General Methods. All reactions were carried out under a nitrogen or argon atmosphere. Melting points are uncorrected. The column chromatographic separations were performed with Woelm silica gel (230-400 mesh). Solvents were reagent grade and in most cases dried prior to use. The purity of all compounds was shown to be >95% by TLC and high field ^{1}H and ^{13}C NMR. The high-resolution mass spectra were recorded at The Ohio State University Campus Chemical Instrumentation Center. Elemental analyses were performed at Atlantic Microlab, Inc., Norcross, Georgia.

Dialkylations.

B. From 600 mg (3.57 mmol) of **8** and 1.80 g (8.57 mmol) of 1-iodo-5-hexene, there was isolated 800 mg (66%) of **3b** as a colorless oil; IR (neat, cm^{-1}) 1641, 1462, 1285, 1123; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.90-5.70 (m, 2 H), 5.10-4.85 (m, 4 H), 2.15-1.20 (series of m, 28 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.8, 114.7, 64.0, 36.5, 34.5, 33.6, 31.2, 29.5, 24.1, 23.6; HRMS (EI) *m/z* (M^+) calcd for $C_{20}H_{34}O_2S$ 338.2279, obsd 338.2274.

C. From 745 mg (4.40 mmol) of **8** and 2.00 g (8.90 mmol) of 1-iodo-6-heptene, there was isolated 1.08 g (74%) of **3c** as a colorless oil; IR (neat, cm^{-1}) 1290, 1125; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.86-5.71 (m, 2 H), 5.02-4.88 (m, 4 H), 2.10-1.23 (series of m, 32 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.9, 114.3, 63.8, 36.5, 34.3, 33.6, 31.1, 29.6, 28.6, 24.0, 23.8; HRMS (EI) *m/z* (M^+) calcd 366.2592, obsd 366.2578.

Anal. Calcd for $C_{22}H_{38}O_2S$: C, 72.08; H, 10.45. Found: C, 72.21; H, 10.31.

D. From 500 mg (3.00 mmol) of **8** and 1.86 g (7.00 mmol) of 1-iodo-9-decene, there was isolated 1.00 g (75%) of **3d** as colorless crystals, mp 38 °C; IR (neat, cm^{-1}) 1505, 1280, 1120; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.88-5.73 (m, 2 H), 5.03-4.89 (m, 4 H), 2.09-1.21 (series of m, 44 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.2, 114.1, 63.8, 36.5, 34.3, 33.8, 31.1, 30.1, 29.4, 29.3, 29.1, 28.9, 24.0, 23.9; HRMS (EI) *m/z* (M^+) calcd 450.3532, obsd 450.3540.

Anal. Calcd for $C_{28}H_{50}O_2S$: C, 74.61; H, 11.18. Found: C, 74.42; H, 11.28.

Ring Closing Metathesis of 3b. A solution of Grubbs' catalyst (100 mg, 0.11 mmol) in refluxing dry CH_2Cl_2 (100 mL) under N_2 was slowly treated with a solution of **3b** (500 mg, 1.48 mmol) in dry CH_2Cl_2 (200 mL) in a high dilution apparatus. The addition required 30 h. After 4 h of additional heating, the predescribed workup afforded 110 mg (24%) of an inseparable 3.5:1 mixture (^{13}C NMR analysis) of **15** and **16**, along with 90 mg (20%) of **19**.

For **15/16**: colorless crystals, mp 204-207 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 5.39-5.29 (m, 4 H), 2.18-1.19 (series of m, 56 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (major isomer) 130.6, 63.5, 35.6, 34.4, 31.9, 30.4, 29.7, 23.9, 22.8; FAB MS *m/z* (M^+ + H) calcd for $C_{36}H_{60}O_4S_2$ 621.39, obsd 621.38.

For **19**: colorless oil; ^1H NMR (300 MHz, $CDCl_3$) δ 5.40-5.33 (m, 6 H), 2.12-1.21 (series of m, 84 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 130.3 (m), 63.8 (s), 36.0 (m), 34.2 (s), 31.8 (m), 30.9 (m), 29.7 (m), 23.9 (m), 22.9 (m); FAB MS *m/z* (M^+ + H) calcd for $C_{54}H_{90}O_6S_3$ 931.59, obsd 931.57.

This material was directly hydrogenated.

Hydrogenation of 15/16. A solution of the dimer mixture (50 mg, 0.16 mmol) in ethyl acetate (50 mL) containing 5% palladium on charcoal (100 mg) was stirred under an atm of H_2 for 24 h and processed as described above to give 50 mg (100%) of **21** as colorless crystals, mp 273-275 °C (dec) (from CH_2Cl_2/hexanes); ^1H NMR (300 MHz, $CDCl_3$) δ 2.14-1.45 (series of m, 34 H), 1.45-1.14 (series of m, 30 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 63.8, 35.5, 34.3, 30.8, 29.2, 28.7, 27.9, 24.0, 23.2; FAB MS *m/z* (M^+ + H) calcd for $C_{36}H_{64}O_4S_2$ 625.42, obsd 625.49.

Hydrogenation of 19. Catalytic reduction of **19** (40 mg, 0.13 mmol) as described above gave **20** (40 mg, 100%) as a colorless crystalline solid, mp 209-210 °C (from CH_2Cl_2/hexanes); ^1H NMR (300 MHz, $CDCl_3$) δ 2.06-1.35 (series of m, 56 H), 1.35-0.97 (series of m, 40 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 63.8 (s), 36.3 (m), 34.3 (s), 31.0 (m), 29.8 (s), 28.9 (m), 28.8 (m), 24.0 (s), 23.7 (m); FAB MS *m/z* (M^+ + H) calcd for $C_{54}H_{96}O_6S_3$ 937.64, obsd 937.73.

Ring Closing Metathesis of 3c. Exposure of **3c** (490 mg, 1.34 mmol) to Grubbs' catalyst (100 mg, 0.11 mmol) in dry CH_2Cl_2 (300 mL) under N_2 in a high dilution apparatus during 30 h was followed by chromatography on silica gel. Gradient elution with 10-20% ethyl acetate in hexanes gave 140 mg (30%) of **22** (or **23**) and 50 mg (11%) of **24**.

For **22** (or **23**): colorless crystals, mp 262-265 °C; IR (neat, cm^{-1}) 1274, 1112; ^1H NMR (300 MHz, $CDCl_3$) δ 5.39-5.30 (m, 4 H), 2.09-1.23 (series of m, 64 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 130.4, 63.7, 36.1, 34.3, 32.2, 31.0, 29.1, 28.8, 24.0, 23.8; FAB MS *m/z* (M^+ + H) calcd 677.46, obsd 677.39.

Anal. Calcd for $C_{40}H_{68}O_4S_2$: C, 70.69; H, 10.12. Found: C, 70.57; H, 10.04.

For **24**: colorless crystals, mp 188-190 °C; IR (neat, cm^{-1}) 1275, 1110; ^1H NMR (300 MHz, $CDCl_3$) δ 5.41-5.30 (m, 6 H), 2.10-1.21 (series of m, 96 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 130.3, 63.8, 36.4, 32.3, 31.1, 29.4, 29.1, 24.0, 23.8; FAB MS *m/z* (M^+ + H) calcd 1015.68, obsd 1015.89.

Anal. Calcd for $C_{60}H_{102}O_6S_3$: C, 70.69; H, 10.12. Found: C, 70.53; H, 10.13.

Ring Closing Metathesis of 3d. Reaction of **3b** (620 mg, 1.4 mmol) with 100 mg (0.11 mmol) of Grubbs' catalyst as described above afforded 150 mg (25%) of a 6.5:3.5 mixture of **29** and **30**, 170 mg (29%) of **31**, 100 mg (17%) of **32**, and 50 mg (8%) of a tetramer from the group **33-36**.

For the **29/30** mixture: white solid, mp 60-61 °C; IR (neat, cm^{-1}) 1455, 1280, 1120; ^1H NMR (300 MHz, $CDCl_3$) δ 5.40-5.36 (*E*, m, 1.3 H), 5.30 (*Z*, t, *J* = 4.8 Hz, 0.7 H), 2.13-1.12 (series of m, 44 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 130.5 (*E*), 130.0 (*Z*), 64.3 (*Z*), 64.2 (*E*), 37.0 (*Z*), 36.3 (*E*), 34.1 (*Z*), 34.0 (*E*), 33.0 (*Z*), 32.4 (*E*), 32.4 (*E*), 30.2 (*Z*), 29.3 (*E*), 29.1 (*Z*), 28.1 (*E*), 28.1 (*Z*), 27.9 (*E*), 27.6 (*E*), 27.4 (*Z*), 27.2 (*Z*), 27.2 (*Z*), 26.9 (*E*), 24.1 (*Z*), 24.1 (*E*), 22.0 (*E*), 21.6 (*Z*); FAB MS *m/z* (M^+ + H) calcd 423.32, obsd 423.28.

Anal. Calcd for $C_{26}H_{46}O_2S$: C, 73.88; H, 10.97. Found: C, 73.90; H, 10.92.

For **31**: colorless crystals, mp 160-163 °C; IR (neat, cm^{-1}) 1455, 1280, 1120; ^1H NMR (300 MHz, $CDCl_3$) δ 5.37-5.32 (m, 4 H), 2.04-1.43 (series of m, 44 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 130.3, 63.7, 36.3, 34.2, 32.3, 31.0, 29.9, 29.2, 29.2, 29.0, 28.6, 23.9, 23.8; FAB MS *m/z* (M^+ + H) calcd 845.64, obsd 845.64.

Anal. Calcd for $C_{52}H_{92}O_4S_2$: C, 73.88; H, 10.97. Found: C, 73.93; H, 10.71.

For **32**: waxy white solid; IR (neat, cm^{-1}) 1275, 1120; ^1H NMR (300 MHz, $CDCl_3$) δ 5.39-5.34 (m, 6 H), 2.09-1.44 (series of m, 66 H), 1.42-1.20 (series of m, 66 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 130.3, 63.8, 36.4, 34.3, 32.5, 31.1, 30.1, 29.6, 29.4, 29.3, 28.9, 24.0, 23.8; FAB MS *m/z* (M^+ + H) calcd 1267.97, obsd 1268.05.

Anal. Calcd for $C_{78}H_{138}O_6S_3$: C, 73.88; H, 10.97. Found: C, 74.02; H, 11.08.

For the tetramer: waxy white solid; IR (neat, cm^{-1}) 1280, 1120; ^1H NMR (300 MHz, $CDCl_3$) δ 5.40-5.34 (m, 8 H), 2.08-1.42 (series of m, 88 H), 1.41-1.18 (series of m, 88 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 130.3, 63.8, 36.4, 34.3, 32.5, 31.0, 30.2, 29.6, 29.4, 29.3, 29.1, 24.0, 23.9; FAB MS *m/z* (M^+ + H) calcd 1691.29, obsd 1691.24.

