(8)	-2.5	-1.2	-1.3
C(2)-C(1)-C(7)-O(9)	178.0	-179.2	-2.8
C(2)-C(3)-C(4)-C(5)	1.2	0.7	0.5
C(2)-C(3)-C(4)-N(10)	179.2	179.8	-0.6
C(3)-C(2)-C(1)-C(6)	-0.4	-0.3	-0.1
C(3)-C(2)-C(1)-C(7)	-179.6	180.0	0.4
C(3)-C(4)-C(5)-C(6)	-1.4	-0.7	-0.7
C(3)-C(4)-N(10)-H(22)	171.3	153.6	17.7
C(3)-C(4)-N(10)-H(23)	10.9	27.5	-16.6
C(5)-C(4)-N(10)-H(22)	-10.7	-27.3	16.6
C(5)-C(4)-N(10)-H(23)	-171.2	-153.4	-17.8
C(5)-C(6)-C(1)-C(7)	179.4	-180.0	-0.6
C(6)-C(1)-C(7)-O(8)	178.3	179.1	-0.8
C(6)-C(1)-C(7)-O(9)	-1.3	1.1	-2.4
C(6)-C(5)-C(4)-N(10)	-179.4	-179.8	0.4
C(7)-O(8)-C(11)-C(12)	147.1	175.6	-28.5
O(8)-C(11)-C(12)-N(13)	-82.6	-77.1	-5.5
O(8)-C(11)-C(12)-H(26)	43.8	48.3	-4.5
O(8)-C(11)-C(12)-H(27)	156.7	162.5	-5.8
O(9)-C(7)-O(8)-C(11)	-1.9	7.4	-9.3
C(11)-C(12)-N(13)-C(14)	-156.8	-168.8	12.0
C(11)-C(12)-N(13)-C(16)	72.4	61.3	11.1
C(12)-N(13)-C(14)-C(15)	72.7	69.0	3.7
C(12)-N(13)-C(14)-H(28)	-55.4	-54.6	-0.8
C(12)-N(13)-C(14)-H(29)	-156.7	-171.2	14.5
C(12)-N(13)-C(16)-C(17)	62.7	64.3	-1.6
C(12)-N(13)-C(16)-H(33)	-165.9	-173.2	7.3
C(12)-N(13)-C(16)-H(34)	-65.2	-59.7	-5.5
C(14)-N(13)-C(12)-H(26)	76.9	66.1	10.8
C(14)-N(13)-C(12)-H(27)	-32.5	-49.4	16.9
C(14)-N(13)-C(16)-C(17)	-68.5	-66.1	-2.4
C(14)-N(13)-C(16)-H(33)	62.9	56.4	6.5
C(14)-N(13)-C(16)-H(34)	163.5	169.9	-6.4
C(15)-C(14)-N(13)-C(16)	-155.2	-159.3	4.1
C(16)-N(13)-C(12)-H(26)	-53.9	-63.7	9.8

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(16)-N(13)-C(12)-H(27)	-163.3	-179.3	16.0
C(16)-N(13)-C(14)-H(28)	76.7	77.2	-0.5
C(16)-N(13)-C(14)-H(29)	-24.5	-39.5	15.0
		RMS value:	9.7

Table 12. Mepivicaine

I. Missing parameters

A. Missing for atoms 8-3-1-2 (type 162-1-39-1)
Missing for atoms 8-3-1-7 (type 162-1-39-1)
Missing for atoms 10-11-12-18 (type 151-2-2-1)
Missing for atoms 10-11-16-17 (type 151-2-2-1)

B. Estimated Parameters

2 torsional parameters are read in

Atom type numbers	V1	V2	V3
162 1 39 1	0.000	0.000	0.270
1 2 2 151	0.000	11.600	0.000

II. Bond angles

	Length		Difference
Bond	Crystal	MM3	(in Å)
N+(1)-C(2)	1.4913	1.5081	-0.0168
N+(1)-C(3)	1.4985	1.5152	-0.0167
N+(1)-C(7)	1.5066	1.5058	0.0008
N+(1)-H(19)	1.0188	1.0216	-0.0028
C(3)-C(4)	1.5148	1.5221	-0.0073
C(3)-C(8)	1.5217	1.5277	-0.0060
C(3)-H(23)	0.9993	1.0982	-0.0989
C(4)-C(5)	1.5287	1.5240	0.0047
C(4)-H(24)	0.9999	1.1087	-0.1088
C(4)-H(25)	1.0003	1.1083	-0.1080
C(5)-C(6)	1.5137	1.5266	-0.0129
C(5)-H(26)	1.0005	1.1143	-0.1138
C(5)-H(27)	0.9997	1.1146	-0.1149
C(6)-C(7)	1.4963	1.5176	-0.0213
C(8)-O(9)	1.2316	1.2194	0.0122
C(8)-N(10)	1.3341	1.3734	-0.0393
N(10)-C(11)	1.4374	1.4137	0.0237
N(10)-H(32)	0.8888	1.0282	-0.1394
C(11)-C(12)	1.3896	1.4039	-0.0143
C(11)-C(16)	1.3951	1.4021	-0.0070
C(12)-C(13)	1.3898	1.3996	-0.0098
C(12)-C(18)	1.5023	1.5091	-0.0068
C(15)-C(16)	1.3961	1.4010	-0.0049
C(16)-C(17)	1.5042	1.5090	-0.0048

Bond	Length Crystal	MM3	Difference (in Å)
C(18)-H(39)	1.1000	1.1121	-0.0121
C(18)-H(40)	1.1000	1.1123	-0.0123
C(18)-H(41)	1.1000	1.1123	-0.0123

RMS value: 0.0566

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(2)-N+(1)-C(3)	110.497	112.179	-1.682
C(2)-N+(1)-C(7)	109.560	109.758	-0.198
C(2)-N+(1)-H(19)	102.859	106.721	-3.862
C(3)-N+(1)-C(7)	112.952	113.697	-0.745
C(3)-N+(1)-H(19)	110.789	104.684	6.105
C(7)-N+(1)-H(19)	109.711	109.428	0.283
N+(1)-C(3)-C(4)	111.066	113.290	-2.224
N+(1)-C(3)-C(8)	107.742	107.747	-0.005
N+(1)-C(3)-H(23)	109.016	105.493	3.523
C(4)-C(3)-C(8)	108.147	108.142	0.005
C(4)-C(3)-H(23)	108.818	110.670	-1.852
C(8)-C(3)-H(23)	112.066	111.499	0.567
C(3)-C(4)-C(5)	112.790	112.709	0.081
C(3)-C(4)-H(24)	108.696	109.521	-0.825
C(3)-C(4)-H(25)	108.572	109.783	-1.211
C(5)-C(4)-H(24)	108.610	108.610	0.000
C(5)-C(4)-H(25)	108.619	109.664	-1.045
H(24)-C(4)-H(25)	109.518	106.347	3.171
C(4)-C(5)-C(6)	108.227	109.780	-1.553
C(4)-C(5)-H(26)	109.723	109.921	-0.198
C(4)-C(5)-H(27)	109.790	110.086	-0.296
C(6)-C(5)-H(26)	109.755	109.962	-0.207
C(6)-C(5)-H(27)	109.845	110.119	-0.274
H(26)-C(5)-H(27)	109.484	106.934	2.550
C(5)-C(6)-C(7)	110.622	110.564	0.058
N+(1)-C(7)-C(6)	111.820	111.381	0.439
C(3)-C(8)-O(9)	120.102	117.516	2.586
C(3)-C(8)-N(10)	115.101	117.298	-2.197
O(9)-C(8)-N(10)	124.626	125.182	-0.556
C(8)-N(10)-C(11)	123.285	121.167	2.118
C(8)-N(10)-H(32)	114.432	125.787	-11.355

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(11)-N(10)-H(32)	121.852	113.033	8.819
N(10)-C(11)-C(12)	119.052	119.820	-0.768
N(10)-C(11)-C(16)	118.396	118.809	-0.413
C(12)-C(11)-C(16)	122.520	121.332	1.188
C(11)-C(12)-C(13)	117.850	118.708	-0.858
C(11)-C(12)-C(18)	121.991	121.698	0.293
C(13)-C(12)-C(18)	120.157	119.584	0.573
C(11)-C(16)-C(15)	117.289	118.783	-1.494
C(11)-C(16)-C(17)	120.802	121.249	-0.447
C(15)-C(16)-C(17)	121.908	119.959	1.949
C(12)-C(18)-H(39)	121.991	111.912	10.079
C(12)-C(18)-H(40)	109.728	111.126	-1.398
C(12)-C(18)-H(41)	99.944	111.691	-11.747
H(39)-C(18)-H(40)	109.728	107.621	2.107
H(39)-C(18)-H(41)	99.943	106.732	-6.789
H(40)-C(18)-H(41)	115.018	107.869	7.149

RMS value: 3.831

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
N+(1)-C(3)-C(4)-C(5)	-53.1	-48.4	-4.7
N+(1)-C(3)-C(4)-H(24)	67.4	72.6	-5.2
N+(1)-C(3)-C(4)-H(25)	-173.5	-171.0	-2.5
N+(1)-C(3)-C(8)-O(9)	-40.0	-29.1	-10.9
N+(1)-C(3)-C(8)-N(10)	144.5	150.3	-5.8
N+(1)-C(7)-C(6)-C(5)	58.1	58.0	0.1
C(2)-N+(1)-C(3)-C(4)	173.2	172.0	1.2
C(2)-N+(1)-C(3)-C(8)	-68.5	-68.4	-0.1
C(2)-N+(1)-C(3)-H(23)	53.3	50.8	2.5
C(2)-N+(1)-C(7)-C(6)	-177.0	-178.1	1.1
C(3)-N+(1)-C(7)-C(6)	-53.4	-51.6	-1.8
C(3)-C(4)-C(5)-C(6)	57.4	54.5	2.9
C(3)-C(4)-C(5)-H(26)	-62.4	-66.5	4.1
C(3)-C(4)-C(5)-H(27)	177.2	175.9	1.3
C(3)-C(8)-N(10)-C(11)	170.6	179.9	-9.3
C(3)-C(8)-N(10)-H(32)	-16.8	-1.5	-15.3
C(4)-C(3)-N+(1)-C(7)	50.1	46.8	3.3
C(4)-C(3)-N+(1)-H(19)	-73.5	-72.6	-0.9

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(4)-C(3)-C(8)-O(9)	80.1	93.7	-13.6
C(4)-C(3)-C(8)-N(10)	-95.4	-86.9	-8.5
C(4)-C(5)-C(6)-C(7)	-59.1	-59.3	0.2
C(5)-C(4)-C(3)-C(8)	-171.1	-167.8	-3.3
C(5)-C(4)-C(3)-H(23)	66.9	69.8	-2.9
C(6)-C(5)-C(4)-H(24)	-63.2	-67.0	3.8
C(6)-C(5)-C(4)-H(25)	177.8	177.2	0.6
C(6)-C(7)-N+(1)-H(19)	70.8	65.1	5.7
C(7)-N+(1)-C(3)-C(8)	168.4	166.4	2.0
C(7)-N+(1)-C(3)-H(23)	-69.8	-74.4	4.6
C(7)-C(6)-C(5)-H(26)	60.6	61.8	-1.2
C(7)-C(6)-C(5)-H(27)	-178.9	179.4	1.7
C(8)-C(3)-N+(1)-H(19)	44.8	47.0	-2.2
C(8)-C(3)-C(4)-H(24)	-50.6	-46.8	-3.8
C(8)-C(3)-C(4)-H(25)	68.4	69.6	-1.2
C(8)-N(10)-C(11)-C(12)	-69.5	-76.0	6.5
C(8)-N(10)-C(11)-C(16)	112.5	106.2	6.3
O(9)-C(8)-C(3)-H(23)	-160.0	-144.4	-15.6
O(9)-C(8)-N(10)-C(11)	-4.6	-0.9	-3.7
O(9)-C(8)-N(10)-H(32)	168.0	177.7	-9.7
N(10)-C(8)-C(3)-H(23)	24.6	34.9	-10.3
N(10)-C(11)-C(12)-C(13)	-178.0	-179.2	1.2
N(10)-C(11)-C(12)-C(18)	1.5	-0.4	1.9
N(10)-C(11)-C(16)-C(15)	177.6	179.1	-1.5
N(10)-C(11)-C(16)-C(17)	-2.8	-1.9	-0.9
C(11)-C(12)-C(18)-H(40)	49.7	79.0	-29.3
C(11)-C(12)-C(18)-H(41)	-71.6	-41.5	-30.1
C(12)-C(11)-N(10)-H(32)	118.4	105.2	13.2
C(12)-C(11)-C(16)-C(15)	-0.3	1.4	-1.7
C(12)-C(11)-C(16)-C(17)	179.3	-179.6	-1.1
C(12)-C(13)-C(14)-C(15)	-0.9	0.3	-1.2
C(13)-C(12)-C(11)-C(16)	-0.2	-1.5	1.3
C(13)-C(12)-C(18)-H(39)	-0.5	17.7	-18.2
C(13)-C(12)-C(18)-H(40)	-130.8	-102.2	-28.6
C(13)-C(12)-C(18)-H(41)	107.9	137.3	-29.4
C(16)-C(11)-N(10)-H(32)	-59.5	-72.6	13.1
C(16)-C(11)-C(12)-C(18)	179.3	177.3	2.0
H(19)-N+(1)-C(3)-H(23)	166.6	166.2	0.4
H(19)-N+(1)-C(7)-H(30)	-49.7	-57.5	7.8
H(19)-N+(1)-C(7)-H(31)	-168.9	-173.1	4.2

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
H(23)-C(3)-C(4)-H(24)	-172.6	-169.2	-3.4
H(23)-C(3)-C(4)-H(25)	-53.5	-52.7	-0.8
H(24)-C(4)-C(5)-H(26)	177.1	171.9	5.2
H(24)-C(4)-C(5)-H(27)	56.7	54.4	2.3
H(25)-C(4)-C(5)-H(26)	58.0	56.1	1.9
H(25)-C(4)-C(5)-H(27)	-62.3	-61.5	-0.8
		RMS value:	9.5

Table 13. Demeclocycline

I. Missing parameters

A. Pi-atom parameter of type (96-151) is missing.
Pi-atom parameter of type (81-151) is missing.
Pi-atom parameter of type (101-151) is missing.
Pi-atom parameter of type (151-3) is missing.
Pi-atom parameter of type (151-162) is missing.
Missing for atoms 9-29-12-2 (type 6-1-2-41).
Missing for atoms 16-29-12-2 (type 1-1-2-41).
Missing for atoms 28-29-12-2 (type 2-1-2-41).
Missing for atoms 14-13-30-3 (type 3-2-162-96).
Missing for atoms 30-13-14-4 (type 162-2-3-81).
Missing for atoms 9-29-28-8 (type 6-1-2-41).
Missing for atoms 12-29-28-8 (type 2-1-2-41).
Missing for atoms 16-29-28-8 (type 1-1-2-41).
Missing for atoms 14-13-30-10 (type 3-2-162-151).
Missing for atoms 11-15-14-13 (type 39-1-3-2).
Missing for atoms 14-15-11-31 (type 3-1-39-1).
Missing for atoms 14-15-11-32 (type 3-1-39-1).
Missing for atoms 30-13-14-15 (type 162-2-3-1).
Missing for atoms 29-12-2-39 (type 1-2-41-73).
Missing for atoms 14-13-30 (type 3-2-162) angle type 1.
Missing for atoms 13-30-10 (type 2-162-151) angle type 1.

B. Estimated Parameters
Pi-atom parameters of type (7-7) is used for type (96-81).
Pi-atom parameters of type (7-7) is used for type (96-101).
Pi-atom parameters of type (2-2) is used for type (96-151).
Pi-atom parameters of type (2-2) is used for type (101-151).
Pi-atom parameters of type (2-2) is used for type (151-3).
Pi-atom parameters of type (2-2) is used for type (151-162).
Pi-atom parameters of type (7-2) is used for type (81-2).
Pi-atom parameters of type (81-3) is used for type (81-162).
Pi-atom parameters of type (7-2) is used for type (101-2).
Pi-atom parameters of type (7-3) is used for type (101-3).
Pi-atom parameters of type (7-3) is used for type (101-162).
Pi-atom parameters of type (40-2) is used for type (151-2).
Pi-atom parameters of type (2-3) is used for type (2-162).
Pi-atom parameters of type (3-3) is used for type (3-162).

Estimated parameters continued on next page

10 torsional parameters are read in

Atom type numbers	V1	V2	V3
6 1 1 41	0.000	0.160	0.090
1 1 2 41	0.000	0.160	0.090
2 1 2 41	0.000	0.160	0.090
3 2 162 96	0.000	11.600	0.000
162 2 3 81	0.000	11.600	0.000
3 2 162 151	0.000	11.600	0.000
39 1 3 2	0.000	0.160	0.090
3 1 39 1	0.000	0.000	0.270
162 2 3 1	0.000	11.600	0.000
1 2 41 73	0.000	11.600	0.000

2 bending parameters are read in

Atom type numbers	Kb	Theta
3 2 162	0.695	120.000
2 162 151	0.696	120.000

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
Cl(1)-C(21)	1.7607	1.7373	0.0234
O(2)-C(12)	1.2408	1.2461	-0.0053
O(2)-H(39)	1.1997	0.9645	0.2352
O(3)-C(30)	1.3099	1.2467	0.0632
O(4)-C(14)	1.2240	1.2177	0.0063
O(5)-C(19)	1.4359	1.4299	0.0060
O(5)-H(38)	0.8196	0.9483	-0.1287
O(6)-C(24)	1.3505	1.2443	0.1062
O(6)-H(35)	0.9682	0.9632	0.0050
O(7)-C(26)	1.2566	1.2299	0.0267
O(8)-C(28)	1.3301	1.2474	0.0827
O(8)-H(37)	0.8673	0.9623	-0.0950
O(9)-C(29)	1.4140	1.4299	-0.0159
O(9)-H(36)	0.7959	0.9459	-0.1500
N(10)-C(30)	1.3108	1.3783	-0.0675
N(10)-H(33)	0.8823	1.0320	-0.1497
N(10)-H(34)	0.8926	1.0282	-0.1356
N+(11)-C(15)	1.5049	1.5249	-0.0200
N+(11)-C(31)	1.4806	1.5055	-0.0249
N+(11)-C(32)	1.4883	1.5037	-0.0154
N+(11)-H(54)	1.1000	1.0253	0.0747

Bond	Length Crystal	MM3	Difference (in Å)
C(12)-C(13)	1.4287	1.3539	0.0748
C(12)-C(29)	1.5398	1.5275	0.0123
C(13)-C(14)	1.4169	1.5018	-0.0849
C(13)-C(30)	1.4367	1.5186	-0.0819
C(14)-C(15)	1.5285	1.5256	0.0029
C(15)-C(16)	1.5397	1.5403	-0.0006
C(16)-C(17)	1.5368	1.5309	0.0059
C(16)-C(29)	1.5258	1.5348	-0.0090
C(16)-H(41)	1.0954	1.1088	-0.0134
C(17)-C(18)	1.5188	1.5374	-0.0186
C(17)-H(43)	0.9999	1.1126	-0.1127
C(18)-C(19)	1.5129	1.5356	-0.0227
C(18)-C(27)	1.5022	1.5096	-0.0074
C(18)-H(44)	0.9912	1.1150	-0.1238
C(19)-C(20)	1.5156	1.5095	0.0061
C(19)-H(45)	0.9683	1.1177	-0.1494
C(20)-C(21)	1.3711	1.4033	-0.0322
C(20)-C(25)	1.4107	1.4130	-0.0023
C(21)-C(22)	1.3927	1.3941	-0.0014
C(22)-C(23)	1.3557	1.3895	-0.0338
C(23)-C(24)	1.3803	1.3961	-0.0158
C(24)-C(25)	1.4048	1.4163	-0.0115
C(25)-C(26)	1.4678	1.5150	-0.0472
C(26)-C(27)	1.4518	1.5115	-0.0597
C(27)-C(28)	1.3525	1.3603	-0.0078
C(28)-C(29)	1.5154	1.5260	-0.0106

RMS value: 0.0743

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(12)-O(2)-H(39)	106.402	110.601	-4.199
C(19)-O(5)-H(38)	116.267	108.640	7.627
C(24)-O(6)-H(35)	118.701	109.955	8.746
C(28)-O(8)-H(37)	109.193	110.021	-0.828
C(29)-O(9)-H(36)	113.164	108.750	4.414
C(30)-N(10)-H(33)	116.828	119.556	-2.728
C(30)-N(10)-H(34)	113.461	118.529	-5.068
H(33)-N(10)-H(34)	127.987	121.914	6.073

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(15)-N+(11)-C(31)	112.171	112.389	-0.218
C(15)-N+(11)-C(32)	115.607	116.159	-0.552
C(15)-N+(11)-H(54)	103.279	104.132	-0.853
C(31)-N+(11)-C(32)	110.290	111.188	-0.898
C(31)-N+(11)-H(54)	109.435	107.146	2.289
C(32)-N+(11)-H(54)	105.463	104.871	0.592
O(2)-C(12)-C(13)	123.562	122.715	0.847
O(2)-C(12)-C(29)	120.079	115.793	4.286
C(13)-C(12)-C(29)	116.174	121.469	-5.295
C(12)-C(13)-C(14)	121.021	116.126	4.895
C(12)-C(13)-C(30)	117.378	122.830	-5.452
C(14)-C(13)-C(30)	121.571	121.012	0.559
O(4)-C(14)-C(13)	125.260	122.136	3.124
O(4)-C(14)-C(15)	116.835	118.533	-1.698
C(13)-C(14)-C(15)	117.478	119.282	-1.804
N+(11)-C(15)-C(14)	108.627	109.290	-0.663
N+(11)-C(15)-C(16)	115.506	117.131	-1.625
C(14)-C(15)-C(16)	117.106	114.179	2.927
C(15)-C(16)-C(17)	110.235	111.635	-1.400
C(15)-C(16)-C(29)	111.917	112.737	-0.820
C(15)-C(16)-H(41)	109.484	108.683	0.801
C(17)-C(16)-C(29)	109.474	107.120	2.354
C(17)-C(16)-H(41)	110.442	107.392	3.050
C(29)-C(16)-H(41)	105.185	109.124	-3.939
C(16)-C(17)-C(18)	111.425	110.775	0.650
C(17)-C(18)-C(19)	113.426	110.187	3.239
C(17)-C(18)-C(27)	112.887	113.443	-0.556
C(17)-C(18)-H(44)	108.322	107.640	0.682
C(19)-C(18)-C(27)	110.508	109.659	0.849
C(19)-C(18)-H(44)	106.768	108.712	-1.944
C(27)-C(18)-H(44)	104.304	107.034	-2.730
O(5)-C(19)-C(18)	112.658	108.813	3.845
O(5)-C(19)-C(20)	103.973	108.356	-4.383
O(5)-C(19)-H(45)	109.858	110.099	-0.241
C(18)-C(19)-C(20)	110.437	110.031	0.406
C(18)-C(19)-H(45)	114.037	108.179	5.858
C(20)-C(19)-H(45)	105.141	111.331	-6.190
C(19)-C(20)-C(21)	122.621	120.554	2.067
C(19)-C(20)-C(25)	118.345	120.224	-1.879
C(21)-C(20)-C(25)	118.815	119.151	-0.336

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
Cl(1)-C(21)-C(20)	121.012	121.812	-0.800
Cl(1)-C(21)-C(22)	117.613	117.262	0.351
C(20)-C(21)-C(22)	121.368	120.925	0.443
C(21)-C(22)-C(23)	120.005	119.864	0.141
C(22)-C(23)-C(24)	120.532	120.699	-0.167
O(6)-C(24)-C(23)	117.472	116.495	0.977
O(6)-C(24)-C(25)	122.318	123.762	-1.444
C(23)-C(24)-C(25)	120.196	119.741	0.455
C(20)-C(25)-C(24)	119.014	119.611	-0.597
C(20)-C(25)-C(26)	119.803	118.914	0.889
C(24)-C(25)-C(26)	121.167	121.466	-0.299
O(7)-C(26)-C(25)	119.779	120.864	-1.085
O(7)-C(26)-C(27)	121.250	121.183	0.067
C(25)-C(26)-C(27)	118.946	117.952	0.994
C(18)-C(27)-C(26)	118.262	114.260	4.002
C(18)-C(27)-C(28)	122.295	122.150	0.145
C(26)-C(27)-C(28)	119.414	123.564	-4.150
O(8)-C(28)-C(27)	124.604	123.153	1.451
O(8)-C(28)-C(29)	112.058	114.612	-2.554
C(27)-C(28)-C(29)	123.338	122.224	1.114
O(9)-C(29)-C(12)	106.435	106.091	0.344
O(9)-C(29)-C(16)	108.591	105.834	2.757
O(9)-C(29)-C(28)	112.022	109.376	2.646
C(12)-C(29)-C(16)	110.194	109.927	0.267
C(12)-C(29)-C(28)	108.704	115.122	-6.418
C(16)-C(29)-C(28)	110.803	110.019	0.784
O(3)-C(30)-N(10)	118.733	120.736	-2.003
O(3)-C(30)-C(13)	119.429	120.451	-1.022
N(10)-C(30)-C(13)	121.836	118.813	3.023

RMS value: 2.955

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
Cl(1)-C(21)-C(20)-C(19)	5.6	-4.1	9.7
Cl(1)-C(21)-C(20)-C(25)	-179.9	179.0	1.1
Cl(1)-C(21)-C(22)-C(23)	-179.6	-179.9	0.3
O(2)-C(12)-C(13)-C(14)	-176.6	179.1	4.3
O(2)-C(12)-C(13)-C(30)	5.3	1.2	4.1

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
O(2)-C(12)-C(29)-O(9)	-105.9	-107.5	1.6
O(2)-C(12)-C(29)-C(16)	136.6	138.5	-1.9
O(2)-C(12)-C(29)-C(28)	15.0	13.6	1.4
O(3)-C(30)-N(10)-H(33)	171.2	-179.6	-9.2
O(3)-C(30)-N(10)-H(34)	5.0	0.8	4.2
O(3)-C(30)-C(13)-C(12)	-6.3	-27.8	21.5
O(3)-C(30)-C(13)-C(14)	175.7	154.4	21.3
O(4)-C(14)-C(13)-C(12)	-161.7	-150.1	-11.6
O(4)-C(14)-C(13)-C(30)	16.3	27.9	-11.6
O(4)-C(14)-C(15)-N+(11)	34.9	29.1	5.8
O(4)-C(14)-C(15)-C(16)	167.9	162.5	5.4
O(5)-C(19)-C(18)-C(17)	-67.8	-67.3	-0.5
O(5)-C(19)-C(18)-C(27)	60.2	58.2	2.0
O(5)-C(19)-C(18)-H(44)	173.0	174.9	-1.9
O(5)-C(19)-C(20)-C(21)	94.6	97.3	-2.7
O(5)-C(19)-C(20)-C(25)	-79.9	-85.8	5.9
O(6)-C(24)-C(23)-C(22)	178.8	179.7	-0.9
O(6)-C(24)-C(25)-C(20)	-178.3	178.8	2.9
O(6)-C(24)-C(25)-C(26)	0.3	-2.3	2.6
O(7)-C(26)-C(25)-C(20)	168.1	163.3	4.8
O(7)-C(26)-C(25)-C(24)	-10.4	-15.6	5.2
O(7)-C(26)-C(27)-C(18)	174.5	167.7	6.8
O(7)-C(26)-C(27)-C(28)	-3.6	-10.4	6.8
O(8)-C(28)-C(27)-C(18)	-174.8	179.5	5.7
O(8)-C(28)-C(27)-C(26)	3.2	-2.5	5.7
O(8)-C(28)-C(29)-O(9)	35.4	39.1	-3.7
O(8)-C(28)-C(29)-C(12)	-81.9	-80.2	-1.7
O(8)-C(28)-C(29)-C(16)	156.9	155.0	1.9
O(9)-C(29)-C(12)-C(13)	69.3	70.8	-1.5
O(9)-C(29)-C(16)-C(15)	-64.0	-61.9	-2.1
O(9)-C(29)-C(16)-C(17)	173.4	174.9	-1.5
O(9)-C(29)-C(16)-H(41)	54.8	59.0	-4.2
O(9)-C(29)-C(28)-C(27)	-144.5	-142.0	-2.5
N(10)-C(30)-C(13)-C(12)	174.2	152.3	21.9
N(10)-C(30)-C(13)-C(14)	-3.9	-25.5	21.6
N+(11)-C(15)-C(14)-C(13)	-152.2	-153.4	1.2
N+(11)-C(15)-C(16)-C(17)	-128.5	-132.5	4.0
N+(11)-C(15)-C(16)-C(29)	109.4	106.9	2.5
N+(11)-C(15)-C(16)-H(41)	-6.8	-14.3	7.5
C(12)-C(13)-C(14)-C(15)	26.1	32.5	-6.4

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(12)-C(29)-O(9)-H(36)	108.3	71.9	36.4
C(12)-C(29)-C(16)-C(15)	52.2	52.3	-0.1
C(12)-C(29)-C(16)-C(17)	-70.3	-70.9	0.6
C(12)-C(29)-C(16)-H(41)	171.0	173.1	-2.1
C(12)-C(29)-C(28)-C(27)	98.2	98.7	-0.5
C(13)-C(12)-O(2)-H(39)	-0.1	2.3	-2.4
C(13)-C(12)-C(29)-C(16)	-48.2	-43.2	-5.0
C(13)-C(12)-C(29)-C(28)	-169.8	-168.1	-1.7
C(13)-C(14)-C(15)-C(16)	-19.2	-20.0	0.8
C(13)-C(30)-N(10)-H(33)	-9.2	0.3	-9.5
C(13)-C(30)-N(10)-H(34)	-175.4	-179.2	3.8
C(14)-C(13)-C(12)-C(29)	8.3	0.9	7.4
C(14)-C(15)-N+(11)-C(31)	-159.5	-153.2	-6.3
C(14)-C(15)-N+(11)-C(32)	72.9	77.1	-4.2
C(14)-C(15)-N+(11)-H(54)	-41.8	-37.6	-4.2
C(14)-C(15)-C(16)-C(17)	101.6	97.9	3.7
C(14)-C(15)-C(16)-C(29)	-20.5	-22.7	2.2
C(14)-C(15)-C(16)-H(41)	-136.7	-143.8	7.1
C(15)-C(14)-C(13)-C(30)	-156.0	-149.6	-6.4
C(15)-C(16)-C(17)-C(18)	174.1	170.6	3.5
C(15)-C(16)-C(17)-H(43)	-60.9	-67.0	6.1
C(15)-C(16)-C(29)-C(28)	172.5	-180.0	-7.5
C(16)-C(15)-N+(11)-C(31)	66.6	74.9	-8.3
C(16)-C(15)-N+(11)-C(32)	-61.1	-54.7	-6.4
C(16)-C(15)-N+(11)-H(54)	-175.7	-169.5	-6.2
C(16)-C(17)-C(18)-C(19)	170.2	163.8	6.4
C(16)-C(17)-C(18)-C(27)	43.5	40.4	3.1
C(16)-C(17)-C(18)-H(44)	-71.5	-77.8	6.3
C(16)-C(29)-O(9)-H(36)	-133.1	-171.4	38.3
C(16)-C(29)-C(28)-C(27)	-23.1	-26.2	3.1
C(17)-C(16)-C(29)-C(28)	50.0	56.9	-6.9
C(17)-C(18)-C(19)-C(20)	176.5	174.1	2.4
C(17)-C(18)-C(19)-H(45)	58.3	52.3	6.0
C(17)-C(18)-C(27)-C(26)	166.7	174.0	-7.3
C(17)-C(18)-C(27)-C(28)	-15.3	-7.8	-7.5
C(18)-C(17)-C(16)-C(29)	-62.3	-65.6	3.3
C(18)-C(17)-C(16)-H(41)	53.0	51.5	1.5
C(18)-C(19)-O(5)-H(38)	61.3	-175.7	-123.0
C(18)-C(19)-C(20)-C(21)	-144.3	-143.8	-0.5
C(18)-C(19)-C(20)-C(25)	41.2	33.1	8.1

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(18)-C(27)-C(26)-C(25)	-3.7	-12.5	8.8
C(18)-C(27)-C(28)-C(29)	5.1	0.8	4.3
C(19)-C(18)-C(17)-H(43)	47.8	41.8	6.0
C(19)-C(18)-C(27)-C(26)	38.5	50.4	-11.9
C(19)-C(18)-C(27)-C(28)	-143.5	-131.4	-12.1
C(19)-C(20)-C(21)-C(22)	-173.4	176.3	-349.7
C(19)-C(20)-C(25)-C(24)	172.4	-175.9	-11.7
C(19)-C(20)-C(25)-C(26)	-6.2	5.2	-11.4
C(20)-C(19)-O(5)-H(38)	-179.1	-56.1	-123.0
C(20)-C(19)-C(18)-C(27)	-55.6	-60.4	4.8
C(20)-C(19)-C(18)-H(44)	57.2	56.4	0.8
C(20)-C(21)-C(22)-C(23)	-0.6	-0.3	-0.3
C(20)-C(25)-C(24)-C(23)	3.1	-0.6	3.7
C(20)-C(25)-C(26)-C(27)	-13.7	-16.5	2.8
C(21)-C(20)-C(19)-H(45)	-20.8	-23.9	3.1
C(21)-C(20)-C(25)-C(24)	-2.4	1.1	-3.5
C(21)-C(20)-C(25)-C(26)	179.1	-177.8	-3.1
C(21)-C(22)-C(23)-C(24)	1.3	0.7	0.6
C(22)-C(21)-C(20)-C(25)	1.2	-0.6	1.8
C(22)-C(23)-C(24)-C(25)	-2.6	-0.3	-2.3
C(23)-C(24)-O(6)-H(35)	-169.6	-179.2	9.6
C(23)-C(24)-C(25)-C(26)	-178.4	178.2	3.4
C(24)-C(25)-C(26)-C(27)	167.8	164.6	3.2
C(25)-C(20)-C(19)-H(45)	164.6	153.0	11.6
C(25)-C(24)-O(6)-H(35)	11.7	1.3	10.4
C(25)-C(26)-C(27)-C(28)	178.2	169.3	8.9
C(26)-C(27)-C(18)-H(44)	-76.0	-67.4	-8.6
C(26)-C(27)-C(28)-C(29)	-176.9	178.8	4.3
C(27)-C(18)-C(17)-H(43)	-78.9	-81.6	2.7
C(27)-C(18)-C(19)-H(45)	-173.7	177.8	8.5
C(27)-C(28)-O(8)-H(37)	4.6	-0.6	5.2
C(28)-C(27)-C(18)-H(44)	102.1	110.8	-8.7
C(28)-C(29)-O(9)-H(36)	-10.4	-52.9	42.5
C(28)-C(29)-C(16)-H(41)	-68.7	-59.1	-9.6
C(29)-C(12)-O(2)-H(39)	174.8	-179.4	-5.8
C(29)-C(12)-C(13)-C(30)	-169.7	-177.0	7.3
C(29)-C(16)-C(17)-H(43)	62.7	56.9	5.8
C(29)-C(28)-O(8)-H(37)	-175.3	178.2	6.5
H(38)-O(5)-C(19)-H(45)	-67.0	65.9	227.1
H(41)-C(16)-C(17)-H(43)	178.0	174.0	4.0

	Omega (in degrees)			Difference
Bond	Crystal	MM3		(in degrees)
H(43)-C(17)-C(18)-H(44)	166.1	160.2		5.9
H(44)-C(18)-C(19)-H(45)	-60.9	-65.5		4.6
			RMS value:	41.1

VI. Other

1. In crystal structure pi-system is found to be nonplanar.
   In MM3 pi-system is found to be nonplanar.

Table 14. Streptomycin

I. Missing parameters

A. Missing for atoms 14-15-20-21 (type 6-1-1-40).
Missing for atoms 15-20-21-22 (type 1-1-40-2).
Missing for atoms 15-20-21-59 (type 1-1-40-23).
Missing for atoms 16-15-20-21 (type 1-1-1-40).
Missing for atoms 16-17-18-26 (type 1-1-1-40).
Missing for atoms 17-18-26-27 (type 1-1-40-2).
Missing for atoms 18-19-20-21 (type 1-1-1-40).
Missing for atoms 28-27-26-18 (type 37-2-40-1).
Missing for atoms 29-27-26-18 (type 40-2-40-1).
Missing for atoms 19-18-26-27 (type 1-1-40-2).
Missing for atoms 19-20-21-22 (type 1-1-40-2).
Missing for atoms 20-19-18-26 (type 1-1-1-40).
Missing for atoms 23-22-21-20 (type 37-2-40-1).
Missing for atoms 24-22-21-20 (type 40-2-40-1).
Missing for atoms 21-20-15-53 (type 20-1-1-5).
Missing for atoms 21-20-19-25 (type 40-1-1-6).
Missing for atoms 21-22-23-60 (type 40-2-37-23).
Missing for atoms 21-22-24-62 (type 40-2-40-23).
Missing for atoms 21-22-24-82 (type 40-2-40-23).
Missing for atoms 24-22-21-59 (type 40-2-40-23).
Missing for atoms 24-22-23-60 (type 40-2-37-23).
Missing for atoms 25-19-18-26 (type 6-1-1-40).
Missing for atoms 26-18-17-30 (type 40-1-1-6).
Missing for atoms 26-27-28-61 (type 40-2-37-23).
Missing for atoms 26-27-29-65 (type 40-2-40-23).
Missing for atoms 26-27-29-66 (type 40-2-40-23).
Missing for atoms 29-27-26-64 (type 40-2-40-23).
Missing for atoms 29-27-28-61 (type 40-2-37-23).
Missing for atoms 33-10-34-35 (type 6-1-2-108).
Missing for atoms 70-36-35-34 (type 73-41-108-2).
Missing for atoms 56-18-26-64 (type 5-1-40-23).
Missing for bond 35-36 (type 41-108).
Missing for atoms 17-18-26 (type 1-1-40) angle type 2.
Missing for atoms 19-18-26 (type 1-1-40) angle type 1.
Missing for atoms 15-20-21 (type 1-1-40) angle type 2.
Missing for atoms 19-20-21 (type 1-1-40) angle type 1.
Missing for atoms 20-21-59 (type 1-40-23) angle type 1.
Missing for atoms 21-22-24 (type 40-2-40) angle type 1.

Missing parameters continued

Missing for atoms 62-24-82 (type 23-40-23) angle type 1.
Missing for atoms 18-26-64 (type 1-40-23) angle type 1.
Missing for atoms 26-27-29 (type 40-2-40) angle type 1.
Missing for atoms 65-29-66 (type 23-40-23) angle type 1.
Missing for atoms 34-35-36 (type 2-108-41) angle type 1.
Missing for atoms 70-36-35 (type 73-41-108) angle type 1.

