

Electronic Supplementary Materials for

meso-meso 1,3-bis(*E*-vinyl) azulene bridged tetrathiaoctaphyrins: Synthesis, Spectroscopic and Theoretical Characterization

Sumit Sahoo,^a Gunasekaran Velmurugan,^b Peter Comba^{*b} and Harapriya Rath^{*a}

^a School of Chemical Sciences, Indian Association for The Cultivation of Science, 2A/2B Raja S. C. Mullick Road, Jadavpur, Kolkata 700 032, India, E-mail: ichr@iacs.res.in

^b1Heidelberg University, Institute of Inorganic Chemistry and Interdisciplinary Center for Scientific Computing, Im Neuenheimer Feld 270, 69120 Heidelberg, GERMANY. E-mail: peter.comba@aci.uni-heidelberg.de

Table of Contents

Materials and Methods	S2-S4
General Synthetic Procedure	S5-S7
Spectroscopic Data	S8-S23
X-ray crystal Data	S24
Electrochemistry Data	S25-S26
Theoretical Calculations	S27-S59
X,Y,Z Coordinates	S60-S112

Materials and Methods:

1.1 Electronic absorption spectra were measured with a Perkin Elmer Lambda 950 UV-visible-NIR spectrophotometer. ^1H NMR spectra were recorded on a Bruker AVIII 500 MHz spectrometer, Bruker AVIII 400 MHz, Bruker DPX-300 MHz spectrometer and chemical shifts were reported as the delta scale in ppm relative to CHCl_3 ($\delta = 7.26$ ppm) and CH_2Cl_2 ($\delta = 5.32$ ppm) as internal reference for ^1H and ^{13}C NMR CHCl_3 ($\delta = 77.00$ ppm) and CH_2Cl_2 ($\delta = 55.00$ ppm). MALDI-TOF MS data were recorded using Bruker Daltonics flex Analyser and ESI HR-MS data were recorded using Waters QTOF Micro YA263 spectrometer. All solvents and chemicals were of reagent grade quality, obtained commercially and used without further purification except as noted. For spectral measurements, anhydrous dichloromethane was obtained by refluxing and distillation over CaH_2 . Dry THF was obtained by refluxing and distillation over pressed Sodium metal. Thin layer chromatography (TLC) was carried out on alumina sheets coated with silica gel 60 F_{254} (Merck 5554) and gravity column chromatography were performed using Merck Silica Gel 230-400 mesh. Aluminum Oxide (Basic) grade II was purchased from Sigma Aldrich.

1.2 X-Ray structure determination.

A specimen of $\text{C}_{72}\text{H}_{61}\text{S}_4\text{O}_2\text{N}_4$, approximate dimensions 0.100 mm x 0.100 mm x 0.100 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured ($\lambda = 0.71073$ Å).

The total exposure time was 1.2 hours. The frames were integrated with the Bruker SAINT Software package using a narrow-frame algorithm. The integration of the data using triclinic unit cell yielded a total of 30809 reflections to a maximum θ angle of 28.37° (0.75 Å resolution), of which 11760 were independent (average redundancy 2.620, completeness = 99.0%, $R_{\text{int}} = 3.45\%$, $R_{\text{sig}} = 4.45\%$) and 8752 (74.42%) were greater than 2σ (F^2). The final cell constants of $a = 12.5941(7)$ Å, $b = 13.3888(8)$ Å, $c = 14.2293(8)$ Å, volume = $2376.1(2)$ Å³, are based upon the refinement of the XYZ-centroids of 9933 reflections above 20σ (I) with $4.599^\circ < 2\theta < 56.68^\circ$. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.829. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9200 and 0.9380. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P-1$, with $Z = 1$ for the formula unit, $\text{C}_{78}\text{H}_{66}\text{Cl}_{18}\text{N}_4\text{O}_2\text{S}_4$. The final anisotropic full-matrix least-squares refinement on F^2 with 484 variables converged at $R1 = 6.87\%$, for the observed data and $wR2 = 20.49\%$ for all data. The goodness-of-fit was 1.043. The largest peak in the final difference electron density synthesis was $1.168 \text{ e}/\text{\AA}^3$ and the largest hole was $-1.220 \text{ e}/\text{\AA}^3$ with an RMS deviation of $0.085 \text{ e}/\text{\AA}^3$. On the basis of the final model, the calculated density was $1.298 \text{ g}/\text{cm}^3$ and $F(000)$, 948 e⁻.

The structure have been squeezed out of the solvent apart from three CHCl_3 which could be located properly. However, there is one B alert due to large ellipsoid of Oxygen atom.

1.3 Computational details

All the calculations have been computed using the Gaussian16 program¹ at B3LYP/6-31G(d,p) level of theory.² The electronic absorption spectra, singlet vertical excitation energies and oscillator strengths on the ground state optimized geometries have been computed using time dependent density functional

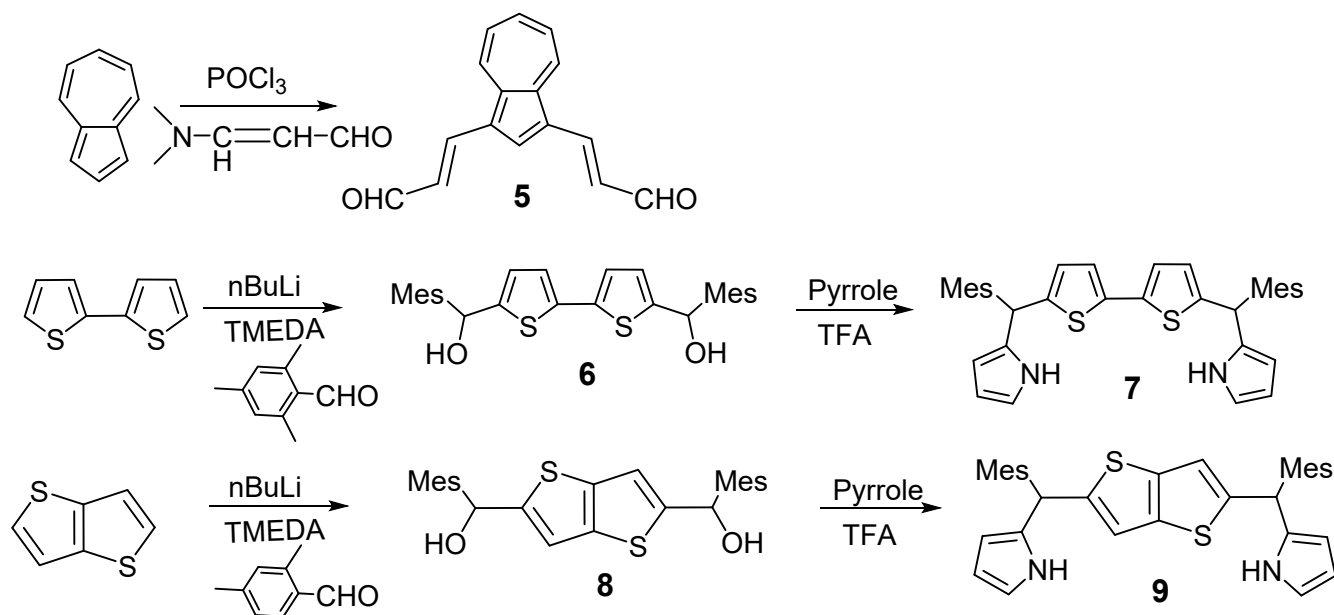
theory (TD-DFT).³ We have used dichloromethane as solvent using the polarized continuum model (PCM).⁴ The contribution of various fragments of the macrocycles have been analyzed using the QMForge program.⁵ The nucleus independent chemical shift (NICS) values were calculated at the non-weighted mass of the conjugation π -pathway of the macrocycle (1-8 Å above and below the molecular plane).⁶ The NICS values are scanned along the trajectory orthogonal to the plane of macrocycle based on the Stranger method.⁷ The NMR shielding tensors were computed using the Gauge-Independent Atomic Orbital (GIAO) at the non-weighted mass of conjugation π -pathway of the macrocycles.⁸ The harmonic oscillator model of aromaticity (HOMA) index, the electron localization function (ELF), multi center index (MCI), AV1245, AVmin and localized orbital locator (LOL) topology analysis, the NBO analysis based -decomposition of Wiberg bond index have been calculated using Multiwfn.⁹ The anisotropy of the current (induced) density (ACID) has been done using ACID plot.¹⁰

References:

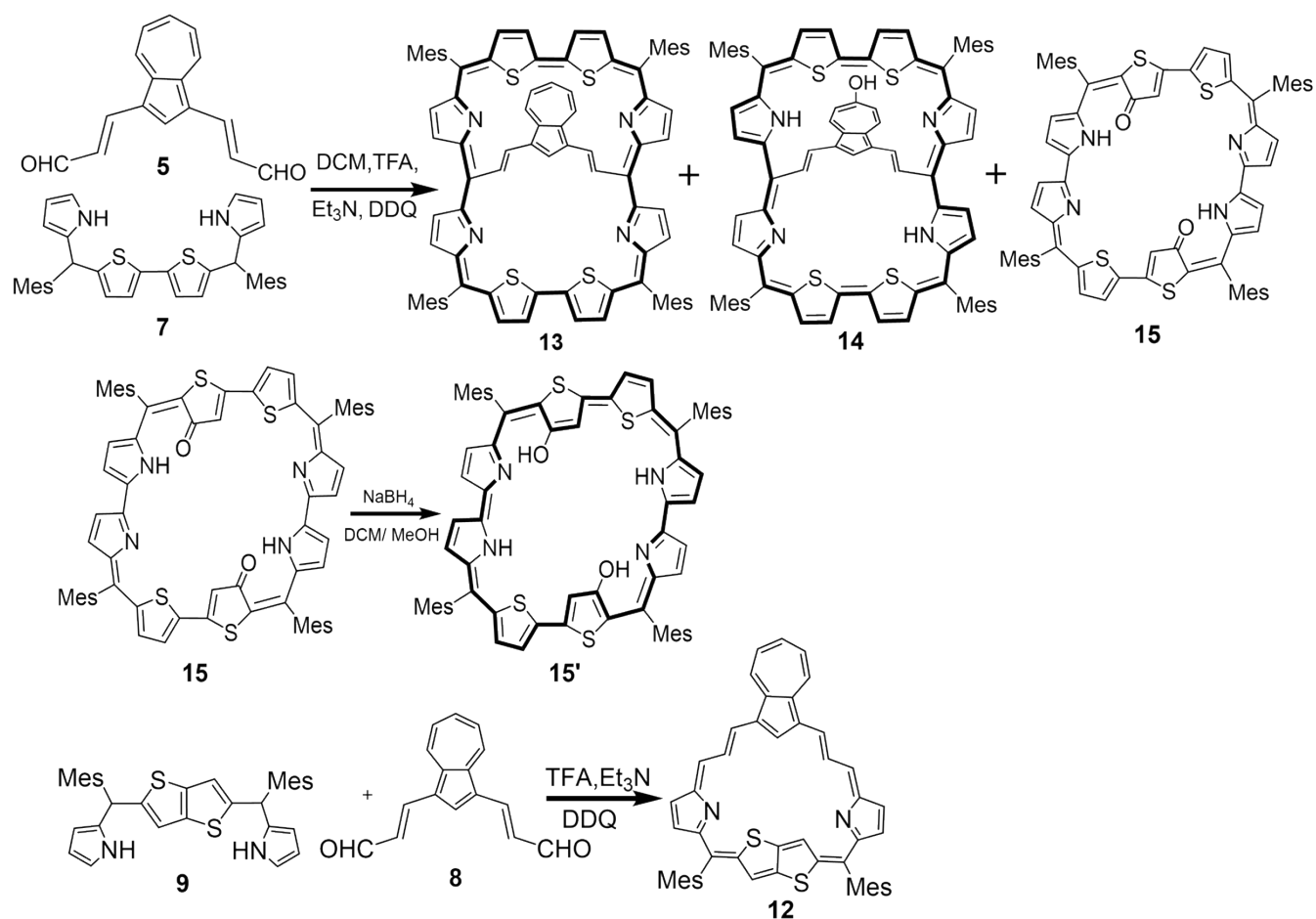
1. M. Frisch, G. Trucks, H. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. Hratchian, A. Izmaylov, J. Bloino, G. Zheng, J. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. Montgomery, Jr, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. Burant, S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. Stratmann, O. Yazyev, A. Austin, R. Cammi, C. Pomelli, J. Ochterski, R. L. Martin, K. Morokuma, V. Zakrzewski, G. Voth, P. Salvador, J. Dannenberg, S. Dapprich, A. Daniels, Ö. Farkas, J. Foresman, J. Ortiz, J. Cioslowski, D. Fox, Gaussian 16, revision C. 01, Gaussian, Inc., Wallingford, CT 2010.
2. (a) A. D. Becke, Density-Functional Thermochemistry. III. The Role of Exact Exchange, *J. Chem. Phys.*, 1993, **98**, 5648—5652; (b) J. P. Perdew, Density-functional approximation for the correlation energy of the inhomogeneous electron gas, *Phys. Rev. B*, 1986, **33**, 8822—1824; (c) A. D. Becke, Density-functional exchange-energy approximation with correct asymptotic behaviour, *Phys. Rev. A.*, 1988, **38**, 3098—3100; (d) C. Lee, W. Yang and R. G. Parr, Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density, *Phys. Rev. B*, 1988, **37**, 785—789.
3. (a) E. Runge and E. K. U. Gross, Density-Functional Theory for Time-Dependent Systems, *Phys. Rev. Lett.*, 1984, **52**, 997—1000; (b) R. E. Stratmann, G. E. Scuseria and M. J. Frisch, An efficient implementation of time-dependent density-functional theory for the calculation of excitation energies of large molecules, *J. Chem. Phys.*, 1998, **109**, 8218—8224; (c) R. Bauernschmitt and R. Ahlrichs, Treatment of Electronic Excitations within the Adiabatic Approximation of Time Dependent Density Functional Theory, *Chem. Phys. Lett.*, 1996, **256**, 454—464.
4. (a) M. Cossi, G. Scalmani, N. Rega and V. Barone, New Developments in the Polarizable Continuum Model for Quantum Mechanical and Classical Calculations on Molecules in Solution, *J. Chem. Phys.*, 2002, **117**, 43—54; (b) E. Cancès, B. Mennucci and J. Tomasi, A New Integral Equation Formalism for the Polarizable Continuum Model: Theoretical Background and Applications to Isotropic and Anisotropic Dielectrics, *J. Chem. Phys.*, 1997, **107**, 3032—3041; (c) B. Mennucci and J. Tomasi, Continuum solvation models: A New Approach to the Problem of Solute's Charge Distribution and Cavity Boundaries, *J. Chem. Phys.*, 1997, **106**, 5151—5158.
5. (a) A. Tenderholt, "QMForge: A Program to Analyze Quantum Chemistry Calculations", Version 2.3.2, <http://qmforge.sourceforge.net>; (b) G. Velmurugan and P. Venuvanalingam, Luminescent

- Re(I) Terpyridine Complexes for OLEDs: What Does the DFT/TD-DFT Probe Reveal?, *Dalton Trans.*, 2015, **44**, 8529—8542; (c) G. Velmurugan, B. K. Ramamoorthi and P. Venuvanalingam, Are Re(I) Phenanthroline Complexes Suitable Candidates for OLEDs? Answers from DFT and TD-DFT investigations, *Phys. Chem. Chem. Phys.*, 2014, **16**, 21157—21171; (d) G. Velmurugan, S. A. Vedha and P. Venuvanalingam, Computational Evaluation of Optoelectronic and Photophysical Properties of Unsymmetrical Distyrylbiphenyls, *RSC Adv.*, 2014, **4**, 53060—53071.
6. (a) P. V. R. Schleyer, C. Maerker, A. Dransfeld, H. Jiao and N. J. R. V. E. Hommes, Nucleus-Independent Chemical Shifts: A Simple and Efficient Aromaticity Probe, *J. Am. Chem. Soc.*, 1996, **118**, 6317—6318; (b) K. K. Zborowski, I. Alkorta, J. Elguero and L. M. Proniewicz, Calculation of the HOMA Model Parameters for the Carbon-Boron Bond, *Struct. Chem.*, 2012, **23**, 595—600.
 7. A. Stanger, Nucleus-independent chemical shifts (NICS): distance dependence and revised criteria for aromaticity and antiaromaticity, *J. Org. Chem.*, **2006**, *71*, 883—893.
 8. K. Wolinski, J. F. Hinton and P. Pulay, Efficient Implementation of the Gauge-Independent Atomic Orbital Method for NMR Chemical Shift Calculations, *J. Am. Chem. Soc.*, 1990, **112**, 8251—8260.
 9. (a) S. Ostrowski and J. C. Dobrowolski, What Does the HOMA Index Really Measure?, *RSC Adv.*, 2014, **4**, 44158—44161; (b) T. Lu and F. Chen, Multiwfn: A Multifunctional Wavefunction Analyzer, *J. Comput. Chem.*, 2012, **33**, 580—592.
 10. (a) D. Geuenich, K. Hess, F. Köhler and R. Herges, Anisotropy of the Induced Current Density (ACID), a General Method to Quantify and Visualize Electronic Delocalization, *Chem. Rev.*, 2005, **105**, 3758—3772; (b) R. Herges and D. Geuenich, Delocalization of Electrons in Molecules, *J. Phys. Chem. A*, 2001, **105**, 3214—3220.
 11. A. Mallick, J. Oh, D. Kim, H. Rath, Aromatic Fused [30] Heteroannulenes with NIR Absorption and NIR Emission: Synthesis, Characterization, and Excited-State Dynamics, *Chem. Eur. J.*, 2016, **22**, 8026-8031.

1.4 Synthesis:



Scheme S1. Synthesis of all precursors used for the macrocycles reported in the manuscript ^{S11}



Scheme S2. Synthesis of porphyrinoids **13-15** reported in the manuscript

General Synthesis of **13/14/15**:

Tetrapyrane **7** (0.280 g, 0.5 mmol) was taken in a round bottom flask; to it 250 mL of dry DCM was added and stirred for 15 minutes under nitrogen atmosphere to get a clear solution. Azulene-1, 3-bisacrylaldehyde **5** (0.118 g, 0.5 mmol) was added to the reaction mixture and stirred for 15 minutes under dark condition. To this, 0.192 mL (2.5 mmol) CF₃COOH was added and reaction mixture was stirred under nitrogen atmosphere in dark for overnight. The reaction mixture was then neutralised with 0.174 mL (1.25 mmol) triethylamine followed by oxidation with 283 mg (1.25 mmol) of DDQ in open air. After complete removal of solvent from crude mixture by rotary evaporator, the compound was purified using basic alumina grade III where a violet colour band was eluted using dichloromethane as eluent while a deep violet colour band using 5% EtOAc- dichloromethane as eluent and a deep red band using 15% EtOAc- dichloromethane was obtained. These three fractions were further purified by repeated PTLCs. The desired macrocycles **13**, **14** and **15** were isolated as extra pure crystalline violet, green and deep blue solids, respectively upon further recrystallization.

Compound **13**: Yield. ~65mg (10%). R_f = 0.2 (CH₂Cl₂/ Hexane = (6:4). Mp > 350°C

HR-ESI-TOF MS (*m/z*): calcd. for [M]⁺ [C₈₈H₇₀S₄N₄]⁺ 1310.4483, found 1310.4485. Elemental analysis Calcd. for C₈₈H₇₀S₄N₄: C, 80.57; H, 5.38; N, 4.27. Found: C, 80.88; H, 4.40; N, 4.26.

UV-vis-NIR (CH₂Cl₂, λ [nm], (ε [M⁻¹ cm⁻¹]), 298K): 552.82 (4.32 x 10⁵), 587.59 (shoulder), 678.28 (2.26 x 10³), 744.16 (2.92 x 10³), 919.36 (3.55 x 10³). ¹H NMR (500 MHz, CDCl₃, 298 K, δ [ppm], TMS): 10.39 (d, ³J = 3.5Hz, 4H, thiophene β -CHs), 9.82 (d, ³J = 3.5Hz, 4H, thiophene β -CHs), 9.74 (d, ³J = 4Hz, 4H, pyrrole β -CHs), 9.11 (d, ³J = 4Hz, 4H, pyrrole β -CHs), 7.29 (s, 8H, mesityl-CHs), 6.47 (m, 1H, azulene-CH), 5.85 (d, ³J = 9.5 Hz, 2H, azulene-CHs), 5.38 (d, ³J = 9 Hz, 2H, azulene-CHs), 3.68 (d, 2H, ³J = 14.5 Hz, bridge-outer meso CHs), 2.65 (s, 12H, mesityl -CH₃), 2.21 (s, 24H, mesityl -CH₃), -3.93 (s, 1H, inner azulene CH), -5.44 (d, 2H, ³J = 14.5 Hz, bridge-inner meso CHs).

Compound **14**: Yield. ~32.5 mg (5%).

R_f = 0.3 (CH₂Cl₂/ Hexane = (9:1). Mp > 350°C

HR-ESI-TOF MS (*m/z*): calcd. for [M]⁺ [C₈₈H₇₂S₄ON₄]⁺ 1328.4586, found. 1328.4588. Elemental analysis Calcd. for C₈₈H₇₀S₄ON₄: C, 79.60; H, 5.31; N, 4.22. Found: C, 80.00; H, 5.40; N, 4.20.

UV-vis-NIR (CH₂Cl₂, λ [nm], (ε [M⁻¹ cm⁻¹]), 298K): 353.25 (5.6 x 10³), 480.35 (1.31 x 10⁴), 638.12 (1.42 x 10³), 850-1300. UV-vis-NIR (10 % TFA/CH₂Cl₂, λ [nm], (ε [M⁻¹ cm⁻¹]), 298K): 360.13 (2.8 x 10³), 491.03 (8.43 x 10³), 649.74 (1.12 x 10³), 784.62 (1.03 x 10³).

¹H NMR (600 MHz, CDCl₃, 298 K) δ = 12.08 (br, 1H, -NH), 10.53 (br, 1H, -NH), 10.37 (d, ³J = 13.2 Hz, 1H, vinylogous-CH), 10.15 (d, ³J = 13.8 Hz, 1H, vinylogous CH), 9.62 (m, 4H, inner seven-member CHs), 8.94 (m, 2H, thiophene β -CHs), 8.77 (s, 1H, inner five-member CH), 8.66 (d, ³J = 4.2 Hz, 1H, thiophene β -CH), 8.57 (d, ³J = 3.6 Hz, 1H, thiophene β -CH), 8.14 (d, ³J = 4.2Hz, 1H, thiophene β -CH), 7.99 (d, ³J = 13.6 Hz, 1H, vinylogous CH), 7.80 (d, ³J = 13.2 Hz, 1H, vinylogous CH), 7.76 (d, ³J = 3.6 Hz, 1H, thiophene β -CH), 7.72 (m, 2H, thiophene β -CHs), 7.19 (m, 3H, pyrrole β -H), 6.82 (d, 1H, ³J = 3.2 Hz, pyrrole β -H), 6.96 (s, 8H, mes-CH), 6.75 (d, ³J = 3 Hz, 1H, pyrrole β -H), 6.69 (d, ³J = 3.6 Hz, 1H,

pyrrole β -H), 6.58 (m, 2H, pyrrole β -H), 6.25 (br, 1H, inner OH), 2.37 (s, 12H, -CH₃), 2.12 (s, 24H, -CH₃).
¹³C NMR (125 MHz, CDCl₃) δ = 167.41, 154.31, 150.15, 149.30, 146.00, 145.05, 144.47, 142.51, 142.45, 142.27, 142.01, 141.75, 141.37, 141.22, 141.17, 138.41, 138.39, 138.23, 138.13, 136.92, 136.82, 136.79, 136.58, 135.83, 135.67, 135.45, 134.97, 134.95, 134.76, 133.65, 131.44, 128.58, 128.32, 128.28, 128.26, 125.92, 125.51, 108.33, 21.30, 20.09, 20.03.

IR (neat) $\nu_{\max}$ 3480.42 cm⁻¹ (OH), 3298.94 cm⁻¹ (NH), 2924.18 cm⁻¹ (CH), 2853.65 cm⁻¹ (CH), 2807.67 cm⁻¹ (-CH), 1593.25 cm⁻¹ (C=N), 1521.05 cm⁻¹ (C=C).

Compound **15**: Yield. ~6 mg (~1%).

R_f = 0.3 (CH₂Cl₂/ EtOAc = (95:5). Mp > 350°C

HR-ESI-TOF MS (*m/z*): calcd. for [M+H]⁺ [C₇₂H₆₁S₄O₂N₄]⁺ 1141.3672, found 114.3678.

Elemental analysis Calc. for C₇₂H₆₂S₄O₂N₄: C, 75.76; H, 5.30; N, 4.91, Found: C, 76.04; H, 5.47; N, 5.27.

UV-vis-NIR (CH₂Cl₂, λ [nm], (ϵ [M⁻¹ cm⁻¹]), 298K): 412.85 (2.51 x 10³), 595.94 (6.38 x 10³).

IR (neat) $\nu_{\max}$ 2924.61 cm⁻¹ (CH), 2857.2 cm⁻¹ (CH), 1709.44 cm⁻¹ (C=O), 1623.63 cm⁻¹ (C=N), 1534.5 cm⁻¹ (C=C).

Compound **15'**: 12 mg (10.5 μ mol) of **15** was dissolved in 5 mL of CH₂Cl₂, to this was added 4.35 mg (105 μ mol) NaBH₄ followed by addition of 3 mL of MeOH. The reaction mixture was stirred under nitrogen atmosphere for 30-40 min. Extraction of the reaction mixture from dichloromethane and subsequent evaporation of the solvent followed by recrystallization from CH₂Cl₂/hexane gave **15'**.

Yield. 10.8 mg (90%).

HR-ESI-TOF MS (*m/z*): calcd. for [M]⁺ [C₇₂H₆₂S₄O₂N₄]⁺ 1142.3756, found 1142.3758.

Elemental analysis Calc. for C₇₂H₆₂S₄O₂N₄: C, 75.62; H, 5.47; N, 4.90. Found: C, 76.02; H, 5.53; N, 5.44.

UV-vis-NIR (CH₂Cl₂, λ [nm], (ϵ [M⁻¹ cm⁻¹]), 298K): 480.55 (3.44 x 10³), 649.75 (2.21 x 10⁵), 1050.35 (3.21 x 10³), 1267.65 (3.28 x 10³).

¹H NMR (400 MHz, CDCl₃, 298 K) δ = 12.06 (d, ³J = 4.4 Hz, 2H, thiophene β -H), 11.23 (d, ³J = 4.4 Hz, 2H, thiophene β -H), 11.12 (d, 2H, ³J = 3.2 Hz, pyrrole β -H), 11.06 (d, ³J = 3.2 Hz, 2H, pyrrole β -H), 10.30 (d, ³J = 3.2 Hz, 2H, pyrrole β -H), 10.23 (d, ³J = 3.2 Hz, 2H, pyrrole β -H), 6.99 (s, 8H, mesityl-CHs), 2.61 (s, 6H, -CH₃), 7.69 (br, 2H, -OH), 2.59 (s, 6H, -CH₃), 2.08 (s, 12H, -CH₃), 2.05 (s, 12H, -CH₃), -3.61 (br, 2H, -NH), -5.77 (s, 2H, thiophene β -H). ¹³C NMR (100 MHz, CDCl₃) δ = 139.30, 138.11, 133.08, 131.26, 130.68, 130.58, 130.38, 130.13, 130.13, 129.24, 129.24, 128.98, 128.33, 127.94, 127.94, 127.56, 127.42, 126.16, 125.62, 125.13, 124.50, 124.44, 124.44, 123.67, 104.68, 90.28, 22.83, 22.11.

IR (neat) $\nu_{\max}$ 3361.76 cm⁻¹ (OH), 3097.1 cm⁻¹ (NH), 2938.2 cm⁻¹ (CH), 2925.4 cm⁻¹ (CH), 2850.7 cm⁻¹ (CH), 1628.06 cm⁻¹ (C=N), 1586.46 cm⁻¹ (C=C).

2. Supplementary Data:

2.1 Mass Spectra

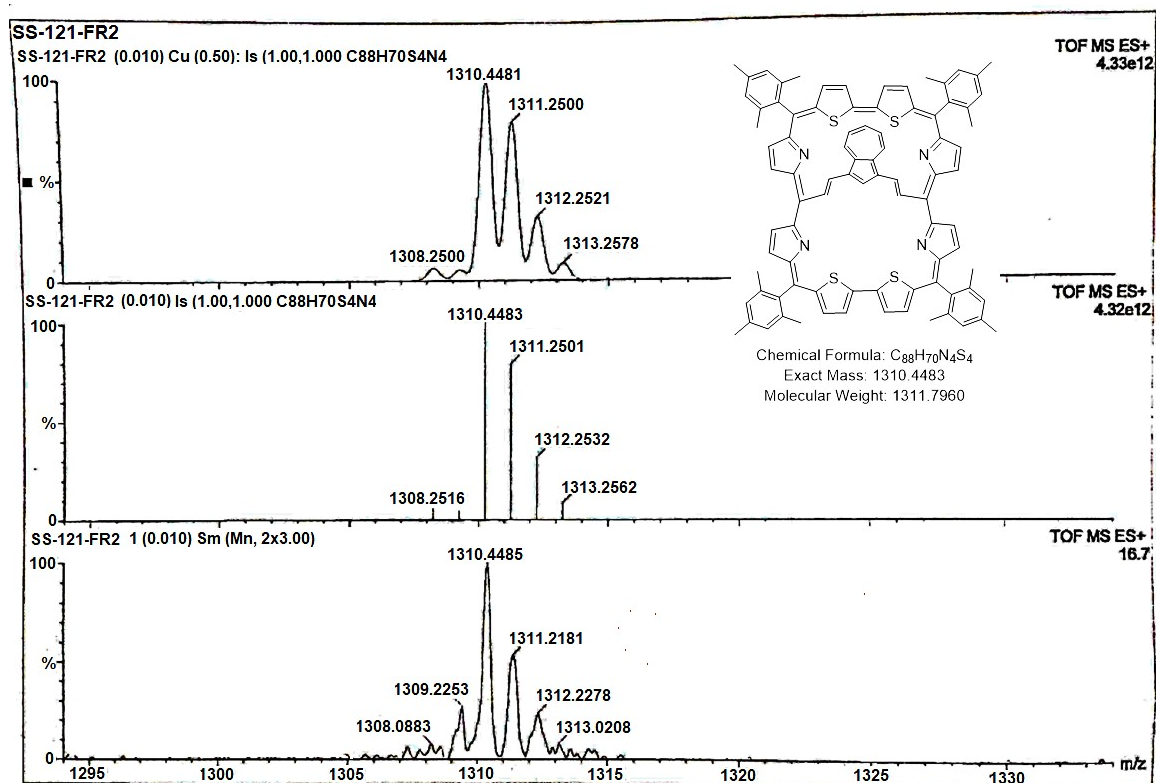


Fig. S1 HRMS Spectra of 13

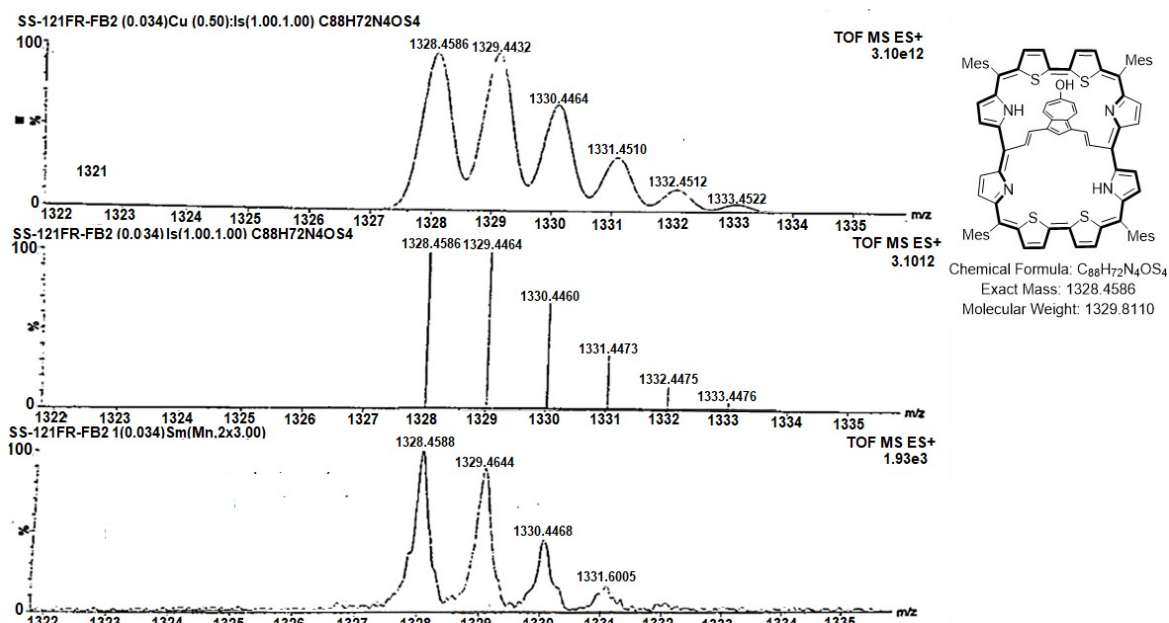


Fig. S2 HRMS Spectra of **14**

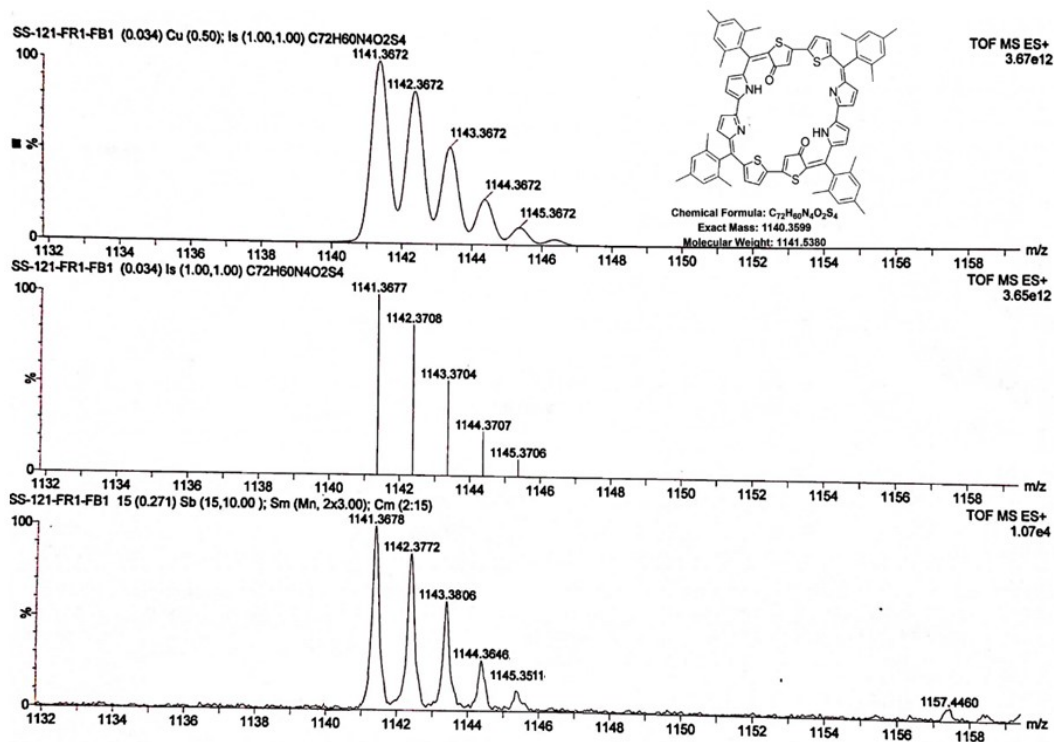


Fig. S3 HRMS Spectra of **15**

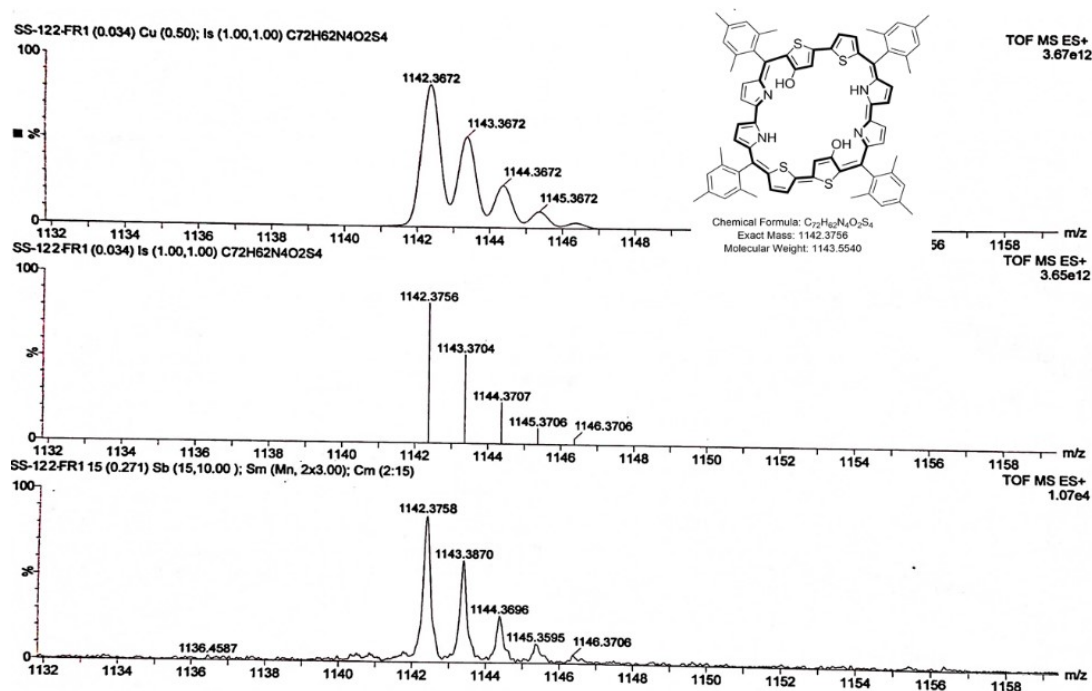


Fig. S4 HRMS Spectra of **15'**

2.2 IR spectra:

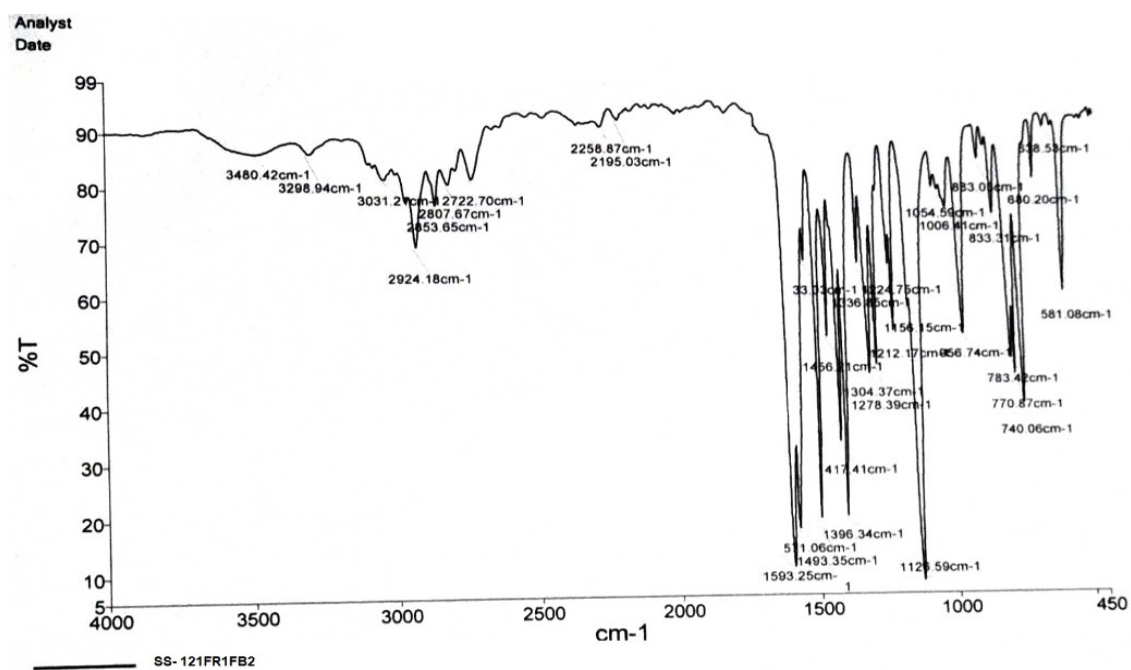


Fig. S5 IR Spectrum of **14**

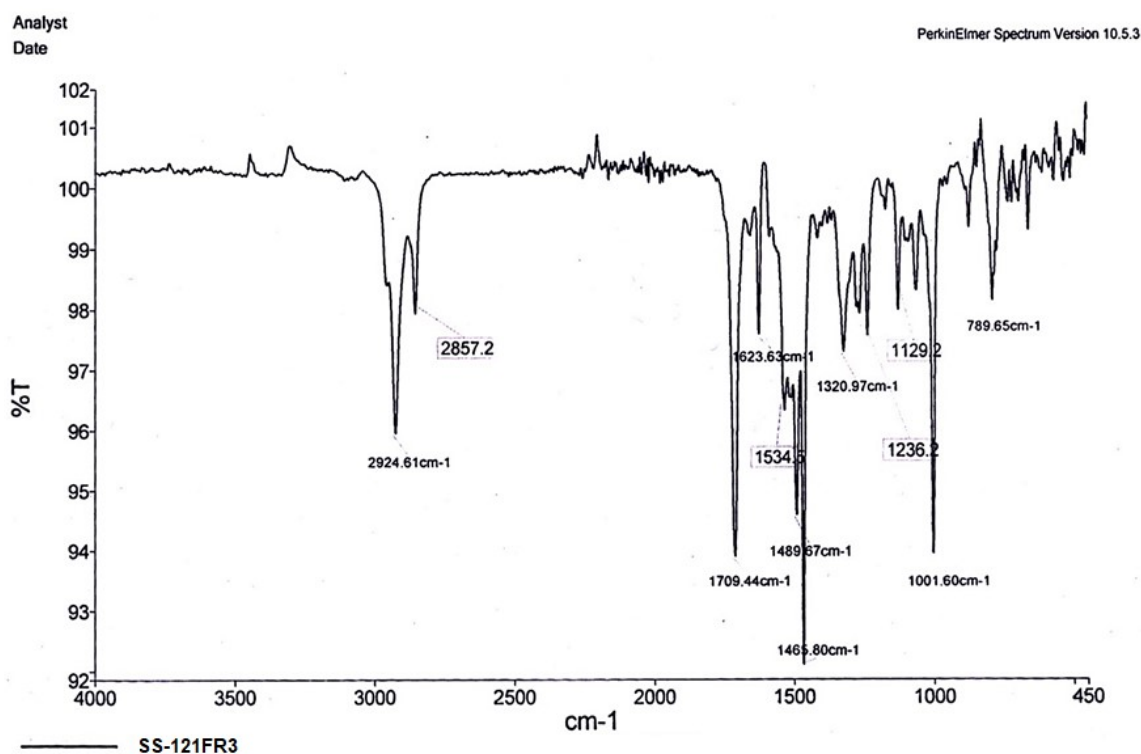


Fig. S6 IR Spectrum of **15**

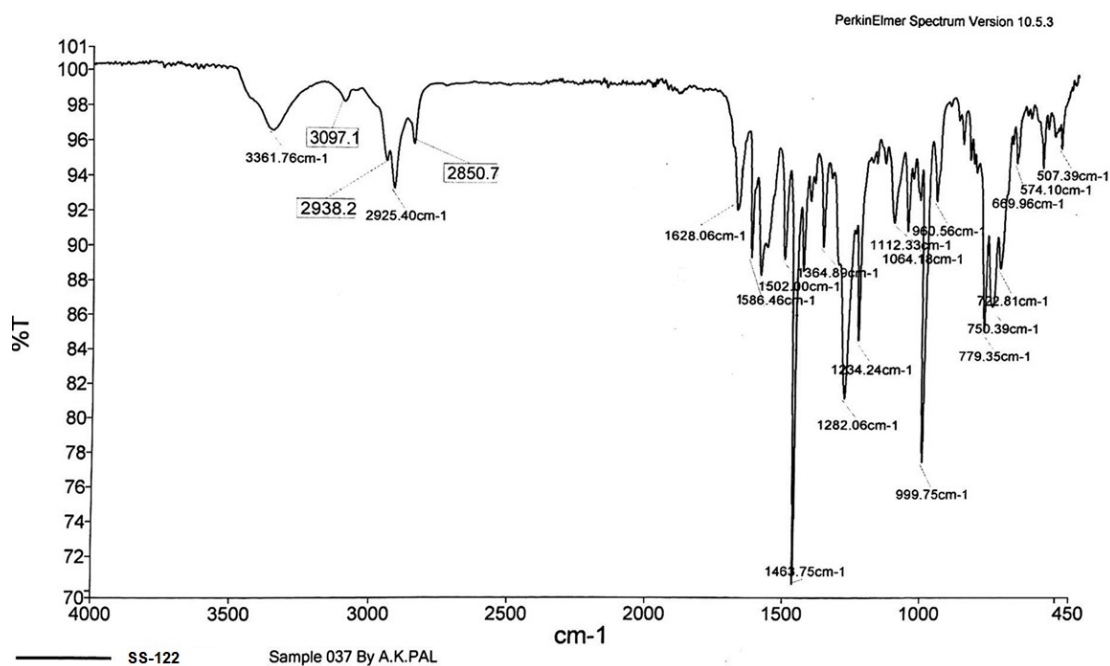


Fig. S7 IR Spectrum of **15'**

2.3 UV-vis spectra:

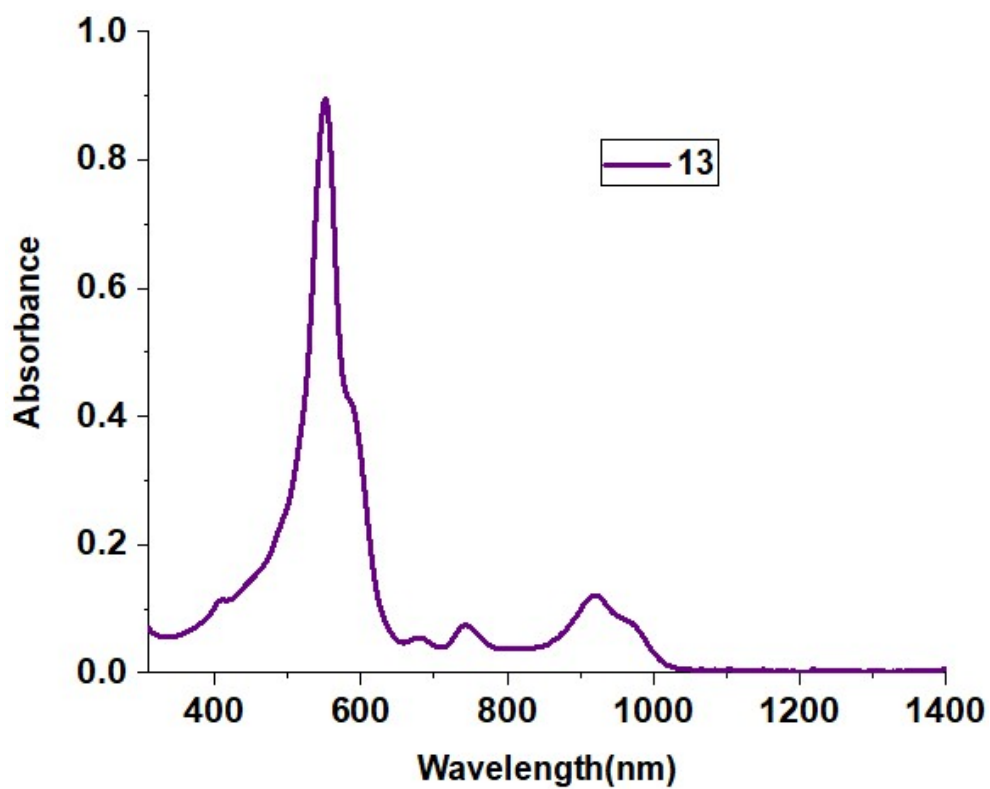


Fig. S8 UV-vis-NIR Spectrum of **13** in CH_2Cl_2 at 298 K

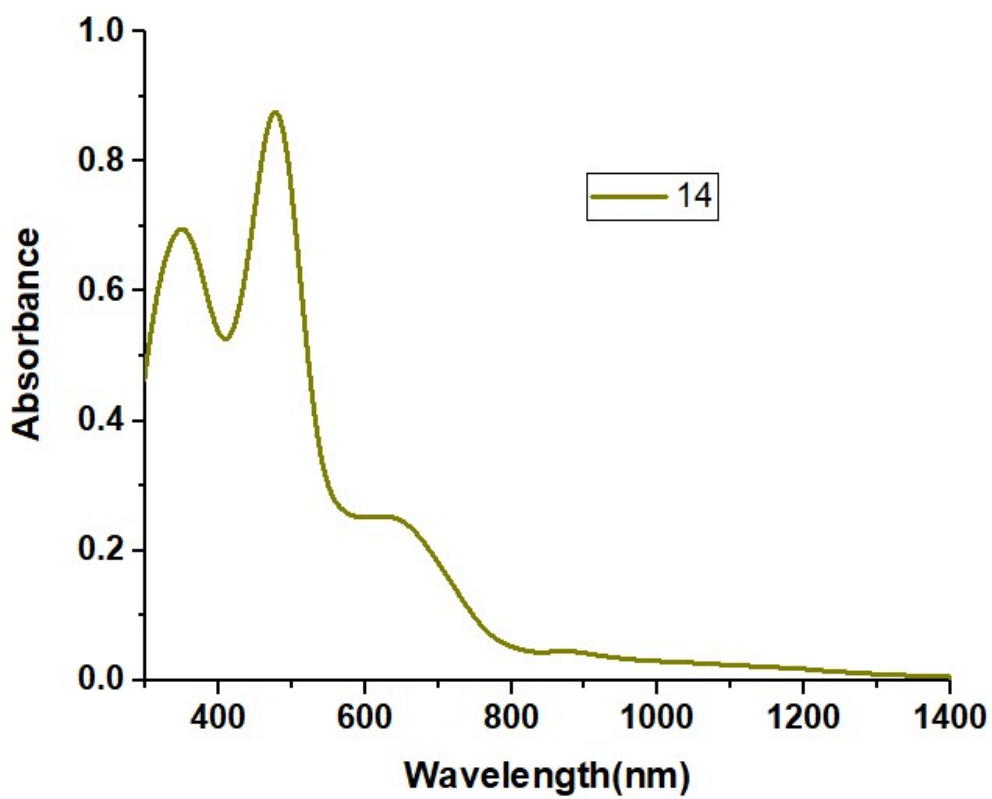


Fig. S9 UV-vis Spectra of **14** in CH_2Cl_2 at 298 K

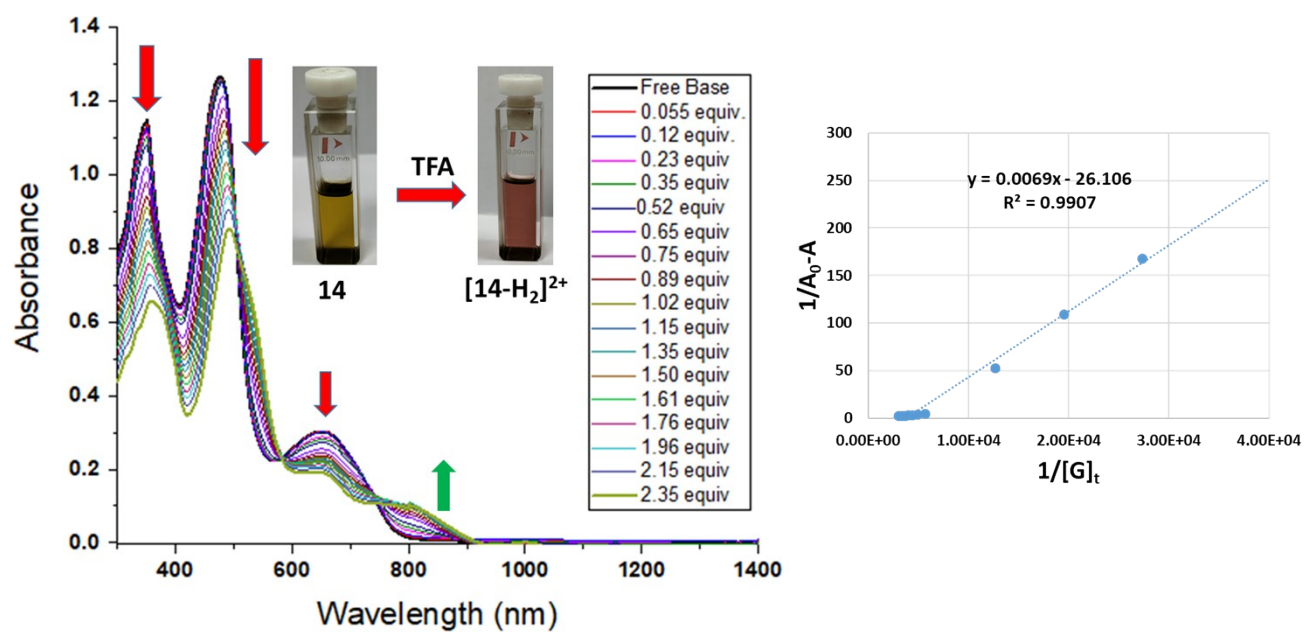


Fig. S10 Acid titration UV-vis Spectra of **14** (1.38×10^{-5} M) using 1×10^{-3} M TFA. Association Constant (K_a) = $3.78 \times 10^{-3} \text{ M}^{-1}$