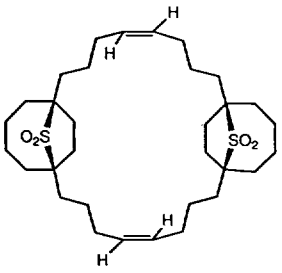
Anal. Calcd for $C_{104}H_{184}O_8S_4$: C, 73.88 H, 10.97. Found: C, 74.06; H, 10.83.

Energy Minimization Study

The following structures were minimized using the MonteCarlo conformational searching method. Energies for each unique conformer were calculated using the MM3 force field. Each conformational search was allowed 1000 iterations to locate the global minimum.

Conformers of interest were selected by scanning the local minima found by the conformational searching protocol. All conformers of interest were again minimized using the Full-Matrix Newton Raphson method to ensure accurate relative energies were found.

Below the data is summarized. Two dimensional representations of the coordinates found for each conformer of interest are included and can be correlated with the summary data below by way of file name. The energy output files are also included.



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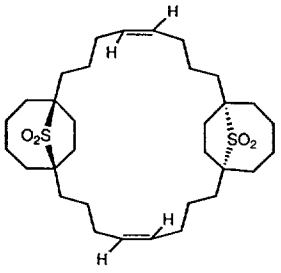
Aligned Double Bonds



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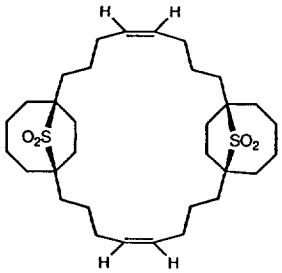
Aligned Double Bonds



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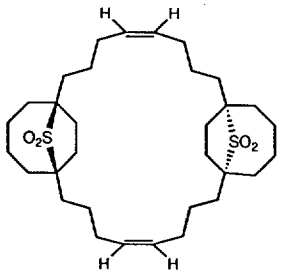

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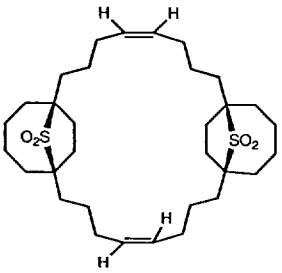

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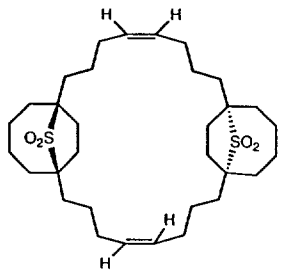

Structure 6
File Name: 100699jstf.*

E (Kcal/mole): 90.78

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up       up
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Aligned Double Bonds

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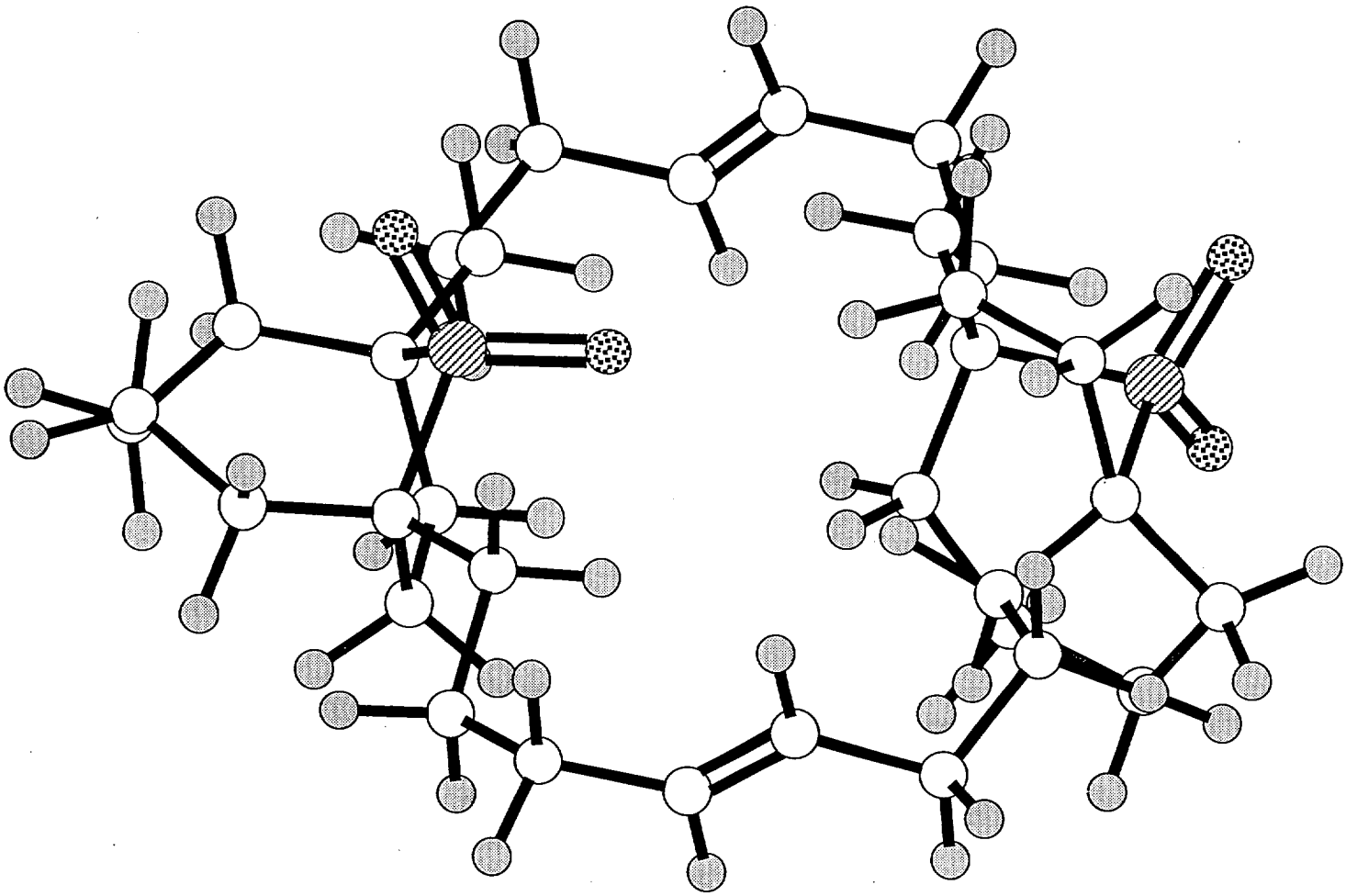

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092899jstf1.*
Orthoganol Double bonds

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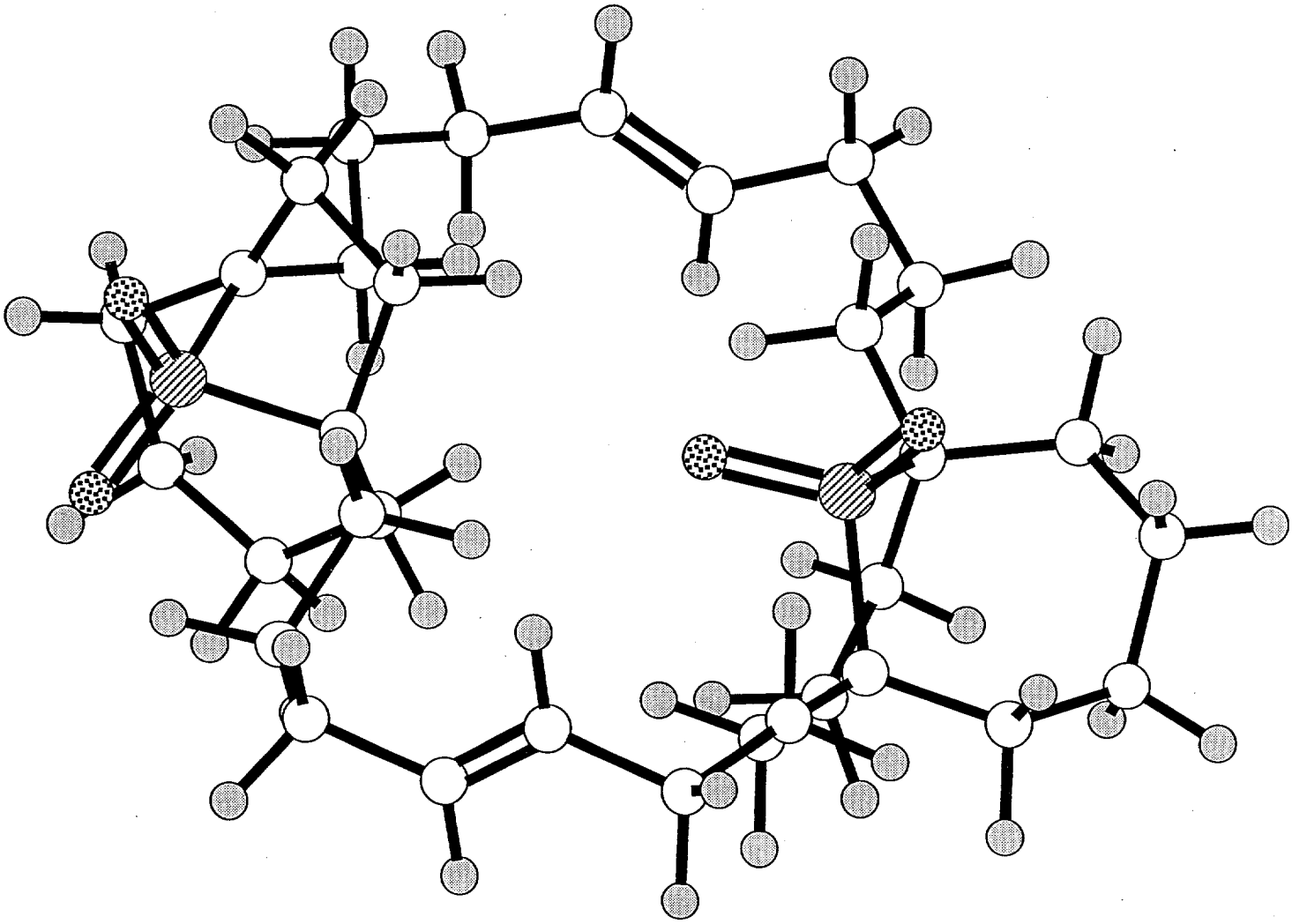