B. Estimated Parameters

12 torsional parameters are read in

Atom type numbers	V1	V2	V3
6 1 1 40	0.000	0.000	0.270
1 1 40 2	0.000	0.160	0.090
1 1 40 23	0.000	0.160	0.090
1 1 1 40	0.000	0.000	0.270
37 2 40 1	0.000	11.600	0.000
40 2 40 1	0.000	11.600	0.000
5 1 1 40	0.000	0.000	0.270
40 2 37 23	0.000	11.600	0.000
40 2 40 23	0.000	11.600	0.000
6 1 2 108	0.000	0.160	0.090
73 41 108 2	0.000	11.600	0.000
5 1 40 23	0.000	0.160	0.090

1 stretching parameter is read in

Bond type	Ks	L(0)
41-108	5.1261	1.3940

1 dipole parameter is read in

Bond type	Moment
41-108	-0.4500

6 bending parameters are read in

Atom type numbers	Kb	Theta
1 1 40	0.695	109.500
1 40 23	0.543	120.000
40 2 40	0.695	120.000
23 40 23	0.493	120.000
2 108 41	0.695	120.000
73 41 108	0.543	120.000

Bond lengths begin on next page

II. Bond lengths

Bond	Length		Difference
	Crystal	MM3	(in Å)
O(1)-C(2)	1.3959	1.4333	-0.0374
C(2)-C(3)	1.5428	1.5291	0.0137
C(3)-C(4)	1.4850	1.5389	-0.0539
C(3)-O(37)	1.4625	1.4462	0.0163
C(4)-C(5)	1.5241	1.5100	0.0141
C(4)-O(38)	1.4191	1.4351	-0.0160
C(5)-C(6)	1.4854	1.5108	-0.0254
C(5)-O(39)	1.4143	1.4329	-0.0186
C(6)-C(7)	1.5156	1.5073	0.0083
C(6)-N+(40)	1.4836	1.5119	-0.0283
C(7)-O(8)	1.4433	1.4130	0.0303
C(7)-O(37)	1.4073	1.4230	-0.0157
O(8)-C(9)	1.3977	1.4305	-0.0328
C(9)-C(10)	1.5612	1.5219	0.0393
C(9)-C(13)	1.5109	1.5399	-0.0290
C(9)-H(50)	1.0843	1.1154	-0.0311
C(10)-C(11)	1.5813	1.5340	0.0473
C(10)-O(33)	1.4320	1.4427	-0.0107
C(10)-O(34)	1.4905	1.5175	-0.0270
C(11)-O(12)	1.4228	1.4431	-0.0203
C(11)-C(32)	1.5160	1.5235	-0.0075
O(12)-C(13)	1.4159	1.4300	-0.0141
C(13)-O(14)	1.4608	1.4127	0.0481
C(13)-H(52)	1.0889	1.1160	-0.0271
O(14)-C(15)	1.4445	1.4451	-0.0006
C(15)-C(16)	1.5142	1.5268	-0.0126
C(15)-C(20)	1.5058	1.5376	-0.0318
C(15)-H(53)	1.0808	1.1158	-0.0350
C(16)-C(17)	1.5620	1.5243	0.0377
C(16)-O(31)	1.3945	1.4365	-0.0420
C(16)-H(54)	1.0871	1.1192	-0.0321
C(17)-C(18)	1.5450	1.5327	0.0123
C(17)-O(30)	1.3973	1.4348	-0.0375
C(17)-H(55)	1.0645	1.1187	-0.0542
C(18)-C(19)	1.5445	1.5407	0.0038
C(18)-N(26)	1.4984	1.5132	-0.0148
C(18)-H(56)	1.0786	1.1129	-0.0343
C(19)-C(20)	1.5292	1.5399	-0.0107

Bond	Length Crystal	MM3	Difference (in Å)
C(19)-O(25)	1.4408	1.4375	0.0033
C(19)-H(57)	0.7948	1.1202	-0.3254
C(20)-N(21)	1.4555	1.5124	-0.0569
C(20)-H(58)	1.0823	1.1119	-0.0296
N(21)-C(22)	1.3139	1.4069	-0.0930
N(21)-H(59)	1.0798	1.0315	0.0483
C(22)-N(23)	1.3124	1.2985	0.0139
C(22)-N(24)	1.3851	1.3978	-0.0127
N(23)-H(60)	0.9025	1.0256	-0.1231
N(24)-H(62)	0.9977	1.0300	-0.0323
N(24)-H(82)	1.1000	1.0302	0.0698
O(25)-H(63)	0.9940	0.9474	0.0466
N(26)-C(27)	1.3422	1.4106	-0.0684
N(26)-H(64)	1.0026	1.0325	-0.0299
C(27)-N(28)	1.4440	1.3005	0.1435
C(27)-N(29)	1.3120	1.3921	-0.0801
N(28)-H(61)	0.9980	1.0278	-0.0298
N(29)-H(65)	0.9984	1.0290	-0.0306
N(29)-H(66)	1.0011	1.0299	-0.0288
O(30)-H(75)	0.9500	0.9499	0.0001
O(31)-H(67)	0.9994	0.9507	0.0487
O(33)-H(68)	0.9943	0.9484	0.0459
C(34)-N(35)	1.2683	1.2744	-0.0061
C(34)-H(69)	1.1056	1.0995	0.0061
N(35)-O(36)	1.3806	1.4020	-0.0214
O(36)-H(70)	1.0003	0.9607	0.0396
O(38)-H(71)	1.0031	0.9501	0.0530
O(39)-H(72)	1.0029	0.9471	0.0558
N+(40)-C(41)	1.4491	1.5017	-0.0526
N+(40)-H(73)	1.0017	1.0538	-0.0521
N+(40)-H(74)	1.0061	1.0347	-0.0286

RMS value: 0.0578

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
O(1)-C(2)-C(3)	111.562	109.492	2.070
C(2)-C(3)-C(4)	114.575	112.717	1.858
C(2)-C(3)-O(37)	107.396	105.735	1.661

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(4)-C(3)-O(37)	109.875	109.994	-0.119
C(3)-C(4)-C(5)	113.609	106.795	6.814
C(3)-C(4)-O(38)	107.581	111.627	-4.046
C(5)-C(4)-O(38)	111.212	105.127	6.085
C(4)-C(5)-C(6)	111.119	107.943	3.176
C(4)-C(5)-O(39)	111.302	116.350	-5.048
C(6)-C(5)-O(39)	108.987	103.506	5.481
C(5)-C(6)-C(7)	111.314	108.892	2.422
C(5)-C(6)-N+(40)	106.436	104.721	1.715
C(7)-C(6)-N+(40)	113.483	115.119	-1.636
C(6)-C(7)-O(8)	106.618	103.214	3.404
C(6)-C(7)-O(37)	112.023	109.738	2.285
O(8)-C(7)-O(37)	113.047	112.380	0.667
C(7)-O(8)-C(9)	115.234	119.130	-3.896
O(8)-C(9)-C(10)	113.291	111.796	1.495
O(8)-C(9)-C(13)	107.910	107.463	0.447
O(8)-C(9)-H(50)	108.187	111.794	-3.607
C(10)-C(9)-C(13)	103.091	101.976	1.115
C(10)-C(9)-H(50)	108.526	111.909	-3.383
C(13)-C(9)-H(50)	115.942	111.414	4.528
C(9)-C(10)-C(11)	100.205	99.202	1.003
C(9)-C(10)-O(33)	111.962	107.042	4.920
C(9)-C(10)-C(34)	111.675	116.770	-5.095
C(11)-C(10)-O(33)	110.615	112.798	-2.183
C(11)-C(10)-C(34)	112.668	112.642	0.026
O(33)-C(10)-C(34)	109.489	108.198	1.291
C(10)-C(11)-O(12)	103.013	105.108	-2.095
C(11)-O(12)-C(13)	109.847	116.548	-6.701
C(9)-C(13)-O(12)	108.949	106.487	2.462
C(9)-C(13)-O(14)	102.457	107.604	-5.147
C(9)-C(13)-H(52)	110.743	110.867	-0.124
O(12)-C(13)-O(14)	111.769	108.952	2.817
O(12)-C(13)-H(52)	108.408	110.022	-1.614
O(14)-C(13)-H(52)	114.332	112.684	1.648
C(13)-O(14)-C(15)	115.009	114.785	0.224
O(14)-C(15)-C(16)	105.256	104.321	0.935
O(14)-C(15)-C(20)	110.159	109.420	0.739
O(14)-C(15)-H(53)	110.628	111.740	-1.112
C(16)-C(15)-C(20)	111.686	110.703	0.983
C(16)-C(15)-H(53)	110.265	109.623	0.642

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(20)-C(15)-H(53)	108.825	110.858	-2.033
C(15)-C(16)-C(17)	110.725	111.743	-1.018
C(15)-C(16)-O(31)	113.405	107.666	5.739
C(15)-C(16)-H(54)	109.374	110.204	-0.830
C(17)-C(16)-O(31)	109.131	107.093	2.038
C(17)-C(16)-H(54)	107.472	109.931	-2.459
O(31)-C(16)-H(54)	106.486	110.128	-3.642
C(16)-C(17)-C(18)	108.398	110.603	-2.205
C(16)-C(17)-O(30)	111.232	106.523	4.709
C(16)-C(17)-H(55)	110.408	110.703	-0.295
C(18)-C(17)-O(30)	108.118	108.351	-0.233
C(18)-C(17)-H(55)	109.040	110.047	-1.007
O(30)-C(17)-H(55)	109.582	110.533	-0.951
C(17)-C(18)-C(19)	112.299	110.241	2.058
C(17)-C(18)-N(26)	108.149	110.334	-2.185
C(17)-C(18)-H(56)	109.226	109.334	-0.108
C(19)-C(18)-N(26)	108.560	108.437	0.123
C(19)-C(18)-H(56)	108.937	108.074	0.863
N(26)-C(18)-H(56)	109.640	110.387	-0.747
C(18)-C(19)-C(20)	109.234	113.514	-4.280
C(18)-C(19)-O(25)	108.868	107.807	1.061
C(18)-C(19)-H(57)	113.082	109.856	3.226
C(20)-C(19)-O(25)	108.428	106.157	2.271
C(20)-C(19)-H(57)	105.248	109.161	-3.913
O(25)-C(29)-H(57)	111.817	110.264	1.553
C(15)-C(20)-C(19)	112.169	111.268	0.901
C(15)-C(20)-N(21)	111.329	109.439	1.890
C(15)-C(20)-H(58)	109.081	107.737	1.344
C(19)-C(20)-N(21)	109.059	108.084	0.975
C(19)-C(20)-H(58)	108.505	109.011	-0.506
N(21)-C(20)-H(58)	106.500	111.324	-4.824
C(20)-N(21)-C(22)	126.012	126.235	-0.223
C(20)-N(21)-H(59)	115.900	117.712	-1.812
C(22)-N(21)-H(59)	118.087	115.923	2.164
N(21)-C(22)-N(23)	123.466	125.720	-2.254
N(21)-C(22)-N(24)	117.406	117.078	0.328
N(23)-C(22)-N(24)	119.094	117.201	1.893
C(22)-N(23)-H(60)	129.241	112.288	16.953
C(22)-N(24)-H(62)	123.935	121.358	2.577
C(22)-N(24)-H(82)	118.032	118.221	-0.189

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
H(62)-N(24)-H(82)	118.033	120.180	-2.147
C(19)-O(25)-H(63)	108.675	109.145	-0.470
C(18)-N(26)-C(27)	122.600	125.396	-2.796
C(18)-N(26)-H(64)	122.540	118.205	4.335
C(27)-N(26)-H(64)	113.849	116.399	-2.550
N(26)-C(27)-N(28)	117.455	121.684	-4.229
N(26)-C(27)-N(29)	125.085	120.568	4.517
N(28)-C(27)-N(29)	117.459	117.747	-0.288
C(27)-N(28)-H(61)	120.005	112.773	7.232
C(27)-N(29)-H(65)	125.094	120.709	4.385
C(27)-N(29)-H(66)	132.946	119.109	13.837
H(65)-N(29)-H(66)	101.722	119.933	-18.211
C(17)-O(30)-H(75)	109.471	106.890	2.581
C(16)-O(31)-H(67)	118.620	107.087	11.533
C(10)-O(33)-H(68)	118.041	107.050	10.991
C(10)-C(34)-N(35)	122.090	121.181	0.909
C(10)-C(34)-H(69)	117.564	118.517	-0.953
N(35)-C(34)-H(69)	120.321	120.291	0.030
C(34)-N(35)-O(36)	111.980	124.463	-12.483
N(35)-O(36)-H(70)	120.054	122.574	-2.520
C(3)-O(37)-C(7)	111.912	117.970	-6.058
C(4)-O(38)-H(71)	120.005	108.144	11.861
C(5)-O(39)-H(72)	93.195	105.533	-12.338
C(6)-N+(40)-C(41)	117.687	115.656	2.031
C(6)-N+(40)-H(73)	114.454	107.864	6.590
C(6)-N+(40)-H(74)	107.646	103.384	4.262
C(41)-N+(40)-H(73)	117.139	111.229	5.910
C(41)-N+(40)-H(74)	107.224	109.143	-1.919
H(73)-N+(40)-H(74)	87.357	109.165	-21.808

RMS value: 5.1114

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
O(1)-C(2)-C(3)-C(4)	-52.3	61.4	-113.7
O(1)-C(2)-C(3)-O(37)	70.0	-178.4	-111.6
C(2)-C(3)-C(4)-C(5)	173.6	173.7	-0.1
C(2)-C(3)-C(4)-O(38)	-62.9	-71.9	9.0
C(2)-C(3)-O(37)-C(7)	175.7	-174.5	-9.8

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(3)-C(4)-C(5)-C(6)	-48.4	-63.9	15.5
C(3)-C(4)-C(5)-O(39)	-170.1	-179.6	9.5
C(3)-C(4)-O(38)-H(71)	152.5	43.1	109.4
C(3)-O(37)-C(7)-C(6)	60.8	52.0	8.8
C(3)-O(37)-C(7)-O(8)	-59.7	-62.2	2.5
C(4)-C(3)-O(37)-C(7)	-59.1	-52.5	-6.6
C(4)-C(5)-C(6)-C(7)	47.6	64.8	-17.2
C(4)-C(5)-C(6)-N+(40)	171.8	-171.5	-16.7
C(4)-C(5)-O(39)-H(72)	-126.5	-40.0	-86.5
C(5)-C(4)-C(3)-O(37)	52.6	56.0	-3.4
C(5)-C(4)-O(38)-H(71)	-82.5	158.5	119.0
C(5)-C(6)-C(7)-O(8)	69.0	63.9	5.1
C(5)-C(6)-C(7)-O(37)	-55.2	-56.1	0.9
C(5)-C(6)-N+(40)-C(41)	170.2	139.0	31.2
C(5)-C(6)-N+(40)-H(73)	-46.3	-95.8	49.5
C(5)-C(6)-N+(40)-H(74)	49.0	19.8	29.2
C(6)-C(5)-C(4)-O(38)	-170.0	177.4	12.6
C(6)-C(5)-O(39)-H(72)	110.6	-158.2	-91.2
C(6)-C(7)-O(8)-C(9)	173.0	139.8	33.2
C(7)-C(6)-C(5)-O(39)	170.6	-171.3	341.9
C(7)-C(6)-N+(40)-H(73)	76.5	23.8	52.7
C(7)-C(6)-N+(40)-H(74)	171.8	139.3	32.5
C(7)-O(8)-C(9)-C(10)	-88.5	-75.8	-12.7
C(7)-O(8)-C(9)-C(13)	158.0	173.1	-15.1
C(7)-O(8)-C(9)-H(50)	31.9	50.5	-18.6
O(8)-C(7)-C(6)-N+(40)	-51.1	-53.3	2.2
O(8)-C(9)-C(10)-C(11)	-146.5	-154.8	8.3
O(8)-C(9)-C(10)-O(33)	-29.3	-37.4	8.1
O(8)-C(9)-C(10)-C(34)	93.9	84.0	9.9
O(8)-C(9)-C(13)-O(12)	133.0	145.2	-12.2
O(8)-C(9)-C(13)-O(14)	-108.5	-98.1	-10.4
O(8)-C(9)-C(13)-H(52)	13.9	25.5	-11.6
C(9)-O(8)-C(7)-O(37)	-63.5	-102.1	38.6
C(9)-C(10)-C(11)-O(12)	38.1	40.8	-2.7
C(9)-C(10)-C(11)-C(32)	157.5	161.7	-4.2
C(9)-C(10)-C(11)-H(51)	-77.6	-75.1	-2.5
C(9)-C(10)-O(33)-H(68)	-53.0	-168.7	115.7
C(9)-C(10)-C(34)-N(35)	-105.3	-134.5	29.2
C(9)-C(10)-C(34)-H(69)	72.9	46.7	26.2
C(9)-C(13)-O(12)-C(11)	12.7	-1.7	14.4

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(9)-C(13)-O(14)-C(15)	-176.5	169.3	14.2
C(10)-C(9)-C(13)-O(12)	12.9	27.5	-14.6
C(10)-C(9)-C(13)-O(14)	131.4	144.2	-12.8
C(10)-C(9)-C(13)-H(52)	-106.3	-92.2	-14.1
C(10)-C(11)-O(12)-C(13)	-32.4	-24.9	-7.5
C(10)-C(34)-N(35)-O(36)	175.0	-179.2	-5.8
C(11)-C(10)-C(9)-C(13)	-30.2	-40.3	10.1
C(11)-C(10)-C(9)-H(50)	93.3	78.9	14.4
C(11)-C(10)-O(33)-H(68)	57.9	-60.7	118.6
C(11)-C(10)-C(34)-N(35)	142.8	111.7	31.1
C(11)-C(10)-C(34)-H(69)	-39.0	-67.1	28.1
C(11)-O(12)-C(13)-O(14)	-99.8	-117.5	17.7
C(11)-O(12)-C(13)-H(52)	133.3	118.5	14.8
O(12)-C(11)-C(10)-O(33)	-80.1	-72.2	-7.9
O(12)-C(11)-C(10)-C(34)	157.0	165.0	-8.0
O(12)-C(13)-C(9)-H(50)	-105.5	-92.0	-13.5
O(12)-C(13)-O(14)-C(15)	-60.0	-75.7	15.7
C(13)-C(9)-C(10)-O(33)	87.1	77.1	10.0
C(13)-C(9)-C(10)-C(34)	-149.7	-161.5	11.8
C(13)-O(12)-C(11)-C(32)	-154.7	-150.5	-4.2
C(13)-O(12)-C(11)-H(51)	84.0	91.2	-7.2
C(13)-O(14)-C(15)-C(16)	136.8	148.3	-11.5
C(13)-O(14)-C(15)-C(20)	-102.7	-93.2	-9.5
C(13)-O(14)-C(15)-H(53)	17.7	29.9	-12.2
O(14)-C(13)-C(9)-H(50)	13.0	24.7	-11.7
O(14)-C(15)-C(16)-C(17)	177.1	175.1	2.0
O(14)-C(15)-C(16)-O(31)	-59.8	-67.6	7.8
O(14)-C(15)-C(16)-H(54)	58.9	52.5	6.4
O(14)-C(15)-C(20)-C(19)	-173.9	-167.3	-6.6
O(14)-C(15)-C(20)-N(21)	63.5	73.4	-9.9
C(14)-C(15)-C(20)-H(58)	-53.7	-47.8	-5.9
C(15)-O(14)-C(13)-H(52)	63.6	46.7	16.9
C(15)-C(16)-C(17)-C(18)	-56.6	-59.2	2.6
C(15)-C(16)-C(17)-O(30)	-175.4	-176.8	1.4
C(15)-C(16)-C(17)-H(55)	62.8	63.0	-0.2
C(15)-C(16)-O(31)-H(67)	-63.0	49.5	-112.5
C(15)-C(20)-C(19)-C(18)	55.4	51.8	3.6
C(15)-C(20)-C(19)-O(25)	173.9	170.0	3.9
C(15)-C(20)-C(19)-H(57)	-66.3	-71.1	4.8
C(15)-C(20)-N(21)-C(22)	-119.7	-136.6	16.9

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(15)-C(20)-N(21)-H(59)	60.7	47.8	12.9
C(16)-C(15)-C(20)-C(19)	-57.3	-52.8	-4.5
C(16)-C(15)-C(20)-N(21)	-179.9	-172.2	-7.7
C(16)-C(15)-C(20)-H(58)	62.9	66.6	-3.7
C(16)-C(17)-C(18)-C(19)	57.0	55.7	1.3
C(16)-C(17)-C(18)-N(26)	176.8	175.4	1.4
C(16)-C(17)-C(18)-H(56)	-64.0	-63.0	-1.0
C(16)-C(17)-O(30)-H(75)	-61.1	-58.0	-3.1
C(17)-C(16)-C(15)-C(20)	57.6	57.5	0.1
C(17)-C(16)-C(15)-H(53)	-63.5	-65.1	1.6
C(17)-C(16)-O(31)-H(67)	60.9	169.8	-108.9
C(17)-C(18)-C(19)-C(20)	-56.4	-53.0	-3.4
C(17)-C(18)-C(19)-O(25)	-174.6	-170.3	-4.3
C(17)-C(18)-C(19)-H(57)	60.4	69.6	-9.2
C(17)-C(18)-N(26)-C(27)	97.3	92.3	5.0
C(17)-C(18)-N(26)-H(64)	-70.5	-87.5	17.0
C(18)-C(17)-C(16)-O(31)	177.9	-176.9	-5.2
C(18)-C(17)-C(16)-H(54)	62.8	63.5	-0.7
C(18)-C(17)-O(30)-H(75)	180.0	-177.1	-2.9
C(18)-C(19)-C(20)-N(21)	179.2	171.9	7.3
C(18)-C(19)-C(20)-H(58)	-65.2	-66.9	1.7
C(18)-C(19)-O(25)-H(63)	-94.0	-56.3	-37.7
C(18)-N(26)-C(27)-N(28)	-179.3	175.0	5.7
C(18)-N(26)-C(27)-N(29)	0.7	-5.5	6.2
C(19)-C(18)-C(17)-O(30)	177.7	172.1	5.6
C(19)-C(18)-C(17)-H(55)	-63.2	-66.9	3.7
C(19)-C(18)-N(26)-C(27)	-140.7	-146.8	6.1
C(19)-C(18)-N(26)-H(64)	51.6	33.3	18.3
C(19)-C(20)-C(15)-H(53)	64.6	69.0	-4.4
C(19)-C(20)-N(21)-C(22)	116.0	102.1	13.9
C(19)-C(20)-N(21)-H(59)	-63.6	-73.6	10.0
C(20)-C(15)-C(16)-O(31)	-179.3	174.8	5.9
C(20)-C(15)-C(16)-H(54)	-60.6	-65.1	4.5
C(20)-C(19)-C(18)-N(26)	-175.9	-173.8	-2.1
C(20)-C(19)-C(18)-H(56)	64.7	66.5	-1.8
C(20)-C(19)-O(25)-H(63)	147.3	-178.3	-34.4
C(20)-N(21)-C(22)-N(23)	-7.4	-1.6	-5.8
C(20)-N(21)-C(22)-N(24)	170.4	178.2	-7.8
N(21)-C(20)-C(15)-H(53)	-57.9	-50.3	-7.6
N(21)-C(20)-C(19)-O(25)	-62.3	-69.8	7.5

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
N(21)-C(20)-C(19)-H(57)	57.5	49.0	8.5
N(21)-C(22)-N(23)-H(60)	17.4	-4.2	21.6
N(21)-C(22)-N(24)-H(62)	-16.8	3.5	-20.3
N(21)-C(22)-N(24)-H(82)	163.2	177.9	-14.7
C(22)-N(21)-C(20)-H(58)	-0.9	-17.6	16.7
N(23)-C(22)-N(21)-H(59)	172.2	174.1	-1.9
N(23)-C(22)-N(24)-H(62)	161.1	-176.7	337.8
N(23)-C(22)-N(24)-H(82)	-18.9	-2.3	-16.6
N(24)-C(22)-N(21)-H(59)	-9.9	-6.1	-3.8
N(24)-C(22)-N(23)-H(60)	-160.4	176.0	23.6
O(25)-C(19)-C(18)-N(26)	65.8	68.9	-3.1
O(25)-C(19)-C(18)-H(56)	-53.5	-50.8	-2.7
O(25)-C(19)-C(20)-H(58)	53.3	51.3	2.0
N(26)-C(18)-C(17)-O(30)	-62.6	-68.2	5.6
N(26)-C(18)-C(17)-H(55)	56.5	52.8	3.7
N(26)-C(18)-C(19)-H(57)	-59.1	-51.3	-7.8
N(26)-C(27)-N(28)-H(61)	0.0	-0.1	0.1
N(26)-C(27)-N(29)-H(65)	6.2	-6.3	12.5
N(26)-C(27)-N(29)-H(66)	179.5	179.4	0.1
C(27)-N(26)-C(18)-H(56)	-21.8	-28.6	6.8
N(28)-C(27)-N(26)-H(64)	-10.6	-5.2	-5.4
N(28)-C(27)-N(29)-H(65)	-173.8	173.2	13.0
N(28)-C(27)-N(29)-H(66)	-0.5	-1.0	0.5
N(29)-C(27)-N(26)-H(64)	169.4	174.4	-5.0
N(29)-C(27)-N(28)-H(61)	180.0	-179.6	-0.4
O(30)-C(17)-C(16)-O(31)	59.1	65.6	-6.5
O(30)-C(17)-C(16)-H(54)	-55.9	-54.1	-1.8
O(30)-C(17)-C(18)-H(56)	56.7	53.4	3.3
O(31)-C(16)-C(15)-H(53)	59.5	52.2	7.3
O(31)-C(16)-C(17)-H(55)	-62.7	-54.6	-8.1
C(32)-C(11)-C(10)-O(33)	39.2	48.7	-9.5
C(32)-C(11)-C(10)-C(34)	-83.7	-74.1	-9.6
O(33)-C(10)-C(9)-H(50)	-149.4	-163.7	14.3
O(33)-C(10)-C(11)-H(51)	164.1	171.9	-7.8
O(33)-C(10)-C(34)-N(35)	19.3	-13.7	33.0
O(33)-C(10)-C(34)-H(69)	-162.5	167.5	30.0
C(34)-C(10)-C(9)-H(50)	-26.3	-42.3	16.0
C(34)-C(10)-C(11)-H(51)	41.2	49.1	-7.9
C(34)-C(10)-O(33)-H(68)	-177.4	64.6	118.0
C(34)-N(35)-O(36)-H(70)	0.5	1.4	-0.9

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
O(36)-N(35)-C(34)-H(69)	-3.1	-0.4	-2.7
O(37)-C(3)-C(4)-O(38)	176.1	170.4	5.7
O(37)-C(7)-C(6)-N+(40)	-175.2	-173.3	-1.9
O(38)-C(4)-C(5)-O(39)	68.4	61.7	6.7
O(39)-C(5)-C(6)-N+(40)	-65.2	-47.6	-17.6
H(50)-C(9)-C(13)-H(52)	135.3	148.3	-13.0
H(53)-C(15)-C(16)-H(54)	178.2	172.3	5.9
H(53)-C(15)-C(20)-H(58)	-175.1	-171.5	-3.6
H(54)-C(16)-C(17)-H(55)	-177.8	-174.3	-3.5
H(54)-C(16)-O(31)-H(67)	176.7	-70.7	-112.6
H(55)-C(17)-C(18)-H(56)	175.8	174.4	1.4
H(55)-C(17)-O(30)-H(75)	61.3	62.3	-1.0
H(56)-C(18)-C(19)-H(57)	-178.4	-171.0	-7.4
H(56)-C(18)-N(26)-H(64)	170.5	151.5	19.0
H(57)-C(19)-C(20)-H(58)	173.1	170.2	2.9
H(57)-C(19)-O(25)-H(63)	31.7	63.6	-31.9
H(58)-C(20)-N(21)-H(59)	179.5	166.7	12.8
		RMS value:	47.5

V. Other

1. In crystal structure pi-system is found to be nonplanar.
   In MM3 pi-system is found to be nonplanar.
2. Geometry optimization can not be accomplished in MM3. Optimization switches to energy minimization.
3. Energy minimization was not accomplished under 11 iterations in 3 VESCF cycles. Minimization stopped.

Table 15. Clavulante

Generic name: clavulanate

I. Missing parameters

A. Missing for atoms 4-3-2-1 (type 8-1-2-41) [5-membered ring].
Missing for atoms 10-3-2-1 (type 3-1-2-41).
Missing for atoms 3-4-5-1 (type 1-8-56-41) [5-membered ring].
Missing for atoms 7-4-5-1 (type 58-8-56-41).
Missing for atoms 1-5-6-7 (type 41-56-56-58).
Missing for atoms 2-1-5-4 (type 2-41-56-8) [5-membered ring].
Missing for atoms 2-3-4-7 (type 2-1-8-58).
Missing for atoms 3-4-7-6 (type 1-8-58-56).
Missing for atoms 3-4-7-18 (type 1-8-58-79).
Missing for atoms 4-3-10-21 (type 8-1-3-75).
Missing for atoms 5-6-7-4 (type 56-56-58-8) [4-membered ring].
Missing for atoms 25-6-7-4 (type 5-56-58-8).
Missing for atoms 5-4-7-6 (type 56-8-58-56) [4-membered ring].
Missing for atoms 5-4-7-18 (type 56-8-58-79).
Missing for atoms 7-4-5-6 (type 58-8-56-56) [4-membered ring].
Missing for atoms 10-3-4-7 (type 3-1-8-58).
Missing for atoms 23-3-4-7 (type 5-1-8-58).
Missing for atoms 7-4-5-24 (type 58-8-56-5).
Missing for bond 4-7 (type 8-58) [4-membered ring].
Missing for atoms 3-4-7 (type 1-8-58) angle type 1.
Missing for atoms 5-4-7 (type 56-8-58) angle type 1 [4-membered ring].
Missing for atoms 4-5-1 (type 8-56-41) angle type 1 [5-membered ring].
Missing for atoms 4-7-6 (type 8-58-56) angle type 1 [4-membered ring].
Missing for atoms 4-7-18 (type 8-58-79) angle type 1.

B. Estimated Parameters

18 torsional parameters are read in

Atom type numbers				V1	V2	V3
8	1	2	41	0.000	0.160	0.090
3	1	2	41	0.000	0.160	0.090
1	8	56	41	0.000	0.000	0.360
58	8	56	41	0.000	0.000	0.360
41	56	56	58	0.000	0.000	0.270
2	41	56	8	0.000	0.160	0.090
2	1	8	58	0.000	0.000	0.360
1	8	58	56	0.000	0.000	0.000
1	8	58	79	0.000	0.000	0.000
8	1	3	75	0.000	0.160	0.090

Torsional parameters (cont.)

Atom type numbers				V1	V2	V3	
56	56	58	8	0.000	0.160	0.690	[4-memb. ring]
5	56	58	8	0.000	0.160	0.090	
56	8	58	56	0.000	0.000	0.600	[4-memb. ring]
56	8	58	79	0.000	0.000	0.000	
58	8	56	56	0.000	0.000	0.960	[4-memb. ring]
3	1	8	58	0.000	0.000	0.360	
5	1	8	58	0.000	0.000	0.360	
58	8	56	5	0.000	0.000	0.360	

1 stretching parameter is read in

Bond type	Ks	L(0)	
8-58	5.3477	1.4340	[4-memb. ring]

1 dipole parameter is read in

Bond type	Moment	
8-58	-0.4500	[4-memb. ring]

5 bending parameters are read in

Atom type numbers			Kb	Theta	
1	8	58	0.695	110.000	
56	8	58	0.521	110.000	[4-memb. ring]
8	56	41	0.695	109.500	
8	58	56	0.521	120.000	[4-memb. ring]
8	58	79	0.695	120.000	

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
O(1)-C(2)	1.4008	1.2322	0.1686
O(1)-C(5)	1.4460	1.4296	0.0164
C(2)-C(3)	1.5671	1.5296	0.0375
C(2)-C(8)	1.3448	1.3378	0.0070
C(3)-N(4)	1.4928	1.4594	0.0334
C(3)-C(10)	1.5716	1.5076	0.0640
C(3)-H(23)	1.1000	1.1105	-0.0105
N(4)-C(5)	1.5258	1.5121	0.0137
N(4)-C(7)	1.4191	1.4338	-0.0147
C(5)-C(6)	1.5630	1.5613	0.0017
C(5)-H(24)	1.1000	1.1085	-0.0085
C(6)-C(7)	1.5121	1.5165	-0.0044

Bond	Length Crystal	MM3	Difference (in Å)
C(6)-H(25)	1.1000	1.1077	-0.0077
C(6)-H(26)	1.1000	1.1067	-0.0067
C(7)-O(18)	1.1516	1.2051	-0.0535
C(8)-C(9)	1.4520	1.5047	-0.0527
C(8)-H(27)	1.0890	1.1020	-0.0130
C(9)-O(19)	1.4999	1.4292	0.0707
C(10)-O(20)	1.1397	1.2158	-0.0761
C(10)-O(21)	1.3601	1.3575	0.0026
C(11)-C(12)	1.5472	1.5078	0.0394
C(11)-O(21)	1.5217	1.4424	0.0793
C(12)-C(13)	1.4264	1.3962	0.0302
C(12)-C(17)	1.3451	1.4075	-0.0624
C(13)-C(14)	1.5042	1.4020	0.1022
C(14)-C(15)	1.3105	1.3877	-0.0772
C(14)-H(33)	1.0840	1.1930	-0.1090
C(15)-C(16)	1.4030	1.3991	0.0039
C(15)-Br(22)	1.8897	1.8931	-0.0034
C(16)-C(17)	1.4047	1.3907	0.0140
O(19)-H(36)	0.9500	0.9532	-0.0032
		RMS value:	0.0550

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(2)-O(1)-C(5)	113.498	108.758	4.740
O(1)-C(2)-C(3)	109.286	113.038	-3.752
O(1)-C(2)-C(8)	121.353	119.419	1.934
C(3)-C(2)-C(8)	129.358	127.536	1.822
C(2)-C(3)-N(4)	98.221	104.790	-6.569
C(2)-C(3)-C(10)	110.834	110.260	0.574
C(2)-C(3)-H(23)	113.714	111.569	2.145
N(4)-C(3)-C(10)	106.251	109.413	-3.162
N(4)-C(3)-H(23)	114.715	110.548	4.167
C(10)-C(3)-H(23)	112.125	110.131	1.994
C(3)-N(4)-C(5)	112.140	101.376	10.764
C(3)-N(4)-C(7)	123.569	115.149	8.420
C(5)-N(4)-C(7)	91.739	89.847	1.892
O(1)-C(5)-N(4)	100.957	110.495	-9.538
O(1)-C(5)-C(6)	113.568	110.338	3.230

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
O(1)-C(5)-H(24)	114.408	114.037	0.371
N(4)-C(5)-C(6)	87.174	89.997	-2.823
N(4)-C(5)-H(24)	120.081	113.520	6.561
C(6)-C(5)-H(24)	116.988	116.088	0.900
C(5)-C(6)-C(7)	86.896	85.073	1.823
C(5)-C(6)-H(25)	114.785	114.860	-0.075
C(5)-C(6)-H(26)	114.783	116.322	-1.539
C(7)-C(6)-H(25)	114.777	114.059	0.718
C(7)-C(6)-H(26)	114.780	114.243	0.537
H(25)-C(6)-H(26)	109.471	110.362	-0.891
N(4)-C(7)-C(6)	93.146	94.857	-1.711
N(4)-C(7)-O(18)	127.123	129.359	-2.236
C(6)-C(7)-O(18)	139.723	135.777	3.946
C(2)-C(8)-C(9)	123.757	126.779	-3.022
C(2)-C(8)-H(27)	118.122	118.162	-0.040
C(9)-C(8)-H(27)	118.121	115.034	3.087
C(8)-C(9)-O(19)	106.508	108.602	-2.094
C(3)-C(10)-O(20)	127.868	125.405	2.463
C(3)-C(10)-O(21)	104.202	111.983	-7.781
O(20)-C(10)-O(21)	127.881	122.610	5.271
C(12)-C(11)-O(21)	101.380	107.197	-5.817
C(11)-C(12)-C(13)	113.132	120.489	-7.357
C(11)-C(12)-C(17)	122.357	120.501	1.856
C(13)-C(12)-C(17)	124.038	118.937	5.101
C(12)-C(13)-C(14)	113.243	120.579	-7.336
C(13)-C(14)-C(15)	120.142	119.776	0.366
C(13)-C(14)-H(33)	119.932	119.592	0.340
C(15)-C(14)-H(33)	119.926	120.631	-0.705
C(14)-C(15)-C(16)	123.780	120.359	3.421
C(14)-C(15)-Br(22)	118.100	119.842	-1.742
C(16)-C(15)-Br(22)	117.923	119.798	-1.875
C(15)-C(16)-C(17)	117.702	119.749	-2.047
C(15)-C(16)-H(34)	121.148	120.595	0.553
C(17)-C(16)-H(34)	121.150	119.656	1.494
C(12)-C(17)-C(16)	120.272	120.600	-0.328
C(9)-O(19)-H(36)	109.471	107.801	1.670
C(10)-O(21)-C(11)	111.280	115.772	-4.492

RMS value: 4.0072

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
O(1)-C(2)-C(3)-N(4)	-18.5	-13.0	-5.5
O(1)-C(2)-C(3)-C(10)	92.5	104.7	-12.2
O(1)-C(2)-C(3)-H(23)	-140.1	-132.6	-7.5
O(1)-C(2)-C(8)-C(9)	177.9	174.8	3.1
O(1)-C(2)-C(8)-H(27)	-2.1	-3.3	1.2
O(1)-C(5)-N(4)-C(3)	-21.9	-7.5	-14.4
O(1)-C(5)-N(4)-C(7)	105.7	108.2	-2.5
O(1)-C(5)-C(6)-C(7)	-93.4	-108.5	15.1
O(1)-C(5)-C(6)-H(25)	150.6	137.2	13.4
O(1)-C(5)-C(6)-H(26)	22.5	6.2	16.3
C(2)-O(1)-C(5)-N(4)	8.6	-0.3	8.9
C(2)-O(1)-C(5)-C(6)	100.3	97.7	2.6
C(2)-O(1)-C(5)-H(24)	-121.9	-129.6	7.7
C(2)-C(3)-N(4)-C(5)	24.6	11.0	13.6
C(2)-C(3)-N(4)-C(7)	-83.5	-84.3	0.8
C(2)-C(3)-C(10)-O(20)	-100.7	-100.8	0.1
C(2)-C(3)-C(10)-O(21)	81.7	79.9	1.8
C(2)-C(8)-C(9)-O(19)	128.2	107.7	20.5
C(3)-C(2)-O(1)-C(5)	6.5	8.0	-1.5
C(3)-C(2)-C(8)-C(9)	-1.4	-4.2	2.8
C(3)-C(2)-C(8)-H(27)	178.6	177.7	0.9
C(3)-N(4)-C(5)-C(6)	-135.3	-119.3	-16.0
C(3)-N(4)-C(5)-H(24)	104.9	122.1	-17.2
C(3)-N(4)-C(7)-C(6)	126.2	106.2	20.0
C(3)-N(4)-C(7)-O(18)	-54.6	-72.9	18.3
C(3)-C(10)-O(21)-C(11)	-178.3	-179.8	1.5
N(4)-C(3)-C(2)-C(8)	160.8	166.1	-5.3
N(4)-C(3)-C(10)-O(20)	5.0	14.0	-9.0
N(4)-C(3)-C(10)-O(21)	-172.6	-165.4	-7.2
N(4)-C(5)-C(6)-C(7)	7.3	3.4	3.9
N(4)-C(5)-C(6)-H(25)	-108.6	-110.8	2.2
N(4)-C(5)-C(6)-H(26)	123.2	118.1	5.1
N(4)-C(7)-C(6)-C(5)	-7.8	-3.6	-4.2
N(4)-C(7)-C(6)-H(25)	108.1	111.4	-3.3
N(4)-C(7)-C(6)-H(26)	-123.8	-120.3	-3.5
C(5)-O(1)-C(2)-C(8)	-172.9	-171.1	-1.8
C(5)-N(4)-C(3)-C(10)	-90.0	-107.2	17.2
C(5)-N(4)-C(3)-H(23)	145.5	131.3	14.2
C(5)-N(4)-C(7)-C(6)	8.0	3.7	4.3

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(5)-N(4)-C(7)-O(18)	-172.8	-175.4	2.6
C(5)-C(6)-C(7)-O(18)	173.2	175.4	-2.2
C(6)-C(5)-N(4)-C(7)	-7.8	-3.6	-4.2
C(7)-N(4)-C(3)-C(10)	161.9	157.5	4.4
C(7)-N(4)-C(3)-H(23)	37.5	36.1	1.4
C(7)-N(4)-C(5)-H(24)	-127.5	-122.3	-5.2
C(7)-C(6)-C(5)-H(24)	129.8	119.8	10.0
C(8)-C(2)-C(3)-C(10)	-88.2	-76.3	-11.9
C(8)-C(2)-C(3)-H(23)	39.2	46.4	-7.2
C(8)-C(9)-O(19)-H(36)	-180.0	-84.7	-95.3
C(10)-O(21)-C(11)-C(12)	175.8	169.9	5.9
C(11)-C(12)-C(13)-C(14)	179.5	177.0	2.5
C(11)-C(12)-C(17)-C(16)	177.9	-177.0	-5.1
C(11)-C(12)-C(17)-H(35)	-2.1	2.8	-4.9
C(11)-O(21)-C(10)-O(20)	4.2	0.8	3.4
C(12)-C(13)-C(14)-C(15)	9.1	-0.1	9.2
C(12)-C(13)-C(14)-H(33)	-170.9	-179.7	8.8
C(12)-C(17)-C(16)-C(15)	-4.4	0.1	-4.5
C(12)-C(17)-C(16)-H(34)	175.6	179.8	-4.2
C(13)-C(12)-C(11)-O(21)	-98.1	-130.8	32.7
C(13)-C(12)-C(17)-C(16)	6.3	-0.1	6.4
C(13)-C(14)-C(15)-C(16)	-8.5	0.1	-8.6
C(13)-C(14)-C(15)-Br(22)	176.8	-179.8	-3.4
C(14)-C(13)-C(12)-C(17)	-8.2	0.1	-8.3
C(14)-C(15)-C(16)-C(17)	5.9	-0.1	6.0
C(14)-C(15)-C(16)-H(34)	-174.1	-179.9	5.8
C(16)-C(15)-C(14)-H(33)	171.5	179.7	-8.2
C(17)-C(12)-C(11)-O(21)	89.5	46.1	43.4
C(17)-C(16)-C(15)-Br(22)	-179.3	179.8	0.9
O(18)-C(7)-C(6)-H(25)	-70.8	-69.5	-1.3
O(18)-C(7)-C(6)-H(26)	57.3	58.7	-1.4
O(19)-C(9)-C(8)-H(27)	-51.8	-74.2	22.4
O(20)-C(10)-C(3)-H(23)	131.0	135.7	-4.7
O(21)-C(10)-C(3)-H(23)	-46.5	-43.7	-2.8
Br(22)-C(15)-C(14)-H(33)	-3.2	-0.2	-3.0
Br(22)-C(15)-C(16)-H(34)	0.7	0.0	0.7
H(24)-C(5)-C(6)-H(25)	13.9	5.5	8.4
H(24)-C(5)-C(6)-H(26)	-114.2	-125.5	11.3
		RMS value:	15.2

VI. Other

1. In crystal structure pi-system is found to be nonplanar.
   In MM3 pi-system is found to be nonplanar.
2. Geometry optimization can not be accomplished in MM3. Optimization switches to energy minimization.

Table 16. Cephalosporin

I. Missing parameters

A. Missing for atoms 1-13-34-16 (type 3-1-8-58).
Missing for atoms 2-12-6-40 (type 1-2-2-15).
Missing for atoms 3-4-38-5 (type 3-1-41-2).
Missing for atoms 6-40-14-15 (type 2-15-56-56).
Missing for atoms 6-40-14-31 (type 2-15-56-5).
Missing for atoms 6-40-14-34 (type 2-15-56-8)
Missing for atoms 12-6-40-14 (type 2-2-15-56).
Missing for atoms 12-13-34-16 (type 2-1-8-58).
Missing for atoms 13-12-6-40 (type 1-2-2-15).
Missing for atoms 13-34-14-40 (type 1-8-56-15).
Missing for atoms 13-34-16-15 (type 1-8-58-56).
Missing for atoms 13-34-16-39 (type 1-8-58-79).
Missing for atoms 14-15-16-34 (type 56-56-58-8) [4-membered ring].
Missing for atoms 14-34-16-15 (type 56-8-58-56) [4-membered ring].
Missing for atoms 14-34-16-39 (type 56-8-58-79).
Missing for atoms 25-6-40-14 (type 5-2-15-56).
Missing for atoms 16-34-14-15 (type 58-8-56-56) [4-membered ring].
Missing for atoms 30-13-34-16 (type 5-1-8-58).
Missing for atoms 16-34-14-31 (type 58-8-56-5).
Missing for atoms 16-34-14-40 (type 58-8-56-15).
Missing for atoms 32-15-16-34 (type 5-56-58-8).
Missing for atoms 38-4-3-33 (type 41-1-3-9).
Missing for atoms 33-15-16-34 (type 9-56-58-8).
Missing for atoms 34-13-1-36 (type 8-1-3-75).
Missing for atoms 38-4-3-37 (type 41-1-3-79).
Missing for bond 6-40 (type 2-15).
Missing for bond 16-34 (type 8-58) [4-membered ring].
Missing for atoms 3-4-38 (type 3-1-41) angle type 2.
Missing for atoms 12-6-40 (type 2-2-15) angle type 1.
Missing for atoms 25-6-40 (type 5-2-15) angle type 1.
Missing for atoms 34-14-40 (type 8-56-15) angle type 1.
Missing for atoms 34-16-15 (type 8-58-56) angle type 2 [4-membered ring].
Missing for atoms 34-16-39 (type 8-58-79) angle type 2.
Missing for atoms 13-34-16 (type 1-8-58) angle type 1.
Missing for atoms 14-34-16 (type 56-8-58) angle type 1 [4-membered ring].
Missing for atoms 6-40-14 (type 2-15-56) angle type 1.