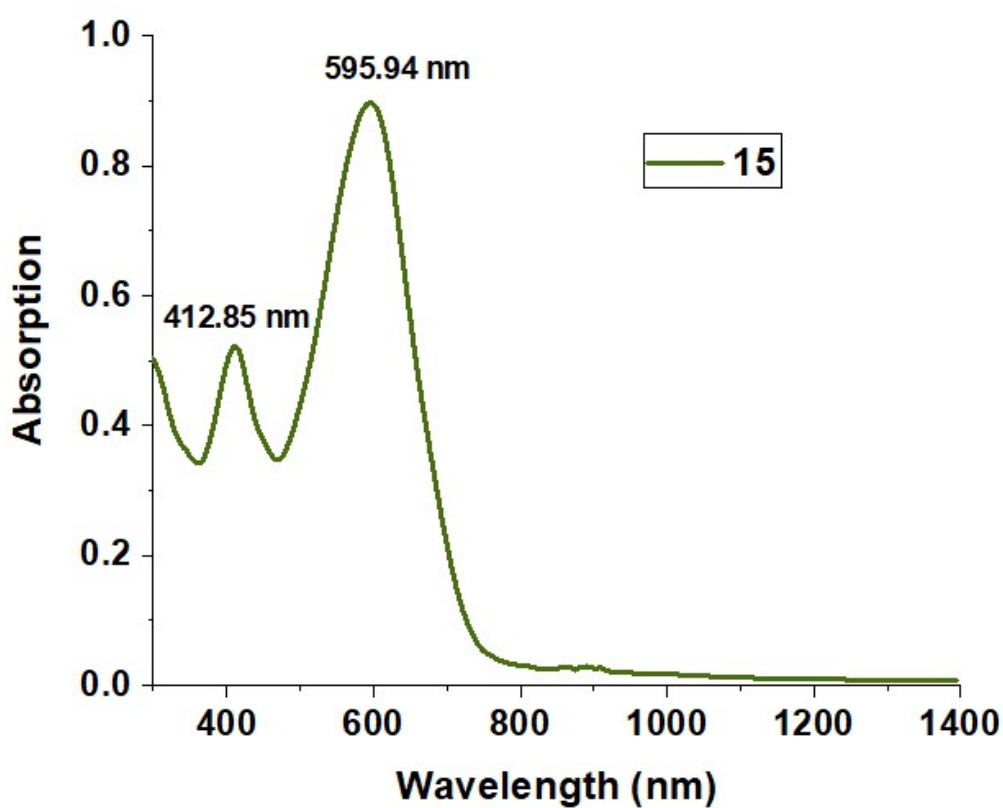


Fig. S11 UV-vis Spectra of **15** in CH_2Cl_2 at 298 K

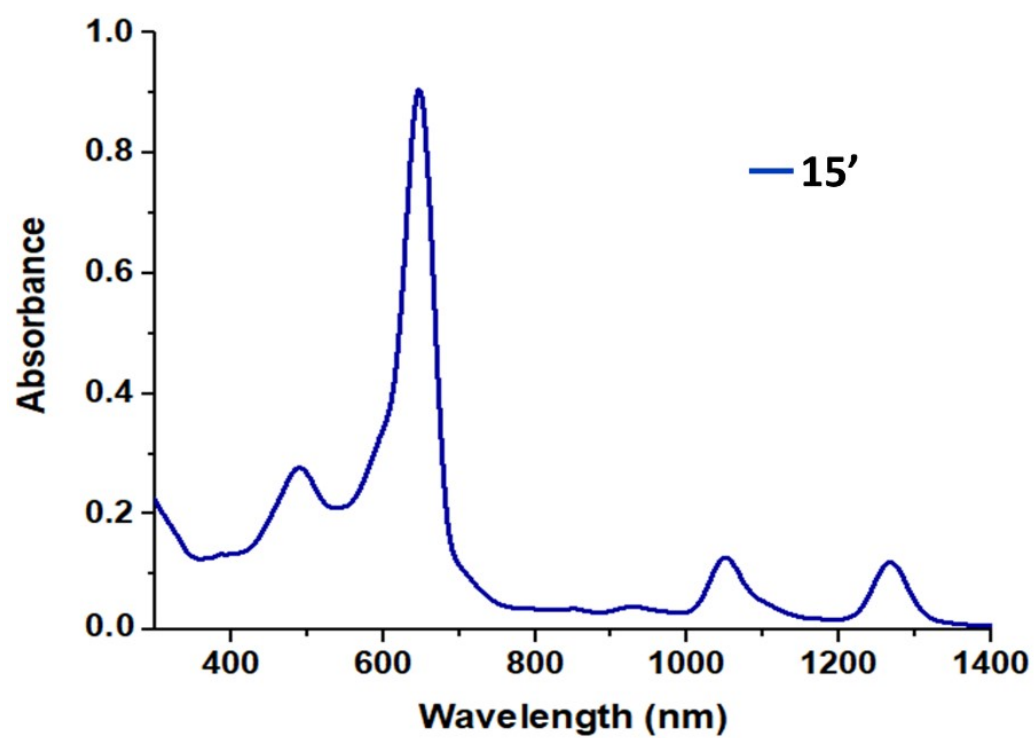


Fig. S12 UV-vis Spectra of **15'** in CH_2Cl_2 at 298 K

2.4 NMR spectra:

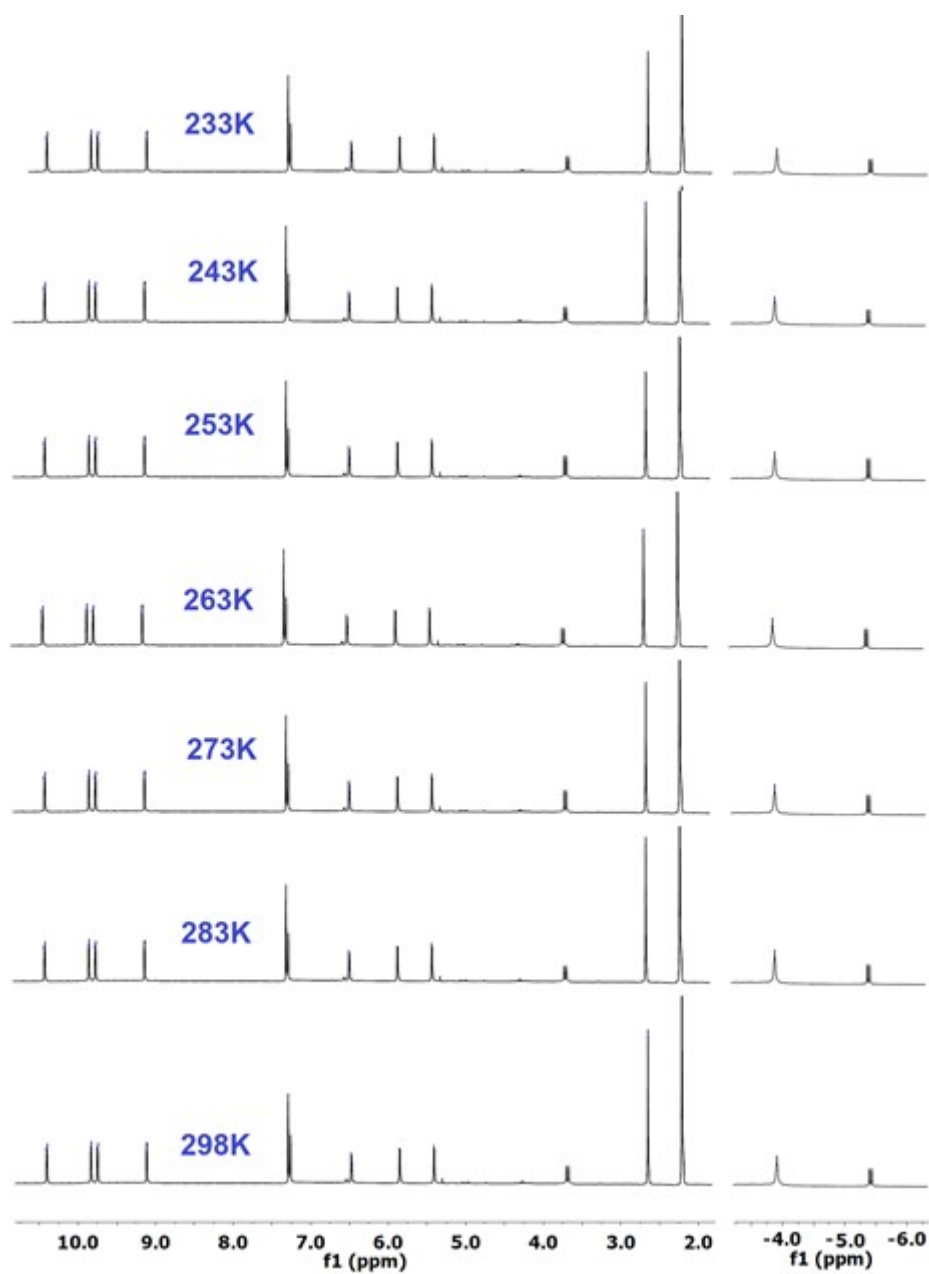


Fig. S13 Low VT ^1H NMR spectra of **13** in CDCl_3

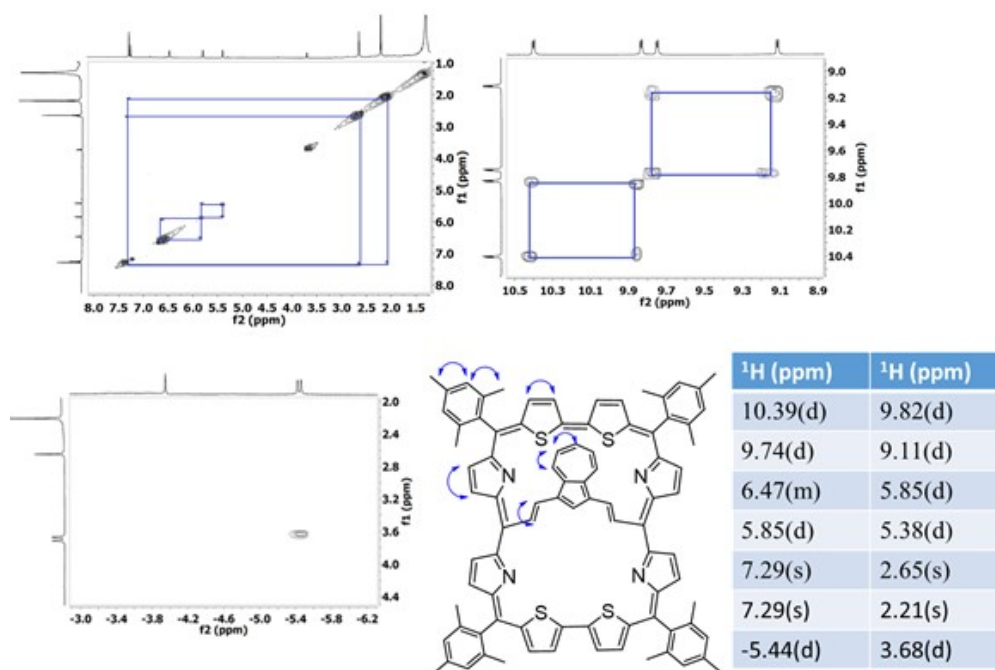


Fig. S14 ^1H - ^1H 2D COSY NMR spectra of **13** in CDCl_3 at 298 K

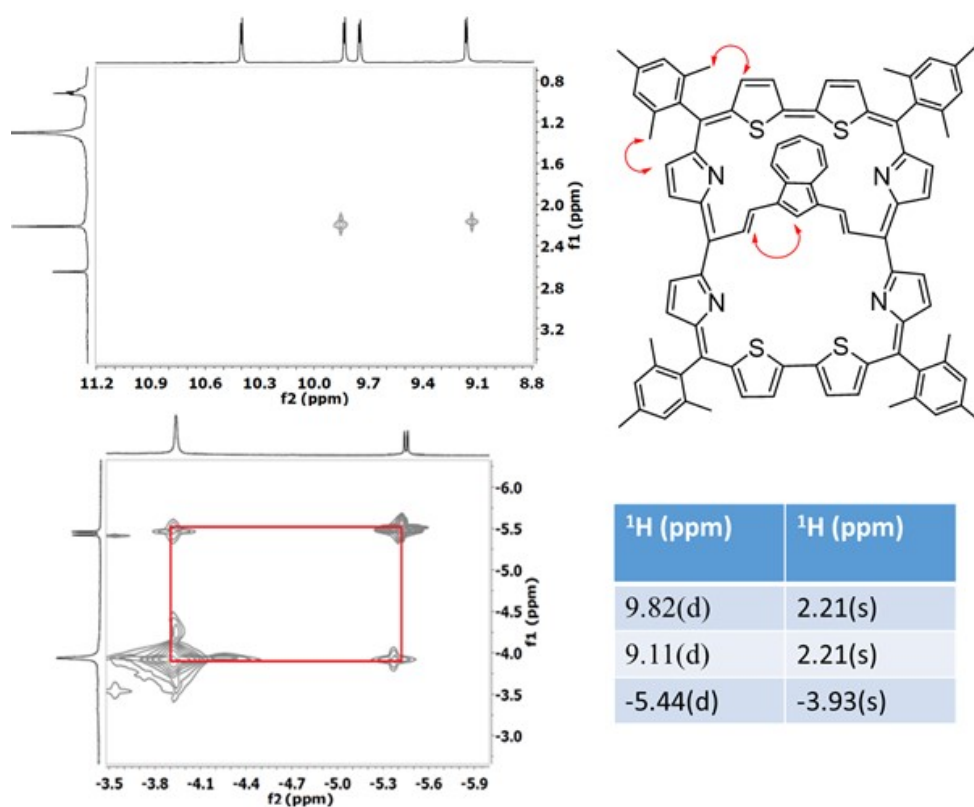


Fig. S15 ^1H - ^1H 2D ROESY NMR spectra of **13** in CDCl_3 at 298 K

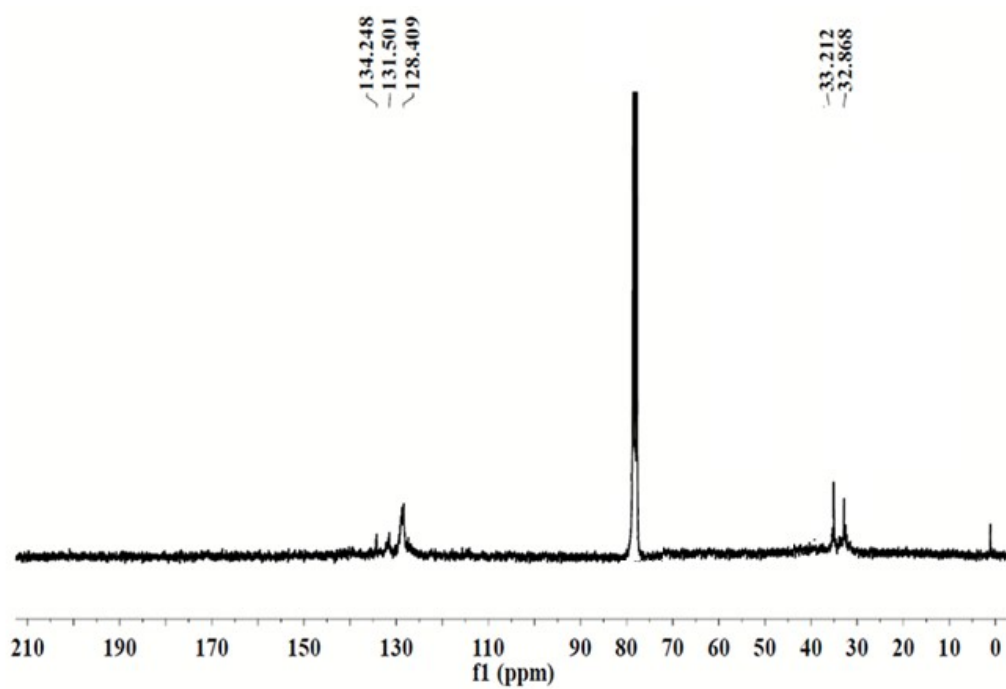


Fig. S16 ^{13}C NMR spectra of **15''** in CDCl_3 at 298 K

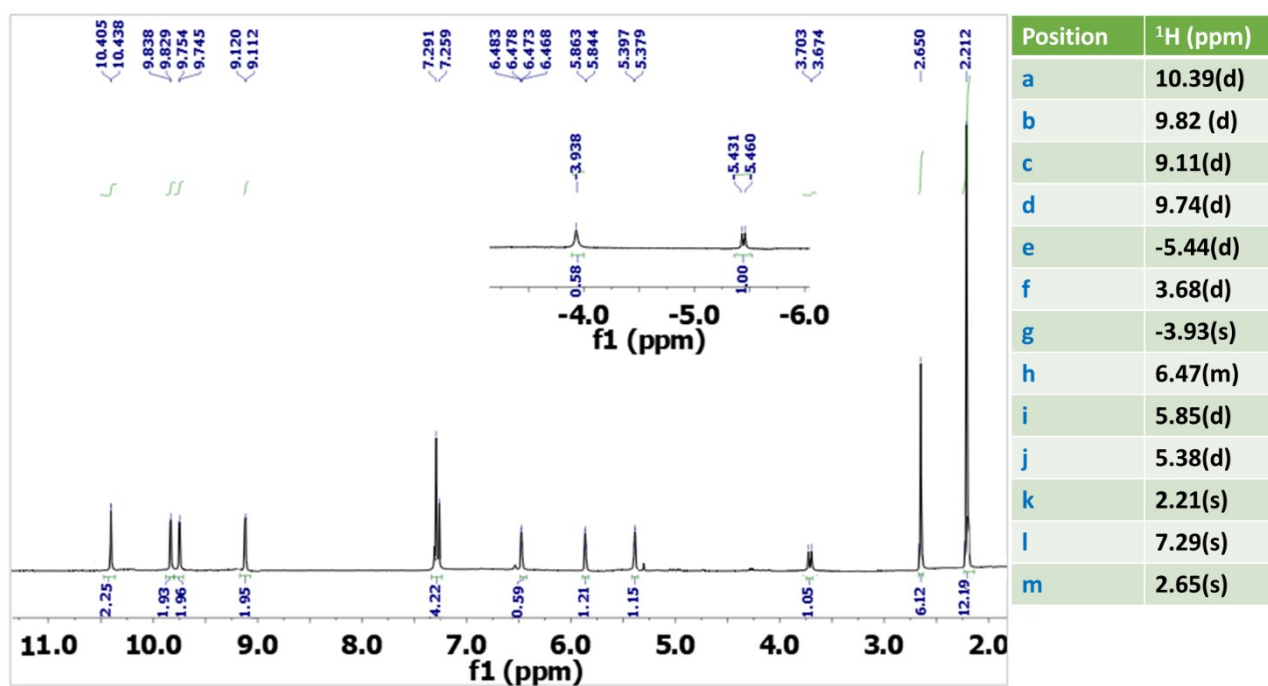


Fig. S17 Complete ^1H NMR spectral assignment of **13** in CDCl_3 at 298 K

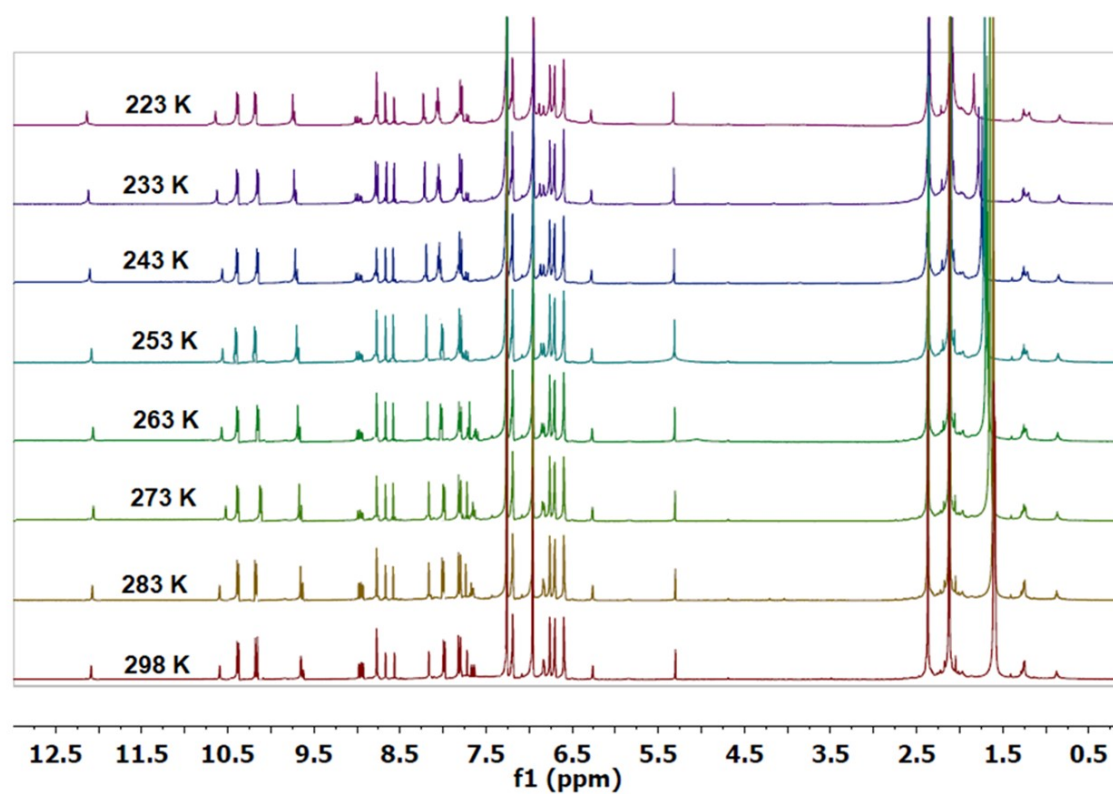


Fig. S18 Low VT ^1H NMR spectra of **14** in CDCl_3

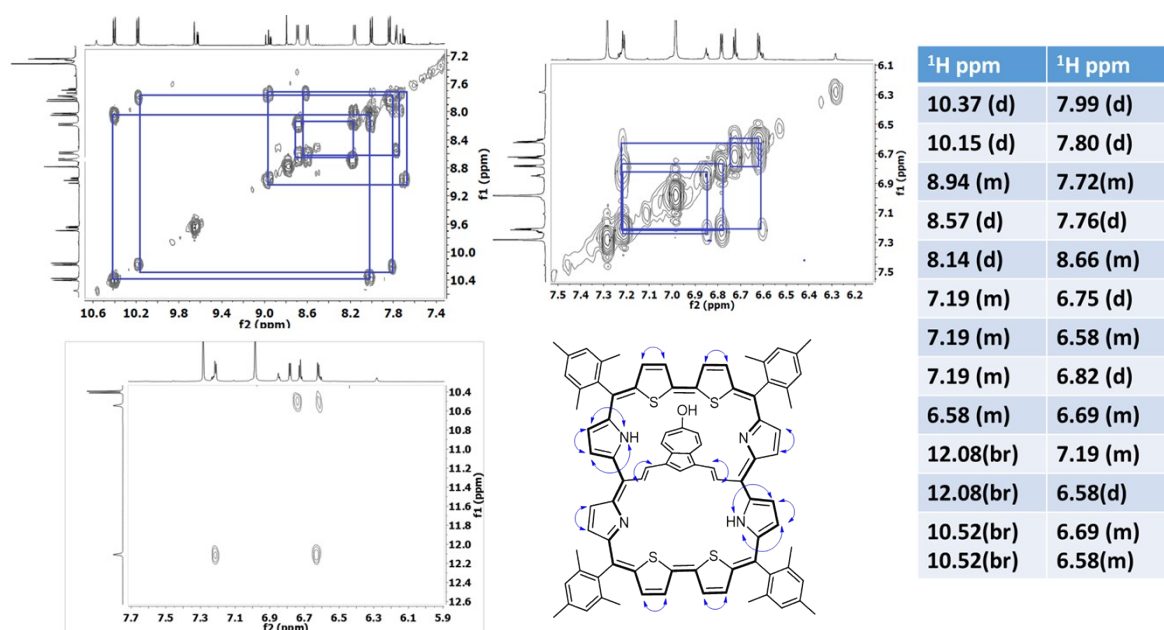


Fig. S19 ^1H - ^1H 2D COSY NMR spectra of **14** in CDCl_3 at 298 K

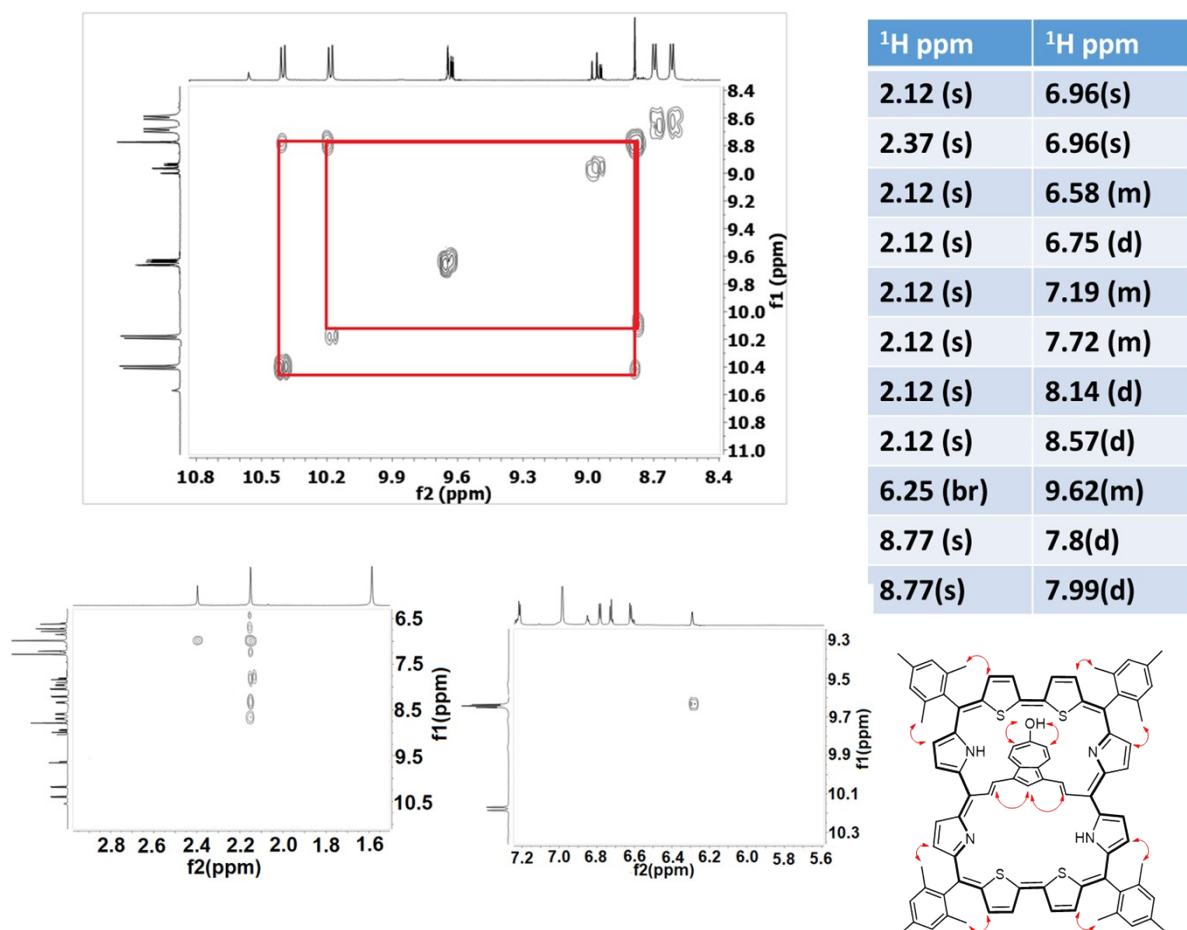


Fig. S20 ¹H -¹H 2D ROESY NMR spectra of **14** in CDCl₃ at 298 K

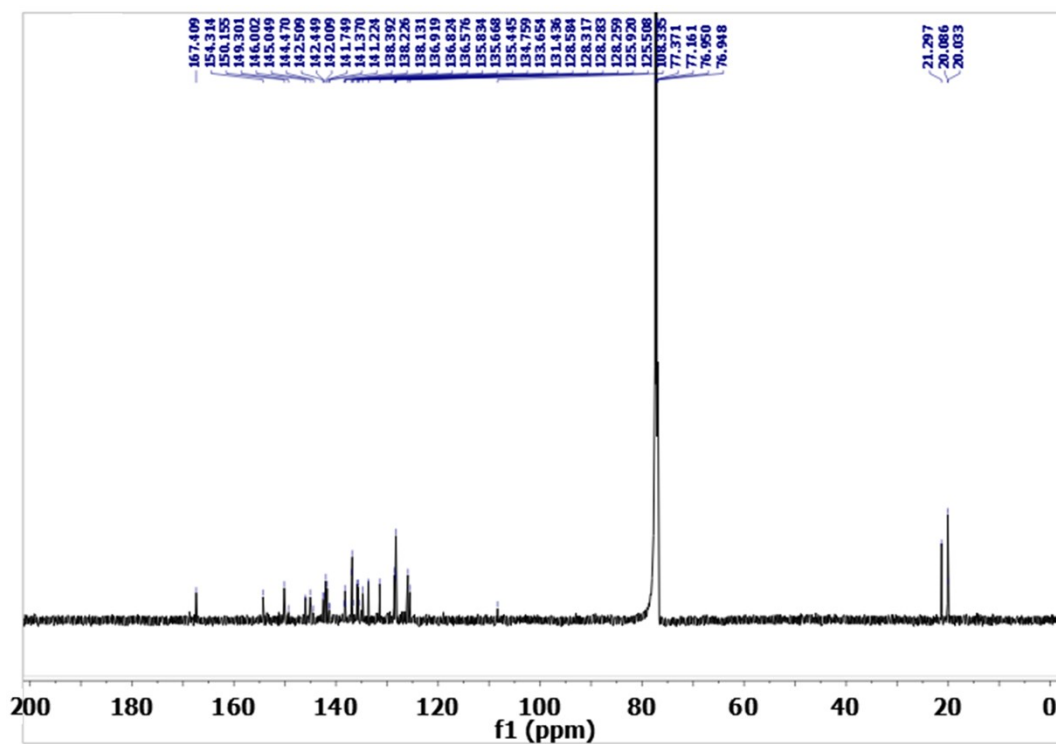


Fig. S21 ¹³C NMR spectra of **14** in CDCl₃ at 298 K

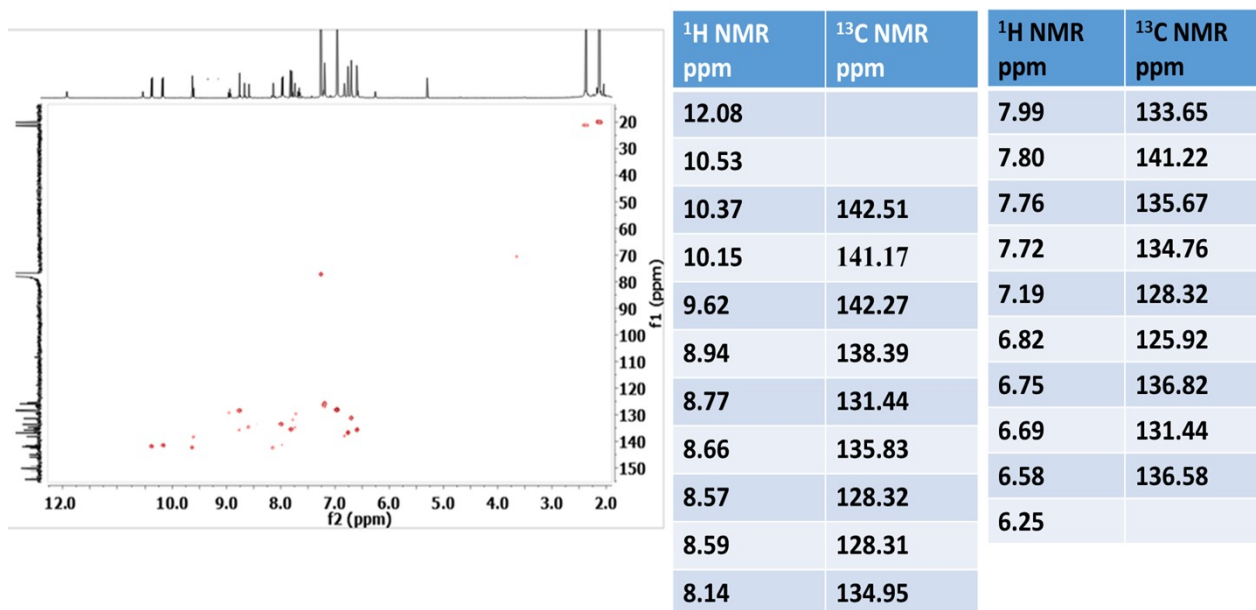


Fig. S22 HSQC NMR spectra of **14** in CDCl₃ at 298 K

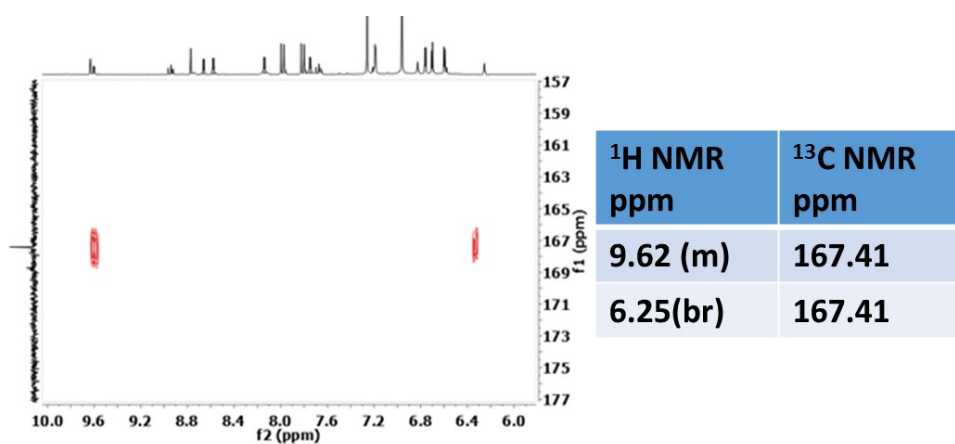


Fig. S23 HMBC NMR spectra of **14** in CDCl₃ at 298 K

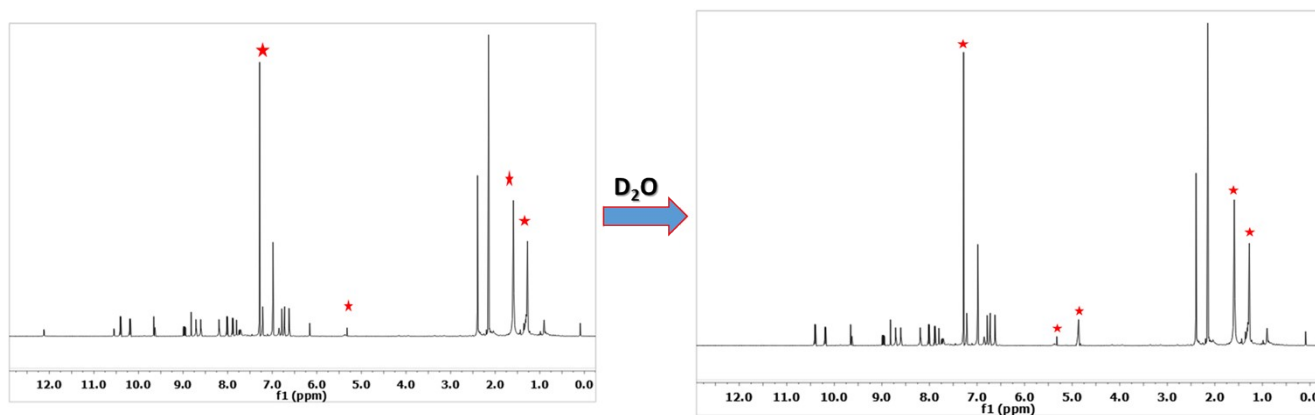


Fig. S24 D₂O exchange ¹H NMR spectrum of **14** in CDCl₃ at 298 K

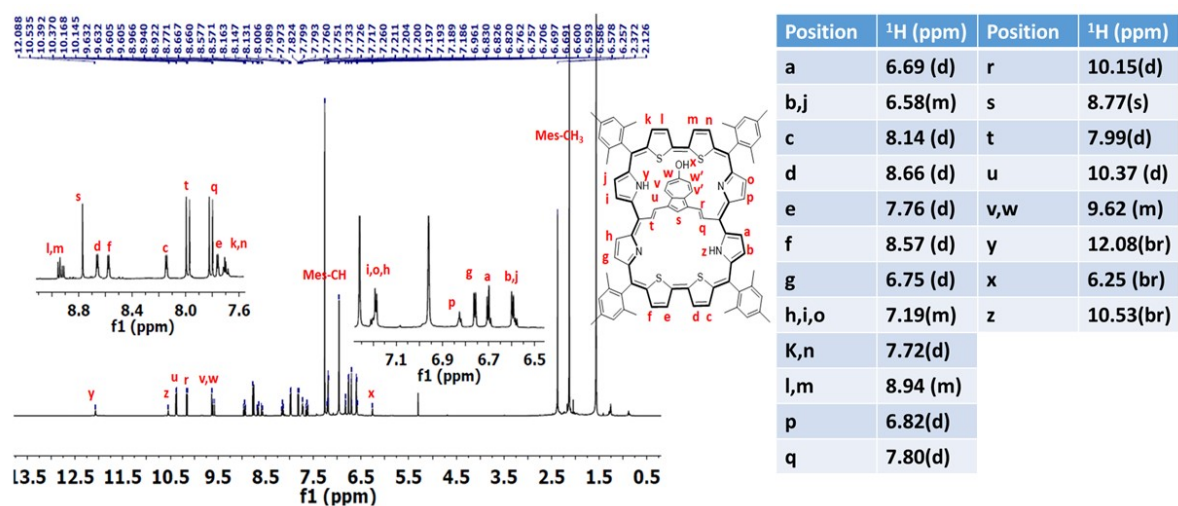


Fig. S25 Complete ¹H NMR spectral assignment of **14** in CDCl₃ at 298 K

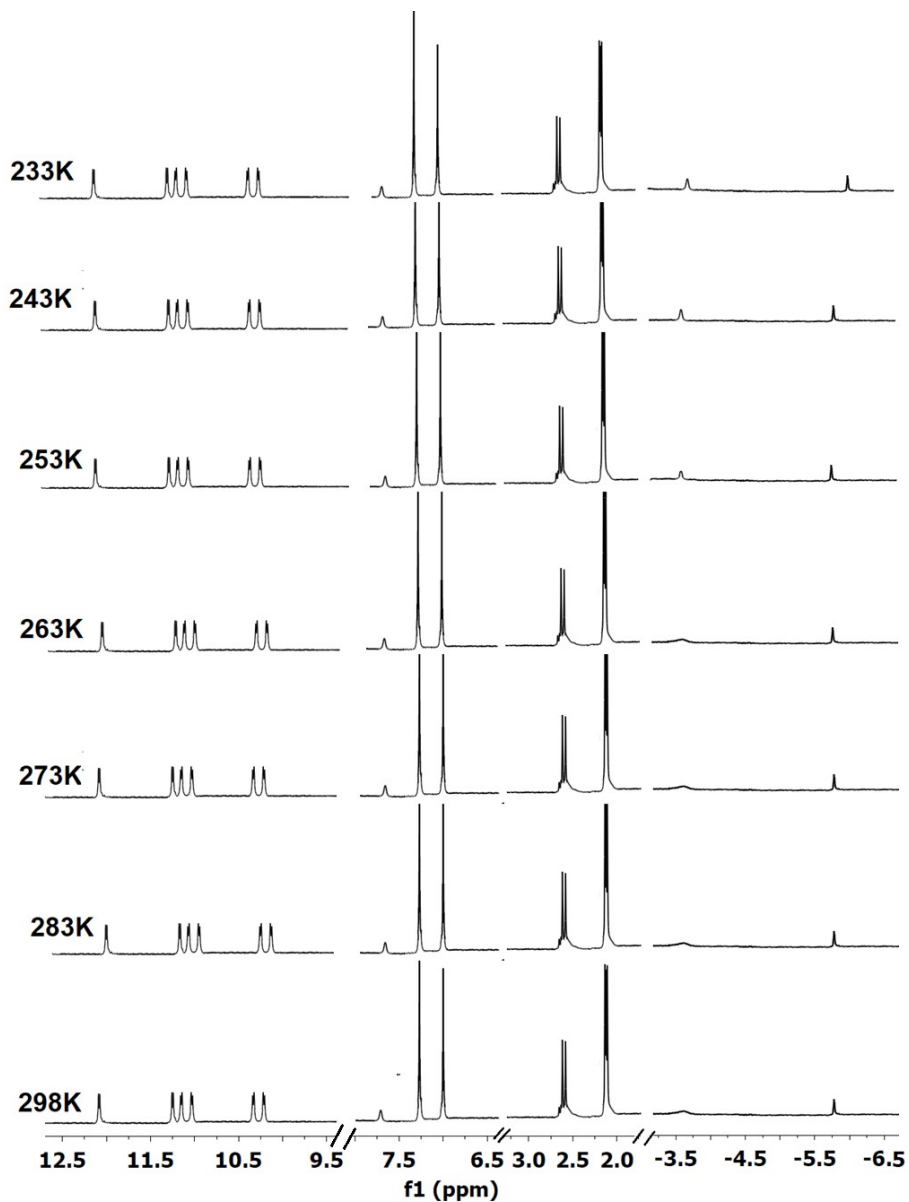


Fig. S26 Low VT ¹H NMR spectra of **15'** in CDCl₃

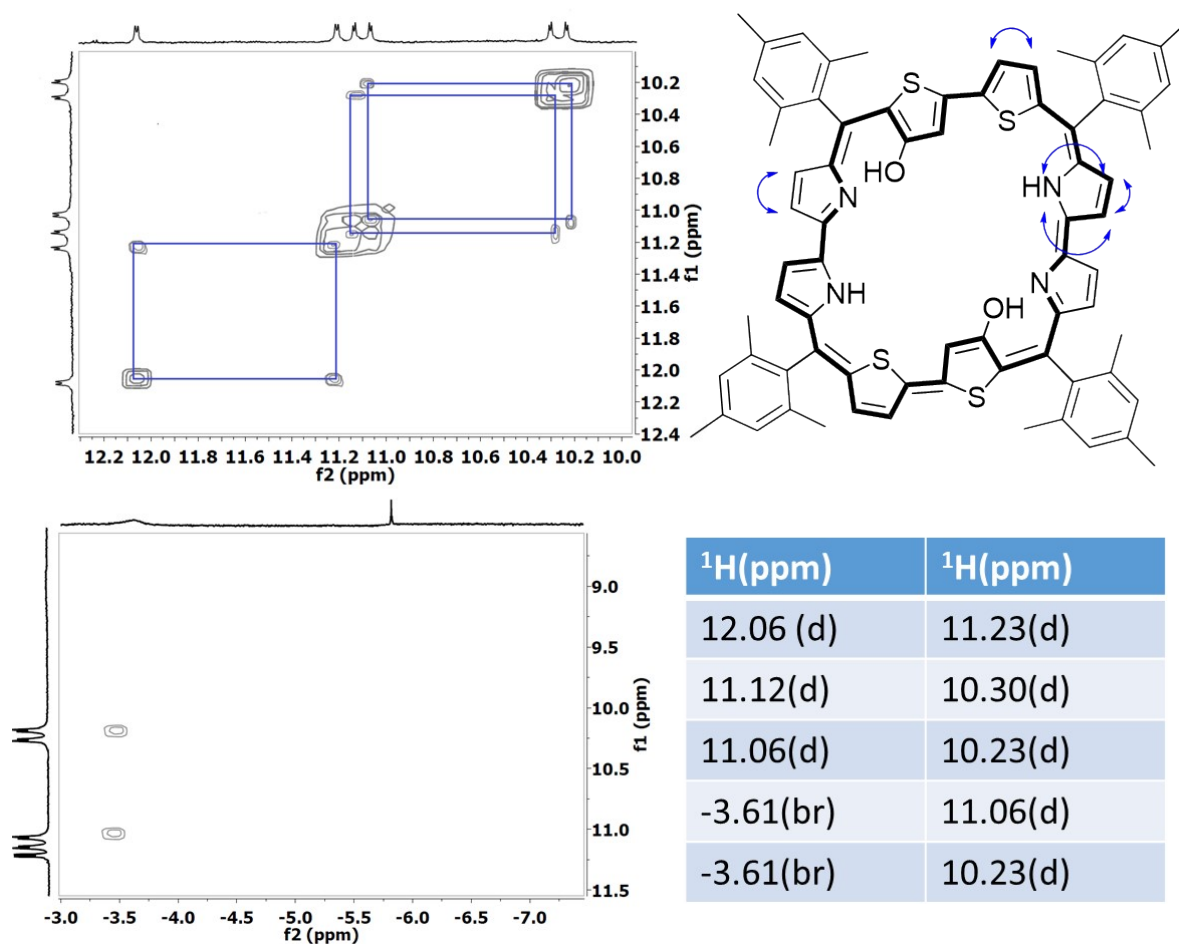


Fig. S27 ^1H - ^1H 2D COSY NMR spectra of **15'** in CDCl_3 at 298 K

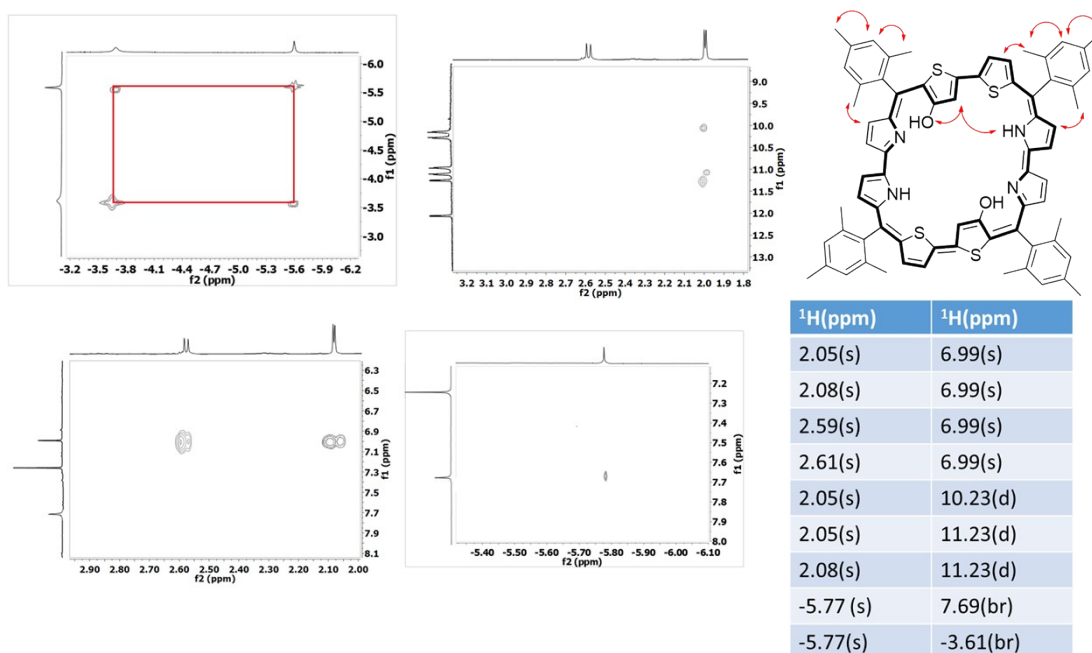


Fig. S28 ^1H - ^1H 2D ROESY NMR spectra of **15'** in CDCl_3 at 298 K

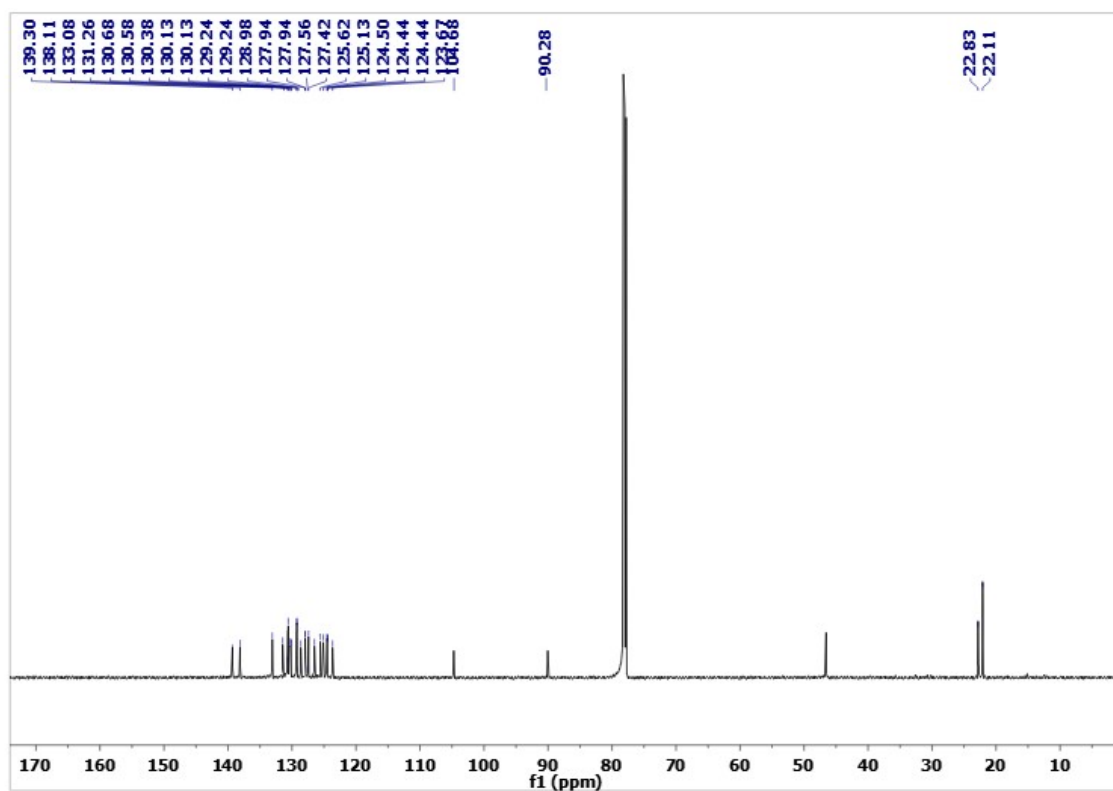


Fig. S29 ^{13}C NMR spectra of **15'** in CDCl_3 at 298 K

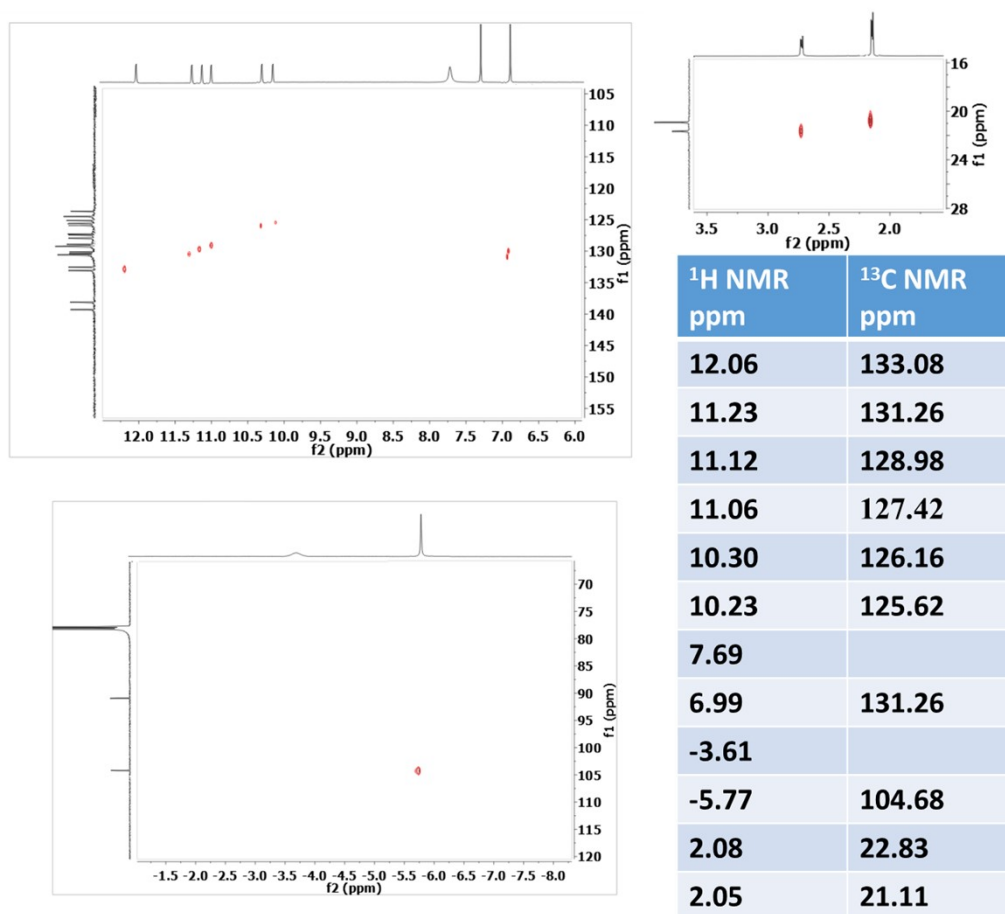


Fig. S30 HSQC NMR spectra of **15'** in CDCl_3 at 298 K

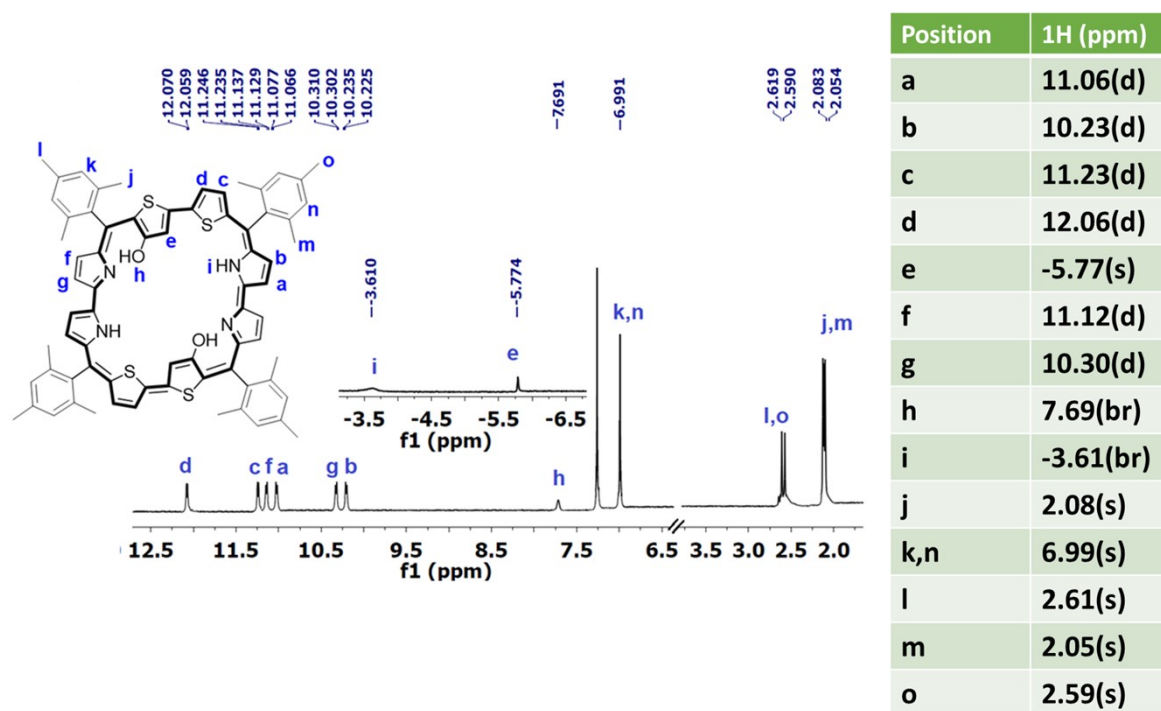


Fig. S31 Complete ^1H NMR spectral assignment of **15'** in CDCl_3 at 298 K

4. Crystal Data

Table S1. Crystallographic data

Parameters	15
Chemical formula	C ₇₂ H ₆ N ₄ O ₂ S ₄
Formula weight	1140.3599
Temperature	145K
Crystal system	triclinic
Space group	P-1
a(Å); α(°)	12.5941(7); 91.61
b(Å), β(°)	13.3888(8); 97.04
c(Å), γ(°)	14.2293(8); 93.22
Volume(Å ³); Z	2376.0(2); 1
ρ _{calc} /cm ³	1.298
μ(Mo Kα) mm ⁻¹	0.649
2θ max (°)	56.742
R(int)	0.0920
Completeness to θ	99
Data/parameters	11760/484
GOF	1.043
R1 [F>4σ (F)]	0.0687
wR ₂ [all data]	11760
Max.peak/hole / e Å ⁻³	1.17/-1.22
CCDC	2274626

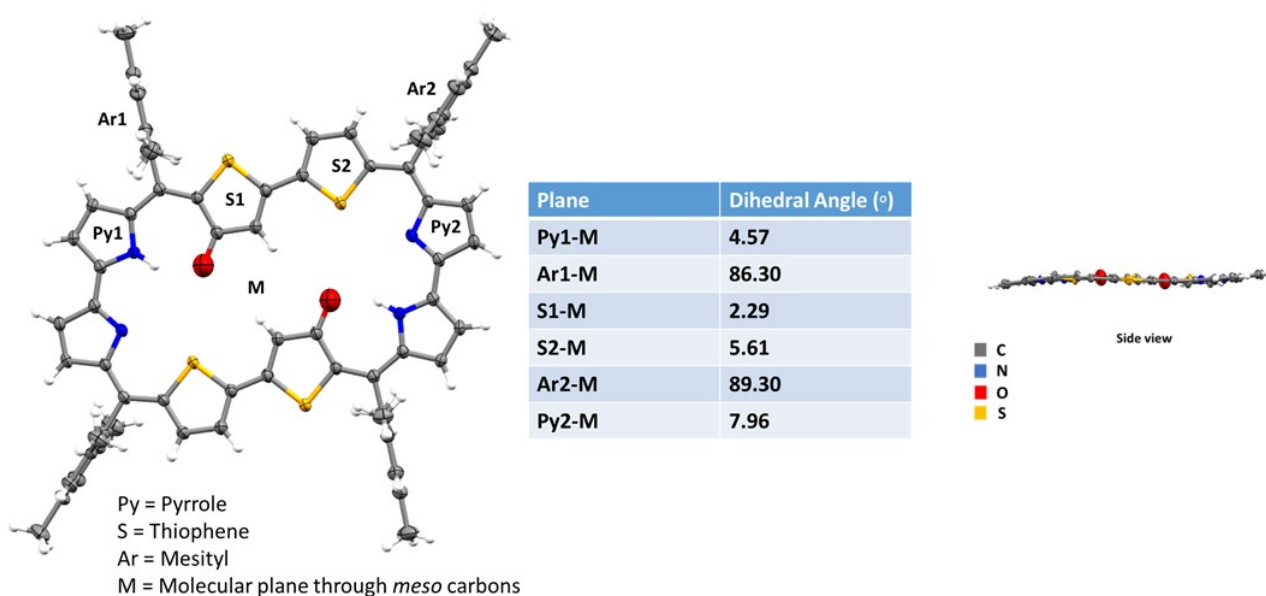


Fig. S32 Crystal structure of 15 (A: top view; B-side view)

5. Electrochemical Studies

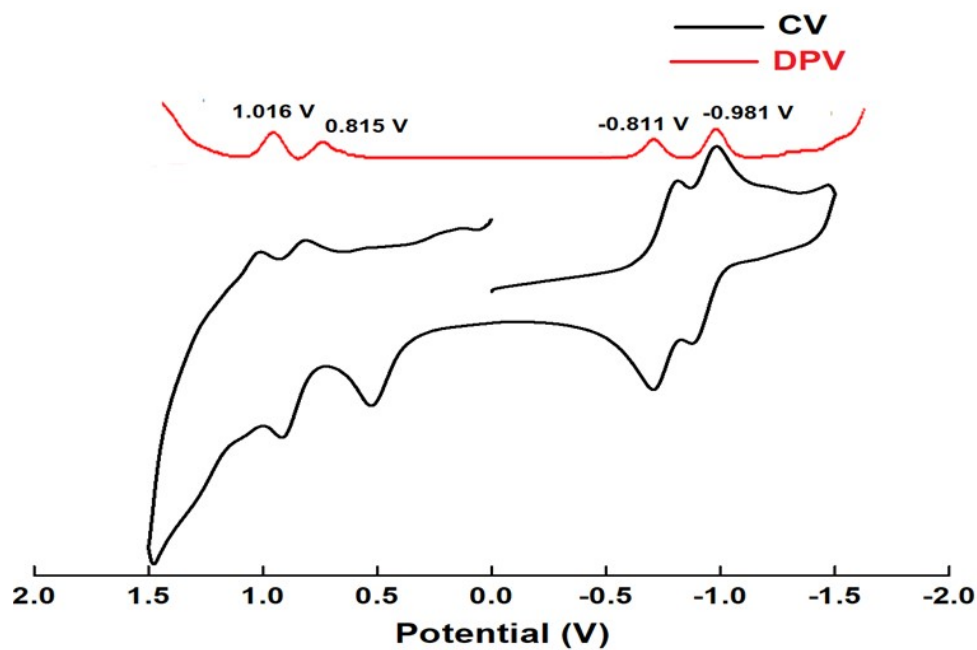


Fig. S33 Cyclic voltammogram of **13** (~10⁻⁴M) in dichloromethane containing tetrabutylammonium hexafluorophosphate (0.01M) recorded at 100 mVs⁻¹.

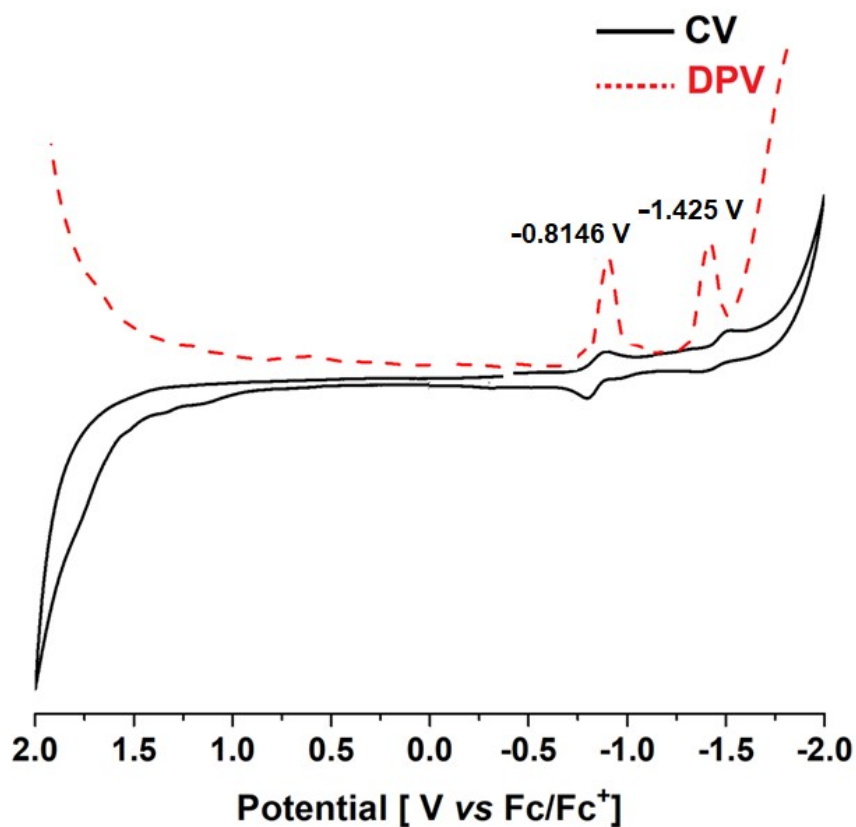


Fig. S34 Cyclic voltammogram of **14** (~10⁻⁴M) in dichloromethane containing tetrabutylammonium hexafluorophosphate (0.01M) recorded at 100 mVs⁻¹.

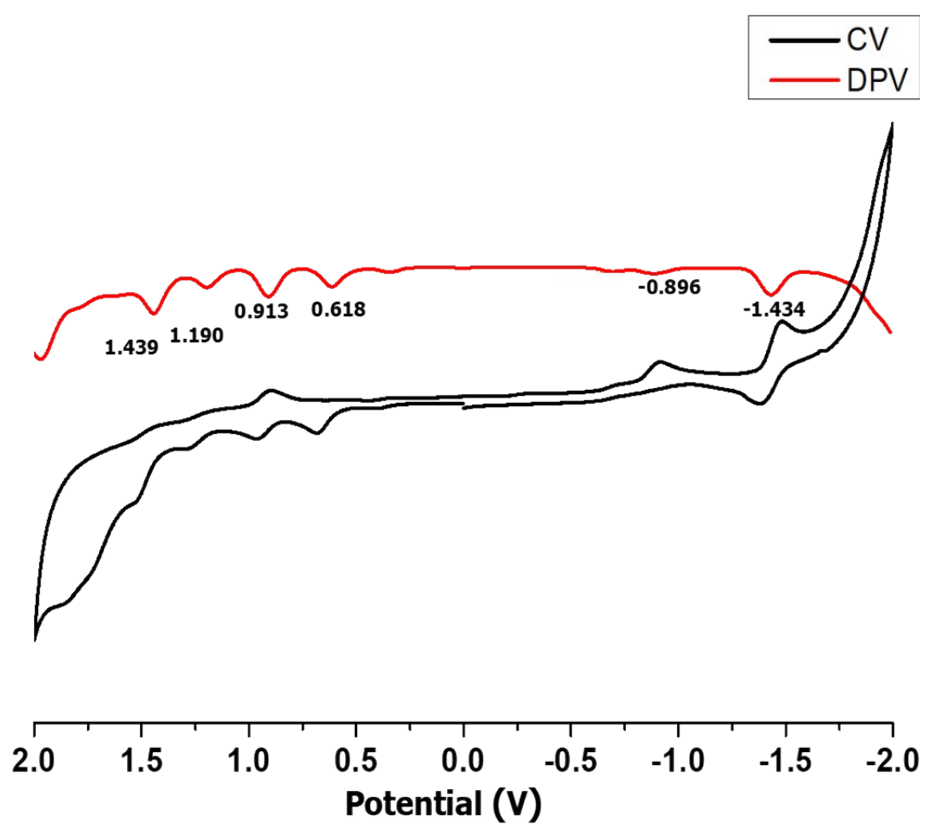


Fig. S35 Cyclic voltammogram of **15'** ($\sim 10^{-4}$ M) in dichloromethane containing tetrabutylammonium hexafluorophosphate (0.01M) recorded at 100 mVs^{-1} .

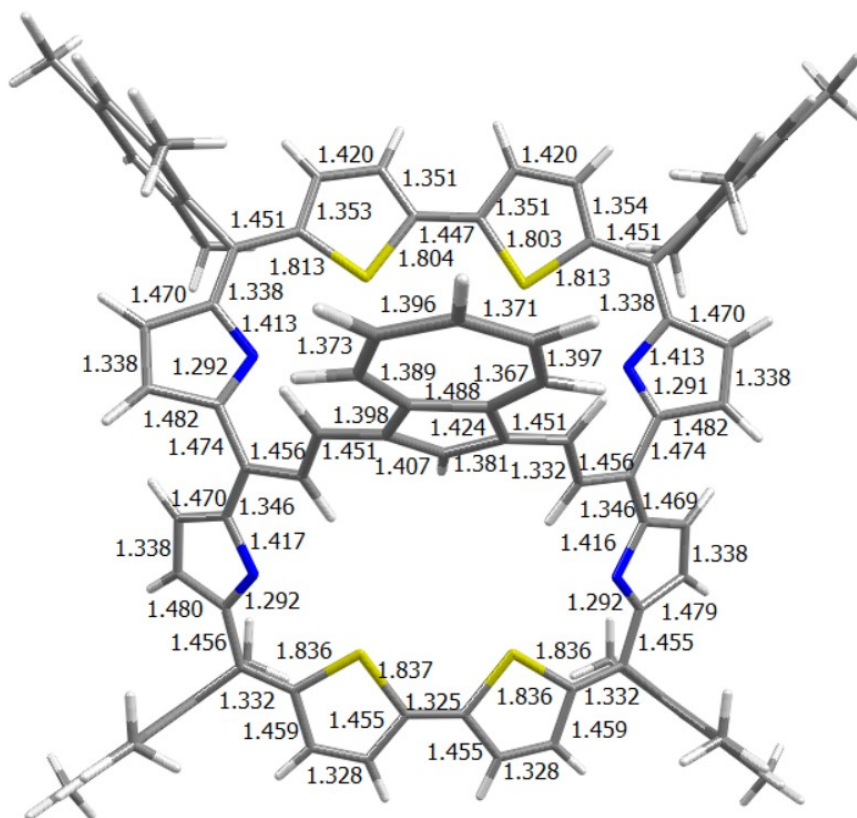


Fig. S36 Optimized geometry of **13** with selected bond length (Å).

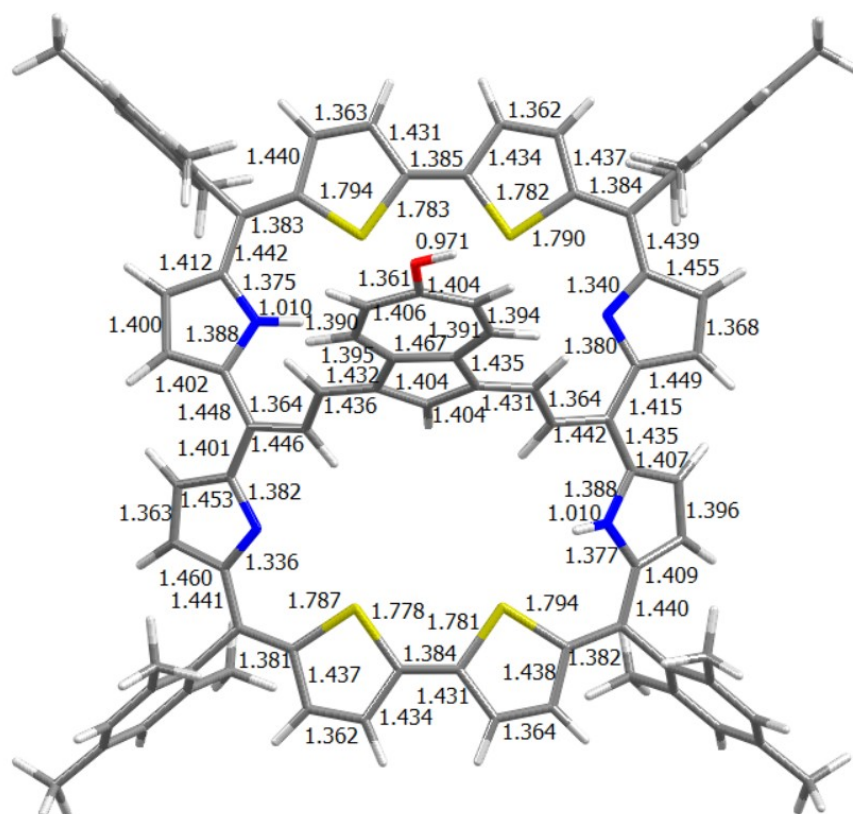


Fig. S37 Optimized geometry of **14** with selected bond length (Å).

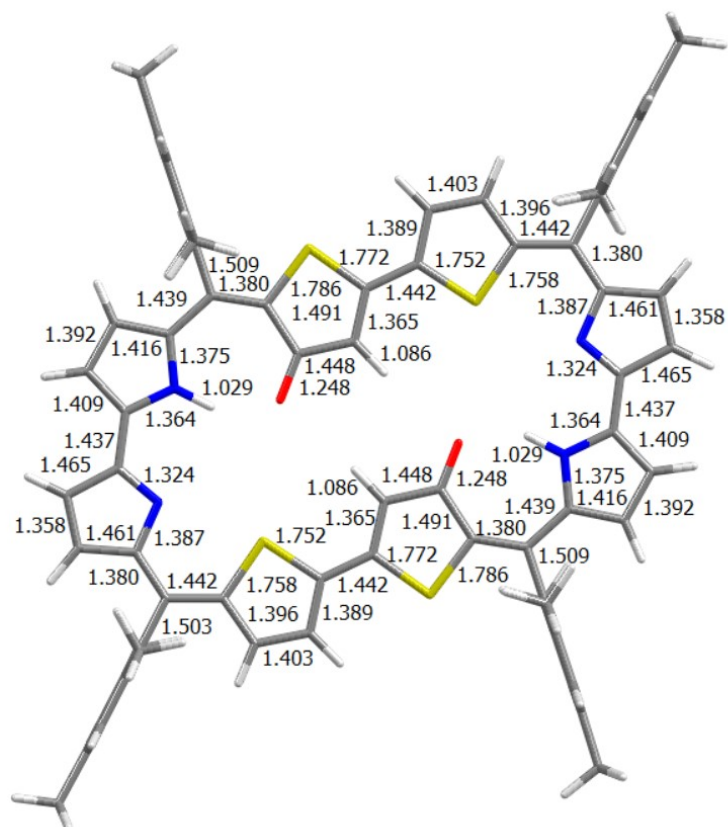


Fig. S38 Optimized geometry of **15** with selected bond length (Å).

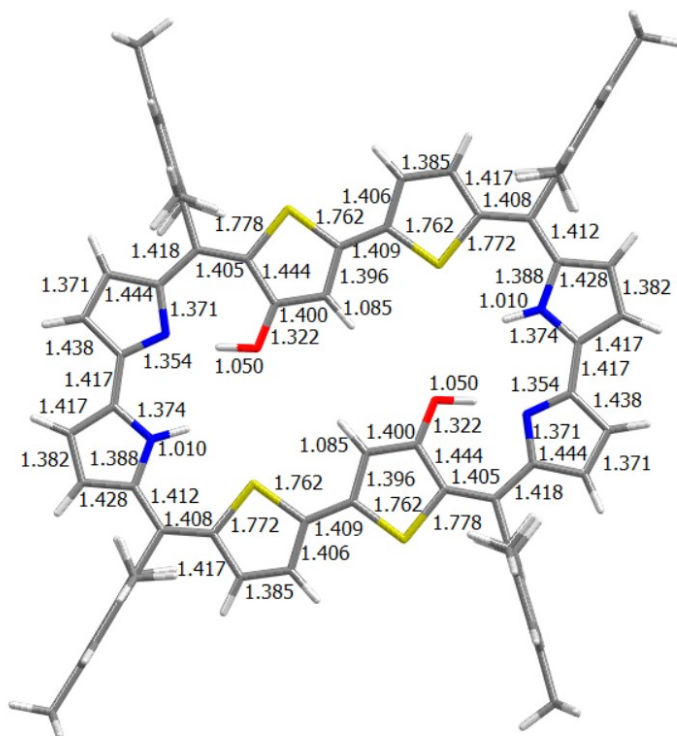
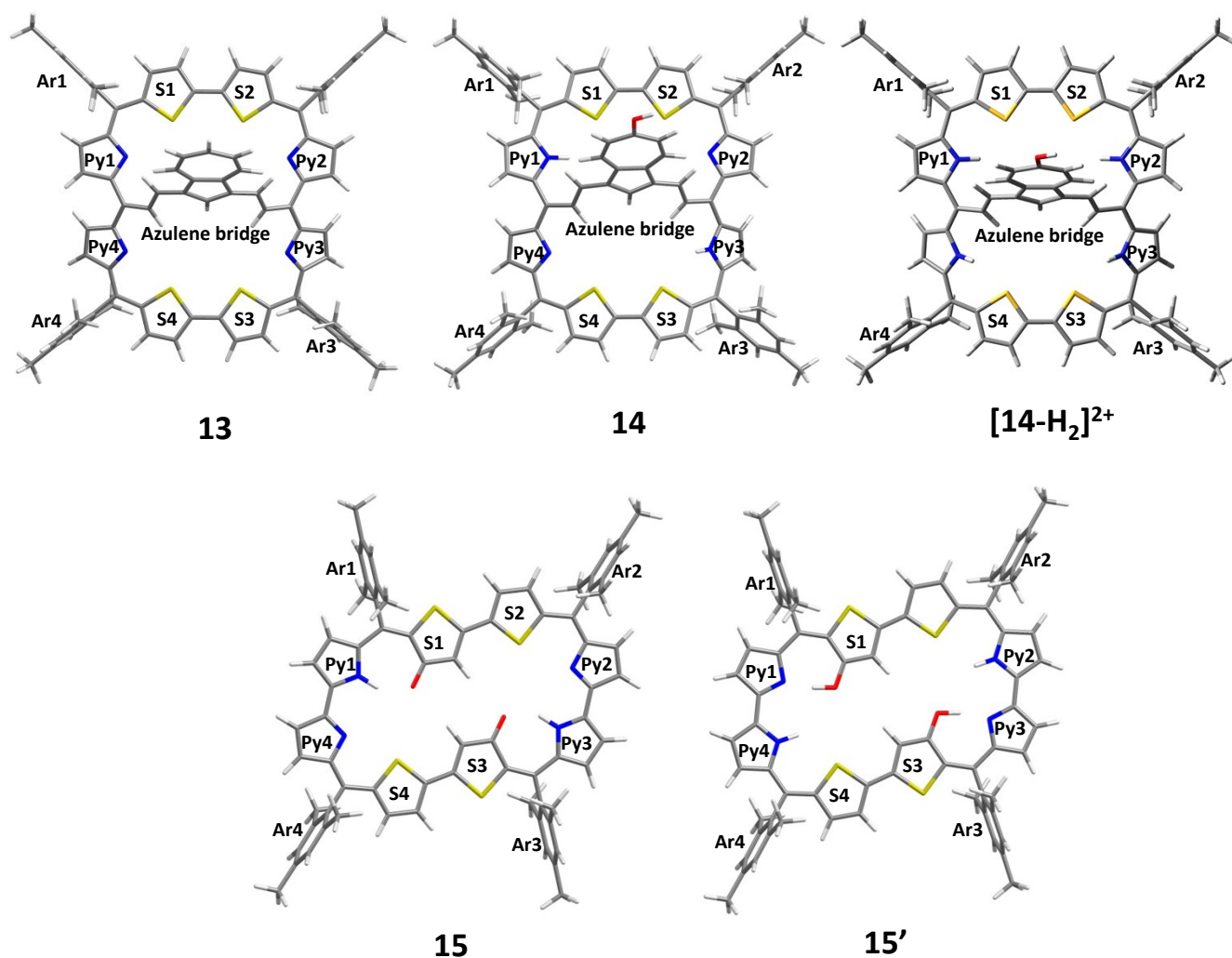


Fig. S39 Optimized geometry of **15'** with selected bond length (Å)



Plane	Dihedral Angle (°)				
	13	14	[14-H ₂] ²⁺	15	15'
Py1-M	8.86	9.27	8.76	0.00	1.20
Ar1-M	83.33	82.48	81.26	90.00	89.71