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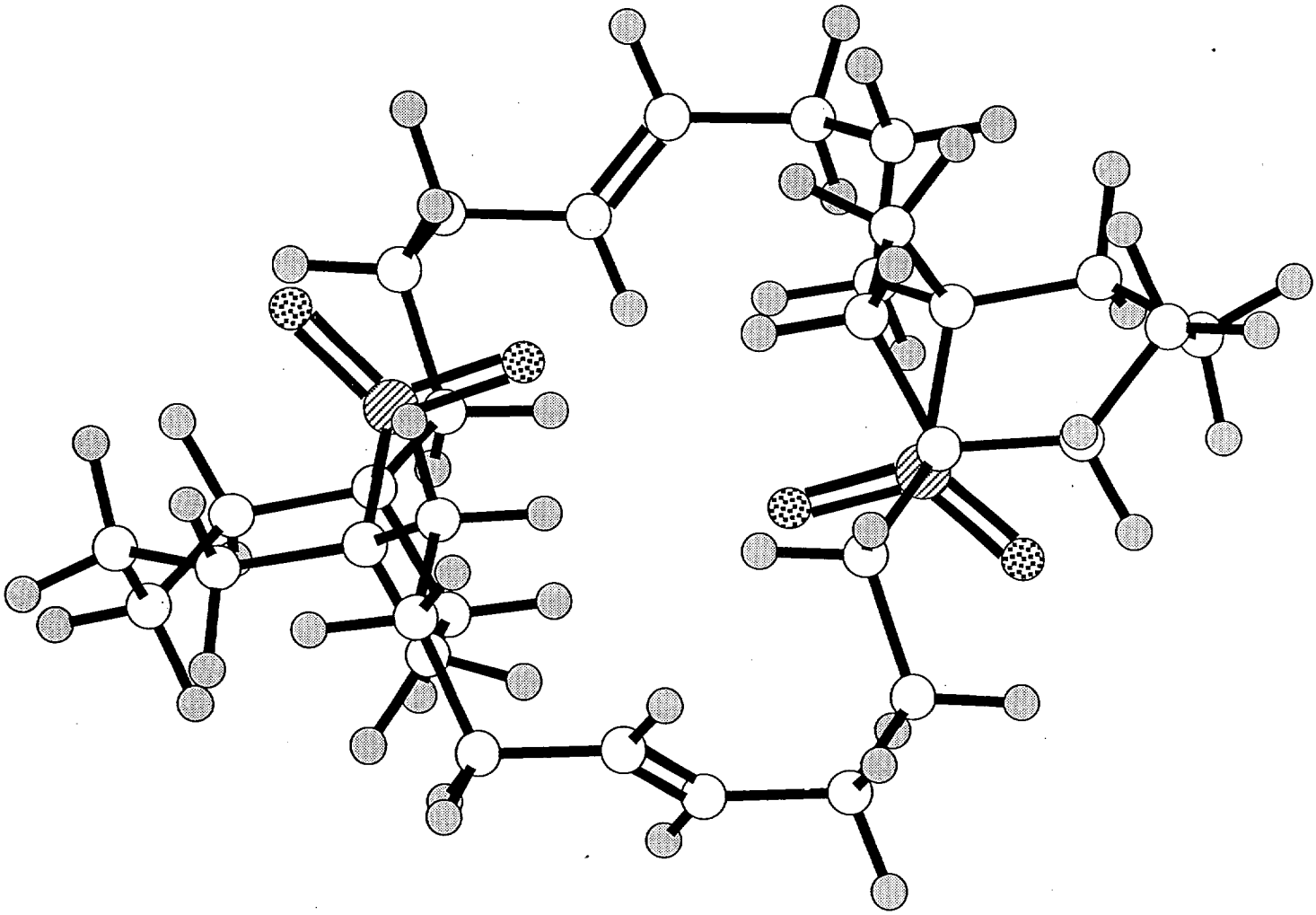

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up    down
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100599jstf.*
double bonds aligned

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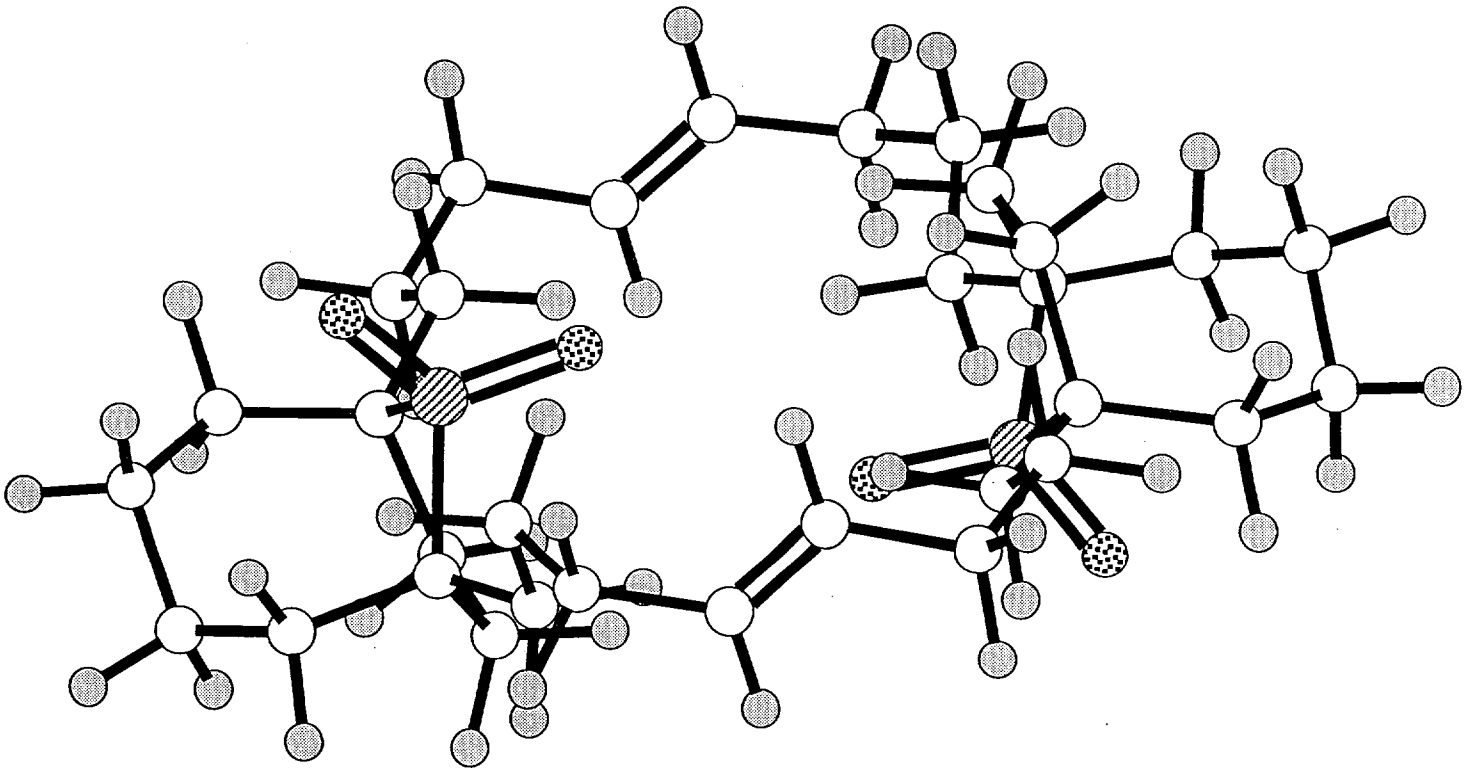
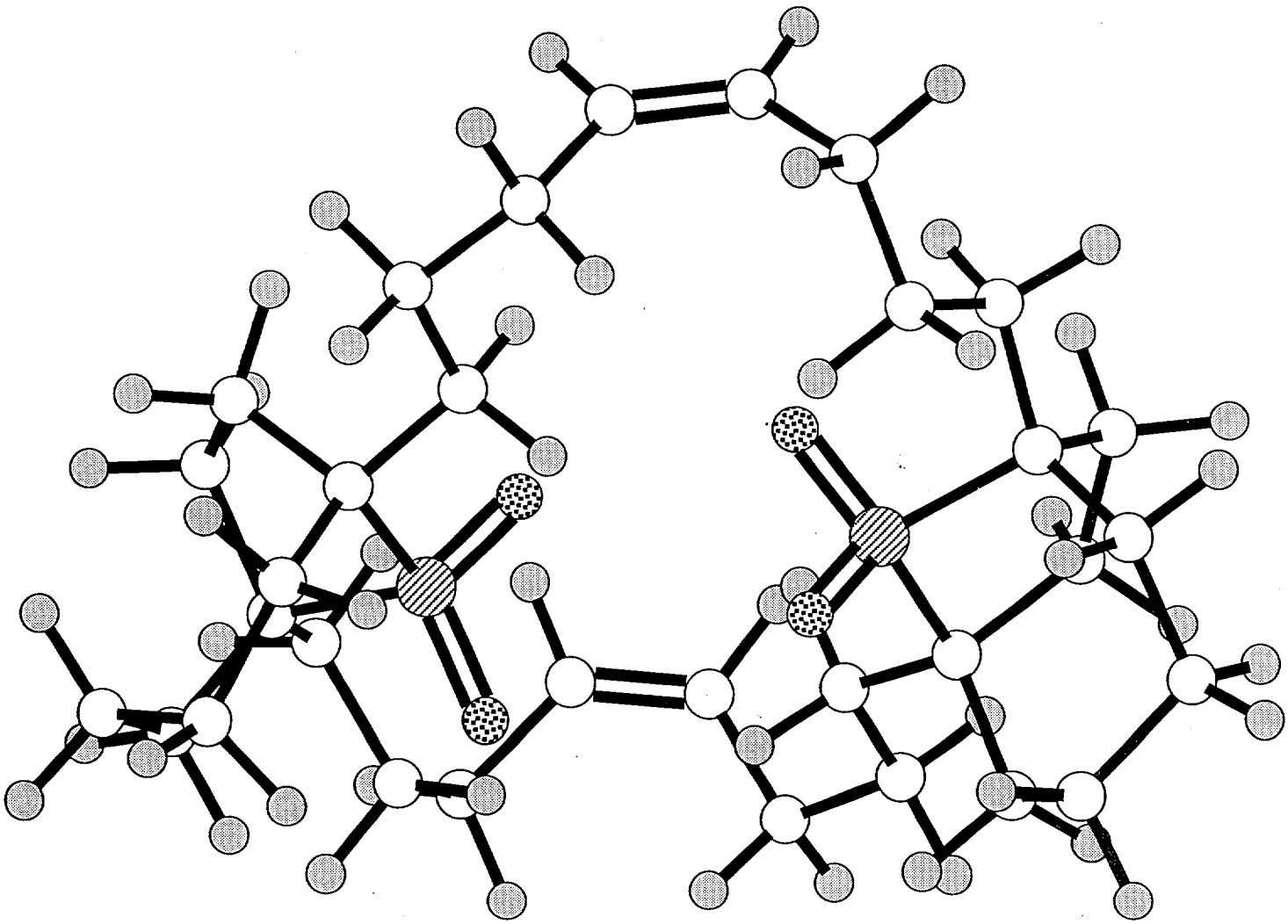
 DONE  001
```