Estimated parameters begin on next page.

B. Estimated Parameters

24 torsional parameters are read in

Atom type numbers				V1	V2	V3	
3	1	8	58	0.000	0.000	0.360	
1	2	2	15	0.000	11.600	0.000	
3	1	41	2	0.000	0.160	0.090	
2	15	56	56	0.000	0.000	0.300	
2	15	56	5	0.000	0.000	0.300	
2	15	56	8	0.000	0.000	0.300	
2	2	15	56	0.000	1.700	0.200	
2	1	8	58	0.000	0.000	0.360	
1	8	56	15	0.000	0.000	0.360	
1	8	58	56	0.000	0.000	0.000	
1	8	58	79	0.000	0.000	0.000	
56	56	58	8	0.000	0.160	0.690	[4-memb. ring]
56	8	58	56	0.000	0.000	0.600	[4-memb. ring]
56	8	58	79	0.000	0.000	0.000	
5	2	15	56	0.000	1.700	0.200	
58	8	56	56	0.000	0.000	0.960	[4-memb. ring]
5	1	8	58	0.000	0.000	0.360	
58	8	56	5	0.000	0.000	0.360	
58	8	56	15	0.000	0.000	0.360	
5	56	58	8	0.000	0.160	0.090	
41	1	3	9	0.000	0.160	0.090	
9	56	58	8	0.000	0.160	0.090	
8	1	3	75	0.000	0.160	0.090	
41	1	3	79	0.000	0.160	0.090	

2 stretching parameters are read in

Bond type	Ks	L(0)	
2-15	2.9868	1.8000	
8-58	5.3477	1.4340	[4-memb. ring]

2 dipole parameters are read in

Bond type	Moment	
2-15	0.0000	
8-58	-0.4500	[4-memb. ring]

11 bending parameters are read in

Atom type numbers			Kb	Theta
3	1	41	0.695	109.500
2	2	15	0.695	120.000

Atom type numbers			Kb	Theta	
5	2	15	0.543	120.000	
8	56	15	0.695	109.500	
8	58	56	0.521	120.000	[4-memb. ring]
8	58	79	0.695	120.000	
1	8	58	0.695	110.000	
56	8	58	0.521	110.000	[4-memb. ring]
2	15	56	0.695	110.000	

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(13)	1.5127	1.5075	0.0052
C(1)-O(35)	1.1892	1.2134	-0.0242
C(1)-O(36)	1.3170	1.3654	-0.0484
C(2)-C(12)	1.5054	1.5094	-0.0040
C(3)-C(4)	1.5176	1.5247	-0.0071
C(3)-N(33)	1.3415	1.3798	-0.0383
C(3)-O(37)	1.2104	1.2193	-0.0089
C(4)-H(22)	1.0421	1.1143	-0.0722
C(4)-H(23)	1.0499	1.1096	-0.0597
C(4)-O(38)	1.4058	1.4290	-0.0232
C(5)-C(7)	1.3776	1.4015	-0.0239
C(5)-C(11)	1.3740	1.4027	-0.0287
C(5)-O(38)	1.3762	1.2256	0.1506
C(6)-C(12)	1.3312	1.3500	-0.0188
C(6)-H(25)	1.2307	1.1022	0.1285
C(6)-S(40)	1.7881	1.8085	-0.0204
C(7)-C(8)	1.3692	1.3938	-0.0246
C(7)-H(24)	1.1866	1.1017	0.0849
C(10)-C(11)	1.3988	1.4000	-0.0012
C(12)-C(13)	1.5305	1.5190	0.0115
C(13)-H(30)	0.9375	1.1074	-0.1699
C(13)-N(34)	1.4496	1.4474	0.0022
C(14)-C(15)	1.5507	1.5791	-0.0284
C(14)-H(31)	1.0321	1.1145	-0.0824
C(14)-N(34)	1.4509	1.4907	-0.0398
C(14)-S(40)	1.7952	1.7866	0.0086
C(15)-C(16)	1.5388	1.5291	0.0097
C(15)-H(32)	1.0873	1.1047	-0.0174
C(15)-N(33)	1.4385	1.4527	-0.0142
C(16)-N(34)	1.3407	1.4176	-0.0769

Bond	Crystal	MM3	Difference (in Å)
C(16)-O(39)	1.2230	1.2049	0.0181
H(17)-O(36)	1.0670	0.9737	0.0933
H(21)-N(33)	0.9403	1.0299	-0.0896
		RMS value:	0.0615

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(13)-C(1)-O(35)	123.590	126.561	-2.971
C(13)-C(1)-O(36)	112.235	111.941	0.294
O(35)-C(1)-O(36)	124.168	121.492	2.676
C(4)-C(3)-N(33)	115.162	114.577	0.585
C(4)-C(3)-O(37)	122.644	121.687	0.957
N(33)-C(3)-O(37)	122.114	123.732	-1.618
C(3)-C(4)-H(22)	114.069	108.395	5.674
C(3)-C(4)-H(23)	106.964	109.482	-2.518
C(3)-C(4)-O(38)	107.674	109.474	-1.800
H(22)-C(4)-H(23)	113.169	108.934	4.235
H(22)-C(4)-O(38)	99.525	110.272	-10.747
H(23)-C(4)-O(38)	115.440	110.252	5.188
C(7)-C(5)-C(11)	121.584	118.933	2.651
C(7)-C(5)-O(38)	115.307	116.896	-1.589
C(11)-C(5)-O(38)	123.110	124.171	-1.061
C(12)-C(6)-H(25)	112.984	119.895	-6.911
C(12)-C(6)-S(40)	131.189	121.966	9.223
H(25)-C(6)-S(40)	115.570	118.139	-2.569
C(5)-C(7)-C(8)	118.582	120.794	-2.212
C(5)-C(7)-H(24)	106.374	119.782	-13.408
C(8)-C(7)-H(24)	134.785	119.423	15.362
C(5)-C(11)-C(10)	117.653	120.191	-2.538
C(5)-C(11)-H(29)	84.306	122.121	-37.815
C(10)-C(11)-H(29)	148.802	117.687	31.115
C(2)-C(12)-C(6)	121.289	120.406	0.883
C(2)-C(12)-C(13)	116.847	114.557	2.290
C(6)-C(12)-C(13)	121.733	125.023	-3.290
C(1)-C(13)-C(12)	112.661	112.174	0.487
C(1)-C(13)-H(30)	116.193	108.607	7.586
C(1)-C(13)-N(34)	108.211	111.745	-3.534
C(12)-C(13)-H(30)	104.760	106.990	-2.230

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(12)-C(13)-N(34)	110.557	110.185	0.372
H(30)-C(13)-N(34)	104.098	106.869	-2.771
C(15)-C(14)-H(31)	122.938	111.976	10.962
C(15)-C(14)-N(34)	87.517	87.684	-0.167
C(15)-C(14)-S(40)	115.794	124.232	-8.438
H(31)-C(14)-N(34)	111.525	111.841	-0.316
H(31)-C(14)-S(40)	106.885	113.454	-6.569
N(34)-C(14)-S(40)	110.488	103.528	6.960
C(14)-C(15)-C(16)	84.189	84.971	-0.782
C(14)-C(15)-H(32)	120.927	116.164	4.763
C(14)-C(15)-N(33)	121.112	113.767	7.345
C(16)-C(15)-H(32)	108.681	112.749	-4.068
C(16)-C(15)-N(33)	119.073	110.654	8.419
H(32)-C(15)-N(33)	102.534	114.851	-12.317
C(15)-C(16)-N(34)	92.075	92.351	-0.276
C(15)-C(16)-O(39)	134.566	137.307	-2.741
N(34)-C(16)-O(39)	133.357	130.338	3.019
C(3)-N(33)-C(15)	120.936	122.129	-1.193
C(3)-N(33)-H(21)	133.057	119.741	13.316
C(15)-N(33)-H(21)	106.006	117.733	-11.727
C(13)-N(34)-C(14)	127.156	118.374	8.782
C(13)-N(34)-C(16)	136.419	136.861	-0.442
C(14)-N(34)-C(16)	95.707	92.394	3.313
C(1)-O(36)-H(17)	119.953	107.531	12.422
C(4)-O(38)-C(5)	117.550	120.722	-3.172
C(6)-S(40)-C(14)	97.213	103.147	-5.934
		RMS value:	8.903

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(13)-C(12)-C(2)	68.2	71.5	-3.3
C(1)-C(13)-C(12)-C(6)	-115.9	-109.8	-6.1
C(1)-C(13)-N(34)-C(14)	83.1	65.9	17.2
C(1)-C(13)-N(34)-C(16)	-109.2	-64.3	-44.9
C(2)-C(12)-C(6)-H(25)	3.3	0.5	2.8
C(2)-C(12)-C(6)-S(40)	177.1	-179.3	-3.6
C(2)-C(12)-C(13)-H(30)	-59.0	-47.5	-11.5
C(2)-C(12)-C(13)-N(34)	-170.5	-163.3	-7.2

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(3)-C(4)-O(38)-C(5)	169.0	178.0	-9.0
C(3)-N(33)-C(15)-C(14)	-98.4	-132.5	34.1
C(3)-N(33)-C(15)-C(16)	160.0	133.9	26.1
C(3)-N(33)-C(15)-H(32)	40.1	4.8	35.3
C(4)-C(3)-N(33)-C(15)	-177.7	177.1	5.2
C(4)-C(3)-N(33)-H(21)	2.6	4.5	-1.9
C(4)-O(38)-C(5)-C(7)	-179.1	-179.5	0.4
C(4)-O(38)-C(5)-C(11)	0.7	0.4	0.3
C(5)-O(38)-C(4)-H(22)	49.8	58.9	-9.1
C(5)-O(38)-C(4)-H(23)	-71.6	-61.5	-10.1
C(6)-C(12)-C(13)-H(30)	116.9	131.2	-14.3
C(6)-C(12)-C(13)-N(34)	5.3	15.4	-10.1
C(6)-S(40)-C(14)-C(15)	-135.2	-139.8	4.6
C(6)-S(40)-C(14)-H(31)	83.8	78.1	5.7
C(6)-S(40)-C(14)-N(34)	-37.7	-43.3	5.6
C(7)-C(5)-C(11)-C(10)	0.9	0.1	0.8
C(7)-C(5)-C(11)-H(29)	-155.7	-179.7	24.0
C(8)-C(7)-C(5)-C(11)	-1.2	-0.1	-1.1
C(8)-C(7)-C(5)-O(38)	178.7	179.8	-1.1
C(10)-C(11)-C(5)-O(38)	-178.9	-179.8	0.9
C(11)-C(5)-C(7)-H(24)	173.8	179.8	-6.0
C(12)-C(6)-S(40)-C(14)	14.8	13.0	1.8
C(12)-C(13)-C(1)-O(35)	108.8	47.5	61.3
C(12)-C(13)-C(1)-O(36)	-72.1	-131.6	59.5
C(12)-C(13)-N(34)-C(14)	-40.8	-59.5	18.7
C(12)-C(13)-N(34)-C(16)	127.0	170.3	-43.3
C(13)-C(1)-O(36)-H(17)	-179.4	179.8	0.8
C(13)-C(12)-C(6)-H(25)	-172.4	-178.0	5.6
C(13)-C(12)-C(6)-S(40)	1.4	2.1	-0.7
C(13)-N(34)-C(14)-C(15)	177.2	-160.9	-21.9
C(13)-N(34)-C(14)-H(31)	-58.2	-48.1	-10.1
C(13)-N(34)-C(14)-S(40)	60.6	74.4	-13.8
C(13)-N(34)-C(16)-C(15)	-175.9	150.5	33.6
C(13)-N(34)-C(16)-O(39)	3.6	-28.8	32.4
C(14)-C(15)-C(16)-N(34)	5.3	-12.1	17.4
C(14)-C(15)-C(16)-O(39)	-174.2	167.2	18.6
C(14)-C(15)-N(33)-H(21)	81.3	40.3	41.0
C(14)-N(34)-C(13)-H(30)	-152.8	-175.4	22.6
C(14)-N(34)-C(16)-C(15)	-5.7	12.8	-18.5
C(14)-N(34)-C(16)-O(39)	173.9	-166.6	-19.5

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(14)-S(40)-C(6)-H(25)	-171.5	-166.9	-4.6
C(15)-C(14)-N(34)-C(16)	5.7	-12.4	18.1
C(15)-N(33)-C(3)-O(37)	-0.8	-3.6	2.8
C(16)-C(15)-C(14)-H(31)	-119.1	-101.2	-17.9
C(16)-C(15)-C(14)-N(34)	-4.9	11.5	-16.4
C(16)-C(15)-C(14)-S(40)	106.7	116.3	-9.6
C(16)-C(15)-N(33)-H(21)	-20.2	-53.4	33.2
C(16)-N(34)-C(13)-H(30)	15.0	54.4	-39.4
C(16)-N(34)-C(14)-H(31)	130.3	100.4	29.9
C(16)-N(34)-C(14)-S(40)	-111.0	-137.1	26.1
H(17)-O(36)-C(1)-O(35)	-0.3	0.6	-0.9
H(21)-N(33)-C(3)-O(37)	179.5	-176.2	-4.3
H(21)-N(33)-C(15)-H(32)	-140.2	177.6	42.2
H(22)-C(4)-C(3)-N(33)	63.7	75.7	-12.0
H(22)-C(4)-C(3)-O(37)	-113.1	-103.6	-9.5
H(23)-C(4)-C(3)-N(33)	-170.4	-165.6	-4.8
H(23)-C(4)-C(3)-O(37)	12.8	15.1	-2.3
H(24)-C(7)-C(5)-O(38)	-6.3	-0.3	-6.0
H(24)-C(7)-C(8)-H(26)	8.2	0.0	8.2
H(29)-C(11)-C(5)-O(38)	24.4	0.4	24.0
H(30)-C(13)-C(1)-O(35)	-130.3	165.6	64.1
H(30)-C(13)-C(1)-O(36)	48.7	-13.6	62.3
H(31)-C(14)-C(15)-H(32)	-10.8	11.7	-22.5
H(31)-C(14)-C(15)-N(33)	120.3	148.4	-28.1
H(32)-C(15)-C(14)-N(34)	103.4	124.4	-21.0
H(32)-C(15)-C(14)-S(40)	-145.0	-130.8	-14.2
H(32)-C(15)-C(16)-N(34)	-115.4	-128.4	13.0
H(32)-C(15)-C(16)-O(39)	65.0	50.9	14.1
N(33)-C(3)-C(4)-O(38)	-45.7	-44.6	-1.1
N(33)-C(15)-C(14)-N(34)	-125.5	-98.9	-26.6
N(33)-C(15)-C(14)-S(40)	-13.9	5.9	-19.8
N(33)-C(15)-C(16)-N(34)	127.9	101.5	26.4
N(33)-C(15)-C(16)-O(39)	-51.7	-79.3	27.6
N(34)-C(13)-C(1)-O(35)	-13.8	-76.8	63.0
N(34)-C(13)-C(1)-O(36)	165.3	104.1	61.2
O(37)-C(3)-C(4)-O(38)	137.5	136.0	1.5
		RMS value:	24.8

VI. Other

1. In crystal structure pi-system is found to be nonplanar. In MM3 pi-system is found to be planar.
2. In MM3 geometry optimization can not be accomplished. Optimization switches to energy minimization.

Table 17. Sulfanilamide

I. Missing parameters

A. Missing for atoms 1-8-11-18 (type 2-154-155-23).
Missing for atoms 2-1-8-11 (type 2-2-154-155).
Missing for atoms 6-1-8-11 (type 2-2-154-155).
Missing for atoms 1-8-11 (type 2-154-155) angle type 1.

B. Estimated parameters

2 torsional parameters are read in

Atom type numbers	V1	V2	V3
2 154 155 23	0.000	0.000	0.360
2 2 154 155	0.000	-0.060	0.340

1 bending parameter is read in

Atom type numbers	Kb	Theta
2 154 155	0.695	109.500

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(2)	1.3795	1.3945	-0.0150
C(1)-C(6)	1.3794	1.3948	-0.0154
C(1)-S(8)	1.7528	1.7840	-0.0312
C(2)-C(3)	1.3914	1.3967	-0.0053
C(3)-C(4)	1.3930	1.4032	-0.0102
C(4)-C(5)	1.4064	1.4035	0.0029
C(4)-N(7)	1.3691	1.3973	-0.0282
C(5)-C(6)	1.3860	1.3963	-0.0103
N(7)-H(16)	0.9349	1.0154	-0.0805
N(7)-H(17)	1.0215	1.0154	0.0061
S(8)-O(9)	1.4445	1.4624	-0.0179
S(8)-O(10)	1.4284	1.4624	-0.0340
S(8)-N(11)	1.5902	1.6702	-0.0800
N(11)-H(18)	0.9200	1.0186	-0.0986
N(11)-H(19)	1.0045	1.0186	-0.0141

RMS value: 0.0423

Bond angles begin on next page

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(2)-C(1)-C(6)	120.364	120.332	0.032
C(2)-C(1)-S(8)	119.797	118.796	1.001
C(6)-C(1)-S(8)	119.828	118.796	1.032
C(1)-C(2)-C(3)	120.184	119.595	0.589
C(2)-C(3)-C(4)	120.425	120.705	-0.280
C(3)-C(4)-C(5)	118.472	118.766	-0.294
C(3)-C(4)-N(7)	119.864	120.618	-0.754
C(5)-C(4)-N(7)	121.650	120.616	1.034
C(4)-C(5)-C(6)	120.604	120.705	-0.101
C(1)-C(6)-C(5)	119.939	119.595	0.344
C(4)-N(7)-H(16)	112.628	114.247	-1.619
C(4)-N(7)-H(17)	113.174	114.248	-1.074
H(16)-N(7)-H(17)	121.594	109.631	11.963
C(1)-S(8)-O(9)	108.627	107.095	1.532
C(1)-S(8)-O(10)	106.958	107.094	-0.136
C(1)-S(8)-N(11)	109.456	106.728	2.728
O(9)-S(8)-O(10)	118.218	121.111	-2.893
O(9)-S(8)-N(11)	105.862	107.022	-1.160
O(10)-S(8)-N(11)	107.530	107.022	0.508
S(8)-N(11)-H(18)	109.432	114.974	-5.542
S(8)-N(11)-H(19)	129.230	114.974	14.256
H(18)-N(11)-H(19)	115.285	115.811	-0.526

RMS value: 4.292

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(2)-C(3)-C(4)	0.9	3.0	-2.1
C(1)-C(6)-C(5)-C(4)	-0.3	-3.0	2.7
C(1)-S(8)-N(11)-H(18)	67.1	69.2	-2.1
C(1)-S(8)-N(11)-H(19)	-83.6	-69.2	-14.4
C(2)-C(1)-C(6)-C(5)	-0.2	6.3	-6.5
C(2)-C(1)-S(8)-O(9)	-25.9	-32.5	6.6
C(2)-C(1)-S(8)-O(10)	-154.6	-163.8	9.2
C(2)-C(1)-S(8)-N(11)	89.2	81.8	7.4
C(2)-C(3)-C(4)-C(5)	-1.3	0.3	-1.6
C(2)-C(3)-C(4)-N(7)	180.0	-179.5	-0.5
C(3)-C(2)-C(1)-C(6)	-0.1	-6.3	6.2

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(3)-C(2)-C(1)-S(8)	-178.9	-169.8	-9.1
C(3)-C(4)-C(5)-C(6)	1.0	-0.3	1.3
C(3)-C(4)-N(7)-H(16)	-164.7	-153.8	-10.9
C(3)-C(4)-N(7)-H(17)	-22.0	-26.4	4.4
C(5)-C(4)-N(7)-H(16)	16.6	26.4	-9.8
C(5)-C(4)-N(7)-H(17)	159.4	153.8	5.6
C(5)-C(6)-C(1)-S(8)	178.6	169.8	8.8
C(6)-C(1)-S(8)-O(9)	155.3	163.8	-8.5
C(6)-C(1)-S(8)-O(10)	26.7	32.5	-5.8
C(6)-C(1)-S(8)-N(11)	-89.6	-81.8	-7.8
C(6)-C(5)-C(4)-N(7)	179.7	179.5	0.2
O(9)-S(8)-N(11)-H(18)	-175.9	-176.4	0.5
O(9)-S(8)-N(11)-H(19)	33.3	45.2	-11.9
O(10)-S(8)-N(11)-H(18)	-48.7	-45.2	-3.5
O(10)-S(8)-N(11)-H(19)	160.5	176.4	-15.9
		RMS value:	7.6

VI. Other

1. In crystal structure pi-system is found to be planar.
   In MM3 pi-system is found to be nonplanar.

Table 18. Trimethoprim

I. Missing parameters

A. Missing for atoms 15-34-19 (type 23-40-23) angle type 3.
Missing for atoms 21-36-22 (type 23-40-23) angle type 3.

B. Estimated parameters

1 bending parameter is read in

Atom type numbers	Kb	Theta
23 40 23	0.493	120.000

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(4)	1.3950	1.3963	-0.0013
C(1)-C(11)	1.3945	1.3969	-0.0024
C(1)-C(12)	1.5167	1.5113	0.0054
C(2)-O(39)	1.4121	1.4273	-0.0152
C(3)-N(33)	1.3430	1.3547	-0.0117
C(3)-N(34)	1.3493	1.3689	-0.0196
C(3)-N(35)	1.3461	1.3591	-0.0130
C(4)-C(5)	1.3999	1.4015	-0.0016
C(5)-C(7)	1.3998	1.4092	-0.0094
C(5)-O(37)	1.3596	1.2278	0.1318
C(6)-C(8)	1.4178	1.4137	0.0041
C(6)-N(35)	1.3427	1.3466	-0.0039
C(6)-N(36)	1.3508	1.3809	-0.0301
C(7)-C(9)	1.3983	1.4160	-0.0177
C(7)-O(38)	1.3707	1.2287	0.1420
C(8)-C(10)	1.3791	1.3859	-0.0068
C(8)-C(12)	1.5025	1.5066	-0.0041
C(9)-C(11)	1.3976	1.4039	-0.0063
C(9)-O(39)	1.3623	1.2263	0.1360
C(10)-H(23)	1.0929	1.1024	-0.0095
C(10)-H(33)	1.3427	1.3414	0.0013
C(11)-H(24)	1.0853	1.0984	-0.0131
C(13)-O(37)	1.4104	1.4275	-0.0171
C(14)-H(30)	1.0610	1.1127	-0.0517
C(14)-H(31)	1.0378	1.1127	-0.0749
C(14)-H(32)	1.0544	1.1122	-0.0578

Bond	Length Crystal	MM3	Difference (in Å)
C(14)-O(38)	1.4224	1.4253	-0.0029
H(15)-N(34)	1.0197	1.0295	-0.0098
H(19)-N(34)	0.9928	1.0294	-0.0366
H(21)-N(36)	1.0205	1.0298	-0.0093
H(22)-N(36)	0.9905	1.0297	-0.0392

RMS value: 0.0488

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(4)-C(1)-C(11)	120.119	118.985	1.134
C(4)-C(1)-C(12)	118.673	120.195	-1.522
C(11)-C(1)-C(12)	121.014	120.789	0.225
N(33)-C(3)-N(34)	116.734	118.398	-1.664
N(33)-C(3)-N(35)	125.352	123.141	2.211
N(34)-C(3)-N(35)	117.904	118.461	-0.557
C(1)-C(4)-C(5)	119.950	120.883	-0.933
C(4)-C(5)-C(7)	120.130	119.994	0.136
C(4)-C(5)-O(37)	124.739	122.757	1.982
C(7)-C(5)-O(37)	115.130	117.248	-2.118
C(8)-C(6)-N(35)	121.603	120.226	1.377
C(8)-C(6)-N(36)	121.631	120.508	1.123
N(35)-C(6)-N(36)	116.753	119.264	-2.511
C(5)-C(7)-C(9)	119.553	119.529	0.024
C(5)-C(7)-O(38)	119.733	115.611	4.122
C(9)-C(7)-O(38)	120.688	124.860	-4.172
C(6)-C(8)-C(10)	114.761	117.393	-2.632
C(6)-C(8)-C(12)	123.074	122.851	0.223
C(10)-C(8)-C(12)	122.018	119.755	2.263
C(7)-C(9)-C(11)	120.289	119.069	1.220
C(7)-C(9)-O(39)	115.180	119.334	-4.154
C(11)-C(9)-O(39)	124.526	121.597	2.929
C(8)-C(10)-H(23)	119.539	120.489	-0.950
C(8)-C(10)-N(33)	124.811	122.143	2.668
H(23)-C(10)-N(33)	115.637	117.368	-1.731
C(1)-C(11)-C(9)	119.944	121.523	-1.579
C(1)-C(11)-H(24)	119.372	117.406	1.966
C(9)-C(11)-H(24)	120.669	121.070	-0.401
C(1)-C(12)-C(8)	117.902	115.639	2.263

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
H(30)-C(14)-H(31)	107.300	111.456	-4.156
H(30)-C(14)-H(32)	108.326	107.135	1.191
H(30)-C(14)-O(38)	110.743	111.177	-0.434
H(31)-C(14)-H(32)	110.083	107.127	2.956
H(31)-C(14)-O(38)	111.867	111.190	0.677
H(32)-C(14)-O(38)	108.465	108.542	-0.077
C(3)-N(33)-C(10)	115.413	118.108	-2.695
C(3)-N(33)-H(15)	118.609	119.751	-1.142
C(3)-N(34)-H(19)	121.005	119.728	1.277
H(15)-N(34)-H(19)	117.801	120.521	-2.720
C(3)-N(35)-C(6)	117.518	118.984	-1.466
C(6)-N(36)-H(21)	118.851	118.422	0.429
C(6)-N(36)-H(22)	120.888	122.287	-1.399
H(21)-N(36)-H(22)	118.819	119.259	-0.440
C(5)-O(37)-C(13)	117.748	121.131	-3.383
C(7)-O(38)-C(14)	114.538	124.211	-9.673
C(2)-O(39)-C(9)	118.255	121.574	-3.319
		RMS value:	2.524

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(4)-C(5)-C(7)	-0.9	0.2	-1.1
C(1)-C(4)-C(5)-O(37)	179.4	-179.6	1.0
C(1)-C(11)-C(9)-C(7)	-0.9	1.4	-2.3
C(1)-C(11)-C(9)-O(39)	178.2	-178.4	3.4
C(1)-C(12)-C(8)-C(6)	-89.5	-65.4	-24.1
C(1)-C(12)-C(8)-C(10)	95.2	114.3	-19.1
C(2)-O(39)-C(9)-C(7)	-172.3	-178.9	6.6
C(2)-O(39)-C(9)-C(11)	8.6	0.8	7.8
C(3)-N(33)-C(10)-C(8)	-3.4	-0.2	-3.2
C(3)-N(33)-C(10)-H(23)	175.3	179.9	-4.6
C(3)-N(35)-C(6)-C(8)	-3.2	-0.7	-2.5
C(3)-N(35)-C(6)-N(36)	178.2	178.8	-0.6
C(4)-C(1)-C(11)-C(9)	1.0	-1.6	2.6
C(4)-C(1)-C(11)-H(24)	179.6	178.9	0.7
C(4)-C(1)-C(12)-C(8)	153.4	146.7	6.7
C(4)-C(5)-C(7)-C(9)	1.0	-0.4	1.4
C(4)-C(5)-C(7)-O(38)	-177.2	179.7	-3.1

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(4)-C(5)-O(37)-C(13)	-4.8	0.3	-5.1
C(5)-C(4)-C(1)-C(11)	-0.1	0.7	-0.8
C(5)-C(4)-C(1)-C(12)	174.9	178.7	-3.8
C(5)-C(7)-C(9)-C(11)	-0.1	-0.4	0.3
C(5)-C(7)-C(9)-O(39)	-179.3	179.4	-1.3
C(5)-C(7)-O(38)-C(14)	-101.1	179.8	-79.1
C(6)-C(8)-C(10)-H(23)	178.4	179.6	-1.2
C(6)-C(8)-C(10)-N(33)	-3.0	-0.4	-2.6
C(6)-N(35)-C(3)-N(33)	-4.2	0.0	-4.2
C(6)-N(35)-C(3)-N(34)	174.7	-179.8	5.5
C(7)-C(5)-C(4)-H(20)	177.5	179.7	-2.2
C(7)-C(5)-O(37)-C(13)	175.6	-179.6	4.8
C(7)-C(9)-C(11)-H(24)	-179.5	-179.1	-0.4
C(7)-O(38)-C(14)-H(30)	57.1	62.7	-5.6
C(7)-O(38)-C(14)-H(31)	-62.6	-62.1	-0.5
C(7)-O(38)-C(14)-H(32)	175.8	-179.7	4.5
C(8)-C(6)-N(36)-H(21)	178.1	179.7	-1.6
C(8)-C(6)-N(36)-H(22)	12.0	1.8	10.2
C(8)-C(12)-C(1)-C(11)	-31.7	-35.3	3.6
C(9)-C(7)-C(5)-O(37)	-179.3	179.4	-1.3
C(9)-C(7)-O(38)-C(14)	80.8	0.0	80.8
C(9)-C(11)-C(1)-C(12)	-173.9	-179.5	5.6
C(10)-C(8)-C(6)-N(35)	6.4	0.8	5.6
C(10)-C(8)-C(6)-N(36)	-175.0	-178.6	3.6
C(10)-N(33)-C(3)-N(34)	-171.5	-179.8	8.3
C(10)-N(33)-C(3)-N(35)	7.3	0.4	6.9
C(11)-C(9)-C(7)-O(38)	178.1	179.5	-1.4
C(12)-C(1)-C(11)-H(24)	4.8	0.9	3.9
C(12)-C(8)-C(6)-N(35)	-169.2	-179.5	10.3
C(12)-C(8)-C(6)-N(36)	9.4	1.1	8.3
C(12)-C(8)-C(10)-H(23)	-5.9	-0.2	-5.7
C(12)-C(8)-C(10)-N(33)	172.7	179.9	-7.2
H(15)-N(34)-C(3)-N(33)	-14.1	0.1	-14.2
H(15)-N(34)-C(3)-N(35)	167.0	180.0	-13.0
H(19)-N(34)-C(3)-N(33)	-175.5	-179.9	4.4
H(19)-N(34)-C(3)-N(35)	5.6	-0.1	5.7
H(21)-N(36)-C(6)-N(35)	-3.2	0.3	-3.5
H(22)-N(36)-C(6)-N(35)	-169.3	-177.6	8.3
H(24)-C(11)-C(9)-O(39)	-0.4	1.2	-1.6
O(37)-C(5)-C(7)-O(38)	2.5	-0.5	3.0

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
O(38)-C(7)-C(9)-O(39)	-1.1	-0.7	-0.4

RMS value: 16.2

V. Other

1. In both crystal structure and MM3 pi-system is found to be non-planar.
2. Geometry optimization can not be accomplished in MM3. Optimization switches to energy minimization.

Table 19. Griseofulvin

I. Missing parameters

A. Pi-atom parameter of type (2-81) is missing.
Pi-atom parameter of type (81-81) is missing.
Missing for atoms 1-7-6-22 (type 12-2-2-41).
Missing for atoms 1-7-8-19 (type 12-2-2-41).
Missing for atoms 3-2-13-24 (type 3-1-2-41).
Missing for atoms 3-2-19-8 (type 3-1-41-2) [5-membered ring].
Missing for atoms 19-2-3-9 (type 41-1-3-2) [5-membered ring].
Missing for atoms 19-2-13-14 (type 41-1-2-2).
Missing for atoms 17-2-13-24 (type 1-1-2-41).
Missing for atoms 19-2-3-21 (type 41-1-3-81).
Missing for atoms 19-2-13-24 (type 41-1-2-41).
Missing for atoms 3-2-19 (type 3-1-41) angle type 1 [5-membered ring].
Missing for atoms 13-2-19 (type 2-1-41) angle type 1.

B. Estimated parameters
Pi-atom parameters of type (2-7) is used for type (2-81).
Pi-atom parameters of type (7-7) is used for type (81-81).

9 torsional parameters are read in

Atom type numbers				V1	V2	V3
12	2	2	41	0.000	11.600	0.000
3	1	2	41	0.000	0.160	0.090
3	1	41	2	0.000	0.160	0.090
2	1	41	2	0.000	0.160	0.090
41	1	3	2	0.000	0.160	0.090
41	1	2	2	0.000	0.160	0.090
1	1	2	41	0.000	0.160	0.090
41	1	3	81	0.000	0.160	0.090
41	1	2	41	0.000	0.160	0.090

2 bending parameters are read in

Atom type numbers			Kb	Theta
3	1	41	0.695	109.500
2	1	41	0.695	109.500

Bond lengths begin on next page

II. Bond lengths

Bond	Length Crystal	Length MM3	Difference (in Å)
Cl(1)-C(7)	1.7224	1.7422	-0.0198
C(2)-C(3)	1.5556	1.5303	0.0253
C(2)-C(13)	1.5099	1.5189	-0.0090
C(2)-C(17)	1.5422	1.5494	-0.0072
C(2)-O(19)	1.4509	1.4422	0.0087
C(3)-C(9)	1.4478	1.4673	-0.0195
C(3)-O(21)	1.2060	1.2170	-0.0110
C(4)-C(5)	1.3862	1.4060	-0.0198
C(4)-C(9)	1.4051	1.3902	0.0149
C(4)-O(20)	1.3431	1.2252	0.1179
C(5)-C(6)	1.3870	1.4114	-0.0244
C(5)-H(25)	0.8459	1.0956	-0.2497
C(6)-C(7)	1.3986	1.4071	-0.0085
C(6)-O(22)	1.3524	1.2266	0.1258
C(7)-C(8)	1.3743	1.3940	-0.0197
C(8)-C(9)	1.3899	1.3919	-0.0020
C(8)-O(19)	1.3619	1.2369	0.1250
C(10)-C(17)	1.5132	1.5362	-0.0230
C(11)-O(24)	1.4443	1.4274	0.0169
C(12)-O(20)	1.4434	1.4269	0.0165
C(13)-C(14)	1.3379	1.3472	-0.0093
C(13)-O(24)	1.3299	1.2284	0.1015
C(14)-C(15)	1.4513	1.4910	-0.0397
C(15)-C(16)	1.4924	1.5205	-0.0281
C(15)-O(23)	1.2187	1.2180	0.0007
C(16)-C(17)	1.5209	1.5307	-0.0098
C(16)-H(36)	0.8820	1.1125	-0.2305
C(16)-H(37)	0.9487	1.1108	-0.1621
C(17)-H(38)	0.8716	1.1152	-0.2436
C(18)-O(22)	1.4316	1.4268	0.0048
		RMS value:	0.0938

III. Bond angles

Bond	Theta (in degrees) Crystal	Theta (in degrees) MM3	Difference (in degrees)
C(3)-C(2)-C(13)	111.301	109.630	1.671
C(3)-C(2)-C(17)	113.127	113.567	-0.440
C(3)-C(2)-O(19)	105.300	104.194	1.106

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(13)-C(2)-C(17)	109.707	111.233	-1.526
C(13)-C(2)-O(19)	110.003	110.694	-0.691
C(17)-C(2)-O(19)	107.214	107.558	-0.344
C(2)-C(3)-C(9)	104.980	104.456	0.524
C(2)-C(3)-O(21)	123.937	120.601	3.336
C(9)-C(3)-O(21)	131.030	125.920	5.110
C(5)-C(4)-C(9)	118.509	117.607	0.902
C(5)-C(4)-O(20)	124.722	124.726	-0.004
C(9)-C(4)-O(20)	116.769	117.667	-0.898
C(4)-C(5)-C(6)	120.877	121.030	-0.153
C(4)-C(5)-H(25)	119.897	119.317	0.580
C(6)-C(5)-H(25)	119.224	119.654	-0.430
C(5)-C(6)-C(7)	121.161	119.499	1.662
C(5)-C(6)-O(22)	123.306	123.263	0.043
C(7)-C(6)-O(22)	115.520	117.238	-1.718
Cl(1)-C(7)-C(6)	122.481	120.742	1.739
Cl(1)-C(7)-C(8)	120.111	119.565	0.546
C(6)-C(7)-C(8)	117.389	119.693	-2.304
C(7)-C(8)-C(9)	122.673	119.568	3.105
C(7)-C(8)-O(19)	122.397	122.806	-0.409
C(9)-C(8)-O(19)	114.895	117.625	-2.730
C(3)-C(9)-C(4)	133.568	133.288	0.280
C(3)-C(9)-C(8)	106.972	104.109	2.863
C(4)-C(9)-C(8)	119.380	122.603	-3.223
C(17)-C(10)-H(26)	110.058	111.911	-1.853
C(2)-C(13)-C(14)	119.740	121.157	-1.417
C(2)-C(13)-O(24)	112.537	115.150	-2.613
C(14)-C(13)-O(24)	127.664	123.684	3.980
C(13)-C(14)-C(15)	122.388	122.390	-0.002
C(14)-C(15)-C(16)	118.329	118.155	0.174
C(14)-C(15)-O(23)	121.087	120.436	0.651
C(16)-C(15)-O(23)	120.583	121.408	-0.825
C(15)-C(16)-C(17)	115.219	111.991	3.228
C(2)-C(17)-C(10)	113.081	117.729	-4.648
C(2)-C(17)-C(16)	109.341	110.706	-1.365
C(2)-C(17)-H(38)	104.635	107.798	-3.163
C(10)-C(17)-C(16)	112.524	110.050	2.474
C(10)-C(17)-H(38)	107.851	107.738	0.113
C(16)-C(17)-H(38)	109.035	107.618	1.417
C(2)-O(19)-C(8)	107.153	109.613	-2.460

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(4)-O(20)-C(12)	117.545	120.454	-2.909
C(6)-O(22)-C(18)	118.202	121.070	-2.868
C(11)-O(24)-C(13)	117.939	121.014	-3.075

RMS value: 2.139

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
Cl(1)-C(7)-C(6)-C(5)	179.0	179.8	-0.8
Cl(1)-C(7)-C(6)-O(22)	0.2	-0.1	0.3
Cl(1)-C(7)-C(8)-C(9)	-178.2	-179.8	1.6
Cl(1)-C(7)-C(8)-O(19)	-0.5	-0.2	-0.3
C(2)-C(3)-C(9)-C(4)	173.0	179.5	-6.5
C(2)-C(3)-C(9)-C(8)	-3.6	-0.6	-3.0
C(2)-C(13)-C(14)-C(15)	2.5	-0.3	2.8
C(2)-C(13)-O(24)-C(11)	178.8	179.2	-0.4
C(2)-C(17)-C(16)-C(15)	-43.7	-52.2	8.5
C(2)-C(17)-C(16)-H(36)	77.4	69.6	7.8
C(2)-C(17)-C(16)-H(37)	-163.8	-173.5	9.7
C(2)-O(19)-C(8)-C(7)	-171.1	-179.8	8.7
C(2)-O(19)-C(8)-C(9)	6.7	-0.1	6.8
C(3)-C(2)-C(13)-C(14)	87.8	98.3	-10.5
C(3)-C(2)-C(13)-O(24)	-89.6	-80.6	-9.0
C(3)-C(2)-C(17)-C(10)	58.3	53.6	4.7
C(3)-C(2)-C(17)-C(16)	-68.0	-70.2	2.2
C(3)-C(2)-C(17)-H(38)	175.4	172.4	3.0
C(3)-C(2)-O(19)-C(8)	-8.4	-0.2	-8.2
C(3)-C(9)-C(4)-C(5)	-175.1	179.8	5.1
C(3)-C(9)-C(4)-O(20)	4.7	-0.2	4.9
C(3)-C(9)-C(8)-C(7)	176.1	-179.9	-4.0
C(3)-C(9)-C(8)-O(19)	-1.8	0.5	-2.3
C(4)-C(5)-C(6)-C(7)	-0.5	0.0	-0.5
C(4)-C(5)-C(6)-O(22)	178.2	179.9	-1.7
C(4)-C(9)-C(3)-O(21)	-4.3	1.1	-5.4
C(4)-C(9)-C(8)-C(7)	-1.1	0.1	-1.2
C(4)-C(9)-C(8)-O(19)	-179.0	-179.6	0.6
C(5)-C(4)-C(9)-C(8)	1.2	-0.1	1.3
C(5)-C(4)-O(20)-C(12)	-1.5	-0.1	-1.4
C(5)-C(6)-C(7)-C(8)	0.6	0.0	0.6

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(5)-C(6)-O(22)-C(18)	3.1	0.1	3.0
C(6)-C(5)-C(4)-C(9)	-0.4	0.1	-0.5
C(6)-C(5)-C(4)-O(20)	179.8	-179.9	-0.3
C(6)-C(7)-C(8)-C(9)	0.2	0.0	0.2
C(6)-C(7)-C(8)-O(19)	177.9	179.6	-1.7
C(7)-C(6)-C(5)-H(25)	-180.0	-180.0	0.0
C(7)-C(6)-O(22)-C(18)	-178.2	-180.0	1.8
C(8)-C(7)-C(6)-O(22)	-178.2	-180.0	1.8
C(8)-C(9)-C(3)-O(21)	179.1	-179.0	-1.9
C(8)-C(9)-C(4)-O(20)	-179.0	179.9	1.1
C(8)-O(19)-C(2)-C(13)	-128.4	-117.7	-10.7
C(8)-O(19)-C(2)-C(17)	112.4	120.6	-8.2
C(9)-C(3)-C(2)-C(13)	126.5	118.9	7.6
C(9)-C(3)-C(2)-C(17)	-109.5	-116.2	6.7
C(9)-C(3)-C(2)-O(19)	7.3	0.5	6.8
C(9)-C(4)-C(5)-H(25)	179.1	-179.9	-1.0
C(9)-C(4)-O(20)-C(12)	178.6	179.9	-1.3
C(10)-C(17)-C(2)-C(13)	-176.8	177.5	5.7
C(10)-C(17)-C(2)-O(19)	-57.4	-61.1	3.7
C(10)-C(17)-C(16)-C(15	-170.2	-177.5	7.3
C(10)-C(17)-C(16)-H(36	-49.2	-55.7	6.5
C(10)-C(17)-C(16)-H(37	69.7	61.2	8.5
C(11)-O(24)-C(13)-C(14	1.7	0.3	1.4
C(13)-C(2)-C(3)-O(21)	-55.9	-62.8	6.9
C(13)-C(2)-C(17)-C(16)	57.0	53.7	3.3
C(13)-C(2)-C(17)-H(38)	-59.7	-63.7	4.0
C(13)-C(14)-C(15)-C(16	13.2	2.1	11.1
C(13)-C(14)-C(15)-O(23	-166.4	-177.6	11.2
C(14)-C(13)-C(2)-C(17)	-38.2	-27.9	-10.3
C(14)-C(13)-C(2)-O(19)	-155.9	-147.5	-8.4
C(14)-C(15)-C(16)-C(17	9.4	25.0	-15.6
C(14)-C(15)-C(16)-H(36	-114.1	-97.7	-16.4
C(14)-C(15)-C(16)-H(37	136.0	146.4	-10.4
C(15)-C(14)-C(13)-O(24	179.5	178.6	0.9
C(15)-C(16)-C(17)-H(38	70.2	65.3	4.9
C(16)-C(15)-C(14)-H(35	-169.2	-178.7	9.5
C(16)-C(17)-C(2)-O(19)	176.4	175.1	1.3
C(17)-C(2)-C(3)-O(21)	68.1	62.1	6.0
C(17)-C(2)-C(13)-O(24)	144.4	153.1	-8.7
C(17)-C(16)-C(15)-O(23	-171.0	-155.4	-15.6

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
O(19)-C(2)-C(3)-O(21)	-175.1	178.8	6.1
O(19)-C(2)-C(13)-O(24)	26.7	33.6	-6.9
O(19)-C(2)-C(17)-H(38)	59.7	57.6	2.1
O(20)-C(4)-C(5)-H(25)	-0.8	0.1	-0.9
O(22)-C(6)-C(5)-H(25)	-1.3	-0.1	-1.2
O(23)-C(15)-C(16)-H(36	65.5	82.0	-16.5
O(23)-C(15)-C(16)-H(37	-44.4	-34.0	-10.4
H(36)-C(16)-C(17)-H(38	-168.8	-172.8	4.0
H(37)-C(16)-C(17)-H(38	-49.9	-56.0	6.1
		RMS value:	6.6

V. Other

1. In crystal structure the pi-system is found to be nonplanar.
   In the MM3 structure the pi-system is found to be nonplanar.