S1-M	9.93	11.51	16.31	0.00	1.04
S2-M	9.93	8.61	16.39	0.00	4.72
Ar2-M	83.34	87.84	81.19	90.00	86.39
Py2-M	8.86	8.94	8.90	0.00	2.92
Py3-M	28.93	38.57	36.34	0.01	1.21
Ar3-M	76.59	68.95	69.61	89.98	89.71
S3-M	6.50	7.05	6.40	0.01	1.04
S4-M	6.53	4.98	6.41	0.00	4.72
Ar4-M	76.65	74.99	69.52	90.00	86.39
Py4-M	28.92	28.36	36.20	0.00	2.92
Azulene bridge-M	53.07	56.82	60.82	-	-

Fig. S40 Important dihedral between the macrocyclic mean plane (M) and the rings of **13**, **14**, **[14-H₂]²⁺**, **15** and **15'**

Table S2. Calculated energies of the optimized structures and relative energies (ΔE) for plausible isomers of **13**.

	Energy (hartree)	ΔE (kJ/mol)
13	-5207.188172	0.00
Conformer-1	-5207.125010	165.83
Conformer-2	-5207.125010	165.83
Conformer-3	-5207.168040	52.86
Conformer-4	-5207.168040	52.86
Conformer-5	-5207.090339	256.86
Conformer-6	-5207.159220	76.014
Conformer-7	-5207.159220	76.01
Conformer-8	-5207.175167	34.15
Conformer-9	-5207.175167	34.15
Conformer-10	-5207.131486	148.83
Conformer-11	-5207.127956	158.10
Conformer-12	-5207.139626	127.46
Conformer-13	-5207.144938	113.51
Conformer-14	-5207.161649	69.64

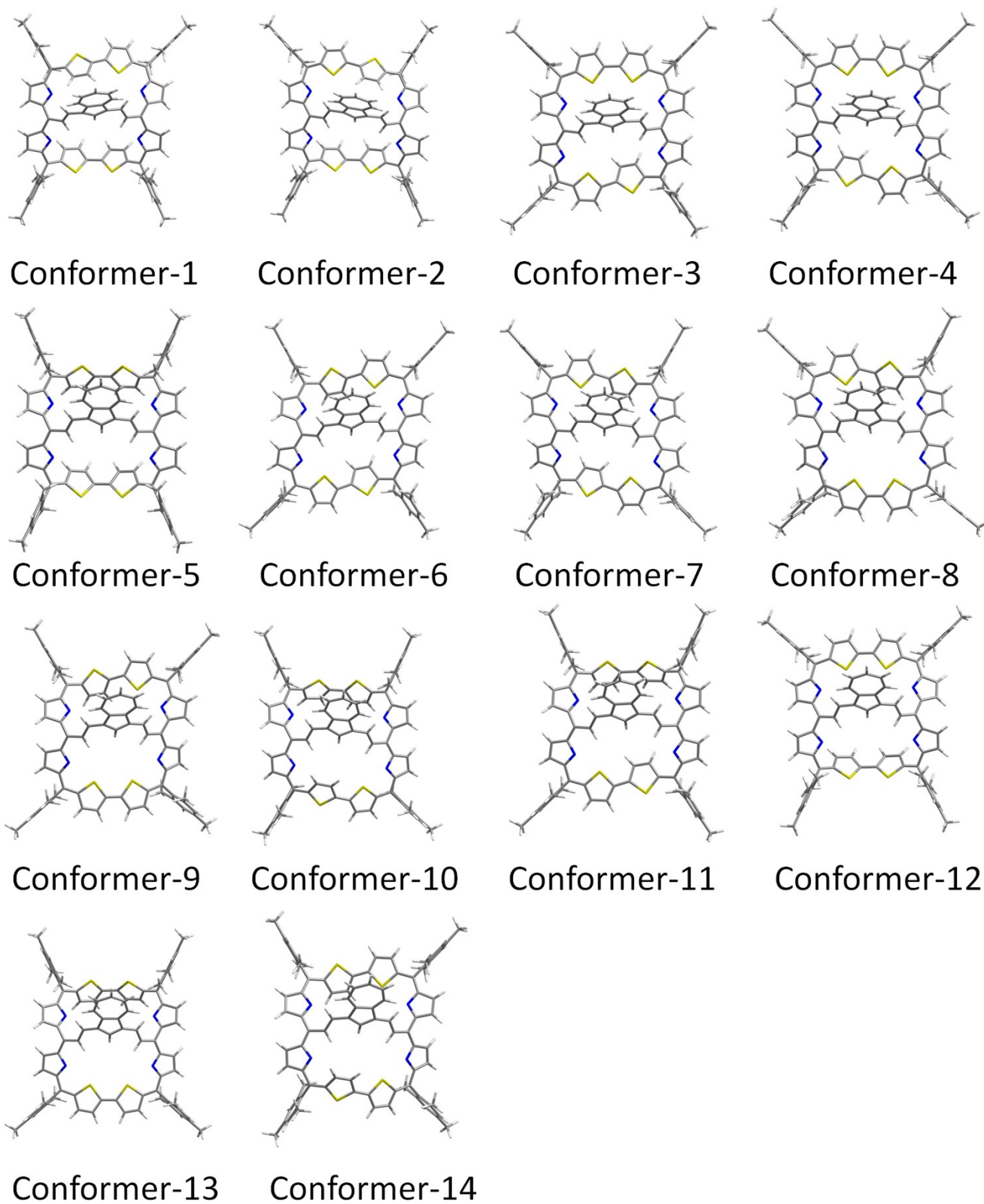


Fig. S41 Optimized geometry of all the possible conformers of **13**

Table S3. Calculated energies of the optimized structures and relative energies (ΔE) for plausible isomers of **14**.

	Energy (hartree)	ΔE (kJ/mol)
14	-5283.636455	0.00
Conformer-1	-5283.626579	25.93
Conformer-2	-5283.610400	68.41
Conformer-3	-5283.627248	24.17
Conformer-4	-5283.617156	50.67
Conformer-5	-5283.607963	74.81
Conformer-6	-5283.606322	79.11
Conformer-7	-5283.601150	92.69
Conformer-8	-5283.617619	49.45
Conformer-9	-5283.621145	40.20
Conformer-10	-5283.577150	155.71
Conformer-11	-5283.600540	94.29
Conformer-12	-5283.607963	74.81
Conformer-13	-5283.603027	87.77

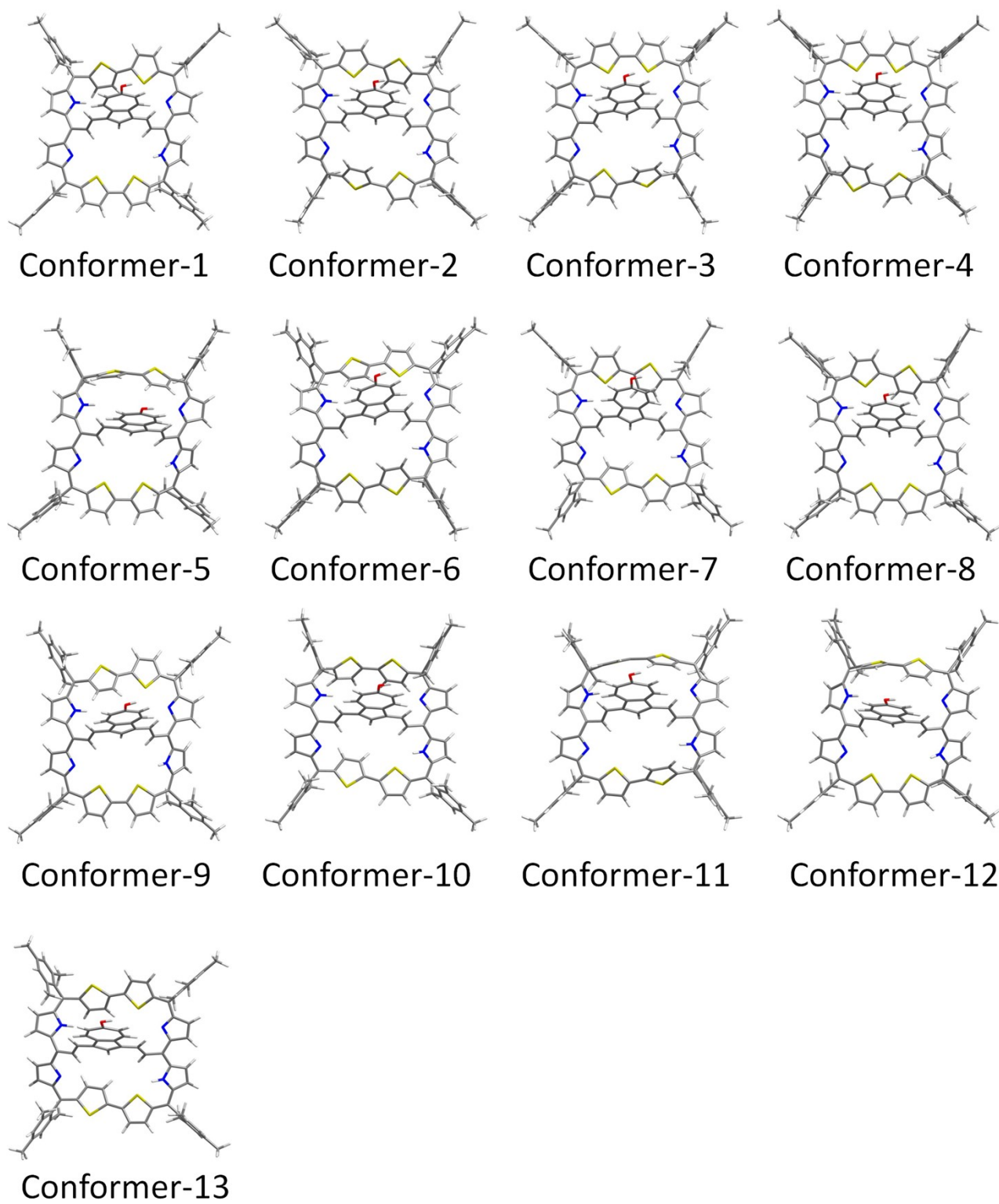


Fig. S42 Optimized geometry of all the possible conformers **14**

Table S4. Calculated energies of the optimized structures and relative energies (ΔE) for plausible isomers of **15** and **15'**

	15		15'	
	Energy (hartree)	ΔE (kJ/mol)	Energy (hartree)	ΔE (kJ/mol)
15	-4742.0533363	0.00	-4743.2536316	0.00
Conformer-1	-4742.0279447	66.67	-4743.2348475	49.32
Conformer-2	-4742.0025597	133.31	-4743.2127673	107.29
Conformer-3	-4742.0134092	104.83	-	-
Conformer-4	-4741.9992970	141.88	-4743.1905828	165.53
Conformer-5	-4742.0092364	115.78	-4743.2228661	80.77
Conformer-6	-4742.0026949	132.96	-4743.1828036	185.96
Conformer-7	-4742.0101016	113.51	-4743.2167111	96.93
Conformer-8	-4741.9994241	141.55	-4743.1905828	165.53
Conformer-9	-4742.0134091	104.83	-	-
Conformer-10	-4742.0025596	133.31	-4743.2127673	107.29
Conformer-11	-4742.0279444	66.67	-4743.2348475	49.32
Conformer-12	-4741.9906914	164.47	-4743.1888097	170.19
Conformer-13	-4741.9906913	164.47	-4743.1888098	170.19
Conformer-14	-4742.0187237	90.88	-	-

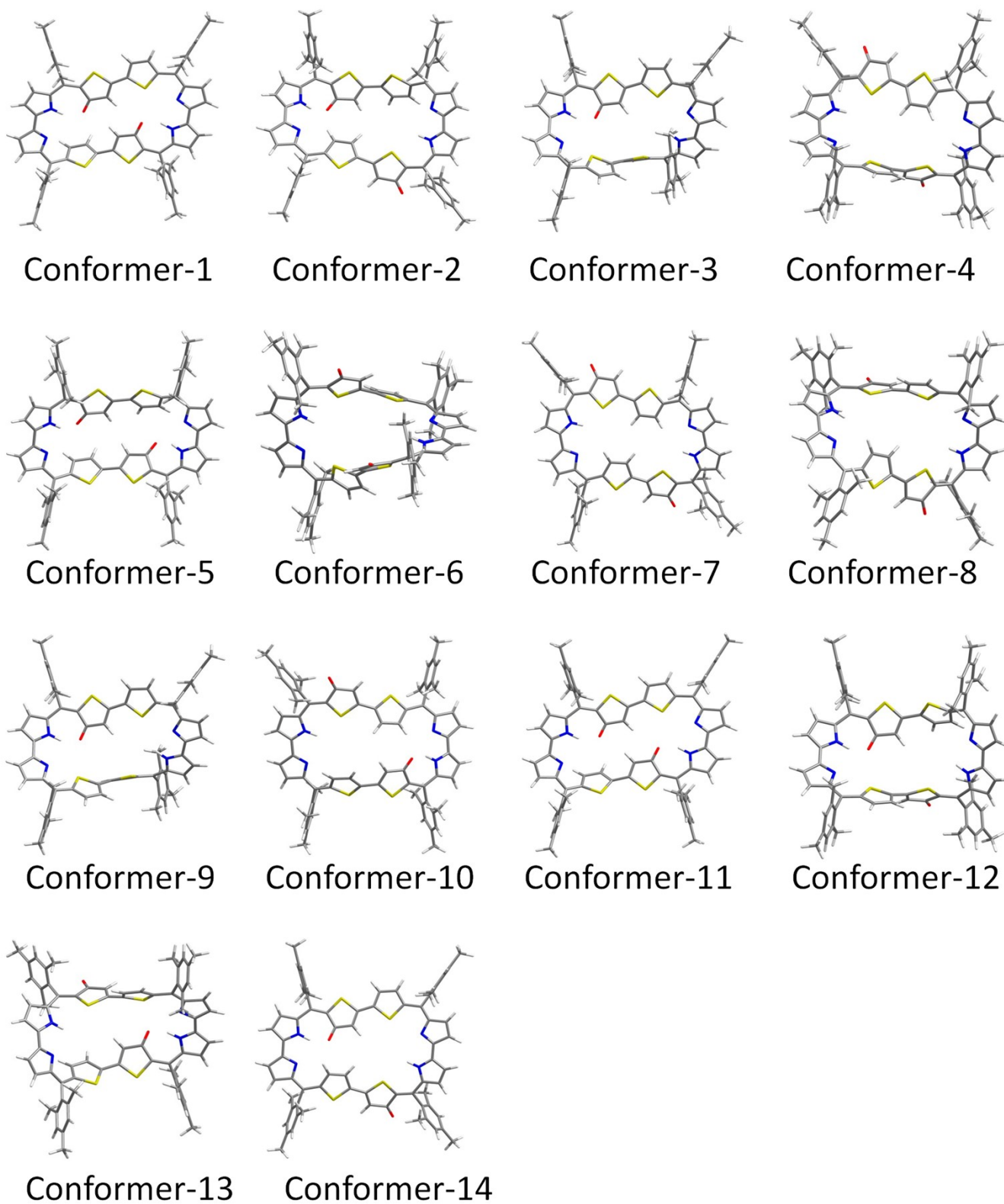


Fig. S43 Optimized geometry of all the possible conformers of **15**

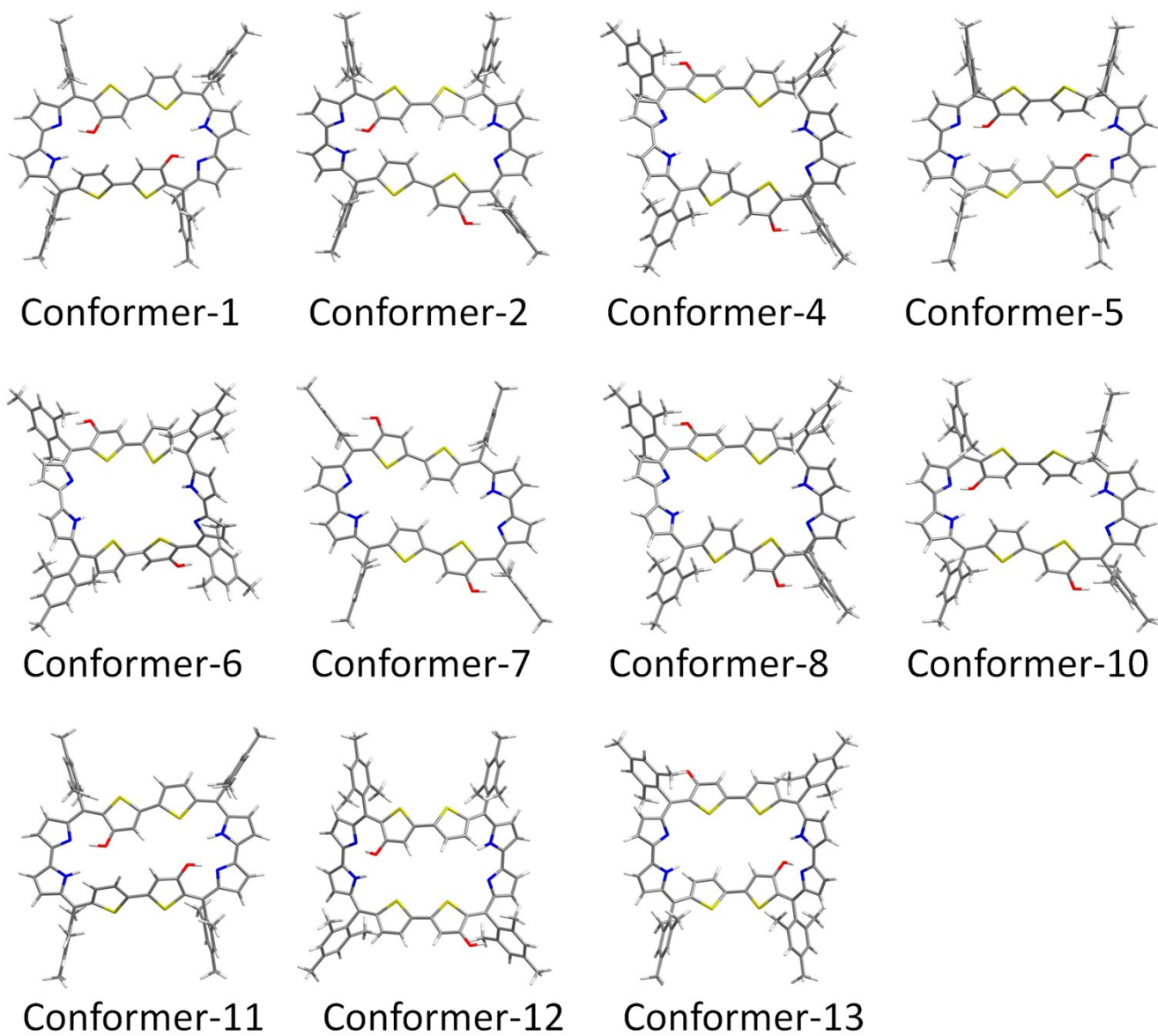


Fig. S44 Optimized geometry of all the possible conformers of **15'**

Table S5. Frontier Molecular Orbital compositions (%) in the ground state for **13**

	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3
Energy (eV)	-5.715	-4.986	-4.698	-4.17	-2.925	-2.841	-2.242	-1.943
Thiophene-1	0.79	18.94	0.42	4.61	13.62	4.74	0.07	5.06
Thiophene-2	0.79	18.94	0.42	4.61	13.62	4.74	0.07	5.05
Thiophene-3	7.12	1.62	11.36	10.79	7.40	8.04	0.03	8.64
Thiophene-4	7.11	1.62	11.36	10.79	7.40	8.04	0.03	8.65
Pyrrole-1	3.78	15.73	1.48	3.97	11.17	3.36	0.04	5.84
Pyrrole-2	3.78	15.73	1.48	3.96	11.17	3.36	0.04	5.82
Pyrrole-3	16.68	2.34	13.94	5.03	6.57	4.72	0.08	9.81
Pyrrole-4	16.69	2.34	13.94	5.03	6.57	4.72	0.08	9.83
Mesitylene-1	0.77	1.00	0.05	4.81	6.59	4.33	0.02	0.55
Mesitylene-2	0.77	1.00	0.05	4.81	6.59	4.33	0.02	0.54
Mesitylene-3	5.10	0.09	0.84	8.92	3.06	5.02	0.01	1.06
Mesitylene-4	5.12	0.09	0.84	8.92	3.07	5.02	0.01	1.07
Azulene	31.52	20.56	43.8	23.74	3.19	39.6	99.5	38.07

Table S6. Frontier Molecular Orbital compositions (%) in the ground state for **14**.