```
  Cis
up   up
  Cis

100199jstf.*

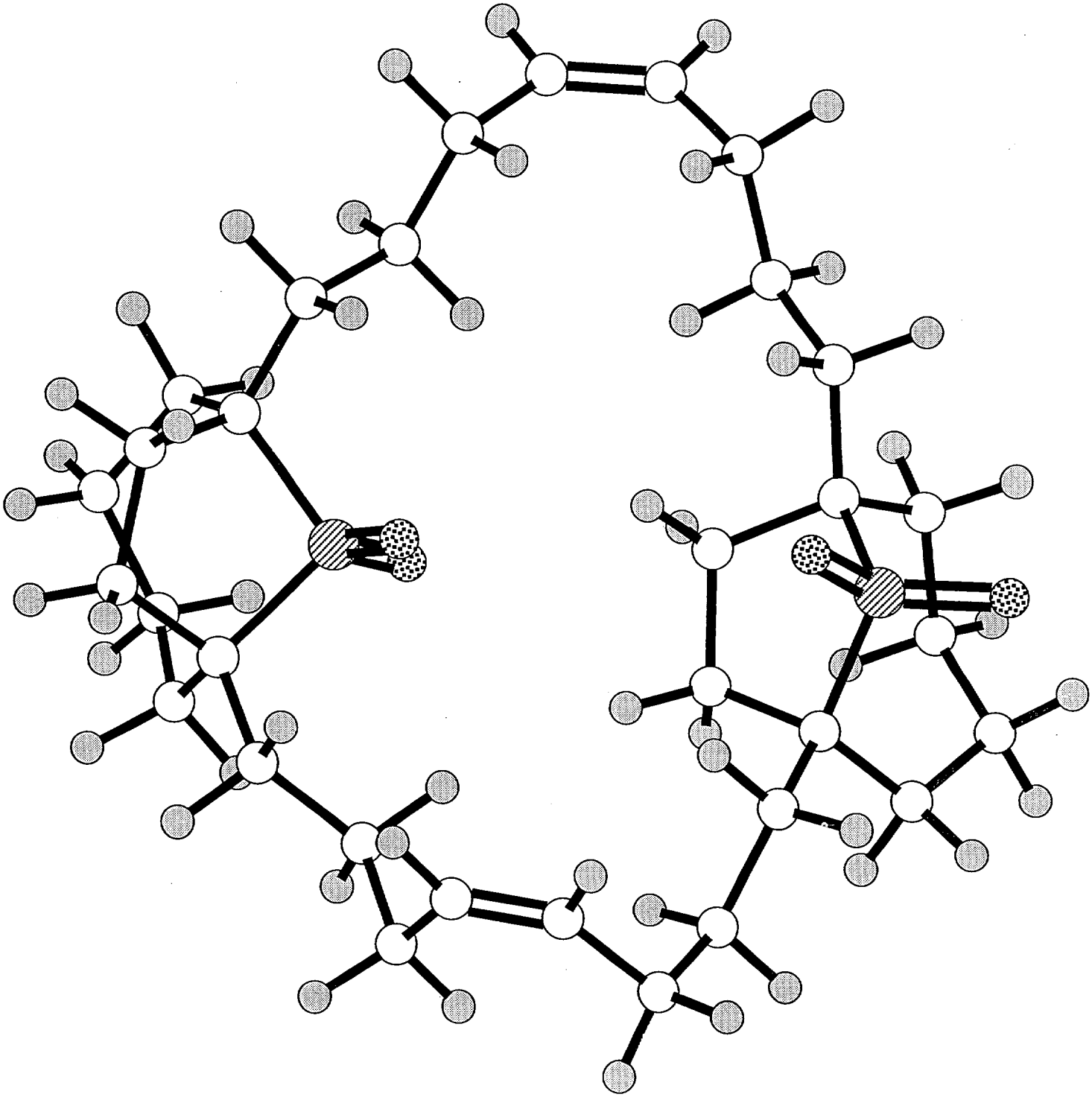
 STRT  001 BatchMin V5.0 : Job started
 STRT  002 Reading force field...
 STRT  003 Generating interactions...
 STRT  004 Loading parameters from force field...
 FFLD  002 WARNING - Conformational Energies May Not Be Accurate
 FFLD  001 Low quality force field parameters in use:
 FFLD  001 Number of low quality stretches, bends & torsions =  16  24  68
 STRT  005 Simulation initiated...
 MINI  010          Total Energy = 0.3907987E+03 kJ/mol
 MINI  011               Stretch = 0.1674799E+02 kJ/mol
 MINI  012                 Bend = 0.7989955E+02 kJ/mol
 MINI  013               Torsion = 0.1030677E+03 kJ/mol
 MINI  014      Improper Torsion = 0.8256868E-03 kJ/mol
 MINI  015                 VDW = 0.1585043E+03 kJ/mol
 MINI  016         Electrostatic = 0.3012663E+02 kJ/mol
 MINI  017 Explicit Hydrogen Bonds = 0.0000000E+00 kJ/mol
 MINI  021           Cross Terms = 0.2451735E+01 kJ/mol
 MINI  040  No more updates
 MINI  003 Iter     1  Movt 0.000000A  Energy     390.795 kJ/mol
 MINI  005 Minimization converged; gradient = 0.191E-01 .LT.  0.500E-01
 MINI  008 Computing final energy, standby...
 MINI  009 Final Gradient =  0.191E-01 kJ/A-mol    CPU Time =      1.0 sec
 MINI  010          Total Energy = 0.3907439E+03 kJ/mol
 MINI  011               Stretch = 0.1672766E+02 kJ/mol
 MINI  012                 Bend = 0.7988091E+02 kJ/mol
 MINI  013               Torsion = 0.1030905E+03 kJ/mol
 MINI  014      Improper Torsion = 0.7872430E-03 kJ/mol
 MINI  015                 VDW = 0.1584818E+03 kJ/mol
 MINI  016         Electrostatic = 0.3011526E+02 kJ/mol
 MINI  017 Explicit Hydrogen Bonds = 0.0000000E+00 kJ/mol
 MINI  021           Cross Terms = 0.2446979E+01 kJ/mol
 MINI  040  No more updates
 DONE  001
```



```
  cis
up  down
  cis

100299jstf.*

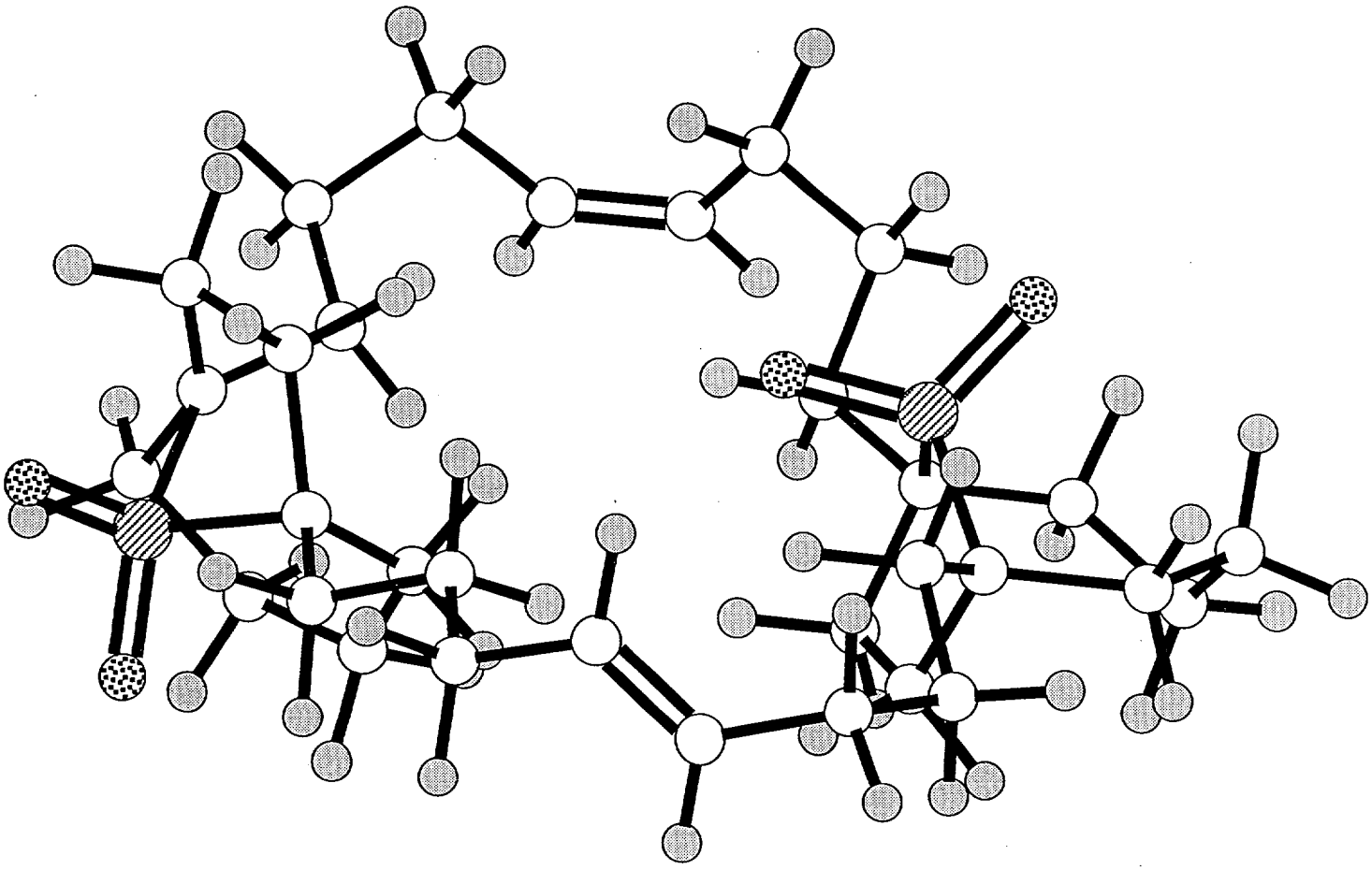
 STRT  001 BatchMin V5.0 : Job started
 STRT  002 Reading force field...
 STRT  003 Generating interactions...
 STRT  004 Loading parameters from force field...
 FFLD  002 WARNING - Conformational Energies May Not Be Accurate
 FFLD  001 Low quality force field parameters in use:
 FFLD  001 Number of low quality stretches, bends & torsions =  16  24  68
 STRT  005 Simulation initiated...
 MINI  010          Total Energy = 0.3842549E+03 kJ/mol
 MINI  011               Stretch = 0.1579288E+02 kJ/mol
 MINI  012                 Bend = 0.8328587E+02 kJ/mol
 MINI  013               Torsion = 0.9806135E+02 kJ/mol
 MINI  014      Improper Torsion = 0.3214357E-01 kJ/mol
 MINI  015                 VDW = 0.1665658E+03 kJ/mol
 MINI  016         Electrostatic = 0.1748298E+02 kJ/mol
 MINI  017 Explicit Hydrogen Bonds = 0.0000000E+00 kJ/mol
 MINI  021          Cross Terms = 0.3033883E+01 kJ/mol
 MINI  040  No more updates
 MINI  003 Iter     1  Movt 0.000000A  Energy     384.255 kJ/mol
 MINI  005 Minimization converged; gradient = 0.101E-03 .LT.  0.500E-01
 MINI  008 Computing final energy, standby...
 MINI  009 Final Gradient =  0.101E-03 kJ/A-mol    CPU Time =     1.0 sec
 MINI  010          Total Energy = 0.3842162E+03 kJ/mol
 MINI  011               Stretch = 0.1577544E+02 kJ/mol
 MINI  012                 Bend = 0.8328439E+02 kJ/mol
 MINI  013               Torsion = 0.9806608E+02 kJ/mol
 MINI  014      Improper Torsion = 0.3214420E-01 kJ/mol
 MINI  015                 VDW = 0.1665481E+03 kJ/mol
 MINI  016         Electrostatic = 0.1747964E+02 kJ/mol
 MINI  017 Explicit Hydrogen Bonds = 0.0000000E+00 kJ/mol
 MINI  021          Cross Terms = 0.3030449E+01 kJ/mol
 MINI  040  No more updates
 DONE  001
```