Table 20. Ketoconazole

I. Missing parameters

A. Missing for atoms 1-6-7-8 (type 40-1-1-6).
Missing for atoms 1-6-7-11 (type 40-1-1-6).
Missing for atoms 1-6-7-12 (type 40-1-1-2).
Missing for atoms 7-6-1-2 (type 1-1-40-2).
Missing for atoms 3-2-1-6 (type 37-2-40-1).
Missing for atoms 7-6-1-5 (type 1-1-40-2).
Missing for atoms 8-9-19-20 (type 6-1-1-41).
Missing for atoms 7-6-1 (type 1-1-40) angle type 1.

B. Estimated parameters

5 torsional parameters are read in

Atom type numbers	V1	V2	V3
6 1 1 40	0.000	0.000	0.270
2 1 1 40	0.000	0.000	0.270
1 1 40 2	0.000	0.160	0.090
37 2 40 1	0.000	11.600	0.000
6 1 1 41	0.000	0.000	0.270

1 bending parameter is read in

Atom type numbers	Kb	Theta
1 1 40	0.695	109.500

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
N(1)-C(2)	1.3554	1.3692	-0.0138
N(1)-C(5)	1.3709	1.3775	-0.0066
N(1)-C(6)	1.4466	1.5014	-0.0548
C(2)-N(3)	1.3138	1.3265	-0.0127
C(2)-H(36)	1.0634	1.0790	-0.0156
N(3)-C(4)	1.3580	1.3806	-0.0226
C(4)-C(5)	1.3567	1.3759	-0.0192
C(4)-H(37)	0.9547	1.0998	-0.1451
C(5)-H(38)	1.0478	1.0960	-0.0482
C(6)-C(7)	1.5156	1.5499	-0.0343
C(7)-O(8)	1.4204	1.4347	-0.0143
C(7)-O(11)	1.4052	1.4247	-0.0195

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(7)-C(12)	1.5447	1.5196	0.0251
O(8)-C(9)	1.5257	1.4479	0.0778
C(9)-C(10)	1.5207	1.5219	-0.0012
C(9)-C(19)	1.5212	1.5306	-0.0094
C(10)-O(11)	1.3753	1.4405	-0.0652
C(12)-C(13)	1.3825	1.4069	-0.0244
C(12)-C(17)	1.4045	1.4086	-0.0041
C(13)-C(14)	1.3827	1.3993	-0.0166
C(13)-Cl(64)	1.7475	1.7376	0.0099
C(14)-C(15)	1.3802	1.3909	-0.0107
C(15)-C(16)	1.3782	1.3933	-0.0151
C(15)-Cl(18)	1.7407	1.7314	0.0093
C(16)-C(17)	1.3733	1.3933	-0.0200
C(19)-O(20)	1.4339	1.4290	0.0049
O(20)-C(21)	1.4177	1.2262	0.1915
C(21)-C(22)	1.3706	1.4056	-0.0350
C(21)-C(26)	1.3062	1.3930	-0.0868
C(22)-C(23)	1.3984	1.3938	0.0046
C(23)-C(24)	1.3635	1.4070	-0.0435
C(24)-C(25)	1.3735	1.4013	-0.0278
C(24)-N(27)	1.4210	1.3930	0.0280
C(25)-C(26)	1.3876	1.3993	-0.0117
N(27)-C(28)	1.4628	1.4699	-0.0071
N(27)-C(32)	1.4705	1.4668	0.0037
C(28)-C(29)	1.5083	1.5205	-0.0122
C(28)-H(53)	1.1599	1.1269	0.0330
C(28)-H(54)	0.9779	1.1126	-0.1347
C(29)-N(30)	1.4639	1.4591	0.0048
C(29)-H(55)	0.9759	1.1088	-0.1329
C(29)-H(56)	1.0960	1.1125	-0.0165
N(30)-C(31)	1.4701	1.4568	0.0133
N(30)-C(33)	1.3375	1.3904	-0.0529
C(31)-C(32)	1.5133	1.5196	-0.0063
C(31)-H(57)	1.1564	1.1113	0.0451
C(31)-H(58)	1.0602	1.1125	-0.0523
C(32)-H(59)	1.1065	1.1268	-0.0203
C(32)-H(60)	0.9846	1.1141	-0.1295
C(33)-O(34)	1.2195	1.2202	-0.0007
C(33)-C(35)	1.4896	1.5209	-0.0313

RMS value: 0.0551

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(2)-N(1)-C(5)	106.302	106.990	-0.688
C(2)-N(1)-C(6)	125.574	126.735	-1.161
C(5)-N(1)-C(6)	128.120	126.273	1.847
N(1)-C(2)-N(3)	112.373	112.006	0.367
N(1)-C(2)-H(36)	116.488	120.558	-4.070
N(3)-C(2)-H(36)	131.135	127.434	3.701
C(2)-N(3)-C(4)	104.488	104.682	-0.194
N(3)-C(4)-H(37)	123.508	123.566	-0.058
C(5)-C(4)-H(37)	125.090	125.525	-0.435
N(1)-C(5)-C(4)	105.442	105.414	0.028
N(1)-C(5)-H(38)	117.630	122.491	-4.861
C(4)-C(5)-H(38)	136.506	132.093	4.413
N(1)-C(6)-C(7)	113.272	112.237	1.035
C(6)-C(7)-O(8)	109.202	108.087	1.115
C(6)-C(7)-O(11)	110.771	109.636	1.135
C(6)-C(7)-C(12)	108.517	110.998	-2.481
O(8)-C(7)-O(11)	106.382	106.055	0.327
O(8)-C(7)-C(12)	109.322	110.243	-0.921
O(11)-C(7)-C(12)	112.586	111.646	0.940
C(7)-O(8)-C(9)	104.134	106.612	-2.478
O(8)-C(9)-C(10)	105.527	103.567	1.960
O(8)-C(9)-C(19)	105.341	107.589	-2.248
C(10)-C(9)-C(19)	115.770	113.760	2.010
C(9)-C(10)-O(11)	98.730	100.806	-2.076
C(7)-O(11)-C(10)	112.319	102.329	9.990
C(7)-C(12)-C(13)	124.957	123.517	1.440
C(7)-C(12)-C(17)	118.373	118.685	-0.312
C(13)-C(12)-C(17)	116.357	117.734	-1.377
C(12)-C(13)-C(14)	122.602	120.921	1.681
C(12)-C(13)-Cl(64)	121.803	122.436	-0.633
C(14)-C(13)-Cl(64)	115.591	116.637	-1.046
C(13)-C(14)-C(15)	118.718	120.118	-1.400
C(14)-C(15)-C(16)	121.037	120.000	1.037
C(14)-C(15)-Cl(18)	119.389	120.045	-0.656
C(16)-C(15)-Cl(18)	119.566	119.955	-0.389
C(15)-C(16)-C(17)	118.858	119.832	-0.974
C(12)-C(17)-C(16)	122.404	121.394	1.010

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(9)-C(19)-O(20)	105.002	107.866	-2.864
C(19)-O(20)-C(21)	114.815	119.836	-5.021
O(20)-C(21)-C(22)	122.331	124.318	-1.987
O(20)-C(21)-C(26)	111.750	117.185	-5.435
C(22)-C(21)-C(26)	125.838	118.497	7.341
C(21)-C(22)-C(23)	117.757	120.295	-2.538
C(22)-C(23)-C(24)	118.405	121.558	-3.153
C(23)-C(24)-C(25)	118.200	117.589	0.611
C(23)-C(24)-N(27)	117.042	118.991	-1.949
C(25)-C(24)-N(27)	123.129	123.415	-0.286
C(24)-C(25)-C(26)	122.772	120.963	1.809
C(21)-C(26)-C(25)	114.641	121.077	-6.436
C(24)-N(27)-C(28)	116.833	112.356	4.477
C(24)-N(27)-C(32)	116.586	117.466	-0.880
C(28)-N(27)-C(32)	109.688	109.226	0.462
N(27)-C(28)-C(29)	111.137	111.650	-0.513
N(27)-C(28)-H(53)	104.593	109.842	-5.249
N(27)-C(28)-H(54)	111.868	110.753	1.115
C(29)-C(28)-H(53)	113.140	109.869	3.271
C(29)-C(28)-H(54)	107.650	108.150	-0.500
H(53)-C(28)-H(54)	108.484	106.428	2.056
C(28)-C(29)-N(30)	110.565	109.801	0.764
C(28)-C(29)-H(55)	111.500	108.409	3.091
C(28)-C(29)-H(56)	105.564	109.007	-3.443
N(30)-C(29)-H(55)	109.686	113.141	-3.455
N(30)-C(29)-H(56)	111.388	110.099	1.289
H(55)-C(29)-H(56)	108.061	106.255	1.806
C(29)-N(30)-C(31)	112.399	115.960	-3.561
C(29)-N(30)-C(33)	125.799	123.086	2.713
C(31)-N(30)-C(33)	120.445	120.618	-0.173
N(30)-C(31)-C(32)	109.766	109.755	0.011
N(30)-C(31)-H(57)	102.812	112.405	-9.593
N(30)-C(31)-H(58)	111.328	110.223	1.105
C(32)-C(31)-H(57)	110.813	108.860	1.953
C(32)-C(31)-H(58)	110.596	109.152	1.444
H(57)-C(31)-H(58)	111.288	106.347	4.941
N(27)-C(32)-C(31)	110.717	111.245	-0.528
N(27)-C(32)-H(59)	106.082	110.497	-4.415
N(27)-C(32)-H(60)	106.498	109.792	-3.294
C(31)-C(32)-H(59)	114.057	109.373	4.684

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(31)-C(32)-H(60)	104.577	108.212	-3.635
H(59)-C(32)-H(60)	114.727	107.624	7.103
N(30)-C(33)-O(34)	121.505	122.466	-0.961
N(30)-C(33)-C(35)	117.904	117.867	0.037
O(34)-C(33)-C(35)	120.590	119.667	0.923

RMS value: 3.083

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
N(1)-C(2)-N(3)-C(4)	-0.4	-0.3	-0.1
N(1)-C(5)-C(4)-N(3)	0.1	0.0	0.1
N(1)-C(5)-C(4)-H(37)	-178.9	-179.6	0.7
N(1)-C(6)-C(7)-O(8)	-55.4	-57.5	2.1
N(1)-C(6)-C(7)-O(11)	61.5	57.7	3.8
N(1)-C(6)-C(7)-C(12)	-174.5	-178.5	4.0
C(2)-N(1)-C(5)-C(4)	-0.3	-0.1	-0.2
C(2)-N(1)-C(5)-H(38)	-174.1	-179.7	5.6
C(2)-N(1)-C(6)-C(7)	90.0	93.4	-3.4
C(2)-N(3)-C(4)-C(5)	0.2	0.2	0.0
C(2)-N(3)-C(4)-H(37)	179.2	179.8	-0.6
N(3)-C(2)-N(1)-C(5)	0.5	0.3	0.2
N(3)-C(2)-N(1)-C(6)	-178.8	-179.3	0.5
N(3)-C(4)-C(5)-H(38)	172.0	179.4	-7.4
C(4)-N(3)-C(2)-H(36)	-179.6	-179.7	0.1
C(4)-C(5)-N(1)-C(6)	178.9	179.4	-0.5
C(5)-N(1)-C(2)-H(36)	179.8	179.7	0.1
C(5)-N(1)-C(6)-C(7)	-89.2	-86.0	-3.2
C(6)-N(1)-C(2)-H(36)	0.5	0.2	0.3
C(6)-N(1)-C(5)-H(38)	5.2	-0.2	5.4
C(6)-C(7)-O(8)-C(9)	126.4	135.4	-9.0
C(6)-C(7)-O(11)-C(10)	-148.2	-156.6	8.4
C(6)-C(7)-C(12)-C(13)	-73.9	-81.9	8.0
C(6)-C(7)-C(12)-C(17)	99.4	101.1	-1.7
C(7)-O(8)-C(9)-C(10)	14.5	10.1	4.4
C(7)-O(8)-C(9)-C(19)	-108.4	-110.6	2.2
C(7)-O(11)-C(10)-C(9)	36.9	44.8	-7.9
C(7)-C(12)-C(13)-C(14)	175.1	-177.3	-7.6
C(7)-C(12)-C(13)-Cl(64)	-5.6	3.6	-9.2

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(7)-C(12)-C(17)-C(16)	-174.9	177.4	7.7
O(8)-C(7)-O(11)-C(10)	-29.7	-40.1	10.4
O(8)-C(7)-C(12)-C(13)	167.0	158.4	8.6
O(8)-C(7)-C(12)-C(17)	-19.6	-18.6	-1.0
O(8)-C(9)-C(10)-O(11)	-30.0	-33.8	3.8
O(8)-C(9)-C(19)-O(20)	-167.9	-178.1	10.2
C(9)-O(8)-C(7)-C(12)	-115.0	-103.1	-11.9
C(9)-C(19)-O(20)-C(21)	170.0	179.2	-9.2
C(10)-C(9)-C(19)-O(20)	76.0	67.8	8.2
C(10)-O(11)-C(7)-C(12)	90.1	80.0	10.1
O(11)-C(7)-C(12)-C(13)	49.0	40.8	8.2
O(11)-C(7)-C(12)-C(17)	-137.6	-136.2	-1.4
O(11)-C(10)-C(9)-C(19)	86.0	82.6	3.4
C(12)-C(13)-C(14)-C(15)	-1.0	0.2	-1.2
C(12)-C(17)-C(16)-C(15)	-0.3	-0.2	-0.1
C(13)-C(12)-C(17)-C(16)	-1.0	0.2	-1.2
C(13)-C(14)-C(15)-C(16)	-0.4	-0.2	-0.2
C(13)-C(14)-C(15)-Cl(18)	-179.4	179.9	0.7
C(14)-C(13)-C(12)-C(17)	1.7	-0.3	2.0
C(14)-C(15)-C(16)-C(17)	1.1	0.1	1.0
C(15)-C(14)-C(13)-Cl(64)	179.6	179.4	0.2
C(17)-C(12)-C(13)-Cl(64)	-179.0	-179.4	0.4
C(17)-C(16)-C(15)-Cl(18)	-180.0	-180.0	0.0
C(19)-O(20)-C(21)-C(22)	11.8	0.4	11.4
C(19)-O(20)-C(21)-C(26)	-171.3	-179.6	8.3
O(20)-C(21)-C(22)-C(23)	-178.7	-179.1	0.4
O(20)-C(21)-C(26)-C(25)	176.0	179.2	-3.2
O(20)-C(21)-C(26)-H(52)	12.9	-0.3	13.2
C(21)-C(22)-C(23)-C(24)	-8.2	0.2	-8.4
C(21)-C(26)-C(25)-C(24)	13.9	-0.5	14.4
C(22)-C(21)-C(26)-C(25)	-7.3	-0.8	-6.5
C(22)-C(21)-C(26)-H(52)	-170.3	179.7	10.0
C(22)-C(23)-C(24)-C(25)	14.6	-1.4	-16.0
C(22)-C(23)-C(24)-N(27)	-179.5	179.4	1.1
C(23)-C(22)-C(21)-C(26)	4.9	0.9	4.0
C(23)-C(24)-C(25)-C(26)	-18.1	1.5	19.6
C(23)-C(24)-N(27)-C(28)	-10.5	-64.0	53.5
C(23)-C(24)-N(27)-C(32)	-143.0	168.1	48.9
C(24)-C(25)-C(26)-H(52)	178.4	179.1	-0.7
C(24)-N(27)-C(28)-C(29)	166.1	168.4	-2.3

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(24)-N(27)-C(28)-H(53)	-71.5	-69.4	-2.1
C(24)-N(27)-C(28)-H(54)	45.7	47.9	-2.2
C(24)-N(27)-C(32)-C(31)	-165.2	-170.6	5.4
C(24)-N(27)-C(32)-H(59)	70.6	67.7	2.9
C(24)-N(27)-C(32)-H(60)	-52.1	-50.9	-1.2
C(25)-C(24)-N(27)-C(28)	154.7	116.9	37.8
C(25)-C(24)-N(27)-C(32)	22.2	-11.1	33.3
C(26)-C(25)-C(24)-N(27)	176.9	-179.3	-3.8
N(27)-C(28)-C(29)-N(30)	56.0	53.7	2.3
N(27)-C(28)-C(29)-H(55)	178.3	177.8	0.5
N(27)-C(28)-C(29)-H(56)	-64.6	-66.9	2.3
N(27)-C(32)-C(31)-N(30)	-57.2	-55.1	-2.1
N(27)-C(32)-C(31)-H(57)	-170.1	-178.5	8.4
N(27)-C(32)-C(31)-H(58)	66.0	65.8	0.2
C(28)-N(27)-C(32)-C(31)	59.2	59.9	-0.7
C(28)-N(27)-C(32)-H(59)	-65.1	-61.8	-3.3
C(28)-N(27)-C(32)-H(60)	172.3	179.7	-7.4
C(28)-C(29)-N(30)-C(31)	-54.7	-50.9	-3.8
C(28)-C(29)-N(30)-C(33)	138.7	135.8	2.9
C(29)-C(28)-N(27)-C(32)	-58.4	-59.4	1.0
C(29)-N(30)-C(31)-C(32)	55.3	51.5	3.8
C(29)-N(30)-C(31)-H(57)	173.2	172.8	0.4
C(29)-N(30)-C(31)-H(58)	-67.5	-68.7	1.2
C(29)-N(30)-C(33)-O(34)	165.2	176.0	-10.8
C(29)-N(30)-C(33)-C(35)	-14.5	-4.1	-10.4
N(30)-C(29)-C(28)-H(53)	-61.4	-68.4	7.0
N(30)-C(29)-C(28)-H(54)	178.8	175.8	3.0
N(30)-C(31)-C(32)-H(59)	62.3	67.3	-5.0
N(30)-C(31)-C(32)-H(60)	-171.6	-175.8	4.2
C(31)-N(30)-C(29)-H(55)	-178.1	-172.1	-6.0
C(31)-N(30)-C(29)-H(56)	62.4	69.2	-6.8
C(31)-N(30)-C(33)-O(34)	-0.5	2.9	-3.4
C(31)-N(30)-C(33)-C(35)	179.8	-177.2	-3.0
C(32)-N(27)-C(28)-H(53)	64.0	62.8	1.2
C(32)-N(27)-C(28)-H(54)	-178.7	-180.0	1.3
C(32)-C(31)-N(30)-C(33)	-137.3	-134.9	-2.4
C(33)-N(30)-C(29)-H(55)	15.3	14.5	0.8
C(33)-N(30)-C(29)-H(56)	-104.3	-104.2	-0.1
C(33)-N(30)-C(31)-H(57)	-19.3	-13.6	-5.7
C(33)-N(30)-C(31)-H(58)	99.9	104.8	-4.9

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
H(37)-C(4)-C(5)-H(38)	-6.9	-0.2	-6.7
H(53)-C(28)-C(29)-H(55)	61.0	55.7	5.3
H(53)-C(28)-C(29)-H(56)	178.1	170.9	7.2
H(54)-C(28)-C(29)-H(55)	-58.9	-60.1	1.2
H(54)-C(28)-C(29)-H(56)	58.2	55.2	3.0
H(57)-C(31)-C(32)-H(59)	-50.6	-56.1	5.5
H(57)-C(31)-C(32)-H(60)	75.6	60.8	14.8
H(58)-C(31)-C(32)-H(59)	-174.5	-171.8	-2.7
H(58)-C(31)-C(32)-H(60)	-48.3	-54.9	6.6
		RMS value:	10.2

V. Other

1. In crystal structure the pi system is found to be nonplanar.
   In MM3 the pi system is determined to be nonplanar.

Table 21. Pyrazinamide

I. Missing parameters

A. Pi-atom parameter of type (37-162) is missing.
Pi-atom parameter of type (37-151) is missing.
Pi-atom parameter of type (2-162) is missing.
Pi-atom parameter of type (2-151) is missing.
Pi-atom parameter of type (162-151) is missing.
Pi-atom parameter of type (162-96) is missing.
Pi-atom parameter of type (151-96) is missing.
Missing for atoms 1-5-10-11 (type 37-2-162-151).
Missing for atoms 1-5-10-12 (type 37-2-162-96).
Missing for atoms 7-6-5-10 (type 37-2-2-162).
Missing for atoms 10-5-1-9 (type 162-2-37-2).
Missing for atoms 1-5-10 (type 37-2-162) angle type 1.
Missing for atoms 5-10-11 (type 2-162-151) angle type 1.

B. Estimated parameters
Pi-atom parameters of type (2-2) is used for type (37-162).
Pi-atom parameters of type (37-40) is used for type (37-151).
Pi-atom parameters of type (2-3) is used for type (2-162).
Pi-atom parameters of type (2-40) is used for type (2-151).
Pi-atom parameters of type (2-2) is used for type (162-151).
Pi-atom parameters of type (3-96) is used for type (162-96).
Pi-atom parameters of type (2-2) is used for type (151-96).

4 torsional parameters are read in

Atom type numbers	V1	V2	V3
37 2 162 151	0.000	11.600	0.000
37 2 162 96	0.000	11.600	0.000
37 2 2 162	0.000	11.600	0.000
162 2 37 2	0.000	11.600	0.000

2 bending parameters are read in

Atom type numbers	Kb	Theta
37 2 162	0.695	120.000
2 162 151	0.695	120.000

Bond lengths begin on next page

II. Bond lengths

Bond	Length Crystal	Length MM3	Difference (in Å)
N(1)-C(5)	1.3437	1.3411	0.0026
N(1)-C(9)	1.3537	1.3400	0.0137
H(2)-C(9)	0.9182	1.1028	-0.1846
H(3)-N(11)	0.8659	1.0295	-0.1636
H(4)-N(11)	0.8709	1.0285	-0.1576
C(5)-C(6)	1.3830	1.4044	-0.0214
C(5)-C(10)	1.4998	1.5039	-0.0041
C(6)-N(7)	1.3289	1.3372	-0.0083
C(6)-H(13)	1.0009	1.1020	-0.1011
N(7)-C(8)	1.3527	1.3421	0.0106
C(8)-C(9)	1.3747	1.3954	-0.0207
C(8)-H(14)	1.0189	1.1028	-0.0839
C(10)-N(11)	1.3094	1.3771	-0.0677
C(10)-O(12)	1.2408	1.2461	-0.0053

RMS value: 0.0882

III. Bond angles

Bond	Theta (in degrees) Crystal	Theta (in degrees) MM3	Difference (in degrees)
C(5)-N(1)-C(9)	115.447	115.221	0.226
N(1)-C(5)-C(6)	121.916	122.230	-0.314
N(1)-C(5)-C(10)	117.223	119.011	-1.788
C(6)-C(5)-C(10)	120.861	118.759	2.102
C(5)-C(6)-N(7)	122.574	122.347	0.227
C(5)-C(6)-H(13)	115.355	120.396	-5.041
N(7)-C(6)-H(13)	121.250	117.257	3.993
C(6)-N(7)-C(8)	116.055	115.270	0.785
N(7)-C(8)-C(9)	121.601	122.420	-0.819
N(7)-C(8)-H(14)	117.255	117.745	-0.490
C(9)-C(8)-H(14)	120.358	119.835	0.523
N(1)-C(9)-H(2)	114.067	117.778	-3.711
N(1)-C(9)-C(8)	122.398	122.512	-0.114
H(2)-C(9)-C(8)	123.414	119.711	3.703
C(5)-C(10)-N(11)	117.510	116.855	0.655
C(5)-C(10)-O(12)	119.115	120.909	-1.794
N(11)-C(10)-O(12)	123.240	122.235	1.005
H(3)-N(11)-H(4)	118.898	122.780	-3.882
H(3)-N(11)-C(10)	117.181	118.111	-0.930

Bond	Theta (in degrees) Crystal	MM3		Difference (in degrees)
H(4)-N(11)-C(10)	121.585	119.109		2.476
			RMS value:	2.293

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
N(1)-C(5)-C(6)-C(7)	-0.8	0.0	-0.8
N(1)-C(5)-C(6)-H(13)	-170.6	180.0	9.4
N(1)-C(5)-C(10)-N(11)	-1.9	0.0	-1.9
N(1)-C(5)-C(10)-O(12)	174.0	180.0	-6.0
N(1)-C(9)-C(8)-N(7)	0.6	0.0	0.6
N(1)-C(9)-C(8)-H(14)	-169.0	180.0	11.0
H(2)-C(9)-N(1)-C(5)	-176.6	180.0	3.4
H(2)-C(9)-C(8)-N(7)	176.4	180.0	-3.6
H(2)-C(9)-C(8)-H(14)	6.8	0.0	6.8
H(3)-N(11)-C(10)-C(5)	-20.5	0.0	-20.5
H(3)-N(11)-C(10)-O(12)	163.8	180.0	-16.2
H(4)-N(11)-C(10)-C(5)	177.1	180.0	-2.9
H(4)-N(11)-C(10)-O(12)	1.3	0.0	1.3
C(5)-N(1)-C(9)-C(8)	-0.4	0.0	-0.4
C(5)-C(6)-N(7)-C(8)	0.9	0.0	0.9
C(6)-C(5)-N(1)-C(9)	0.5	0.0	0.5
C(6)-C(5)-C(10)-N(11)	178.2	180.0	-1.8
C(6)-C(5)-C(10)-O(12)	-5.9	0.0	-5.9
C(6)-N(7)-C(8)-C(9)	-0.8	0.0	-0.8
C(6)-N(7)-C(8)-H(14)	169.1	180.0	-10.9
N(7)-C(6)-C(5)-C(10)	179.1	-180.0	-0.9
C(8)-N(7)-C(6)-H(13)	170.0	-180.0	-10.0
C(9)-N(1)-C(5)-C(10)	-179.4	180.0	0.6
C(10)-C(5)-C(6)-H(13)	9.4	0.0	9.4
		RMS value:	7.5

V. Other

1. In crystal structure the pi system is found to be nonplanar.
   In MM3 the pi system is determined to be planar.

Table 22. Isoniazid

I. Missing parameters

A. Pi-atom parameter of type (3-37) is missing.

Missing for atoms 1-17-2-6 (type 3-150-150-23).
Missing for atoms 7-1-17-2 (type 2-3-150-150).
Missing for atoms 13-1-17-2 (type 96-3-150-150).
Missing for atoms 7-1-17-4 (type 2-3-150-23).
Missing for atoms 13-1-17-4 (type 96-3-150-23).
Missing for atoms 5-7-1-17 (type 2-2-3-150).
Missing for atoms 9-7-1-17 (type 2-2-3-150).
Missing for bond 1-17 (type 3-150).
Missing for atoms 7-1-17 (type 2-3-150) angle type 1.
Missing for atoms 13-1-17 (type 96-3-150) angle type 1.
Missing for atoms 1-17-2 (type 3-150-150) angle type 1.
Missing for atoms 1-17-4 (type 3-150-23) angle type 1.

B. Estimated parameters

Pi-atom parameters of type (2-2) is used for type (3-37).

6 torsional parameters are read in

Atom type numbers	V1	V2	V3
3 150 150 23	0.000	0.000	0.000
2 3 150 150	0.000	0.000	0.000
96 3 150 150	0.000	0.000	0.000
2 3 150 23	0.000	0.000	0.000
96 3 150 23	0.000	0.000	0.000
2 2 3 150	0.000	11.600	0.000

1 stretching parameter is read in

Bond type	Ks	L(0)
3-150	5.3477	1.4340

1 dipole parameter is read in

Bond type	Moment
3-150	0.4500

4 bending parameters are read in

Atom type numbers	Kb	Theta
2 3 150	0.695	120.000
96 3 150	0.695	120.000

Bending parameters cont.

Atom type numbers	Kb	Theta
3 150 150	0.695	110.000
3 150 23	0.543	110.000

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(7)	1.4852	1.4923	-0.0071
C(1)-O(13)	1.2321	1.2176	0.0145
C(1)-N(17)	1.3325	1.4406	-0.1081
N(2)-H(6)	1.0706	1.0237	0.0469
N(2)-H(16)	1.0170	1.0287	-0.0117
N(2)-N(17)	1.4127	1.4342	-0.0215
C(3)-C(5)	1.3942	1.3964	-0.0022
C(3)-H(14)	1.0747	1.1032	-0.0285
C(3)-N(15)	1.3354	1.3465	-0.0111
H(4)-N(17)	1.0957	1.0238	0.0719
C(5)-C(7)	1.3877	1.3913	-0.0036
C(7)-C(9)	1.4023	1.3931	0.0092
C(9)-C(11)	1.3860	1.3948	-0.0088
H(10)-C(11)	1.0563	1.1032	-0.0469
C(11)-N(15)	1.0563	1.3486	-0.2923
		RMS value:	0.0394

III. Bond angles

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(7)-C(1)-O(13)	122.288	121.714	0.574
C(7)-C(1)-N(17)	115.556	119.896	-4.340
O(13)-C(1)-N(17)	122.052	118.390	3.662
H(6)-N(2)-H(16)	103.159	108.200	-5.041
H(6)-N(2)-N(17)	108.780	107.815	0.965
H(16)-N(2)-N(17)	100.609	108.804	-8.195
C(5)-C(3)-H(14)	122.239	119.493	2.746
C(5)-C(3)-N(15)	123.561	123.003	0.558
H(14)-C(3)-N(15)	114.042	117.504	-3.462
C(3)-C(5)-C(7)	119.781	119.135	0.646
C(1)-C(7)-C(5)	125.169	120.961	4.208
C(1)-C(7)-C(9)	118.280	120.807	-2.527
C(5)-C(7)-C(9)	116.551	118.232	-1.681
C(7)-C(9)-C(11)	119.398	119.126	0.272
C(9)-C(11)-H(10)	118.702	119.502	-0.800

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(9)-C(11)-N(15)	124.080	122.991	1.089
H(10)-C(11)-N(15)	117.216	117.507	-0.291
C(3)-N(15)-C(11)	116.536	117.513	-0.977
C(1)-N(17)-N(2)	120.713	116.155	4.558
C(1)-N(17)-H(4)	128.072	114.892	13.180
N(2)-N(17)-H(4)	110.975	105.846	5.129
		RMS value:	4.348

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(7)-C(5)-C(3)	-178.7	-180.0	1.3
C(1)-C(7)-C(9)-C(11)	-179.8	179.9	-0.3
C(1)-N(17)-N(2)-H(6)	-84.2	-94.6	10.4
C(1)-N(17)-N(2)-H(16)	23.7	22.5	1.2
N(2)-N(17)-C(1)-C(7)	-173.7	112.1	-74.2
N(2)-N(17)-C(1)-O(13)	2.7	-67.9	70.6
C(3)-C(5)-C(7)-C(9)	1.6	0.0	1.6
C(3)-N(15)-C(11)-C(9)	-2.0	0.0	-2.0
C(3)-N(15)-C(11)-H(10)	177.7	-180.0	2.3
H(4)-N(17)-C(1)-C(7)	0.2	-123.6	123.8
H(4)-N(17)-C(1)-O(13)	176.5	56.3	120.2
H(4)-N(17)-N(2)-H(6)	101.0	136.6	-35.6
H(4)-N(17)-N(2)-H(16)	-151.1	-106.3	-44.8
C(5)-C(3)-N(15)-C(11)	3.6	0.0	3.6
C(5)-C(7)-C(1)-O(13)	-160.5	-179.6	19.1
C(5)-C(7)-C(1)-N(17)	15.9	0.4	15.5
C(5)-C(7)-C(9)-H(8)	-179.3	180.0	-0.7
C(5)-C(7)-C(9)-C(11)	-0.1	0.0	-0.1
C(7)-C(5)-C(3)-H(14)	-178.7	-180.0	1.3
C(7)-C(5)-C(3)-N(15)	-3.5	0.0	-3.5
C(7)-C(9)-C(11)-H(10)	-179.4	-180.0	0.6
C(7)-C(9)-C(11)-N(15)	0.3	0.0	0.3
C(9)-C(7)-C(1)-N(17)	-164.4	-179.6	15.2
C(11)-N(15)-C(3)-H(14)	179.1	180.0	-0.9
		RMS value:	43.1

V. Other

1. In crystal structure the pi system is found to be nonplanar.

Other cont.

In MM3 the pi system is determined to be planar.

2. In MM3 geometry optimization can not be accomplished and optimization switches to energy minimization.

Table 23. Ribavarin

I. Missing parameters

A. Pi-atom parameter of type (2-162) is missing.
Pi-atom parameter of type (2-151) is missing.
Pi-atom parameter of type (2-79) is missing.
Pi-atom parameter of type (162-40) is missing.
Pi-atom parameter of type (162-37) is missing.
Pi-atom parameter of type (162-151) is missing.
Pi-atom parameter of type (162-79) is missing.
Pi-atom parameter of type (40-151) is missing.
Pi-atom parameter of type (40-79) is missing.
Pi-atom parameter of type (37-151) is missing.
Pi-atom parameter of type (37-79) is missing.
Pi-atom parameter of type (151-79) is missing.
Missing for atoms 23-6-21-1 (type 37-2-40-1).
Missing for atoms 3-22-21-1 (type 2-37-40-1).
Missing for atoms 2-1-21-6 (type 1-1-40-2).
Missing for atoms 2-1-21-22 (type 1-1-40-37).
Missing for atoms 4-2-1-21 (type 1-1-1-40).
Missing for atoms 21-1-25-5 (type 40-1-6-1).
Missing for atoms 25-1-21-6 (type 6-1-40-2).
Missing for atoms 8-3-23-6 (type 162-2-37-2).
Missing for atoms 8-3-22-21 (type 162-2-37-40).
Missing for atoms 9-1-21-22 (type 5-1-40-37).
Missing for atoms 10-2-1-21 (type 5-1-1-40).
Missing for atoms 21-1-2-26 (type 40-1-1-6).
Missing for atoms 22-3-8-24 (type 37-2-162-151).
Missing for atoms 22-3-8-29 (type 37-2-162-79).
Missing for atoms 25-1-21-22 (type 6-1-40-37).
Missing for atoms 23-3-8-24 (type 37-2-162-151).
Missing for atoms 23-3-8-29 (type 37-2-162-79).
Missing for atoms 2-1-21 (type 1-1-40) angle type 1.
Missing for atoms 25-1-21 (type 6-1-40) angle type 1.
Missing for atoms 22-3-8 (type 37-2-162) angle type 1.
Missing for atoms 23-3-8 (type 37-2-162) angle type 1.
Missing for atoms 3-8-24 (type 2-162-151) angle type 2.
Missing for atoms 1-21-22 (type 1-40-37) angle type 1.

B. Estimated parameters
Pi-atom parameters of type (2-3) is used for type (2-162).
Pi-atom parameters of type (2-40) is used for type (2-151).

Pi-atom parameters of type (2-7) is used for type (2-79).
Pi-atom parameters of type (2-2) is used for type (162-40).
Pi-atom parameters of type (2-2) is used for type (162-37).
Pi-atom parameters of type (2-2) is used for type (162-151).
Pi-atom parameters of type (3-7) is used for type (162-79).
Pi-atom parameters of type (40-40) is used for type (40-151).
Pi-atom parameters of type (2-2) is used for type (40-79).
Pi-atom parameters of type (37-40) is used for type (37-151).
Pi-atom parameters of type (37-7) is used for type (37-79).
Pi-atom parameters of type (2-2) is used for type (151-79).