	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3
Energy (eV)	-5.037	-4.978	-4.556	-3.838	-2.848	-2.265	-2.083	-1.887
Thiophene-1	11.67	0.45	8.37	13.44	5.52	5.30	0.21	6.68
Thiophene-2	13.63	0.47	7.52	12.26	5.70	4.42	0.13	7.91
Thiophene-3	3.33	7.24	12.04	8.30	8.37	6.34	0.07	14.18
Thiophene-4	3.20	6.30	13.18	9.02	8.30	7.47	0.07	12.19
Pyrrole-1	5.23	13.27	3.78	6.01	6.39	9.61	0.14	8.21
Pyrrole-2	15.61	2.00	3.21	8.78	4.18	6.59	0.09	4.19
Pyrrole-3	19.43	1.34	3.42	8.02	5.98	7.81	0.07	3.99
Pyrrole-4	6.71	9.90	4.57	6.83	6.33	9.11	0.09	6.28
Mesitylene-1	1.99	0.23	5.66	6.85	2.69	1.89	0.10	4.56
Mesitylene-2	0.74	0.39	5.81	6.01	2.30	0.68	0.06	5.41
Mesitylene-3	0.29	0.73	8.56	3.84	4.01	1.08	0.02	9.05
Mesitylene-4	0.30	1.32	8.67	4.30	3.87	2.31	0.01	8.49
Azulene	17.88	56.35	15.21	6.36	36.35	37.4	98.95	8.88

Table S7. Frontier Molecular Orbital compositions (%) in the ground state for **15**

	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3
Energy (eV)	-5.813	-5.716	-5.169	-4.798	-3.022	-2.479	-2.091	-1.463
Thiophene-1	9.31	36.07	23.21	12.12	12.78	6.85	18.08	12.26
Thiophene-2	18.94	6.46	4.09	9.17	10.61	13.82	5.92	6.42
Thiophene-3	18.93	6.47	4.09	9.17	10.61	13.82	5.92	6.42
Thiophene-4	9.31	36.07	23.21	12.12	12.78	6.86	18.08	12.26
Pyrrole-1	12.95	3.94	5.17	7.68	10.07	13.81	3.45	8.40
Pyrrole-2	4.59	1.43	12.65	15.97	3.79	5.65	7.57	6.77
Pyrrole-3	12.95	3.94	5.17	7.68	10.07	13.8	3.45	8.40
Pyrrole-4	4.60	1.43	12.65	15.96	3.79	5.65	7.57	6.77
Mesitylene-1	3.71	1.92	0.77	1.17	4.91	0.86	11.02	8.99
Mesitylene-2	0.50	0.17	4.11	3.89	7.84	9.00	3.97	7.17
Mesitylene-3	3.71	1.92	0.77	1.17	4.91	0.86	11.02	8.99
Mesitylene-4	0.50	0.17	4.11	3.89	7.84	9.00	3.97	7.17

Table S8. Frontier Molecular Orbital compositions (%) in the ground state for **15'**

	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3
Energy (eV)	-5.917	-5.520	-4.69	-4.081	-2.924	-2.398	-1.663	-0.948
Thiophene-1	11.03	19.58	13.68	10.12	8.21	14.7	11.39	14.24
Thiophene-2	13.28	6.12	9.91	12.05	13.38	8.22	7.48	16.15
Thiophene-3	13.28	6.12	9.91	12.05	13.38	8.22	7.48	16.15
Thiophene-4	11.03	19.58	13.68	10.12	8.2	14.7	11.39	14.24
Pyrrole-1	8.10	12.29	15.34	3.48	7.94	7.25	8.66	5.89
Pyrrole-2	12.38	5.17	8.89	9.42	11.38	5.70	6.80	8.45
Pyrrole-3	12.38	5.17	8.89	9.42	11.38	5.70	6.80	8.45
Pyrrole-4	8.10	12.29	15.34	3.48	7.94	7.25	8.66	5.89
Mesitylene-1	4.48	1.42	0.52	6.13	0.47	11.24	9.08	3.78
Mesitylene-2	0.72	5.42	1.67	8.8	8.62	2.89	6.60	1.49
Mesitylene-3	0.72	5.42	1.67	8.8	8.62	2.89	6.60	1.49
Mesitylene-4	4.48	1.42	0.52	6.13	0.47	11.24	9.08	3.78

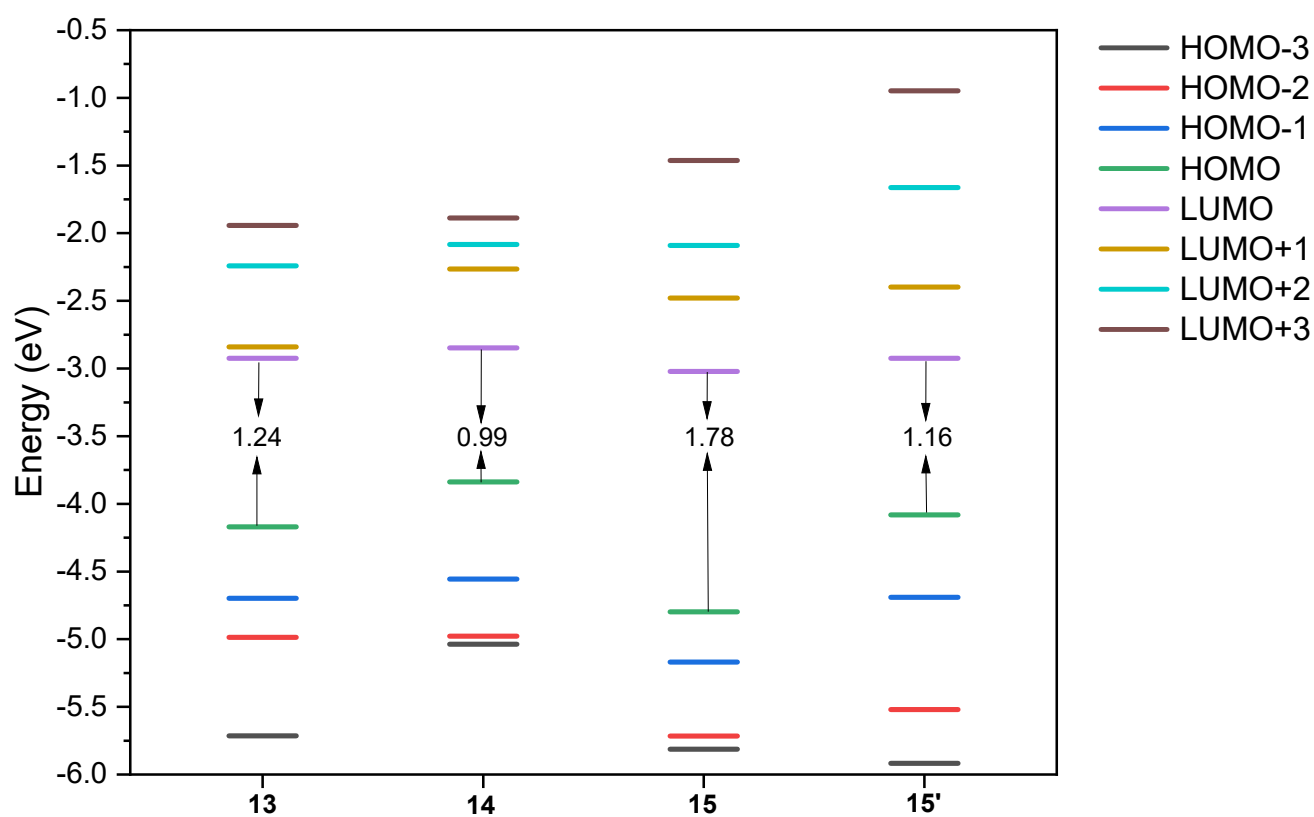


Fig. S45 FMO energy levels of **13**, **14**, **15** and **15'**

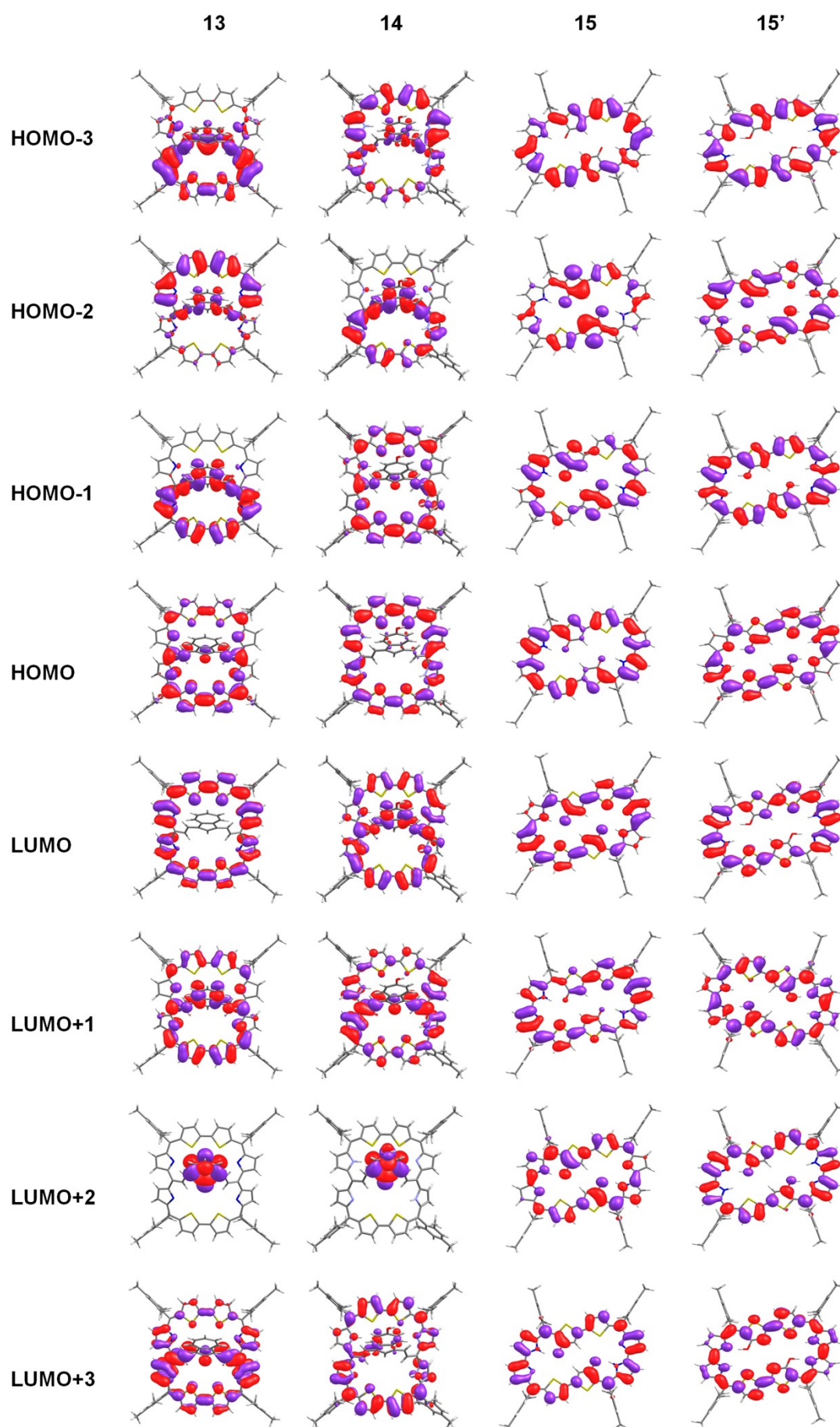


Fig. S46 Highest occupied molecular orbital and lowest unoccupied molecular orbitals of **13**, **14**, **15** and **15'**

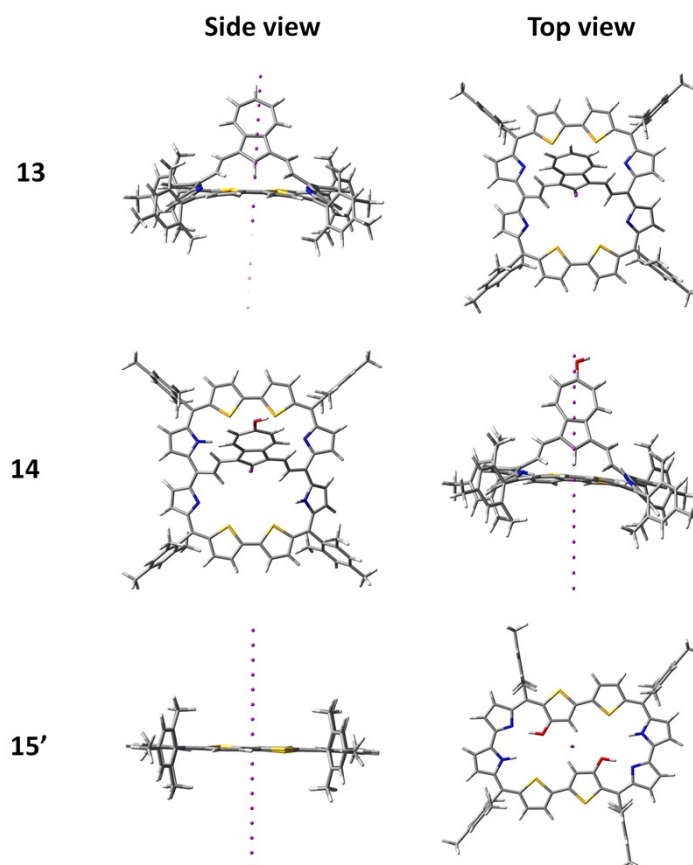


Fig. S47 The centers of macrocycles **13**, **14** and **15'** for the NICS values were designated at the non-weighted mass of π conjugation pathway of the macrocycles.

Table S9. The calculated nucleus-independent chemical shifts (NICS) values for **13**, **14** and **15'**

Distance (Å)	Macrocycle				
	13	13-withoutazulene-bridge	14	14-without-azulene-bridge	15'
-8	-2.1940	-2.3561	2.2970	4.0131	-2.2060
-7	-2.8037	-3.0026	2.9551	5.1531	-2.8368
-6	-3.6008	-3.8447	3.8348	6.6693	-3.6843
-5	-4.6245	-4.9213	4.9976	8.6608	-4.8208
-4	-5.8908	-6.2454	6.4903	11.1974	-6.3242
-3	-7.3472	-7.7566	8.2950	14.2320	-8.2346
-2	-8.8026	-9.2524	10.2417	17.4487	-10.4157
-1	-9.8687	-10.3558	11.9439	20.1311	-12.3880
0	-10.4177	-10.6589	12.2899	21.3472	-13.3789
1	-26.4467	-10.0464	11.1924	20.5850	-12.3880
2	-18.4986	-8.7916	2.4550	18.1825	-10.4156
3	-29.3402	-7.2873	10.6299	15.0098	-8.2346
4	-15.1389	-5.8303	2.0622	11.8663	-6.3242
5	-8.1994	-4.5761	1.4098	9.1777	-4.8208
6	-5.2153	-3.5674	1.9840	7.0497	-3.6843
7	-3.6730	-2.7848	1.9300	5.4283	-2.8368
8	-2.6154	-2.1872	1.8157	4.2118	-2.2060

Table S10. Harmonic oscillator model of aromaticity (HOMA), multi-center indices (MCI), approximate multi-center bond order for large rings (AV1245 index) and Avmin index values for **13**, **14** and **15'**

	HOMA	MCI	AV1245	AVmin
13	0.8221	0.562	2.040	0.264
14	0.7009	0.569	1.943	0.896
15'	0.8319	0.574	2.194	0.314

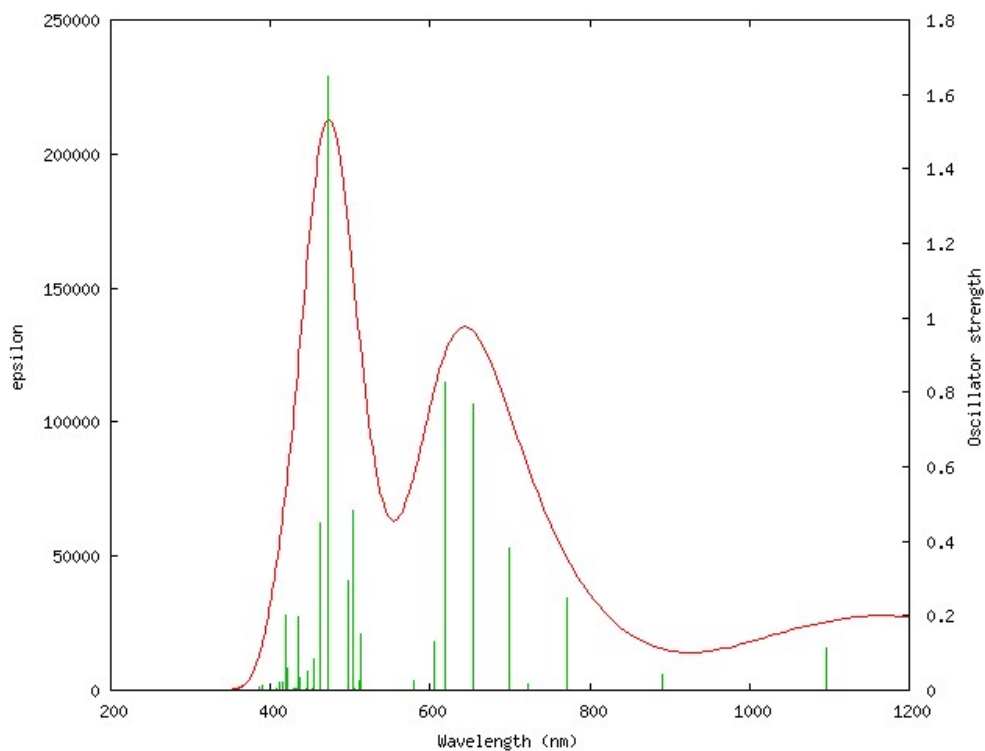


Fig. S48 Computed absorption spectrum of **13** in solvent phase (CH_2Cl_2)

Table S11. Computed absorption maxima (λ_{max} nm), Electronic excitation energies (E, eV), and Oscillator strength (f) of **13** in solvent phase (CH₂Cl₂).

No.	Cal. λ_{max} (nm)	Oscillator Strength f	E (eV)	Main Contributing Configurations
1	1205.13	0.2823	1.0288	HOMO→LUMO (88%)
2	1096.81	0.1119	1.1304	HOMO→LUMO+1 (87%)
3	890.30	0.0407	1.3926	HOMO-1→LUMO (86%)
4	770.90	0.2478	1.6083	HOMO-1→LUMO+1 (61%), HOMO→LUMO+3 (27%)
5	721.71	0.0160	1.7179	HOMO→LUMO+2 (96%)
6	698.81	0.3805	1.7742	HOMO-2→LUMO (73%)
7	654.23	0.7659	1.8951	HOMO-2→LUMO+1 (90%)
8	626.65	0.0017	1.9785	HOMO-1→LUMO+2 (88%)
9	618.46	0.8259	2.0047	HOMO-1→LUMO+1 (28%), HOMO→LUMO+3 (65%)
10	604.41	0.1296	2.0513	HOMO→LUMO+4 (86%)
11	580.23	0.0249	2.1368	HOMO-1→LUMO+3 (24%), HOMO→LUMO+5 (71%)
12	512.88	0.1503	2.4174	HOMO-3→LUMO (88%)
13	511.44	0.0272	2.4242	HOMO-4→LUMO (44%), HOMO-3→LUMO+1 (41%), HOMO-1→LUMO+3 (12%)
14	505.68	0.0029	2.4518	HOMO-2→LUMO+2 (90%)
15	503.14	0.4832	2.4642	HOMO-4→LUMO (38%), HOMO-1→LUMO+3 (35%)
16	496.57	0.2955	2.4968	HOMO-1→LUMO+4 (91%)
17	471.58	0.0123	2.6291	HOMO-5→LUMO (22%), HOMO-4→LUMO+1 (67%)
18	471.33	1.6472	2.6305	HOMO-3→LUMO+1 (11%), HOMO-2→LUMO+3 (64%)
19	462.57	0.4506	2.6803	HOMO-5→LUMO+1 (25%), HOMO-3→LUMO+1 (20%), HOMO-2→LUMO+3 (22%)
20	461.83	0.0252	2.6846	HOMO-5→LUMO (44%), HOMO-4→LUMO+1 (11%), HOMO-2→LUMO+4 (19%), HOMO-1→LUMO+5 (19%)
21	453.54	0.0836	2.7337	HOMO-12→LUMO (13%), HOMO-2→LUMO+4 (27%), HOMO-1→LUMO+5 (40%)
22	452.46	0.0038	2.7402	HOMO-8→LUMO (85%)
23	451.52	0.0027	2.7459	HOMO-9→LUMO (86%)
24	447.43	0.0202	2.7710	HOMO-15→LUMO (10%), HOMO-13→LUMO (33%), HOMO-6→LUMO (49%)
25	446.42	0.0508	2.7773	HOMO-7→LUMO (70%)
26	445.17	0.0044	2.7851	HOMO-13→LUMO (31%), HOMO-6→LUMO (40%)
27	437.24	0.0323	2.8356	HOMO-16→LUMO (58%), HOMO-12→LUMO (20%)
28	436.91	0.0022	2.8377	HOMO-7→LUMO+1 (10%), HOMO-5→LUMO+1 (58%)
29	434.92	0.1981	2.8507	HOMO-16→LUMO (19%), HOMO-12→LUMO (50%)
30	432.66	0.0000	2.8656	HOMO-15→LUMO (72%), HOMO-13→LUMO (20%)
31	432.48	0.0041	2.8668	HOMO-16→LUMO (11%), HOMO-14→LUMO (81%)
32	431.25	0.0032	2.8750	HOMO-6→LUMO+1 (88%)
33	429.38	0.0048	2.8875	HOMO-10→LUMO (84%)
34	429.07	0.0018	2.8896	HOMO-11→LUMO (91%)
35	428.05	0.0002	2.8965	HOMO-7→LUMO+1 (72%)
36	421.88	0.0579	2.9388	HOMO-2→LUMO+5 (82%)
37	418.51	0.2021	2.9625	HOMO-15→LUMO+1 (12%), HOMO-13→LUMO+1 (37%)
38	418.21	0.1125	2.9646	HOMO-12→LUMO+1 (66%)
39	415.70	0.0022	2.9825	HOMO-10→LUMO+1 (54%), HOMO-8→LUMO+1 (38%)
40	415.45	0.0060	2.9843	HOMO-11→LUMO+1 (67%), HOMO-8→LUMO+1 (16%)
41	415.26	0.0190	2.9857	HOMO-12→LUMO+1 (23%), HOMO-11→LUMO+1 (25%), HOMO-10→LUMO+1 (20%), HOMO-8→LUMO+1 (27%)
42	414.63	0.0222	2.9902	HOMO-9→LUMO+1 (80%)

43	412.15	0.0223	3.0082	HOMO-13→LUMO+1 (31%), HOMO-2→LUMO+4 (10%)
44	408.03	0.0033	3.0386	HOMO-16→LUMO+1 (79%)
45	402.87	0.0003	3.0775	HOMO-14→LUMO+1 (82%)
46	402.82	0.0000	3.0779	HOMO-15→LUMO+1 (73%), HOMO-13→LUMO+1 (21%)
47	401.75	0.0000	3.0861	HOMO-17→LUMO (40%), HOMO-16→LUMO+1 (14%)
48	390.77	0.0109	3.1728	HOMO→LUMO+6 (78%)
49	385.94	0.0098	3.2125	HOMO-17→LUMO+1 (59%), HOMO-3→LUMO+2 (16%)
50	384.22	0.0017	3.2269	HOMO-20→LUMO (11%), HOMO-18→LUMO (65%)

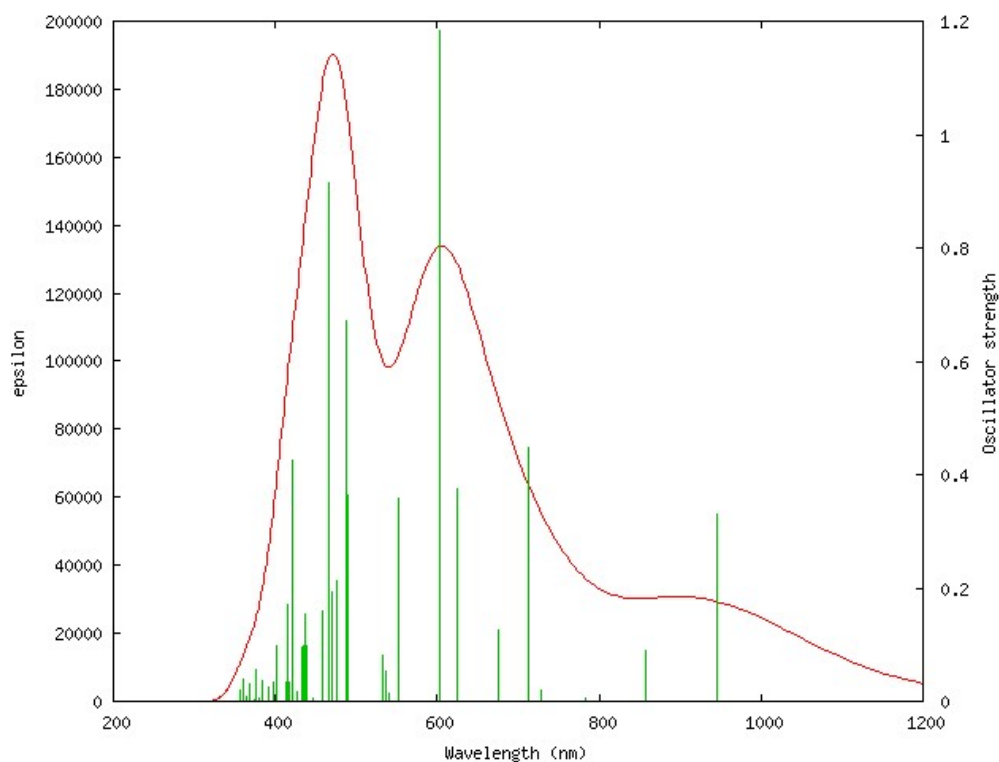


Fig. S49 Computed absorption spectrum of **14** in solvent phase (CH₂Cl₂).

Table S12. Computed absorption maxima (λ_{max} nm), Electronic excitation energies (E, eV), and Oscillator strength (*f*) of **14** in solvent phase (CH₂Cl₂).

1	2052.70	0.0027	0.6040	HOMO→LUMO (100%)
2	944.63	0.3298	1.3125	HOMO→LUMO+1 (93%)
3	858.43	0.0898	1.4443	HOMO-1→LUMO (84%), HOMO→LUMO+2 (11%)
4	783.91	0.0058	1.5816	HOMO→LUMO+3 (91%)
5	727.94	0.0188	1.7032	HOMO-2→LUMO (25%), HOMO→LUMO+4 (66%)
6	713.49	0.4473	1.7377	HOMO-2→LUMO+1 (16%), HOMO→LUMO+2 (63%)
7	675.77	0.1256	1.8347	HOMO-2→LUMO (44%), HOMO-1→LUMO+1 (22%), HOMO→LUMO+4 (30%)
8	625.29	0.3751	1.9828	HOMO-3→LUMO (53%), HOMO-1→LUMO+1 (31%)
9	603.53	1.1828	2.0543	HOMO-3→LUMO (36%), HOMO-2→LUMO (19%), HOMO- 1→LUMO+1 (37%)
10	551.38	0.3567	2.2486	HOMO-2→LUMO+1 (46%), HOMO-2→LUMO+3 (11%), HOMO-1→LUMO+3 (11%), HOMO-1→LUMO+4 (18%)
11	540.21	0.0128	2.2951	HOMO-3→LUMO+1 (26%), HOMO-1→LUMO+2 (59%)
12	536.56	0.0539	2.3107	HOMO-1→LUMO+3 (74%)
13	531.84	0.0803	2.3312	HOMO-2→LUMO+3 (58%), HOMO-1→LUMO+4 (12%)
14	490.34	0.3638	2.5285	HOMO-3→LUMO+1 (40%), HOMO-1→LUMO+2 (16%), HOMO-1→LUMO+4 (10%), HOMO→LUMO+5 (22%)
15	487.93	0.6704	2.5410	HOMO-4→LUMO (26%), HOMO-2→LUMO+1 (15%), HOMO- 1→LUMO+4 (34%)
16	475.63	0.2130	2.6067	HOMO-4→LUMO (18%), HOMO→LUMO+5 (50%)
17	471.01	0.1917	2.6323	HOMO-5→LUMO (27%), HOMO-2→LUMO+2 (56%)
18	466.33	0.9146	2.6587	HOMO-5→LUMO (36%), HOMO-4→LUMO (11%), HOMO- 2→LUMO+2 (24%), HOMO-1→LUMO+4 (10%)
19	458.15	0.1586	2.7062	HOMO-6→LUMO (30%), HOMO-4→LUMO (30%)
20	445.92	0.0066	2.7804	HOMO-3→LUMO+2 (10%), HOMO-3→LUMO+3 (77%)
21	439.24	0.0990	2.8227	HOMO-3→LUMO+2 (50%), HOMO-2→LUMO+4 (35%)
22	435.82	0.1534	2.8448	HOMO-9→LUMO (30%), HOMO-3→LUMO+2 (17%), HOMO- 3→LUMO+3 (13%), HOMO-2→LUMO+4 (17%)
23	434.57	0.0966	2.8530	HOMO-9→LUMO (22%), HOMO-8→LUMO (24%), HOMO- 2→LUMO+4 (17%)
24	433.13	0.0231	2.8625	HOMO-8→LUMO (35%), HOMO-7→LUMO (35%), HOMO- 6→LUMO (12%)
25	432.30	0.0964	2.8680	HOMO-9→LUMO (21%), HOMO-7→LUMO (52%)
26	427.75	0.0165	2.8985	HOMO-3→LUMO+4 (63%), HOMO→LUMO+6 (20%)
27	421.68	0.4247	2.9402	HOMO-3→LUMO+4 (25%), HOMO→LUMO+6 (46%)
28	419.57	0.0010	2.9550	HOMO-10→LUMO (95%)
29	416.61	0.0344	2.9760	HOMO-13→LUMO (25%), HOMO-8→LUMO (14%), HOMO- 6→LUMO (25%)
30	415.05	0.1704	2.9872	HOMO-13→LUMO (25%), HOMO-12→LUMO (37%)
31	413.62	0.0104	2.9975	HOMO-13→LUMO (16%), HOMO-12→LUMO (40%), HOMO- 11→LUMO (37%)
32	413.26	0.0338	3.0001	HOMO-13→LUMO (15%), HOMO-12→LUMO (16%), HOMO- 11→LUMO (55%)
33	405.88	0.0004	3.0547	HOMO-14→LUMO (98%)
34	405.00	0.0009	3.0613	HOMO-15→LUMO (98%)
35	401.59	0.0969	3.0873	HOMO-16→LUMO (31%), HOMO→LUMO+7 (29%)
36	398.17	0.0347	3.1138	HOMO-17→LUMO (26%), HOMO-5→LUMO+1 (28%), HOMO- 4→LUMO+1 (15%), HOMO→LUMO+7 (10%)
37	391.30	0.0240	3.1685	HOMO-5→LUMO+1 (11%), HOMO-4→LUMO+1 (63%)
38	384.91	0.0354	3.2211	HOMO-17→LUMO (33%), HOMO-5→LUMO+1 (44%)
39			3.2707	HOMO-20→LUMO (14%), HOMO-19→LUMO (22%), HOMO-

				18→LUMO (39%)
40	377.00	0.0555	3.2887	HOMO-16→LUMO (34%), HOMO→LUMO+7 (10%), HOMO→LUMO+8 (14%)
41	375.23	0.0060	3.3042	HOMO-1→LUMO+5 (78%)
42	373.80	0.0021	3.3168	HOMO→LUMO+8 (44%), HOMO→LUMO+9 (31%)
43	369.22	0.0077	3.3580	HOMO-6→LUMO+1 (73%)
44	367.43	0.0301	3.3743	HOMO-9→LUMO+1 (59%), HOMO→LUMO+9 (14%)
45	365.34	0.0081	3.3936	HOMO-19→LUMO (28%), HOMO-18→LUMO (41%)
46	361.44	0.0398	3.4303	HOMO→LUMO+8 (16%), HOMO→LUMO+9 (26%)
47	360.64	0.0012	3.4379	HOMO-7→LUMO+1 (84%)
48	360.58	0.0028	3.4384	HOMO-8→LUMO+1 (75%)
49	356.59	0.0195	3.4769	HOMO-20→LUMO (22%), HOMO-19→LUMO (30%)
50	354.52	0.0002	3.4972	HOMO-10→LUMO+1 (94%)

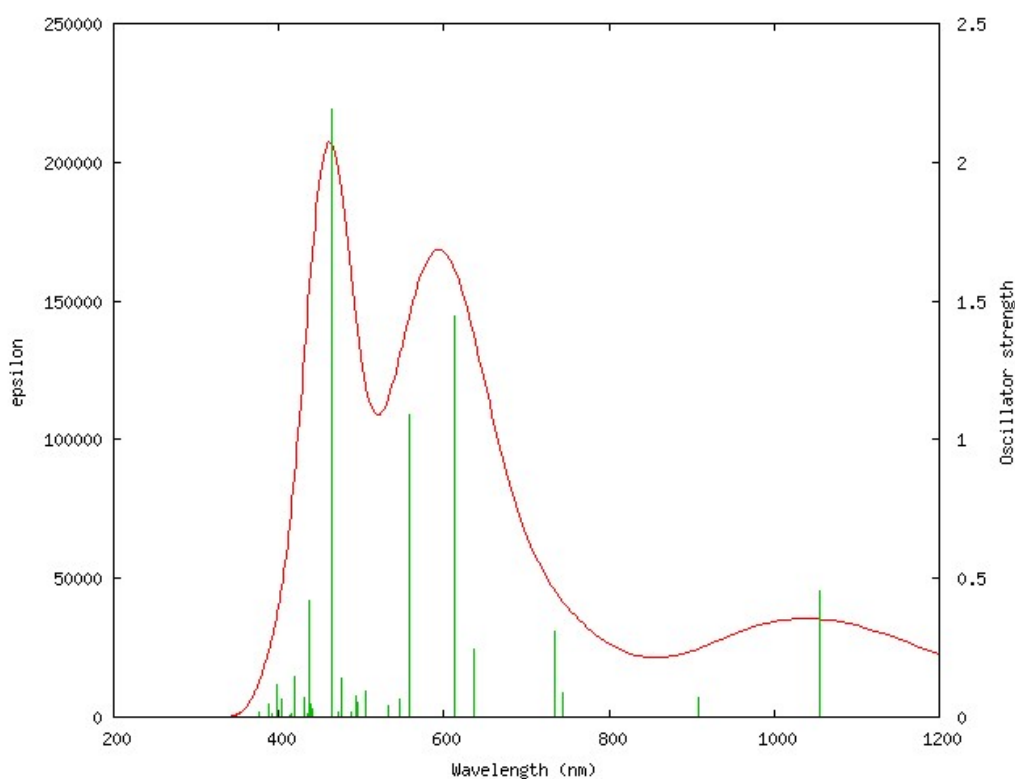


Fig. S50 Computed absorption spectrum of **[14-H₂]²⁺** in solvent phase (CH₂Cl₂).

Table S13. Computed absorption maxima (λ_{max} nm), Electronic excitation energies (E, eV), and Oscillator strength (*f*) of **[14-H₂]²⁺** in solvent phase (CH₂Cl₂).

1	2745.42	0.0002	0.4516	HOMO→LUMO (100%)
2	1055.72	0.4527	1.1744	HOMO→LUMO+1 (95%)
3	907.51	0.0698	1.3662	HOMO-1→LUMO (87%)
4	743.48	0.0864	1.6676	HOMO-2→LUMO (61%), HOMO-1→LUMO+1 (37%)
5	734.67	0.3063	1.6876	HOMO-2→LUMO+1 (27%), HOMO→LUMO+2 (69%)
6	703.21	0.0012	1.7631	HOMO→LUMO+3 (91%)
7	677.80	0.0022	1.8292	HOMO→LUMO+4 (90%)
8	636.96	0.2475	1.9465	HOMO-3→LUMO (33%), HOMO-2→LUMO (23%), HOMO-1→LUMO+1 (42%)
9	613.17	1.4444	2.0220	HOMO-3→LUMO (61%), HOMO-2→LUMO (15%), HOMO-1→LUMO+1 (18%)
10	557.88	1.0889	2.2224	HOMO-2→LUMO+1 (56%), HOMO→LUMO+2 (15%)
11	547.07	0.0638	2.2663	HOMO-3→LUMO+1 (54%), HOMO-1→LUMO+2 (42%)
12	539.50	0.0007	2.2981	HOMO-4→LUMO (98%)
13	537.91	0.0006	2.3049	HOMO-5→LUMO (98%)
14	531.77	0.0397	2.3315	HOMO-6→LUMO (97%)
15	528.69	0.0026	2.3451	HOMO-9→LUMO (93%)
16	523.18	0.0000	2.3698	HOMO-7→LUMO (98%)
17	521.99	0.0000	2.3752	HOMO-8→LUMO (98%)
18	520.92	0.0000	2.3801	HOMO-10→LUMO (98%)
19	520.57	0.0001	2.3817	HOMO-11→LUMO (97%)
20	505.72	0.0912	2.4516	HOMO-12→LUMO (54%), HOMO-2→LUMO+3 (16%), HOMO-1→LUMO+3 (14%)
21	495.46	0.0503	2.5024	HOMO-3→LUMO+1 (31%), HOMO-1→LUMO+2 (37%), HOMO→LUMO+5 (25%)
22	492.84	0.0751	2.5157	HOMO-1→LUMO+3 (62%), HOMO-1→LUMO+4 (31%)
23	486.97	0.0189	2.5460	HOMO-12→LUMO (18%), HOMO-2→LUMO+3 (47%), HOMO-2→LUMO+4 (19%), HOMO-1→LUMO+4 (10%)
24	476.05	0.1370	2.6044	HOMO-2→LUMO+2 (89%)
25	472.62	0.0188	2.6233	HOMO-13→LUMO (30%), HOMO→LUMO+5 (58%)
26	463.59	2.1907	2.6744	HOMO-12→LUMO (16%), HOMO-1→LUMO+3 (15%), HOMO-1→LUMO+4 (46%)
27	445.57	0.0004	2.7826	HOMO-4→LUMO+1 (98%)
28	444.56	0.0019	2.7889	HOMO-5→LUMO+1 (97%)
29	441.10	0.0293	2.8108	HOMO-6→LUMO+1 (94%)
30	438.86	0.0438	2.8251	HOMO-9→LUMO+1 (82%), HOMO→LUMO+6 (11%)
31	436.85	0.4207	2.8381	HOMO-9→LUMO+1 (12%), HOMO→LUMO+6 (69%)
32	435.27	0.0144	2.8484	HOMO-3→LUMO+2 (35%), HOMO-2→LUMO+4 (13%), HOMO→LUMO+7 (35%)
33	434.85	0.0001	2.8512	HOMO-7→LUMO+1 (98%)
34	434.43	0.0005	2.8539	HOMO-10→LUMO+1 (98%)
35	434.15	0.0009	2.8558	HOMO-11→LUMO+1 (97%)
36	434.05	0.0001	2.8564	HOMO-8→LUMO+1 (98%)
37	431.16	0.0713	2.8756	HOMO-14→LUMO (29%), HOMO-3→LUMO+2 (12%), HOMO-2→LUMO+3 (13%), HOMO-2→LUMO+4 (29%)
38	420.08	0.1459	2.9514	HOMO-14→LUMO (41%), HOMO-3→LUMO+2 (27%), HOMO→LUMO+7 (15%)
39	414.80	0.0137	2.9890	HOMO-12→LUMO+1 (83%)
40	412.63	0.0033	3.0047	HOMO-13→LUMO (58%), HOMO-1→LUMO+2 (11%), HOMO→LUMO+5 (14%)
41	404.12	0.0613	3.0680	HOMO-3→LUMO+3 (95%)

42	398.39	0.1160	3.1121	HOMO-3→LUMO+4 (92%)
43	392.10	0.0105	3.1620	HOMO-15→LUMO (93%)
44	388.44	0.0491	3.1918	HOMO-17→LUMO (72%)
45	384.89	0.0003	3.2213	HOMO-4→LUMO+2 (88%)
46	383.98	0.0010	3.2289	HOMO-5→LUMO+2 (88%)
47	381.64	0.0000	3.2487	HOMO-16→LUMO (86%)
48	378.76	0.0020	3.2734	HOMO-13→LUMO+1 (86%)
49	375.79	0.0177	3.2993	HOMO-17→LUMO (20%), HOMO-14→LUMO (12%), HOMO→LUMO+7 (13%), HOMO→LUMO+8 (20%)
50	374.26	0.0001	3.3128	HOMO-7→LUMO+2 (90%)

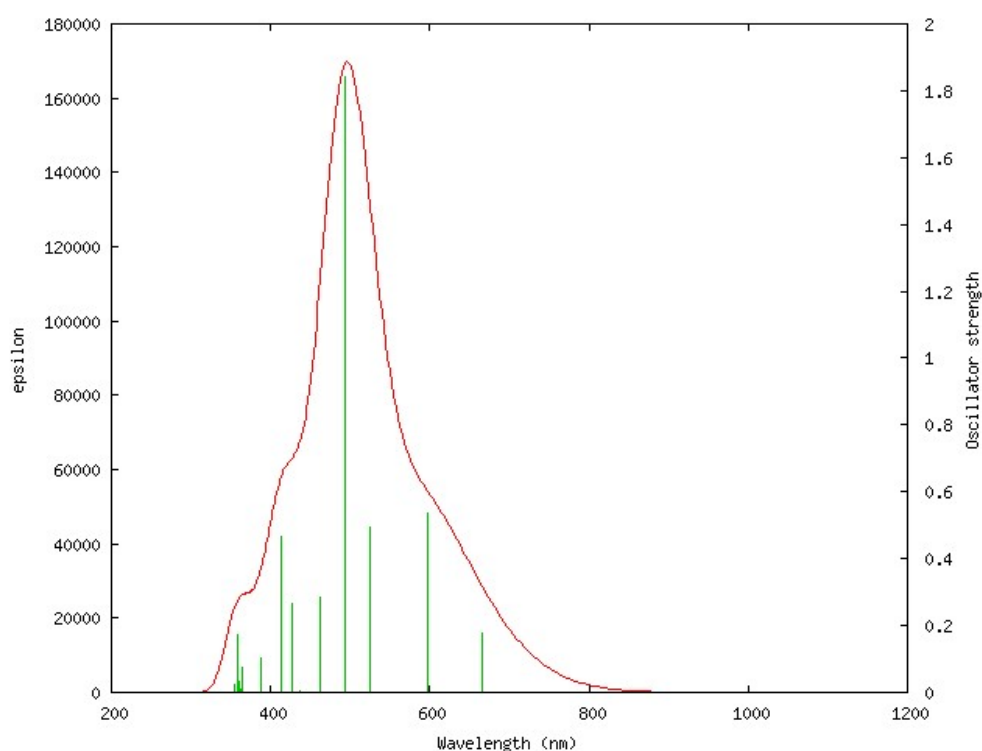


Fig. S51 Computed absorption spectrum of **15** in solvent phase (CH_2Cl_2).

Table S14. Computed absorption maxima (λ_{max} nm), Electronic excitation energies (E, eV), and Oscillator strength (f) of **15** in solvent phase (CH_2Cl_2).

1	987.13	0.0000	1.2560	HOMO→LUMO (99%)
2	666.00	0.1789	1.8616	HOMO-1→LUMO (94%)
3	596.70	0.5353	2.0778	HOMO→LUMO+1 (87%)
4	539.03	0.0000	2.3001	HOMO-2→LUMO (72%), HOMO-1→LUMO+1 (24%)
5	525.06	0.4959	2.3613	HOMO-3→LUMO (17%), HOMO→LUMO+2 (73%)
6	513.32	0.0000	2.4153	HOMO-2→LUMO (21%), HOMO-1→LUMO+1 (72%)
7	493.82	1.8409	2.5107	HOMO-3→LUMO (74%), HOMO→LUMO+2 (21%)
8	466.65	0.0000	2.6569	HOMO-4→LUMO (90%)
9	463.19	0.0000	2.6767	HOMO-6→LUMO (87%)
10	461.63	0.0000	2.6858	HOMO-8→LUMO (89%)
11	461.44	0.2835	2.6869	HOMO-5→LUMO (95%)
12	458.08	0.0000	2.7066	HOMO-7→LUMO (91%)
13	455.35	0.0000	2.7228	HOMO-3→LUMO+1 (16%), HOMO-1→LUMO+2 (66%)
14	444.69	0.0000	2.7881	HOMO-9→LUMO (92%)
15	444.58	0.0006	2.7888	HOMO-10→LUMO (92%)
16	437.39	0.0000	2.8346	HOMO-11→LUMO (89%)
17	436.27	0.0069	2.8419	HOMO-12→LUMO (97%)
18	433.55	0.0000	2.8597	HOMO-13→LUMO (77%)
19	426.21	0.2637	2.9090	HOMO-14→LUMO (11%), HOMO-2→LUMO+1 (85%)
20	413.39	0.4642	2.9992	HOMO-14→LUMO (77%), HOMO-2→LUMO+1 (12%)
21	413.18	0.0000	3.0007	HOMO-3→LUMO+1 (35%), HOMO→LUMO+3 (54%)
22	405.12	0.0000	3.0604	HOMO-16→LUMO (86%)
23	401.67	0.0000	3.0867	HOMO-3→LUMO+1 (40%), HOMO→LUMO+3 (34%)
24	399.12	0.0000	3.1064	HOMO-19→LUMO (84%)
25	387.82	0.1010	3.1969	HOMO-2→LUMO+2 (95%)
26	382.29	0.0000	3.2432	HOMO-5→LUMO+1 (67%), HOMO-3→LUMO+2 (29%)
27	377.55	0.0000	3.2839	HOMO-23→LUMO+1 (13%), HOMO-22→LUMO (74%)
28	376.47	0.0000	3.2933	HOMO-23→LUMO (52%), HOMO-22→LUMO+1 (10%), HOMO-4→LUMO+1 (34%)
29	374.99	0.0000	3.3063	HOMO-23→LUMO (30%), HOMO-4→LUMO+1 (60%)
30	372.60	0.0000	3.3275	HOMO-6→LUMO+1 (87%)
31	371.95	0.0000	3.3333	HOMO-8→LUMO+1 (89%)
32	371.51	0.0000	3.3373	HOMO-15→LUMO (91%)
33	370.89	0.0000	3.3429	HOMO-7→LUMO+1 (86%)
34	370.64	0.0005	3.3451	HOMO-17→LUMO (78%), HOMO-1→LUMO+3 (18%)
35	365.69	0.0000	3.3904	HOMO-18→LUMO (36%), HOMO-5→LUMO+1 (12%), HOMO-3→LUMO+2 (30%)
36	364.79	0.0741	3.3988	HOMO-17→LUMO (12%), HOMO-13→LUMO+1 (13%), HOMO-1→LUMO+3 (54%)
37	363.28	0.0101	3.4129	HOMO-9→LUMO+1 (86%)
38	363.24	0.0000	3.4133	HOMO-10→LUMO+1 (91%)
39	361.60	0.0000	3.4287	HOMO-18→LUMO (43%), HOMO-12→LUMO+1 (24%), HOMO-5→LUMO+1 (14%), HOMO-3→LUMO+2 (15%)
40	360.89	0.0324	3.4355	HOMO-11→LUMO+1 (85%)
41	358.89	0.0000	3.4546	HOMO-18→LUMO (13%), HOMO-12→LUMO+1 (72%), HOMO-3→LUMO+2 (10%)
42	358.31	0.1741	3.4602	HOMO-20→LUMO (48%), HOMO-13→LUMO+1 (21%), HOMO-11→LUMO+1 (10%), HOMO-1→LUMO+3 (11%)
43	355.32	0.0237	3.4893	HOMO-20→LUMO (39%), HOMO-13→LUMO+1 (49%)
44	352.86	0.0000	3.5137	HOMO-21→LUMO (67%), HOMO-14→LUMO+1 (11%), HOMO→LUMO+4 (15%)

45	348.30	0.0000	3.5597	HOMO-5→LUMO+2 (80%)
46	347.38	0.0000	3.5691	HOMO-8→LUMO+2 (12%), HOMO-4→LUMO+2 (75%)
47	344.66	0.0000	3.5973	HOMO-7→LUMO+2 (86%)
48	340.16	0.0000	3.6448	HOMO-21→LUMO (15%), HOMO-14→LUMO+1 (69%)
49	333.70	0.0000	3.7154	HOMO-6→LUMO+2 (93%)
50	333.31	0.0000	3.7164	HOMO-8→LUMO+2 (83%), HOMO-4→LUMO+2 (14%)
1	1172.20	0.4243	1.0577	HOMO-1→LUMO+1 (10%), HOMO→LUMO (85%)
2	951.45	0.0928	1.3031	HOMO-1→LUMO (40%), HOMO→LUMO+1 (53%)

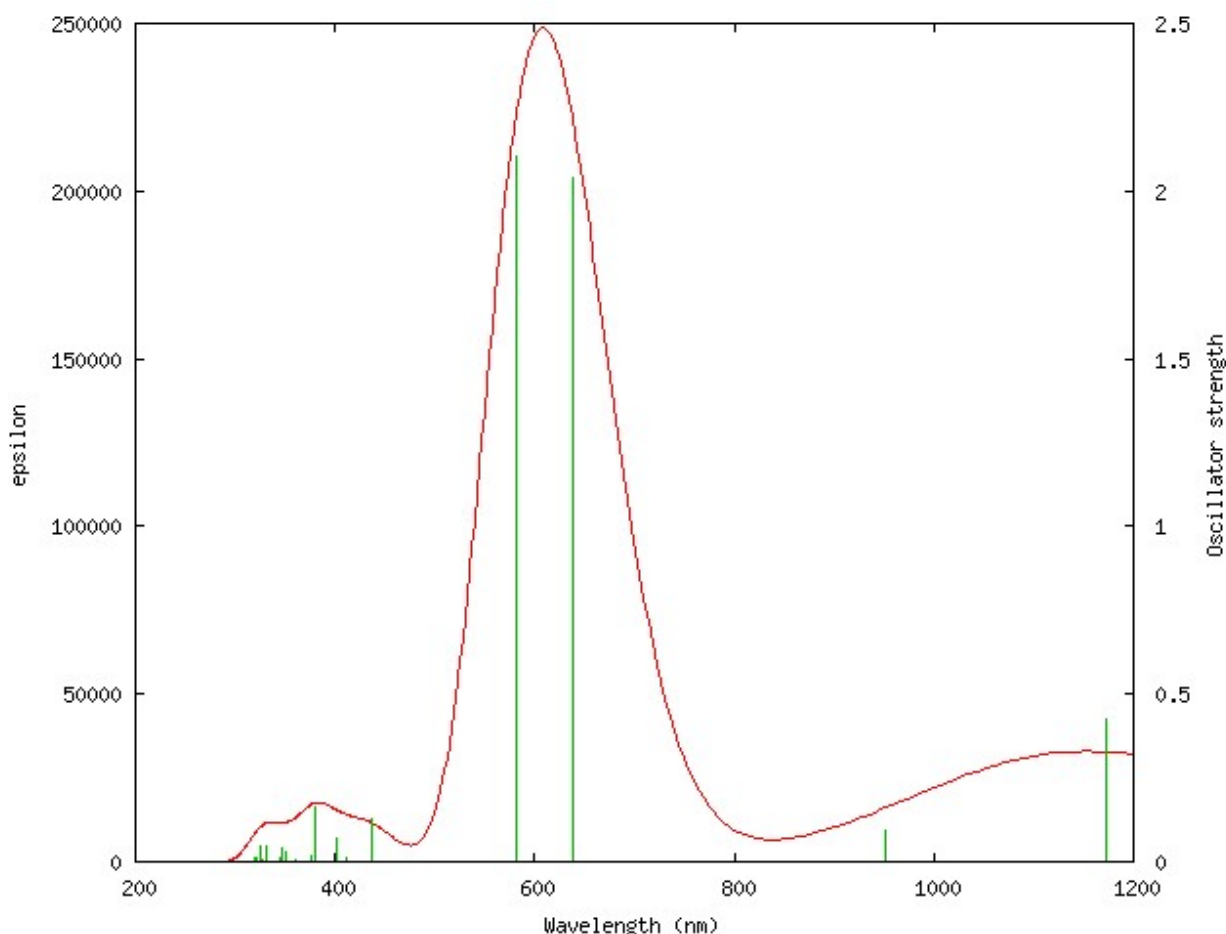


Fig. S52 Computed absorption spectrum of **15'** in solvent phase (CH_2Cl_2).