```
  cis
up   up
 trans

100799jstf.*

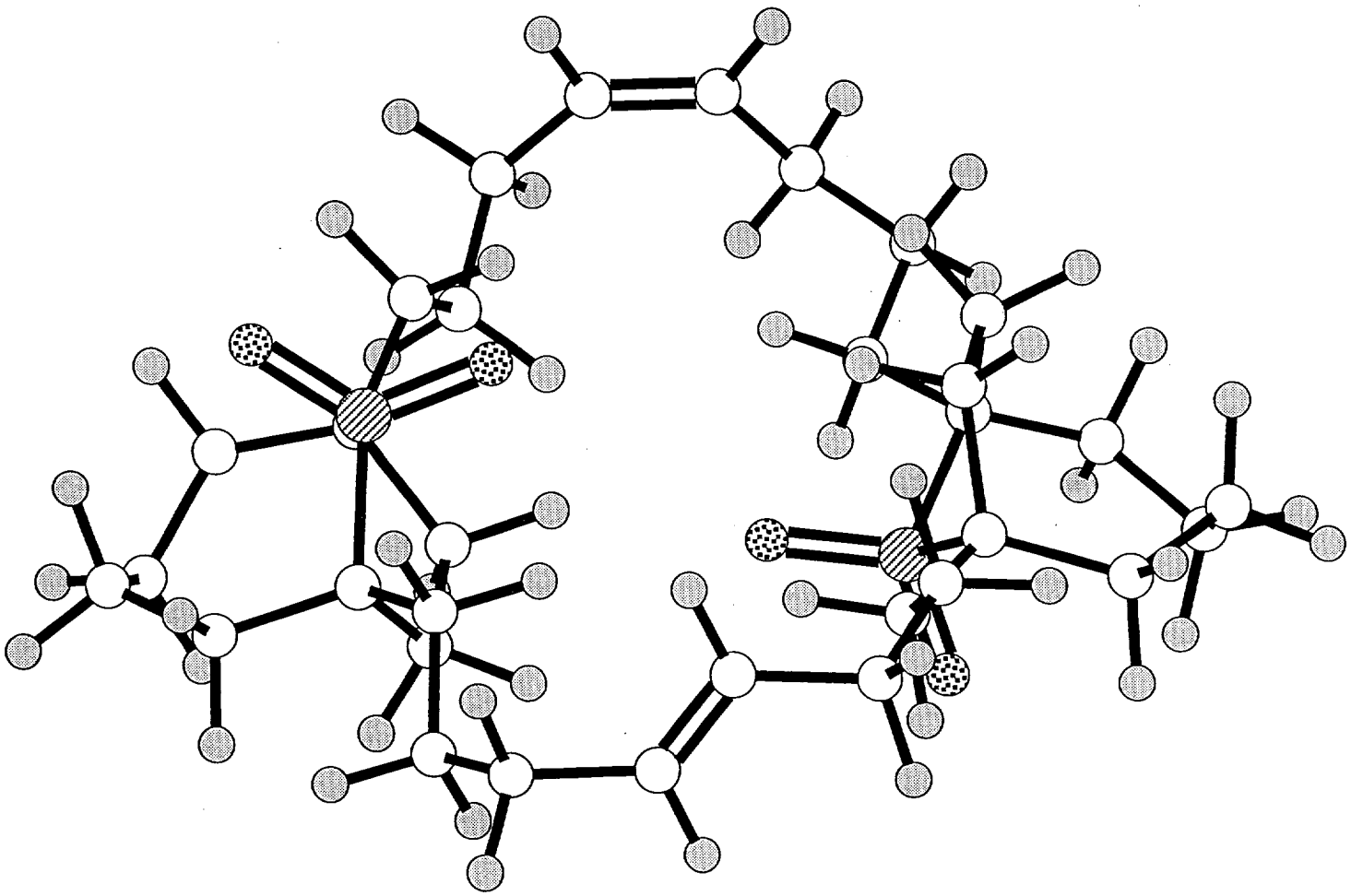
 STRT  001 BatchMin V5.0 : Job started
 STRT  002 Reading force field...
 STRT  003 Generating interactions...
 STRT  004 Loading parameters from force field...
 FFLD  002 WARNING - Conformational Energies May Not Be Accurate
 FFLD  001 Low quality force field parameters in use:
 FFLD  001 Number of low quality stretches, bends & torsions =  16  24  68
 STRT  005 Simulation initiated...
 MINI  010          Total Energy = 0.7065717E+03 kJ/mol
 MINI  011               Stretch = 0.4911411E+02 kJ/mol
 MINI  012                 Bend = 0.2567321E+03 kJ/mol
 MINI  013               Torsion = 0.1150200E+03 kJ/mol
 MINI  014      Improper Torsion = 0.1754528E+00 kJ/mol
 MINI  015                 VDW = 0.2536398E+03 kJ/mol
 MINI  016         Electrostatic = 0.1639255E+02 kJ/mol
 MINI  017 Explicit Hydrogen Bonds = 0.0000000E+00 kJ/mol
 MINI  021          Cross Terms = 0.1549763E+02 kJ/mol
 MINI  040  No more updates
 MINI  003 Iter     1  Movt 0.000000A  Energy     706.552 kJ/mol
 MINI  003 Iter     2  Movt 0.000845A  Energy     706.552 kJ/mol
 MINI  005 Minimization converged; gradient = 0.468E-04 .LT.  0.500E-01
 MINI  008 Computing final energy, standby...
 MINI  009 Final Gradient =  0.468E-04 kJ/A-mol    CPU Time =     1.9 sec
 MINI  010          Total Energy = 0.7065128E+03 kJ/mol
 MINI  011               Stretch = 0.4905172E+02 kJ/mol
 MINI  012                 Bend = 0.2568141E+03 kJ/mol
 MINI  013               Torsion = 0.1149620E+03 kJ/mol
 MINI  014      Improper Torsion = 0.1738813E+00 kJ/mol
 MINI  015                 VDW = 0.2535941E+03 kJ/mol
 MINI  016         Electrostatic = 0.1641054E+02 kJ/mol
 MINI  017 Explicit Hydrogen Bonds = 0.0000000E+00 kJ/mol
 MINI  021          Cross Terms = 0.1550662E+02 kJ/mol
 MINI  040  No more updates
 DONE  001
```

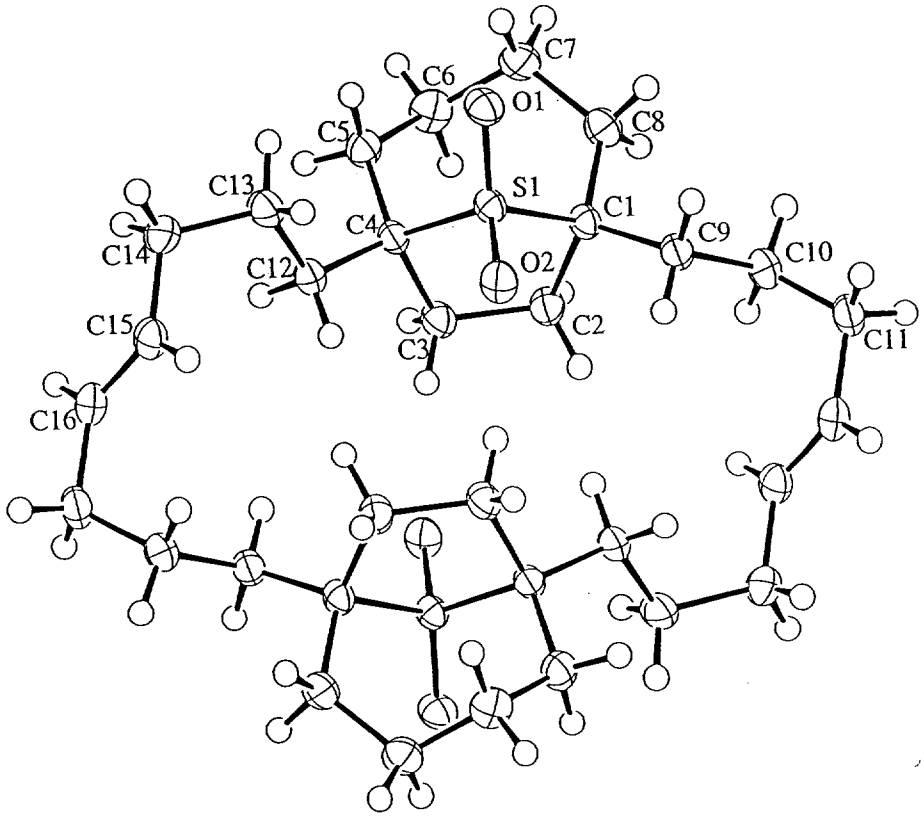