15 torsional parameters are read in

Atom type numbers				V1	V2	V3
37	2	40	1	0.000	11.600	0.000
2	37	40	1	0.000	11.600	0.000
1	1	40	2	0.000	0.160	0.090
1	1	40	37	0.000	0.160	0.090
1	1	1	40	0.000	0.000	0.270
40	1	6	1	0.000	0.000	0.200
6	1	40	2	0.000	0.160	0.090
162	2	37	2	0.000	11.600	0.000
162	2	37	40	0.000	11.600	0.000
5	1	40	37	0.000	0.160	0.090
5	1	1	40	0.000	0.000	0.270
6	1	1	40	0.000	0.000	0.270
37	2	162	151	0.000	11.600	0.000
37	2	162	79	0.000	11.600	0.000
6	1	40	37	0.000	0.160	0.090

5 bending parameters are read in

Atom type numbers			Kb	Theta
1	1	40	0.695	109.500
6	1	40	0.695	109.500
37	2	162	0.695	120.000
2	162	151	0.695	120.000
1	40	37	0.695	120.000

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(2)	1.5288	1.5383	-0.0095
C(1)-H(9)	0.9466	1.1178	-0.1712

Bond	Length Crystal	MM3		Difference (in Å)
C(1)-N(21)	1.4747	1.5008		-0.0261
C(1)-O(25)	1.3936	1.4366		-0.0430
C(2)-C(4)	1.5226	1.5161		0.0065
C(2)-H(10)	0.9798	1.1154		-0.1356
C(2)-O(26)	1.4268	1.4352		-0.0084
C(3)-C(8)	1.4865	1.4975		-0.0110
C(3)-N(22)	1.3222	1.3250		-0.0028
C(3)-N(23)	1.3600	1.3677		-0.0077
C(4)-C(5)	1.5189	1.5229		-0.0040
C(4)-H(14)	0.8175	1.1157		-0.2982
C(4)-O(27)	1.4188	1.4340		-0.0152
C(5)-C(7)	1.5098	1.5240		-0.0142
C(5)-H(15)	0.8955	1.1186		-0.2231
C(5)-O(25)	1.4641	1.4335		0.0306
C(6)-H(16)	0.8887	1.0964		-0.2077
C(6)-N(21)	1.3274	1.3588		-0.0314
C(6)-N(23)	1.3319	1.3153		0.0166
C(7)-O(28)	1.4347	1.4329		0.0018
C(8)-N(24)	1.3281	1.3772		-0.0491
C(8)-O(29)	1.2350	1.2453		-0.0103
H(11)-O(26)	0.7446	0.9503		-0.2057
H(12)-O(27)	1.2504	0.9476		0.3028
H(13)-O(28)	0.7022	0.9478		-0.2456
H(19)-N(24)	0.7076	1.0295		-0.3219
H(20)-N(24)	0.9162	1.0281		-0.1119
N(21)-N(22)	1.3684	1.3568		0.0116
			RMS value:	0.1481

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(2)-C(1)-H(9)	112.800	111.132	1.668
C(2)-C(1)-N(21)	111.441	110.621	0.820
C(2)-C(1)-O(25)	107.720	106.632	1.088
H(9)-C(1)-N(21)	93.134	108.339	-15.205
H(9)-C(1)-O(25)	122.651	110.149	12.502
N(21)-C(1)-O(25)	108.000	109.969	-1.969
C(1)-C(2)-C(4)	101.254	100.518	0.736
C(1)-C(2)-H(10)	115.147	113.945	1.202
C(1)-C(2)-O(26)	111.681	107.353	4.328
C(4)-C(2)-H(10)	105.511	113.676	-8.165

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(4)-C(2)-O(26)	111.681	109.368	2.313
H(10)-C(2)-O(26)	116.351	111.318	5.033
C(8)-C(3)-N(22)	122.337	121.962	0.375
C(8)-C(3)-N(23)	122.184	123.367	-1.183
N(22)-C(3)-N(23)	115.479	114.671	0.808
C(2)-C(4)-C(5)	101.630	100.529	1.101
C(2)-C(4)-H(14)	99.950	109.901	-9.951
C(2)-C(4)-O(27)	109.663	110.173	-0.510
C(5)-C(4)-H(14)	105.207	112.086	-6.879
C(5)-C(4)-O(27)	113.522	112.473	1.049
H(14)-C(4)-O(27)	123.934	111.189	12.745
C(4)-C(5)-C(7)	117.688	115.011	2.677
C(4)-C(5)-H(15)	83.607	109.984	-26.377
C(4)-C(5)-O(25)	104.017	104.625	-0.608
C(7)-C(5)-H(15)	122.073	108.834	13.239
C(7)-C(5)-O(25)	108.248	109.543	-1.295
H(15)-C(5)-O(25)	117.983	108.637	9.346
H(16)-C(6)-N(21)	126.470	121.364	5.106
H(16)-C(6)-N(23)	123.027	127.560	-4.533
N(21)-C(6)-N(23)	110.502	111.076	-0.574
C(5)-C(7)-O(28)	110.255	110.115	0.140
C(3)-C(8)-N(24)	116.757	117.100	-0.343
C(3)-C(8)-O(29)	119.407	120.517	-1.110
N(24)-C(8)-O(29)	123.835	122.383	1.452
C(1)-N(21)-C(6)	130.778	128.351	2.427
C(1)-N(21)-N(22)	118.947	122.969	-4.022
C(6)-N(21)-N(22)	110.269	108.679	1.590
C(3)-N(22)-N(21)	101.585	103.101	-1.516
C(3)-N(23)-C(6)	102.157	102.473	-0.316
C(8)-N(24)-H(19)	135.033	118.798	16.235
C(8)-N(24)-H(20)	107.443	118.761	-11.318
H(19)-N(24)-H(20)	115.213	122.440	-7.227
C(1)-O(25)-C(5)	109.741	108.531	1.210
C(2)-O(26)-H(11)	115.103	106.435	8.668
C(4)-O(27)-H(12)	136.375	107.956	28.419
C(7)-O(28)-H(13)	93.656	108.420	-14.764
		RMS value:	8.621

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(2)-C(4)-C(5)	37.9	41.2	-3.3
C(1)-C(2)-C(4)-H(14)	-70.1	-77.1	7.0
C(1)-C(2)-C(4)-O(27)	158.3	160.1	-1.8
C(1)-C(2)-O(26)-H(11)	137.5	-156.9	65.6
C(1)-N(21)-C(6)-H(16)	-0.4	0.1	-0.5
C(1)-N(21)-C(6)-N(23)	179.2	-180.0	0.8
C(1)-N(21)-N(22)-C(3)	-178.8	179.9	-1.3
C(1)-O(25)-C(5)-C(4)	20.1	23.4	-3.3
C(1)-O(25)-C(5)-C(7)	146.0	147.2	-1.2
C(1)-O(25)-C(5)-H(15)	-70.0	-94.0	24.0
C(2)-C(1)-N(21)-C(6)	-107.7	-114.3	6.6
C(2)-C(1)-N(21)-N(22)	71.3	65.9	5.4
C(2)-C(1)-O(25)-C(5)	4.6	3.6	1.0
C(2)-C(4)-C(5)-C(7)	-155.9	-161.1	5.2
C(2)-C(4)-C(5)-H(15)	81.1	75.6	5.5
C(2)-C(4)-C(5)-O(25)	-36.2	-40.9	4.7
C(2)-C(4)-O(27)-H(12)	173.1	159.5	13.6
C(3)-C(8)-N(24)-H(19)	-29.1	0.2	-29.3
C(3)-C(8)-N(24)-H(20)	169.7	179.9	-10.2
C(3)-N(22)-N(21)-C(6)	0.5	0.2	0.3
C(3)-N(23)-C(6)-H(16)	179.0	-179.9	1.1
C(3)-N(23)-C(6)-N(21)	-0.6	0.2	-0.8
C(4)-C(2)-C(1)-H(9)	-165.6	-148.9	-16.7
C(4)-C(2)-C(1)-N(21)	91.1	90.7	0.4
C(4)-C(2)-C(1)-O(25)	-27.2	-28.8	1.6
C(4)-C(2)-O(26)-H(11)	-113.1	-48.7	-64.4
C(4)-C(5)-C(7)-O(28)	55.1	49.4	5.7
C(5)-C(4)-C(2)-H(10)	158.2	163.4	-5.2
C(5)-C(4)-C(2)-O(26)	-74.5	-71.6	-2.9
C(5)-C(4)-O(27)-H(12)	-74.0	-89.2	15.2
C(5)-C(7)-O(28)-H(13)	156.8	171.0	-14.2
C(5)-O(25)-C(1)-H(9)	138.1	124.3	13.8
C(5)-O(25)-C(1)-N(21)	-115.9	-116.4	0.5
C(6)-N(21)-C(1)-H(9)	136.3	123.6	12.7
C(6)-N(21)-C(1)-O(25)	10.4	3.2	7.2
C(6)-N(23)-C(3)-C(8)	-179.1	-180.0	0.9
C(6)-N(23)-C(3)-N(22)	0.9	-0.1	1.0
C(7)-C(5)-C(4)-H(14)	-52.1	-44.5	-7.6
C(7)-C(5)-C(4)-O(27)	86.5	81.7	4.8

Bond	Crystal	MM3	Difference (in degrees)
C(8)-C(3)-N(22)-N(21)	179.2	179.9	-0.7
H(9)-C(1)-C(2)-H(10)	81.1	89.2	-8.1
H(9)-C(1)-C(2)-O(26)	-49.0	-34.6	-14.4
H(9)-C(1)-N(21)-N(22)	-44.7	-56.1	11.4
H(10)-C(2)-C(1)-N(21)	-22.1	-31.2	9.1
H(10)-C(2)-C(1)-O(25)	-140.4	-150.8	10.4
H(10)-C(2)-C(4)-H(14)	50.2	45.1	5.1
H(10)-C(2)-C(4)-O(27)	-81.4	-77.8	-3.6
H(10)-C(2)-O(26)-H(11)	8.1	77.8	-69.7
H(12)-O(27)-C(4)-H(14)	55.6	37.4	18.2
H(14)-C(4)-C(2)-O(26)	177.5	170.2	7.3
H(14)-C(4)-C(5)-H(15)	-175.1	-167.7	-7.4
H(14)-C(4)-C(5)-O(25)	67.6	75.8	-8.2
H(15)-C(5)-C(4)-O(27)	-36.5	-41.6	5.1
H(15)-C(5)-C(7)-O(28)	155.5	173.3	-17.8
H(16)-C(6)-N(21)-N(22)	-179.5	179.8	-0.8
H(19)-N(24)-C(8)-O(29)	151.1	-179.8	29.2
H(20)-N(24)-C(8)-O(29)	-10.1	-0.1	-10.0
N(21)-C(1)-C(2)-O(26)	-152.2	-155.0	2.8
N(21)-N(22)-C(3)-N(23)	-0.9	-0.1	-0.8
N(22)-C(3)-C(8)-N(24)	1.5	0.6	0.9
N(22)-C(3)-C(8)-O(29)	-178.8	-179.4	0.6
N(22)-N(21)-C(1)-O(25)	-170.6	-176.5	5.9
N(22)-N(21)-C(6)-N(23)	0.1	-0.2	0.3
N(23)-C(3)-C(8)-N(24)	-178.5	-179.5	1.0
N(23)-C(3)-C(8)-O(29)	1.3	0.5	0.8
O(25)-C(1)-C(2)-O(26)	89.5	85.5	4.0
O(25)-C(5)-C(4)-O(27)	-153.8	-158.1	4.3
O(25)-C(5)-C(7)-O(28)	-62.3	-68.1	5.8
O(26)-C(2)-C(4)-O(27)	45.9	47.3	-1.4
		RMS value:	16.6

V. Other

1. The pi-system in the crystal structure is found to be nonplanar. The pi-system in the MM3 structure is found to be planar.

Table 24. Amiodarone

I. Missing parameters

A. Missing for atoms 21-20-4-3 (type 1-1-2-41)
Missing for atoms 24-25-26-27 (type 41-1-1-39)

B. Estimated Parameters

2 torsional parameters are read in

Atom type numbers				V1	V2	V3
1	1	2	41	0.0000	0.1600	0.0900
39	1	1	41	0.0000	0.0000	0.2700

1 bending parameter is read in

Atom type numbers		KB
2	14	0.1000

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
I(1)-C(16)	2.1105	2.1052	0.0053
I(2)-C(18)	2.0913	2.0921	-0.0008
O(3)-C(4)	1.3600	1.3942	-0.0342
O(3)-C(11)	1.3744	1.3714	0.0030
C(4)-C(5)	1.3551	1.3726	-0.0175
C(4)-C(20)	1.5068	1.5087	-0.0019
C(5)-C(6)	1.4595	1.4499	0.0096
C(5)-C(12)	1.4633	1.4888	-0.0255
C(6)-C(7)	1.3848	1.4019	-0.0171
C(6)-C(11)	1.3877	1.3921	-0.0044
C(7)-C(8)	1.3972	1.3928	0.0044
C(8)-C(9)	1.3928	1.4141	-0.0213
C(9)-C(10)	1.3658	1.3917	-0.0259
C(10)-C(11)	1.3738	1.3982	-0.0244
C(12)-O(13)	1.1995	1.2242	-0.0247
C(12)-C(14)	1.4965	1.5044	-0.0079
C(14)-C(15)	1.3950	1.3929	0.0021
C(14)-C(19)	1.3759	1.3859	-0.0100
C(15)-C(16)	1.3936	1.4007	-0.0071
C(15)-H(36)	0.8031	1.1029	-0.2998
C(16)-C(17)	1.3966	1.4225	-0.0259
C(17)-C(18)	1.3756	1.4075	-0.0319
C(17)-O(24)	1.3867	1.2280	0.1587

Bond	Length Crystal	MM3	Difference (in Å)
C(18)-C(19)	1.4095	1.3971	0.0124
C(19)-H(37)	1.1292	1.1024	0.0268
C(20)-C(21)	1.5124	1.5413	-0.0289
C(21)-C(22)	1.5237	1.5386	-0.0149
C(22)-C(23)	1.5079	1.5353	-0.0274
O(24)-C(25)	1.4346	1.4225	0.0121
C(25)-C(26)	1.5203	1.5279	-0.0076
C(26)-N+(27)	1.4840	1.5148	-0.0308
N+(27)-C(28)	1.5012	1.5080	-0.0068
N+(27)-C(30)	1.4991	1.5054	-0.0063
N+(27)-H(51)	0.6261	1.0167	-0.3906
C(28)-C(29)	1.4897	1.5227	-0.033
C(30)-C(31)	1.4736	1.5224	-0.0488

RMS value: 0.0873

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(4)-O(3)-C(11)	107.240	105.587	1.653
O(3)-C(4)-C(5)	111.518	111.363	0.155
O(3)-C(4)-C(20)	113.409	118.320	-4.911
C(5)-C(4)-C(20)	134.689	130.111	4.578
C(4)-C(5)-C(6)	106.009	106.060	-0.051
C(4)-C(5)-C(12)	129.126	130.647	-1.521
C(6)-C(5)-C(12)	123.749	123.128	0.621
C(5)-C(6)-C(7)	135.749	133.909	1.840
C(5)-C(6)-C(11)	105.378	105.543	-0.165
C(7)-C(6)-C(11)	118.867	120.547	-1.680
C(6)-C(7)-C(8)	117.688	118.163	-0.475
C(7)-C(8)-C(9)	121.274	120.957	0.317
C(8)-C(9)-C(10)	121.477	120.702	0.775
C(9)-C(10)-C(11)	116.394	117.845	-1.451
O(3)-C(11)-C(6)	109.853	111.447	-1.594
O(3)-C(11)-C(10)	125.848	126.763	-0.915
C(6)-C(11)-C(10)	124.294	121.785	2.509
C(5)-C(12)-O(13)	120.403	121.552	-1.149
C(5)-C(12)-C(14)	120.802	117.561	3.241
O(13)-C(12)-C(14)	118.732	120.879	-2.147
C(12)-C(14)-C(15)	116.853	118.703	-1.850

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(12)-C(14)-C(19)	122.226	120.936	1.290
C(15)-C(14)-C(19)	120.877	120.361	0.516
C(14)-C(15)-C(16)	119.324	121.031	-1.707
C(14)-C(15)-H(36)	116.559	118.037	-1.478
C(16)-C(15)-H(36)	124.116	120.922	3.194
I(1)-C(16)-C(15)	116.100	109.469	6.631
I(1)-C(16)-C(17)	123.624	131.220	-7.596
C(15)-C(16)-C(17)	120.273	119.311	0.962
C(16)-C(17)-C(18)	119.641	118.182	1.459
C(16)-C(17)-O(24)	119.772	126.592	-6.820
C(18)-C(17)-O(24)	120.483	115.204	5.279
I(2)-C(18)-C(17)	120.729	122.872	-2.143
I(2)-C(18)-C(19)	118.638	115.320	3.318
C(17)-C(18)-C(19)	120.613	121.777	-1.164
C(14)-C(19)-C(18)	119.186	119.245	-0.059
C(14)-C(19)-H(37)	125.612	119.706	5.906
C(18)-C(19)-H(37)	115.203	121.033	-5.830
C(4)-C(20)-C(21)	112.246	112.392	-0.146
C(20)-C(21)-C(22)	113.159	113.336	-0.177
C(21)-C(22)-C(23)	113.024	113.802	-0.778
C(17)-O(24)-C(25)	113.299	125.515	-12.216
O(24)-C(25)-C(26)	109.110	109.466	-0.356
C(25)-C(26)-N+(27)	115.115	117.079	-1.964
C(26)-N+(27)-C(28)	112.892	111.897	0.995
C(26)-N+(27)-C(30)	115.821	115.265	0.556
C(26)-N+(27)-H(51)	99.394	105.088	-5.694
C(28)-N+(27)-C(30)	112.279	112.622	-0.343
C(28)-N+(27)-H(51)	101.970	105.746	-3.776
C(30)-N+(27)-H(51)	112.928	105.205	7.723
N+(27)-C(28)-C(29)	114.905	112.640	2.265
N+(27)-C(30)-C(31)	112.737	112.136	0.601

RMS value: 3.471

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
I(1)-C(16)-C(15)-C(14)	-178.6	-179.9	1.3
I(1)-C(16)-C(15)-H(36)	1.7	-1.1	2.8
I(1)-C(16)-C(17)-C(18)	-178.7	-177.7	-1.0

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
I(1)-C(16)-C(17)-O(24)	-2.4	4.0	-6.4
I(2)-C(18)-C(17)-C(16)	176.0	-179.8	4.2
I(2)-C(18)-C(17)-O(24)	-0.3	-1.3	1.0
I(2)-C(18)-C(19)-C(14)	-176.8	177.4	5.8
I(2)-C(18)-C(19)-H(37)	3.2	-1.2	4.4
O(3)-C(4)-C(5)-C(6)	-0.1	0.1	-0.2
O(3)-C(4)-C(5)-C(12)	168.0	175.5	-7.5
O(3)-C(4)-C(20)-C(21)	-92.0	-83.1	-8.9
O(3)-C(11)-C(6)-C(5)	-0.5	0.2	-0.7
O(3)-C(11)-C(6)-C(7)	178.8	-179.6	-1.6
O(3)-C(11)-C(10)-C(9)	-178.2	179.4	2.4
O(3)-C(11)-C(10)-H(32)	-2.4	-0.4	-2.0
C(4)-O(3)-C(11)-C(6)	0.4	-0.1	0.5
C(4)-O(3)-C(11)-C(10)	179.6	-179.4	-1.0
C(4)-C(5)-C(6)-C(7)	-178.7	179.6	1.7
C(4)-C(5)-C(6)-C(11)	0.4	-0.2	0.6
C(4)-C(5)-C(12)-O(13)	-145.8	-148.5	2.7
C(4)-C(5)-C(12)-C(14)	31.3	30.5	0.8
C(4)-C(20)-C(21)-C(22)	-176.5	179.1	4.4
C(5)-C(4)-O(3)-C(11)	-0.2	0.0	-0.2
C(5)-C(4)-C(20)-C(21)	80.1	91.3	-11.2
C(5)-C(6)-C(7)-C(8)	178.6	-179.5	-1.9
C(5)-C(6)-C(11)-C(10)	-179.7	179.5	0.8
C(5)-C(12)-C(14)-C(15)	-136.7	-129.9	-6.8
C(5)-C(12)-C(14)-C(19)	45.7	50.4	-4.7
C(6)-C(5)-C(4)-C(20)	-172.3	-174.6	2.3
C(6)-C(5)-C(12)-O(13)	20.4	26.2	-5.8
C(6)-C(5)-C(12)-C(14)	-162.5	-154.8	-7.7
C(6)-C(7)-C(8)-C(9)	0.7	0.0	0.7
C(6)-C(11)-C(10)-C(9)	0.8	0.2	0.6
C(7)-C(6)-C(5)-C(12)	12.4	3.8	8.6
C(7)-C(6)-C(11)-C(10)	-0.4	-0.3	-0.1
C(7)-C(8)-C(9)-C(10)	-0.3	-0.1	-0.2
C(8)-C(7)-C(6)-C(11)	-0.4	0.2	-0.6
C(8)-C(9)-C(10)-C(11)	-0.5	0.0	-0.5
C(11)-O(3)-C(4)-C(20)	173.8	175.4	-1.6
C(11)-C(6)-C(5)-C(12)	-168.5	-176.0	7.5
C(12)-C(5)-C(4)-C(20)	-4.2	0.8	-5.0
C(12)-C(14)-C(15)-C(16)	179.4	177.4	2.0
C(12)-C(14)-C(15)-H(36)	-0.9	-1.4	0.5

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(12)-C(14)-C(19)-C(18)	178.6	-177.3	-4.1
C(12)-C(14)-C(19)-H(37)	-1.4	1.3	-2.7
O(13)-C(12)-C(14)-C(15)	40.4	49.1	-8.7
O(13)-C(12)-C(14)-C(19)	-137.2	-130.6	-6.6
C(14)-C(15)-C(16)-C(17)	2.1	0.3	1.8
C(14)-C(19)-C(18)-C(17)	1.6	-0.6	2.2
C(15)-C(14)-C(19)-C(18)	1.1	3.0	-1.9
C(15)-C(14)-C(19)-H(37)	-178.9	-178.4	-0.5
C(15)-C(16)-C(17)-C(18)	0.5	2.0	-1.5
C(15)-C(16)-C(17)-O(24)	176.8	-176.2	-7.0
C(16)-C(15)-C(14)-C(19)	-2.9	-2.8	-0.1
C(16)-C(17)-C(18)-C(19)	-2.4	-1.9	-0.5
C(16)-C(17)-O(24)-C(25)	92.9	5.1	87.8
C(17)-C(16)-C(15)-H(36)	-177.6	179.1	3.3
C(17)-C(18)-C(19)-H(37)	-178.4	-179.2	0.8
C(17)-O(24)-C(25)-C(26)	163.9	173.9	-10.0
C(18)-C(17)-O(24)-C(25)	-90.8	-173.2	82.4
C(19)-C(14)-C(15)-H(36)	176.8	178.3	-1.5
C(19)-C(18)-C(17)-O(24)	-178.7	176.6	4.7
C(20)-C(21)-C(22)-C(23)	71.3	64.8	6.5
O(24)-C(25)-C(26)-N+(27)	66.0	73.6	-7.6
C(25)-C(26)-N+(27)-C(28)	55.0	57.0	-2.0
C(25)-C(26)-N+(27)-C(30)	-76.4	-73.4	-3.0
C(25)-C(26)-N+(27)-H(51)	162.3	171.3	-9.0
C(26)-N+(27)-C(28)-C(29)	155.5	152.6	2.9
C(26)-N+(27)-C(30)-C(31)	-54.1	-69.0	14.9
C(28)-N+(27)-C(30)-C(31)	174.2	161.0	13.2
C(29)-C(28)-N+(27)-C(30)	-71.3	-75.7	4.4
C(29)-C(28)-N+(27)-H(51)	49.8	38.7	11.1
C(31)-C(30)-N+(27)-H(51)	59.6	46.3	13.3
		RMS value:	14.9

Table 25. Methyl-dopa

I. Missing parameters

A. Missing for atoms 15-8-10-12 (type 39-1-3-75)

B. Estimated Parameters

1 torsional parameters is read in

Atom type numbers				V1	V2	V3
39	1	3	75	0.0000	0.1600	0.0900

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(2)	1.3898	1.4020	-0.0122
C(1)-C(6)	1.3868	1.4012	-0.0144
C(1)-C(7)	1.5148	1.5116	0.0032
C(2)-C(3)	1.3843	1.4017	-0.0174
C(3)-C(4)	1.3991	1.4029	-0.0038
C(3)-O(13)	1.3795	1.2448	0.1347
C(4)-C(5)	1.3890	1.4007	-0.0117
C(4)-O(14)	1.3722	1.2447	0.1275
C(5)-C(6)	1.3849	1.3961	-0.0112
C(7)-C(8)	1.5390	1.5596	-0.0206
C(7)-H(19)	1.0077	1.1073	-0.0996
C(7)-H(20)	0.8963	1.1069	-0.2106
C(8)-C(9)	1.5267	1.5377	-0.0110
C(8)-C(10)	1.5374	1.4999	0.0375
C(8)-N+(15)	1.5056	1.5153	-0.0097
C(10)-O(11)	1.2304	1.2123	0.0181
C(10)-O(12)	1.2800	1.3642	-0.0842
O(12)-H(29)	1.1000	0.9736	0.1264
O(13)-H(24)	0.7702	0.9602	-0.1900
O(14)-H(25)	0.8160	0.9601	-0.1441
N+(15)-H(26)	0.9060	1.0203	-0.1143
N+(15)-H(27)	0.8897	1.0194	-0.1297
N+(15)-H(28)	0.9034	1.0190	-0.1156

RMS value: 0.0967

Bond angles begin on next page.

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(2)-C(1)-C(6)	118.654	118.821	-0.167
C(2)-C(1)-C(7)	121.250	120.711	0.539
C(6)-C(1)-C(7)	120.075	120.467	-0.392
C(1)-C(2)-C(3)	121.527	120.850	0.677
C(2)-C(3)-C(4)	119.408	119.777	-0.369
C(2)-C(3)-O(13)	123.276	121.197	2.079
C(4)-C(3)-O(13)	117.309	119.025	-1.716
C(3)-C(4)-C(5)	119.157	119.532	-0.375
C(3)-C(4)-O(14)	117.724	119.143	-1.419
C(5)-C(4)-O(14)	123.119	121.323	1.796
C(4)-C(5)-C(6)	120.732	120.310	0.422
C(1)-C(6)-C(5)	120.486	120.657	-0.171
C(1)-C(7)-C(8)	115.495	112.918	2.577
C(1)-C(7)-H(19)	107.223	109.014	-1.791
C(1)-C(7)-H(20)	112.282	109.577	2.705
C(8)-C(7)-H(19)	109.997	109.276	0.721
C(8)-C(7)-H(20)	106.291	110.255	-3.964
H(19)-C(7)-H(20)	105.079	105.527	-0.448
C(7)-C(8)-C(9)	110.362	109.258	1.104
C(7)-C(8)-C(10)	112.161	111.892	0.269
C(7)-C(8)-N+(15)	108.427	108.773	-0.346
C(9)-C(8)-C(10)	110.220	110.575	-0.355
C(9)-C(8)-N+(15)	107.364	107.602	-0.238
C(10)-C(8)-N+(15)	108.146	108.627	-0.481
C(8)-C(10)-O(11)	118.651	123.628	-4.977
C(8)-C(10)-O(12)	115.221	113.561	1.660
O(11)-C(10)-O(12)	126.079	122.812	3.267
C(10)-O(12)-H(29)	115.221	108.445	6.776
C(3)-O(13)-H(24)	109.811	110.808	-0.997
C(4)-O(14)-H(25)	112.498	110.721	1.777
C(8)-N+(15)-H(26)	115.486	110.513	4.973
C(8)-N+(15)-H(27)	111.293	111.535	-0.242
C(8)-N+(15)-H(28)	110.524	114.667	-4.143
H(26)-N+(15)-H(27)	99.864	104.764	-4.900
H(26)-N+(15)-H(28)	107.269	107.454	-0.185
H(27)-N+(15)-H(28)	111.989	107.344	4.645

RMS value: 2.501

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(2)-C(3)-C(4)	1.0	1.3	-0.3
C(1)-C(2)-C(3)-O(13)	180.0	-178.8	-1.2
C(1)-C(6)-C(5)-C(4)	-0.6	-0.3	-0.3
C(1)-C(7)-C(8)-C(9)	-169.7	-164.9	-4.8
C(1)-C(7)-C(8)-C(10)	67.0	72.3	-5.3
C(1)-C(7)-C(8)-N+(15)	-52.4	-47.7	-4.7
C(2)-C(1)-C(6)-C(5)	-0.6	2.2	-2.8
C(2)-C(1)-C(7)-C(8)	-85.1	-74.2	-10.9
C(2)-C(1)-C(7)-H(19)	151.9	164.2	-12.3
C(2)-C(1)-C(7)-H(20)	37.0	49.2	-12.2
C(2)-C(3)-C(4)-C(5)	-2.2	0.6	-2.8
C(2)-C(3)-C(4)-O(14)	177.7	-179.9	-2.4
C(2)-C(3)-O(13)-H(24)	0.1	-0.9	1.0
C(3)-C(2)-C(1)-C(6)	0.4	-2.7	3.1
C(3)-C(2)-C(1)-C(7)	-177.9	177.6	4.5
C(3)-C(4)-C(5)-C(6)	2.0	-1.1	3.1
C(3)-C(4)-O(14)-H(25)	174.8	-178.8	-6.4
C(4)-C(3)-O(13)-H(24)	179.1	179.1	0.0
C(5)-C(4)-C(3)-O(13)	178.8	-179.3	-1.9
C(5)-C(4)-O(14)-H(25)	-5.3	0.7	-6.0
C(5)-C(6)-C(1)-C(7)	177.7	-178.1	-4.2
C(6)-C(1)-C(7)-C(8)	96.6	106.1	-9.5
C(6)-C(1)-C(7)-H(19)	-26.4	-15.6	-10.8
C(6)-C(1)-C(7)-H(20)	-141.3	-130.6	-10.7
C(6)-C(5)-C(4)-O(14)	-177.9	179.4	2.7
C(7)-C(8)-C(10)-O(11)	-114.7	-115.6	0.9
C(7)-C(8)-C(10)-O(12)	67.7	64.5	3.2
C(7)-C(8)-N+(15)-H(26)	68.1	70.3	-2.2
C(7)-C(8)-N+(15)-H(27)	-179.0	-173.6	-5.4
C(7)-C(8)-N+(15)-H(28)	-53.9	-51.4	-2.5
C(8)-C(10)-O(12)-H(29)	180.0	179.5	0.5
C(9)-C(8)-C(7)-H(19)	-48.2	-43.4	-4.8
C(9)-C(8)-C(7)-H(20)	65.1	72.2	-7.1
C(9)-C(8)-C(10)-O(11)	121.9	122.3	-0.4
C(9)-C(8)-C(10)-O(12)	-55.7	-57.6	1.9
C(9)-C(8)-N+(15)-H(26)	-172.7	-171.5	-1.2
C(9)-C(8)-N+(15)-H(27)	-59.8	-55.4	-4.4
C(9)-C(8)-N+(15)-H(28)	65.3	66.9	-1.6
C(10)-C(8)-C(7)-H(19)	-171.5	-166.1	-5.4

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(10)-C(8)-C(7)-H(20)	-58.3	-50.6	-7.7
C(10)-C(8)-N+(15)-H(26)	-53.8	-51.8	-2.0
C(10)-C(8)-N+(15)-H(27)	59.2	64.4	-5.2
C(10)-C(8)-N+(15)-H(28)	-175.7	-173.4	-2.3
O(11)-C(10)-C(8)-N+(15)	4.8	4.4	0.4
O(11)-C(10)-O(12)-H(29)	2.6	-0.3	2.9
O(12)-C(10)-C(8)-N+(15)	-172.8	-175.4	2.6
O(13)-C(3)-C(4)-O(14)	-1.3	0.1	-1.4
N+(15)-C(8)-C(7)-H(19)	69.1	73.8	-4.7
N+(15)-C(8)-C(7)-H(20)	-177.6	-170.6	-7.0
		RMS value:	5.2

Table 26. Captopril

I. Missing parameters

No missing parameters

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(2)	1.5250	1.5376	-0.0126
C(1)-S(10)	1.8270	1.8350	-0.008
C(2)-C(3)	1.5224	1.5436	-0.0212
C(2)-C(4)	1.5256	1.5351	-0.0095
C(2)-H(17)	1.1000	1.1114	-0.0114
C(3)-H(18)	1.1000	1.1087	-0.0087
C(4)-N(11)	1.3093	1.3876	-0.0783
C(4)-O(12)	1.2601	1.2201	0.04
C(5)-C(6)	1.4820	1.5231	-0.0411
C(5)-N(11)	1.4874	1.4817	0.0057
C(5)-H(21)	1.1000	1.1086	-0.0086
C(5)-H(22)	1.1000	1.1115	-0.0115
C(6)-C(7)	1.5082	1.5305	-0.0223
C(6)-H(23)	1.1000	1.1129	-0.0129
C(6)-H(24)	1.1000	1.115	-0.015
C(7)-C(8)	1.5086	1.5425	-0.0339
C(7)-H(25)	1.1000	1.1116	-0.0116
C(7)-H(26)	1.1000	1.1110	-0.011
C(8)-C(9)	1.5289	1.5107	0.0182
C(8)-N(11)	1.4815	1.4840	-0.0025
C(8)-H(27)	1.1000	1.1072	-0.0072
C(9)-O(13)	1.2990	1.3650	-0.066
C(9)-O(14)	1.2012	1.2136	-0.0124
S(10)-H(28)	1.1000	1.3424	-0.2424
O(13)-H(29)	1.1000	0.9736	0.1264
		RMS value:	0.0608

III. Bond angles

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(2)-C(1)-S(10)	112.132	112.259	-0.127
C(1)-C(2)-C(3)	112.492	110.734	1.758

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(2)-C(4)	108.355	110.769	-2.414
C(1)-C(2)-H(17)	107.478	107.319	0.159
C(3)-C(2)-C(4)	107.170	109.738	-2.568
C(3)-C(2)-H(17)	108.657	109.491	-0.834
C(4)-C(2)-H(17)	112.771	108.730	4.041
C(2)-C(3)-H(18)	112.492	111.954	0.538
C(2)-C(4)-N(11)	118.939	118.210	0.729
C(2)-C(4)-O(12)	121.598	120.244	1.354
N(11)-C(4)-O(12)	119.342	121.547	-2.205
C(6)-C(5)-N(11)	103.252	101.721	1.531
C(6)-C(5)-H(21)	118.912	110.385	8.527
C(6)-C(5)-H(22)	111.627	109.975	1.652
N(11)-C(5)-H(21)	118.913	114.599	4.314
N(11)-C(5)-H(22)	111.626	111.279	0.347
H(21)-C(5)-H(22)	92.429	108.699	-16.27
C(5)-C(6)-C(7)	106.910	104.463	2.447
C(5)-C(6)-H(23)	117.130	112.339	4.791
C(5)-C(6)-H(24)	109.169	109.889	-0.72
C(7)-C(6)-H(23)	117.130	112.444	4.686
C(7)-C(6)-H(24)	109.169	109.653	-0.484
H(23)-C(6)-H(24)	96.555	108.017	-11.462
C(6)-C(7)-C(8)	107.283	104.775	2.508
C(6)-C(7)-H(25)	116.947	109.314	7.633
C(6)-C(7)-H(26)	108.921	111.965	-3.044
C(8)-C(7)-H(25)	116.948	111.141	5.807
C(8)-C(7)-H(26)	108.922	112.001	-3.079
H(25)-C(7)-H(26)	96.984	107.655	-10.671
C(7)-C(8)-C(9)	111.950	111.154	0.796
C(7)-C(8)-N(11)	104.215	104.059	0.156
C(7)-C(8)-H(27)	111.728	109.430	2.298
C(9)-C(8)-N(11)	110.611	110.629	-0.018
C(9)-C(8)-H(27)	105.467	110.851	-5.384
N(11)-C(8)-H(27)	113.040	110.522	2.518
C(8)-C(9)-O(13)	115.588	112.024	3.564
C(8)-C(9)-O(14)	122.517	126.309	-3.792
O(13)-C(9)-O(14)	121.885	121.664	0.221
C(1)-S(10)-H(28)	112.132	96.632	15.5
C(4)-N(11)-C(5)	127.046	125.712	1.334
C(4)-N(11)-C(8)	121.761	122.601	-0.84
C(5)-N(11)-C(8)	111.158	111.627	-0.469

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(9)-O(13)-H(29)	115.588	107.540	8.048

RMS value: 4.966

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(2)-C(3)-H(18)	-180.0	178.7	1.3
C(1)-C(2)-C(4)-N(11)	138.2	160.5	-22.3
C(1)-C(2)-C(4)-O(12)	-45.8	-19.4	-26.4
C(2)-C(1)-S(10)-H(28)	-180.0	-179.8	-0.2
C(2)-C(4)-N(11)-C(5)	-4.3	-6.1	1.8
C(2)-C(4)-N(11)-C(8)	173.3	177.0	-3.7
C(3)-C(2)-C(1)-S(10)	71.1	66.9	4.2
C(3)-C(2)-C(4)-N(11)	-100.1	-76.9	-23.2
C(3)-C(2)-C(4)-O(12)	75.8	103.2	-27.4
C(4)-C(2)-C(1)-S(10)	-170.6	-171.1	0.5
C(4)-C(2)-C(3)-H(18)	61.0	56.1	4.9
C(4)-N(11)-C(5)-C(6)	-159.0	-150.3	-8.7
C(4)-N(11)-C(5)-H(21)	-24.8	-31.2	6.4
C(4)-N(11)-C(5)-H(22)	80.9	92.6	-11.7
C(4)-N(11)-C(8)-C(7)	172.2	170.5	1.7
C(4)-N(11)-C(8)-C(9)	-67.3	-70.0	2.7
C(4)-N(11)-C(8)-H(27)	50.7	53.1	-2.4
C(5)-C(6)-C(7)-C(8)	22.0	33.0	-11
C(5)-C(6)-C(7)-H(25)	-111.7	-86.2	-25.5
C(5)-C(6)-C(7)-H(26)	139.7	154.6	-14.9
C(5)-N(11)-C(4)-O(12)	179.6	173.8	5.8
C(5)-N(11)-C(8)-C(7)	-9.8	-6.8	-3
C(5)-N(11)-C(8)-C(9)	110.7	112.6	-1.9
C(5)-N(11)-C(8)-H(27)	-131.3	-124.2	-7.1
C(6)-C(5)-N(11)-C(8)	23.1	27.0	-3.9
C(6)-C(7)-C(8)-C(9)	-127.0	-135.4	8.4
C(6)-C(7)-C(8)-N(11)	-7.4	-16.3	8.9
C(6)-C(7)-C(8)-H(27)	115.0	101.8	13.2
C(7)-C(6)-C(5)-N(11)	-26.9	-36.1	9.2
C(7)-C(6)-C(5)-H(21)	-161.2	-158.1	-3.1
C(7)-C(6)-C(5)-H(22)	93.1	81.9	11.2
C(7)-C(8)-C(9)-O(13)	-82.4	-131.8	49.4
C(7)-C(8)-C(9)-O(14)	98.8	48.8	50

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(8)-C(7)-C(6)-H(23)	155.7	155.1	0.6
C(8)-C(7)-C(6)-H(24)	-96.0	-84.8	-11.2
C(8)-C(9)-O(13)-H(29)	180.0	-178.2	-1.8
C(8)-N(11)-C(4)-O(12)	-2.7	-3.1	0.4
C(8)-N(11)-C(5)-H(21)	157.4	146.1	11.3
C(8)-N(11)-C(5)-H(22)	-96.9	-90.1	-6.8
C(9)-C(8)-C(7)-H(25)	6.7	-17.4	24.1
C(9)-C(8)-C(7)-H(26)	115.2	103.0	12.2
S(10)-C(1)-C(2)-H(17)	-48.4	-52.5	4.1
N(11)-C(4)-C(2)-H(17)	19.4	42.8	-23.4
N(11)-C(5)-C(6)-H(23)	-160.7	-158.2	-2.5
N(11)-C(5)-C(6)-H(24)	91.0	81.5	9.5
N(11)-C(8)-C(7)-H(25)	126.2	101.7	24.5
N(11)-C(8)-C(7)-H(26)	-125.2	-137.9	12.7
N(11)-C(8)-C(9)-O(13)	161.9	113.1	48.8
N(11)-C(8)-C(9)-O(14)	-17.0	-66.3	49.3
O(12)-C(4)-C(2)-H(17)	-164.7	-137.1	-27.6
O(13)-C(9)-C(8)-H(27)	39.3	-9.9	49.2
O(14)-C(9)-C(8)-H(27)	-139.5	170.8	50
O(14)-C(9)-O(13)-H(29)	-1.2	1.2	-2.4
H(17)-C(2)-C(3)-H(18)	-61.1	-63.1	2
H(21)-C(5)-C(6)-H(23)	65.1	79.7	-14.6
H(21)-C(5)-C(6)-H(24)	-43.2	-40.6	-2.6
H(22)-C(5)-C(6)-H(23)	-40.6	-40.2	-0.4
H(22)-C(5)-C(6)-H(24)	-148.9	-160.5	11.6
H(23)-C(6)-C(7)-H(25)	22.0	35.9	-13.9
H(23)-C(6)-C(7)-H(26)	-86.5	-83.3	-3.2
H(24)-C(6)-C(7)-H(25)	130.3	156.1	-25.8
H(24)-C(6)-C(7)-H(26)	21.8	36.9	-15.1
H(25)-C(7)-C(8)-H(27)	-111.4	-140.2	28.8
H(26)-C(7)-C(8)-H(27)	-2.8	-19.7	16.9
		RMS value:	19.7

Table 27. Fosinopril

I. Missing parameters

A. Missing for atoms 7-26-6-1 (type 75-1-159-153)
Missing for atoms 1-16-15-4 (type 153-1-3-79)
Missing for atoms 1-16-15-9 (type 153-1-3-9)
Missing for atoms 15-16-1-5 (type 3-1-153-7)
Missing for atoms 15-16-1-6 (type 3-1-153-159)
Missing for atoms 6-27-7-31 (type 159-1-75-3)
Missing for atoms 15-16-1-17 (type 3-1-153-1)

B. Estimated Parameters

7 torsional parameters are read in

Atom type numbers				V1	V2	V3
75	1	159	153	0.0000	0.0000	0.2000
153	1	3	79	0.0000	0.1600	0.0900
153	1	3	9	0.0000	0.1600	0.0900
3	1	153	7	0.0000	0.0000	0.2700
3	1	153	159	0.0000	0.0000	0.2700
159	1	75	3	0.0000	0.0000	0.2000
3	1	153	1	0.0000	0.0000	0.2700

1 bending parameter is read in

Atom type numbers			KB	Theta
3	1	153	0.6950	109.5000

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
P(1)-O(5)	1.4610	1.4774	-0.0164
P(1)-O(6)	1.6061	1.6231	-0.017
P(1)-C(16)	1.8110	1.8187	-0.0077
P(1)-C(17)	1.7739	1.8196	-0.0457
O(2)-C(14)	1.2494	1.2547	-0.0053
O(3)-C(14)	1.2323	1.2555	-0.0232
O(4)-C(15)	1.2904	1.2194	0.071
O(6)-C(27)	1.4296	1.4335	-0.0039
O(7)-C(27)	1.4136	1.4449	-0.0313
O(7)-C(31)	1.3331	1.3592	-0.0261
N(9)-C(10)	1.4859	1.4857	0.0002
N(9)-C(13)	1.4670	1.4787	-0.0117

	Length		Difference
Bond	Crystal	MM3	(in Å)
N(9)-C(15)	1.2864	1.3855	-0.0991
C(10)-C(11)	1.5163	1.5309	-0.0146
C(10)-C(14)	1.5279	1.5433	-0.0154
C(10)-H(40)	0.9619	1.1084	-0.1465
C(11)-C(12)	1.5163	1.5354	-0.0191
C(11)-H(41)	0.9618	1.1127	-0.1509
C(11)-H(42)	0.9486	1.1101	-0.1615
C(12)-C(13)	1.5202	1.5294	-0.0092
C(12)-C(34)	1.5476	1.5397	0.0079
C(12)-H(43)	0.9692	1.1165	-0.1473
C(13)-H(44)	0.9684	1.1117	-0.1433
C(13)-H(45)	0.9695	1.1109	-0.1414
C(15)-C(16)	1.4761	1.5253	-0.0492
C(16)-H(46)	0.9687	1.1101	-0.1414
C(16)-H(47)	0.9646	1.1096	-0.145
C(17)-C(18)	1.4876	1.5352	-0.0476
C(18)-C(19)	1.5466	1.5371	0.0095
C(19)-C(20)	1.4984	1.5485	-0.0501
C(20)-C(21)	1.5461	1.5106	0.0355
C(21)-C(22)	1.4049	1.4033	0.0016
C(21)-C(26)	1.3636	1.4003	-0.0367
C(22)-C(23)	1.3818	1.3952	-0.0134
C(22)-H(56)	1.0001	1.1031	-0.103
C(26)-H(60)	0.9636	1.1033	-0.1397
C(27)-C(28)	1.5019	1.5315	-0.0296
C(27)-H(61)	0.9614	1.1070	-0.1456
C(28)-C(29)	1.5374	1.5359	0.0015
C(28)-C(30)	1.5412	1.5359	0.0053
C(31)-C(32)	1.5040	1.4964	0.0076
C(32)-C(33)	1.4256	1.5252	-0.0996
C(32)-H(70)	0.9775	1.1122	-0.1347
C(34)-C(35)	1.5026	1.5437	-0.0411
C(34)-C(39)	1.5317	1.5438	-0.0121
C(35)-C(36)	1.5324	1.5359	-0.0035
C(36)-C(37)	1.5263	1.5339	-0.0076
C(37)-C(38)	1.4818	1.5338	-0.052
C(38)-C(39)	1.5117	1.5358	-0.0241
C(39)-H(84)	0.9588	1.1143	-0.1555