Table S15. Computed absorption maxima (λ_{max} nm), Electronic excitation energies (E, eV), and Oscillator strength (*f*) of **15'** in solvent phase (CH_2Cl_2).

3	639.09	2.0392	1.9400	HOMO-1→LUMO (59%), HOMO→LUMO+1 (44%)
4	582.44	0.0000	2.1287	HOMO-2→LUMO (14%), HOMO→LUMO+2 (81%)
5	580.99	2.1042	2.1340	HOMO-1→LUMO+1 (88%), HOMO→LUMO (14%)
6	531.66	0.0000	2.3320	HOMO-2→LUMO (77%), HOMO→LUMO+2 (12%)
7	484.94	0.0000	2.5567	HOMO-3→LUMO (30%), HOMO-2→LUMO+1 (11%), HOMO-1→LUMO+2 (25%), HOMO→LUMO+3 (33%)
8	474.98	0.0000	2.6103	HOMO-3→LUMO (40%), HOMO-2→LUMO+1 (16%), HOMO-1→LUMO+2 (25%), HOMO→LUMO+3 (17%)
9	436.27	0.1302	2.8419	HOMO-4→LUMO (97%)
10	435.89	0.0000	2.8444	HOMO-3→LUMO+1 (10%), HOMO-2→LUMO+1 (32%), HOMO-1→LUMO+2 (20%), HOMO→LUMO+3 (19%)
11	431.52	0.0004	2.8732	HOMO-8→LUMO (69%), HOMO-5→LUMO (29%)
12	431.26	0.0000	2.8749	HOMO-7→LUMO (91%)
13	426.24	0.0000	2.9088	HOMO-8→LUMO (29%), HOMO-5→LUMO (70%)
14	426.02	0.0000	2.9103	HOMO-6→LUMO (93%)
15	419.81	0.0000	2.9533	HOMO-9→LUMO (33%), HOMO-3→LUMO+1 (21%), HOMO-1→LUMO+2 (11%)
16	417.28	0.0001	2.9712	HOMO-10→LUMO (99%)
17	417.28	0.0000	2.9712	HOMO-11→LUMO (98%)
18	413.61	0.0000	2.9976	HOMO-9→LUMO (55%), HOMO-2→LUMO+1 (15%)
19	411.48	0.0122	3.0131	HOMO-12→LUMO (98%)
20	407.63	0.0000	3.0416	HOMO-13→LUMO (85%)
21	401.06	0.0678	3.0914	HOMO-14→LUMO (96%)
22	387.82	0.0000	3.1969	HOMO-15→LUMO (74%), HOMO-1→LUMO+3 (13%)
23	379.82	0.1605	3.2643	HOMO-4→LUMO+1 (64%), HOMO→LUMO+4 (29%)
24	375.78	0.0012	3.2994	HOMO-5→LUMO+1 (78%)
25	375.34	0.0000	3.3032	HOMO-6→LUMO+1 (93%)
26	375.29	0.0189	3.3037	HOMO-5→LUMO+1 (10%), HOMO-4→LUMO+1 (27%), HOMO→LUMO+4 (55%)
27	372.79	0.0000	3.3258	HOMO-13→LUMO+1 (16%), HOMO-9→LUMO+1 (26%), HOMO-3→LUMO+1 (31%)
28	361.37	0.0000	3.4309	HOMO-9→LUMO+1 (13%), HOMO-7→LUMO+1 (66%)
29	360.97	0.0004	3.4347	HOMO-8→LUMO+1 (87%)
30	360.69	0.0000	3.4374	HOMO-9→LUMO+1 (54%), HOMO-7→LUMO+1 (26%)
31	360.62	0.0056	3.4381	HOMO-12→LUMO+1 (91%)
32	357.69	0.0000	3.4662	HOMO-13→LUMO+1 (44%), HOMO-3→LUMO+1 (10%), HOMO-1→LUMO+3 (30%)
33	352.58	0.0001	3.5165	HOMO-10→LUMO+1 (95%)
34	352.58	0.0000	3.5165	HOMO-11→LUMO+1 (95%)
35	351.16	0.0299	3.5307	HOMO-2→LUMO+2 (88%)
36	349.28	0.0000	3.5497	HOMO-13→LUMO+1 (25%), HOMO-1→LUMO+3 (38%)
37	346.24	0.0403	3.5809	HOMO-16→LUMO (69%), HOMO-14→LUMO+1 (17%)
38	343.95	0.0091	3.6047	HOMO-16→LUMO (11%), HOMO-14→LUMO+1 (70%)
39	343.75	0.0003	3.6068	HOMO→LUMO+5 (95%)
40	343.14	0.0000	3.6132	HOMO→LUMO+6 (89%)
41	341.62	0.0000	3.6293	HOMO→LUMO+7 (86%)
42	341.09	0.0029	3.6349	HOMO→LUMO+8 (93%)
43	340.19	0.0000	3.6445	HOMO-17→LUMO (83%), HOMO-15→LUMO+1 (12%)
44	334.94	0.0000	3.7017	HOMO-15→LUMO+1 (78%)
45	330.68	0.0442	3.7494	HOMO-18→LUMO (70%)

46	326.56	0.0061	3.7967	HOMO-19→LUMO (43%), HOMO-1→LUMO+4 (19%), HOMO→LUMO+9 (24%)
47	325.20	0.0491	3.8125	HOMO-19→LUMO (51%), HOMO→LUMO+9 (25%)
48	323.48	0.0000	3.8328	HOMO-20→LUMO (90%)
49	321.38	0.0105	3.8578	HOMO-21→LUMO (20%), HOMO-3→LUMO+2 (52%), HOMO→LUMO+9 (15%)
50	318.67	0.0136	3.8907	HOMO-21→LUMO (42%), HOMO-3→LUMO+2 (16%), HOMO- 1→LUMO+4 (23%)

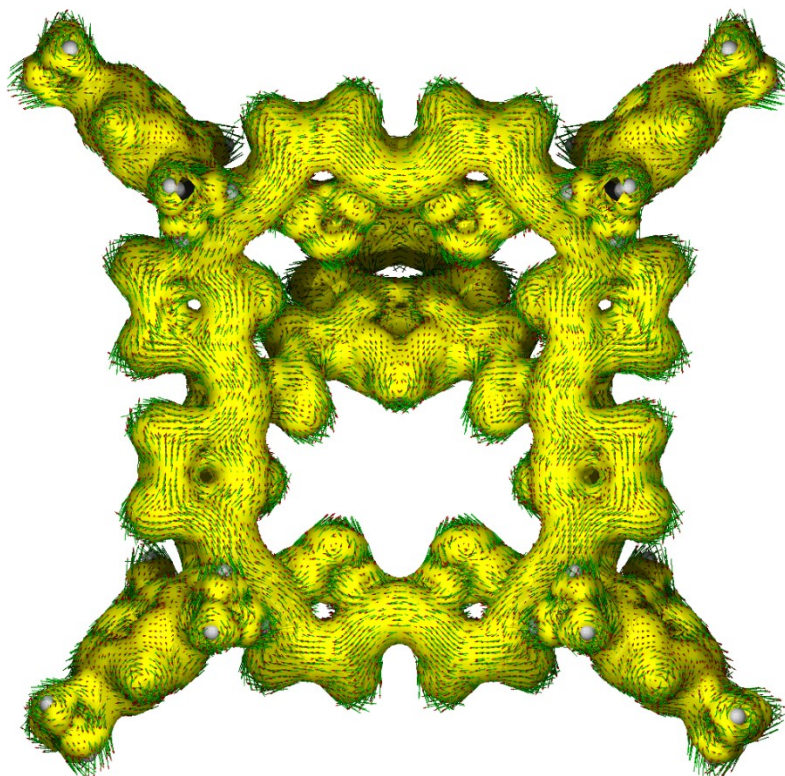


Fig. S53 The Anisotropy of Induced Current Density (AICD) plot of **13**. A continuous clock-wise ring current along the macrocycle indicating the aromatic nature of macrocycles (isovalue = 0.02).

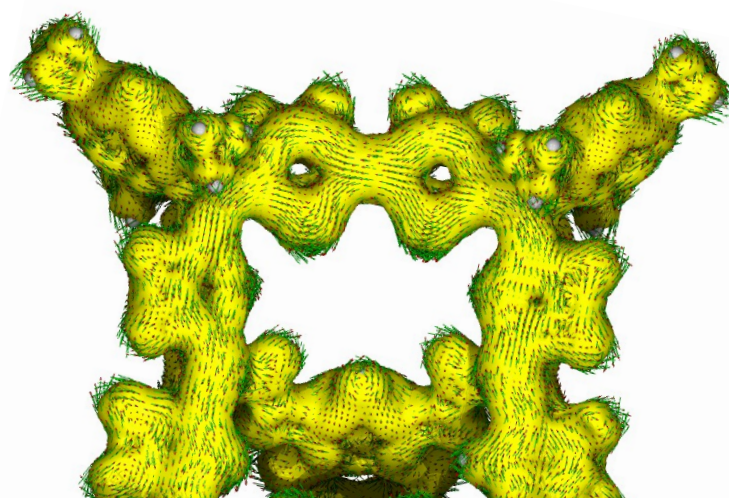


Fig. S54 The Anisotropy of Induced Current Density (AICD) plot of **14**. A continuous anti clock-wise ring current along the macrocycle indicating the anti-aromatic nature of macrocycle (isovalue = 0.02).

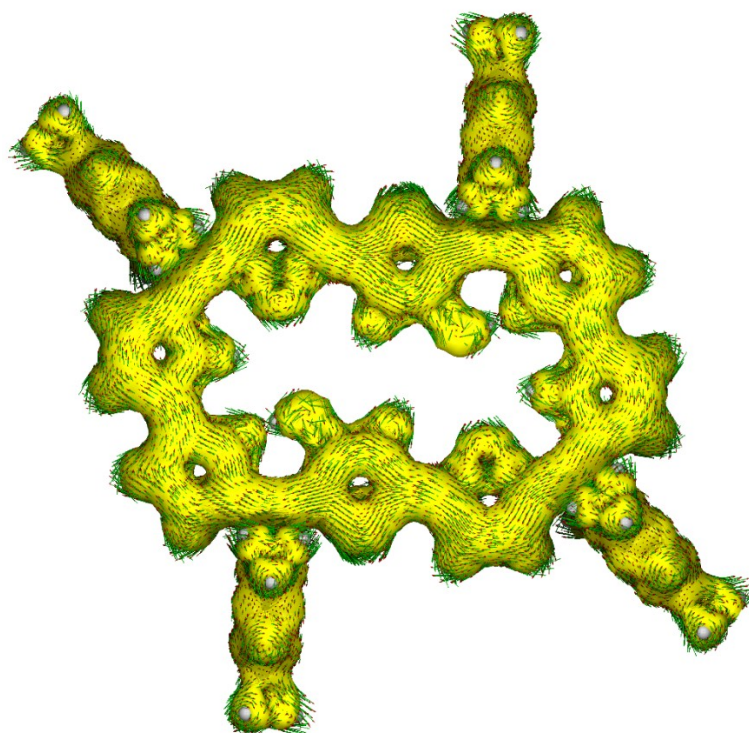


Fig. S55 The Anisotropy of Induced Current Density (AICD) plot of **15'**. A continuous clock-wise ring current along the macrocycle indicating the aromatic nature of macrocycles (isovalue = 0.02).

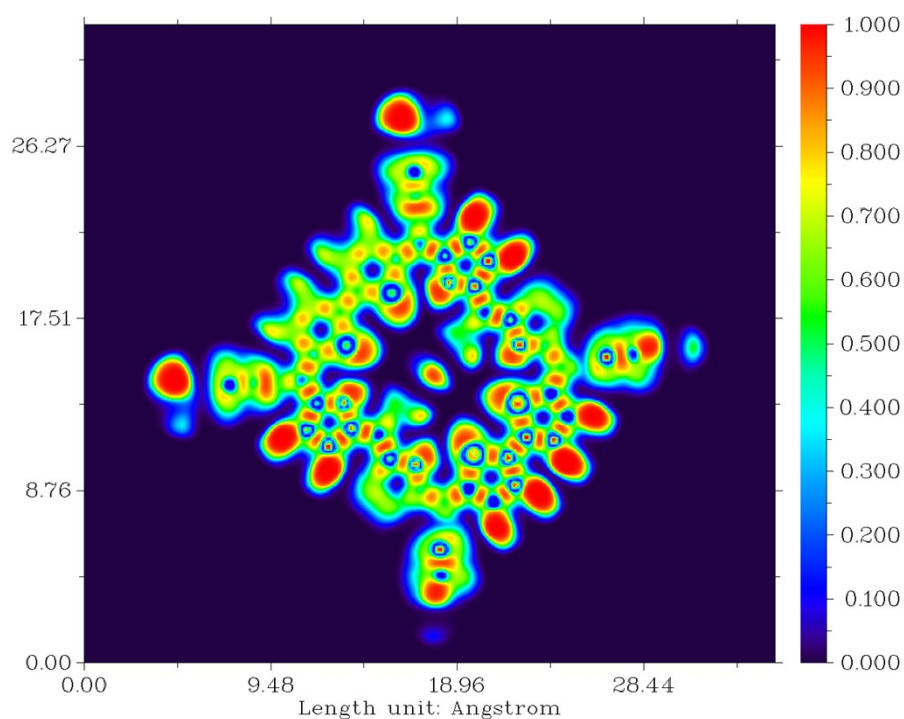


Fig. S56 Color-filled map of the electron localization function of **13**.

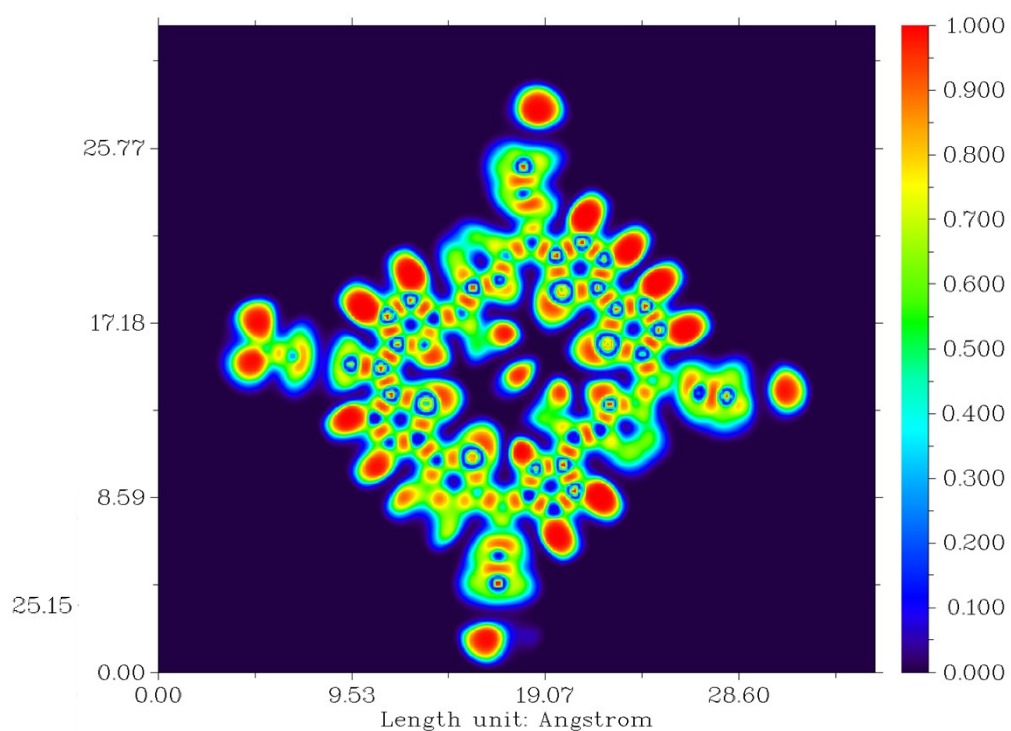
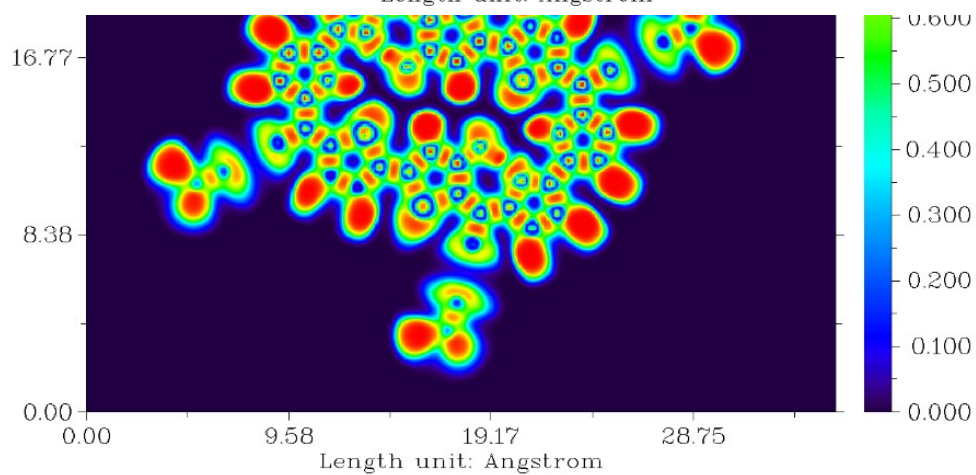


Fig.S57
map of
function



Color-filled
the electron
localization
of **14**.

Fig. S58 Color-filled map of the electron localization function of **15'**.

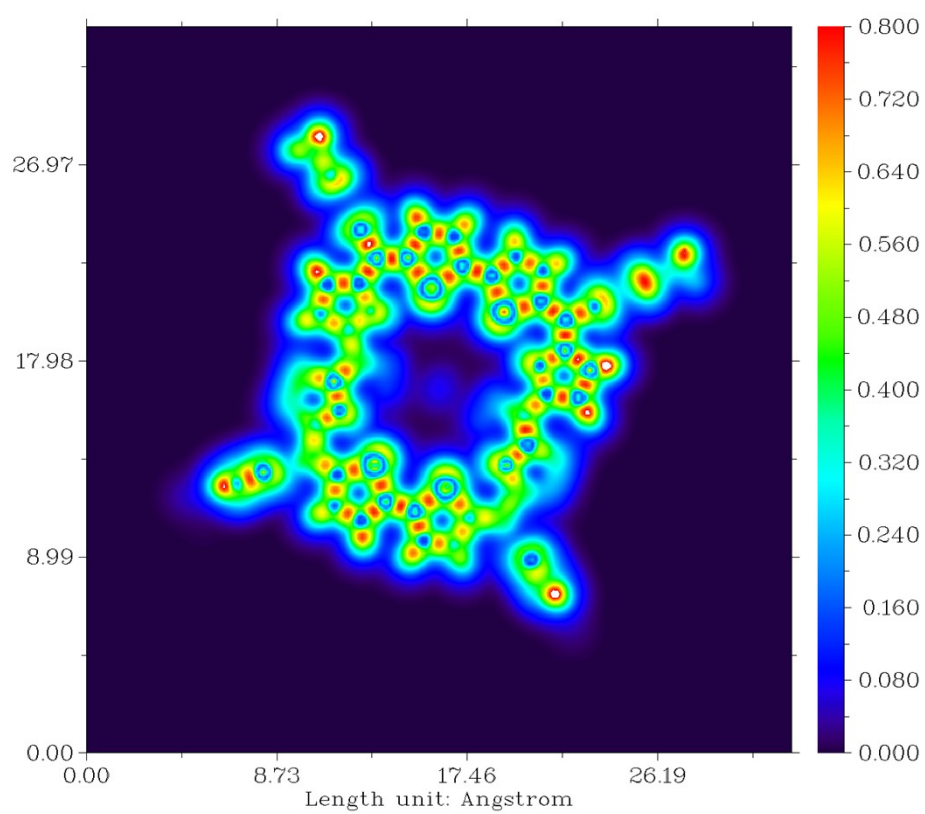


Fig. S59 Computed contour map of the π -localized orbital locator of **13**.

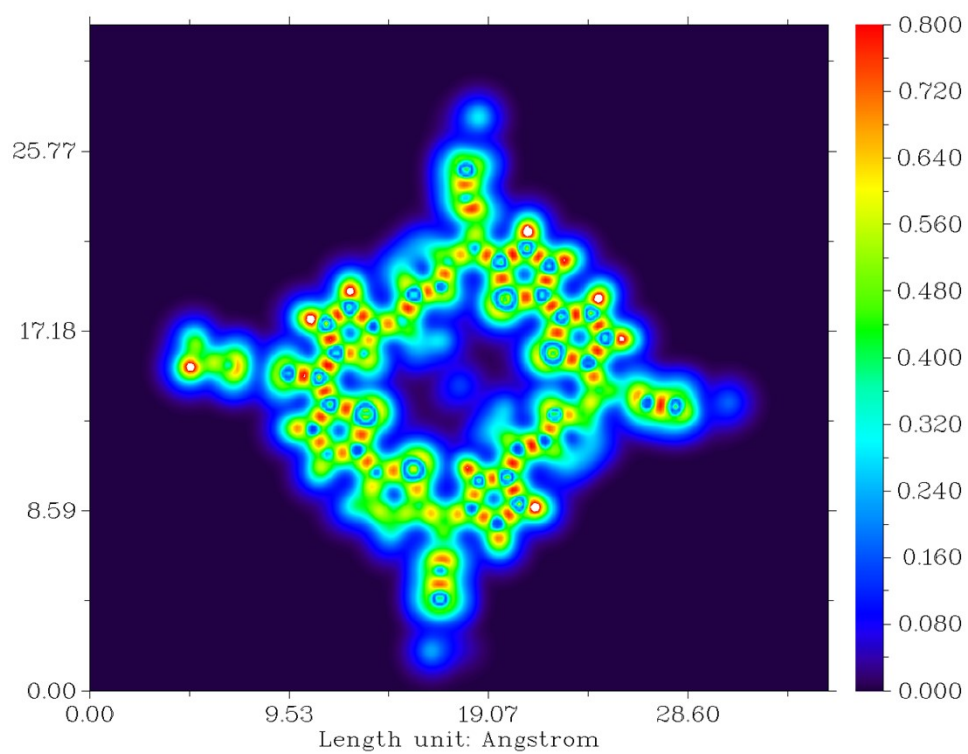


Fig. S60 Computed contour map of the π -localized orbital locator of **14**.

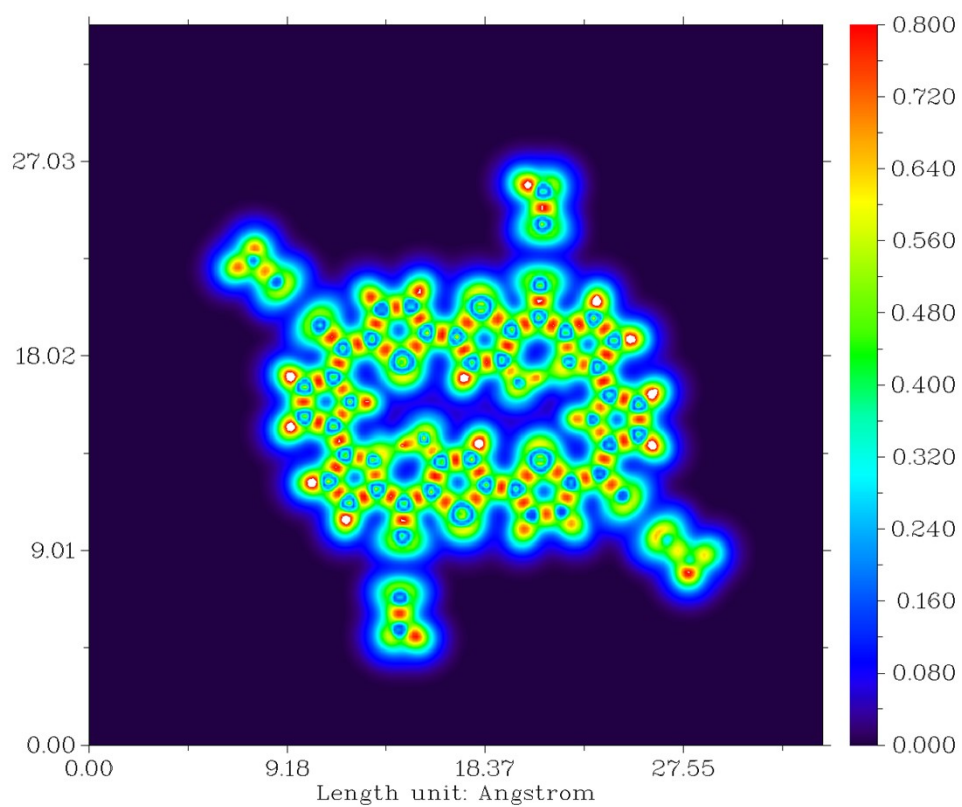


Fig. S61 Computed contour map of the π -localized orbital locator of **15'**.

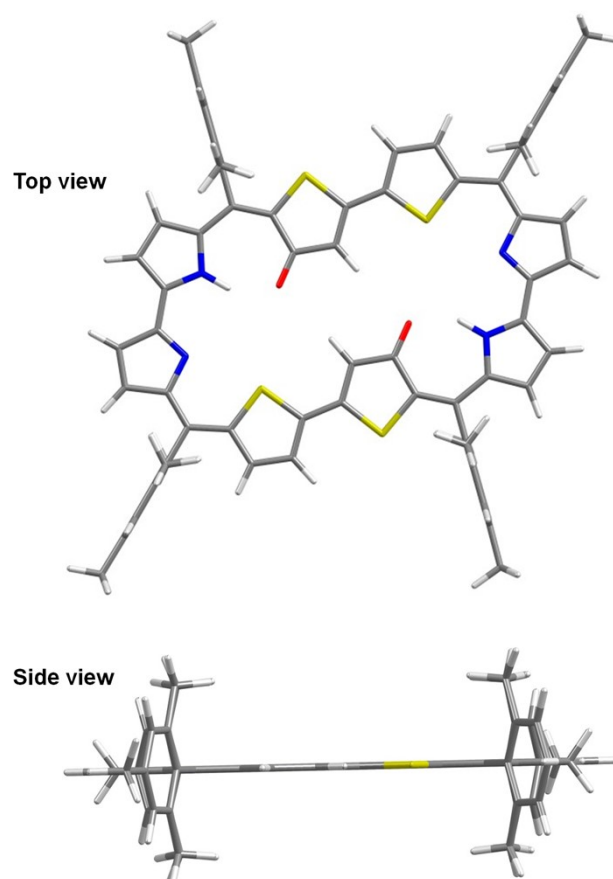


Fig. S62 Overlay plot (DFT and XRD) of structure **15**.

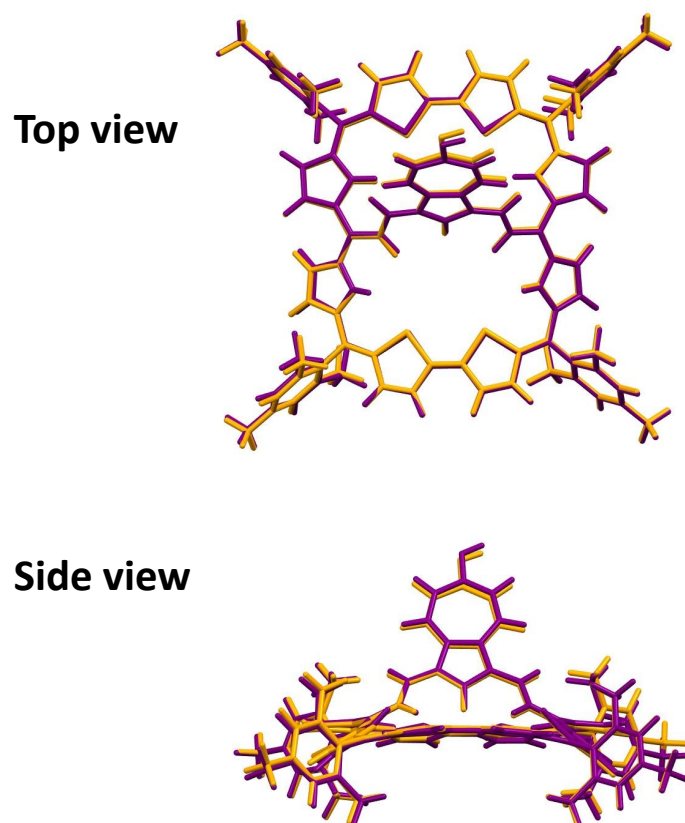
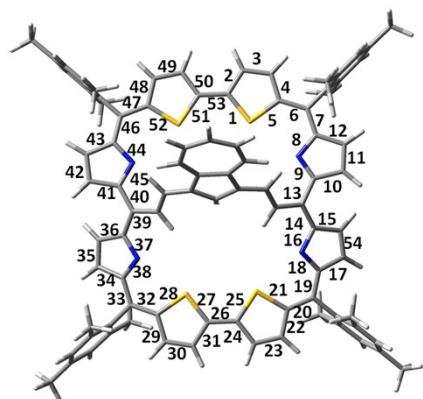
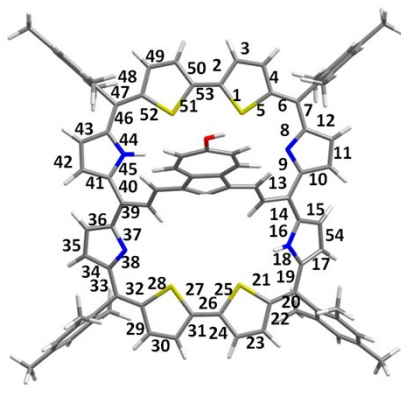


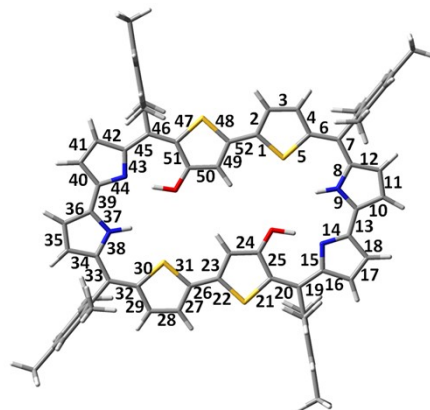
Fig. S63 Overlay plot (DFT) of structure **14** (orange) and **[14-H₂]²⁺** (purple)



13



14



15'

Number of Bond	13		14		15'	
	Wieberg Bond Index	π -character of the bond	Wieberg Bond Index	π -character of the bond	Wieberg Bond Index	π -character of the bond
1	1.151	0.189	1.088	0.198	1.105	0.486
2	1.368	0.327	1.203	0.200	1.338	0.345
3	1.439	0.406	1.617	0.570	1.482	0.480
4	1.357	0.303	1.203	0.194	1.306	0.353
5	1.136	0.222	1.309	0.223	1.111	0.518
6	1.264	0.262	1.483	0.299	1.340	0.361
7	1.382	0.335	1.175	0.211	1.302	0.332
8	1.238	0.213	1.408	0.356	1.137	0.229
9	1.431	0.398	1.244	0.255	1.170	0.383
10	1.141	0.345	1.179	0.259	1.287	0.360
11	1.685	0.593	1.638	0.588	1.530	0.531
12	1.130	0.278	1.161	0.337	1.263	0.288
13	1.155	0.204	1.295	0.264	1.210	0.239
14	1.282	0.200	1.192	0.141	1.304	0.339
15	1.137	0.194	1.355	0.355	1.245	0.286
16	1.310	0.211	1.137	0.274	1.199	0.231
17	1.130	0.148	1.352	0.270	1.601	0.611
18	1.340	0.177	1.173	0.142	1.200	0.393
19	1.274	0.315	1.160	0.345	1.277	0.361
20	1.361	0.310	1.498	0.415	1.386	0.406
21	1.118	0.218	1.075	0.372	1.087	0.546
22	1.282	0.304	1.201	0.336	1.100	0.499
23	1.517	0.494	1.612	0.565	1.370	0.381
24	1.291	0.311	1.216	0.232	1.360	0.379
25	1.125	0.193	1.078	0.323	1.201	0.341
26	1.303	0.330	1.427	0.419	1.275	0.280
27	1.125	0.208	1.090	0.212	1.338	0.345
28	1.118	0.219	1.086	0.228	1.482	0.480
29	1.282	0.305	1.200	0.213	1.306	0.353
30	1.517	0.494	1.620	0.592	1.111	0.518
31	1.292	0.311	1.203	0.227	1.105	0.486
32	1.361	0.310	1.491	0.431	1.340	0.361
33	1.274	0.315	1.165	0.247	1.302	0.332
34	1.130	0.162	1.143	0.168	1.263	0.288
35	1.686	0.432	1.666	0.426	1.530	0.531
36	1.137	0.193	1.154	0.179	1.287	0.360
37	1.310	0.197	1.221	0.140	1.170	0.382
38	1.340	0.177	1.437	0.248	1.137	0.229

39	1.281	0.200	1.355	0.200	1.211	0.239
40	1.155	0.205	1.142	0.138	1.200	0.393
41	1.141	0.345	1.386	0.371	1.610	0.610
42	1.685	0.593	1.434	0.366	1.200	0.231
43	1.130	0.278	1.351	0.341	1.245	0.286
44	1.238	0.213	1.176	0.204	1.304	0.340
45	1.431	0.398	1.143	0.187	1.277	0.361
46	1.382	0.335	1.171	0.290	1.386	0.406
47	1.264	0.262	1.499	0.462	1.087	0.546
48	1.357	0.302	1.198	0.305	1.100	0.499
49	1.439	0.406	1.615	0.550	1.370	0.381
50	1.368	0.327	1.216	0.187	1.360	0.379
51	1.151	0.189	1.076	0.285	1.207	0.341
52	1.136	0.221	1.076	0.357	1.274	0.280
53	1.217	0.340	1.427	0.392	-	-
54	1.686	0.431	1.448	0.197	-	-

Fig. S64 Computed Weiberg Bond Index and π -character of each bond.

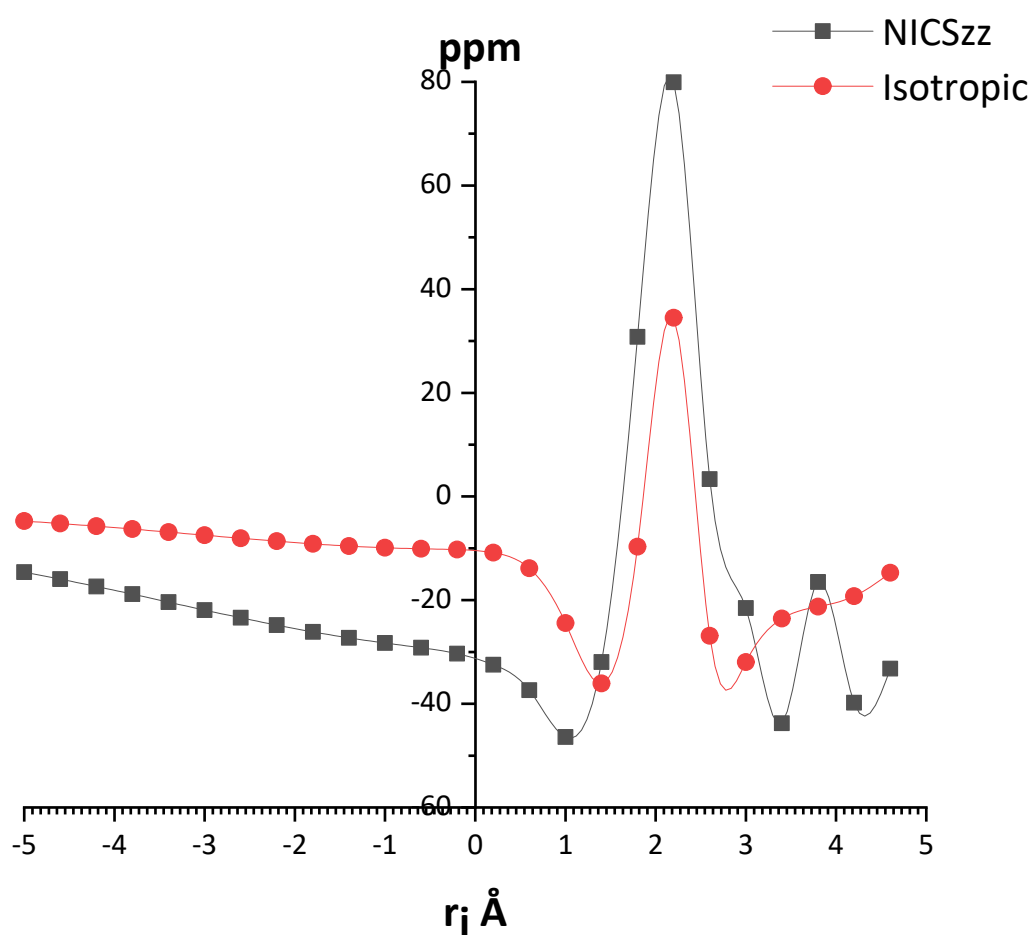


Fig. S65 Isotropic NICS and NICSzz scan plot of **13** where NICSzz is the out of plane contribution.

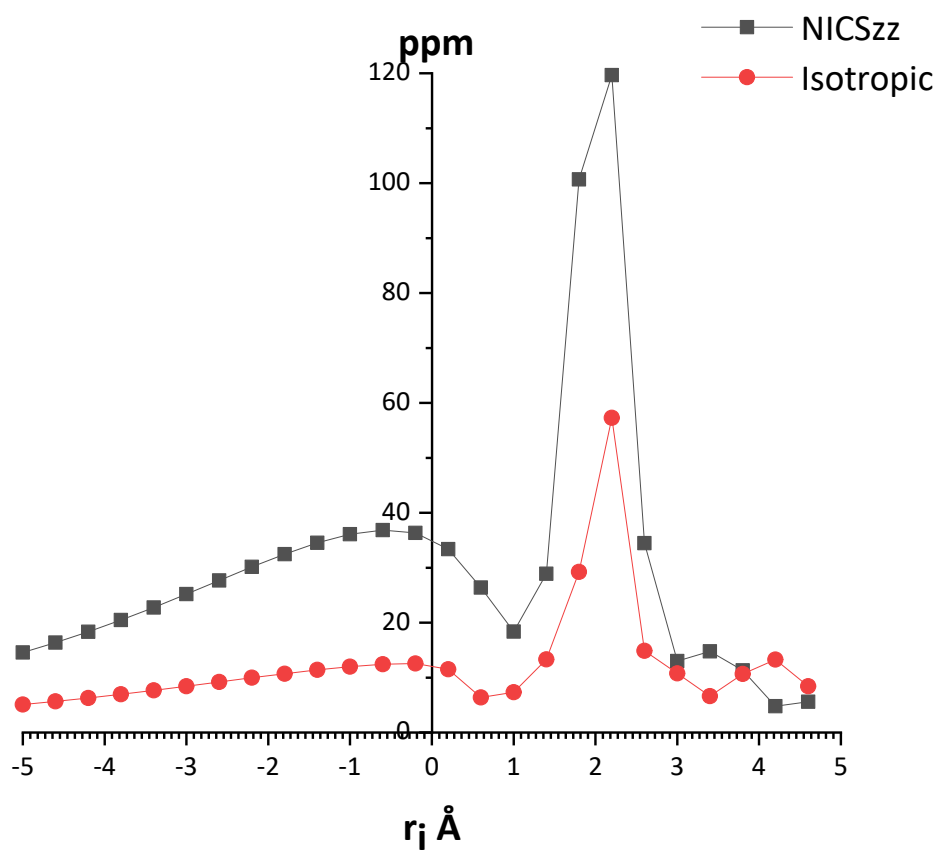


Fig. S66 Isotropic NICS and NICSzz scan plot of **14** where NICSzz is the out of plane contribution.

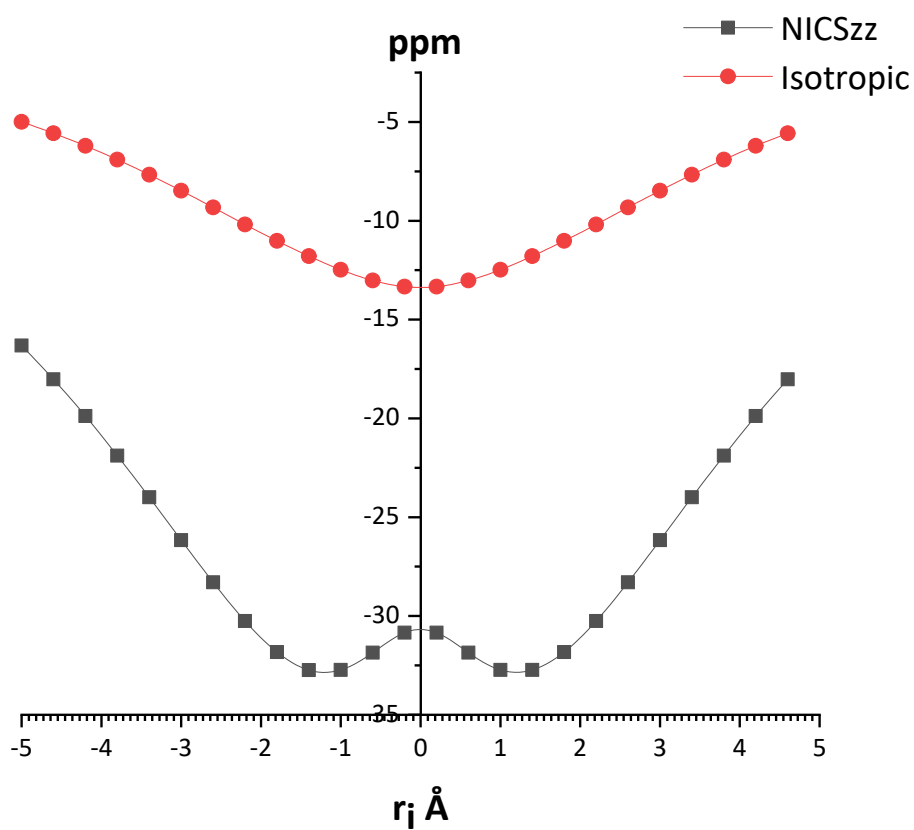


Fig. S67 Isotropic NICS and NICSzz scan plot of **15'** where NICSzz is the out of plane contribution.

7. X,Y,Z Coordinates

Cartesian Coordinates			
13			
C	5.48570900	-3.19580100	0.20898200
C	6.86045700	-2.85777400	0.31012000
H	7.63317800	-3.61349900	0.23783800
C	7.11104400	-1.51386200	0.46723400
H	8.11043300	-1.10006400	0.53011600
C	5.94624200	-0.70933900	0.49136500
C	5.94741900	0.69962300	0.49140800
C	7.11356100	1.50222300	0.46773800
H	8.11223900	1.08676500	0.53100400
C	6.86524700	2.84655700	0.31068000
H	7.63922600	3.60101200	0.23869200
C	5.49109700	3.18687700	0.20905000
C	5.00484100	4.46437100	-0.10943800
C	3.63306500	4.80322400	-0.18275000
C	3.09424700	6.01480200	-0.79422500
H	3.67152600	6.80149400	-1.26177300
C	1.74178600	5.91091700	-0.70406500
H	1.00894200	6.59648800	-1.10245200
C	1.47337200	4.66743600	0.01522600
C	0.22520900	4.14091600	0.43670700
C	0.21558100	2.88569300	1.12920400
C	-0.78963700	2.48430400	1.96268300
H	-1.58146500	3.19079500	2.18946000
C	-0.93479300	1.15951300	2.48094600
C	-0.93663900	-1.15731000	2.48146700
C	-0.79362300	-2.48255300	1.96377500
H	-1.58654500	-3.18768700	2.19094500
C	0.21085700	-2.88590400	1.13034700
C	0.21836300	-4.14142000	0.43836900
C	1.46559100	-4.67008600	0.01679100
C	1.73180600	-5.91429700	-0.70207100
H	0.99774500	-6.59893400	-1.09982500
C	3.08406200	-6.02029800	-0.79269700
H	3.65995700	-6.80813000	-1.26002400
C	3.62499400	-4.80929700	-0.18194500
C	4.99728700	-4.47251400	-0.10938100
C	-1.04685400	-4.78357800	0.14266700
C	-1.33040100	-6.21431300	0.02015700
H	-0.62892100	-7.01927600	0.18842400
C	-2.66058700	-6.32124300	-0.24522400
H	-3.24079800	-7.22410300	-0.38262400
C	-3.16845100	-4.95530700	-0.30749000
C	-4.47118000	-4.56517900	-0.61840000
C	-4.92776700	-3.21770400	-0.71161800
C	-6.25163400	-2.85831500	-1.01720600
H	-7.01599000	-3.60367300	-1.19963500
C	-6.48295000	-1.49118200	-1.06428800
H	-7.45339900	-1.06577600	-1.28880200
C	-5.34686500	-0.71214400	-0.79917000
C	-5.34567600	0.72015800	-0.79949500
C	-6.48048000	1.50096100	-1.06491000
H	-7.45166100	1.07706500	-1.28911400
C	-6.24687700	2.86772900	-1.01852600
H	-7.01000000	3.61427100	-1.20128000
C	-4.92239500	3.22506000	-0.71318900
C	-4.46355800	4.57181800	-0.62067700
C	-3.16019900	4.95995500	-0.30990600
C	-2.65010000	6.32508700	-0.24830300
H	-3.22881600	7.22882700	-0.38623000
C	-1.32011800	6.21611500	0.01726400
H	-0.61734200	7.02002200	0.18517700
C	-1.03892600	4.78498100	0.14053400
C	6.01180800	5.53578600	-0.42913500
C	6.56105200	5.63171100	-1.72580100
C	7.48103400	6.64973600	-1.99917800
C	7.87919100	7.56927300	-1.02510500
C	7.31994700	7.45718900	0.25071500
C	6.39126100	6.46024900	0.56738600
C	6.16202900	4.66744300	-2.82095500
H	6.47969600	3.64315200	-2.59284700
H	6.61432200	4.95440300	-3.77529500
H	5.07491100	4.63763000	-2.95515000
C	8.90132500	8.63824200	-1.33541500
H	8.87020000	8.92849800	-2.39110700
H	9.92104800	8.28803300	-1.12520000
H	8.73750900	9.53736400	-0.73162100
C	5.81063400	6.38938000	1.96229400
H	4.72986300	6.57274500	1.95671100
H	6.27616100	7.13357100	2.61594400
H	5.95866000	5.40112400	2.41236900
C	6.00233100	-5.54552300	-0.42982400
C	6.38370300	-6.46760700	0.56587000
C	7.31404600	-7.46481800	0.24811900
C	7.86920200	-7.57900900	-1.02756500
C	7.47089400	-6.65765600	-2.00213600
C	6.55126900	-5.64152800	-1.72835800
C	5.80838300	-6.39510800	1.96290300
H	5.95817800	-5.40651700	2.41164400
H	6.27608300	-7.13881300	2.61555800
H	4.72757700	-6.57840400	1.96144100
C	8.87175800	-8.66210100	-1.35296800
H	8.53189600	-9.28401300	-2.19041000
H	9.04131900	-9.32071000	-0.49528900
H	9.84092900	-8.23696200	-1.64341800
C	6.15221700	-4.67516600	-2.82164300
H	5.06511600	-4.64619800	-2.95628800
H	6.60523000	-4.95976000	-3.77634700
H	6.46863700	-3.65104400	-2.59114900
C	-5.48361600	-5.64674600	-0.88782100
C	-6.24167100	-6.18216900	0.17435700
C	-7.17313000	-7.18984400	-0.09800600
C	-7.37192500	-7.68422500	-1.38981300
C	-6.61075500	-7.13673300	-2.42622700
C	-5.66820800	-6.12784100	-2.20131600
C	-6.06166500	-5.68810400	1.59270900
H	-5.04198800	-5.86840100	1.95264200
H	-6.75419000	-6.19453000	2.27204500
H	-6.23870300	-4.60908600	1.67047500
C	-8.36095400	-8.79564600	-1.65451500
H	-8.79313900	-8.71765500	-2.65796000
H	-9.18190800	-8.78341700	-0.92962000
H	-7.88046800	-9.78083600	-1.58440000
C	-4.86621400	-5.57543900	-3.35851000
H	-5.16061500	-6.05170000	-4.29863200
H	-3.79204200	-5.74112400	-3.21675400
H	-5.00645300	-4.49393200	-3.46837000
C	-5.47417000	5.65492900	-0.89075300
C	-5.65793400	6.13553900	-2.20460000
C	-6.59871700	7.14586300	-2.43015000
C	-7.35899300	7.69531400	-1.39404500
C	-7.16105500	7.20141800	-0.10197700
C	-6.23129200	6.19228600	0.17104400
C	-4.85684000	5.58102800	-3.36140900
H	-4.99900300	4.49970700	-3.47064100
H	-3.78238500	5.74487800	-3.21966700
H	-5.15032200	6.05726000	-4.30183200
C	-8.34610900	8.80820700	-1.65969900
H	-8.78648300	8.72394300	-2.65910500
H	-7.86154000	9.79215700	-1.60129400
H	-9.16134200	8.80460100	-0.92832900
C	-6.05218600	5.69882400	1.58972100
H	-6.23113500	4.62017000	1.66818400
H	-6.74383300	6.20691100	2.26871200
H	-5.03220300	5.87755300	1.94956700
N	2.63978700	4.01603000	0.28837800
N	2.63309900	-4.02037700	0.28924600
N	-2.16356800	-4.06025800	-0.04529200
N	-2.15680300	4.06339200	-0.04716900
S	4.50464700	-1.72805800	0.39427100
S	4.50754600	1.72072600	0.39387400
S	-3.95736200	-1.75218900	-0.48229300
S	-3.95442900	1.75804000	-0.48317400
H	-6.73952800	7.51236000	-3.44528500
H	-7.74550100	7.61138200	0.71962400
H	-6.75221200	-7.50362000	-3.44112300
H	-7.75828400	-7.59827700	0.72386300
H	7.88601600	-6.73171200	-3.00587600
H	7.60883900	-8.17166500	1.02135100
H	7.89471900	6.72596400	-3.00310800
H	7.61038300	8.16707900	1.02308600
C	-0.38809500	0.00054200	1.90495500
C	-1.83132500	0.74008600	3.51850400
C	-2.54834500	1.58867600	4.35404500
C	-3.43537600	1.26607600	5.38782900
C	-1.83249200	-0.73599500	3.51883700
C	-3.82259100	0.00415800	5.84545800
C	-2.55084900	-1.58306600	4.35478300
C	-3.43735500	-1.25858700	5.38841800
H	-2.39617600	2.65288600	4.18602300
H	-3.88033600	2.11309700	5.90488700
H	-4.52904600	0.00490400	6.67361800
H	-2.40035800	-2.64759200	4.18725400
H	-3.88364200	-2.10466200	5.90588200
H	1.09858800	2.26531000	1.01056100
H	1.09483800	-2.26698400	1.01131900
H	0.26568300	-0.00017000	1.04188700