```
 Trans
up   down
 cis

100699jstf.*

 STRT  001 BatchMin V5.0 : Job started
 STRT  002 Reading force field...
 STRT  003 Generating interactions...
 STRT  004 Loading parameters from force field...
 FFLD  002 WARNING - Conformational Energies May Not Be Accurate
 FFLD  001 Low quality force field parameters in use:
 FFLD  001 Number of low quality stretches, bends & torsions =  16  24  68
 STRT  005 Simulation initiated...
 MINI  010          Total Energy = 0.3798779E+03 kJ/mol
 MINI  011               Stretch = 0.1558002E+02 kJ/mol
 MINI  012                 Bend = 0.7818662E+02 kJ/mol
 MINI  013               Torsion = 0.1001260E+03 kJ/mol
 MINI  014      Improper Torsion = 0.2539926E-01 kJ/mol
 MINI  015                 VDW = 0.1651895E+03 kJ/mol
 MINI  016         Electrostatic = 0.1787363E+02 kJ/mol
 MINI  017 Explicit Hydrogen Bonds = 0.0000000E+00 kJ/mol
 MINI  021          Cross Terms = 0.2896641E+01 kJ/mol
 MINI  040  No more updates
 MINI  003 Iter     1  Movt 0.000000A  Energy     379.873 kJ/mol
 MINI  005 Minimization converged; gradient = 0.354E-01 .LT.  0.500E-01
 MINI  008 Computing final energy, standby...
 MINI  009 Final Gradient =  0.354E-01 kJ/A-mol    CPU Time =      1.0 sec
 MINI  010          Total Energy = 0.3798372E+03 kJ/mol
 MINI  011               Stretch = 0.1560551E+02 kJ/mol
 MINI  012                 Bend = 0.7823550E+02 kJ/mol
 MINI  013               Torsion = 0.9998875E+02 kJ/mol
 MINI  014      Improper Torsion = 0.2665216E-01 kJ/mol
 MINI  015                 VDW = 0.1651879E+03 kJ/mol
 MINI  016         Electrostatic = 0.1787999E+02 kJ/mol
 MINI  017 Explicit Hydrogen Bonds = 0.0000000E+00 kJ/mol
 MINI  021          Cross Terms = 0.2912913E+01 kJ/mol
 MINI  040  No more updates
 DONE  001
```





ORTEP drawing of **9**. The molecular structure is drawn with 50% probability displacement ellipsoids for the nonhydrogen atoms. The hydrogen atoms are drawn with circles of arbitrary radii.

The data collection crystal was a clear,colorless, square plate. All work was done at 203 K using an Oxford Cryosystems Cryostream Cooler. Examination of the diffraction pattern on a Nonius Kappa CCD diffractometer indicated a monoclinic crystal system. Almost a whole sphere of reciprocal space was measured using omega scans with a frame width of 1.0°. Data integration was done with Denzo[1], and scaling and merging of the data was done with Scalepack[1]. Merging the data and averaging the symmetry equivalent reflections (including the Friedel pairs) resulted in an Rint value of 0.035. The teXsan[2] package was used to determine the space group as $P2_1/c$.

The structure was solved by the direct methods procedure in SHELXS-86[3]. The molecule is centered about a crystallographic inversion center. Full-matrix least-squares refinements based on F^2 were performed in SHELXL-93[4].

The hydrogen atoms were included in the model at calculated positions using a riding model with U(H) = 1.2 * Ueq(attached atom). The final refinement cycle was based on all the 3357 intensities and 172 variables and resulted in agreement factors of R1(F) = 0.042 and wR2(F^2) = 0.095. For the subset of data with $I > 2\sigma(I)$, the R1(F) value is 0.036 for 2923 reflections. The final difference electron density map contains maximum and minimum peak heights of 0.24 and -0.36 e/$\AA^3$. Neutral atom scattering factors were used and include terms for anomalous dispersion[5].

References

(1) DENZO: Otwinowski, Z. & Minor, W., Methods in Enzymology, Vol 276: Macromolecular Crystallography, part A, 307-326, (1997), Carter, Jr., C. W. & Sweet, R. M., Eds., Academic Press.

(2) teXsan: Crystal Structure Analysis Package, version 1.7-2, Molecular Structure Corporation, The Woodlands, TX (1995).

(3) SHELXS-86: Sheldrick, G. M., Acta Cryst., (1990), A46, 467-473.

(4) SHELXL-93: Sheldrick, G. M., Universitat Gottingen, Germany, 1993.

(5) International Tables for Crystallography (1992). Volume C. Dordrecht: Kluwer Academic Publishers.

Table 1. Crystallographic Details for **9**.

Empirical formula	C32 H52 O4 S2
Formula weight	564.86
Temperature	203 K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 11.9779(1) A b = 10.1304(1) A c = 13.4330(2) A beta = 116.063(1) deg.
Volume	1464.22(3) A^3
Z	2
Density (calculated)	1.281 Mg/m^3
Absorption coefficient	0.218 mm^-1
F(000)	616
Crystal size	0.12 x 0.27 x 0.27 mm
Theta range for data collection	2.63 to 27.48 deg.
Index ranges	0<=h<=15, 0<=k<=13, -17<=l<=15
Reflections collected	36022
Independent reflections	3357 [R(int) = 0.035]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3357 / 0 / 172
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.036, wR2 = 0.091
R indices (all data)	R1 = 0.042, wR2 = 0.095
Largest diff. peak and hole	0.24 and -0.36 e/A^3

Table 2. Bond Lengths (Å) and Angles (°) for **9**.

S(1)-O(1)	1.445(1)
S(1)-O(2)	1.446(1)
S(1)-C(4)	1.813(1)
S(1)-C(1)	1.819(1)
C(1)-C(9)	1.539(2)
C(1)-C(8)	1.542(2)
C(1)-C(2)	1.549(2)
C(2)-C(3)	1.549(2)
C(2)-H(2A)	0.97
C(2)-H(2B)	0.97
C(3)-C(4)	1.540(2)
C(3)-H(3A)	0.97
C(3)-H(3B)	0.97
C(4)-C(5)	1.534(2)
C(4)-C(12)	1.539(2)
C(5)-C(6)	1.529(2)
C(5)-H(5A)	0.97
C(5)-H(5B)	0.97
C(6)-C(7)	1.527(2)
C(6)-H(6A)	0.97
C(6)-H(6B)	0.97
C(7)-C(8)	1.539(2)
C(7)-H(7A)	0.97
C(7)-H(7B)	0.97
C(8)-H(8A)	0.97
C(8)-H(8B)	0.97
C(9)-C(10)	1.532(2)
C(9)-H(9A)	0.97
C(9)-H(9B)	0.97
C(10)-C(11)	1.528(2)
C(10)-H(10A)	0.97
C(10)-H(10B)	0.97
C(11)-C(16)'	1.502(2)
C(11)-H(11A)	0.97
C(11)-H(11B)	0.97
C(12)-C(13)	1.532(2)
C(12)-H(12A)	0.97
C(12)-H(12B)	0.97
C(13)-C(14)	1.535(2)
C(13)-H(13A)	0.97
C(13)-H(13B)	0.97
C(14)-C(15)	1.496(2)
C(14)-H(14A)	0.97
C(14)-H(14B)	0.97
C(15)-C(16)	1.326(2)
C(15)-H(15)	0.93
C(16)-H(16)	0.93
O(1)-S(1)-O(2)	117.30(6)
O(1)-S(1)-C(4)	112.83(6)
O(2)-S(1)-C(4)	107.87(6)
O(1)-S(1)-C(1)	111.48(6)
O(2)-S(1)-C(1)	108.51(6)
C(4)-S(1)-C(1)	96.85(6)
C(9)-C(1)-C(8)	110.15(11)
C(9)-C(1)-C(2)	112.10(11)
C(8)-C(1)-C(2)	113.25(11)
C(9)-C(1)-S(1)	107.02(9)

Table 2 (continued)

C(8)-C(1)-S(1)	111.79(9)
C(2)-C(1)-S(1)	102.14(8)
C(3)-C(2)-C(1)	112.34(10)
C(4)-C(3)-C(2)	111.83(10)
C(5)-C(4)-C(12)	110.86(11)
C(5)-C(4)-C(3)	113.64(11)
C(12)-C(4)-C(3)	110.29(10)
C(5)-C(4)-S(1)	109.96(9)
C(12)-C(4)-S(1)	110.57(9)
C(3)-C(4)-S(1)	101.14(8)
C(6)-C(5)-C(4)	118.56(11)
C(7)-C(6)-C(5)	115.04(12)
C(6)-C(7)-C(8)	117.44(12)
C(7)-C(8)-C(1)	121.12(11)
C(10)-C(9)-C(1)	113.66(11)
C(11)-C(10)-C(9)	112.07(12)
C(16)'-C(11)-C(10)	115.60(11)
C(13)-C(12)-C(4)	116.92(11)
C(12)-C(13)-C(14)	112.06(12)
C(15)-C(14)-C(13)	112.80(12)
C(16)-C(15)-C(14)	125.91(14)
C(15)-C(16)-C(11)'	126.86(13)

The primed atoms are related to the corresponding unprimed atoms by the symmetry operation: -x,-y,-z+1