RMS value: 0.0793

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
O(5)-P(1)-O(6)	115.855	114.428	1.427
O(5)-P(1)-C(16)	113.170	115.837	-2.667
O(5)-P(1)-C(17)	111.506	114.318	-2.812
O(6)-P(1)-C(16)	98.131	100.564	-2.433
O(6)-P(1)-C(17)	106.914	102.140	4.774
C(16)-P(1)-C(17)	110.407	107.864	2.543
P(1)-O(6)-C(27)	126.333	125.277	1.056
C(27)-O(7)-C(31)	117.886	117.141	0.745
C(10)-N(9)-C(13)	111.794	111.650	0.144
C(10)-N(9)-C(15)	126.054	125.315	0.739
C(13)-N(9)-C(15)	122.084	122.190	-0.106
N(9)-C(10)-C(11)	102.012	103.363	-1.351
N(9)-C(10)-C(14)	113.330	113.348	-0.018
N(9)-C(10)-H(40)	114.500	111.000	3.5
C(11)-C(10)-C(14)	111.184	111.154	0.03
C(11)-C(10)-H(40)	113.337	108.732	4.605
C(14)-C(10)-H(40)	102.852	109.075	-6.223
C(10)-C(11)-C(12)	105.106	104.879	0.227
C(10)-C(11)-H(41)	110.354	109.563	0.791
C(10)-C(11)-H(42)	111.585	112.339	-0.754
C(12)-C(11)-H(41)	109.544	109.558	-0.014
C(12)-C(11)-H(42)	111.701	112.847	-1.146
H(41)-C(11)-H(42)	108.522	107.620	0.902
C(11)-C(12)-C(13)	102.914	102.515	0.399
C(11)-C(12)-C(34)	115.450	114.187	1.263
C(11)-C(12)-H(43)	109.947	108.526	1.421
C(13)-C(12)-C(34)	114.734	114.048	0.686
C(13)-C(12)-H(43)	111.705	108.456	3.249
C(34)-C(12)-H(43)	102.324	108.787	-6.463
N(9)-C(13)-C(12)	104.356	103.465	0.891
N(9)-C(13)-H(44)	110.644	110.844	-0.2
N(9)-C(13)-H(45)	111.691	112.341	-0.65
C(12)-C(13)-H(44)	111.411	110.311	1.1
C(12)-C(13)-H(45)	112.597	111.402	1.195
H(44)-C(13)-H(45)	106.251	108.441	-2.19
O(2)-C(14)-O(3)	124.385	125.243	-0.858
O(2)-C(14)-C(10)	119.627	118.020	1.607
O(3)-C(14)-C(10)	115.959	116.736	-0.777
O(4)-C(15)-N(9)	120.264	122.112	-1.848

Bond	Crystal	MM3	Difference (in degrees)
O(4)-C(15)-C(16)	117.599	121.742	-4.143
N(9)-C(15)-C(16)	122.134	116.117	6.017
P(1)-C(16)-C(15)	112.800	114.680	-1.88
P(1)-C(16)-H(46)	108.928	106.916	2.012
P(1)-C(16)-H(47)	109.005	108.449	0.556
C(15)-C(16)-H(46)	109.894	108.846	1.048
C(15)-C(16)-H(47)	109.369	109.928	-0.559
H(46)-C(16)-H(47)	106.653	107.777	-1.124
P(1)-C(17)-C(18)	117.934	114.891	3.043
C(17)-C(18)-C(19)	112.703	111.993	0.71
C(18)-C(19)-C(20)	112.125	112.380	-0.255
C(19)-C(20)-C(21)	113.841	111.767	2.074
C(20)-C(21)-C(22)	117.769	120.825	-3.056
C(20)-C(21)-C(26)	120.628	120.257	0.371
C(22)-C(21)-C(26)	121.299	118.915	2.384
C(21)-C(22)-C(23)	119.370	120.537	-1.167
C(21)-C(22)-H(56)	120.997	119.861	1.136
C(23)-C(22)-H(56)	119.632	119.602	0.03
C(21)-C(26)-H(60)	120.264	119.830	0.434
O(6)-C(27)-O(7)	108.392	107.060	1.332
O(6)-C(27)-C(28)	113.700	112.841	0.859
O(6)-C(27)-H(61)	107.479	108.074	-0.595
O(7)-C(27)-C(28)	107.397	109.276	-1.879
O(7)-C(27)-H(61)	111.435	111.038	0.397
C(28)-C(27)-H(61)	108.493	108.565	-0.072
C(27)-C(28)-C(29)	110.196	110.711	-0.515
C(27)-C(28)-C(30)	110.506	110.594	-0.088
C(29)-C(28)-C(30)	108.935	109.443	-0.508
O(7)-C(31)-C(32)	112.661	111.141	1.52
C(31)-C(32)-C(33)	117.843	112.951	4.892
C(31)-C(32)-H(70)	108.806	109.138	-0.332
C(33)-C(32)-H(70)	109.337	109.335	0.002
C(12)-C(34)-C(35)	112.976	110.988	1.988
C(12)-C(34)-C(39)	111.851	110.927	0.924
C(35)-C(34)-C(39)	111.311	109.243	2.068
C(34)-C(35)-C(36)	112.290	112.147	0.143
C(35)-C(36)-C(37)	109.986	111.314	-1.328
C(36)-C(37)-C(38)	112.187	110.751	1.436
C(37)-C(38)-C(39)	112.026	111.280	0.746
C(34)-C(39)-C(38)	111.707	112.142	-0.435

Bond	Crystal	MM3	Difference (in degrees)
C(34)-C(39)-H(84)	111.505	109.606	1.899
C(38)-C(39)-H(84)	110.360	109.302	1.058

RMS value: 6.637

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
P(1)-O(6)-C(27)-O(7)	55.0	48.2	6.8
P(1)-O(6)-C(27)-C(28)	-64.3	-72.1	7.8
P(1)-O(6)-C(27)-H(61)	175.6	167.8	7.8
P(1)-C(16)-C(15)-O(4)	-47.0	0.2	-47.2
P(1)-C(16)-C(15)-N(9)	133.5	178.3	-44.8
P(1)-C(17)-C(18)-C(19)	174.1	169.9	4.2
O(2)-C(14)-C(10)-N(9)	-11.4	-72.1	60.7
O(2)-C(14)-C(10)-C(11)	102.9	43.8	59.1
O(2)-C(14)-C(10)-H(40)	-135.5	163.7	61.8
O(3)-C(14)-C(10)-N(9)	170.5	108.1	62.4
O(3)-C(14)-C(10)-C(11)	-75.3	-136.0	60.7
O(3)-C(14)-C(10)-H(40)	46.3	-16.1	62.4
O(4)-C(15)-N(9)-C(10)	177.6	-162.2	20.2
O(4)-C(15)-N(9)-C(13)	0.9	6.4	-5.5
O(4)-C(15)-C(16)-H(46)	-168.8	-119.5	-49.3
O(4)-C(15)-C(16)-H(47)	74.4	122.7	-48.3
O(5)-P(1)-O(6)-C(27)	30.8	16.5	14.3
O(5)-P(1)-C(16)-C(15)	-52.4	-63.0	10.6
O(5)-P(1)-C(16)-H(46)	69.9	57.7	12.2
O(5)-P(1)-C(16)-H(47)	-174.1	173.7	12.2
O(5)-P(1)-C(17)-C(18)	177.7	-171.7	-10.6
O(6)-P(1)-C(16)-C(15)	-175.1	173.1	11.8
O(6)-P(1)-C(16)-H(46)	-52.8	-66.2	13.4
O(6)-P(1)-C(16)-H(47)	63.2	49.8	13.4
O(6)-P(1)-C(17)-C(18)	-54.8	-47.5	-7.3
O(6)-C(27)-O(7)-C(31)	94.7	79.8	14.9
O(6)-C(27)-C(28)-C(29)	-55.2	-58.1	2.9
O(6)-C(27)-C(28)-C(30)	-175.6	-179.6	4
O(7)-C(27)-C(28)-C(29)	-175.1	-177.1	2
O(7)-C(27)-C(28)-C(30)	64.5	61.4	3.1
O(7)-C(31)-C(32)-C(33)	-179.7	175.0	5.3
O(7)-C(31)-C(32)-H(70)	-54.6	-63.1	8.5

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
N(9)-C(10)-C(11)-C(12)	31.8	25.9	5.9
N(9)-C(10)-C(11)-H(41)	-86.3	-91.6	5.3
N(9)-C(10)-C(11)-H(42)	153.0	148.8	4.2
N(9)-C(13)-C(12)-C(11)	28.3	33.8	-5.5
N(9)-C(13)-C(12)-C(34)	154.5	157.8	-3.3
N(9)-C(13)-C(12)-H(43)	-89.6	-80.8	-8.8
N(9)-C(15)-C(16)-H(46)	11.7	58.6	-46.9
N(9)-C(15)-C(16)-H(47)	-105.0	-59.2	-45.8
C(10)-N(9)-C(13)-C(12)	-8.9	-18.8	9.9
C(10)-N(9)-C(13)-H(44)	111.0	99.5	11.5
C(10)-N(9)-C(13)-H(45)	-130.9	-139.0	8.1
C(10)-N(9)-C(15)-C(16)	-2.9	19.8	-22.7
C(10)-C(11)-C(12)-C(13)	-37.8	-37.4	-0.4
C(10)-C(11)-C(12)-C(34)	-163.6	-161.3	-2.3
C(10)-C(11)-C(12)-H(43)	81.3	77.2	4.1
C(11)-C(10)-N(9)-C(13)	-14.1	-4.4	-9.7
C(11)-C(10)-N(9)-C(15)	168.9	165.2	3.7
C(11)-C(12)-C(13)-H(44)	-91.2	-84.8	-6.4
C(11)-C(12)-C(13)-H(45)	149.6	154.7	-5.1
C(11)-C(12)-C(34)-C(35)	-64.7	-60.8	-3.9
C(11)-C(12)-C(34)-C(39)	168.7	177.6	-8.9
C(12)-C(11)-C(10)-C(14)	-89.3	-96.0	6.7
C(12)-C(11)-C(10)-H(40)	155.4	143.9	11.5
C(12)-C(13)-N(9)-C(15)	168.2	171.2	-3
C(12)-C(34)-C(35)-C(36)	-179.7	-177.9	-1.8
C(12)-C(34)-C(39)-C(38)	179.9	178.0	1.9
C(12)-C(34)-C(39)-H(84)	55.9	56.4	-0.5
C(13)-N(9)-C(10)-C(14)	105.5	116.0	-10.5
C(13)-N(9)-C(10)-H(40)	-136.9	-120.8	-16.1
C(13)-N(9)-C(15)-C(16)	-179.7	-171.6	-8.1
C(13)-C(12)-C(11)-H(41)	80.8	80.1	0.7
C(13)-C(12)-C(11)-H(42)	-159.0	-160.0	1
C(13)-C(12)-C(34)-C(35)	175.8	-178.2	-6
C(13)-C(12)-C(34)-C(39)	49.3	60.1	-10.8
C(14)-C(10)-N(9)-C(15)	-71.5	-74.4	2.9
C(14)-C(10)-C(11)-H(41)	152.6	146.5	6.1
C(14)-C(10)-C(11)-H(42)	31.9	26.9	5
C(15)-N(9)-C(10)-H(40)	46.1	48.8	-2.7
C(15)-N(9)-C(13)-H(44)	-71.8	-70.5	-1.3
C(15)-N(9)-C(13)-H(45)	46.3	51.0	-4.7

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(15)-C(16)-P(1)-C(17)	73.3	66.5	6.8
C(16)-P(1)-O(6)-C(27)	151.5	141.3	10.2
C(16)-P(1)-C(17)-C(18)	50.9	57.9	-7
C(17)-P(1)-O(6)-C(27)	-94.2	-107.6	13.4
C(17)-P(1)-C(16)-H(46)	-164.4	-172.7	8.3
C(17)-P(1)-C(16)-H(47)	-48.3	-56.7	8.4
C(17)-C(18)-C(19)-C(20)	167.3	-176.8	-15.9
C(18)-C(19)-C(20)-C(21)	178.7	176.2	2.5
C(19)-C(20)-C(21)-C(22)	66.0	93.5	-27.5
C(19)-C(20)-C(21)-C(26)	-120.2	-87.1	-33.1
C(20)-C(21)-C(22)-C(23)	174.2	179.6	-5.4
C(20)-C(21)-C(22)-H(56)	-6.1	-0.6	-5.5
C(20)-C(21)-C(26)-H(60)	15.8	0.6	15.2
C(22)-C(21)-C(26)-H(60)	-170.7	-180.0	9.3
C(23)-C(22)-C(21)-C(26)	0.5	0.2	0.3
C(26)-C(21)-C(22)-H(56)	-179.8	-180.0	0.2
C(27)-O(7)-C(31)-C(32)	179.6	-177.9	-2.5
C(28)-C(27)-O(7)-C(31)	-142.1	-157.7	15.6
C(29)-C(28)-C(27)-H(61)	64.3	61.6	2.7
C(30)-C(28)-C(27)-H(61)	-56.1	-59.9	3.8
C(31)-O(7)-C(27)-H(61)	-23.4	-37.9	14.5
C(34)-C(12)-C(11)-H(41)	-45.0	-43.7	-1.3
C(34)-C(12)-C(11)-H(42)	75.3	76.1	-0.8
C(34)-C(12)-C(13)-H(44)	35.1	39.2	-4.1
C(34)-C(12)-C(13)-H(45)	-84.2	-81.3	-2.9
C(34)-C(35)-C(36)-C(37)	53.6	56.3	-2.7
C(34)-C(39)-C(38)-C(37)	-54.5	-56.3	1.8
C(35)-C(34)-C(12)-H(43)	54.7	60.6	-5.9
C(35)-C(34)-C(39)-C(38)	52.5	55.4	-2.9
C(35)-C(34)-C(39)-H(84)	-71.5	-66.2	-5.3
C(35)-C(36)-C(37)-C(38)	-54.8	-55.3	0.5
C(36)-C(35)-C(34)-C(39)	-52.9	-55.3	2.4
C(36)-C(37)-C(38)-C(39)	56.2	55.3	0.9
C(37)-C(38)-C(39)-H(84)	70.1	65.4	4.7
C(39)-C(34)-C(12)-H(43)	-71.9	-61.1	-10.8
H(40)-C(10)-C(11)-H(41)	37.4	26.4	11
H(40)-C(10)-C(11)-H(42)	-83.4	-93.2	9.8
H(41)-C(11)-C(12)-H(43)	-160.1	-165.3	5.2
H(42)-C(11)-C(12)-H(43)	-39.8	-45.4	5.6
H(43)-C(12)-C(13)-H(44)	150.9	160.6	-9.7

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
H(43)-C(12)-C(13)-H(45)	31.7	40.1	-8.4

RMS value: 19.8

Table 28. Timolol

I. Missing parameters

A. Missing for atoms 1-6-16-3 (type 42-37-161-41)
Missing for atoms 8-17-7-1 (type 40-2-37-42)
Missing for atoms 2-14-15-3 (type 6-1-1-41)
Missing for atoms 7-17-16-3 (type 37-2-161-41)
Missing for atoms 8-17-16-3 (type 40-2-161-41)
Missing for atoms 4-19-18-8 (type 6-1-1-40)
Missing for atoms 15-3-16-6 (type 1-41-161-37)
Missing for atoms 7-17-8-18 (type 37-2-40-1)
Missing for atoms 7-17-8-21 (type 37-2-40-1)
Missing for atoms 19-18-8-17 (type 1-1-40-2)
Missing for atoms 20-21-8-17 (type 1-1-40-2)
Missing for atoms 20-21-8-18 (type 1-1-40-1)
Missing for atoms 44-21-8-18 (type 5-1-40-1)
Missing for atoms 19-18-8-21 (type 1-1-40-1)
Missing for 18-8-21 (type 1-40-1) angle type 1
Missing for 6-16-3 (type 37-161-41) angle type 1
Missing for 19-18-8 (type 1-1-40) angle type 1
Missing for 20-21-8 (type 1-1-40) angle type 1

B. Estimated Parameters

12 torsional parameters are read in

Atom type numbers				V1	V2	V3
42	37	161	41	0.0000	11.6000	0.0000
40	2	37	42	0.0000	11.6000	0.0000
6	1	1	41	0.0000	0.0000	0.2700
37	2	161	41	0.0000	11.6000	0.0000
40	2	161	41	0.0000	11.6000	0.0000
6	1	1	40	0.0000	0.0000	0.2700
1	41	161	37	0.0000	11.6000	0.0000
37	2	40	1	0.0000	11.6000	0.0000
5	1	1	40	0.0000	11.6000	0.0000
1	1	40	2	0.0000	0.1600	0.0900
1	1	40	1	0.0000	0.1600	0.0900
5	1	40	1	0.0000	0.1600	0.0900

3 bending parameters are read in

Atom type numbers			Kb	Theta
1	40	1	0.6950	120.000
37	161	41	0.6950	120.000
1	1	40	0.6950	109.500

II. Bond lengths

Bond	Length		Difference
	Crystal	MM3	(in Å)
S(1)-N(6)	1.6539	1.6170	0.0369
S(1)-N(7)	1.6433	1.6360	0.0073
O(2)-C(14)	1.4203	1.4367	-0.0164
O(2)-H(23)	0.8034	0.9517	-0.1483
O(3)-C(15)	1.4406	1.4308	0.0098
O(3)-C(16)	1.3509	1.2194	0.1315
O(4)-C(19)	1.4132	1.4192	-0.0060
O(4)-C(20)	1.4144	1.4191	-0.0047
N(5)-C(9)	1.4949	1.4761	0.0188
N(5)-C(13)	1.4708	1.4689	0.0019
N(5)-H(22)	1.0458	1.0177	0.0281
N(6)-C(16)	1.3095	1.3245	-0.0150
N(7)-C(17)	1.3156	1.3368	-0.0212
N(8)-C(17)	1.3817	1.4073	-0.0256
N(8)-C(18)	1.4696	1.5027	-0.0331
N(8)-C(21)	1.4824	1.5026	-0.0202
C(9)-C(10)	1.5379	1.5407	-0.0028
C(9)-C(11)	1.5144	1.5386	-0.0242
C(9)-C(12)	1.5282	1.5379	-0.0097
C(13)-C(14)	1.5128	1.5324	-0.0196
C(14)-C(15)	1.5192	1.5321	-0.0129
C(14)-H(35)	1.1000	1.1205	-0.0205
C(15)-H(36)	1.1000	1.1138	-0.0138
C(15)-H(37)	1.1000	1.1137	-0.0137
C(16)-C(17)	1.4373	1.4880	-0.0507
C(18)-C(19)	1.5091	1.5283	-0.0192
C(18)-H(38)	1.1000	1.1116	-0.0116
C(18)-H(39)	1.1000	1.1134	-0.0134
C(19)-H(40)	1.1000	1.1107	-0.0107
C(19)-H(41)	1.1000	1.1175	-0.0175
C(20)-C(21)	1.4975	1.5306	-0.0331
C(20)-H(42)	1.1000	1.1177	-0.0177
C(20)-H(43)	1.1000	1.1108	-0.0108
C(21)-H(44)	1.1000	1.1109	-0.0109
C(21)-H(45)	1.1000	1.1109	-0.0109

RMS value: 0.0388

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
N(6)-S(1)-N(7)	98.823	99.303	-0.480
C(14)-O(2)-H(23)	105.772	106.439	-0.667
C(15)-O(3)-C(16)	116.811	116.084	0.727
C(19)-O(4)-C(20)	109.104	110.909	-1.805
C(9)-N(5)-C(13)	114.837	117.366	-2.529
C(9)-N(5)-H(22)	108.401	109.590	-1.189
C(13)-N(5)-H(22)	107.072	109.446	-2.374
S(1)-N(6)-C(16)	105.295	108.302	-3.007
S(1)-N(7)-C(17)	107.840	108.651	-0.811
C(17)-N(8)-C(18)	114.455	118.613	-4.158
C(17)-N(8)-C(21)	116.172	125.306	-9.134
C(18)-N(8)-C(21)	112.072	115.909	-3.837
N(5)-C(9)-C(10)	105.809	107.924	-2.115
N(5)-C(9)-C(11)	109.204	110.847	-1.643
N(5)-C(9)-C(12)	112.680	111.669	1.011
C(10)-C(9)-C(11)	110.064	107.799	2.265
C(10)-C(9)-C(12)	108.927	108.710	0.217
C(11)-C(9)-C(12)	110.064	109.771	0.293
N(5)-C(13)-C(14)	110.673	110.862	-0.189
O(2)-C(14)-C(13)	111.741	107.581	4.160
O(2)-C(14)-C(15)	108.060	107.854	0.206
O(2)-C(14)-H(35)	109.284	110.064	-0.780
C(13)-C(14)-C(15)	110.572	111.739	-1.167
C(13)-C(14)-H(35)	106.709	109.840	-3.131
C(15)-C(14)-H(35)	110.482	109.715	0.767
O(3)-C(15)-C(14)	107.045	108.426	-1.381
O(3)-C(15)-H(36)	117.064	110.082	6.982
O(3)-C(15)-H(37)	109.079	110.444	-1.365
C(14)-C(15)-H(36)	117.064	109.393	7.671
C(14)-C(15)-H(37)	109.079	110.054	-0.975
H(36)-C(15)-H(37)	96.710	108.433	-11.723
O(3)-C(16)-N(6)	122.159	124.639	-2.480
O(3)-C(16)-C(17)	121.750	122.282	-0.532
N(6)-C(16)-C(17)	116.090	113.074	3.016
N(7)-C(17)-N(8)	121.493	123.784	-2.291
N(7)-C(17)-C(16)	111.820	110.667	1.153
N(8)-C(17)-C(16)	126.639	125.547	1.092

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
N(8)-C(18)-C(19)	110.390	110.654	-0.264
N(8)-C(18)-H(38)	115.427	112.443	2.984
N(8)-C(18)-H(39)	106.880	108.386	-1.506
C(19)-C(18)-H(38)	115.426	109.059	6.367
C(19)-C(18)-H(39)	106.880	109.595	-2.715
H(38)-C(18)-H(39)	100.640	106.595	-5.955
O(4)-C(19)-C(18)	112.828	110.008	2.820
O(4)-C(19)-H(40)	114.229	108.733	5.496
O(4)-C(19)-H(41)	105.319	110.246	-4.927
C(18)-C(19)-H(40)	114.229	109.947	4.282
C(18)-C(19)-H(41)	105.319	111.040	-5.721
H(40)-C(19)-H(41)	103.581	106.790	-3.209
O(4)-C(20)-C(21)	112.392	110.685	1.707
O(4)-C(20)-H(42)	114.444	110.049	4.395
O(4)-C(20)-H(43)	105.596	108.664	-3.068
C(21)-C(20)-H(42)	114.445	110.843	3.602
C(21)-C(20)-H(43)	105.596	109.850	-4.254
H(42)-C(20)-H(43)	103.049	106.644	-3.595
N(8)-C(21)-C(20)	110.116	110.601	-0.485
N(8)-C(21)-H(44)	115.560	108.478	7.082
N(8)-C(21)-H(45)	107.058	113.317	-6.259
C(20)-C(21)-H(44)	115.561	109.725	5.836
C(20)-C(21)-H(45)	107.058	107.802	-0.744
H(44)-C(21)-H(45)	100.312	106.819	-6.507

RMS value: 2.748

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
S(1)-N(6)-C(16)-O(3)	176.6	-178.9	4.5
S(1)-N(6)-C(16)-C(17)	-3.8	0.3	-4.1
S(1)-N(7)-C(17)-N(8)	-179.4	-179.9	0.5
S(1)-N(7)-C(17)-C(16)	-1.7	0.5	-2.2
O(2)-C(14)-C(13)-N(5)	-75.7	-59.2	-16.5
O(2)-C(14)-C(15)-O(3)	81.6	64.4	17.2
O(2)-C(14)-C(15)-H(36)	-144.6	-175.5	30.9
O(2)-C(14)-C(15)-H(37)	-36.2	-56.5	20.3
O(3)-C(15)-C(14)-C(13)	-155.8	-177.5	21.7
O(3)-C(15)-C(14)-H(35)	-37.9	-55.5	17.6

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
O(3)-C(16)-C(17)-N(7)	-176.6	178.7	-4.7
O(3)-C(16)-C(17)-N(8)	0.9	-0.9	1.8
O(4)-C(19)-C(18)-N(8)	54.8	53.0	1.8
O(4)-C(19)-C(18)-H(38)	-172.0	177.2	-10.8
O(4)-C(19)-C(18)-H(39)	-61.0	-66.5	5.5
O(4)-C(20)-C(21)-N(8)	-56.7	-51.4	-5.3
O(4)-C(20)-C(21)-H(44)	76.5	68.2	8.3
O(4)-C(20)-C(21)-H(45)	-172.7	-175.8	3.1
N(5)-C(13)-C(14)-C(15)	163.9	-177.4	18.7
N(5)-C(13)-C(14)-H(35)	43.7	60.6	-16.9
N(6)-S(1)-N(7)-C(17)	-0.3	-0.3	0.0
N(6)-C(16)-O(3)-C(15)	10.9	-1.1	12.0
N(6)-C(16)-C(17)-N(7)	3.9	-0.6	4.5
N(6)-C(16)-C(17)-N(8)	-178.7	179.8	-1.5
N(7)-S(1)-N(6)-C(16)	2.4	-0.1	2.5
N(7)-C(17)-N(8)-C(18)	-5.7	-5.1	-0.6
N(7)-C(17)-N(8)-C(21)	-138.8	179.9	-41.3
N(8)-C(18)-C(19)-H(40)	-172.5	172.7	-14.8
N(8)-C(18)-C(19)-H(41)	-59.5	-69.3	9.8
N(8)-C(21)-C(20)-H(42)	76.1	71.0	5.1
N(8)-C(21)-C(20)-H(43)	-171.3	-171.4	0.1
C(9)-N(5)-C(13)-C(14)	-172.8	172.5	-14.7
C(10)-C(9)-N(5)-C(13)	174.4	179.9	-5.5
C(10)-C(9)-N(5)-H(22)	54.7	54.3	0.4
C(11)-C(9)-N(5)-C(13)	-67.2	-62.2	-5.0
C(11)-C(9)-N(5)-H(22)	173.1	172.2	0.9
C(12)-C(9)-N(5)-C(13)	55.4	60.5	-5.1
C(12)-C(9)-N(5)-H(22)	-64.2	-65.1	0.9
C(13)-C(14)-O(2)-H(23)	94.1	39.6	54.5
C(13)-C(14)-C(15)-H(36)	-22.1	-57.5	35.4
C(13)-C(14)-C(15)-H(37)	86.3	61.6	24.7
C(14)-C(13)-N(5)-H(22)	-52.4	-61.9	9.5
C(14)-C(15)-O(3)-C(16)	-179.1	179.4	-1.5
C(15)-O(3)-C(16)-C(17)	-168.6	179.7	-11.7
C(15)-C(14)-O(2)-H(23)	-144.0	160.3	-45.7
C(16)-O(3)-C(15)-H(36)	47.2	59.8	-12.6
C(16)-O(3)-C(15)-H(37)	-61.2	-59.9	-1.3
C(16)-C(17)-N(8)-C(18)	177.1	174.5	2.6
C(16)-C(17)-N(8)-C(21)	44.0	-0.5	44.5
C(17)-N(8)-C(18)-C(19)	175.3	141.8	33.5

	Omega (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(17)-N(8)-C(18)-H(38)	42.1	19.5	22.6
C(17)-N(8)-C(18)-H(39)	-68.8	-98.1	29.3
C(17)-N(8)-C(21)-C(20)	-175.1	-143.0	-32.1
C(17)-N(8)-C(21)-H(44)	51.7	96.6	-44.9
C(17)-N(8)-C(21)-H(45)	-59.0	-21.8	-37.2
C(18)-N(8)-C(21)-C(20)	50.8	41.9	8.9
C(18)-N(8)-C(21)-H(44)	-82.4	-78.5	-3.9
C(18)-N(8)-C(21)-H(45)	166.8	163.0	3.8
C(18)-C(19)-O(4)-C(20)	-59.8	-66.1	6.3
C(19)-O(4)-C(20)-C(21)	60.9	65.5	-4.6
C(19)-O(4)-C(20)-H(42)	-71.9	-57.4	-14.5
C(19)-O(4)-C(20)-H(43)	175.5	-173.8	10.7
C(19)-C(18)-N(8)-C(21)	-49.7	-42.8	-6.9
C(20)-O(4)-C(19)-H(40)	167.5	173.4	-5.9
C(20)-O(4)-C(19)-H(41)	54.6	56.7	-2.1
C(21)-N(8)-C(18)-H(38)	177.2	-165.0	17.8
C(21)-N(8)-C(18)-H(39)	66.2	77.4	-11.2
H(23)-O(2)-C(14)-H(35)	-23.7	-80.0	56.3
H(34)-C(13)-C(14)-H(35)	-72.0	-61.3	-10.7
H(35)-C(14)-C(15)-H(36)	95.8	64.6	31.2
H(35)-C(14)-C(15)-H(37)	-155.8	-176.4	20.6
H(38)-C(18)-C(19)-H(40)	-39.3	-63.1	23.8
H(38)-C(18)-C(19)-H(41)	73.6	54.8	18.8
H(39)-C(18)-C(19)-H(40)	71.6	53.2	18.4
H(39)-C(18)-C(19)-H(41)	-175.4	171.2	-13.4
H(42)-C(20)-C(21)-H(44)	-150.7	-169.4	18.7
H(42)-C(20)-C(21)-H(45)	-40.0	-53.4	13.4
H(43)-C(20)-C(21)-H(44)	-38.1	-51.8	13.7
H(43)-C(20)-C(21)-H(45)	72.6	64.2	8.4

RMS value: 19.6

Table 29. Dopamine

I. Missing parameters

No missing parameters

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(2)	1.4249	1.3979	0.0270
C(1)-C(6)	1.3870	1.3996	-0.0126
C(2)-C(3)	1.3917	1.4060	-0.0143
C(2)-O(10)	1.3610	1.2448	0.1162
C(3)-C(4)	1.3894	1.4032	-0.0138
C(3)-O(11)	1.3942	1.2450	0.1492
C(4)-C(5)	1.4086	1.3957	0.0129
C(5)-C(6)	1.3910	1.4008	-0.0098
C(6)-C(7)	1.5279	1.5110	0.0169
C(7)-C(8)	1.5090	1.5356	-0.0266
C(8)-N+(9)	1.5090	1.5172	-0.0082
N+(9)-H(19)	1.1000	1.0212	0.0788
N+(9)-H(20)	1.1000	1.0213	0.0787
N+(9)-H(21)	1.1000	1.0213	0.0787
O(10)-H(22)	1.1000	0.9589	0.1411
O(11)-H(23)	1.1000	0.9593	0.1407
		RMS value:	0.0777

III. Bond angles

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(2)-C(1)-C(6)	118.615	121.147	-2.532
C(1)-C(2)-C(3)	120.721	119.732	0.989
C(1)-C(2)-O(10)	117.297	117.836	-0.539
C(3)-C(2)-O(10)	121.982	122.432	-0.450
C(2)-C(3)-C(4)	120.178	119.295	0.883
C(2)-C(3)-O(11)	117.173	119.602	-2.429
C(4)-C(3)-O(11)	122.641	121.104	1.537
C(3)-C(4)-C(5)	119.060	120.414	-1.354
C(4)-C(5)-C(6)	121.013	120.601	0.412
C(1)-C(6)-C(5)	120.372	118.811	1.561
C(1)-C(6)-C(7)	119.406	120.149	-0.743

Bond	Theta (in degrees) Crystal	MM3		Difference (in degrees)
C(5)-C(6)-C(7)	120.190	121.038		-0.848
C(6)-C(7)-C(8)	110.693	111.140		-0.447
C(7)-C(8)-N+(9)	110.529	110.531		-0.002
C(8)-N+(9)-H(19)	110.529	111.550		-1.021
C(8)-N+(9)-H(20)	115.358	111.947		3.411
C(8)-N+(9)-H(21)	106.790	112.054		-5.264
H(19)-N+(9)-H(20)	115.358	107.026		8.332
H(19)-N+(9)-H(21)	106.791	107.108		-0.317
H(20)-N+(9)-H(21)	100.805	106.839		-6.034
C(2)-O(10)-H(22)	117.297	110.000		7.297
C(3)-O(11)-H(23)	117.173	110.260		6.913
			RMS value:	3.427

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3		Difference (in degrees)
C(1)-C(2)-C(3)-C(4)	-0.5	0.0		-0.5
C(1)-C(2)-C(3)-O(11)	178.5	-180.0		-1.5
C(1)-C(2)-O(10)-H(22)	180.0	179.8		0.2
C(1)-C(6)-C(5)-C(4)	-1.0	-0.3		-0.7
C(1)-C(6)-C(7)-C(8)	79.2	84.9		-5.7
C(2)-C(1)-C(6)-C(5)	2.1	0.5		1.6
C(2)-C(1)-C(6)-C(7)	-175.9	179.9		4.2
C(2)-C(3)-C(4)-C(5)	1.6	0.1		1.5
C(2)-C(3)-O(11)-H(23)	180.0	179.8		0.2
C(3)-C(2)-C(1)-C(6)	-1.3	-0.3		-1.0
C(3)-C(2)-O(10)-H(22)	0.1	-0.2		0.3
C(3)-C(4)-C(5)-C(6)	-0.9	0.1		-1.0
C(4)-C(3)-C(2)-O(10)	179.4	180.0		-0.6
C(4)-C(3)-O(11)-H(23)	-1.0	-0.1		-0.9
C(4)-C(5)-C(6)-C(7)	176.9	-179.7		-3.4
C(5)-C(4)-C(3)-O(11)	-177.3	-179.9		2.6
C(5)-C(6)-C(7)-C(8)	-98.8	-95.7		-3.1
C(6)-C(1)-C(2)-O(10)	178.8	179.7		-0.9
C(6)-C(7)-C(8)-N+(9)	174.2	-178.0		-7.8
C(7)-C(8)-N+(9)-H(19)	-180.0	-179.9		-0.1
C(7)-C(8)-N+(9)-H(20)	46.9	60.2		-13.3
C(7)-C(8)-N+(9)-H(21)	-64.2	-59.8		-4.4
O(10)-C(2)-C(3)-O(11)	-1.6	0.0		-1.6
			RMS value:	3.9

Table 30. Atenolol

I. Missing parameters

A. Missing for atoms 36-3-4-37 (type 41-1-1-6)

B. Estimated Parameters

1 torsional parameter is read in

Atom type numbers	V1	V2	V3
6 1 1 41	0.0000	0.0000	0.2700

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(9)	1.3597	1.3979	-0.0382
C(1)-C(13)	1.3849	1.4076	-0.0227
C(1)-C(14)	1.5145	1.5042	0.0103
C(2)-C(15)	1.1913	1.3390	-0.1477
C(2)-H(38)	1.1000	1.1022	-0.0022
C(2)-H(39)	1.1000	1.1016	-0.0016
C(3)-C(4)	1.5617	1.5303	0.0314
C(3)-O(36)	1.4231	1.4295	-0.0064
C(4)-(5)	1.3725	1.5276	-0.1551
C(4)-H(22)	1.0551	1.1155	-0.0604
C(4)-O(37)	1.4481	1.4418	0.0063
C(5)-N+(35)	1.6839	1.5085	0.1754
C(6)-C(7)	1.5126	1.5291	-0.0165
C(6)-C(8)	1.5020	1.5299	-0.0279
C(6)-H(27)	0.9554	1.1034	-0.1480
C(6)-N+(35)	1.4649	1.5152	-0.0503
C(9)-H(16)	0.9944	1.1030	-0.1086
C(11)-C(12)	1.3806	1.3992	-0.0186
C(12)-C(13)	1.3772	1.4024	-0.0252
C(12)-H(19)	0.8640	1.0998	-0.2358
C(13)-O(36)	1.3465	1.2259	0.1206
C(14)-C(15)	1.3699	1.5055	-0.1356
C(14)-H(33)	0.9292	1.1038	-0.1746
C(14)-H(34)	0.8249	1.1036	-0.2787
C(15)-H(41)	1.1000	1.1043	-0.0043
H(25)-N+(35)	1.1119	1.0166	0.0953
H(26)-N+(35)	0.9564	1.0337	-0.0773

Bond	Length Crystal	MM3		Difference (in Å)
O(37)-H(42)	1.1000	0.9453		0.1547
			RMS value =	0.1130

III. Bond angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(9)-C(1)-C(13)	118.676	119.855	-1.179
C(9)-C(1)-C(14)	120.879	119.841	1.038
C(13)-C(1)-C(14)	120.435	120.280	0.155
C(15)-C(2)-H(38)	147.128	120.921	26.207
C(15)-C(2)-H(39)	106.436	121.014	-14.578
H(38)-C(2)-H(39)	106.436	118.065	-11.629
C(4)-C(3)-O(36)	102.417	106.825	-4.408
C(3)-C(4)-C(5)	103.087	112.138	-9.051
C(3)-C(4)-H(22)	118.352	110.144	8.208
C(3)-C(4)-O(37)	106.527	110.368	-3.841
C(5)-C(4)-H(22)	100.947	110.138	-9.191
C(5)-C(4)-O(37)	107.472	104.118	3.354
H(22)-C(4)-O(37)	118.622	109.777	8.845
C(4)-C(5)-N+(35)	104.176	104.797	-0.621
C(7)-C(6)-C(8)	113.633	109.986	3.647
C(7)-C(6)-H(27)	118.210	109.331	8.879
C(7)-C(6)-N+(35)	110.492	112.078	-1.586
C(8)-C(6)-H(27)	109.131	108.797	0.334
C(8)-C(6)-N+(35)	107.687	111.273	-3.586
H(27)-C(6)-N+(35)	95.917	105.213	-9.296
C(1)-C(9)-H(16)	104.375	119.936	-15.561
C(11)-C(12)-C(13)	121.144	120.342	0.802
C(11)-C(12)-H(19)	118.997	117.455	1.542
C(13)-C(12)-H(19)	119.856	122.202	-2.346
C(1)-C(13)-C(12)	119.117	119.283	-0.166
C(1)-C(13)-O(36)	115.626	116.926	-1.300
C(12)-C(13)-O(36)	125.256	123.792	1.464
C(1)-C(14)-C(15)	119.680	107.005	12.675
C(1)-C(14)-H(33)	107.993	89.168	18.825
C(1)-C(14)-H(34)	113.226	163.756	-50.530
C(15)-C(14)-H(33)	106.198	163.582	-57.384
C(15)-C(14)-H(34)	116.569	89.101	27.468
H(33)-C(14)-H(34)	87.292	74.647	12.645
C(2)-C(15)-C(14)	147.127	123.789	23.338

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(2)-C(15)-H(41)	106.436	119.294	-12.858
C(14)-C(15)-H(41)	106.436	116.915	-10.479
C(5)-N+(35)-C(6)	124.578	116.967	7.611
C(5)-N+(35)-H(25)	107.345	110.569	-3.224
C(5)-N+(35)-H(26)	113.357	103.313	10.044
C(6)-N+(35)-H(25)	107.345	109.959	-2.614
C(6)-N+(35)-H(26)	106.523	109.503	-2.980
H(25)-N+(35)-H(26)	92.934	105.773	-12.839
C(3)-O(36)-C(13)	118.765	120.722	-1.957
C(4)-O(37)-H(42)	106.527	108.300	-1.773

RMS value = 15.297

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(13)-C(12)-C(11)	0.8	-0.2	1.0
C(1)-C(13)-C(12)-H(19)	-179.9	180.0	0.1
C(1)-C(13)-O(36)-C(3)	-178.7	179.7	1.6
C(1)-C(14)-C(15)-C(2)	-116.7	-79.7	-37.0
C(1)-C(14)-C(15)-H(41)	63.3	99.8	-36.5
C(2)-C(15)-C(14)-H(33)	5.7	90.1	-84.4
C(2)-C(15)-C(14)-H(34)	100.9	98.2	2.7
C(3)-C(4)-C(5)-N+(35)	169.6	-156.3	-34.1
C(3)-C(4)-O(37)-H(42)	-180.0	-58.8	-121.2
C(3)-O(36)-C(13)-C(12)	1.7	-0.3	2.0
C(4)-C(3)-O(36)-C(13)	-173.2	-179.4	6.2
C(4)-C(5)-N+(35)-C(6)	-58.4	-88.9	30.5
C(4)-C(5)-N+(35)-H(25)	175.1	144.2	30.9
C(4)-C(5)-N+(35)-H(26)	73.9	31.4	42.5
C(5)-C(4)-C(3)-O(36)	-78.3	-59.1	-19.2
C(5)-C(4)-O(37)-H(42)	70.1	-179.3	-110.6
C(5)-N+(35)-C(6)-C(7)	-46.9	-74.4	27.5
C(5)-N+(35)-C(6)-C(8)	-171.6	162.0	26.4
C(5)-N+(35)-C(6)-H(27)	76.1	44.3	31.8
C(7)-C(6)-N+(35)-H(25)	79.5	52.8	26.7
C(7)-C(6)-N+(35)-H(26)	178.1	168.6	9.5
C(8)-C(6)-N+(35)-H(25)	-45.1	-70.9	25.8
C(8)-C(6)-N+(35)-H(26)	53.4	45.0	8.4
C(9)-C(1)-C(13)-C(12)	-1.9	0.5	-2.4