C	6.072000157	-2.277066663	0.186250174
C	7.374171909	-1.690864448	0.349823106
H	8.266026659	-2.306042477	0.336094612
C	7.383745201	-0.335341021	0.485280704
H	8.291938723	0.247925822	0.583739662
C	6.084646647	0.269975155	0.431190805
C	5.848749590	1.633207115	0.412914331
C	6.839588003	2.662714341	0.494929658
H	7.885792538	2.433712537	0.661755878
C	6.371756156	3.933005555	0.330293249
H	6.996902292	4.817363885	0.355650008
C	4.957970312	4.036583095	0.091554613
C	4.281143483	5.195667551	-0.236300251
C	2.857851124	5.309330591	-0.426335218
C	2.150972196	6.235480472	-1.219043276
H	2.612363295	7.008231871	-1.817298260
C	0.792094234	5.922194047	-1.149889499
H	-0.007461669	6.390224865	-1.704231703
C	0.633612512	4.826461680	-0.281041641
C	-0.520105323	4.093825034	0.155791265
C	-0.298742874	2.825614969	0.805840714
C	-1.144962060	2.290630851	1.731600803
H	-1.982180053	2.898246742	2.058749133
C	-0.221567823	-2.602032591	1.785411213
C	0.798912699	-2.814245484	0.905505359
C	1.043136525	-4.075589142	0.241059207
C	2.351831301	-4.388785782	-0.147661404
C	2.842390136	-5.565968222	-0.843238655
H	2.239654339	-6.359896394	-1.261742890
C	4.200407312	-5.449638182	-0.873753227
H	4.916466793	-6.131560538	-1.313523572
C	4.510929945	-4.170753473	-0.242116560
C	5.828685411	-3.605507947	-0.103584639
C	-0.093169501	-4.931600410	-0.029251151
C	-0.259606810	-6.321475162	-0.111491579
H	0.510741883	-7.051255780	0.091746302
C	-1.601296430	-6.582596511	-0.412672316
H	-2.065490491	-7.552335675	-0.518031474
C	-2.280957142	-5.350592499	-0.531266462
C	-3.673631332	-5.133605067	-0.834676519
C	-4.357125964	-3.931818737	-0.876020185
C	-5.753625216	-3.788402580	-1.195001309
H	-6.360344342	-4.653251907	-1.432886951
C	-6.227609543	-2.510821108	-1.180386195
H	-7.257242046	-2.261946074	-1.409011294
C	-5.266054100	-1.499985049	-0.860132061
C	-5.504995996	-0.136500242	-0.815930685
C	-6.786410875	0.466312116	-1.044550454
H	-7.673662789	-0.118312360	-1.257627568
C	-6.787560301	1.826521020	-0.971659797
H	-7.668543899	2.439280408	-1.121727157
C	-5.511972880	2.425847799	-0.692684198
C	-5.276631200	3.788340915	-0.635717325
C	-3.988026637	4.383884108	-0.399888893
C	-3.666103267	5.799572619	-0.492507917
H	-4.366504043	6.604110689	-0.675626550
C	-2.313276494	5.892734591	-0.312125368
H	-1.717860235	6.794694457	-0.266097425
C	-1.840945217	4.543206609	-0.077571878
C	5.074790334	6.449077048	-0.483538869
C	5.767881146	6.622152140	-1.701355805
C	6.484420532	7.806065053	-1.912010261
C	6.536929256	8.821156930	-0.954014572
C	5.845993740	8.627531610	0.246058123
C	5.110898230	7.465545156	0.496664094
C	5.750223824	5.561001999	-2.779976098
H	6.342639500	4.683355933	-2.494073563
H	6.164658459	5.952350747	-3.714278616
H	4.734392226	5.204257273	-2.980470234
C	7.294163907	10.102282614	-1.215867218
H	6.631702626	10.881177972	-1.616974751
H	8.097241183	9.951833818	-1.944986221
H	7.739780100	10.499892640	-0.297397639
C	4.380458014	7.310375040	1.811597819
H	3.293602373	7.292615270	1.665800269
H	4.613930571	8.138818322	2.487448534
H	4.649380653	6.374749552	2.315132843
C	7.001161428	-4.524547221	-0.311559482
C	7.434880604	-5.358024370	0.741921870
C	8.518801454	-6.215583937	0.528861090
C	9.179524918	-6.281123492	-0.701196209
C	8.731934735	-5.450190748	-1.731385746
C	7.655332830	-4.572440805	-1.561055686
C	6.752965656	-5.327358443	2.091425336

H	6.761029100	-4.320856859	2.525397157
H	7.248297151	-6.004692833	2.794130939
H	5.701202113	-5.627043531	2.015792624
C	10.325173712	-7.242608655	-0.917975855
H	9.962784982	-8.228552761	-1.239209808
H	10.901119540	-7.394520150	0.001467666
H	11.011052304	-6.881682889	-1.691882601
C	7.212029407	-3.697678543	-2.713139270
H	6.138371738	-3.799859898	-2.906495711
H	7.749296135	-3.960683821	-3.629722394
H	7.395421921	-2.635913720	-2.509421958
C	-4.457130256	-6.386701973	-1.133838442
C	-5.128571194	-7.065486944	-0.095370794
C	-5.842183558	-8.231342636	-0.394346678
C	-5.907406295	-8.745893743	-1.691927951
C	-5.237655962	-8.055588795	-2.706076829
C	-4.511524762	-6.887245917	-2.451997050
C	-5.093875513	-6.550121433	1.326262392
H	-4.064701002	-6.436846174	1.685777218
H	-5.615468996	-7.235421211	2.001666148
H	-5.569827035	-5.565934354	1.410140447
C	-6.657292791	-10.024596484	-1.985770912
H	-7.072658195	-10.022348062	-2.999357184
H	-7.482208895	-10.176958150	-1.281545253
H	-5.998097591	-10.899775166	-1.907978909
C	-3.807457877	-6.177774434	-3.586760679
H	-3.954123034	-6.711350945	-4.530903111
H	-2.729209812	-6.102964170	-3.404184447
H	-4.179195311	-5.154504562	-3.714855409
C	-6.433669735	4.722628071	-0.869020472
C	-6.765121545	5.129497710	-2.178906987
C	-7.835491171	6.010727835	-2.367133043
C	-8.585117154	6.504596685	-1.296052097
C	-8.240387757	6.088375018	-0.007345582
C	-7.177148847	5.209786313	0.226347712
C	-5.985278749	4.627002768	-3.373423485
H	-6.073481801	3.539971091	-3.485294297
H	-4.916254688	4.847215139	-3.274869715
H	-6.344768963	5.091667717	-4.296907826
C	-9.716132821	7.481141385	-1.522570779
H	-10.198253142	7.318885216	-2.492728834
H	-9.355974626	8.518825267	-1.509547944
H	-10.482626698	7.395082930	-0.744750873
C	-6.843479096	4.791443550	1.641077738
H	-6.931317915	3.706418397	1.771770352
H	-7.513102104	5.275306140	2.359245450
H	-5.812997263	5.058293148	1.903319599
N	1.913939609	4.469501246	0.120455795
N	3.403533162	-3.553751888	0.179646281
N	-1.341934294	-4.378840054	-0.276732723
N	-2.896540675	3.656103759	-0.127738340
S	4.837232628	-0.991081200	0.305267130
S	4.256128015	2.386340971	0.152210644
S	-3.702198886	-2.295448439	-0.540248807
S	-4.294038125	1.129576231	-0.492620632
H	-8.088258135	6.319330777	-3.380007381
H	-8.813280233	6.456964276	0.841829958
H	-5.280445229	-8.434956336	-3.725423502
H	-6.360485791	-8.750030481	0.410136920
H	9.232241555	-5.484555836	-2.697538257
H	8.854427203	-6.849866795	1.347438425
H	7.014108649	7.936677693	-2.853842304
H	5.879715825	9.402132906	1.010083923
H	0.598703689	2.271280427	0.535819635
H	-1.482708788	-3.383728180	-0.375301049
H	2.104934426	3.808250881	0.859757187
H	-0.823553388	-3.453956076	2.093567170
H	1.519474573	-2.025509118	0.713710378
C	-0.340624274	-0.094005037	1.641930337
C	-1.048598565	0.957593974	2.244273077
C	-0.614307030	-1.313193640	2.282602259
C	-1.780843927	0.403056557	3.347037204
C	-1.502556189	-1.037065946	3.371226796
C	-2.600374155	1.116422054	4.215926403
C	-1.995280592	-1.976951919	4.277125609
C	-3.345140136	0.671484203	5.306903149
H	-2.676208678	2.184086516	4.021665996
C	-2.855470985	-1.810808461	5.356057895
H	-1.654237153	-2.998860361	4.123868713
C	-3.459952506	-0.629694198	5.821559404
H	-3.915856381	1.437612858	5.831426866
H	-3.109794904	-2.696574626	5.930705704
O	-4.249857545	-0.832537161	6.911728991
H	-4.649532521	0.007401979	7.188699463
H	0.242171379	-0.001581927	0.734108632

S	1.90319700	4.16559800	-0.21218100
S	3.97593900	0.31389000	0.16646200
N	-2.80881600	4.00927000	0.00994200
N	5.12478300	-2.23042800	0.06945800
C	-2.02388600	5.14816100	0.09989000
C	-4.06103300	4.43813700	-0.00715900
C	-4.14639200	5.89989000	0.06278000
H	-5.05156800	6.49398700	0.07242000
C	-2.86484000	6.34537500	0.12106900
H	-2.51612000	7.36677800	0.19315400
C	-0.63654700	5.15071300	0.14910400
C	0.21126200	4.00013700	0.29181400
C	0.02161200	2.71667100	0.83638200
C	1.18497700	1.90732500	0.80937800
H	1.21725000	0.90429700	1.22563000
C	2.29632500	2.54139500	0.28526900
C	5.20880200	-3.55075300	0.05902400
C	6.60819300	-4.00110200	0.06175000
H	6.94800100	-5.02891300	0.05859400
C	7.37084400	-2.87806100	0.06495800
H	8.44989100	-2.79936000	0.06597500
C	6.42951100	-1.76133500	0.06643800
C	0.06302200	6.47748500	0.01207600
C	0.19842900	7.07671800	-1.25865600
C	0.85786200	8.30729200	-1.35690000
H	0.96725600	8.76427700	-2.33851600
C	1.37190300	8.96484600	-0.23730600
C	1.21079300	8.35888600	1.01266600
H	1.59053500	8.86110500	1.90047900
C	0.57322300	7.12459400	1.15986300
C	3.64104600	2.03713000	0.15830000
C	5.71037600	0.61358400	0.05346900
C	5.96005000	1.98381100	-0.01137800
H	6.96561800	2.38108400	-0.08121400
C	4.80608000	2.78149600	0.04199400
H	4.82196200	3.86621100	0.03219700
C	6.72136200	-0.41377700	0.04243100
C	8.15587900	0.03056500	-0.00161000
C	8.84932900	0.28809600	1.19974500
C	10.18393700	0.70134000	1.13419400
H	10.71617600	0.90049200	2.06242700
C	10.84942600	0.86554200	-0.08380000
C	10.13964900	0.60858100	-1.25982200
H	10.63658000	0.73585200	-2.21971700
C	8.80444400	0.19156500	-1.24392100
C	-0.35579300	6.42677900	-2.50814100
H	0.02204500	6.92961800	-3.40371700
H	-1.45071600	6.47466100	-2.53150300
H	-0.08386500	5.36796900	-2.57398900
C	2.10138000	10.28097000	-0.37286900
H	1.92441300	10.92868900	0.49275400
H	1.78831800	10.82245300	-1.27169200
H	3.18659900	10.12804300	-0.44576500
C	0.41880400	6.51748700	2.53590000
H	0.77312600	7.20806200	3.30716900
H	0.99003800	5.58631700	2.63153200
H	-0.62693000	6.27166100	2.75221000
C	8.17786800	0.11894400	2.54442500
H	8.86075400	0.38537100	3.35677700
H	7.85115200	-0.91538100	2.70240900
H	7.28517500	0.74897100	2.63265400
C	12.30086400	1.28368800	-0.12664700
H	12.53258200	1.83527400	-1.04403400
H	12.96707500	0.41101500	-0.09553000
H	12.56065900	1.91950700	0.72652400
C	8.08509500	-0.08155300	-2.54621200
H	8.72202300	0.16441200	-3.40127200
H	7.16324100	0.50524600	-2.63045900
H	7.79716100	-1.13583500	-2.63173100
S	-1.90319200	-4.16563200	0.21209100
S	-3.97594500	-0.31388600	-0.16632400
N	2.80881600	-4.00927100	-0.00994200
N	-5.12478700	2.23042300	-0.06945800
C	2.02388900	-5.14815500	-0.09989000
C	4.06103400	-4.43813800	0.00704700
C	4.14639600	-5.89988400	-0.06278000
H	5.05157200	-6.49397900	-0.07242800
C	2.86484500	-6.34536400	-0.12106900
H	2.51612700	-7.36675900	-0.19360500
C	0.63654900	-5.15070200	-0.14929000
C	-0.21126000	-4.00011600	-0.29189900
C	-0.02162100	-2.71660200	-0.83635900
C	-1.18499400	-1.90727300	-0.80929000
H	-1.21727800	-0.90421500	-1.22547000

C	-2.29633100	-2.54138300	-0.28520400
C	-5.20880500	3.55075000	-0.05903200
C	-6.60819600	4.00109900	-0.06171200
H	-6.94800300	5.02891000	-0.05858900
C	-7.37084700	2.87805800	-0.06481900
H	-8.44989500	2.79935800	-0.06577700
C	-6.42951500	1.76133200	-0.06629600
C	-0.06301900	-6.47748800	-0.01238600
C	-0.19842900	-7.07683600	1.25829200
C	-0.85785600	-8.30742400	1.35642000
H	-0.96725700	-8.76449500	2.33799500
C	-1.37188600	-8.96488000	0.23676500
C	-1.21077600	-8.35880400	-1.01315200
H	-1.59050800	-8.86094600	-1.90101200
C	-0.57321800	-7.12449300	-1.16023400
C	-3.64104500	-2.03712600	-0.15816300
C	-5.71037700	-0.61358400	-0.05326000
C	-5.96004000	-1.98381100	0.01165700
H	-6.96560200	-2.38108500	0.08156000
C	-4.80607100	-2.78149200	-0.04175900
H	-4.82195100	-3.86620700	-0.03192600
C	-6.72136400	0.41377400	-0.04222200
C	-8.15587800	-0.03056900	0.00190500
C	-8.84938300	-0.28815600	-1.19940700
C	-10.18398700	-0.70140100	-1.13377600
H	-10.71626900	-0.90059500	-2.06197500
C	-10.84941800	-0.86555000	0.08425600
C	-10.13958900	-0.60853500	1.26023400
H	-10.63647400	-0.73576500	2.22015800
C	-8.80438600	-0.19151500	1.24425300
C	0.35578400	-6.42701900	2.50784400
H	-0.02234100	-6.92972400	3.40337500
H	1.45069000	-6.47523300	2.53138200
H	0.08416800	-5.36812800	2.57361900
C	-2.10135300	-10.28102200	0.37220500
H	-1.92438400	-10.92865700	-0.49348100
H	-1.78828600	-10.82258900	1.27097500
H	-3.18657300	-10.12810900	0.44511700
C	-0.41883100	-6.51725000	-2.53621400
H	-0.77283800	-7.20789300	-3.30756700
H	-0.99037400	-5.58626700	-2.63185300
H	0.62684300	-6.27105800	-2.75239000
C	-8.17798400	-0.11906400	-2.54412600
H	-8.86091500	-0.38550700	-3.35643500
H	-7.85125500	0.91524900	-2.70216300
H	-7.28530800	-0.74911200	-2.63237600
C	-12.30085400	-1.28369900	0.12718900
H	-12.53252700	-1.83524600	1.04461000
H	-12.96706800	-0.41102900	0.09606600
H	-12.56068700	-1.91955400	-0.72594300
C	-8.08497800	0.08166400	2.54649800
H	-8.72186200	-0.16427100	3.40159900
H	-7.16311400	-0.50512300	2.63072600
H	-7.79704900	1.13595200	2.63195900
O	1.12924200	-2.33243600	-1.41770200
H	1.02644400	-1.43385800	-1.76979400
O	-1.12927700	2.33253900	1.41769900
H	-1.02650700	1.43396800	1.76981500

S	1.880340000	-4.434888000	-0.024324000
S	3.895930000	-0.503455000	-0.142408000
N	-2.918598000	-4.146851000	-0.008723000
N	5.149439000	2.285793000	-0.000323000
C	-2.140091000	-5.275431000	-0.007556000
C	-4.210601000	-4.552215000	0.021137000
C	-4.283690000	-5.988590000	0.037924000
H	-5.190159000	-6.579617000	0.059252000
C	-2.990473000	-6.442030000	0.018746000
H	-2.650855000	-7.468334000	0.024224000
C	-0.722369000	-5.285096000	-0.015039000
C	0.123241000	-4.163469000	-0.029044000
C	-0.135997000	-2.742599000	-0.049175000
C	1.031154000	-1.969121000	-0.062336000
H	1.001965000	-0.884553000	-0.068950000
C	2.216412000	-2.705777000	-0.045334000
C	5.303600000	3.650462000	-0.039571000
C	6.696393000	3.901716000	-0.110753000
H	7.146957000	4.882771000	-0.168481000
C	7.350750000	2.683928000	-0.106015000
H	8.416374000	2.514877000	-0.160996000
C	6.378237000	1.641248000	-0.034310000
C	-0.063100000	-6.640362000	-0.001765000
C	0.239715000	-7.264835000	1.227284000
C	0.844311000	-8.525834000	1.214127000

H	1.073776000	-9.006149000	2.163437000
C	1.157133000	-9.184467000	0.021967000
C	0.839504000	-8.550515000	-1.182271000
H	1.065171000	-9.050271000	-2.122412000
C	0.235096000	-7.289943000	-1.218885000
C	3.541209000	-2.226490000	-0.036799000
C	5.644111000	-0.767586000	-0.020387000
C	5.885827000	-2.161694000	0.062285000
H	6.890582000	-2.558650000	0.139902000
C	4.745584000	-2.947116000	0.052230000
H	4.764817000	-4.029852000	0.121054000
C	6.616688000	0.249884000	-0.017298000
C	8.059086000	-0.182662000	0.007172000
C	8.730742000	-0.465709000	-1.201311000
C	10.069744000	-0.868075000	-1.155088000
H	10.583918000	-1.085944000	-2.089322000
C	10.762072000	-0.998664000	0.051966000
C	10.075063000	-0.719306000	1.236448000
H	10.592663000	-0.822377000	2.188330000
C	8.736786000	-0.311538000	1.238145000
C	-0.086644000	-6.600160000	2.545697000
H	0.226675000	-7.227950000	3.385399000
H	-1.162028000	-6.412644000	2.645432000
H	0.416590000	-5.631244000	2.642946000
C	1.840178000	-10.532232000	0.034401000
H	1.568426000	-11.127992000	-0.843629000
H	1.577763000	-11.106893000	0.929150000
H	2.933179000	-10.423834000	0.027272000
C	-0.095898000	-6.652065000	-2.549338000
H	0.208752000	-7.299520000	-3.377207000
H	0.412228000	-5.688378000	-2.670539000
H	-1.170796000	-6.460535000	-2.646543000
C	8.029134000	-0.342619000	-2.535588000
H	8.717699000	-0.557013000	-3.358578000
H	7.624551000	0.664795000	-2.686057000
H	7.184684000	-1.037429000	-2.612771000
C	12.217198000	-1.405537000	0.073836000
H	12.472461000	-1.932785000	0.999247000
H	12.876282000	-0.529412000	0.007087000
H	12.463475000	-2.060369000	-0.768893000
C	8.041705000	-0.022657000	2.550091000
H	8.706748000	-0.223995000	3.395419000
H	7.141738000	-0.635874000	2.673629000
H	7.723036000	1.024369000	2.614085000
S	-1.880342000	4.434883000	0.024269000
S	-3.895924000	0.503446000	0.142364000
N	2.918586000	4.146847000	0.008754000
N	-5.149446000	-2.285800000	0.000349000
C	2.140086000	5.275431000	0.007594000
C	4.210591000	4.552208000	-0.021082000
C	4.283687000	5.988583000	-0.037788000
H	5.190159000	6.579606000	-0.059047000
C	2.990470000	6.442026000	-0.018765000
H	2.650855000	7.468331000	-0.024296000
C	0.722365000	5.285099000	0.015060000
C	-0.123242000	4.163472000	0.029050000
C	0.136003000	2.742604000	0.049187000
C	-1.031144000	1.969121000	0.062324000
H	-1.001951000	0.884553000	0.068943000
C	-2.216406000	2.705771000	0.045298000
C	-5.303610000	-3.650469000	0.039632000
C	-6.696402000	-3.901717000	0.110865000
H	-7.146967000	-4.882769000	0.168635000
C	-7.350756000	-2.683927000	0.106108000
H	-8.416379000	-2.514872000	0.161114000
C	-6.378242000	-1.641252000	0.034352000
C	0.063097000	6.640365000	0.001749000
C	-0.239671000	7.264826000	-1.227318000
C	-0.844267000	8.525825000	-1.214197000
H	-1.073696000	9.006130000	-2.163520000
C	-1.157134000	9.184470000	-0.022055000
C	-0.839551000	8.550530000	1.182201000
H	-1.065253000	9.050296000	2.122328000
C	-0.235145000	7.289959000	1.218851000
C	-3.541202000	2.226481000	0.036746000
C	-5.644107000	0.767579000	0.020359000
C	-5.885819000	2.161684000	-0.062363000
H	-6.890573000	2.558640000	-0.139994000
C	-4.745575000	2.947105000	-0.052323000
H	-4.764807000	4.029839000	-0.121172000
C	-6.616688000	-0.249887000	0.017312000
C	-8.059085000	0.182664000	-0.007147000
C	-8.730727000	0.465724000	1.201342000
C	-10.069728000	0.868094000	1.155129000
H	-10.583892000	1.085971000	2.089367000
C	-10.762069000	0.998675000	-0.051918000

C	-10.075073000	0.719305000	-1.236406000
H	-10.592682000	0.822371000	-2.188283000
C	-8.736798000	0.311532000	-1.238114000
C	0.086739000	6.600138000	-2.545710000
H	-0.226549000	7.227918000	-3.385431000
H	1.162127000	6.412623000	-2.645403000
H	-0.416489000	5.631219000	-2.642969000
C	-1.840179000	10.532235000	-0.034530000
H	-1.568460000	11.128004000	0.843505000
H	-1.577730000	11.106887000	-0.929275000
H	-2.933179000	10.423838000	-0.027440000
C	0.095798000	6.652095000	2.549324000
H	-0.208883000	7.299560000	3.377173000
H	-0.412333000	5.688411000	2.670516000
H	1.170693000	6.460566000	2.646572000
C	-8.029108000	0.342638000	2.535613000
H	-8.717662000	0.557045000	3.358608000
H	-7.624533000	-0.664780000	2.686086000
H	-7.184649000	1.037439000	2.612782000
C	-12.217193000	1.405553000	-0.073777000
H	-12.472464000	1.932795000	-0.999189000
H	-12.876280000	0.529431000	-0.007015000
H	-12.463460000	2.060392000	0.768950000
C	-8.041730000	0.022641000	-2.550065000
H	-8.706783000	0.223969000	-3.395387000
H	-7.141767000	0.635862000	-2.673618000
H	-7.723057000	-1.024383000	-2.614053000
O	1.328602000	2.171845000	0.050877000
H	2.081809000	2.902581000	0.024406000
O	-1.328592000	-2.171833000	-0.050834000
H	-2.081799000	-2.902571000	-0.024339000
H	-4.249230000	-1.848388000	-0.132839000
H	4.249219000	1.848375000	0.132827000

13

Conformer-1

C	-5.387260000	1.924229000	-1.440609000
C	-4.270885000	1.878610000	-2.262885000
H	-3.748538000	2.776450000	-2.564760000
C	-3.876088000	0.587500000	-2.623294000
H	-2.990962000	0.383931000	-3.212977000
C	-4.656165000	-0.416517000	-2.059335000
C	-4.268278000	-1.805287000	-2.037903000
C	-3.153667000	-2.309754000	-2.699376000
H	-2.606010000	-1.746031000	-3.444721000
C	-2.758926000	-3.576618000	-2.256306000
H	-1.883718000	-4.099779000	-2.618034000
C	-3.580163000	-4.115915000	-1.278115000
C	-3.313961000	-5.320879000	-0.522003000
C	-2.003416000	-5.524499000	-0.111431000
C	-1.367986000	-6.740578000	0.384311000
H	-1.841825000	-7.708795000	0.485448000
C	-0.069439000	-6.413051000	0.637920000
H	0.704506000	-7.055884000	1.037987000
C	0.052572000	-4.975070000	0.360167000
C	1.158094000	-4.061371000	0.680509000
C	0.730083000	-2.788075000	1.208103000
C	1.450948000	-2.006198000	2.060862000
H	2.428401000	-2.368093000	2.363525000
C	1.031892000	-0.740217000	2.604137000
C	0.152564000	1.407710000	2.774720000
C	-0.353417000	2.691700000	2.372019000
H	0.134915000	3.548679000	2.826000000
C	-1.305455000	2.967074000	1.433903000
C	-1.545773000	4.286119000	0.895147000
C	-2.913092000	4.527729000	0.428524000
C	-3.740127000	5.736795000	0.513322000
H	-3.422999000	6.707645000	0.873692000
C	-4.997199000	5.364264000	0.134058000
H	-5.883784000	5.982995000	0.074864000
C	-4.904200000	3.961694000	-0.255246000
C	-5.875691000	3.110075000	-0.771296000
C	-0.471216000	5.173793000	0.672990000
C	-0.450462000	6.514464000	0.086412000
H	-1.307940000	7.137585000	-0.131467000
C	0.860379000	6.808482000	-0.152645000
H	1.262883000	7.707970000	-0.601607000
C	1.630550000	5.632098000	0.266023000
C	3.017888000	5.354209000	0.001177000
C	3.585226000	4.137644000	0.398872000
C	3.066045000	3.199939000	1.332367000
H	2.234825000	3.456128000	1.965296000
C	3.675920000	1.973961000	1.313170000

H	3.377774000	1.146878000	1.946869000
C	4.743811000	1.855639000	0.390938000
C	5.371184000	0.646825000	0.064149000
C	6.566374000	0.375231000	-0.642182000
H	7.223475000	1.159753000	-1.004184000
C	6.821904000	-0.971838000	-0.797246000
H	7.698895000	-1.367300000	-1.296736000
C	5.809604000	-1.838120000	-0.282815000
C	5.751109000	-2.231260000	-0.430941000
C	4.593310000	-3.989277000	-0.091467000
C	4.343159000	-5.390232000	-0.434811000
H	5.055798000	-6.072412000	-0.880034000
C	3.034411000	-5.622285000	-0.146574000
H	2.480839000	-6.535630000	-0.315847000
C	2.502026000	-4.375403000	0.406617000
C	-4.141722000	-6.257424000	-0.156514000
C	-5.108701000	-6.966378000	-1.168073000
C	-6.138508000	-7.834675000	-0.803832000
C	-6.520128000	-8.014504000	0.530166000
C	-5.834905000	-7.295148000	1.509936000
C	-4.783636000	-6.424632000	1.198567000
C	-4.737149000	-6.830474000	-2.628176000
H	-4.991692000	-5.840366000	-3.023180000
H	-5.264583000	-7.576340000	-2.230646000
H	-3.661222000	-6.967435000	-2.785174000
C	-7.630176000	-8.971978000	0.894403000
H	-7.287031000	-10.014119000	0.847664000
H	-8.478888000	-8.882367000	0.206760000
H	-7.996729000	-8.792586000	1.910139000
C	-4.103100000	-5.672113000	2.323434000
H	-3.139762000	-6.122971000	2.588766000
H	-4.730917000	-5.679665000	3.220019000
H	-3.900619000	-4.629963000	2.058242000
C	-7.332528000	3.368576000	-0.607724000
C	-7.904159000	3.409007000	0.686160000
C	-9.280001000	3.634792000	0.810280000
C	-10.103825000	3.837654000	-0.297455000
C	-9.518383000	3.794934000	-1.567472000
C	-8.155478000	3.555921000	-1.746720000
C	-7.089196000	3.181764000	1.942876000
H	-6.352386000	2.382738000	1.817258000
H	-7.745268000	2.912941000	2.776811000
H	-6.533241000	4.080323000	2.234541000
C	-11.580390000	4.111353000	-0.135767000
H	-11.805627000	5.175550000	-0.286447000
H	-11.930900000	3.840223000	0.865150000
H	-12.174504000	3.550989000	-0.866682000
C	-7.588295000	3.540442000	-3.149254000
H	-6.707748000	4.186726000	-3.236439000
H	-8.335554000	3.887945000	-3.869231000
H	-7.275121000	2.534800000	-3.451902000
C	3.809206000	6.310627000	-0.839591000
C	4.725298000	7.190176000	-0.221429000
C	5.451109000	8.084326000	-1.013944000
C	5.305248000	8.126747000	-2.403207000
C	4.394637000	7.247807000	-2.994875000
C	3.641398000	6.340930000	-2.241768000
C	4.920184000	7.189064000	1.278722000
H	3.970211000	7.322346000	1.809101000
H	5.595188000	7.994901000	1.583483000
H	5.348015000	6.242206000	1.628902000
C	6.128186000	9.076143000	-3.242746000
H	7.080197000	8.618177000	-3.543582000
H	6.369622000	9.992141000	-2.692642000
H	5.601517000	9.360209000	-4.160168000
C	2.670174000	5.414207000	-2.939118000
H	2.785448000	5.479636000	-4.025584000
H	1.630508000	5.662551000	-2.695098000
H	2.825472000	4.371080000	-2.643105000
C	6.916552000	-3.934732000	-1.067761000
C	6.969063000	-4.110624000	-2.467230000
C	8.063107000	-4.779288000	-3.027488000
C	9.106876000	-5.278044000	-2.243567000
C	9.031778000	-5.098315000	-0.859717000
C	7.957838000	-4.434894000	-0.257280000
C	5.863842000	-3.596605000	-3.362918000
H	5.730635000	-2.513621000	-3.259503000
H	4.900105000	-4.056940000	-3.116116000
H	6.082659000	-3.811782000	-4.413485000
C	10.293292000	-5.968920000	-2.875265000
H	11.091325000	-5.252814000	-3.114044000
H	10.016027000	-6.467768000	-3.810156000
H	10.723727000	-6.720617000	-2.204743000
C	7.923353000	-4.269094000	1.245812000
H	7.907125000	-3.211455000	1.534057000
H	8.799615000	-4.732648000	1.709730000

H	7.026931000	-4.726798000	1.680213000
N	-1.085806000	-4.478669000	-0.092597000
N	-3.611231000	3.504365000	-0.034476000
N	0.809730000	4.704719000	0.777998000
N	3.494504000	-3.428000000	0.445357000
S	-5.987847000	0.287528000	-1.157428000
S	-4.909493000	-3.008314000	-0.931844000
S	5.022523000	3.422183000	-0.395442000
S	4.539025000	-0.872223000	0.469645000
H	8.097335000	-4.915045000	-4.106985000
H	9.829643000	-5.485983000	-0.228756000
H	4.264631000	7.265179000	-4.075426000
H	6.148374000	8.766566000	-0.530999000
H	-10.141955000	3.952544000	-2.445515000
H	-9.718545000	3.646204000	1.806092000
H	-6.658548000	-8.386748000	-1.584518000
H	-6.127489000	-7.407451000	2.552015000
C	0.164574000	0.209927000	2.027181000
C	1.555921000	-0.159890000	3.807568000
C	2.424605000	-0.791447000	4.691886000
C	2.972070000	-0.313364000	5.888351000
C	0.988376000	1.197820000	3.922324000
C	2.773524000	0.922462000	6.507985000
C	1.198632000	2.118125000	4.944085000
C	1.990643000	2.002100000	6.092381000
H	2.720046000	-1.801948000	4.419233000
H	3.638168000	-1.000165000	6.405240000
H	3.306878000	1.065924000	7.445984000
H	0.666243000	3.061620000	4.843994000
H	1.994714000	2.869662000	6.748094000
H	-0.300645000	-2.526140000	0.983602000
H	-1.970930000	2.185794000	1.075209000
H	-0.329048000	0.082816000	1.070680000

Conformer-2

C	3.580432000	-4.115738000	-1.278310000
C	2.759161000	-3.576542000	-2.256517000
H	1.883999000	-4.099790000	-2.618228000
C	3.153741000	-2.309615000	-2.699554000
H	2.606042000	-1.745973000	-3.444932000
C	4.268272000	-1.805004000	-2.038055000
C	4.656115000	-0.416228000	-2.059573000
C	3.876082000	0.587778000	-2.623618000
H	2.990993000	0.384216000	-3.213358000
C	4.270864000	1.878906000	-2.263222000
H	3.748527000	2.776740000	-2.565147000
C	5.387145000	1.924534000	-1.440833000
C	5.875541000	3.110373000	-0.771498000
C	4.903992000	3.962006000	-0.255570000
C	4.996888000	5.364568000	0.133772000
H	5.883417000	5.983382000	0.074575000
C	3.739759000	5.737034000	0.512910000
H	3.422572000	6.707876000	0.873245000
C	2.912805000	4.527907000	0.428092000
C	1.545484000	4.286241000	0.894634000
C	1.305230000	2.967141000	1.433401000
C	0.353311000	2.691722000	2.371632000
H	-0.135074000	3.548686000	2.825587000
C	-0.152544000	1.407713000	2.774448000
C	-1.031698000	-0.740275000	2.603955000
C	-1.450681000	-2.006295000	2.060632000
H	-2.428014000	-2.368377000	2.363473000
C	-0.729849000	-2.788014000	1.207730000
C	-1.157851000	-4.061457000	0.680289000
C	-0.052234000	-4.975052000	0.360021000
C	0.069914000	-6.412986000	0.638059000
H	-0.703962000	-7.055790000	1.038295000
C	1.368487000	-6.740429000	0.384478000
H	1.842416000	-7.708598000	0.485700000
C	2.003780000	-5.524401000	-0.111555000
C	3.314309000	-5.320660000	-0.522059000
C	-2.501722000	-4.375631000	0.406524000
C	-3.034094000	-5.622546000	-0.146578000
H	-2.480449000	-6.535843000	-0.315899000
C	-4.342863000	-5.390583000	-0.434776000
H	-5.055503000	-6.072844000	-0.879880000
C	-4.593091000	-3.989611000	-0.091481000
C	-5.750997000	-3.231684000	-0.430957000
C	-5.809564000	-1.838566000	-0.282885000
C	-6.821999000	-0.972332000	-0.797200000
H	-7.699052000	-1.367862000	-1.296533000
C	-6.566544000	0.374737000	-0.642184000
H	-7.223714000	1.159214000	-1.004159000
C	-5.371254000	0.646420000	0.064012000
C	-4.743950000	1.855252000	0.390740000

C	-3.675914000	1.973565000	1.312842000
H	-3.377566000	1.146411000	1.946356000
C	-3.066166000	3.199573000	1.332136000
H	-2.234910000	3.455752000	1.965017000
C	-3.585576000	4.137409000	0.398851000
C	-3.018402000	5.354049000	0.001283000
C	-1.630996000	5.632001000	0.265965000
C	-0.861012000	6.808643000	-0.152355000
H	-1.263696000	7.708259000	-0.600905000
C	0.449892000	6.514706000	0.086478000
H	1.307272000	7.138043000	-0.131180000
C	0.470879000	5.173857000	0.672609000
C	7.332349000	3.368866000	-0.607787000
C	8.155458000	3.556252000	-1.746733000
C	9.518282000	3.795343000	-1.567343000
C	10.103604000	3.838059000	-0.297218000
C	9.279663000	3.635296000	0.810383000
C	7.903801000	3.409396000	0.686117000
C	7.588395000	3.540903000	-3.149323000
H	7.275265000	2.535299000	-3.452128000
H	8.335714000	3.888508000	-3.869190000
H	6.707840000	4.187183000	-3.236514000
C	11.580315000	4.111027000	-0.135626000
H	11.808042000	5.172690000	-0.299628000
H	12.174998000	3.540096000	-0.857927000
H	11.928017000	3.851955000	0.869433000
C	7.088750000	3.182169000	1.942778000
H	6.532957000	4.080792000	2.234598000
H	7.744747000	2.913067000	2.776683000
H	6.351788000	2.383323000	1.816985000
C	4.415165000	-6.257060000	-0.156461000
C	4.784205000	-6.423873000	1.198650000
C	5.835576000	-7.294183000	1.510176000
C	6.520781000	-8.013769000	0.530540000
C	6.139064000	-7.834305000	-0.803465000
C	5.109126000	-6.966203000	-1.167872000
C	4.103699000	-5.671070000	2.323344000
H	3.901288000	-4.628966000	2.057921000
H	4.731497000	-5.678473000	3.219943000
H	3.140311000	-6.121792000	2.588761000
C	7.630715000	-8.971266000	0.895067000
H	7.285680000	-10.013066000	0.854740000
H	8.001440000	-8.787652000	1.908545000
H	8.476879000	-8.886340000	0.203739000
C	4.737449000	-6.830776000	-2.627984000
H	3.661590000	-6.968411000	-2.784903000
H	5.265282000	-7.576462000	-3.230332000
H	4.991371000	-5.840601000	-3.023204000
C	-6.916393000	-3.935272000	-1.067718000
C	-7.957259000	-4.436069000	-0.257166000
C	-9.031193000	-5.099609000	-0.859589000
C	-9.106623000	-5.278819000	-2.243440000
C	-8.063183000	-4.779439000	-3.027488000
C	-6.969237000	-4.110668000	-2.467284000
C	-7.922424000	-4.270916000	1.245989000
H	-7.026160000	-4.729270000	1.680038000
H	-8.798834000	-4.734231000	1.709866000
H	-7.905598000	-3.213410000	1.534687000
C	-10.292961000	-5.969706000	-2.875271000
H	-11.087522000	-5.252396000	-3.121917000
H	-10.728558000	-6.715541000	-2.201591000
H	-10.013829000	-6.475543000	-3.805871000
C	-5.864397000	-3.595931000	-3.363033000
H	-6.082944000	-3.811595000	-4.413559000
H	-4.900268000	-4.055316000	-3.116013000
H	-5.732182000	-2.512789000	-3.259925000
C	-3.809874000	6.310579000	-0.839208000
C	-3.642003000	6.341358000	-2.241346000
C	-4.395336000	7.248393000	-2.994207000
C	-5.306092000	8.126997000	-2.402315000
C	-5.452036000	8.084092000	-1.013055000
C	-4.726160000	7.189793000	-0.220804000
C	-2.670629000	5.415005000	-2.938980000
H	-2.825484000	4.371817000	-2.642974000
H	-1.630978000	5.663699000	-2.695219000
H	-2.786196000	5.480453000	-4.025416000
C	-6.129224000	9.076524000	-3.241518000
H	-7.083090000	8.620076000	-3.538785000
H	-5.604431000	9.357585000	-4.160923000
H	-6.367163000	9.994154000	-2.692587000
C	-4.921116000	7.188172000	1.279340000
H	-5.348898000	6.241166000	1.629193000
H	-5.596200000	7.993859000	1.584330000
H	-3.971180000	7.321355000	1.809807000
N	3.611039000	3.504576000	-0.034848000
N	1.086052000	-4.478642000	-0.092888000

N	-3.494357000	-3.428239000	0.445288000
N	-0.810021000	4.704557000	0.777495000
S	4.909615000	-3.007981000	-0.932018000
S	5.987744000	0.287862000	-1.157619000
S	-4.538969000	-0.872570000	0.469450000
S	-5.022950000	3.421910000	-0.395359000
H	-4.265283000	7.266127000	-4.074744000
H	-6.149424000	8.766080000	-0.529924000
H	-8.097634000	-4.914840000	-4.107028000
H	-9.828768000	-5.487760000	-0.228568000
H	6.659145000	-8.386497000	-1.584035000
H	6.128271000	-7.406144000	2.552263000
H	10.141914000	3.953076000	-2.445328000
H	9.718068000	3.646894000	1.806247000
C	-0.164542000	0.209963000	2.026897000
C	-0.988119000	1.197698000	3.922202000
C	-1.198384000	2.118000000	4.943935000
C	-1.990281000	2.001912000	6.092327000
C	-1.555512000	-0.160097000	3.807498000
C	-2.772803000	0.922111000	6.508134000
C	-2.423919000	-0.791792000	4.692014000
C	-2.971177000	-0.313809000	5.888592000
H	-0.666150000	3.061574000	4.843731000
H	-1.994508000	2.869551000	6.747936000
H	-3.306039000	1.065495000	7.446212000
H	-2.719267000	-1.802334000	4.419401000
H	-3.637000000	-1.000740000	6.405664000
H	1.970809000	2.185913000	1.074791000
H	0.300795000	-2.525961000	0.983014000
H	0.328940000	0.082965000	1.070310000

Conformer-3

C	-6.338690000	1.080175000	-0.034456000
C	-7.372237000	0.119783000	-0.074944000
H	-8.417181000	0.408701000	-0.069127000
C	-6.932584000	-1.200783000	-0.175806000
H	-7.598888000	-2.053033000	-0.262452000
C	-5.538194000	-1.308527000	-0.244269000
C	-4.668383000	-2.409700000	-0.464922000
C	-3.364096000	-2.276967000	-0.960384000
H	-2.976504000	-1.328223000	-1.312563000
C	-2.649709000	-3.460007000	-1.003425000
H	-1.644458000	-3.544557000	-1.386654000
C	-3.356999000	-4.580662000	-0.537869000
C	-2.820742000	-5.886031000	-0.366951000
C	-1.428381000	-5.982786000	-0.151049000
C	-0.533970000	-7.098436000	-0.436388000
H	-0.829003000	-8.077107000	-0.793684000
C	0.733429000	-6.618110000	-0.271013000
H	1.651153000	-7.157036000	-0.456805000
C	0.594896000	-5.238157000	0.201490000
C	1.562625000	-4.232370000	0.554449000
C	1.038700000	-3.007066000	1.097522000
C	1.750512000	-2.146311000	1.882780000
H	2.757986000	-2.432799000	2.164732000
C	1.306485000	-0.857727000	2.321709000
C	0.331178000	1.248406000	2.279118000
C	-0.323421000	2.423025000	1.786293000
H	0.148187000	3.360832000	2.059062000
C	-1.413902000	2.503838000	0.966805000
C	-1.852827000	3.756619000	0.403596000
C	-3.244903000	3.911576000	0.093582000
C	-3.967276000	5.080826000	-0.416279000
H	-3.542144000	6.024234000	-0.721729000
C	-5.282926000	4.735030000	-0.461062000
H	-6.117160000	5.340710000	-0.790718000
C	-5.346510000	3.337038000	-0.054433000
C	-6.467972000	2.491441000	-0.089757000
C	-0.868146000	4.770050000	0.139617000
C	-1.050963000	6.219368000	0.065397000
H	-1.962353000	6.762742000	0.266323000
C	0.175145000	6.750708000	-0.185618000
H	0.436454000	7.795733000	-0.286564000
C	1.092636000	5.619403000	-0.287865000
C	2.462793000	5.703914000	-0.591763000
C	3.367849000	4.619620000	-0.692882000
C	4.738670000	4.774674000	-0.998658000
H	5.170776000	5.750515000	-1.181719000
C	5.460197000	3.599557000	-1.038443000
H	6.520610000	3.570375000	-1.255703000
C	4.701284000	2.442386000	-0.767302000
C	5.254845000	1.132055000	-0.757514000
C	6.609487000	0.860312000	-1.044751000
H	7.324007000	1.632530000	-1.301104000
C	6.946317000	-0.476104000	-0.978834000

H	7.941957000	-0.855277000	-1.173870000
C	5.881666000	-1.339846000	-0.636949000
C	6.010684000	-2.744509000	-0.527640000
C	4.972462000	-3.631570000	-0.190082000
C	5.052810000	-5.088101000	-0.147276000
H	5.941077000	-5.683848000	-0.311706000
C	3.792121000	-5.526376000	0.122951000
H	3.479419000	-6.550056000	0.271364000
C	2.965047000	-4.333065000	0.280229000
C	-3.686849000	-7.098925000	-0.398639000
C	-4.344506000	-7.476712000	-1.594045000
C	-5.147052000	-8.620402000	-1.594365000
C	-5.330176000	-9.398591000	-0.447837000
C	-4.678992000	-9.004346000	0.723411000
C	-3.853284000	-7.876955000	0.771566000
C	-4.175970000	-6.692980000	-2.877379000
H	-4.699330000	-5.730423000	-2.839087000
H	-4.577627000	-7.254963000	-3.726224000
H	-3.122354000	-6.474636000	-3.082526000
C	-6.185662000	-10.643179000	-0.482116000
H	-5.598343000	-11.520541000	-0.785249000
H	-7.010367000	-10.543897000	-1.196125000
H	-6.612746000	-10.863175000	0.502011000
C	-3.185656000	-7.508022000	2.079324000
H	-2.115019000	-7.742980000	2.067013000
H	-3.638459000	-8.059776000	2.909130000
H	-3.270311000	-6.437902000	2.294035000
C	-7.837790000	3.081029000	-0.255331000
C	-8.532892000	3.559822000	0.875851000
C	-9.810101000	4.104080000	0.706953000
C	-10.414375000	4.197611000	-0.549676000
C	-9.706923000	3.718952000	-1.655648000
C	-8.430140000	3.160290000	-1.534175000
C	-7.923267000	3.485701000	2.258246000
H	-7.626916000	2.462303000	2.515446000
H	-8.632537000	3.833945000	3.015421000
H	-7.019764000	4.101938000	2.332214000
C	-11.780673000	4.822697000	-0.711103000
H	-11.705968000	5.906710000	-0.871876000
H	-12.399523000	4.669942000	0.179672000
H	-12.314533000	4.404016000	-1.570965000
C	-7.707631000	2.664800000	-2.767447000
H	-6.723981000	3.136152000	-2.873496000
H	-8.286633000	2.881677000	-3.670362000
H	-7.536637000	1.582642000	-2.728951000
C	3.027892000	7.080053000	-0.835810000
C	3.548476000	7.830555000	0.239104000
C	4.053604000	9.111612000	-0.008429000
C	4.060315000	9.669382000	-1.289643000
C	3.534429000	8.909754000	-2.338317000
C	3.018281000	7.625145000	-2.137229000
C	3.558248000	7.278161000	1.647252000
H	2.543003000	7.059790000	1.998567000
H	4.010629000	7.992155000	2.342452000
H	4.122880000	6.340559000	1.709065000
C	4.640484000	11.042417000	-1.538432000
H	5.705671000	10.983840000	-1.800239000
H	4.559682000	11.678866000	-0.650748000
H	4.131953000	11.548777000	-2.365971000
C	2.453722000	6.849734000	-3.306609000
H	2.551687000	7.419791000	-4.235566000
H	1.392031000	6.619857000	-3.160263000
H	2.967709000	5.891073000	-3.441475000
C	7.367469000	-3.334430000	-0.808937000
C	7.712680000	-3.717957000	-2.122300000
C	8.972608000	-4.279399000	-2.355440000
C	9.900533000	-4.469857000	-1.327799000
C	9.534510000	-4.087740000	-0.034502000
C	8.285488000	-3.522960000	0.245321000
C	6.743560000	-3.541404000	-3.269970000
H	6.455621000	-2.491515000	-3.397634000
H	5.817700000	-4.103924000	-3.103335000
H	7.185472000	-3.887285000	-4.209423000
C	11.267161000	-5.049146000	-1.611386000
H	11.985678000	-4.262814000	-1.879709000
H	11.237106000	-5.757657000	-2.446206000
H	11.670459000	-5.571885000	-0.737516000
C	7.937535000	-3.133290000	1.664888000
H	7.687448000	-2.068652000	1.741046000
H	8.775189000	-3.333361000	2.340160000
H	7.066748000	-3.689581000	2.030996000
N	-0.706013000	-4.907431000	0.273064000
N	-4.105289000	2.887177000	0.284006000
N	0.434090000	4.449264000	-0.068963000
N	3.710708000	-3.215532000	0.091817000
S	-4.778239000	0.269807000	-0.058552000

S	-5.008307000	-4.099834000	-0.102773000
S	3.015452000	2.893111000	-0.461430000
S	4.405375000	-0.378088000	-0.396743000
H	9.232973000	-4.578199000	-3.369184000
H	10.238165000	-4.234668000	0.782846000
H	3.521353000	9.327682000	-3.343265000
H	4.449915000	9.688750000	0.825035000
H	-10.159279000	3.781030000	-2.643706000
H	-10.345960000	4.464493000	1.583136000
H	-5.641629000	-8.912201000	-2.518941000
H	-4.819171000	-9.588466000	1.630946000
C	0.330556000	-0.040849000	1.715569000
C	1.923851000	-0.085269000	3.361169000
C	2.913339000	-0.545486000	4.223917000
C	3.560887000	0.127665000	5.265512000
C	1.303816000	1.250088000	3.337121000
C	3.370369000	1.437958000	5.711046000
C	1.577328000	2.324694000	4.176066000
C	2.495487000	2.413616000	5.229072000
H	3.226995000	-1.575929000	4.073276000
H	4.310803000	-0.449604000	5.801354000
H	3.993809000	1.741952000	6.549937000
H	0.992791000	3.223934000	3.996084000
H	2.528459000	3.372578000	5.740989000
H	-0.017622000	-2.826913000	0.929729000
H	-2.033283000	1.631003000	0.783998000
H	-0.259051000	-0.330275000	0.853892000