Table 3. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters (Å^2 x 10^3) for **9**.

	x	y	z	U(eq)
S(1)	2589(1)	636(1)	5897(1)	22(1)
O(1)	3573(1)	1515(1)	5971(1)	30(1)
O(2)	1379(1)	1213(1)	5601(1)	30(1)
C(1)	3034(1)	-314(1)	7164(1)	23(1)
C(2)	2268(1)	-1597(1)	6730(1)	29(1)
C(3)	1813(1)	-1784(1)	5467(1)	27(1)
C(4)	2385(1)	-754(1)	4983(1)	23(1)
C(5)	3644(1)	-1170(1)	5042(1)	29(1)
C(6)	4601(1)	-1803(2)	6110(1)	34(1)
C(7)	5191(1)	-865(2)	7096(1)	33(1)
C(8)	4448(1)	-557(1)	7756(1)	30(1)
C(9)	2617(1)	480(1)	7918(1)	26(1)
C(10)	2919(1)	-195(2)	9028(1)	30(1)
C(11)	2301(1)	498(2)	9667(1)	32(1)
C(12)	1461(1)	-407(1)	3786(1)	27(1)
C(13)	1805(1)	750(2)	3241(1)	31(1)
C(14)	1171(1)	652(2)	1972(1)	34(1)
C(15)	-213(1)	550(1)	1504(1)	29(1)
C(16)	-911(1)	-389(1)	831(1)	30(1)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

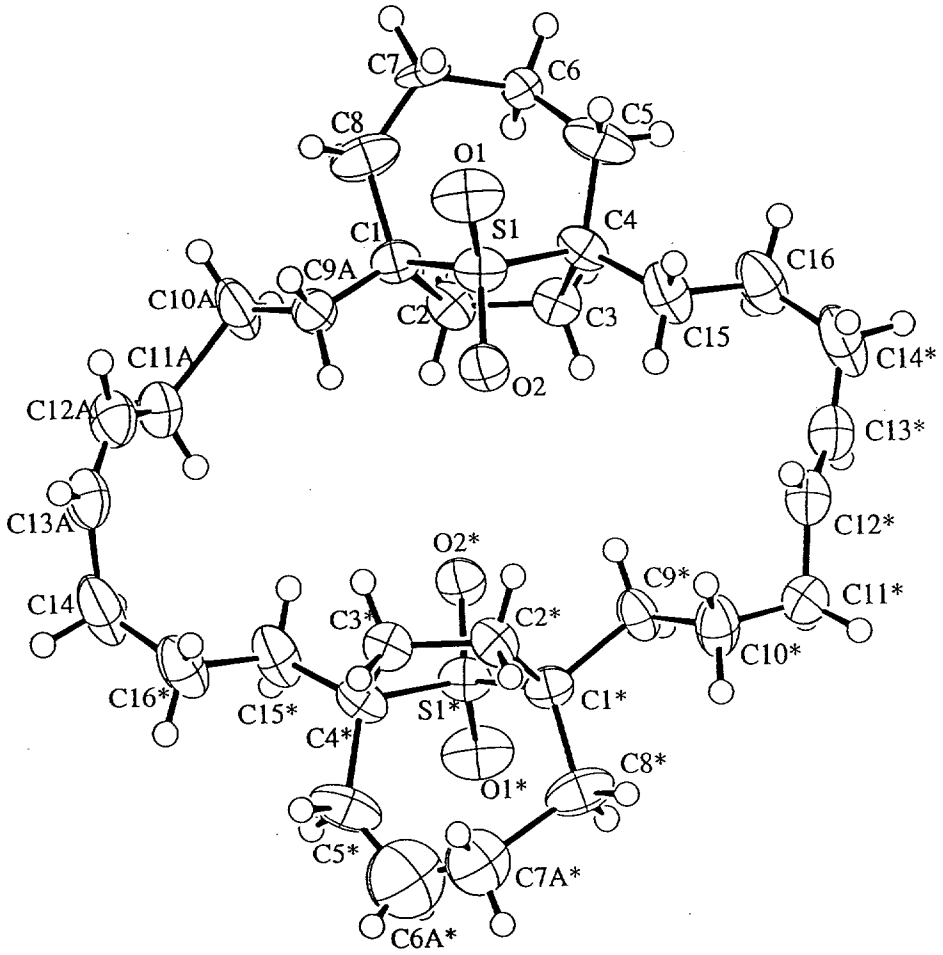
Table 4. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **9**.

	U11	U22	U33	U23	U13	U12
S(1)	23(1)	21(1)	20(1)	1(1)	7(1)	0(1)
O(1)	33(1)	26(1)	30(1)	1(1)	11(1)	-7(1)
O(2)	27(1)	34(1)	27(1)	4(1)	9(1)	10(1)
C(1)	24(1)	23(1)	19(1)	2(1)	7(1)	0(1)
C(2)	36(1)	26(1)	25(1)	-1(1)	14(1)	-7(1)
C(3)	30(1)	26(1)	24(1)	-1(1)	10(1)	-5(1)
C(4)	23(1)	24(1)	20(1)	-1(1)	7(1)	-2(1)
C(5)	28(1)	31(1)	28(1)	-2(1)	13(1)	2(1)
C(6)	31(1)	35(1)	38(1)	4(1)	15(1)	10(1)
C(7)	23(1)	41(1)	31(1)	5(1)	8(1)	5(1)
C(8)	24(1)	35(1)	24(1)	4(1)	6(1)	3(1)
C(9)	28(1)	26(1)	22(1)	-1(1)	10(1)	-2(1)
C(10)	28(1)	36(1)	20(1)	2(1)	6(1)	0(1)
C(11)	36(1)	36(1)	19(1)	-4(1)	10(1)	-5(1)
C(12)	26(1)	34(1)	19(1)	0(1)	7(1)	-4(1)
C(13)	28(1)	38(1)	24(1)	3(1)	7(1)	-6(1)
C(14)	33(1)	45(1)	25(1)	5(1)	14(1)	-2(1)
C(15)	31(1)	33(1)	20(1)	4(1)	10(1)	3(1)
C(16)	36(1)	34(1)	21(1)	1(1)	14(1)	3(1)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

Table 5. Calculated Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for **9**.

	x	y	z	U(eq)
H(2A)	2776(1)	-2347(1)	7117(1)	34
H(2B)	1555(1)	-1571(1)	6891(1)	34
H(3A)	2035(1)	-2662(1)	5327(1)	33
H(3B)	915(1)	-1711(1)	5096(1)	33
H(5A)	3484(1)	-1786(1)	4441(1)	34
H(5B)	4024(1)	-394(1)	4897(1)	34
H(6A)	4201(1)	-2516(2)	6313(1)	41
H(6B)	5256(1)	-2187(2)	5964(1)	41
H(7A)	5360(1)	-36(2)	6826(1)	40
H(7B)	5985(1)	-1234(2)	7604(1)	40
H(8A)	4822(1)	219(1)	8202(1)	35
H(8B)	4586(1)	-1283(1)	8267(1)	35
H(9A)	3017(1)	1338(1)	8061(1)	31
H(9B)	1727(1)	623(1)	7530(1)	31
H(10A)	2639(1)	-1105(2)	8894(1)	35
H(10B)	3812(1)	-199(2)	9475(1)	35
H(11A)	2644(1)	137(2)	10411(1)	38
H(11B)	2521(1)	1426(2)	9730(1)	38
H(12A)	1351(1)	-1184(1)	3330(1)	33
H(12B)	664(1)	-213(1)	3778(1)	33
H(13A)	2699(1)	767(2)	3500(1)	38
H(13B)	1563(1)	1571(2)	3464(1)	38
H(14A)	1383(1)	1426(2)	1665(1)	41
H(14B)	1488(1)	-116(2)	1748(1)	41
H(15)	-621(1)	1204(1)	1704(1)	34
H(16)	-495(1)	-1050(1)	647(1)	36



ORTEP drawing of **10**. The molecular structure is drawn with 50% probability displacement ellipsoids for the nonhydrogen atoms. The hydrogen atoms are drawn with circles of arbitrary radii. The molecule is shown as the cis-trans isomer. All of the disordered atoms are shown.

The data collection crystal was a clear,colorless plate. All work was done at 203 K using an Oxford Cryosystems Cryostream Cooler. Examination of the diffraction pattern on a Nonius Kappa CCD diffractometer indicated a monoclinic crystal system. Almost a whole sphere of reciprocal space was measured using omega scans with a frame width of 1.0°. Data integration was done with Denzo[1], and scaling and merging of the data was done with Scalepack[1]. Merging the data and averaging the symmetry equivalent reflections (including the Friedel pairs) resulted in an Rint value of 0.032. The teXsan[2] package was used to determine the space group as $P2_1/c$.

The structure was solved by the direct methods procedure in SHELXS-86[3]. With Z=2, the molecule is centered about a crystallographic inversion center. Full-matrix least-squares refinements based on F^2 were performed in SHELXL-93[4]. There is disorder in the region of the double bonds and in the seven membered ring which contains the sulfur atom. This disorder might be explained by assuming that this molecule is the cis-trans isomer and that it is enantiomerically disordered. Since the cis-trans isomer cannot contain an inversion center and this molecule is centered about an inversion center, enantiomeric disorder is invoked to resolve this discrepancy. The following atoms constitute the disordered region and each has an occupancy factor of 0.5: C6, C7, C6A, C7A (for the disorder in the seven membered ring) and C9, C10, C11, C12, C13, C9A, C10A, C11A, C12A, C13A (for the disorder about the cis-trans double bonds). Atoms C12 and C13 make up the trans double bond, while C12A and C13A are the cis double bond. Atoms C6, C6A and C7A were kept isotropic, while all the other non-hydrogen atoms were refined anisotropically.

The hydrogen atoms were included in the model at calculated positions using a riding model with U(H) = 1.2 * Ueq(attached atom). The final refinement cycle was based on all the 3498 intensities and 220 variables and resulted in agreement factors of R1(F) = 0.074 and wR2(F^2) = 0.173. For the subset of data with $I > 2\sigma(I)$, the R1(F) value is 0.067 for 3082 reflections. The final difference electron density map contains maximum and minimum peak heights of 0.55 and -0.52 e/$\AA^3$. Neutral atom scattering factors were used and include terms for anomalous dispersion[5].

References

(1) DENZO: Otwinowski, Z. & Minor, W., Methods in Enzymology, Vol 276: Macromolecular Crystallography, part A, 307-326, (1997), Carter, Jr., C. W. & Sweet, R. M., Eds., Academic Press.

(2) teXsan: Crystal Structure Analysis Package, version 1.7-2, Molecular Structure Corporation, The Woodlands, TX (1995).

(3) SHELXS-86: Sheldrick, G. M., Acta Cryst., (1990), A46, 467-473.

(4) SHELXL-93: Sheldrick, G. M., Universitat Gottingen, Germany, 1993.

(5) International Tables for Crystallography (1992). Volume C. Dordrecht: Kluwer Academic Publishers.

Table 6. Crystallographic Details for **10**.

Empirical formula	C32 H52 O4 S2
Formula weight	564.86
Temperature	203.0(1) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 12.3313(2) A b = 10.3494(1) A c = 12.9137(2) A beta = 111.318(1)
Volume	1535.30(4) A^3
Z	2
Density (calculated)	1.222 Mg/m^3
Absorption coefficient	0.208 mm^-1
F(000)	616
Crystal size	0.19 x 0.31 x 0.35 mm
Theta range for data collection	2.60 to 27.43 deg.
Index ranges	0<=h<=15, 0<=k<=13, -16<=l<=15
Reflections collected	35553
Independent reflections	3498 [R(int) = 0.032]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3498 / 0 / 220
Goodness-of-fit on F^2	1.112
Final R indices [I>2sigma(I)]	R1 = 0.067, wR2 = 0.168
R indices (all data)	R1 = 0.074, wR2 = 0.173
Largest diff. peak and hole	0.55 and -0.52 e/A^3