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(9)-C(1)-C(13)-O(36)	178.5	-179.4	-2.1
C(9)-C(1)-C(14)-C(15)	67.4	93.4	-26.0
C(9)-C(1)-C(14)-H(33)	-54.2	-83.8	29.6
C(9)-C(1)-C(14)-H(34)	-149.1	-79.0	-70.1
C(11)-C(12)-C(13)-O(36)	-179.6	179.8	0.6
C(12)-C(13)-C(1)-C(14)	177.0	178.8	-1.8
C(13)-C(1)-C(9)-H(16)	166.6	179.3	-12.7
C(13)-C(1)-C(14)-C(15)	-111.5	-84.9	-26.6
C(13)-C(1)-C(14)-H(33)	127.0	98.0	29.0
C(13)-C(1)-C(14)-H(34)	32.1	102.8	-70.7
C(14)-C(1)-C(9)-H(16)	-12.3	1.1	-13.4
C(14)-C(1)-C(13)-O(36)	-2.6	-1.2	-1.4
C(14)-C(15)-C(2)-H(38)	180.0	179.5	0.5
C(14)-C(15)-C(2)-H(39)	0.0	-0.4	0.4
H(19)-C(12)-C(13)-O(36)	-0.3	0.0	-0.3
H(22)-C(4)-C(3)-O(36)	32.0	64.0	-32.0
H(22)-C(4)-C(5)-N+(35)	46.8	80.7	-33.9
H(22)-C(4)-O(37)-H(42)	-43.4	62.8	253.8
H(25)-N+(35)-C(6)-H(27)	-157.4	171.5	31.1
H(26)-N+(35)-C(6)-H(27)	-58.8	-72.7	13.9
H(33)-C(14)-C(15)-H(41)	-174.3	-90.4	-83.9
H(34)-C(14)-C(15)-H(41)	-79.1	-82.3	3.2
N+(35)-C(5)-C(4)-O(37)	-78.1	-37.0	-41.1
O(36)-C(3)-C(4)-O(37)	168.7	-174.7	-16.6
H(38)-C(2)-C(15)-H(41)	0.0	0.1	-0.1
H(39)-C(2)-C(15)-H(41)	-180.0	-179.9	-0.1
		RMS value =	52.2

Table 31. Phenyl-propanolamine

I. Missing parameters

No missing parameters

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(2)	1.5630	1.5433	0.0197
C(1)-C(4)	1.5166	1.5118	0.0048
C(1)-O(11)	1.4171	1.4395	-0.0224
C(1)-H(13)	1.1000	1.1146	-0.0146
C(2)-C(3)	1.5297	1.5234	0.0063
C(2)-N+(10)	1.5250	1.5181	0.0069
C(2)-H(14)	1.1000	1.1009	-0.0009
C(3)-O(12)	1.4255	1.4411	-0.0156
C(4)-C(5)	1.3825	1.4056	-0.0231
C(4)-C(9)	1.4059	1.4008	0.0051
C(5)-C(6)	1.3976	1.3943	0.0033
C(8)-C(9)	1.4157	1.3986	0.0171
C(9)-H(21)	1.1000	1.1033	-0.0033
N+(10)-H(22)	1.1000	1.0199	0.0801
N+(10)-H(23)	1.1000	1.0371	0.0629
N+(10)-H(24)	1.1000	1.0369	0.0631
O(11)-H(25)	1.1000	0.9461	0.1539
O(12)-H(26)	1.1000	0.9458	0.1542
		RMS value=	0.0597

III. Bond angles

	Theta (in degrees)		Difference
Bond	Crystal	MM3	(in degrees)
C(2)-C(1)-C(4)	108.914	111.566	-2.652
C(2)-C(1)-O(11)	104.944	104.277	0.667
C(2)-C(1)-H(13)	113.397	110.151	3.246
C(4)-C(1)-O(11)	111.344	111.504	-0.16
C(4)-C(1)-H(13)	107.235	110.374	-3.139
O(11)-C(1)-H(13)	111.054	108.786	2.268
C(1)-C(2)-C(3)	114.704	113.979	0.725
C(1)-C(2)-N+(10)	108.453	106.246	2.207
C(1)-C(2)-H(14)	106.611	110.950	-4.339

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(3)-C(2)-N+(10)	109.515	106.776	2.739
C(3)-C(2)-H(14)	105.484	112.123	-6.639
N+(10)-C(2)-H(14)	112.094	106.187	5.907
C(2)-C(3)-O(12)	116.311	105.057	11.254
C(1)-C(4)-C(5)	122.705	121.422	1.283
C(1)-C(4)-C(9)	116.974	119.864	-2.89
C(5)-C(4)-C(9)	120.288	118.648	1.64
C(4)-C(5)-C(6)	120.776	120.648	0.128
C(4)-C(9)-C(8)	118.085	120.686	-2.601
C(4)-C(9)-H(21)	120.957	120.404	0.553
C(8)-C(9)-H(21)	120.957	118.909	2.048
C(2)-N+(10)-H(22)	108.453	114.934	-6.481
C(2)-N+(10)-H(23)	116.376	105.039	11.337
C(2)-N+(10)-H(24)	108.148	106.266	1.882
H(22)-N+(10)-H-23	116.375	109.201	7.174
H(22)-N+(10)-H(24)	108.147	111.172	-3.025
H(23)-N+(10)-H(24)	98.346	109.994	-11.648
C(1)-O(11)-H(25)	104.944	107.615	-2.671
C(3)-O(12)-H(26)	116.311	107.716	8.595

RMS value= 5.161

IV. Dihedral angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(2)-C(3)-O(12)	-51.1	-86.4	35.3
C(1)-C(2)-N+(10)-H(22)	180.0	-146.4	33.6
C(1)-C(2)-N+(10)-H(23)	46.5	93.5	-47
C(1)-C(2)-N+(10)-H(24)	-62.9	-23.0	-39.9
C(1)-C(4)-C(5)-C(6)	177.6	-178.1	4.3
C(1)-C(4)-C(9)-C(8)	-177.5	178.2	-4.3
C(1)-C(4)-C(9)-H(21)	2.5	-1.5	4
C(2)-C(1)-C(4)-C(5)	-89.0	-83.7	-5.3
C(2)-C(1)-C(4)-C(9)	88.9	99.2	-10.3
C(2)-C(1)-O(11)-H(25)	-180.0	168.9	-11.1
C(2)-C(3)-O(12)-H(26)	180.0	169.6	10.4
C(3)-C(2)-C(1)-C(4)	-66.3	-91.0	24.7
C(3)-C(2)-C(1)-O(11)	174.4	148.5	25.9
C(3)-C(2)-C(1)-H(13)	53.0	31.9	21.1
C(3)-C(2)-N+(10)-H(22)	54.1	91.6	-37.5

Bond	Omega (in degrees) Crystal	MM3		Difference (in degrees)
C(3)-C(2)-N+(10)-H(23)	-79.3	-28.5		-50.8
C(3)-C(2)-N+(10)-H(24)	171.2	-145.0		43.8
C(4)-C(1)-C(2)-N+(10)	171.0	151.7		19.3
C(4)-C(1)-C(2)-H(14)	50.1	36.7		13.4
C(4)-C(1)-O(11)-H(25)	62.3	48.4		13.9
C(5)-C(4)-C(1)-O(11)	26.3	32.4		-6.1
C(5)-C(4)-C(1)-H(13)	148.0	153.4		-5.4
C(5)-C(4)-C(9)-C(8)	0.4	1.1		-0.7
C(5)-C(4)-C(9)-H(21)	-179.6	-178.6		-1
C(6)-C(5)-C(4)-C(9)	-0.2	-1.1		0.9
C(9)-C(4)-C(1)-O(11)	-155.8	-144.6		-11.2
C(9)-C(4)-C(1)-H(13)	-34.1	-23.6		-10.5
N+(10)-C(2)-C(1)-O(11)	51.6	31.2		20.4
N+(10)-C(2)-C(1)-H(13)	-69.7	-85.4		15.7
N+(10)-C(2)-C(3)-O(12)	71.1	30.6		40.5
O(11)-C(1)-C(2)-H(14)	-69.3	-83.8		14.5
O(12)-C(3)-C(2)-H(14)	-168.1	146.5		-45.4
H(13)-C(1)-C(2)-H(14)	169.4	159.6		9.8
H(13)-C(1)-O(11)-H(25)	-57.1	-73.5		16.4
H(14)-C(2)-N+(10)-H(22)	-62.6	-28.2		-34.4
H(14)-C(2)-N+(10)-H(23)	163.9	-148.3		47.8
H(14)-C(2)-N+(10)-H(24)	54.5	95.2		-40.7
			RMS value =	26.2

Table 32. Chlorimipramine

I. Missing parameters

A. Missing for atoms 4-17-2-14 (type 2-2-8-2).
Missing for atoms 13-14-2-17 (type 2-2-8-2).
Missing for atoms 16-17-2-14 (type 2-2-8-2).
Missing for atoms 15-14-2-17 (type 2-2-8-2).
Missing for angle 14-2-17 (type 2-8-2).

B. Estimated Parameters

1 torsional parameter is read in

Atom type numbers	V1	V2	V3
2 2 8 2	0.000	0.000	0.000

1 bending parameter is read in

Atom type numbers	Kb	Theta
2 8 2	0.695	110.000

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
Cl(1)-C(5)	1.7414	1.7313	0.0101
N(2)-C(14)	1.4305	1.3833	0.0472
N(2)-C(17)	1.4252	1.3887	0.0365
N(2)-C(18)	1.4692	1.4680	0.0012
N+(3)-C(20)	1.4843	1.5119	-0.0276
N+(3)-C(21)	1.4816	1.5049	-0.0233
N+(3)-C(22)	1.4796	1.5060	-0.0264
N+(3)-H(46)	0.9015	1.0196	-0.1181
C(4)-C(5)	1.3771	1.3932	-0.0161
C(4)-C(17)	1.3929	1.4062	-0.0133
C(5)-C(6)	1.3755	1.1019	0.2736
C(6)-C(7)	1.3723	1.3888	-0.0165
C(7)-C(16)	1.3871	1.3932	-0.0061
C(7)-H(25)	0.8934	1.4047	-0.5113
C(8)-C(9)	1.5250	1.5447	-0.0197
C(8)-C(16)	1.5123	1.5161	-0.0038
C(8)-H(26)	0.9003	1.1153	-0.2150
C(8)-H(27)	0.9990	1.1156	-0.1166
C(9)-C(15)	1.4864	1.5078	-0.0214
C(9)-H(28)	1.0077	1.1136	-0.1059
C(9)-H(29)	0.9777	1.1138	-0.1361

Bond	Length Crystal	MM3	Difference (in Å)
C(10)-C(11)	1.3830	1.3949	-0.0119
C(10)-C(15)	1.3958	1.3996	-0.0038
C(11)-C(12)	1.3666	1.3953	-0.0287
C(12)-C(13)	1.3731	1.3958	-0.0227
C(13)-C(14)	1.3938	1.4030	-0.0092
C(14)-C(15)	1.3932	1.4028	-0.0096
C(16)-C(17)	1.4167	1.4170	-0.0003
C(18)-C(19)	1.5036	1.5352	-0.0316
C(19)-C(20)	1.5226	1.5240	-0.0014
C(21)-H(40)	0.9426	1.1001	-0.1575
C(21)-H(41)	1.0508	1.0997	-0.0489
C(21)-H(42)	0.8995	1.1000	-0.2005
C(22)-H(43)	0.9766	1.0985	-0.1219
C(22)-H(44)	0.9576	1.0995	-0.1419
C(22)-H(45)	0.9481	1.0999	-0.1518

RMS value: 0.1264

III. Bond Angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(14)-N(2)-C(17)	117.745	112.715	5.030
C(14)-N(2)-C(18)	114.695	114.882	-0.187
C(17)-N(2)-C(18)	118.406	118.905	-0.499
C(20)-N^+(3)-C(21)	111.182	111.378	-0.196
C(20)-N^+(3)-C(22)	113.210	112.900	0.310
C(20)-N^+(3)-H(46)	104.896	107.617	-2.721
C(21)-N^+(3)-C(22)	110.622	110.905	-0.283
C(21)-N^+(3)-H(46)	112.689	106.784	5.905
C(22)-N^+(3)-H(46)	103.944	106.908	-2.964
C(5)-C(4)-C(17)	121.394	121.176	0.218
Cl(1)-C(5)-C(4)	118.988	118.129	0.859
Cl(1)-C(5)-C(6)	119.681	120.682	-1.001
C(4)-C(5)-C(6)	121.326	119.789	1.537
C(5)-C(6)-C(7)	116.959	119.911	-2.952
C(6)-C(7)-C(16)	124.632	120.299	4.333
C(6)-C(7)-H(25)	117.089	119.287	-2.198
C(16)-C(7)-H(25)	118.238	121.494	-3.256
C(9)-C(8)-C(16)	117.889	118.522	-0.633
C(9)-C(8)-H(26)	110.931	108.004	2.927

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(9)-C(8)-H(27)	111.028	107.831	3.197
C(16)-C(8)-H(26)	105.069	108.155	-3.086
C(16)-C(8)-H(27)	109.550	107.690	1.860
H(26)-C(8)-H(27)	100.884	105.976	-5.092
C(8)-C(9)-C(15)	110.815	110.990	-0.175
C(8)-C(9)-H(28)	106.188	110.231	-4.043
C(8)-C(9)-H(29)	107.294	109.504	-2.210
C(15)-C(9)-H(28)	109.779	109.970	-0.191
C(15)-C(9)-H(29)	112.537	110.166	2.371
H(28)-C(9)-H(29)	110.010	105.854	4.156
C(11)-C(10)-C(15)	122.173	120.247	1.926
C(10)-C(11)-C(12)	119.394	119.897	-0.503
C(11)-C(12)-C(13)	120.248	120.106	0.142
C(12)-C(13)-C(14)	120.566	120.381	0.185
N(2)-C(14)-C(13)	121.099	124.039	-2.940
N(2)-C(14)-C(15)	118.475	116.656	1.819
C(13)-C(14)-C(15)	120.391	119.293	1.098
C(9)-C(15)-C(10)	123.793	122.220	1.573
C(9)-C(15)-C(14)	118.938	117.705	1.233
C(10)-C(15)-C(14)	117.225	120.075	-2.850
C(7)-C(16)-C(8)	116.286	115.468	0.818
C(7)-C(16)-C(17)	117.200	119.086	-1.886
C(8)-C(16)-C(17)	126.504	125.386	1.118
N(2)-C(17)-C(4)	119.526	121.027	-1.501
N(2)-C(17)-C(16)	122.049	120.387	1.662
C(4)-C(17)-C(16)	118.425	118.585	-0.160
N(2)-C(18)-C(19)	113.585	113.075	0.510
C(18)-C(19)-C(20)	111.170	112.817	-1.647
N^+(3)-C(20)-C(19)	111.973	112.760	-0.787
N^+(3)-C(21)-H(40)	106.577	108.552	-1.975
N^+(3)-C(21)-H(41)	110.110	108.080	2.030
N^+(3)-C(21)-H(42)	103.067	108.492	-5.425
H(40)-C(21)-H(41)	110.892	110.738	0.154
H(40)-C(21)-H(42)	119.664	110.212	9.452
H(41)-C(21)-H(42)	106.103	110.685	-4.582
N^+(3)-C(22)-H(43)	110.447	109.025	1.422
N^+(3)-C(22)-H(44)	106.337	108.193	-1.856
N^+(3)-C(22)-H(45)	109.804	108.402	1.402
H(43)-C(22)-H(44)	107.977	110.719	-2.742
H(43)-C(22)-H(45)	108.493	109.912	-1.419

Bond	Theta (in degrees) Crystal	MM3		Difference (in degrees)
H(44)-C(22)-H(45)	113.755	110.528		3.227
			RMS value:	2.691

IV. Dihedral Angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
Cl(1)-C(5)-C(4)-C(17)	177.2	179.2	-2.0
Cl(1)-C(5)-C(4)-H(23)	-6.3	-2.1	-4.2
Cl(1)-C(5)-C(6)-C(7)	-177.7	178.9	3.4
N(2)-C(14)-C(13)-C(12)	177.7	179.1	-1.4
N(2)-C(14)-C(15)-C(9)	4.9	0.6	4.3
N(2)-C(14)-C(15)-C(10)	-177.4	-179.3	1.9
N(2)-C(17)-C(4)-C(5)	179.8	-176.7	3.5
N(2)-C(17)-C(4)-H(23)	3.6	4.6	-1.0
N(2)-C(17)-C(16)-C(7)	-177.7	176.8	5.5
N(2)-C(17)-C(16)C(8)	3.4	-6.2	9.6
N(2)-C(18)-C(19)-C(20)	71.2	52.1	19.1
N^{+}(3)-C(20)-C(19)-C(18)	167.6	-177.5	14.9
C(4)-C(5)-C(6)-C(7)	1.5	-0.9	2.4
C(4)-C(17)-N(2)-C(14)	-129.6	-111.9	-17.7
C(4)-C(17)-N(2)-C(18)	15.6	26.9	-11.3
C(4)-C(17)-C(16)-C(7)	2.0	-2.9	4.9
C(4)-C(17)-C(16)-C(8)	-176.9	174.1	-9.0
C(5)-C(4)-C(17)-C(16)	0.1	3.0	-2.9
C(5)-C(6)-C(7)-C(16)	0.8	0.9	-0.1
C(6)-C(5)-C(4)-C(17)	-1.9	-1.1	-0.8
C(6)-C(5)-C(4)-H(23)	174.5	177.7	-3.2
C(6)-C(7)-C(16)-C(8)	176.4	-176.3	7.3
C(6)-C(7)-C(16)-C(17)	-2.6	1.0	-3.6
C(7)-C(16)-C(8)-C(9)	-171.8	179.5	-8.7
C(7)-C(16)-C(8)-H(26)	-47.7	-57.3	9.6
C(7)-C(16)-C(8)-H(27)	60.0	56.9	3.1
C(8)-C(9)-C(15)-C(10)	-108.7	-100.2	-8.5
C(8)-C(9)-C(15)-C(14)	68.8	69.9	-1.1
C(9)-C(8)-C(16)-C(17)	7.1	2.4	4.7
C(9)-C(15)-C(10)-C(11)	177.2	-179.6	3.2
C(9)-C(15)-C(14)-C(13)	-177.2	179.4	-3.4
C(10)-C(11)-C(12)-C(13)	0.6	0.0	0.6
C(10)-C(15)-C(9)-H(28)	134.3	127.5	6.8
C(10)-C(15)-C(9)-H(29)	11.4	11.2	0.2

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(10)-C(15)-C(14)-C(13)	0.5	-0.5	1.0
C(11)-C(10)-C(15)-C(14)	-0.3	0.3	-0.6
C(11)-C(12)-C(13)-C(14)	-0.4	-0.2	-0.2
C(12)-C(11)-C(10)-C(15)	-0.2	-0.1	-0.1
C(12)-C(13)-C(14)-C(15)	-0.1	0.4	-0.5
C(13)-C(14)-N(2)-C(17)	109.1	100.8	8.3
C(13)-C(14)-N(2)-C(18)	-37.3	-39.7	2.4
C(14)-N(2)-C(17)-C(16)	50.1	68.4	-18.3
C(14)-N(2)-C(18)-C(19)	-142.5	-164.1	21.6
C(14)-C(15)-C(9)-H(28)	-48.2	-52.4	4.2
C(14)-C(15)-C(9)-H(29)	-171.1	-168.7	-2.4
C(15)-C(9)-C(8)-C(16)	-63.2	-54.5	-8.7
C(15)-C(9)-C(8)-H(26)	175.6	-177.8	6.6
C(15)-C(9)-C(8)-H(27)	64.3	68.0	-3.7
C(15)-C(14)-N(2)-C(17)	-73.0	-80.5	7.5
C(15)-C(14)-N(2)-C(18)	140.5	139.0	1.5
C(16)-C(8)-C(9)-H(28)	56.0	67.6	-11.6
C(16)-C(8)-C(9)-H(29)	173.6	-176.4	10.0
C(16)-C(17)-N(2)-C(18)	-164.7	-152.8	-11.9
C(16)-C(17)-C(4)-H(23)	-176.1	-175.7	-0.4
C(17)-N(2)-C(18)-C(19)	71.3	58.0	13.3
C(17)-C(16)-C(8)-H(26)	131.2	125.6	5.6
C(17)-C(16)-C(8)-H(27)	-121.2	-120.3	-0.9
C(19)-C(20)-N^+(3)-C(21)	-170.0	-163.3	-6.7
C(19)-C(20)-N^+(3)-C(22)	64.8	71.2	-6.4
C(19)-C(20)-N^+(3)-H(46)	-47.9	-46.6	-1.3
C(20)-N^+(3)-C(21)-H(40)	57.1	58.1	-1.0
C(20)-N^+(3)-C(21)-H(41)	-63.3	-62.1	-1.2
C(20)-N^+(3)-C(21)-H(42)	-176.1	177.9	-6.0
C(20)-N^+(3)-C(22)-H(43)	-62.4	-60.9	-1.5
C(20)-N^+(3)-C(22)-H(44)	54.5	59.6	-5.1
C(20)-N^+(3)-C(22)-H(45)	178.0	179.5	-1.5
C(21)-N^+(3)-C(22)-H(43)	172.0	173.3	-1.3
C(21)-N^+(3)-C(22)-H(44)	-71.1	-66.2	-4.9
C(21)-N^+(3)-C(22)-H(45)	52.4	53.7	-1.3
C(22)-N^+(3)-C(21)-H(40)	-176.2	-175.3	-0.9
C(22)-N^+(3)-C(21)-H(41)	63.4	64.6	-1.2
C(22)-N^+(3)-C(21)-H(42)	-49.4	-55.5	6.1
H(26)-C(8)-C(9)-H(28)	-65.2	-55.8	-9.4
H(26)-C(8)-C(9)-H(29)	52.4	60.3	-7.9

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
H(27)-C(8)-C(9)-H(28)	-176.5	-169.9	-6.6
H(27)-C(8)-C(9)-H(29)	-58.9	-53.8	-5.1
H(40)-C(21)-N^+(3)-H(46)	-60.4	-59.1	-1.3
H(41)-C(21)-N^+(3)-H(46)	179.3	-179.3	1.4
H(42)-C(21)-N^+(3)-H(46)	66.5	60.6	5.9
H(43)-C(22)-N^+(3)-H(46)	50.8	57.2	-6.4
H(44)-C(22)-N^+(3)-H(46)	167.7	177.7	-10.0
H(45)-C(22)-N^+(3)-H(46)	-68.8	-62.4	-6.4
		RMS value:	7.1

Table 33. Amoxapine

I. Missing parameters

A. Missing for atoms 18-17-16-8 (type 1-1-40-2).
Missing for atoms 20-21-16-8 (type 1-1-40-2).
Missing for atoms 9-8-16-17 (type 37-2-40-1).
Missing for atoms 9-8-16-21 (type 37-2-40-1).
Missing for atoms 9-10-11-12 (type 37-2-2-41).
Missing for atoms 16-17-18-19 (type 40-1-1-8).
Missing for atoms 16-17-18-37 (type 40-1-1-5).
Missing for atoms 16-21-20-19 (type 40-1-1-8).
Missing for atoms 20-21-16-17 (type 1-1-40-1).
Missing for atoms 29-21-16-17 (type 5-1-40-1).
Missing for atoms 18-17-16-21 (type 1-1-40-1).
Missing for angle 17-16-21 (type 1-40-1).
Missing for angle 18-17-16 (type 1-1-40).
Missing for angle 20-21-16 (type 1-1-40).

B. Estimated Parameters

7 torsional parameters are read in

Atom type numbers	V1	V2	V3
1 1 40 2	0.000	0.160	0.090
37 2 40 1	0.000	11.600	0.000
37 2 2 41	0.000	11.600	0.000
8 1 1 40	0.000	0.000	0.270
5 1 1 40	0.000	0.000	0.270
1 1 40 1	0.000	0.160	0.090
5 1 40 1	0.000	0.160	0.090

2 bending parameters are read in

Atom type numbers	Kb	Theta
1 40 1	0.695	120.000
1 1 40	0.695	109.500

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
Cl(1)-C(2)	1.7446	1.7312	0.0134
C(2)-C(3)	1.3949	1.3938	0.0011
C(2)-C(7)	1.3815	1.3894	-0.0079
C(3)-C(4)	1.3826	1.3907	-0.0081
C(4)-C(5)	1.3762	1.4030	-0.0268

Bond	Length Crystal	MM3	Difference (in Å)
C(5)-C(6)	1.3760	1.4010	-0.0250
C(5)-O(12)	1.3875	1.2410	0.1465
C(6)-C(7)	1.4044	1.4085	-0.0041
C(6)-C(8)	1.4961	1.4825	0.0136
C(8)-N(9)	1.2869	1.2990	-0.0121
C(8)-N(16)	1.3944	1.4076	-0.0132
N(9)-C(10)	1.4008	1.4163	-0.0155
C(10)-C(11)	1.3963	1.4141	-0.0178
C(10)-C(14)	1.4033	1.4037	-0.0004
C(11)-O(12)	1.4094	1.2430	0.1664
C(11)-C(13)	1.3857	1.4013	-0.0156
C(13)-C(22)	1.3922	1.3933	-0.0011
C(14)-C(15)	1.3871	1.3916	-0.0045
C(15)-C(22)	1.3824	1.3925	-0.0101
N(16)-C(17)	1.4637	1.5056	-0.0419
N(16)-C(21)	1.4718	1.5047	-0.0329
C(17)-C(18)	1.5091	1.5315	-0.0224
C(17)-H(35)	1.1000	1.1143	-0.0143
C(17)-H(36)	1.1000	1.1081	-0.0081
C(18)-N(19)	1.4642	1.4644	-0.0002
C(18)-H(37)	1.1000	1.1137	-0.0137
C(18)-H(38)	1.1000	1.1263	-0.0263
N(19)-C(20)	1.4633	1.4644	-0.0011
N(19)-H(33)	1.1051	1.0176	0.0875
C(20)-C(21)	1.5213	1.5333	-0.0120
C(20)-H(31)	1.1223	1.1138	0.0085
C(20)-H(32)	1.1104	1.1268	-0.0164
C(21)-H(29)	1.0974	1.1138	-0.0164
C(21)-H(30)	1.0744	1.1120	-0.0376

RMS value: 0.0442

III. Bond Angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
Cl(1)-C(2)-C(3)	118.402	119.975	-1.573
Cl(1)-C(2)-C(7)	119.899	119.939	-0.040
C(3)-C(2)-C(7)	121.698	120.081	1.617
C(2)-C(3)-C(4)	117.933	119.204	-1.271
C(3)-C(4)-C(5)	120.471	121.076	-0.605

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(4)-C(5)-C(6)	122.071	119.658	2.413
C(4)-C(5)-O(12)	118.301	115.934	2.367
C(6)-C(5)-O(12)	119.619	124.402	-4.783
C(5)-C(6)-C(7)	118.094	118.309	-0.215
C(5)-C(6)-C(8)	121.553	122.701	-1.148
C(7)-C(6)-C(8)	120.348	118.959	1.389
C(2)-C(7)-C(6)	119.586	121.157	-1.571
C(6)-C(8)-N(9)	125.577	122.175	3.402
C(6)-C(8)-N(16)	115.194	119.958	-4.764
N(9)-C(8)-N(16)	118.983	117.849	1.134
C(8)-N(9)-C(10)	122.523	122.746	-0.223
N(9)-C(10)-C(11)	124.659	124.837	-0.178
N(9)-C(10)-C(14)	117.909	115.645	2.264
C(11)-C(10)-C(14)	117.132	118.765	-1.633
C(10)-C(11)-O(12)	119.189	126.007	-6.818
C(10)-C(11)-C(13)	122.901	118.912	3.989
O(12)-C(11)-C(13)	117.886	115.082	2.804
C(5)-O(12)-C(11)	111.338	122.935	-11.597
C(11)-C(13)-C(22)	118.260	121.503	-3.243
C(10)-C(14)-C(15)	120.761	121.594	-0.833
C(14)-C(15)-C(22)	120.374	119.545	0.829
C(8)-N(16)-C(17)	117.918	125.685	-7.767
C(8)-N(16)-C(21)	116.359	119.664	-3.305
C(17)-N(16)-C(21)	112.031	114.277	-2.246
N(16)-C(17)-C(18)	109.731	109.481	0.250
N(16)-C(17)-H(35)	115.749	107.531	8.218
N(16)-C(17)-H(36)	107.309	115.102	-7.793
C(18)-C(17)-H(35)	115.750	108.964	6.786
C(18)-C(17)-H(36)	107.309	110.338	-3.029
H(35)-C(17)-H(36)	99.854	105.168	-5.314
C(17)-C(18)-N(19)	108.647	111.022	-2.375
C(17)-C(18)-H(37)	116.280	109.192	7.088
C(17)-C(18)-H(38)	108.019	109.916	-1.897
N(19)-C(18)-H(37)	116.280	109.301	6.979
N(19)-C(18)-H(38)	108.019	110.205	-2.186
H(37)-C(18)-H(38)	98.576	107.115	-8.539
C(18)-N(19)-C(20)	109.543	110.909	-1.366
C(18)-N(19)-H(33)	108.248	109.754	-1.506
C(20)-N(19)-H(33)	109.984	109.702	0.282
N(19)-C(20)-C(21)	109.302	111.771	-2.469

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
N(19)-C(20)-H(31)	110.328	109.257	1.071
N(19)-C(20)-H(32)	113.000	110.001	2.999
C(21)-C(20)-H(31)	109.792	109.106	0.686
C(21)-C(20)-H(32)	109.392	109.561	-0.169
H(31)-C(20)-H(32)	104.933	107.022	-2.089
N(16)-C(21)-C(20)	108.970	109.298	-0.328
N(16)-C(21)-H(29)	108.338	108.915	-0.577
N(16)-C(21)-H(30)	110.445	113.234	-2.789
C(20)-C(21)-H(29)	108.329	109.755	-1.426
C(20)-C(21)-H(30)	112.437	108.966	3.471
H(29)-C(21)-H(30)	108.216	106.610	1.606
C(13)-C(22)-C(15)	120.520	119.613	0.907

RMS value: 3.821

IV. Dihedral Angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
Cl(1)-C(2)-C(3)-C(4)	176.2	177.9	-1.7
Cl(1)-C(2)-C(7)-C(6)	-178.4	178.9	2.7
C(2)-C(3)-C(4)-C(5)	2.4	0.2	2.2
C(2)-C(7)-C(6)-C(5)	2.0	6.1	-4.1
C(2)-C(7)-C(6)-C(8)	-178.7	-171.9	-6.8
C(3)-C(2)-C(7)-C(6)	1.5	-0.4	1.9
C(3)-C(4)-C(5)-C(6)	1.2	5.6	-4.4
C(3)-C(4)-C(5)-O(12)	-179.9	-173.5	-6.4
C(4)-C(3)-C(2)-C(7)	-3.7	-2.8	-0.9
C(4)-C(5)-C(6)-C(7)	-3.4	-8.6	5.2
C(4)-C(5)-C(6)-C(8)	177.4	169.3	8.1
C(4)-C(5)-O(12)-C(11)	114.4	131.1	-16.7
C(5)-C(6)-C(8)-N(9)	41.9	45.8	-3.9
C(5)-C(6)-C(8)-N(16)	-143.9	-135.8	-8.1
C(5)-O(12)-C(11)-C(10)	68.2	46.6	21.6
C(5)-O(12)-C(11)-C(13)	-113.5	-133.4	19.9
C(6)-C(5)-O(12)-C(11)	-66.6	-48.0	-18.6
C(6)-C(8)-N(9)-C(10)	-0.8	-10.1	9.3
C(6)-C(8)-N(16)-C(17)	51.9	15.1	36.8
C(6)-C(8)-N(16)-C(21)	-170.7	-172.3	1.6
C(7)-C(6)-C(5)-O(12)	177.7	170.4	7.3
C(7)-C(6)-C(8)-N(9)	-137.3	-136.3	-1.0

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(7)-C(6)-C(8)-N(16)	36.9	42.1	-5.2
C(8)-C(6)-C(5)-O(12)	-1.5	-11.7	10.2
C(8)-N(9)-C(10)-C(11)	-40.5	-32.3	-8.2
C(8)-N(9)-C(10)-C(14)	146.0	157.8	-11.8
C(8)-N(16)-C(17)-C(18)	-163.5	-134.9	-28.6
C(8)-N(16)-C(17)-H(35)	63.2	106.9	-43.7
C(8)-N(16)-C(17)-H(36)	-47.2	-10.0	-37.2
C(8)-N(16)-C(21)-C(20)	163.9	135.3	28.6
C(8)-N(16)-C(21)-H(29)	-78.4	-104.8	26.4
C(8)-N(16)-C(21)-H(30)	39.9	13.6	26.3
N(9)-C(8)-N(16)-C(17)	-133.5	-166.4	32.9
N(9)-C(8)-N(16)-C(21)	3.9	6.2	-2.3
N(9)-C(10)-C(11)-O(12)	2.0	12.1	-10.1
N(9)-C(10)-C(11)-C(13)	-176.2	-167.9	-8.3
N(9)-C(10)-C(14)-C(15)	176.5	171.3	5.2
C(10)-N(9)-C(8)-N(16)	-174.9	171.4	-13.7
C(10)-C(11)-C(13)-C(22)	1.6	-2.7	4.3
C(10)-C(14)-C(15)-C(22)	-1.4	-2.2	0.8
C(11)-C(10)-C(14)-C(15)	2.5	0.7	1.8
C(11)-C(13)-C(22)-C(15)	-0.3	1.3	-1.6
O(12)-C(11)-C(10)-C(14)	175.5	-178.3	6.2
O(12)-C(11)-C(13)-C(22)	-176.6	177.2	-7.2
C(13)-C(11)-C(10)-C(14)	-2.7	1.7	-4.4
C(13)-C(22)-C(15)-C(14)	0.2	1.2	-1.0
N(16)-C(17)-C(18)-N(19)	-59.3	-55.4	-3.9
N(16)-C(17)-C(18)-H(37)	167.3	-175.9	16.1
N(16)-C(17)-C(18)-H(38)	57.6	66.8	-9.2
N(16)-C(21)-C(20)-N(19)	58.1	54.1	4.0
N(16)-C(21)-C(20)-H(31)	179.2	175.0	4.2
N(16)-C(21)-C(20)-H(32)	-66.1	-68.1	2.0
C(17)-N(16)-C(21)-C(20)	-56.3	-51.3	-5.0
C(17)-N(16)-C(21)-H(29)	61.4	68.6	-7.2
C(17)-N(16)-C(21)-H(30)	179.8	-173.0	7.2
C(17)-C(18)-N(19)-C(20)	62.7	60.4	2.3
C(17)-C(18)-N(19)-H(33)	-177.4	-178.2	0.8
C(18)-C(17)-N(16)-C(21)	57.3	52.2	5.1
C(18)-N(19)-C(20)-C(21)	-62.4	-60.0	-2.4
C(18)-N(19)-C(20)-H(31)	176.8	179.2	-2.4
C(18)-N(19)-C(20)-H(32)	59.6	62.0	-2.4
N(19)-C(18)-C(17)-H(35)	74.0	62.0	12.0

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
N(19)-C(18)-C(17)-H(36)	-175.6	177.0	-7.4
N(19)-C(20)-C(21)-H(29)	-59.6	-65.3	5.7
N(19)-C(20)-C(21)-H(30)	-179.1	178.3	-2.6
C(20)-N(19)-C(18)-H(37)	-163.9	-179.1	15.2
C(20)-N(19)-C(18)-H(38)	-54.3	-61.6	7.3
C(21)-N(16)-C(17)-H(35)	-76.0	-66.1	-9.9
C(21)-N(16)-C(17)-H(36)	173.6	177.1	-3.5
C(21)-C(20)-N(19)-H(33)	178.7	178.6	0.1
H(29)-C(21)-C(20)-H(31)	61.5	55.7	5.8
H(29)-C(21)-C(20)-H(32)	176.2	172.5	3.7
H(30)-C(21)-C(20)-H(31)	-58.0	-60.7	2.7
H(30)-C(21)-C(20)-H(32)	56.6	56.1	0.5
H(31)-C(20)-N(19)-H(33)	57.9	57.8	0.1
H(32)-C(20)-N(19)-H(33)	-59.2	-59.4	0.2
H(33)-N(19)-C(18)-H(37)	-44.0	-57.7	13.7
H(33)-N(19)-C(18)-H(38)	65.6	59.7	5.9
H(35)-C(17)-C(18)-H(37)	-59.5	-58.6	-0.9
H(35)-C(17)-C(18)-H(38)	-169.1	-175.8	6.7
H(36)-C(17)-C(18)-H(37)	51.0	56.4	-5.4
H(36)-C(17)-C(18)-H(38)	-58.6	-60.8	2.2
		RMS value:	12.7

Table 34. Fluoxetine

I. Missing parameters

A. Missing for atoms 4-3-13-14 (type 41-1-2-2).
Missing for atoms 4-3-13-18 (type 41-1-2-2).
Missing for atoms 13-3-4-5 (type 2-1-41-2).
Missing for angle 13-3-4 (type 2-1-41).

B. Estimated Parameters

7 torsional parameters are read in

Atom type numbers	V1	V2	V3
41 1 2 2	0.000	0.160	0.090
2 1 41 2	0.000	0.160	0.090

1 bending parameters is read in

Atom type numbers	Kb	Theta
2 1 41	0.695	109.500

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(2)	1.5249	1.5253	-0.0004
C(1)-N^+(11)	1.4998	1.5132	-0.0134
C(2)-C(3)	1.5235	1.5531	-0.0296
C(3)-O(4)	1.4284	1.4312	-0.0028
C(3)-C(13)	1.5099	1.5146	-0.0047
C(3)-H(27)	0.9604	1.1153	-0.1549
O(4)-C(5)	1.3786	1.2306	0.1480
C(5)-C(6)	1.3950	1.4024	-0.0074
C(5)-C(10)	1.3774	1.3978	-0.0204
C(6)-C(7)	1.3796	1.3974	-0.0178
C(7)-C(8)	1.3667	1.3957	-0.0290
C(8)-C(9)	1.3935	1.3965	-0.0030
C(8)-C(19)	1.4680	1.5060	-0.0380
C(9)-C(10)	1.3786	1.3950	-0.0164
N^+(11)-C(12)	1.4854	1.5069	-0.0215
N^+(11)-H(32)	0.9606	1.0202	-0.0596
N^+(11)-H(33)	0.9603	1.0196	-0.0593
C(13)-C(14)	1.3840	1.4027	-0.0187
C(13)-C(18)	1.3813	1.4029	-0.0216
C(14)-C(15)	1.3886	1.3961	-0.0075
C(15)-C(16)	1.3777	1.3954	-0.0177

Bond	Length Crystal	MM3	Difference (in Å)
C(16)-C(17)	1.3623	1.3951	-0.0328
C(17)-C(18)	1.3723	1.3965	-0.0242
C(19)-F(20)	1.2227	1.3400	-0.1173
C(19)-F(21)	1.3006	1.3400	-0.0394
C(19)-F(22)	1.2467	1.3403	-0.0936
		RMS value:	0.0571

III. Bond Angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(2)-C(1)-N^+(11)	111.431	111.707	-0.276
C(1)-C(2)-C(3)	110.969	112.698	-1.729
C(2)-C(3)-O(4)	106.349	106.205	0.144
C(2)-C(3)-C(13)	111.090	108.339	2.751
C(2)-C(3)-H(27)	111.040	107.945	3.095
O(4)-C(3)-C(13)	113.323	112.936	0.387
O(4)-C(3)-H(27)	109.305	110.415	-1.110
C(13)-C(3)-H(27)	105.797	110.757	-4.960
C(3)-O(4)-C(5)	118.769	121.248	-2.479
O(4)-C(5)-C(6)	124.715	124.499	0.216
O(4)-C(5)-C(10)	115.030	117.012	-1.982
C(6)-C(5)-C(10)	120.250	118.489	1.761
C(5)-C(6)-C(7)	118.585	120.302	-1.717
C(6)-C(7)-C(8)	121.941	121.108	0.833
C(7)-C(8)-C(9)	118.867	118.409	0.458
C(7)-C(8)-C(19)	121.884	120.537	1.347
C(9)-C(8)-C(19)	119.247	120.528	-1.281
C(8)-C(9)-C(10)	120.305	120.724	-0.419
C(5)-C(10)-C(9)	120.015	120.887	-0.872
C(1)-N^+(11)-C(12)	114.664	115.639	-0.975
C(1)-N^+(11)-H(32)	108.767	108.575	0.192
C(1)-N^+(11)-H(33)	107.734	109.694	-1.960
C(12)-N^+(11)-H(32)	108.170	108.170	0.000
C(12)-N^+(11)-H(33)	107.997	108.884	-0.887
H(32)-N^+(11)-H(33)	109.429	105.377	4.052
C(3)-C(13)-C(14)	121.785	121.176	0.609
C(3)-C(13)-C(18)	119.717	120.052	-0.335
C(14)-C(13)-C(18)	118.476	118.772	-0.296
C(13)-C(14)-C(15)	120.227	120.614	-0.387

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(14)-C(15)-C(16)	119.948	120.105	-0.157
C(15)-C(16)-C(17)	119.936	119.808	0.128
C(16)-C(17)-C(18)	120.280	120.096	0.184
C(13)-C(18)-C(17)	121.113	120.604	0.509
C(8)-C(19)-F(20)	117.601	113.080	4.521
C(8)-C(19)-F(21)	113.307	113.096	0.211
C(8)-C(19)-F(22)	114.815	110.357	4.458
F(20)-C(19)-F(21)	101.632	106.861	-5.229
F(20)-C(19)-F(22)	107.205	106.503	0.702
F(21)-C(19)-F(22)	100.135	106.509	-6.374
		RMS value:	2.262

IV. Dihedral Angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(2)-C(3)-O(4)	60.6	59.7	0.9
C(1)-C(2)-C(3)-C(13)	-175.7	-178.7	3.0
C(1)-C(2)-C(3)-H(27)	-58.3	-58.7	0.4
C(2)-C(1)-N^+(11)-C(12)	77.9	70.3	7.6
C(2)-C(1)-N^+(11)-H(32)	-160.8	-167.9	7.1
C(2)-C(1)-N^+(11)-H(33)	-42.3	-53.2	10.9
C(2)-C(3)-O(4)-C(5)	-161.9	-171.4	9.5
C(2)-C(3)-C(13)-C(14)	-77.6	-85.8	8.2
C(2)-C(3)-C(13)-C(18)	100.6	94.0	6.6
C(3)-C(2)-C(1)-N^+(11)	-180.0	-179.4	-0.6
C(3)-O(4)-C(5)-C(6)	-14.4	0.3	-14.7
C(3)-O(4)-C(5)-C(10)	166.5	180.0	-13.5
C(3)-C(13)-C(14)-C(15)	179.3	-180.0	-0.7
C(3)-C(13)-C(18)-C(17)	-180.0	-180.0	0.0
O(4)-C(3)-C(13)-C(14)	42.0	31.5	10.5
O(4)-C(3)-C(13)-C(18)	-139.7	-148.6	8.9
O(4)-C(5)-C(6)-C(7)	-177.7	-179.8	2.1
O(4)-C(5)-C(10)-C(9)	178.0	179.8	-1.8
C(5)-O(4)-C(3)-C(13)	75.8	70.0	5.8
C(5)-O(4)-C(3)-H(27)	-41.9	-54.6	12.7
C(5)-C(6)-C(7)-C(8)	0.1	1.3	-1.2
C(5)-C(10)-C(9)-C(8)	-0.4	-1.4	1.0
C(6)-C(5)-C(10)-C(9)	-1.2	-0.5	-0.7
C(6)-C(7)-C(8)-C(9)	-1.7	-3.2	1.5

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(6)-C(7)-C(8)-C(19)	177.8	-174.9	7.3
C(7)-C(6)-C(5)-C(10)	1.4	0.6	0.8
C(7)-C(8)-C(9)-C(10)	1.8	3.2	-1.4
C(7)-C(8)-C(19)-F(20)	142.6	146.6	-4.0
C(7)-C(8)-C(19)-F(21)	24.4	25.0	-0.6
C(7)-C(8)-C(19)-F(22)	-89.8	-94.2	4.4
C(9)-C(8)-C(19)-F(20)	-37.8	-24.9	-12.9
C(9)-C(8)-C(19)-F(21)	-156.1	-146.6	-9.5
C(9)-C(8)-C(19)-F(22)	89.7	94.3	-4.6
C(10)-C(9)-C(8)-C(19)	-177.7	175.0	-7.3
C(13)-C(14)-C(15)-C(16)	0.0	-0.1	0.1
C(13)-C(18)-C(17)-C(16)	1.4	0.0	1.4
C(14)-C(13)-C(3)-H(27)	161.8	156.0	5.8
C(14)-C(13)-C(18)-C(17)	-1.7	-0.1	-1.6
C(14)-C(15)-C(16)-C(17)	-0.3	0.0	-0.3
C(15)-C(14)-C(13)-C(18)	1.0	0.2	0.8
C(15)-C(16)-C(17)-C(18)	-0.4	0.0	-0.4
C(18)-C(13)-C(3)-H(27)	-20.0	-24.2	4.2
		RMS value:	6.3

Table 35. Thioridazine

I. Missing parameters

A. Missing for atoms 15-14-26-1 (type 1-1-15-2).
Missing for atoms 49-14-26-1 (type 5-1-15-2).
Missing for atoms 6-5-23-16 (type 1-1-40-2).
Missing for atoms 6-5-23-21 (type 1-1-40-2).
Missing for atoms 7-6-5-23 (type 1-1-1-40).
Missing for atoms 12-1-26-14 (type 2-2-15-1).
Missing for atoms 19-1-26-14 (type 2-2-15-1).
Missing for atoms 16-12-1-26 (type 2-2-2-15).
Missing for atoms 18-19-1-26 (type 2-2-2-15).
Missing for atoms 23-5-6-33 (type 40-1-1-5).
Missing for atoms 23-16-17-27 (type 40-2-2-42).
Missing for atoms 23-21-20-27 (type 40-2-2-42).
Missing for atoms 26-1-12-46 (type 15-2-2-5).
Missing for atoms 26-1-19-55 (type 15-2-2-5).
Missing for bond 1-26 (type 2-15).
Missing for angle 12-1-26 (type 2-2-15).
Missing for angle 19-1-26 (type 2-2-15).
Missing for angle 6-5-23 (type 1-1-40).
Missing for angle 14-26-1 (type 1-15-2).