Conformer-4

C	3.356930000	-4.580631000	-0.537763000
C	2.649592000	-3.459943000	-1.003182000
H	1.644306000	-3.544469000	-1.386320000
C	3.363980000	-2.276908000	-0.960147000
H	2.976346000	-1.328148000	-1.312232000
C	4.668320000	-2.409672000	-0.464837000
C	5.538159000	-1.308513000	-0.244243000
C	6.932551000	-1.200790000	-0.175828000
H	7.598848000	-2.053043000	-0.262507000
C	7.372223000	0.119772000	-0.074960000
H	8.417174000	0.408667000	-0.069188000
C	6.338692000	1.080177000	-0.034422000
C	6.467978000	2.491448000	-0.089699000
C	5.346524000	3.337049000	-0.054343000
C	5.282939000	4.735044000	-0.460958000
H	6.117178000	5.340727000	-0.790596000
C	3.967288000	5.080835000	-0.416200000
H	3.542146000	6.024236000	-0.721656000
C	3.244919000	3.911580000	0.093672000
C	1.852828000	3.756629000	0.403671000
C	1.413884000	2.503863000	0.966878000
C	0.323306000	2.423026000	1.786239000
H	-0.148368000	3.360821000	2.058919000
C	-0.331300000	1.248399000	2.279043000
C	-1.306556000	-0.857756000	2.321633000
C	-1.750584000	-2.146345000	1.882715000
H	-2.758075000	-2.432798000	2.164648000
C	-1.038765000	-3.007160000	1.097544000
C	-1.562694000	-4.232475000	0.554502000
C	-0.594963000	-5.238253000	0.201539000
C	-0.733462000	-6.618140000	-0.271181000
H	-1.651176000	-7.157028000	-0.457124000
C	0.533943000	-7.098455000	-0.436456000
H	0.829003000	-8.077086000	-0.793885000
C	1.428336000	-5.982828000	-0.151011000
C	2.820690000	-5.886026000	-0.366931000
C	-2.965119000	-4.333142000	0.280267000
C	-3.792242000	-5.526426000	0.123038000
H	-3.479573000	-6.550109000	0.271497000
C	-5.052909000	-5.088108000	-0.147218000
H	-5.941192000	-5.683821000	-0.311679000
C	-4.972516000	-3.631584000	-0.190015000
C	-6.010715000	-2.744499000	-0.527584000
C	-5.881675000	-1.339841000	-0.636949000
C	-6.946348000	-0.476078000	-0.978668000
H	-7.942019000	-0.855237000	-1.173870000
C	-6.609511000	0.860332000	-1.044596000
H	-7.324052000	1.632569000	-1.300839000
C	-5.254839000	1.132057000	-0.757470000
C	-4.701272000	2.442383000	-0.767280000
C	-5.460188000	3.599558000	-1.038407000
H	-6.520608000	3.570374000	-1.255635000
C	-4.738659000	4.774671000	-0.998646000
H	-5.170762000	5.750515000	-1.181696000
C	-3.367828000	4.619616000	-0.692904000
C	-2.462774000	5.703909000	-0.591802000

C	-1.092619000	5.619402000	-0.287885000
C	-0.175129000	6.750706000	-0.185674000
H	-0.436435000	7.795726000	-0.286670000
C	1.050969000	6.219375000	0.065412000
H	1.962364000	6.762742000	0.266348000
C	0.868163000	4.770062000	0.139630000
C	7.837815000	3.081004000	-0.255248000
C	8.430086000	3.160480000	-1.534090000
C	9.706930000	3.719063000	-1.655521000
C	10.414485000	4.197409000	-0.549506000
C	9.810276000	4.103654000	0.707161000
C	8.533049000	3.559478000	0.876015000
C	7.707497000	2.665256000	-2.767421000
H	7.536382000	1.583109000	-2.729062000
H	8.286517000	2.882176000	-3.670315000
H	6.723902000	3.136730000	-2.873401000
C	11.780831000	4.822427000	-0.710795000
H	11.706412000	5.907092000	-0.867237000
H	12.313055000	4.406760000	-1.573116000
H	12.401079000	4.665968000	0.178378000
C	7.923533000	3.484939000	2.258433000
H	7.019051000	4.099740000	2.332191000
H	8.632267000	3.834530000	3.015486000
H	7.628816000	2.461143000	2.515992000
C	3.686855000	-7.098886000	-0.398780000
C	3.853501000	-7.876942000	0.771361000
C	4.679345000	-9.004240000	0.723069000
C	5.330440000	-9.398355000	-0.448260000
C	5.147075000	-8.620154000	-1.594754000
C	4.344408000	-7.476563000	-1.594294000
C	3.185975000	-7.508099000	2.079194000
H	3.271319000	-6.438106000	2.294319000
H	3.638339000	-8.060453000	2.908837000
H	2.115191000	-7.742334000	2.066684000
C	6.186127000	-10.642802000	-0.482734000
H	5.599628000	-11.519670000	-0.788860000
H	6.610922000	-10.864493000	0.501994000
H	7.012507000	-10.542170000	-1.194630000
C	4.175618000	-6.692793000	-2.877572000
H	3.121950000	-6.474558000	-3.082571000
H	4.577229000	-7.254695000	-3.726493000
H	4.698877000	-5.730182000	-2.839301000
C	-7.367517000	-3.334397000	-0.808846000
C	-8.285272000	-3.523496000	0.245546000
C	-9.534314000	-4.088236000	-0.034243000
C	-9.900613000	-4.469785000	-1.327634000
C	-8.972952000	-4.278771000	-2.355404000
C	-7.713012000	-3.717329000	-2.122304000
C	-7.936967000	-3.134565000	1.665229000
H	-7.067078000	-3.692251000	2.031380000
H	-8.775016000	-3.333519000	2.340341000
H	-7.685274000	-2.070332000	1.741614000
C	-11.267253000	-5.049090000	-1.611138000
H	-11.986148000	-4.262629000	-1.878052000
H	-11.669894000	-5.573025000	-0.737676000
H	-11.237486000	-5.756565000	-2.446843000
C	-6.744234000	-3.540041000	-3.270149000
H	-7.185695000	-3.887162000	-4.209356000
H	-5.817497000	-4.101010000	-3.103235000
H	-6.457939000	-2.489775000	-3.398504000
C	-3.027856000	7.080050000	-0.835879000
C	-3.018372000	7.625053000	-2.137328000
C	-3.534466000	8.909690000	-2.338435000
C	-4.060169000	9.669415000	-1.289751000
C	-4.053327000	9.111730000	-0.008491000
C	-3.548253000	7.830663000	0.239058000
C	-2.453960000	6.849558000	-3.306722000
H	-2.967825000	5.890802000	-3.441350000
H	-1.392200000	6.619864000	-3.160567000
H	-2.552201000	7.419475000	-4.235737000
C	-4.640341000	11.042450000	-1.538527000
H	-5.706013000	10.984008000	-1.798392000
H	-4.133113000	11.548039000	-2.367329000
C	-4.557794000	11.679528000	-0.651451000
C	-3.557796000	7.278390000	1.647255000
H	-4.121471000	6.340217000	1.709027000
H	-4.011054000	7.991994000	2.342285000
H	-2.542402000	7.061102000	1.998827000
N	4.105299000	2.887194000	0.284105000
N	0.705948000	-4.907532000	0.273207000
N	-3.710749000	-3.215585000	0.091899000
N	-0.434085000	4.449265000	-0.068934000
S	5.008295000	-4.099827000	-0.102847000
S	4.778226000	0.269827000	-0.058517000
S	-4.405353000	-0.378101000	-0.396796000
S	-3.015430000	2.893105000	-0.461444000

H	-3.521484000	9.327555000	-3.343409000
H	-4.449496000	9.688948000	0.824985000
H	-9.233532000	-4.577126000	-3.369222000
H	-10.237774000	-4.235577000	0.783200000
H	5.641567000	-8.911872000	-2.519404000
H	4.819690000	-9.588387000	1.630557000
H	10.159228000	3.781320000	-2.643591000
H	10.346208000	4.463852000	1.583390000
C	-0.330616000	-0.040885000	1.715526000
C	-1.303958000	1.250076000	3.337019000
C	-1.577517000	2.324680000	4.175950000
C	-2.495663000	2.413569000	5.228970000
C	-1.923962000	-0.085293000	3.361072000
C	-3.370520000	1.437893000	5.710946000
C	-2.913440000	-0.545540000	4.223821000
C	-3.561021000	0.127600000	5.265399000
H	-0.993024000	3.223947000	3.995963000
H	-2.528647000	3.372527000	5.740895000
H	-3.993958000	1.741870000	6.549844000
H	-3.227062000	-1.575993000	4.073183000
H	-4.310935000	-0.449679000	5.801234000
H	2.033337000	1.631055000	0.784179000
H	0.017563000	-2.827040000	0.929742000
H	0.259043000	-0.330327000	0.853891000

Conformer-5

C	-4.926408000	3.147346000	-1.134272000
C	-3.901407000	2.749511000	-2.049615000
H	-3.145322000	3.448840000	-2.376836000
C	-3.977712000	1.460334000	-2.474124000
H	-3.267268000	1.025700000	-3.165236000
C	-5.024676000	0.694409000	-1.870662000
C	-5.024599000	-0.694898000	-1.870693000
C	-3.977554000	-1.460662000	-2.474230000
H	-3.267166000	-1.025886000	-3.165308000
C	-3.901080000	-2.749851000	-2.049797000
H	-3.144913000	-3.449073000	-2.377061000
C	-4.925994000	-3.147862000	-1.134435000
C	-4.975489000	-4.378222000	-0.487286000
C	-3.679337000	-5.009534000	-0.288109000
C	-3.277323000	-6.411004000	-0.395479000
H	-3.933004000	-7.250408000	-0.593057000
C	-1.912851000	-6.424803000	-0.283528000
H	-1.259365000	-7.285141000	-0.358273000
C	-1.513461000	-5.048262000	-0.016817000
C	-0.266842000	-4.455076000	0.239601000
C	-0.257471000	-3.073056000	0.672496000
C	0.764973000	-2.523894000	1.388034000
H	1.591556000	-3.176599000	1.646688000
C	0.913455000	-1.161788000	1.819132000
C	0.913286000	1.161863000	1.819218000
C	0.764584000	2.523974000	1.388193000
H	1.591101000	3.176779000	1.646821000
C	-0.257933000	3.073014000	0.672670000
C	-0.267456000	4.455050000	0.239809000
C	-1.514138000	5.048128000	-0.016549000
C	-1.913685000	6.424632000	-0.283223000
H	-1.260288000	7.285042000	-0.357923000
C	-3.278147000	6.410669000	-0.395270000
H	-3.933925000	7.249991000	-0.592880000
C	-3.680008000	5.009153000	-0.287865000
C	-4.976076000	4.377693000	-0.487101000
C	1.038503000	5.086159000	0.012006000
C	1.547812000	6.430419000	0.310641000
H	0.977359000	7.256482000	0.717545000
C	2.889385000	6.396387000	0.055571000
H	3.606075000	7.199570000	0.173694000
C	3.174068000	5.056658000	-0.451611000
C	4.376930000	4.451206000	-0.801860000
C	4.300342000	3.181967000	-1.499668000
C	3.369321000	2.843856000	-2.470133000
H	2.683078000	3.572731000	-2.879650000
C	3.382799000	1.493747000	-2.834829000
H	2.692870000	1.073486000	-3.555916000
C	4.300312000	0.723133000	-2.127143000
C	4.300491000	-0.722765000	-2.127168000
C	3.383325000	-1.493583000	-2.835076000
H	2.693510000	-1.073474000	-3.556360000
C	3.370022000	-2.843690000	-2.470347000
H	2.684011000	-3.572705000	-2.880005000
C	4.300879000	-3.181592000	-1.499665000
C	4.377598000	-4.450800000	-0.801797000
C	3.174773000	-5.056381000	-0.451648000
C	2.890155000	-6.396174000	0.055407000
H	3.606893000	-7.199317000	0.173510000

C	1.548575000	-6.430318000	0.310411000
H	0.978162000	-7.256455000	0.717222000
C	1.039176000	-5.086078000	0.011839000
C	-6.220868000	-4.976242000	0.062309000
C	-7.298822000	-5.305906000	-0.796168000
C	-8.452165000	-5.880164000	-0.252533000
C	-8.581661000	-6.135417000	1.114126000
C	-7.511255000	-5.797976000	1.947282000
C	-6.333710000	-5.232900000	1.452299000
C	-7.234680000	-5.080096000	-2.291262000
H	-7.372017000	-4.023194000	-2.550137000
H	-8.021430000	-5.648031000	-2.798079000
H	-6.269516000	-5.386176000	-2.707551000
C	-9.828823000	-6.778453000	1.673782000
H	-9.703710000	-7.864651000	1.780406000
H	-10.692843000	-6.612812000	1.021696000
H	-10.072279000	-6.383620000	2.666434000
C	-5.226276000	-4.880210000	2.421835000
H	-4.407028000	-5.608257000	2.382828000
H	-5.607798000	-4.864693000	3.447912000
H	-4.786469000	-3.902891000	2.201939000
C	-6.221554000	4.975588000	0.062422000
C	-6.334575000	5.232088000	1.452403000
C	-7.512201000	5.797113000	1.947298000
C	-8.582481000	6.134639000	1.114048000
C	-8.452811000	5.879526000	-0.252639000
C	-7.299410000	5.305339000	-0.796175000
C	-5.227260000	4.879308000	2.422041000
H	-4.787191000	3.902165000	2.201907000
H	-5.608980000	4.863365000	3.448038000
H	-4.408166000	5.607554000	2.383441000
C	-9.829725000	6.777660000	1.673542000
H	-9.705601000	7.864220000	1.777614000
H	-10.071798000	6.384766000	2.667290000
H	-10.694234000	6.609746000	1.022674000
C	-7.235008000	5.079690000	-2.291281000
H	-6.270036000	5.386534000	-2.707476000
H	-8.022135000	5.647094000	-2.798107000
H	-7.371533000	4.022716000	-2.550266000
C	5.697059000	5.032537000	-0.422035000
C	6.074907000	5.117621000	0.937803000
C	7.325174000	5.657664000	1.259349000
C	8.206733000	6.124654000	0.283013000
C	7.809866000	6.037394000	-1.055243000
C	6.580555000	5.491670000	-1.428867000
C	5.184124000	4.619117000	2.057111000
H	4.352490000	5.306457000	2.250985000
H	5.758500000	4.520786000	2.983731000
H	4.745092000	3.642831000	1.825917000
C	9.559894000	6.683307000	0.654907000
H	10.347212000	5.926903000	0.536277000
H	9.583016000	7.018429000	1.696903000
H	9.831427000	7.532911000	0.018601000
C	6.205869000	5.441016000	-2.893524000
H	6.945448000	5.973295000	-3.499262000
H	5.226648000	5.898433000	-3.075779000
H	6.148411000	4.410894000	-3.263056000
C	5.697773000	-5.031973000	-0.421926000
C	6.581436000	-5.490824000	-1.428735000
C	7.810806000	-6.036404000	-1.055072000
C	8.207573000	-6.123776000	0.283196000
C	7.325854000	-5.657042000	1.259523000
C	6.075534000	-5.117160000	0.937944000
C	6.206925000	-5.440013000	-2.893432000
H	6.150062000	-4.409862000	-3.262990000
H	5.227492000	-5.896914000	-3.075799000
H	6.946304000	-5.972680000	-3.499075000
C	9.560787000	-6.682248000	0.655166000
H	10.347836000	-5.925374000	0.537766000
H	9.833001000	-7.531048000	0.018085000
H	9.583532000	-7.018480000	1.696817000
C	5.184629000	-4.618870000	2.057253000
H	4.745564000	-3.642575000	1.826153000
H	5.758934000	-4.520631000	2.983926000
H	4.353018000	-5.306277000	2.250976000
N	-2.622932000	-4.236986000	-0.024829000
N	-2.623516000	4.236726000	-0.024588000
N	2.002241000	4.312822000	-0.462876000
N	2.002878000	-4.312643000	-0.462966000
S	-6.053029000	1.777721000	-0.905042000
S	-6.052790000	-1.778374000	-0.905109000
S	5.250299000	1.753050000	-1.066914000
S	5.250441000	-1.752474000	-1.066699000
H	8.477398000	-6.405353000	-1.832217000
H	7.617707000	-5.710454000	2.306500000
H	8.476334000	6.406546000	-1.832398000

H	7.617100000	5.710999000	2.306310000
H	-9.272709000	6.137457000	-0.920455000
H	-7.598193000	5.971304000	3.018434000
H	-9.272138000	-6.138042000	-0.920275000
H	-7.597110000	-5.972274000	3.018412000
C	0.336887000	0.000006000	1.265898000
C	1.856376000	-0.738072000	2.812527000
C	2.603231000	-1.581621000	3.627530000
C	3.533216000	-1.260670000	4.623919000
C	1.856251000	0.738231000	2.812583000
C	3.940988000	0.000157000	5.064261000
C	2.602923000	1.581839000	3.627706000
C	3.532940000	1.260960000	4.624075000
H	2.438788000	-2.646599000	3.480183000
H	3.993881000	-2.108994000	5.124807000
H	4.680400000	0.000192000	5.863267000
H	2.438270000	2.646800000	3.480477000
H	3.993418000	2.109312000	5.125086000
H	-1.171878000	-2.515402000	0.499291000
H	-1.172262000	2.515244000	0.499433000
H	-0.379894000	-0.000017000	0.452748000

Conformer-6

C	-6.584347000	0.487626000	0.071191000
C	-7.465172000	-0.625260000	-0.011597000
H	-8.541474000	-0.494143000	-0.009073000
C	-6.837731000	-1.854920000	-0.141427000
H	-7.370469000	-2.793344000	-0.258716000
C	-5.431999000	-1.759848000	-0.191020000
C	-4.420871000	-2.712977000	-0.411392000
C	-3.104937000	-2.375760000	-0.796077000
H	-2.828591000	-1.359327000	-1.051347000
C	-2.240456000	-3.439589000	-0.873408000
H	-1.210710000	-3.362167000	-1.184999000
C	-2.814943000	-4.690277000	-0.540992000
C	-2.133486000	-5.917584000	-0.432592000
C	-0.721890000	-5.878962000	-0.225561000
C	0.275939000	-6.894320000	-0.555346000
H	0.074631000	-7.878480000	-0.959834000
C	1.493367000	-6.312774000	-0.342033000
H	2.462282000	-6.750880000	-0.537651000
C	1.223942000	-4.974246000	0.183022000
C	2.086655000	-3.903576000	0.555862000
C	1.442416000	-2.704154000	1.033756000
C	2.033218000	-1.709110000	1.758787000
H	3.078800000	-1.829144000	2.020420000
C	1.414184000	-0.481338000	2.172080000
C	0.116753000	1.452927000	2.165593000
C	-0.726168000	2.526345000	1.714817000
H	-0.325936000	3.513046000	1.921048000
C	-1.899858000	2.492695000	1.013988000
C	-2.509627000	3.687657000	0.467781000
C	-3.909373000	3.693301000	0.240732000
C	-4.785922000	4.777451000	-0.200050000
H	-4.489752000	5.784443000	-0.456380000
C	-6.049160000	4.266252000	-0.227133000
H	-6.964118000	4.773165000	-0.505882000
C	-5.922690000	2.856108000	0.129886000
C	-6.923584000	1.853208000	0.073613000
C	-1.623259000	4.769246000	0.064219000
C	-1.822276000	6.219628000	-0.036794000
H	-2.718853000	6.768612000	-0.218297000
C	-0.620797000	6.748592000	-0.413291000
H	-0.382358000	7.791665000	-0.579936000
C	0.287163000	5.617809000	-0.585259000
C	1.631893000	5.604742000	-0.982620000
C	2.279214000	4.353965000	-1.251198000
C	1.681525000	3.141113000	-1.607955000
H	0.626608000	3.074045000	-1.825074000
C	2.555383000	2.058556000	-1.627571000
H	2.252760000	1.050026000	-1.885524000
C	3.872815000	2.376016000	-1.292661000
C	4.912525000	1.411292000	-1.091632000
C	6.303608000	1.514178000	-1.124798000
H	6.828028000	2.436297000	-1.353816000
C	6.947733000	0.293488000	-0.883342000
H	8.024707000	0.169121000	-0.899072000
C	6.082363000	-0.783615000	-0.624922000
C	6.454258000	-2.138636000	-0.355542000
C	5.513032000	-3.116413000	-0.024439000
C	5.696331000	-4.549410000	0.169752000
H	6.636703000	-5.084104000	0.130586000
C	4.451772000	-5.062903000	0.392593000
H	4.199557000	-6.091301000	0.613430000
C	3.523279000	-3.930970000	0.367711000

C	-2.855624000	-7.222532000	-0.500132000
C	-3.427059000	-7.660669000	-1.717681000
C	-4.091581000	-8.890080000	-1.751961000
C	-4.216117000	-9.697394000	-0.618320000
C	-3.649779000	-9.243825000	0.575865000
C	-2.964520000	-8.028127000	0.657494000
C	-3.315424000	-6.843990000	-2.986528000
H	-3.944573000	-5.946778000	-2.949145000
H	-3.630281000	-7.433757000	-3.853058000
H	-2.288214000	-6.505546000	-3.160368000
C	-4.918455000	-11.033252000	-0.687719000
H	-4.213365000	-11.841493000	-0.924957000
H	-5.692023000	-11.040188000	-1.463018000
H	-5.391961000	-11.287207000	0.266767000
C	-2.377911000	-7.594538000	1.983504000
H	-1.284037000	-7.668350000	1.984339000
H	-2.755822000	-8.223707000	2.795517000
H	-2.622867000	-6.552879000	2.215827000
C	-8.365150000	2.250255000	-0.048823000
C	-9.099961000	2.582121000	1.109871000
C	-10.441984000	2.953373000	0.980276000
C	-11.075595000	3.015126000	-0.263963000
C	-10.329196000	2.684067000	-1.397837000
C	-8.985817000	2.301742000	-1.315527000
C	-8.461488000	2.532366000	2.480146000
H	-8.044796000	1.541747000	2.695800000
H	-9.192307000	2.770133000	3.259333000
H	-7.633129000	3.245405000	2.563786000
C	-12.517033000	3.453515000	-0.381498000
H	-12.594778000	4.544824000	-0.479383000
H	-13.097049000	3.166448000	0.502315000
H	-12.999641000	3.014300000	-1.261157000
C	-8.224692000	1.960151000	-2.577585000
H	-7.310096000	2.556841000	-2.669366000
H	-8.839921000	2.143192000	-3.463993000
H	-7.917302000	0.907906000	-2.592855000
C	2.414299000	6.877712000	-1.060548000
C	2.801127000	7.548738000	0.120569000
C	3.537276000	8.733935000	0.014954000
C	3.893386000	9.278364000	-1.220690000
C	3.491642000	8.602272000	-2.376819000
C	2.766667000	7.409477000	-2.322554000
C	2.449065000	7.014257000	1.492593000
H	1.383576000	7.145199000	1.715164000
H	3.019341000	7.537960000	2.266252000
H	2.663285000	5.943529000	1.578791000
C	4.710358000	10.546177000	-1.308328000
H	5.778935000	10.322511000	-1.428401000
H	4.604583000	11.154972000	-0.404365000
H	4.410844000	11.157755000	-2.166544000
C	2.347801000	6.729174000	-3.606838000
H	2.606615000	7.344818000	-4.473616000
H	1.267619000	6.545221000	-3.631269000
H	2.837879000	5.756158000	-3.728440000
C	7.907183000	-2.504899000	-0.441769000
C	8.469770000	-2.868478000	-1.684005000
C	9.823514000	-3.215410000	-1.737950000
C	10.636532000	-3.206617000	-0.601090000
C	10.056415000	-2.846243000	0.617950000
C	8.706137000	-2.495542000	0.720808000
C	7.632673000	-2.902701000	-2.943221000
H	7.215005000	-1.916561000	-3.177043000
H	6.784025000	-3.589085000	-2.842745000
H	8.231101000	-3.227254000	-3.799854000
C	12.104611000	-3.552628000	-0.692629000
H	12.709129000	-2.665156000	-0.923744000
H	12.294924000	-4.287677000	-1.482068000
H	12.479505000	-3.963460000	0.250821000
C	8.126887000	-2.120306000	2.067014000
H	7.649848000	-1.133772000	2.039746000
H	8.907397000	-2.098309000	2.833750000
H	7.359353000	-2.834887000	2.386723000
N	-0.115775000	-4.771251000	0.250692000
N	-4.639585000	2.559463000	0.428613000
N	-0.369056000	4.455684000	-0.270393000
N	4.188953000	-2.794662000	0.123678000
S	-4.916833000	-0.083712000	0.050324000
S	-4.549612000	-4.464622000	-0.206787000
S	4.021208000	4.105990000	-1.009702000
S	4.412986000	-0.226451000	-0.683822000
H	10.252258000	-3.502495000	-2.696260000
H	10.669459000	-2.838920000	1.517257000
H	3.747650000	9.015439000	-3.350640000
H	3.840642000	9.244031000	0.927213000
H	-10.803297000	2.724156000	-2.376837000
H	-11.006440000	3.200641000	1.877555000

H	-4.522288000	-9.226095000	-2.693367000
H	-3.745981000	-9.851379000	1.473811000
C	0.278533000	0.160804000	1.626388000
C	1.972386000	0.408946000	3.149413000
C	3.076863000	0.133186000	3.950322000
C	3.681268000	0.926654000	4.930858000
C	1.152087000	1.631553000	3.147972000
C	3.321569000	2.204682000	5.366103000
C	1.311206000	2.756734000	3.949137000
C	2.274539000	3.018443000	4.931311000
H	3.536524000	-0.840542000	3.799655000
H	4.545499000	0.485755000	5.422210000
H	3.946030000	2.624493000	6.152639000
H	0.579267000	3.547303000	3.801579000
H	2.190503000	3.984954000	5.422781000
H	0.371673000	-2.665435000	0.866248000
H	-2.455762000	1.566201000	0.907580000
H	-0.327451000	-0.245300000	0.824655000

Conformer-7

C	-2.814873000	4.690229000	-0.541099000
C	-2.240385000	3.439565000	-0.873497000
H	-1.210639000	3.362143000	-1.185086000
C	-3.104880000	2.375719000	-0.796176000
H	-2.828524000	1.359290000	-1.051449000
C	-4.420777000	2.712934000	-0.411456000
C	-5.431948000	1.759807000	-0.191080000
C	-6.837649000	1.854914000	-0.141455000
H	-7.370381000	2.793343000	-0.258740000
C	-7.465123000	0.625248000	-0.011571000
H	-8.541428000	0.494168000	-0.009010000
C	-6.584329000	-0.487621000	0.071240000
C	-6.923586000	-1.853225000	0.073739000
C	-5.922741000	-2.856111000	0.130032000
C	-6.049244000	-4.266298000	-0.226792000
H	-6.964225000	-4.773237000	-0.505415000
C	-4.786008000	-4.777498000	-0.199740000
H	-4.489868000	-5.784521000	-0.455970000
C	-3.909424000	-3.693292000	0.240864000
C	-2.509627000	-3.687663000	0.467850000
C	-1.899856000	-2.492687000	1.014016000
C	-0.726210000	-2.526336000	1.714925000
H	-0.326008000	-3.513039000	1.921204000
C	0.116718000	-1.452928000	2.165692000
C	1.414143000	0.481331000	2.172101000
C	2.033173000	1.709108000	1.758793000
H	3.078719000	1.829207000	2.020557000
C	1.442438000	2.704086000	1.033618000
C	2.086699000	3.903523000	0.555765000
C	1.223954000	4.974223000	0.182970000
C	1.493385000	6.312794000	-0.341996000
H	2.462305000	6.750917000	-0.537563000
C	0.275962000	6.894353000	-0.555280000
H	0.074658000	7.878528000	-0.959731000
C	-0.721868000	5.878972000	-0.225594000
C	-2.133419000	5.917571000	-0.432683000
C	3.523302000	3.930938000	0.367653000
C	4.451769000	5.062888000	0.392496000
H	4.199527000	6.091296000	0.613260000
C	5.696350000	4.549408000	0.169730000
H	6.636708000	5.084124000	0.130538000
C	5.513081000	3.116405000	-0.024426000
C	6.454352000	2.138631000	-0.355507000
C	6.082452000	0.783640000	-0.624874000
C	6.947797000	-0.293523000	-0.883222000
H	8.024777000	-0.169193000	-0.898909000
C	6.303644000	-1.514184000	-1.124654000
H	6.828043000	-2.436332000	-1.353612000
C	4.912545000	-1.411261000	-1.091543000
C	3.872821000	-2.375947000	-1.292526000
C	2.555317000	-2.058439000	-1.627195000
H	2.252676000	-1.049875000	-1.884994000
C	1.681465000	-3.140974000	-1.607609000
H	0.626517000	-3.073871000	-1.824566000
C	2.279194000	-4.353907000	-1.251117000
C	1.631885000	-5.604682000	-0.982650000
C	0.287141000	-5.617755000	-0.585227000
C	-0.620850000	-6.748539000	-0.413429000
H	-0.382427000	-7.791597000	-0.580192000
C	-1.822347000	-6.219586000	-0.036965000
H	-2.718948000	-6.768589000	0.217993000
C	-1.623291000	-4.769230000	0.064276000
C	-8.365173000	-2.250207000	-0.048675000
C	-8.985852000	-2.301696000	-1.315370000
C	-10.329267000	-2.683911000	-1.397652000

C	-11.075688000	-3.014838000	-0.263757000
C	-10.442063000	-2.953078000	0.980474000
C	-9.100005000	-2.581951000	1.110042000
C	-8.224742000	-1.960139000	-2.577446000
H	-7.917964000	-0.907711000	-2.593032000
H	-8.839755000	-2.143815000	-3.463873000
H	-7.309794000	-2.556323000	-2.668905000
C	-12.517157000	-3.453134000	-0.381260000
H	-12.594992000	-4.544463000	-0.478846000
H	-12.999672000	-3.014122000	-1.261071000
H	-13.097204000	-3.165776000	0.502439000
C	-8.461523000	-2.532146000	2.480310000
H	-7.632886000	-3.244868000	2.563840000
H	-9.192240000	-2.770289000	3.259478000
H	-8.045216000	-1.541389000	2.696091000
C	-2.855632000	7.222464000	-0.500278000
C	-2.964572000	8.028113000	0.657328000
C	-3.649936000	9.243731000	0.575664000
C	-4.216335000	9.697204000	-0.618551000
C	-4.091710000	8.889879000	-1.752155000
C	-3.427083000	7.660505000	-1.717836000
C	-2.377863000	7.594624000	1.983326000
H	-2.622662000	6.552933000	2.215674000
H	-2.755825000	8.223756000	2.795343000
H	-1.283996000	7.668581000	1.984118000
C	-4.918839000	11.032979000	-0.687900000
H	-4.213281000	11.841806000	-0.921698000
H	-5.395245000	11.285273000	0.265599000
H	-5.690119000	11.040926000	-1.465453000
C	-3.315365000	6.843817000	-2.986669000
H	-2.288196000	6.505161000	-3.160321000
H	-3.629947000	7.433658000	-3.853249000
H	-3.944713000	5.946736000	-2.949413000
C	7.907278000	2.504909000	-0.441669000
C	8.706119000	2.495810000	0.720983000
C	10.056408000	2.846502000	0.618182000
C	10.636639000	3.206625000	-0.600872000
C	9.823727000	3.215176000	-1.737816000
C	8.469987000	2.868235000	-1.683932000
C	8.126753000	2.120846000	2.067215000
H	7.359484000	2.835720000	2.386908000
H	8.907267000	2.098603000	2.833940000
H	7.649354000	1.134485000	2.039998000
C	12.104722000	3.552630000	-0.692364000
H	12.709179000	2.665261000	-0.924043000
H	12.479726000	3.962923000	0.251273000
H	12.294991000	4.288104000	-1.481421000
C	7.633033000	2.902124000	-2.943252000
H	8.231277000	3.227546000	-3.799685000
H	6.783706000	3.587638000	-2.842656000
H	7.216361000	1.915656000	-3.177495000
C	2.414245000	-6.877671000	-1.060700000
C	2.766442000	-7.409431000	-2.322729000
C	3.491336000	-8.602300000	-2.377084000
C	3.893143000	-9.278431000	-1.221031000
C	3.537178000	-8.733999000	0.014684000
C	2.801144000	-7.548768000	0.120385000
C	2.347426000	-6.729140000	-3.606970000
H	2.837024000	-5.755861000	-3.728368000
H	1.267151000	-6.545725000	-3.631513000
H	2.606650000	-7.344532000	-4.473803000
C	4.710138000	-10.546230000	-1.308646000
H	5.779343000	-10.322523000	-1.422952000
H	4.414472000	-11.155133000	-2.170068000
H	4.599986000	-11.157697000	-0.406994000
C	2.449212000	-7.014288000	1.492443000
H	2.663452000	-5.943566000	1.578627000
H	3.019542000	-7.538008000	2.266052000
H	1.383736000	-7.145214000	1.715099000
N	-4.639575000	-2.559455000	0.428637000
N	-0.115732000	4.771224000	0.250632000
N	4.189029000	2.794620000	0.123670000
N	-0.369017000	-4.455680000	-0.270191000
S	-4.549508000	4.464555000	-0.206794000
S	-4.916810000	0.083667000	0.050198000
S	4.413057000	0.226525000	-0.683784000
S	4.021233000	-4.105976000	-1.009825000
H	3.747223000	-9.015467000	-3.350933000
H	3.840580000	-9.244145000	0.926907000
H	10.252554000	3.502096000	-2.696140000
H	10.669365000	2.839373000	1.517550000
H	-4.522414000	9.225848000	-2.693577000
H	-3.746189000	9.851312000	1.473589000
H	-10.803369000	-2.724033000	-2.376650000
H	-11.006532000	-3.200258000	1.877769000
C	0.278464000	-0.160809000	1.626494000

C	1.152136000	-1.631589000	3.147955000
C	1.311343000	-2.756805000	3.949075000
C	2.274757000	-3.018532000	4.931151000
C	1.972446000	-0.408995000	3.149369000
C	3.321832000	-2.204775000	5.365883000
C	3.076993000	-0.133251000	3.950172000
C	3.681505000	-0.926753000	4.930633000
H	0.579403000	-3.547380000	3.801550000
H	2.190771000	-3.985053000	5.422609000
H	3.946353000	-2.624617000	6.152357000
H	3.536642000	0.840480000	3.799485000
H	4.545788000	-0.485865000	5.421906000
H	-2.455737000	-1.566184000	0.907554000
H	0.371720000	2.665297000	0.865952000
H	-0.327654000	0.245337000	0.824885000

Conformer-8

C	3.982715000	-4.740077000	0.052534000
C	5.395991000	-4.915404000	0.082977000
H	5.842438000	-5.895651000	-0.030053000
C	6.116481000	-3.759572000	0.238506000
H	7.199294000	-3.736640000	0.257769000
C	5.323982000	-2.584142000	0.333644000
C	5.850898000	-1.284447000	0.380505000
C	7.240926000	-0.986533000	0.356113000
H	8.003631000	-1.755740000	0.362603000
C	7.529761000	0.352062000	0.290693000
H	8.534966000	0.752722000	0.240470000
C	6.391727000	1.208412000	0.259595000
C	6.445347000	2.589839000	0.056151000
C	5.305612000	3.440468000	0.026806000
C	5.281104000	4.812910000	-0.477162000
H	6.130136000	5.365650000	-0.857341000
C	3.982192000	5.213201000	-0.414060000
H	3.572305000	6.158969000	-0.739098000
C	3.243396000	4.105216000	0.180938000
C	1.874657000	4.030640000	0.504137000
C	1.386379000	2.841103000	1.149087000
C	0.228835000	2.794115000	1.872621000
H	-0.292778000	3.729384000	2.048862000
C	-0.428479000	1.613341000	2.347858000
C	-1.318883000	-0.529767000	2.329467000
C	-1.672657000	-1.833585000	1.855567000
H	-2.673485000	-2.178609000	2.092403000
C	-0.890386000	-2.635200000	1.073639000
C	-1.320495000	-3.874442000	0.489085000
C	-0.333136000	-4.793107000	0.073802000
C	-0.523740000	-6.093772000	-0.561817000
H	-1.465167000	-6.528401000	-0.865338000
C	0.716420000	-6.627538000	-0.714555000
H	0.980986000	-7.581512000	-1.150937000
C	1.654261000	-5.624117000	-0.210612000
C	3.068760000	-5.765296000	-0.210565000
C	-2.746407000	-4.116913000	0.286679000
C	-3.493890000	-5.376121000	0.366075000
H	-3.083329000	-6.343583000	0.621773000
C	-4.802266000	-5.066033000	0.140060000
H	-5.652296000	-5.736089000	0.135654000
C	-4.839407000	-3.629553000	-0.102197000
C	-5.922712000	-2.820755000	-0.428790000
C	-5.779926000	-1.421091000	-0.715121000
C	-6.814210000	-0.507126000	-0.960650000
H	-7.856029000	-0.807152000	-0.956434000
C	-6.382934000	0.804591000	-1.217465000
H	-7.054836000	1.627334000	-1.439310000
C	-4.996980000	0.928203000	-1.207175000
C	-4.127545000	2.052597000	-1.425597000
C	-2.801259000	1.956862000	-1.835953000
H	-2.360291000	1.019539000	-2.155629000
C	-2.103315000	3.165069000	-1.795057000
H	-1.063787000	3.271896000	-2.065927000
C	-2.862369000	4.246569000	-1.352569000
C	-2.385897000	5.567197000	-1.032511000
C	-1.069576000	5.711568000	-0.591009000
C	-0.266810000	6.917280000	-0.413476000
H	-0.591967000	7.934023000	-0.595247000
C	0.971603000	6.495069000	-0.021962000
H	1.821619000	7.115130000	0.232075000
C	0.894418000	5.033570000	0.088100000
C	7.791862000	3.216882000	-0.185213000
C	8.354550000	3.220272000	-1.479489000
C	9.601445000	3.823872000	-1.676297000
C	10.307551000	4.422694000	-0.629621000
C	9.733300000	4.404259000	0.644383000
C	8.486731000	3.817609000	0.886221000

C	7.633384000	2.589130000	-2.649951000
H	7.525416000	1.505593000	-2.521779000
H	8.178248000	2.764483000	-3.582781000
H	6.621995000	2.994873000	-2.765445000
C	11.639272000	5.094385000	-0.873017000
H	11.510882000	6.158498000	-1.113390000
H	12.172969000	4.635246000	-1.712122000
H	12.284361000	5.038399000	0.010539000
C	7.908721000	3.828138000	2.283901000
H	6.964086000	4.382918000	2.323222000
H	8.603930000	4.293545000	2.989531000
H	7.691521000	2.814253000	2.639244000
C	3.626159000	-7.125894000	-0.537242000
C	3.742317000	-8.099453000	0.477670000
C	4.255776000	-9.360115000	0.154995000
C	4.648209000	-9.688444000	-1.145458000
C	4.523086000	-8.709860000	-2.135224000
C	4.020393000	-7.434155000	-1.856817000
C	3.328013000	-7.798096000	1.900768000
H	3.854354000	-6.922967000	2.298762000
H	3.539202000	-8.648640000	2.556387000
H	2.256445000	-7.576781000	1.967774000
C	5.166388000	-11.068862000	-1.476854000
H	4.3477765000	-11.744760000	-1.759042000
H	5.678536000	-11.521400000	-0.620817000
H	5.868560000	-11.043011000	-2.317159000
C	3.904341000	-6.414317000	-2.967984000
H	2.883338000	-6.025063000	-3.051468000
H	4.179419000	-6.855374000	-3.931103000
H	4.557369000	-5.550931000	-2.794145000
C	-7.300592000	-3.413388000	-0.489535000
C	-8.081531000	-3.501668000	0.681702000
C	-9.360931000	-4.061836000	0.601768000
C	-9.886904000	-4.536738000	-0.602427000
C	-9.091665000	-4.444211000	-1.748200000
C	-7.808721000	-3.888594000	-1.717370000
C	-7.556999000	-3.011060000	2.013196000
H	-6.690314000	-3.596164000	2.342700000
H	-8.327880000	-3.086288000	2.786256000
H	-7.231869000	-1.965737000	1.958463000
C	-11.283141000	-5.110605000	-0.669948000
H	-12.019370000	-4.337276000	-0.927547000
H	-11.586894000	-5.540674000	0.290316000
H	-11.358204000	-5.894321000	-1.431498000
C	-6.986271000	-3.819925000	-2.984714000
H	-7.539095000	-4.238966000	-3.830870000
H	-6.047098000	-4.376162000	-2.884532000
H	-6.716460000	-2.787409000	-3.235081000
C	-3.307749000	6.739832000	-1.117603000
C	-3.727884000	7.214579000	-2.382469000
C	-4.584878000	8.315572000	-2.442348000
C	-5.055686000	8.952017000	-1.289586000
C	-4.632802000	8.463845000	-0.051700000
C	-3.763292000	7.373309000	0.060428000
C	-3.240494000	6.577914000	-3.665041000
H	-3.626537000	5.559043000	-3.784725000
H	-2.147047000	6.507562000	-3.689929000
H	-3.562114000	7.161571000	-4.532888000
C	-6.013643000	10.116315000	-1.383475000
H	-7.048331000	9.769812000	-1.508359000
H	-5.782907000	10.757226000	-2.241566000
H	-5.983562000	10.734460000	-0.480246000
C	-3.351537000	6.896914000	1.437674000
H	-3.411223000	5.807037000	1.526272000
H	-3.998912000	7.335968000	2.203299000
H	-2.318438000	7.179430000	1.671422000
N	4.081685000	3.048529000	0.421678000
N	1.002373000	-4.538729000	0.248253000
N	-3.570933000	-3.105130000	0.015854000
N	-0.317416000	4.606487000	-0.249385000
S	3.604200000	-3.018100000	0.291027000
S	4.915599000	0.221321000	0.388551000
S	-4.227061000	-0.599117000	-0.805367000
S	-4.527409000	3.721845000	-1.048098000
H	-4.891596000	8.687611000	-3.418061000
H	-4.989652000	8.943181000	0.857829000
H	-9.477896000	-4.816382000	-2.695241000
H	-9.960381000	-4.129790000	1.507645000
H	4.824538000	-8.943160000	-3.154845000
H	4.350193000	-10.104986000	0.943146000
H	10.030784000	3.825149000	-2.676579000
H	10.268503000	4.859537000	1.475767000
C	-0.329571000	0.321761000	1.799713000
C	-1.484482000	1.585905000	3.318670000
C	-1.872730000	2.658635000	4.112693000
C	-2.879069000	2.721238000	5.084329000

C	-2.048720000	0.223177000	3.308509000
C	-3.746184000	1.712477000	5.509046000
C	-3.085074000	-0.268222000	4.094976000
C	-3.842378000	0.389091000	5.071292000
H	-1.312348000	3.579521000	3.965580000
H	-2.996654000	3.684229000	5.575859000
H	-4.448946000	1.998353000	6.289653000
H	-3.342682000	-1.312955000	3.935795000
H	-4.607152000	-0.214039000	5.555151000
H	2.024169000	1.964723000	1.084394000
H	0.155268000	-2.385088000	0.921633000
H	0.340522000	0.053535000	0.991771000

Conformer-9

C	-6.391614000	1.208773000	0.259493000
C	-7.529724000	0.352508000	0.290625000
H	-8.534893000	0.753253000	0.240404000
C	-7.241003000	-0.986101000	0.356061000
H	-8.003769000	-1.755245000	0.362520000
C	-5.850992000	-1.284134000	0.380497000
C	-5.324179000	-2.583855000	0.333693000
C	-6.116757000	-3.759250000	0.238640000
H	-7.199567000	-3.736248000	0.257958000
C	-5.396352000	-4.915130000	0.083152000
H	-5.842863000	-5.895353000	-0.029802000
C	-3.983054000	-4.739896000	0.052654000
C	-3.069176000	-5.765163000	-0.210434000
C	-1.654657000	-5.624044000	-0.210560000
C	-0.716890000	-6.627491000	-0.714601000
H	-0.981523000	-7.581444000	-1.150982000
C	0.523304000	-6.093805000	-0.561881000
H	1.464697000	-6.528483000	-0.865427000
C	0.332783000	-4.793123000	0.073741000
C	1.320211000	-3.874567000	0.489036000
C	0.890198000	-2.635292000	1.073732000
C	1.672588000	-1.833774000	1.855619000
H	2.673415000	-2.178874000	2.092337000
C	1.318922000	-0.529971000	2.329653000
C	0.428654000	1.613199000	2.348157000
C	-0.228547000	2.794040000	1.872951000
H	0.293199000	3.729246000	2.049132000
C	-1.386150000	2.841135000	1.149509000
C	-1.874354000	4.030661000	0.504526000
C	-3.243035000	4.105317000	0.181197000
C	-3.981665000	5.213322000	-0.413967000
H	-3.571651000	6.159028000	-0.739026000
C	-5.280603000	4.813141000	-0.477176000
H	-6.129543000	5.365919000	-0.857501000
C	-5.305281000	3.440725000	0.026864000
C	-6.445106000	2.590193000	0.056084000
C	-0.894031000	5.033560000	0.088471000
C	-0.971115000	6.495107000	-0.021276000
H	-1.821065000	7.115158000	0.232991000
C	0.267255000	6.917282000	-0.412927000
H	0.592480000	7.934024000	-0.594570000
C	1.069910000	5.711537000	-0.590809000
C	2.386141000	5.567147000	-1.032430000
C	2.862550000	4.246464000	-1.352630000
C	2.103460000	3.165123000	-1.795348000
H	1.063969000	3.272059000	-2.066322000
C	2.801320000	1.956826000	-1.836284000
H	2.360313000	1.019574000	-2.156116000
C	4.127525000	2.052412000	-1.425736000
C	4.996910000	0.927949000	-1.207292000
C	6.382839000	0.804247000	-1.217740000
H	7.054771000	1.626929000	-1.439702000
C	6.814046000	-0.507514000	-0.960947000
H	7.855840000	-0.807624000	-0.956875000
C	5.779723000	-1.421380000	-0.715287000
C	5.922436000	-2.821071000	-0.428985000
C	4.839114000	-3.629818000	-0.102380000
C	4.801941000	-5.066283000	0.139958000
H	5.651953000	-5.736359000	0.135586000
C	3.493560000	-5.376325000	0.365996000
H	3.082974000	-6.343764000	0.621735000
C	2.746111000	-4.117100000	0.286568000
C	-3.626641000	-7.125766000	-0.536993000
C	-4.020877000	-7.434137000	-1.856506000
C	-4.523615000	-8.709884000	-2.134788000
C	-4.648769000	-9.688346000	-1.144947000
C	-4.256331000	-9.359891000	0.155504000
C	-3.742845000	-8.099235000	0.478040000
C	-3.904779000	-6.414437000	-2.967796000
H	-4.557492000	-5.550831000	-2.793883000
H	-4.180221000	-6.855499000	-3.930808000

H	-2.883674000	-6.025513000	-3.051563000
C	-5.166950000	-11.068829000	-1.476075000
H	-4.347645000	-11.746536000	-1.751864000
H	-5.864240000	-11.043977000	-2.320440000
H	-5.684631000	-11.518672000	-0.621926000
C	-3.328560000	-7.797714000	1.901109000
H	-2.257043000	-7.576153000	1.968074000
H	-3.539544000	-8.648268000	2.556779000
H	-3.855088000	-6.922685000	2.299071000
C	-7.791529000	3.217370000	-0.185425000
C	-8.486011000	3.819001000	0.885718000
C	-9.732526000	4.405771000	0.643735000
C	-10.307029000	4.423481000	-0.630131000
C	-9.601266000	3.823780000	-1.676573000
C	-8.354499000	3.220029000	-1.479618000
C	-7.907633000	3.830616000	2.283238000
H	-7.687798000	2.817233000	2.638319000
H	-8.603747000	4.294234000	2.989153000
H	-6.964359000	4.387756000	2.322367000
C	-11.638619000	5.095318000	-0.873831000
H	-11.509654000	6.157951000	-1.120370000
H	-12.281535000	5.044823000	0.011615000
H	-12.174930000	4.632254000	-1.709122000
C	-7.633771000	2.587862000	-2.649798000
H	-6.621541000	2.991685000	-2.764533000
H	-8.177723000	2.764497000	-3.582919000
H	-7.527978000	1.504074000	-2.521872000
C	3.308056000	6.739725000	-1.117565000
C	3.763639000	7.373211000	0.060413000
C	4.633192000	8.463740000	-0.051775000
C	5.056044000	8.951864000	-1.289661000
C	4.585219000	8.315356000	-2.442411000
C	3.728206000	7.214412000	-2.382478000
C	3.351909000	6.896932000	1.437709000
H	2.319140000	7.180358000	1.671841000
H	3.999916000	7.335290000	2.203199000
H	3.410630000	5.806999000	1.526121000
C	6.013866000	10.116260000	-1.383723000
H	7.047969000	9.769979000	-1.513877000
H	5.987455000	10.731608000	-0.478485000
H	5.779831000	10.759897000	-2.238897000
C	3.240800000	6.577684000	-3.665013000
H	3.562307000	7.161368000	-4.532882000
H	2.147363000	6.507219000	-3.689833000
H	3.626940000	5.558852000	-3.784715000
C	7.300288000	-3.413768000	-0.489799000
C	7.808021000	-3.889713000	-1.717509000
C	9.090953000	-4.445352000	-1.748416000
C	9.886556000	-4.537197000	-0.602840000
C	9.360962000	-4.061589000	0.601241000
C	8.081593000	-3.501358000	0.681245000
C	6.985140000	-3.821849000	-2.984617000
H	6.713953000	-2.789642000	-3.234728000
H	6.046698000	-4.379299000	-2.884272000
H	7.538249000	-4.240070000	-3.830992000
C	11.282792000	-5.111053000	-0.670481000
H	12.018885000	-4.337861000	-0.928886000
H	11.357615000	-5.895281000	-1.431523000
C	11.586923000	-5.540440000	0.289965000
H	7.557496000	-3.009899000	2.012595000
H	7.233851000	-1.964116000	1.957690000
H	8.328127000	-3.086107000	2.785802000
H	6.689925000	-3.593737000	2.341980000
N	-1.002705000	-4.538700000	0.248284000
N	-4.081444000	3.048690000	0.421878000
N	0.317660000	4.606428000	-0.249304000
N	3.570656000	-3.105338000	0.015741000
S	-4.915567000	0.221561000	0.388574000
S	-3.604418000	-3.017927000	0.291051000
S	4.527471000	3.721579000	-1.047953000
S	4.226913000	-0.599276000	-0.805364000
H	9.476887000	-4.818077000	-2.695360000
H	9.960684000	-4.129039000	1.506974000
H	4.891964000	8.687324000	-3.418146000
H	4.990099000	8.943073000	0.857731000
H	-10.030807000	3.824500000	-2.676772000
H	-10.267473000	4.861690000	1.474928000
H	-4.825076000	-8.943279000	-3.154380000
H	-4.350775000	-10.104678000	0.943735000
C	0.329612000	0.321637000	1.800000000
C	2.048871000	0.222884000	3.308652000
C	3.085371000	-0.268550000	4.094929000
C	3.842776000	0.388694000	5.071194000
C	1.484724000	1.585651000	3.318920000
C	3.746560000	1.712035000	5.509139000
C	1.872972000	2.658286000	4.113042000

C	2.879376000	2.720804000	5.084641000
H	3.342987000	-1.313261000	3.935615000
H	4.607659000	-0.214439000	5.554877000
H	4.449401000	1.997823000	6.289708000
H	1.312566000	3.579179000	3.966059000
H	2.996937000	3.683735000	5.576292000
H	-0.155452000	-2.385120000	0.921800000
H	-2.024066000	1.964837000	1.084956000
H	-0.340513000	0.053489000	0.992059000