Table 7. Bond Lengths (Å) and Angles (°) for **10**.

S(1)-O(1)	1.444(2)
S(1)-O(2)	1.445(2)
S(1)-C(1)	1.813(3)
S(1)-C(4)	1.814(3)
C(1)-C(9A)	1.44(2)
C(1)-C(2)	1.538(3)
C(1)-C(8)	1.542(4)
C(1)-C(9)	1.64(2)
C(2)-C(3)	1.540(4)
C(2)-H(2A)	0.97
C(2)-H(2B)	0.97
C(3)-C(4)	1.532(3)
C(3)-H(3A)	0.97
C(3)-H(3B)	0.97
C(4)-C(5)	1.533(4)
C(4)-C(15)	1.540(4)
C(5)-C(6A)	1.325(13)
C(5)-C(6)	1.617(6)
C(5)-H(5A)	0.97
C(5)-H(5B)	0.97
C(5)-H(5C)	0.97
C(5)-H(5D)	0.97
C(6)-C(7)	1.601(7)
C(6)-H(6A)	0.97
C(6)-H(6B)	0.97
C(7)-C(8)	1.433(6)
C(7)-H(7A)	0.97
C(7)-H(7B)	0.97
C(6A)-C(7A)	1.212(14)
C(6A)-H(6C)	0.97
C(6A)-H(6D)	0.97
C(7A)-C(8)	1.836(11)
C(7A)-H(7C)	0.97
C(7A)-H(7D)	0.97
C(8)-H(8A)	0.97
C(8)-H(8B)	0.97
C(8)-H(8C)	0.97
C(8)-H(8D)	0.97
C(9)-C(10)	1.49(3)
C(9)-H(9A)	0.97
C(9)-H(9B)	0.97
C(10)-C(11)	1.43(2)
C(10)-H(10A)	0.97
C(10)-H(10B)	0.97
C(11)-C(12)	1.458(10)
C(11)-H(11A)	0.97
C(11)-H(11B)	0.97
C(12)-C(13)	1.318(12)
C(12)-H(12)	0.93
C(13)-C(14)	1.304(8)
C(13)-H(13)	0.93
C(9A)-C(10A)	1.59(3)
C(9A)-H(9C)	0.97
C(9A)-H(9D)	0.97
C(10A)-C(11A)	1.77(2)
C(10A)-H(10C)	0.97
C(10A)-H(10D)	0.97
C(11A)-C(12A)	1.509(8)
C(11A)-H(11C)	0.97
C(11A)-H(11D)	0.97
C(12A)-C(13A)	1.320(10)
C(12A)-H(12A)	0.93

Table 7 (continued)

C(13A)-C(14)	1.713(9)
C(13A)-H(13A)	0.93
C(14)-C(16)'	1.521(5)
C(14)-H(14A)	0.97
C(14)-H(14B)	0.97
C(14)-H(14C)	0.97
C(14)-H(14D)	0.97
C(15)-C(16)	1.527(4)
C(15)-H(15A)	0.97
C(15)-H(15B)	0.97
C(16)-H(16A)	0.97
C(16)-H(16B)	0.97
O(1)-S(1)-O(2)	116.93(12)
O(1)-S(1)-C(1)	112.86(13)
O(2)-S(1)-C(1)	108.67(11)
O(1)-S(1)-C(4)	111.94(13)
O(2)-S(1)-C(4)	107.98(12)
C(1)-S(1)-C(4)	96.47(11)
C(9A)-C(1)-C(2)	118.6(6)
C(9A)-C(1)-C(8)	106.6(7)
C(2)-C(1)-C(8)	113.7(2)
C(2)-C(1)-C(9)	104.9(6)
C(8)-C(1)-C(9)	112.8(7)
C(9A)-C(1)-S(1)	104.7(7)
C(2)-C(1)-S(1)	101.6(2)
C(8)-C(1)-S(1)	111.3(2)
C(9)-C(1)-S(1)	111.9(6)
C(1)-C(2)-C(3)	112.6(2)
C(4)-C(3)-C(2)	111.9(2)
C(3)-C(4)-C(5)	112.9(2)
C(3)-C(4)-C(15)	112.7(2)
C(5)-C(4)-C(15)	110.3(2)
C(3)-C(4)-S(1)	101.2(2)
C(5)-C(4)-S(1)	111.7(2)
C(15)-C(4)-S(1)	107.6(2)
C(6A)-C(5)-C(4)	131.1(7)
C(4)-C(5)-C(6)	115.3(3)
C(7)-C(6)-C(5)	113.5(4)
C(8)-C(7)-C(6)	111.8(4)
C(7A)-C(6A)-C(5)	119.8(13)
C(6A)-C(7A)-C(8)	130.4(10)
C(7)-C(8)-C(1)	126.1(3)
C(1)-C(8)-C(7A)	109.1(4)
C(10)-C(9)-C(1)	115.4(13)
C(11)-C(10)-C(9)	109.8(12)
C(10)-C(11)-C(12)	103.5(10)
C(13)-C(12)-C(11)	128.3(9)
C(14)-C(13)-C(12)	131.8(9)
C(1)-C(9A)-C(10A)	106.9(14)
C(9A)-C(10A)-C(11A)	116(2)
C(12A)-C(11A)-C(10A)	106.8(9)
C(13A)-C(12A)-C(11A)	127.5(7)
C(12A)-C(13A)-C(14)	124.6(6)
C(13)-C(14)-C(16)'	113.2(4)
C(16)'-C(14)-C(13A)	113.7(4)
C(16)-C(15)-C(4)	114.2(2)
C(14)'-C(16)-C(15)	112.7(2)

The primed atoms are related to the corresponding unprimed atoms by the symmetry transformation: -x,-y,-z+1

Table 8. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$ x 10^3) for **10**.

	x	y	z	U(eq)
S(1)	1403(1)	2363(1)	5479(1)	42(1)
O(1)	1757(2)	3494(2)	6177(2)	66(1)
O(2)	832(2)	1348(2)	5857(1)	47(1)
C(1)	523(2)	2752(2)	4051(2)	41(1)
C(2)	797(2)	1610(3)	3424(2)	44(1)
C(3)	1960(2)	948(3)	4093(2)	44(1)
C(4)	2606(2)	1649(3)	5191(2)	42(1)
C(5)	3454(3)	2679(4)	5086(3)	67(1)
C(6)	2949(5)	3606(5)	4008(4)	36(1)*+
C(7)	2003(5)	4625(4)	4084(4)	41(1) +
C(6A)	3266(11)	3833(13)	4610(12)	130(4)*+
C(7A)	2382(9)	4030(11)	3816(8)	91(2)*+
C(8)	857(4)	4078(3)	3712(3)	68(1)
C(9)	-878(13)	2628(17)	3810(13)	46(3) +
C(10)	-1665(18)	3082(19)	2697(14)	61(4) +
C(11)	-2731(6)	3540(7)	2763(8)	74(2) +
C(12)	-3425(6)	2369(7)	2639(7)	62(2) +
C(13)	-4055(6)	2004(8)	3221(7)	60(2) +
C(9A)	-643(14)	2881(16)	4044(13)	45(3) +
C(10A)	-1462(20)	3188(24)	2798(19)	92(7) +
C(11A)	-2905(6)	2593(7)	2367(5)	50(1) +
C(12A)	-3422(5)	3108(7)	3179(5)	54(1) +
C(13A)	-4180(6)	2532(8)	3529(6)	55(2) +
C(14)	-4765(3)	1035(5)	3106(3)	80(1)
C(15)	3235(2)	713(4)	6148(2)	58(1)
C(16)	4273(2)	16(4)	6025(3)	65(1)

*Refined isotropically.
+Occupancy factor was set to 0.5.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table 9. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **10**.

	U11	U22	U33	U23	U13	U12
S(1)	55(1)	47(1)	31(1)	-4(1)	25(1)	-8(1)
O(1)	103(2)	62(1)	45(1)	-23(1)	41(1)	-21(1)
O(2)	50(1)	58(1)	42(1)	11(1)	27(1)	-2(1)
C(1)	52(1)	42(1)	35(1)	4(1)	23(1)	-4(1)
C(2)	43(1)	54(2)	33(1)	-9(1)	11(1)	-5(1)
C(3)	49(1)	48(1)	35(1)	-7(1)	18(1)	-3(1)
C(4)	40(1)	60(2)	31(1)	-4(1)	18(1)	-12(1)
C(5)	67(2)	91(2)	53(2)	-13(2)	33(2)	-39(2)
C(7)	65(3)	20(2)	53(3)	2(2)	38(3)	-13(2)
C(8)	110(3)	48(2)	54(2)	10(1)	40(2)	-12(2)
C(9)	32(5)	68(8)	39(6)	6(4)	16(5)	4(4)
C(10)	51(9)	84(8)	51(5)	29(5)	23(5)	20(6)
C(11)	48(3)	57(4)	109(6)	30(4)	20(4)	4(3)
C(12)	47(4)	59(4)	74(5)	12(4)	16(3)	10(3)
C(13)	49(4)	56(4)	75(5)	7(4)	23(3)	11(3)
C(9A)	42(7)	50(5)	41(6)	12(4)	11(5)	0(4)
C(10A)	30(5)	127(11)	116(12)	79(9)	21(5)	9(5)
C(11A)	45(3)	60(4)	47(3)	1(3)	17(3)	9(3)
C(12A)	48(3)	56(3)	58(3)	-11(3)	20(3)	9(3)
C(13A)	46(3)	64(4)	58(4)	-7(3)	21(3)	14(3)
C(14)	34(1)	134(3)	70(2)	30(2)	16(1)	12(2)
C(15)	38(1)	99(2)	38(1)	13(2)	15(1)	4(1)
C(16)	39(1)	105(3)	55(2)	13(2)	21(1)	2(2)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

Table 10. Calculated Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for **10**.

	x	y	z	U(eq)
H(2A)	826(2)	1917(3)	2725(2)	53
H(2B)	175(2)	979(3)	3256(2)	53
H(3A)	1812(2)	62(3)	4249(2)	52
H(3B)	2449(2)	930(3)	3650(2)	52
H(5A)	4144(3)	2248(4)	5066(3)	81*
H(5B)	3690(3)	3215(4)	5748(3)	81*
H(5C)	3968(3)	2844(4)	5846(3)	81*
H(5D)	3925(3)	2231(4)	4740(3)	81*
H(6A)	3591(5)	4074(5)	3919(4)	43*
H(6B)	2598(5)	3074(5)	3353(4)	43*
H(7A)	2214(5)	4910(4)	4848(4)	49*
H(7B)	2003(5)	5374(4)	3633(4)	49*
H(6C)	3291(11)	4458(13)	5177(12)	156*
H(6D)	3917(11)	4022(13)	4382(12)	156*
H(7C)	2395(9)	3394(11)	3269(8)	109*
H(7D)	2509(9)	4858(11)	3526(8)	109*
H(8A)	592(4)	4066(3)	2907(3)	81*
H(8B)	374(4)	4705(3)	3900(3)	81*
H(8C)	757(4)	4745(3)	4197(3)	81*
H(8D)	356(4)	4280(3)	2955(3)	81*
H(9A)	-1054(13)	1729(17)	3893(13)	55*
H(9B)	-1048(13)	3117(17)	4374(13)	55*
H(10A)	-1291(18)	3772(19)	2442(14)	73*
H(10B)	-1824(18)	2378(19)	2167(14)	73*
H(11A)	-3110(6)	4151(7)	2172(8)	89*
H(11B)	-2598(6)	3951(7)	3474(8)	89*
H(12)	-3423(6)	1809(7)	2076(7)	74*
H(13)	-3979(6)	2534(8)	3825(7)	72*
H(9C)	-679(14)	3577(16)	4533(13)	54*
H(9D)	-885(14)	2087(16)	4296(13)	54*
H(10C)	-1100(20)	2834(24)	2307(19)	111*
H(10D)	-1497(20)	4118(24)	2700(19)	111*
H(11C)	-3353(6)	2887(7)	1620(5)	60*
H(11D)	-2905(6)	1656(7)	2372(5)	60*
H(12A)	-3178(5)	3927(7)	3466(5)	65*
H(13A)	-4413(6)	2970(8)	4042(6)	66*
H(14A)	-4947(3)	662(5)	2373(3)	96*
H(14B)	-5486(3)	1353(5)	3154(3)	96*
H(14C)	-5601(3)	1080(5)	2917(3)	96*
H(14D)	-4626(3)	797(5)	2438(3)	96*
H(15A)	3504(2)	1194(4)	6840(2)	69
H(15B)	2682(2)	73(4)	6197(2)	69
H(16A)	4034(2)	-368(4)	5290(3)	78
H(16B)	4880(2)	641(4)	6087(3)	78

*Occupancy factor set to 0.5