B. Estimated Parameters

9 torsional parameters are read in

Atom type numbers	V1	V2	V3
1 1 15 2	0.000	0.000	0.300
5 1 15 2	0.000	0.000	0.300
1 1 40 2	0.000	0.160	0.090
1 1 1 40	0.000	0.000	0.270
2 2 15 1	0.000	1.700	0.200
2 2 2 15	0.000	11.600	0.000
5 1 1 40	0.000	0.000	0.270
40 2 2 42	0.000	11.600	0.000
5 2 2 15	0.000	11.600	0.000

2 stretching parameters are read in

Bond type	Kb	L(0)
2-15	2.9868	1.8000
2-15	4.7380	0.1930

3 bending parameters are read in

Atom type numbers			Kb	Theta
2	2	15	0.695	120.000
1	1	40	0.695	109.500
1	15	2	0.695	110.000

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
C(1)-C(12)	1.3988	1.3999	-0.0011
C(1)-C(19)	1.3918	1.3907	0.0011
C(1)-S(26)	1.8118	1.8117	0.0001
C(2)-C(3)	1.3895	1.3892	0.0003
C(2)-C(22)	1.3995	1.3999	-0.0004
C(3)-C(4)	1.3964	1.3967	-0.0003
C(4)-C(20)	1.3975	1.3972	0.0003
C(5)-C(6)	1.5397	1.5397	0.0000
C(5)-N(23)	1.5213	1.5213	0.0000
C(6)-C(7)	1.5345	1.5346	-0.0001
C(8)-C(9)	1.5284	1.5285	-0.0001
C(8)-N(24)	1.4655	1.4655	0.0000
C(9)-N(25)	1.4601	1.4601	0.0000
C(10)-N(25)	1.4594	1.4594	0.0000
C(10)-H(41)	1.1113	1.1113	0.0000
C(10)-H(42)	1.1243	1.1242	0.0001
C(10)-H(43)	1.1113	1.1113	0.0000
C(11)-C(13)	1.5287	1.5287	0.0000
C(11)-N(25)	1.4604	1.4605	-0.0001
C(12)-C(16)	1.4095	1.4085	0.0010
C(13)-N(24)	1.4631	1.4630	0.0001
C(14)-C(15)	1.5329	1.5329	0.0000
C(14)-S(26)	1.8146	1.8144	0.0002
C(14)-H(49)	1.1123	1.1123	0.0000
C(14)-H(50)	1.1136	1.1136	0.0000
C(15)-H(51)	1.1132	1.1132	0.0000
C(15)-H(52)	1.1132	1.1132	0.0000
C(15)-H(53)	1.1131	1.1131	0.0000
C(16)-C(17)	1.4109	1.4120	-0.0011
C(16)-N(23)	1.4558	1.4550	0.0008
C(17)-C(18)	1.3987	1.3978	0.0009
C(17)-S(27)	1.7487	1.7484	0.0003
C(18)-C(19)	1.3944	1.3954	-0.0010

Bond	Length Crystal	MM3	Difference (in Å)
C(20)-C(21)	1.4129	1.4133	-0.0004
C(20)-S(27)	1.7484	1.7483	0.0001
C(21)-C(22)	1.4079	1.4076	0.0003
C(21)-N(23)	1.4549	1.4547	0.0002
		RMS value:	0.0005

III. Bond Angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(12)-C(1)-C(19)	120.100	120.105	-0.005
C(12)-C(1)-S(26)	120.558	120.556	0.002
C(19)-C(1)-S(26)	119.341	119.338	0.003
C(3)-C(2)-C(22)	120.339	120.343	-0.004
C(2)-C(3)-C(4)	119.498	119.497	0.001
C(3)-C(4)-C(20)	120.258	120.257	0.001
C(6)-C(5)-N(23)	110.341	110.382	-0.041
C(5)-C(6)-C(7)	113.008	112.964	0.044
C(6)-C(7)-N(24)	113.613	113.579	0.034
C(9)-C(8)-N(24)	111.533	111.535	-0.002
C(8)-C(9)-N(25)	111.056	111.061	-0.005
N(25)-C(10)-H(41)	110.475	110.476	-0.001
C(13)-C(11)-N(25)	110.780	110.774	0.006
C(1)-C(12)-C(16)	121.487	121.481	0.006
C(11)-C(13)-N(24)	111.175	111.167	0.008
C(15)-C(14)-S(26)	111.152	111.163	-0.011
C(15)-C(14)-H(49)	109.272	109.287	-0.015
C(15)-C(14)-H(50)	109.278	109.268	0.010
S(26)-C(14)-H(49)	110.560	110.558	0.002
S(26)-C(14)-H(50)	109.946	109.943	0.003
H(49)-C(14)-H(50)	106.515	106.503	0.012
C(14)-C(15)-H(51)	111.244	111.243	0.001
C(14)-C(15)-H(52)	111.762	111.759	0.003
C(14)-C(15)-H(53)	111.795	111.801	-0.006
H(51)-C(15)-H(52)	107.150	107.146	0.004
H(51)-C(15)-H(53)	107.116	107.124	-0.008
H(52)-C(15)-H(53)	107.513	107.507	0.006
C(12)-C(16)-C(17)	117.278	117.282	-0.004
C(12)-C(16)-N(23)	120.898	120.902	-0.004
C(17)-C(16)-N(23)	121.823	121.815	0.008

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(16)-C(17)-C(18)	121.197	121.196	0.001
C(16)-C(17)-S(27)	123.996	123.988	0.008
C(18)-C(17)-S(27)	114.807	114.816	-0.009
C(17)-C(18)-C(19)	120.315	120.313	0.002
C(1)-C(19)-C(18)	119.588	119.588	0.000
C(4)-C(20)-C(21)	121.249	121.251	-0.002
C(4)-C(20)-S(27)	114.845	114.836	0.009
C(21)-C(20)-S(27)	123.905	123.912	-0.007
C(20)-C(21)-C(22)	117.293	117.288	0.005
C(20)-C(21)-N(23)	121.860	121.858	0.002
C(22)-C(21)-N(23)	120.845	120.852	-0.007
C(2)-C(22)-C(21)	121.362	121.361	0.001
C(5)-N(23)-C(16)	118.091	118.047	0.044
C(5)-N(23)-C(21)	117.855	117.895	-0.040
C(16)-N(23)-C(21)	124.047	124.051	-0.004
C(7)-N(24)-C(8)	111.829	111.831	-0.002
C(7)-N(24)-C(13)	110.953	110.984	-0.031
C(8)-N(24)-C(13)	108.405	108.409	-0.004
C(9)-N(25)-C(10)	111.591	111.598	-0.007
C(9)-N(25)-C(11)	109.024	109.027	-0.003
C(10)-N(25)-C(11)	111.611	111.618	-0.007
C(1)-S(26)-C(14)	111.469	111.417	0.052
C(17)-S(27)-C(20)	104.305	104.306	-0.001
		RMS value:	0.019

IV. Dihedral Angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(1)-C(12)-C(16)-C(17)	1.5	1.4	0.1
C(1)-C(12)-C(16)-N(23)	-178.7	-178.9	0.2
C(1)-C(19)-C(18)-C(17)	-0.2	-0.3	0.1
C(1)-S(26)-C(14)-H(49)	55.5	55.8	-0.3
C(1)-S(26)-C(14)-H(50)	-61.8	-61.5	-0.3
C(2)-C(3)-C(4)-C(20)	-0.1	-0.1	0.0
C(2)-C(3)-C(4)-H(30)	179.9	179.9	0.0
C(2)-C(22)-C(21)-C(20)	-0.3	-0.4	0.1
C(2)-C(22)-C(21)-N(23)	-179.9	-179.9	0.0
C(3)-C(2)-C(22)-C(21)	0.1	0.1	0.0
C(3)-C(4)-C(20)-C(21)	-0.2	-0.2	0.0

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(3)-C(4)-C(20)-S(27)	-179.9	-179.9	0.0
C(4)-C(3)-C(2)-C(22)	0.1	0.1	0.0
C(4)-C(20)-C(21)-C(22)	0.4	0.4	0.0
C(4)-C(20)-C(21)-N(23)	179.9	180.0	-0.1
C(4)-C(20)-S(27)-C(17)	-178.2	-178.2	0.0
C(5)-C(6)-C(7)-N(24)	-68.3	-68.3	0.0
C(5)-N(23)-C(16)-C(12)	1.2	1.3	-0.1
C(5)-N(23)-C(16)-C(17)	-179.1	-179	-0.1
C(5)-N(23)-C(21)-C(20)	179.1	178.9	0.2
C(5)-N(23)-C(21)-C(22)	-1.4	-1.6	0.2
C(6)-C(5)-N(23)-C(16)	-93.9	-93.5	-0.4
C(6)-C(5)-N(23)-C(21)	85.2	85.6	-0.4
C(6)-C(7)-N(24)-C(8)	-74.7	-75.1	0.4
C(6)-C(7)-N(24)-C(13)	164.1	163.7	0.4
C(7)-C(6)-C(5)-N(23)	171.2	171	0.2
C(7)-N(24)-C(8)-C(9)	-179.6	-179.6	0.0
C(7)-N(24)-C(13)-C(11)	-179.3	-179.2	-0.1
C(8)-C(9)-N(25)-C(10)	179.1	179.1	0.0
C(8)-C(9)-N(25)-C(11)	-57.1	-57.1	0.0
C(8)-N(24)-C(13)-C(11)	57.6	57.6	0.0
C(9)-C(8)-N(24)-C(13)	-57.0	-57.0	0.0
C(9)-N(25)-C(10)-H(41)	-177.9	-177.9	0.0
C(9)-N(25)-C(10)-H(42)	61.5	61.6	-0.1
C(9)-N(25)-C(10)-H(43)	-59.1	-59.1	0.0
C(9)-N(25)-C(11)-C(13)	57.8	57.8	0.0
C(10)-N(25)-C(11)-C(13)	-178.5	-178.5	0.0
C(11)-N(25)-C(10)-H(41)	59.8	59.8	0.0
C(11)-N(25)-C(10)-H(42)	-60.7	-60.7	0.0
C(11)-N(25)-C(10)-H(43)	178.6	178.7	-0.1
C(12)-C(1)-C(19)-C(18)	1.7	1.7	0.0
C(12)-C(1)-S(26)-C(14)	-41.5	-42.1	0.6
C(12)-C(16)-C(17)-C(18)	0.0	0.1	-0.1
C(12)-C(16)-C(17)-S(27)	-179.9	-179.8	-0.1
C(12)-C(16)-N(23)-C(21)	-177.9	-177.8	-0.1
C(14)-S(26)-C(1)-C(19)	138.9	138.3	0.6
C(16)-C(12)-C(1)-C(19)	-2.4	-2.3	-0.1
C(16)-C(12)-C(1)-S(26)	178.1	178.1	0.0
C(16)-C(17)-C(18)-C(19)	-0.6	-0.6	0.0
C(16)-C(17)-S(27)-C(20)	-2.1	-2.2	0.1
C(16)-N(23)-C(21)-C(20)	-1.9	-2.0	0.1

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(16)-N(23)-C(21)-C(22)	177.6	177.5	0.1
C(17)-C(16)-N(23)-C(21)	1.9	1.9	0.0
C(17)-S(27)-C(20)-C(21)	2.1	2.1	0.0
C(18)-C(17)-C(16)-N(23)	-179.8	-179.7	-0.1
C(18)-C(17)-S(27)-C(20)	178.1	177.9	0.2
C(18)-C(19)-C(1)-S(26)	-178.7	-178.7	0.0
C(19)-C(18)-C(17)-S(27)	179.3	179.3	0.0
C(22)-C(21)-C(20)-S(27)	-179.9	-179.9	0.0
N(23)-C(16)-C(17)-S(27)	0.4	0.5	-0.1
N(23)-C(21)-C(20)-S(27)	-0.4	-0.4	0.0
N(24)-C(8)-C(9)-N(25)	58.1	58.1	0.0
N(24)-C(13)-C(11)-N(25)	-59.5	-59.5	0.0
N(24)-C(13)-C(11)-H(45)	62.8	62.8	0.0
S(26)-C(14)-C(15)-H(51)	-179.4	-179.3	-0.1
S(26)-C(14)-C(15)-H(52)	60.9	60.9	0.0
S(26)-C(14)-C(15)-H(53)	-59.6	-59.6	0.0
S(27)-C(20)-C(4)-H(30)	0.1	0.1	0.0
H(49)-C(14)-C(15)-H(51)	-57.1	-57.0	-0.1
H(49)-C(14)-C(15)-H(52)	-176.8	-176.8	0.0
H(49)-C(14)-C(15)-H(53)	62.6	62.7	-0.1
H(50)-C(14)-C(15)-H(51)	59.1	59.1	0.0
H(50)-C(14)-C(15)-H(52)	-60.6	-60.6	0.0
H(50)-C(14)-C(15)-H(53)	178.8	178.8	0.0
		RMS value:	0.2

Table 36. Chlorprothixene

I. Missing parameters

There are no missing parameters for this molecule.

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
Cl(1)-C(12)	1.7489	1.7318	0.0171
C(2)-C(3)	1.4060	1.4034	0.0026
C(2)-C(12)	1.3821	1.3947	-0.0126
C(3)-C(4)	1.4015	1.4045	-0.0030
C(3)-C(19)	1.4747	1.4837	-0.0090
C(4)-C(14)	1.3838	1.3989	-0.0151
C(4)-S(39)	1.7524	1.7621	-0.0097
C(5)-C(6)	1.4008	1.4053	-0.0045
C(5)-C(15)	1.3811	1.3982	-0.0171
C(5)-S(39)	1.7466	1.7629	-0.0163
C(6)-C(18)	1.4010	1.4025	-0.0015
C(6)-C(19)	1.4817	1.4842	-0.0025
C(7)-C(8)	1.4839	1.5085	-0.0246
C(7)-C(19)	1.3379	1.3515	-0.0136
C(8)-C(9)	1.5221	1.5395	-0.0174
C(9)-N(38)	1.4684	1.4661	0.0023
C(10)-H(26)	1.0463	1.1113	-0.0650
C(10)-H(27)	1.0452	1.1114	-0.0662
C(10)-H(28)	1.0525	1.1245	-0.0720
C(10)-N(38)	1.4510	1.461	-0.0100
C(11)-H(29)	1.0503	1.1098	-0.0595
C(11)-H(30)	1.0538	1.1242	-0.0704
C(11)-H(31)	1.0506	1.1115	-0.0609
C(11)-N(38)	1.4229	1.4612	-0.0383
C(12)-C(13)	1.3720	1.3963	-0.0243
C(13)-C(14)	1.3766	1.3939	-0.0173
C(15)-C(16)	1.3749	1.3947	-0.0198
C(16)-C(17)	1.3701	1.3971	-0.0270
C(17)-C(18)	1.3871	1.3967	-0.0096
		RMS value:	0.0333

Bond angles begin on next page.

III. Bond Angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(3)-C(2)-C(12)	119.488	120.402	-0.914
C(2)-C(3)-C(4)	118.002	118.298	-0.296
C(2)-C(3)-C(19)	121.303	121.752	-0.449
C(4)-C(3)-C(19)	120.620	119.795	0.825
C(3)-C(4)-C(14)	120.571	121.235	-0.664
C(3)-C(4)-S(39)	120.771	120.238	0.533
C(14)-C(4)-S(39)	118.685	118.501	0.184
C(6)-C(5)-C(15)	121.447	121.125	0.322
C(6)-C(5)-S(39)	119.634	120.257	-0.623
C(15)-C(5)-S(39)	118.893	118.577	0.316
C(5)-C(6)-C(18)	117.215	118.504	-1.289
C(5)-C(6)-C(19)	121.933	119.717	2.216
C(18)-C(6)-C(19)	120.852	121.761	-0.909
C(8)-C(7)-C(19)	129.077	127.900	1.177
C(7)-C(8)-C(9)	110.266	111.363	-1.097
C(8)-C(9)-N(38)	113.795	113.515	0.280
H(26)-C(10)-H(27)	109.586	107.242	2.344
H(26)-C(10)-H(28)	109.402	108.432	0.970
H(26)-C(10)-N(38)	109.662	110.647	-0.985
H(27)-C(10)-H(28)	109.663	108.408	1.255
H(27)-C(10)-N(38)	108.173	110.605	-2.432
H(28)-C(10)-N(38)	110.337	111.374	-1.037
H(29)-C(11)-H(31)	109.028	106.920	2.108
H(29)-C(11)-N(38)	110.609	110.961	-0.352
H(30)-C(11)-H(31)	109.868	108.308	1.560
H(30)-C(11)-N(38)	104.431	111.408	-6.977
Cl(1)-C(12)-C(2)	117.761	119.637	-1.876
Cl(1)-C(12)-C(13)	119.835	119.679	0.156
C(2)-C(12)-C(13)	122.394	120.682	1.712
C(12)-C(13)-C(14)	118.332	119.608	-1.276
C(4)-C(14)-C(13)	121.193	119.667	1.526
C(5)-C(15)-C(16)	120.250	119.608	0.642
C(15)-C(16)-C(17)	119.502	119.918	-0.416
C(16)-C(17)-C(18)	121.059	120.322	0.737
C(6)-C(18)-C(17)	120.430	120.504	-0.074
C(3)-C(19)-C(6)	115.133	116.957	-1.824
C(3)-C(19)-C(7)	123.834	122.897	0.937
C(6)-C(19)-C(7)	121.028	119.975	1.053
C(9)-N(38)-C(10)	109.405	110.693	-1.288

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(9)-N(38)-C(11)	111.733	112.700	-0.967
C(10)-N(38)-C(11)	108.885	110.194	-1.309
C(4)-S(39)-C(5)	100.983	100.782	0.201

RMS value: 1.589

IV. Dihedral Angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
Cl(1)-C(12)-C(2)-C(3)	178.8	179.4	-0.6
Cl(1)-C(12)-C(13)-C(14)	-179.0	178.6	-2.4
C(2)-C(3)-C(4)-C(14)	-1.7	-3.9	2.2
C(2)-C(3)-C(4)-S(39)	179.9	178.0	1.9
C(2)-C(3)-C(19)-C(6)	-140.8	-137.3	-3.5
C(2)-C(3)-C(19)-C(7)	40.1	47.4	-7.3
C(2)-C(12)-C(13)-C(14)	-0.2	-0.9	0.7
C(3)-C(2)-C(12)-C(13)	0.0	-1.1	1.1
C(3)-C(4)-C(14)-C(13)	1.5	2.0	-0.5
C(3)-C(4)-S(39)-C(5)	-34.1	-34.5	0.4
C(3)-C(19)-C(6)-C(5)	-38.3	-38.2	-0.1
C(3)-C(19)-C(6)-C(18)	141.9	140.2	1.7
C(3)-C(19)-C(7)-C(8)	3.2	5.7	-2.5
C(4)-C(3)-C(2)-C(12)	1.0	3.4	-2.4
C(4)-C(3)-C(19)-C(6)	36.0	38.1	-2.1
C(4)-C(3)-C(19)-C(7)	-143.2	-137.2	-6.0
C(4)-C(14)-C(13)-C(12)	-0.5	0.4	-0.9
C(4)-S(39)-C(5)-C(6)	31.9	34.4	-2.5
C(4)-S(39)-C(5)-C(15)	-149.9	-147.9	-2.0
C(5)-C(6)-C(18)-C(17)	-3.2	-1.0	-2.2
C(5)-C(6)-C(19)-C(7)	140.9	137.2	3.7
C(5)-C(15)-C(16)-C(17)	1.3	0.4	0.9
C(5)-S(39)-C(4)-C(14)	147.7	147.3	0.4
C(6)-C(5)-C(15)-C(16)	-1.2	-1.4	0.2
C(6)-C(18)-C(17)-C(16)	3.5	0.1	3.4
C(6)-C(19)-C(7)-C(8)	-175.9	-169.4	-6.5
C(7)-C(8)-C(9)-N(38)	-172.9	-173.2	0.3
C(7)-C(19)-C(6)-C(18)	-38.9	-44.4	5.5
C(8)-C(9)-N(38)-C(10)	178.0	169.2	8.8
C(8)-C(9)-N(38)-C(11)	-61.3	-66.8	5.5
C(9)-C(8)-C(7)-C(19)	151.4	123.5	27.9

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(9)-N(38)-C(10)-H(26)	-62.9	-58.5	-4.4
C(9)-N(38)-C(10)-H(27)	177.6	-177.2	5.2
C(9)-N(38)-C(10)-H(28)	57.7	62.2	-4.5
C(9)-N(38)-C(11)-H(29)	57.6	62.1	-4.5
C(9)-N(38)-C(11)-H(30)	-59.8	-59.0	-0.8
C(9)-N(38)-C(11)-H(31)	-179.4	-179.4	0.0
C(10)-N(38)-C(11)-H(29)	178.6	-173.7	7.7
C(10)-N(38)-C(11)-H(30)	61.2	65.2	-4.0
C(10)-N(38)-C(11)-H(31)	-58.5	-55.3	-3.2
C(11)-N(38)-C(10)-H(26)	174.7	176.2	-1.5
C(11)-N(38)-C(10)-H(27)	55.3	57.5	-2.2
C(11)-N(38)-C(10)-H(28)	-64.7	-63.1	-1.6
C(12)-C(2)-C(3)-C(19)	177.8	178.9	-1.1
C(13)-C(14)-C(4)-S(39)	179.8	-179.8	0.4
C(14)-C(4)-C(3)-C(19)	-178.6	-179.4	0.8
C(15)-C(5)-C(6)-C(18)	2.1	1.7	0.4
C(15)-C(5)-C(6)-C(19)	-177.7	-179.8	2.1
C(15)-C(16)-C(17)-C(18)	-2.5	0.3	-2.8
C(16)-C(15)-C(5)-S(39)	-179.3	-179.1	-0.2
C(17)-C(18)-C(6)-C(19)	176.5	-179.5	4.0
C(18)-C(6)-C(5)-S(39)	-179.8	179.3	-0.9
C(19)-C(3)-C(4)-S(39)	3.2	2.4	0.8
C(19)-C(6)-C(5)-S(39)	0.5	-2.2	2.7
		RMS value:	5.0

Table 37. Molindone

I. Missing parameters

A. Pi-atom parameter of type (81-40) is missing.
Pi-atom parameter of type (40-3) is missing.
Missing for atoms 9-10-11-3 (type 1-1-160-40).
Missing for atoms 7-12-11-3 (type 3-2-160-40).

B. Estimated parameters
Pi-atom parameters of type (7-2) are used for type (81-2).
Pi-atom parameters of type (7-2) are used for type (81-160).
Pi-atom parameters of type (40-2) are used for type (40-160).
Pi-atom parameters of type (2-2) are used for type (2-160).
Pi-atom parameters of type (3-2) are used for type (3-160).
Pi-atom parameters of type (2-2) are used for type (160-2).
Pi-atom parameters of type (2-2) are used for type (81-40).
Pi-atom parameters of type (2-2) are used for type (40-3).

9 torsional parameters are read in

Atom type numbers	V1	V2	V3
1 1 160 40	0.000	0.160	0.090
3 2 160 40	0.000	11.600	0.000

II. Bond lengths

	Length		Difference
Bond	Crystal	MM3	(in Å)
O(1)-C(7)	1.2276	1.2193	0.0083
O(2)-C(15)	1.4064	1.4176	-0.0112
O(2)-C(16)	1.4163	1.4175	-0.0012
N(3)-C(5)	1.3972	1.3843	0.0129
N(3)-C(11)	1.3435	1.3748	-0.0313
N(3)-H(21)	0.9730	1.0310	-0.0580
N^+(4)-C(13)	1.5049	1.5070	-0.0021
N^+(4)-C(14)	1.5056	1.5958	-0.0902
N^+(4)-C(17)	1.4880	1.5046	-0.0166
N^+(4)-H(22)	0.9559	1.0162	-0.0603
C(5)-C(6)	1.3539	1.3892	-0.0353
C(5)-C(18)	1.4921	1.5117	-0.0196
C(6)-C(12)	1.4451	1.4210	0.0241
C(6)-C(19)	1.5042	1.5039	0.0003
C(7)-C(8)	1.5486	1.5377	0.0109
C(7)-C(12)	1.4329	1.4810	-0.0481

Bond	Length Crystal	MM3	Difference (in Å)
C(8)-C(9)	1.5297	1.5383	-0.0086
C(8)-C(13)	1.5028	1.5335	-0.0307
C(8)-H(23)	1.0097	1.1107	-0.1010
C(9)-C(10)	1.5173	1.5347	-0.0174
C(9)-H(24)	1.0055	1.1129	-0.1074
C(9)-H(25)	1.0132	1.1112	-0.0980
C(10)-C(11)	1.4893	1.5084	-0.0191
C(10)-H(26)	1.0126	1.1134	-0.1008
C(10)-H(27)	1.0176	1.1135	-0.0959
C(11)-C(12)	1.3800	1.3823	-0.0023
C(14)-C(15)	1.5064	1.5171	-0.0107
C(14)-H(30)	1.0160	1.0995	-0.0835
C(14)-H(31)	0.9919	1.0999	-0.1080
C(15)-H(32)	1.0055	1.1123	-0.1068
C(15)-H(33)	1.0129	1.1052	-0.0923
C(16)-C(17)	1.5016	1.5177	-0.0161
C(16)-H(34)	1.0008	1.1052	-0.1044
C(16)-H(35)	1.0177	1.1124	-0.0947
C(17)-H(36)	1.0169	1.0993	-0.0824
C(17)-H(37)	1.0054	1.0985	-0.0931
C(19)-C(20)	1.5027	1.5454	-0.0427
		RMS value:	0.0636

III. Bond Angles

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(15)-O(2)-C(16)	109.377	113.348	-3.971
C(5)-N(3)-C(11)	109.572	110.234	-0.662
C(5)-N(3)-H(21)	125.762	124.517	1.245
C(11)-N(3)-H(21)	124.662	125.249	-0.587
C(13)-N^+(4)-C(14)	108.477	111.547	-3.070
C(13)-N^+(4)-C(17)	113.790	113.263	0.527
C(13)-N^+(4)-H(22)	109.253	107.912	1.341
C(14)-N^+(4)-C(17)	109.039	110.515	-1.476
C(14)-N^+(4)-H(22)	107.983	106.218	1.765
C(17)-N^+(4)-H(22)	108.150	106.995	1.155
N(3)-C(5)-C(6)	108.315	107.505	0.810
N(3)-C(5)-C(18)	120.131	124.926	-4.795
C(6)-C(5)-C(18)	131.553	127.568	3.985

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(5)-C(6)-C(12)	106.665	106.704	-0.039
C(5)-C(6)-C(19)	126.223	125.843	0.380
C(12)-C(6)-C(19)	127.058	127.451	-0.393
O(1)-C(7)-C(8)	120.263	121.947	-1.684
O(1)-C(7)-C(12)	124.722	121.404	3.318
C(8)-C(7)-C(12)	114.988	116.648	-1.660
C(7)-C(8)-C(9)	111.926	110.926	1.000
C(7)-C(8)-C(13)	108.773	109.642	-0.869
C(7)-C(8)-H(23)	106.963	106.259	0.704
C(9)-C(8)-C(13)	114.381	112.674	1.707
C(9)-C(8)-H(23)	108.145	108.447	-0.302
C(13)-C(8)-H(23)	106.242	108.545	-2.303
C(8)-C(9)-C(10)	112.752	112.491	0.261
C(8)-C(9)-H(24)	109.438	109.209	0.229
C(8)-C(9)-H(25)	109.504	110.515	-1.011
C(10)-C(9)-H(24)	107.955	109.418	-1.463
C(10)-C(9)-H(25)	108.870	108.412	0.458
H(24)-C(9)-H(25)	108.212	106.620	1.592
C(9)-C(10)-C(11)	108.780	109.298	-0.518
C(9)-C(10)-H(26)	109.995	110.319	-0.324
C(9)-C(10)-H(27)	109.580	110.329	-0.749
C(11)-C(10)-H(26)	110.784	110.131	0.653
C(11)-C(10)-H(27)	109.965	109.239	0.726
H(26)-C(10)-H(27)	107.725	107.502	0.223
N(3)-C(11)-C(10)	125.117	128.914	-3.797
N(3)-C(11)-C(12)	108.340	106.866	1.474
C(10)-C(11)-C(12)	126.540	124.217	2.323
C(6)-C(12)-C(7)	131.527	130.038	1.489
C(6)-C(12)-C(11)	107.104	108.691	-1.587
C(7)-C(12)-C(11)	121.354	121.268	0.086
N^+(4)-C(13)-C(8)	115.280	117.888	-2.608
N^+(4)-C(14)-C(15)	110.269	109.742	0.527
N^+(4)-C(14)-H(30)	108.250	107.200	1.050
N^+(4)-C(14)-H(31)	110.602	107.710	2.892
C(15)-C(14)-H(30)	108.666	112.001	-3.335
C(15)-C(14)-H(31)	110.395	111.834	-1.439
H(30)-C(14)-H(31)	108.593	108.153	0.440
O(2)-C(15)-C(14)	110.792	108.775	2.017
O(2)-C(15)-H(32)	110.772	110.256	0.516
O(2)-C(15)-H(33)	109.027	108.905	0.122

Bond	Theta (in degrees) Crystal	MM3	Difference (in degrees)
C(14)-C(15)-H(32)	108.885	111.707	-2.822
C(14)-C(15)-H(33)	109.184	110.120	-0.936
H(32)-C(15)-H(33)	108.126	107.036	1.090
O(2)-C(16)-C(17)	111.302	109.024	2.278
O(2)-C(16)-H(34)	109.519	108.887	0.632
O(2)-C(16)-H(35)	109.375	110.193	-0.818
C(17)-C(16)-H(34)	110.701	110.084	0.617
C(17)-C(16)-H(35)	107.134	111.609	-4.475
H(34)-C(16)-H(35)	108.741	106.995	1.746
N^+(4)-C(17)-C(16)	110.995	109.718	1.277
N^+(4)-C(17)-H(36)	110.041	107.159	2.882
N^+(4)-C(17)-H(37)	110.984	107.927	3.057
C(16)-C(17)-H(36)	107.928	112.237	-4.309
C(16)-C(17)-H(37)	109.731	111.334	-1.603
H(36)-C(17)-H(37)	107.035	108.285	-1.250
		RMS value:	1.932

IV. Dihedral Angles

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
O(1)-C(7)-C(8)-C(9)	146.5	148.5	-2.0
O(1)-C(7)-C(8)-C(13)	19.2	23.5	-4.3
O(1)-C(7)-C(8)-H(23)	-95.2	-93.8	-1.4
O(1)-C(7)-C(12)-C(6)	7.0	4.0	3.0
O(1)-C(7)-C(12)-C(11)	-174.6	-176.8	2.2
O(2)-C(15)-C(14)-N^+(4)	59.1	57.2	1.9
O(2)-C(15)-C(14)-H(30)	-59.4	-61.8	2.4
O(2)-C(15)-C(14)-H(31)	-178.4	176.6	5.0
O(2)-C(16)-C(17)-N^+(4)	-57.5	-56.8	-0.7
O(2)-C(16)-C(17)-H(36)	63.1	62.3	0.8
O(2)-C(16)-C(17)-H(37)	179.4	-176.2	-4.4
N(3)-C(5)-C(6)-C(12)	0.7	-0.1	0.8
N(3)-C(5)-C(6)-C(19)	178.1	-179.6	-2.3
N(3)-C(11)-C(10)-C(9)	-161.8	-156.7	-5.1
N(3)-C(11)-C(10)-H(26)	-40.8	-35.3	-5.5
N(3)-C(11)-C(10)-H(27)	78.2	82.5	-4.3
N(3)-C(11)-C(12)-C(6)	0.3	0.0	0.3
N(3)-C(11)-C(12)-C(7)	-178.4	-179.4	1.0
N^+(4)-C(13)-C(8)-C(7)	-162.8	-177.9	15.1

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
N^+(4)-C(13)-C(8)-C(9)	71.2	58.0	13.2
N^+(4)-C(13)-C(8)-H(23)	-48.0	-62.1	14.1
N^+(4)-C(14)-C(15)-H(32)	-63.0	-64.8	1.8
N^+(4)-C(14)-C(15)-H(33)	179.2	176.4	2.8
N^+(4)-C(17)-C(16)-H(34)	-179.6	-176.1	-3.5
N^+(4)-C(17)-C(16)-H(35)	62.0	65.2	-3.2
C(5)-N(3)-C(11)-C(10)	-179.3	179.4	1.3
C(5)-N(3)-C(11)-C(12)	0.1	0.0	0.1
C(5)-C(6)-C(12)-C(7)	177.9	179.3	-1.4
C(5)-C(6)-C(12)-C(11)	-0.6	0.1	-0.7
C(5)-C(6)-C(19)-C(20)	-97.5	-96.1	-1.4
C(6)-C(5)-N(3)-C(11)	-0.5	0.1	-0.6
C(6)-C(5)-N(3)-H(21)	178.8	-180.0	-1.2
C(6)-C(12)-C(7)-C(8)	-171.1	-175.7	4.6
C(6)-C(12)-C(11)-C(10)	179.7	-179.5	-0.8
C(7)-C(8)-C(9)-C(10)	56.7	56.8	-0.1
C(7)-C(8)-C(9)-H(24)	-63.5	-64.9	1.4
C(7)-C(8)-C(9)-H(25)	178.0	178.1	-0.1
C(7)-C(12)-C(6)-C(19)	0.5	-1.2	1.7
C(7)-C(12)-C(11)-C(10)	1.0	1.1	-0.1
C(8)-C(7)-C(12)-C(11)	7.3	3.5	3.8
C(8)-C(9)-C(10)-C(11)	-46.6	-51.2	4.6
C(8)-C(9)-C(10)-H(26)	-168.1	-172.4	4.3
C(8)-C(9)-C(10)-H(27)	73.6	68.9	4.7
C(8)-C(13)-N^+(4)-C(14)	-173.2	-175.7	2.5
C(8)-C(13)-N^+(4)-C(17)	65.2	58.8	6.4
C(8)-C(13)-N^+(4)-H(22)	-55.7	-59.4	3.7
C(9)-C(8)-C(7)-C(12)	-35.2	-31.7	-3.5
C(9)-C(10)-C(11)-C(12)	18.9	22.7	-3.8
C(10)-C(9)-C(8)-C(13)	-179.0	-179.8	0.8
C(10)-C(9)-C(8)-H(23)	-60.9	-59.5	-1.4
C(10)-C(11)-N(3)-H(21)	1.4	-0.5	1.9
C(11)-N(3)-C(5)-C(18)	179.8	179.8	0.0
C(11)-C(10)-C(9)-H(24)	74.4	70.4	4.0
C(11)-C(10)-C(9)-H(25)	-168.4	-173.7	5.3
C(11)-C(12)-C(6)-C(19)	-178.1	179.6	2.3
C(12)-C(6)-C(5)-C(18)	-179.7	-179.8	0.1
C(12)-C(6)-C(19)-C(20)	79.4	84.5	-5.1
C(12)-C(7)-C(8)-C(13)	-162.6	-156.8	-5.8
C(12)-C(7)-C(8)-H(23)	83.0	86.0	-3.0

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
C(12)-C(11)-N(3)-H(21)	-179.2	-180.0	0.8
C(12)-C(11)-C(10)-H(26)	140.0	144.1	-4.1
C(12)-C(11)-C(10)-H(27)	-101.1	-98.1	-3.0
C(13)-N^+(4)-C(14)-C(15)	-177.1	178.5	4.4
C(13)-N^+(4)-C(14)-H(30)	-58.4	-59.7	1.3
C(13)-N^+(4)-C(14)-H(31)	60.5	56.5	4.0
C(13)-N^+(4)-C(17)-C(16)	178.3	-179.7	-2.0
C(13)-N^+(4)-C(17)-H(36)	53.9	58.2	-4.3
C(13)-N^+(4)-C(17)-H(37)	-64.4	-58.2	-6.2
C(13)-C(8)-C(9)-H(24)	60.8	58.5	2.3
C(13)-C(8)-C(9)-H(25)	-57.7	-58.5	0.8
C(14)-N^+(4)-C(17)-C(16)	52.0	54.3	-2.3
C(14)-N^+(4)-C(17)-H(36)	-67.4	-67.8	0.4
C(14)-N^+(4)-C(17)-H(37)	174.3	175.8	-1.5
C(14)-C(15)-O(2)-C(16)	-63.0	-63.1	0.1
C(15)-O(2)-C(16)-C(17)	62.2	62.9	-0.7
C(15)-O(2)-C(16)-H(34)	-175.1	-177.0	1.9
C(15)-O(2)-C(16)-H(35)	-56.0	-59.9	3.9
C(15)-C(14)-N^+(4)-C(17)	-52.7	-54.6	1.9
C(15)-C(14)-N^+(4)-H(22)	64.6	61.1	3.5
C(16)-O(2)-C(15)-H(32)	58.0	59.8	-1.8
C(16)-O(2)-C(15)-H(33)	176.8	176.9	-0.1
C(16)-C(17)-N^+(4)-H(22)	-65.1	-60.9	-4.2
C(17)-N^+(4)-C(14)-H(30)	66.1	67.3	-1.2
C(17)-N^+(4)-C(14)-H(31)	-175.1	-176.6	1.5
C(18)-C(5)-N(3)-H(21)	-0.9	-0.2	-0.7
C(18)-C(5)-C(6)-C(19)	-2.2	0.7	-2.9
H(22)-N^+(4)-C(14)-H(30)	-176.7	-177.0	0.3
H(22)-N^+(4)-C(14)-H(31)	-57.8	-60.8	3.0
H(22)-N^+(4)-C(17)-H(36)	175.5	177.0	-1.5
H(22)-N^+(4)-C(17)-H(37)	57.2	60.5	-3.3
H(23)-C(8)-C(9)-H(24)	178.9	178.8	0.1
H(23)-C(8)-C(9)-H(25)	60.5	61.8	-1.3
H(24)-C(9)-C(10)-H(26)	-47.1	-50.9	3.8
H(24)-C(9)-C(10)-H(27)	-165.4	-169.5	4.1
H(25)-C(9)-C(10)-H(26)	70.1	65.0	5.1
H(25)-C(9)-C(10)-H(27)	-48.1	-53.6	5.5
H(30)-C(14)-C(15)-H(32)	178.5	176.3	2.2
H(30)-C(14)-C(15)-H(33)	60.7	57.5	3.2
H(31)-C(14)-C(15)-H(32)	59.5	54.7	4.8

Bond	Omega (in degrees) Crystal	MM3	Difference (in degrees)
H(31)-C(14)-C(15)-H(33)	-58.3	-64.1	5.8
H(34)-C(16)-C(17)-H(36)	-58.9	-57.1	-1.8
H(34)-C(16)-C(17)-H(37)	57.4	64.5	-7.1
H(35)-C(16)-C(17)-H(36)	-177.3	-175.8	-1.5
H(35)-C(16)-C(17)-H(37)	-61.0	-54.2	-6.8

RMS value: 3.952