Conformer-10

C	4.110753000	-4.098441000	0.931762000
C	3.389034000	-3.174482000	1.737764000
H	2.464728000	-3.460880000	2.213718000
C	3.945446000	-1.921994000	1.803964000
C	3.507822000	-1.098787000	2.358606000
H	5.157756000	-1.773861000	1.087677000
C	5.787920000	-0.552453000	0.820378000
C	7.072287000	-0.270866000	0.299828000
H	7.807008000	-1.045352000	0.103620000
C	7.297931000	1.073388000	0.088180000
H	8.227162000	1.478350000	-0.295789000
C	6.184357000	1.919617000	0.370319000
C	6.092809000	3.289878000	0.093305000
C	4.871033000	4.009830000	0.211018000
C	4.614032000	5.371653000	-0.258697000
H	5.349379000	6.050657000	-0.670536000
C	3.276048000	5.574903000	-0.113309000
H	2.709202000	6.453009000	-0.392937000
C	2.735812000	4.350928000	0.473151000
C	1.390777000	4.026520000	0.726763000
C	1.047254000	2.726823000	1.244325000
C	-0.148138000	2.483745000	1.865059000
H	-0.777549000	3.348921000	2.044316000
C	-0.741959000	1.235458000	2.243006000
C	-1.487340000	-0.965156000	2.141470000
C	-1.698074000	-2.311197000	1.690650000
H	-2.701517000	-2.706088000	1.810813000
C	-0.761204000	-3.112021000	1.106036000
C	-0.996779000	-4.440671000	0.595699000
C	0.131153000	-5.276620000	0.459437000
C	0.292334000	-6.609569000	-0.115618000
H	-0.498291000	-7.256664000	-0.474337000
C	1.636374000	-6.850912000	-0.143315000
H	2.141605000	-7.734482000	-0.512922000
C	2.281671000	-5.653860000	0.407362000
C	3.679788000	-5.335131000	0.430419000
C	-2.350710000	-4.774694000	0.158289000
C	-3.133032000	-6.009078000	0.314391000
H	-2.773928000	-6.945585000	0.724212000
C	-4.405204000	-5.707411000	-0.077765000
H	-5.267734000	-6.362161000	-0.091941000
C	-4.370109000	-6.321115000	-0.538364000
C	-5.378585000	-3.494729000	-1.024187000
C	-4.936038000	-2.291647000	-1.707216000
C	-3.894139000	-2.232053000	-2.618802000
H	-3.417193000	-3.126745000	-2.997554000
C	-3.512133000	-0.934027000	-2.973318000
H	-2.703505000	-0.723833000	-3.662360000
C	-4.209203000	0.063070000	-2.299233000
C	-3.778235000	1.439726000	-2.240839000
C	-2.546930000	1.873673000	-2.724811000
H	-1.878054000	1.234291000	-3.287043000
C	-2.204739000	3.169733000	-2.333393000
H	-1.266381000	3.646323000	-2.579850000
C	-3.164634000	3.802472000	-1.554112000
C	-3.002217000	5.064255000	-0.869798000
C	-1.742481000	5.358068000	-0.351876000
C	-1.198930000	6.617381000	0.147267000
H	-1.709433000	7.572348000	0.159388000
C	0.080361000	6.348250000	0.543054000
H	0.790865000	7.035622000	0.985782000
C	0.279284000	4.907716000	0.341735000
C	7.306736000	4.000849000	-0.434676000
C	7.549984000	4.066011000	-1.823320000
C	8.686956000	4.739747000	-2.282925000
C	9.587419000	5.354046000	-1.408589000
C	9.328340000	5.275289000	-0.037550000
C	8.204804000	4.611764000	0.466272000
C	6.606614000	3.421293000	-2.814494000
H	6.511735000	2.343302000	-2.640148000
H	6.959685000	3.568194000	-3.839984000
H	5.597267000	3.842274000	-2.739861000
C	10.791125000	6.103865000	-1.930940000
H	10.559111000	7.164750000	-2.096299000

H	11.134649000	5.694916000	-2.887233000
H	11.627367000	6.062433000	-1.224572000
C	7.969689000	4.556239000	1.959406000
H	7.001791000	4.993750000	2.230099000
H	8.751093000	5.101482000	2.497894000
H	7.961270000	3.524021000	2.328653000
C	4.658162000	-6.259455000	-0.229034000
C	5.475900000	-7.092831000	0.566484000
C	6.382147000	-7.953999000	-0.058814000
C	6.507794000	-8.011937000	-1.449637000
C	5.696624000	-7.173046000	-2.217502000
C	4.770349000	-6.300250000	-1.636467000
C	5.379746000	-7.073184000	2.076042000
H	5.697324000	-6.108262000	2.488639000
H	6.012913000	-7.850107000	2.515730000
H	4.351267000	-7.239327000	2.416483000
C	7.475756000	-8.970914000	-2.103026000
H	7.015026000	-9.955280000	-2.262652000
H	8.365451000	-9.127533000	-1.483362000
H	7.804288000	-8.604313000	-3.081382000
C	3.921130000	-5.414807000	-2.521673000
H	2.866451000	-5.713438000	-2.497056000
H	4.260968000	-5.467437000	-3.560793000
H	3.962541000	-4.367585000	-2.203268000
C	-6.824204000	-3.780626000	-0.809602000
C	-7.356169000	-3.817598000	0.501068000
C	-8.720478000	-4.077627000	0.671271000
C	-9.573238000	-4.312215000	-0.408466000
C	-9.026530000	-4.277287000	-1.695340000
C	-7.675932000	-4.005801000	-1.919472000
C	-6.507982000	-3.552562000	1.728276000
H	-5.881211000	-4.414314000	1.984850000
H	-7.146887000	-3.336898000	2.590642000
H	-5.835075000	-2.701089000	1.581949000
C	-11.046709000	-4.569998000	-0.199595000
H	-11.636950000	-3.660352000	-0.373531000
H	-11.254672000	-4.904570000	0.821854000
H	-11.421792000	-5.333535000	-0.890205000
C	-7.149799000	-4.001953000	-3.337772000
H	-7.914989000	-4.361127000	-4.032661000
H	-6.268230000	-4.644364000	-3.443394000
H	-6.850501000	-2.997840000	-3.658582000
C	-4.163495000	5.982463000	-0.683702000
C	-4.744509000	6.622579000	-1.805083000
C	-5.827669000	7.481453000	-1.610040000
C	-6.371671000	7.713202000	-0.342606000
C	-5.789370000	7.066029000	0.748549000
C	-4.692191000	6.208956000	0.607734000
C	-4.194274000	6.427303000	-3.200582000
H	-4.369806000	5.409737000	-3.567920000
H	-3.111756000	6.594526000	-3.234772000
H	-4.666517000	7.122030000	-3.901774000
C	-7.569327000	8.616811000	-0.167192000
H	-8.502588000	8.089098000	-0.405228000
H	-7.514545000	9.488048000	-0.829373000
H	-7.651858000	8.978156000	0.862992000
C	-4.125084000	5.536890000	1.841117000
H	-3.913348000	4.476541000	1.668787000
H	-4.832608000	5.610872000	2.673159000
H	-3.185119000	6.002878000	2.159383000
N	3.740179000	3.442752000	0.672169000
N	1.351029000	-4.762262000	0.778364000
N	-3.089652000	-3.811646000	-0.370880000
N	-0.795954000	4.356150000	-0.201737000
S	5.640389000	-3.337149000	0.406637000
S	4.849694000	0.945640000	0.996888000
S	-5.469253000	-0.655745000	-1.305629000
S	-4.568005000	2.739178000	-1.362586000
H	-6.257937000	7.985498000	-2.473350000
H	-6.200588000	7.228913000	1.742871000
H	-9.670496000	-4.469601000	-2.551379000
H	-9.127068000	-4.092948000	1.680571000
H	5.787328000	-7.193172000	-3.301999000
H	7.007236000	-8.596047000	0.559179000
H	8.872277000	4.784045000	-3.354658000
H	10.019122000	5.742389000	0.662164000
C	-0.503835000	-0.048718000	1.711661000
C	-1.890302000	1.132187000	3.101123000
C	-2.422774000	2.168022000	3.860274000
C	-3.526978000	2.160409000	4.722058000
C	-2.364082000	-0.261480000	3.031905000
C	-4.373174000	1.099284000	5.048261000
C	-3.443132000	-0.822570000	3.707817000
C	-4.340624000	-0.222927000	4.598227000
H	-1.906113000	3.121995000	3.784595000
H	-3.750070000	3.109275000	5.204355000

H	-5.170316000	1.334959000	5.751062000
H	-3.613862000	-1.881098000	3.525568000
H	-5.112802000	-0.877177000	4.996250000
H	1.801464000	1.949438000	1.157865000
H	0.272847000	-2.785021000	1.081440000
H	0.263749000	-0.273771000	0.980252000

Conformer-11

C	-6.188487000	1.920907000	0.087361000
C	-7.329498000	1.060670000	0.030398000
H	-8.336201000	1.463363000	0.036757000
C	-7.039804000	-0.283984000	-0.072670000
H	-7.795864000	-1.057689000	-0.163776000
C	-5.650741000	-0.559919000	-0.128535000
C	-4.932639000	-1.740764000	-0.321004000
C	-3.556232000	-1.769802000	-0.669854000
H	-3.015501000	-0.863219000	-0.916067000
C	-3.003989000	-3.016731000	-0.727894000
H	-1.983239000	-3.211894000	-1.015448000
C	-3.896804000	-4.082849000	-0.409169000
C	-3.561312000	-5.432515000	-0.279777000
C	-2.168112000	-5.753928000	-0.083975000
C	-1.438251000	-6.960661000	-0.479113000
H	-1.871851000	-7.856838000	-0.905578000
C	-0.113490000	-6.684562000	-0.282648000
H	0.730761000	-7.323901000	-0.509130000
C	-0.057255000	-5.341384000	0.284100000
C	1.022006000	-4.487977000	0.581445000
C	0.710552000	-3.175652000	-0.1090379000
C	1.603102000	-2.333195000	1.689478000
H	2.613971000	-2.695771000	1.843092000
C	1.362234000	-0.976080000	2.089075000
C	0.637579000	1.234646000	2.051125000
C	0.074983000	2.476322000	1.598280000
H	0.720663000	3.333477000	1.754265000
C	-1.104393000	2.724454000	0.953588000
C	-1.441775000	4.034802000	0.443346000
C	-2.789420000	4.368174000	0.228777000
C	-3.375252000	5.638050000	-0.194048000
H	-2.835786000	6.545271000	-0.431460000
C	-4.724227000	5.447298000	-0.226206000
H	-5.490332000	6.163826000	-0.493890000
C	-4.944563000	4.042648000	0.119465000
C	-6.174701000	3.319100000	0.080481000
C	-0.328076000	4.925266000	0.090010000
C	-0.137798000	6.364620000	0.317150000
H	-0.859618000	7.044400000	0.752629000
C	1.150098000	6.641973000	-0.039632000
H	1.658630000	7.597072000	0.002712000
C	1.713421000	5.389157000	-0.534927000
C	2.997273000	5.099481000	-0.985806000
C	3.207229000	3.826564000	-1.641326000
C	2.306005000	3.176541000	-2.472415000
H	1.385913000	3.645117000	-2.792812000
C	2.676819000	1.872010000	-2.811164000
H	2.052097000	1.220767000	-3.409643000
C	3.869115000	1.451072000	-2.229926000
C	4.306509000	0.074314000	-2.219695000
C	3.647562000	-0.950975000	-2.889563000
H	2.865355000	-0.771691000	-3.616783000
C	4.027964000	-2.233447000	-2.479309000
H	3.577707000	-3.144815000	-2.850543000
C	5.030698000	-2.252264000	-1.523180000
C	5.465651000	-3.425802000	-0.787122000
C	4.461525000	-4.275211000	-0.336706000
C	4.520657000	-5.641309000	0.175158000
H	5.406219000	-6.261661000	0.235411000
C	3.239240000	-5.978695000	0.505883000
H	2.891299000	-6.913569000	0.928810000
C	2.423050000	-4.783819000	0.257295000
C	-4.588233000	-6.515251000	-0.307400000
C	-5.274003000	-6.823551000	-1.505110000
C	-6.222027000	-7.851845000	-1.499728000
C	-6.517961000	-8.581643000	-0.346185000
C	-5.832394000	-8.258982000	0.828485000
C	-4.868736000	-7.248020000	0.870235000
C	-4.993686000	-6.084432000	-2.795358000
H	-5.400016000	-5.066106000	-2.776102000
H	-5.447120000	-6.606062000	-3.644106000
H	-3.918735000	-5.994682000	-2.985211000
C	-7.528920000	-9.704219000	-0.371663000
H	-7.041691000	-10.675581000	-0.532254000
H	-8.258138000	-9.569183000	-1.177424000
H	-8.077264000	-9.771373000	0.574438000
C	-4.165824000	-6.943610000	2.175091000

H	-3.117593000	-7.264475000	2.153747000
H	-4.656493000	-7.458983000	3.006806000
H	-4.160809000	-5.870269000	2.392295000
C	-7.469201000	4.071401000	-0.019639000
C	-8.073118000	4.586745000	1.147671000
C	-9.276583000	5.290621000	1.037806000
C	-9.896423000	5.507461000	-0.195953000
C	-9.281621000	4.990292000	-1.339147000
C	-8.079993000	4.276222000	-1.275651000
C	-7.443713000	4.379490000	2.507238000
H	-7.297508000	3.315489000	2.726115000
H	-8.070926000	4.805840000	3.296406000
H	-6.455428000	4.849872000	2.568672000
C	-11.178751000	6.301293000	-0.293193000
H	-10.975573000	7.374978000	-0.405524000
H	-11.793993000	6.181394000	0.605204000
H	-11.777053000	5.993002000	-1.157335000
C	-7.456175000	3.743919000	-2.547015000
H	-6.419203000	4.080758000	-2.657512000
H	-8.017663000	4.078140000	-3.425084000
H	-7.433736000	2.647857000	-2.558980000
C	4.142555000	6.028139000	-0.753084000
C	4.618296000	6.259507000	0.557519000
C	5.701790000	7.126241000	0.740445000
C	6.321026000	7.777335000	-0.327693000
C	5.829387000	7.539661000	-1.615368000
C	4.761807000	6.671755000	-1.851523000
C	4.008152000	5.583168000	1.767729000
H	3.046903000	6.033857000	2.041332000
H	4.676302000	5.672679000	2.630217000
H	3.823237000	4.518348000	1.591372000
C	7.502821000	8.691805000	-0.106674000
H	8.448502000	8.177648000	-0.324340000
H	7.551443000	9.041125000	0.929755000
H	7.457117000	9.570751000	-0.759388000
C	4.267717000	6.468738000	-3.266656000
H	4.770818000	7.156027000	-3.953526000
H	3.188125000	6.640556000	-3.345421000
H	4.452607000	5.447461000	-3.618830000
C	6.906126000	-3.660326000	-0.487207000
C	7.819081000	-3.902824000	-1.542999000
C	9.163225000	-4.125749000	-1.240161000
C	9.643357000	-4.094556000	0.073110000
C	8.729888000	-3.843770000	1.098212000
C	7.369472000	-3.631250000	0.849044000
C	7.365998000	-3.967963000	-2.984818000
H	7.054444000	-2.986018000	-3.358298000
H	6.510088000	-4.640968000	-3.109515000
H	8.175655000	-4.328600000	-3.626450000
C	11.110613000	-4.300350000	0.366391000
H	11.683535000	-3.380866000	0.186512000
H	11.541914000	-5.078276000	-0.273440000
H	11.274607000	-4.589214000	1.409547000
C	6.450563000	-3.346642000	2.019589000
H	5.765898000	-2.518382000	1.808608000
H	7.036827000	-3.084877000	2.906196000
H	5.832632000	-4.215712000	2.272993000
N	-1.325366000	-4.844759000	0.418378000
N	-3.780868000	3.438165000	0.406391000
N	0.761975000	4.383978000	-0.431845000
N	3.152518000	-3.811111000	-0.262309000
S	-4.719531000	0.941350000	0.075648000
S	-5.526925000	-3.403495000	-0.133814000
S	4.592494000	2.770864000	-1.325745000
S	5.529716000	-0.598385000	-1.151814000
H	9.855619000	-4.331781000	-2.054147000
H	9.083998000	-3.808379000	2.126577000
H	6.289379000	8.045987000	-2.461870000
H	6.072055000	7.293550000	1.749991000
H	-9.748017000	5.146201000	-2.310305000
H	-9.741611000	5.678881000	1.942241000
H	-6.741608000	-8.089306000	-2.426207000
H	-6.056145000	-8.807003000	1.742000000
C	0.400706000	-0.073398000	1.582581000
C	2.215000000	-0.235783000	2.972579000
C	3.263356000	-0.771831000	3.713420000
C	4.135120000	-0.136980000	4.605337000
C	1.753821000	1.163680000	2.953748000
C	4.164088000	1.204895000	4.991886000
C	2.269386000	2.230588000	3.681568000
C	3.340436000	2.255550000	4.583592000
H	3.427981000	-1.839950000	3.591178000
H	4.885633000	-0.777612000	5.062564000
H	4.937091000	1.468256000	5.711641000
H	1.765989000	3.184225000	3.541345000
H	3.554399000	3.224761000	5.028096000

H	-0.335776000	-2.894913000	1.040254000
H	-1.870814000	1.958959000	0.878728000
H	-0.351276000	-0.332012000	0.846104000

Conformer-12

C	4.806046000	-3.149263000	-1.324824000
C	3.880672000	-2.833838000	-2.306381000
H	3.179601000	-3.565239000	-2.686039000
C	3.919303000	-1.497713000	-2.720875000
H	3.231846000	-1.085402000	-3.449071000
C	4.850050000	-0.725598000	-2.035965000
C	4.854327000	0.717594000	-2.036316000
C	3.932859000	1.495349000	-2.727291000
H	3.249624000	1.087711000	-3.462078000
C	3.897940000	2.831172000	-2.311167000
H	3.203317000	3.566683000	-2.694836000
C	4.818206000	3.140708000	-1.323093000
C	4.863975000	4.382666000	-0.578473000
C	3.642906000	4.911094000	-0.187295000
C	3.317543000	6.256575000	0.271101000
H	4.012315000	7.082065000	0.360747000
C	1.973558000	6.264082000	0.499839000
H	1.372638000	7.087698000	0.864427000
C	1.508493000	4.893517000	0.247914000
C	0.203469000	4.284445000	0.546800000
C	0.258221000	2.978536000	1.146029000
C	-0.708162000	2.499786000	1.982969000
H	-1.508522000	3.179524000	2.254076000
C	-0.817326000	1.160516000	2.475554000
C	-0.820424000	-1.157706000	2.477148000
C	-0.714807000	-2.497887000	1.986286000
H	-1.516732000	-3.175338000	2.258488000
C	0.250186000	-2.979826000	1.149577000
C	0.192309000	-4.286039000	0.551366000
C	1.495840000	-4.897514000	0.251072000
C	1.958751000	-6.269247000	0.500142000
H	1.357036000	-7.092291000	0.864696000
C	3.302376000	-6.263964000	0.268910000
H	3.995672000	-7.090974000	0.355954000
C	3.629477000	-4.918466000	-0.188065000
C	4.850665000	-4.392206000	-0.582211000
C	-1.033486000	-4.873993000	0.203450000
C	-1.286312000	-6.222666000	-0.293071000
H	-0.550499000	-7.002657000	-0.434100000
C	-2.624373000	-6.298971000	-0.530022000
H	-3.183079000	-7.143262000	-0.912538000
C	-3.166821000	-4.972045000	-0.230111000
C	-4.514912000	-4.550534000	-0.451155000
C	-4.961006000	-3.229658000	-0.391885000
C	-6.315987000	-2.832583000	-0.613242000
H	-7.092178000	-3.566770000	-0.791828000
C	-6.534002000	-1.482752000	-0.597710000
H	-7.509784000	-1.043997000	-0.766631000
C	-5.369065000	-0.694674000	-0.360885000
C	-5.367205000	0.706022000	-0.361881000
C	-6.530011000	1.496851000	-0.599966000
H	-7.506931000	1.060450000	-0.768413000
C	-6.308412000	2.846078000	-0.617389000
H	-7.082623000	3.582071000	-0.797126000
C	-4.952414000	3.239865000	-0.396378000
C	-4.502856000	4.559500000	-0.457243000
C	-3.153720000	4.977775000	-0.236459000
C	-2.607921000	6.303137000	-0.537309000
H	-3.164450000	7.148473000	-0.920693000
C	-1.270147000	6.223783000	-0.299811000
H	-0.532347000	7.001839000	-0.441201000
C	-1.020785000	4.874873000	0.197871000
C	6.161524000	5.017006000	-0.212490000
C	7.027288000	5.499864000	-1.225127000
C	8.239475000	6.085912000	-0.858987000
C	8.636526000	6.195883000	0.478081000
C	7.777254000	5.699888000	1.459162000
C	6.542657000	5.118964000	1.145988000
C	6.653844000	5.428219000	-2.689361000
H	6.656232000	4.397267000	-3.060947000
H	7.360729000	6.003515000	-3.295016000
H	5.649601000	5.828056000	-2.869944000
C	9.949216000	6.847552000	0.843684000
H	9.882446000	7.941470000	0.773725000
H	10.754878000	6.531454000	0.171282000
H	10.246807000	6.601997000	1.868088000
C	5.679110000	4.593027000	2.274151000
H	4.862777000	5.283387000	2.516320000
H	6.278752000	4.458144000	3.179865000
H	5.216338000	3.633092000	2.025931000

C	6.147728000	-5.030527000	-0.221305000
C	6.533297000	-5.134742000	1.135711000
C	7.767314000	-5.719471000	1.444070000
C	8.621695000	-6.217088000	0.459549000
C	8.220242000	-6.104903000	-0.876030000
C	7.008468000	-5.515063000	-1.237411000
C	5.675007000	-4.607387000	2.267208000
H	5.215161000	-3.645310000	2.021801000
H	6.277735000	-4.476182000	3.171409000
H	4.856767000	-5.295046000	2.510587000
C	9.933895000	-6.872660000	0.819911000
H	9.864996000	-7.966151000	0.745614000
H	10.233984000	-6.631760000	1.844685000
H	10.738816000	-6.555308000	0.147188000
C	6.629961000	-5.441130000	-2.700233000
H	5.624110000	-5.838377000	-2.877578000
H	7.333280000	-6.017543000	-3.308965000
H	6.633499000	-4.409832000	-3.070846000
C	-5.518417000	-5.616952000	-0.802665000
C	-6.153543000	-6.350301000	0.221918000
C	-7.067604000	-7.351728000	-0.122413000
C	-7.369670000	-7.650802000	-1.453658000
C	-6.723020000	-6.918773000	-2.453134000
C	-5.804963000	-5.906089000	-2.154074000
C	-5.858879000	-6.070194000	1.678807000
H	-4.804594000	-6.253886000	1.917077000
H	-6.468311000	-6.705589000	2.329136000
H	-6.062346000	-5.024455000	1.936981000
C	-8.382564000	-8.717070000	-1.801627000
H	-9.394767000	-8.296896000	-1.876670000
H	-8.414755000	-9.503787000	-1.040115000
H	-8.155571000	-9.186895000	-2.764743000
C	-5.130799000	-5.148547000	-3.276425000
H	-5.419929000	-5.556653000	-4.249961000
H	-4.038962000	-5.198979000	-3.196828000
H	-5.398290000	-4.085406000	-3.263462000
C	-5.503538000	5.628109000	-0.810161000
C	-5.788876000	5.916606000	-2.161967000
C	-6.704220000	6.931338000	-2.462377000
C	-7.349332000	7.666045000	-1.463866000
C	-7.048494000	7.367555000	-0.132218000
C	-6.137124000	6.364130000	0.213450000
C	-5.116211000	5.156228000	-3.283298000
H	-5.385552000	4.093582000	-3.268740000
H	-4.024270000	5.204868000	-3.203912000
H	-5.404734000	5.563429000	-4.257392000
C	-8.359400000	8.734518000	-1.813284000
H	-9.372569000	8.316739000	-1.888695000
H	-8.130641000	9.203081000	-2.776597000
H	-8.390189000	9.521864000	-1.052368000
C	-5.843604000	6.084830000	1.670725000
H	-6.049141000	5.039728000	1.929807000
H	-6.452089000	6.722003000	2.320203000
H	-4.789066000	6.266771000	1.909251000
N	2.494180000	4.120515000	-0.166136000
N	2.482470000	-4.125730000	-0.163190000
N	-2.207848000	-4.150523000	0.212810000
N	-2.196892000	4.154259000	0.207377000
S	5.784637000	-1.732008000	-0.943630000
S	5.786318000	1.718014000	-0.936209000
S	-3.970519000	-1.769740000	-0.117422000
S	-3.965829000	1.777721000	-0.119787000
H	-6.915209000	7.154298000	-3.506767000
H	-7.533467000	7.932216000	0.662138000
H	-6.934939000	-7.142255000	-3.497223000
H	-7.553746000	-7.914335000	0.672684000
H	8.870464000	-6.487853000	-1.660390000
H	8.068534000	-5.781168000	2.487894000
H	8.893566000	6.467606000	-1.640734000
H	8.074993000	5.759801000	2.504091000
C	-0.290825000	0.000304000	1.878478000
C	-1.676690000	0.740373000	3.544672000
C	-2.362761000	1.589164000	4.405949000
C	-3.211694000	1.268416000	5.471565000
C	-1.678642000	-0.733819000	3.545693000
C	-3.583240000	0.007448000	5.943820000
C	-2.366959000	-1.579609000	4.408133000
C	-3.215032000	-1.255154000	5.473307000
H	-2.218439000	2.653160000	4.231856000
H	-3.637789000	2.116513000	6.002542000
H	-4.260135000	0.008933000	6.796350000
H	-2.225452000	-2.644220000	4.235496000
H	-3.643367000	-2.101388000	6.005451000
H	1.164609000	2.406962000	0.963244000
H	1.157790000	-2.410484000	0.965915000
H	0.336967000	-0.001123000	0.995345000

Conformer-13

C	-5.599430000	3.063974000	0.232908000
C	-6.964203000	2.640143000	0.240737000
H	-7.773116000	3.357635000	0.175794000
C	-7.147266000	1.286841000	0.309363000
H	-8.126151000	0.822977000	0.302749000
C	-5.940331000	0.529356000	0.360560000
C	-5.893483000	-0.867732000	0.341906000
C	-7.046933000	-1.702413000	0.267492000
H	-8.054602000	-1.304914000	0.270788000
C	-6.773840000	-3.038152000	0.163202000
H	-7.532905000	-3.806130000	0.077549000
C	-5.383811000	-3.369682000	0.149008000
C	-4.885121000	-4.654173000	-0.056536000
C	-3.498506000	-4.996944000	-0.062281000
C	-2.945918000	-6.275539000	-0.517569000
H	-3.516528000	-7.119625000	-0.881963000
C	-1.594373000	-6.157517000	-0.420828000
H	-0.844443000	-6.889608000	-0.690703000
C	-1.342366000	-4.833088000	0.132876000
C	-0.109899000	-4.254059000	0.454669000
C	-0.083415000	-2.951395000	0.105925000
C	0.991201000	-2.458194000	1.739558000
H	1.842121000	-3.115930000	1.885082000
C	1.142929000	-1.119275000	2.220336000
C	1.060990000	1.197731000	2.249246000
C	0.818285000	2.533038000	1.795758000
H	1.628027000	3.240395000	1.944011000
C	-0.290529000	2.967859000	1.126868000
C	-0.394532000	4.269515000	0.531505000
C	-1.661728000	4.779779000	0.225640000
C	-1.998181000	6.088976000	-0.318761000
H	-1.296904000	6.866292000	-0.592351000
C	-3.355570000	6.126422000	-0.401252000
H	-3.979307000	6.936657000	-0.755334000
C	-3.825512000	4.813958000	0.049067000
C	-5.187308000	4.382549000	0.054246000
C	0.859889000	4.951183000	0.167598000
C	1.306069000	6.333549000	0.383712000
H	0.718473000	7.134077000	0.816484000
C	2.618855000	6.374472000	0.009903000
H	3.289604000	7.224213000	0.035494000
C	2.939716000	5.041425000	-0.489660000
C	4.131361000	4.524502000	-0.983110000
C	4.057190000	3.254854000	-1.677566000
C	3.029446000	2.853992000	-2.517092000
H	2.243843000	3.531915000	-2.821511000
C	3.083023000	1.505967000	-2.886827000
H	2.318999000	1.030477000	-3.489022000
C	4.141380000	0.806270000	-2.318580000
C	4.237805000	-0.636233000	-2.328851000
C	3.369840000	-1.465121000	-3.028782000
H	2.674970000	-1.096382000	-3.773229000
C	3.414643000	-2.805205000	-2.622538000
H	2.764312000	-3.577281000	-3.012878000
C	4.353722000	-3.069124000	-1.640861000
C	4.471657000	-4.313623000	-0.897958000
C	3.287413000	-4.883565000	-0.456537000
C	3.018616000	-6.212629000	0.085647000
H	3.732926000	-7.021993000	0.170703000
C	1.694288000	-6.226929000	0.413001000
H	1.131779000	-7.039435000	0.856780000
C	1.184653000	-4.878172000	0.125172000
C	-5.872189000	-5.761325000	-0.314904000
C	-6.356949000	-5.992035000	-1.620039000
C	-7.262069000	-7.037329000	-1.834490000
C	-7.701351000	-7.860943000	-0.794546000
C	-7.211308000	-7.612771000	0.490518000
C	-6.301876000	-6.581932000	0.749776000
C	-5.913631000	-5.132540000	-2.783234000
H	-6.236592000	-4.091712000	-2.662888000
H	-6.328810000	-5.507009000	-3.724169000
H	-4.821846000	-5.114253000	-2.876406000
C	-8.656152000	-9.002856000	-1.056138000
H	-8.114882000	-9.930567000	-1.286470000
H	-9.311614000	-8.790961000	-1.907795000
H	-9.287859000	-9.205405000	-0.184423000
C	-5.800641000	-6.357516000	2.159011000
H	-4.713810000	-6.485529000	2.223270000
H	-6.266175000	-7.062107000	2.855271000
H	-6.017345000	-5.341272000	2.507854000
C	-6.245128000	5.428320000	-0.177832000
C	-6.719368000	6.199170000	0.904990000
C	-7.694847000	7.174078000	0.670856000

C	-8.208284000	7.414836000	-0.606471000	C	5.266412000	-2.854105000	1.067728000
C	-7.723964000	6.641285000	-1.664673000	C	4.330904000	-2.207687000	1.905870000
C	-6.752311000	5.652318000	-1.475597000	H	3.579863000	-2.768327000	2.440011000
C	-6.195675000	5.980208000	2.306892000	C	4.441319000	-0.830748000	1.925922000
H	-6.346199000	4.946007000	2.637355000	H	3.784809000	-0.182251000	2.496371000
H	-6.699719000	6.641061000	3.019041000	C	5.482528000	-0.319830000	1.129897000
H	-5.118564000	6.174635000	2.367748000	C	5.662956000	1.036271000	0.778807000
C	-9.236048000	8.497879000	-0.840483000	C	6.770959000	1.687244000	0.210198000
H	-8.756876000	9.463463000	-1.051942000	H	7.723752000	1.193236000	0.048997000
H	-9.875917000	8.640232000	0.037175000	C	6.526163000	3.015282000	-0.103794000
H	-9.879927000	8.262384000	-1.694760000	H	7.262230000	3.678880000	-0.542258000
C	-6.262520000	4.845630000	-2.657835000	C	5.202054000	3.449354000	0.155625000
H	-5.172278000	4.897696000	-2.756054000	C	4.652523000	4.696205000	-0.209661000
H	-6.705557000	5.212011000	-3.589200000	C	3.278783000	4.997186000	-0.096293000
H	-6.519085000	3.784419000	-2.557218000	C	2.615213000	6.189193000	-0.617478000
C	5.441600000	5.202461000	-0.766246000	H	3.100725000	7.024587000	-1.104613000
C	5.967771000	5.332566000	0.539796000	C	1.285204000	6.001671000	-0.408786000
C	7.206518000	5.960986000	0.709861000	H	0.479404000	6.651489000	-0.717592000
C	7.934011000	6.473550000	-0.365451000	C	1.149854000	4.710289000	0.267707000
C	7.391271000	6.341189000	-1.647681000	C	-0.047897000	4.039617000	0.641996000
C	6.168042000	5.707321000	-1.872100000	C	0.040596000	2.701096000	1.163575000
C	5.249369000	4.792919000	1.759621000	C	-0.949053000	2.120030000	1.910173000
H	4.414593000	5.438443000	2.056642000	H	-1.795800000	2.750043000	2.158671000
H	5.938527000	4.728113000	2.607656000	C	-1.057319000	0.760882000	2.348426000
H	4.834061000	3.795417000	1.582589000	C	-0.980387000	-1.564830000	2.371763000
C	9.279112000	7.128528000	-0.157619000	C	-0.750020000	-2.920999000	1.958271000
H	10.098071000	6.427733000	-0.368068000	H	-1.569821000	-3.613445000	2.118964000
H	9.401862000	7.474464000	0.873825000	C	0.369614000	-3.392268000	1.337805000
H	9.413022000	7.988866000	-0.822754000	C	0.519509000	-4.712482000	0.767641000
C	5.630527000	5.611900000	-3.282865000	C	1.855671000	-5.181886000	0.614050000
H	6.250729000	6.193634000	-3.971507000	C	2.403612000	-6.384576000	-0.013568000
H	4.603911000	5.989572000	-3.350256000	H	1.844189000	-7.219766000	-0.413082000
H	5.611671000	4.576599000	-3.641670000	C	3.758421000	-6.219724000	-0.034533000
C	5.806807000	-4.897355000	-0.583068000	H	4.500813000	-6.900067000	-0.432375000
C	6.633019000	-5.377867000	-1.628502000	C	4.021205000	-4.907536000	0.559936000
C	7.878791000	-5.922405000	-1.313252000	C	5.239845000	-4.178623000	0.571649000
C	8.348466000	-5.988242000	0.002652000	C	-0.654478000	-5.360521000	0.226122000
C	7.523436000	-5.500695000	1.017178000	C	-0.964241000	-6.764370000	-0.061464000
C	6.258908000	-4.961048000	0.755364000	H	-0.330530000	-7.619020000	0.138921000
C	6.179858000	-5.353148000	-3.071439000	C	-2.241170000	-6.785000000	-0.548850000
H	6.111297000	-4.330470000	-3.458909000	H	-2.809333000	-7.647434000	-0.874956000
H	5.188210000	-5.804486000	-3.190841000	C	-2.674369000	-5.391119000	-0.613411000
H	6.880739000	-5.905384000	-3.704747000	C	-3.854864000	-4.828147000	-1.129517000
C	9.717748000	-6.547419000	0.308848000	C	-3.878735000	-3.415393000	-1.366016000
H	10.503273000	-5.808460000	0.101780000	C	-2.780411000	-2.593897000	-1.644676000
H	9.936610000	-7.429281000	-0.303651000	H	-1.800216000	-3.003323000	-1.834955000
H	9.807631000	-6.834614000	1.361426000	C	-3.067685000	-1.234017000	-1.647168000
C	5.434874000	-4.440768000	1.915520000	H	-2.329658000	-0.466309000	-1.850125000
H	4.967069000	-3.477626000	1.686705000	C	-4.402054000	-0.928965000	-1.371133000
H	6.066791000	-4.309144000	2.799669000	C	-4.906166000	0.392787000	-1.163818000
H	4.627684000	-5.132898000	2.182462000	C	-6.201457000	0.911261000	-1.213273000
N	-2.527038000	-4.160052000	0.326649000	H	-7.072149000	0.314533000	-1.465514000
N	-2.801920000	4.035926000	0.426201000	C	-6.251126000	2.284588000	-0.949836000
N	1.823955000	4.219559000	-0.361659000	H	-7.164541000	2.868153000	-0.969867000
N	2.122233000	-4.118469000	-0.407991000	C	-5.005690000	2.869891000	-0.658764000
S	-4.546763000	1.632381000	0.381200000	C	-4.760234000	4.243361000	-0.350942000
S	-4.429195000	-1.875536000	0.335997000	C	-3.497191000	4.721700000	0.006538000
S	5.156455000	1.899075000	-1.392656000	C	-3.086004000	6.095080000	0.270392000
S	5.228099000	-1.590253000	-1.235923000	H	-3.729161000	6.965677000	0.267262000
H	8.500224000	-6.308112000	-2.119189000	C	-1.745138000	6.047016000	0.512442000
H	7.872397000	-5.536882000	2.047287000	H	-1.099263000	6.869334000	0.789066000
H	7.935512000	6.744739000	-2.499385000	C	-1.354703000	4.637129000	0.425500000
H	7.613726000	6.048717000	1.715211000	C	5.570045000	5.718687000	-0.820139000
H	-8.111511000	6.810279000	-2.667792000	C	5.763130000	5.759631000	-2.217544000
H	-8.062075000	7.760763000	1.511065000	C	6.622466000	6.723906000	-2.755297000
H	-7.632643000	-7.211110000	-2.843195000	C	7.292263000	7.650031000	-1.951161000
H	-7.544556000	-8.238166000	1.316858000	C	7.087997000	7.588929000	-0.570092000
C	0.476185000	0.023423000	1.741030000	C	6.238885000	6.641619000	0.011496000
C	2.159060000	-0.672803000	3.128344000	C	5.059797000	4.784267000	-3.135161000
C	3.011372000	-1.498230000	3.852867000	H	5.298503000	3.745251000	-2.880584000
C	4.020758000	-1.150584000	4.758906000	H	5.349547000	4.952216000	-4.177027000
C	2.107483000	0.801968000	3.145979000	H	3.970274000	4.883171000	-3.066666000
C	4.424591000	0.121393000	5.171512000	C	8.190003000	8.702705000	-2.559231000
C	2.902313000	1.668230000	3.887795000	H	7.627200000	9.614114000	-2.802428000
C	3.935035000	1.371349000	4.785637000	H	8.650418000	8.349474000	-3.488231000
H	2.872045000	-2.566790000	3.703129000	H	8.992222000	8.991776000	-1.871726000
H	4.559067000	-1.984719000	5.203000000	C	6.050525000	6.619828000	1.512098000
H	5.237778000	0.141357000	5.894932000	H	4.998504000	6.759149000	1.786539000
H	2.689277000	2.727613000	3.761050000	H	6.633537000	7.413313000	1.989759000
H	4.416114000	2.230658000	5.247063000	H	6.363996000	5.662479000	1.944665000
H	-1.007109000	-2.382801000	1.003248000	C	6.455806000	-4.745128000	-0.096527000
H	-1.179841000	2.346623000	1.078578000	C	7.506807000	-5.257912000	0.697190000
H	-0.300324000	0.005795000	0.985842000	C	8.637358000	-5.786672000	0.069051000
				C	8.763530000	-5.817221000	-1.322942000
				C	7.718290000	-5.295506000	-2.088133000
				C	6.562799000	-4.763319000	-1.504787000

Conformer-14

C	7.420865000	-5.253728000	2.207431000
H	7.399820000	-4.233602000	2.608690000
H	8.280548000	-5.768992000	2.646832000
H	6.509850000	-5.750774000	2.560196000
C	9.985530000	-6.417506000	-1.978357000
H	9.886625000	-7.506430000	-2.083317000
H	10.889727000	-6.231330000	-1.388393000
H	10.144594000	-6.007453000	-2.981210000
C	5.467393000	-4.212953000	-2.391980000
H	4.579076000	-4.855342000	-2.381703000
H	5.813031000	-4.135350000	-3.427544000
H	5.144232000	-3.218319000	-2.067104000
C	-5.068567000	-5.662424000	-1.373216000
C	-5.769169000	-6.233029000	-0.285895000
C	-6.905553000	-7.006991000	-0.543706000
C	-7.364172000	-7.243066000	-1.841394000
C	-6.650864000	-6.677724000	-2.902759000
C	-5.519065000	-5.885746000	-2.696203000
C	-5.336540000	-6.014328000	1.148639000
H	-4.447466000	-6.604945000	1.398407000
H	-6.135395000	-6.305980000	1.837778000
H	-5.085792000	-4.965990000	1.341751000
C	-8.608198000	-8.062543000	-2.092181000
H	-9.492137000	-7.419506000	-2.199495000
H	-8.806717000	-8.753686000	-1.266402000
H	-8.522891000	-8.649351000	-3.013361000
C	-4.782486000	-5.316997000	-3.888889000
H	-5.180978000	-5.729429000	-4.820849000
H	-3.711287000	-5.544030000	-3.847660000
H	-4.873996000	-4.225886000	-3.940473000
C	-5.917950000	5.197425000	-0.419495000
C	-6.246498000	5.819661000	-1.642776000
C	-7.323252000	6.711428000	-1.680813000
C	-8.086525000	7.000221000	-0.546139000
C	-7.740333000	6.374588000	0.654370000
C	-6.669829000	5.478205000	0.740539000
C	-5.448123000	5.548523000	-2.898359000
H	-5.472596000	4.487030000	-3.170716000
H	-4.393217000	5.816570000	-2.768930000
H	-5.842396000	6.122791000	-3.742216000
C	-9.266073000	7.941731000	-0.621632000
H	-10.185798000	7.406837000	-0.894564000
H	-9.109702000	8.720832000	-1.375489000
H	-9.449837000	8.432479000	0.340071000
C	-6.332290000	4.834971000	2.067505000
H	-6.322717000	3.741324000	1.994641000
H	-7.061116000	5.117668000	2.833384000
H	-5.338677000	5.138140000	2.418117000
N	2.372030000	4.141902000	0.441572000
N	2.859090000	-4.348054000	0.964982000
N	-1.691884000	-4.585293000	-0.107084000
N	-2.421240000	3.880186000	0.130816000
S	6.407446000	-1.646709000	0.424718000
S	4.278430000	2.133356000	0.881499000
S	-5.331652000	-2.412940000	-1.177836000
S	-3.745636000	1.641893000	-0.719521000
H	-7.569495000	7.194526000	-2.624535000
H	-8.316873000	6.590042000	1.552069000
H	-6.982613000	-6.860442000	-3.923103000
H	-7.447842000	-7.435513000	0.296975000
H	7.802195000	-5.297277000	-3.173264000
H	9.441698000	-6.184243000	0.685318000
H	6.771340000	6.749761000	-3.833244000
H	7.603348000	8.297421000	0.075877000
C	-0.416696000	-0.388434000	1.836246000
C	-2.036399000	0.308190000	3.299882000
C	-2.852670000	1.130270000	4.069563000
C	-3.822316000	0.780946000	5.016845000
C	-1.990416000	-1.163376000	3.309074000
C	-4.215394000	-0.490665000	5.439105000
C	-2.754713000	-2.031644000	4.081905000
C	-3.747120000	-1.739186000	5.024005000
H	-2.718748000	2.199270000	3.923274000
H	-4.336501000	1.615284000	5.488240000
H	-4.997149000	-0.511688000	6.196221000
H	-2.550311000	-3.090376000	3.939959000
H	-4.211115000	-2.600661000	5.498657000
H	0.976035000	2.177453000	0.985696000
H	1.254413000	-2.765553000	1.296175000
H	0.332555000	-0.373440000	1.053101000

14

Conformer-1

C	6.528864000	-0.601309000	0.377957000
---	-------------	--------------	-------------

C	7.554899000	0.330921000	0.552782000
H	8.586118000	0.026361000	0.684779000
C	7.140916000	1.664535000	0.526444000
H	7.822411000	2.498708000	0.644582000
C	5.771135000	1.822150000	0.315186000
C	5.112978000	3.092398000	0.154798000
C	5.746790000	4.327684000	0.085573000
H	6.820446000	4.437529000	0.185401000
C	4.892487000	5.411844000	-0.152215000
H	5.235095000	6.435252000	-0.244304000
C	3.544558000	5.074263000	-0.279207000
C	2.486453000	5.987616000	-0.616587000
C	1.124991000	5.741438000	-0.525208000
C	0.046866000	6.552569000	-1.041767000
H	0.197039000	7.463112000	-1.604454000
C	-1.142431000	5.942010000	-0.759911000
H	-2.126092000	6.267884000	-1.065814000
C	-0.882303000	4.728529000	-0.030784000
C	-1.738391000	3.751999000	0.468066000
C	-1.164664000	2.529907000	0.992425000
C	-1.753135000	1.696916000	1.892265000
H	-2.713350000	1.992110000	2.304163000
C	0.640892000	-2.716675000	1.651113000
C	1.646081000	-2.638240000	0.743945000
C	2.267764000	-3.826908000	0.143558000
C	3.712378000	-3.810865000	0.072202000
C	4.643935000	-4.920558000	-0.145516000
H	4.394752000	-5.961565000	-0.293758000
C	5.893186000	-4.392083000	-0.059576000
H	6.839734000	-4.907510000	-0.155132000
C	5.715266000	-2.963197000	0.173649000
C	6.724573000	-2.019140000	0.280668000
C	1.434923000	-4.821638000	-0.376441000
C	1.639204000	-6.171728000	-0.865894000
H	2.584563000	-6.691948000	-0.879822000
C	0.441709000	-6.683057000	-1.283169000
H	0.263678000	-7.661625000	-1.708371000
C	-0.576671000	-5.661445000	-1.146359000
C	-1.907591000	-5.645830000	-1.541960000
C	-2.570145000	-4.349816000	-1.628123000
C	-2.017234000	-3.173336000	-2.112958000
H	-1.038901000	-3.146282000	-2.579572000
C	-2.844091000	-2.043637000	-1.980183000
H	-2.565802000	-1.052041000	-2.319187000
C	-4.070935000	-2.309537000	-1.397692000
C	-5.042921000	-1.303380000	-1.032487000
C	-6.427051000	-1.329372000	-0.933011000
H	-7.026817000	-2.209571000	-1.140062000
C	-6.970982000	-0.074480000	-0.591578000
H	-8.035434000	0.112948000	-0.503012000
C	-6.023300000	0.934054000	-0.394709000
C	-6.283349000	2.317614000	-0.088279000
C	-5.263022000	3.223312000	0.162376000
C	-5.323917000	4.663568000	0.368741000
H	-6.222572000	5.265932000	0.406811000
C	-4.030064000	5.081382000	0.493905000
H	-3.680231000	6.086915000	0.690649000
C	-3.193702000	3.882391000	0.384718000
C	2.908412000	7.342528000	-1.117673000
C	3.318340000	7.504596000	-2.460307000
C	3.706730000	8.771673000	-2.905412000
C	3.707892000	9.885543000	-2.060034000
C	3.308397000	9.702633000	-0.734290000
C	2.905490000	8.453571000	-0.247347000
C	3.337222000	6.335826000	-3.419418000
H	4.077840000	5.584202000	-3.121633000
H	3.582897000	6.667416000	-4.433038000
H	2.367451000	5.826779000	-3.453001000
C	4.107451000	11.249361000	-2.573756000
H	3.264247000	11.752448000	-3.066106000
H	4.915453000	11.180156000	-3.310496000
H	4.444909000	11.900900000	-1.760860000
C	2.481949000	8.319341000	1.199138000
H	1.403747000	8.139339000	1.288772000
H	2.714507000	9.231411000	1.757802000
H	2.985594000	7.480283000	1.691449000
C	8.151174000	-2.499910000	0.277678000
C	8.759048000	-2.900279000	1.485931000
C	10.086736000	-3.341775000	1.463020000
C	10.825597000	-3.404772000	0.278909000
C	10.202517000	-3.001807000	-0.905665000
C	8.879481000	-2.548898000	-0.930084000
C	8.003005000	-2.859738000	2.795586000
H	7.577600000	-1.868076000	2.986519000
H	8.660788000	-3.114306000	3.632400000
H	7.165388000	-3.566838000	2.796534000

C	12.247219000	-3.917371000	0.274018000
H	12.280525000	-4.997774000	0.078645000
H	12.738278000	-3.747279000	1.238115000
H	12.846943000	-3.430334000	-0.502634000
C	8.252048000	-2.129594000	-2.240706000
H	7.359087000	-2.724014000	-2.465490000
H	8.958314000	-2.252167000	-3.067596000
H	7.935331000	-1.080441000	-2.218444000
C	-2.632135000	-6.909053000	-1.862974000
C	-2.863770000	-7.879323000	-0.858815000
C	-3.556760000	-9.050579000	-1.186929000
C	-4.029201000	-9.297746000	-2.476578000
C	-3.797624000	-8.325808000	-3.455397000
C	-3.113462000	-7.141431000	-3.176109000
C	-2.411993000	-7.678761000	0.572764000
H	-1.336372000	-7.855847000	0.694492000
H	-2.936275000	-8.370701000	1.239662000
H	-2.605233000	-6.658443000	0.919549000
C	-4.751745000	-10.581045000	-2.813529000
H	-5.599103000	-10.400592000	-3.484766000
H	-5.132380000	-11.074597000	-1.913329000
H	-4.085861000	-11.292440000	-3.320485000
C	-2.875757000	-6.146274000	-4.289307000
H	-3.156438000	-6.573940000	-5.256934000
H	-1.822819000	-5.846925000	-4.340539000
H	-3.457333000	-5.227703000	-4.148143000
C	-7.712034000	2.775978000	-0.061413000
C	-8.347114000	3.179034000	-1.255384000
C	-9.678775000	3.602837000	-1.203003000
C	-10.398945000	3.637085000	-0.005595000
C	-9.750571000	3.227203000	1.162256000
C	-8.418574000	2.799744000	1.159130000
C	-7.611691000	3.165909000	-2.576782000
H	-7.266159000	2.158423000	-2.835547000
H	-6.722871000	3.806668000	-2.547014000
H	-8.257783000	3.520110000	-3.385746000
C	-11.828155000	4.126658000	0.028073000
H	-12.352760000	3.897964000	-0.905900000
H	-11.872754000	5.215385000	0.166406000
H	-12.388620000	3.672104000	0.851941000
C	-7.762393000	2.371696000	2.453332000
H	-7.335979000	1.365031000	2.375740000
H	-8.485870000	2.371904000	3.274479000
H	-6.940438000	3.043701000	2.726729000
N	0.508748000	4.639597000	0.055852000
N	4.371500000	-2.662430000	0.258509000
N	0.079997000	-4.594131000	-0.566353000
N	-3.946712000	2.806056000	0.198969000
S	4.987140000	0.251101000	0.196002000
S	3.378932000	3.315258000	-0.084316000
S	-4.201863000	-4.026717000	-1.027946000
S	-4.405107000	0.276760000	-0.620094000
H	-10.165599000	3.913369000	-2.125622000
H	-10.294727000	3.238444000	2.104827000
H	-4.155472000	-8.497234000	-4.469162000
H	-3.741217000	-9.785221000	-0.405240000
H	-10.760460000	-3.039135000	-1.839574000
H	10.554061000	-3.644214000	2.398382000
H	4.017090000	8.890845000	-3.941982000
H	3.311680000	10.553950000	-0.056024000
H	-0.173585000	2.263966000	0.626487000
H	-0.361710000	-3.715113000	-0.345186000
H	0.974649000	4.036581000	0.717822000
H	0.341201000	-3.710575000	1.981848000
H	2.083834000	-1.675941000	0.492884000
C	-0.285176000	-0.352014000	1.595625000
C	-1.234059000	0.417815000	2.294852000
C	-0.119889000	-1.612823000	2.193774000
C	-1.678507000	-0.366507000	3.407015000
C	-0.966589000	-1.656750000	3.343151000
C	-2.604354000	0.032326000	4.363052000
C	-1.078444000	-2.722262000	4.234048000
C	-3.094875000	-0.650987000	5.476985000
C	-3.013813000	1.032127000	4.232937000
H	-1.866334000	-2.861237000	5.373399000
H	-0.449011000	-3.583015000	4.016233000
C	-2.766452000	-1.937954000	5.930906000
H	-3.828693000	-0.111950000	6.076272000
H	-1.789733000	-3.795944000	5.920990000
O	-3.374865000	-2.403391000	7.059952000
H	-3.983898000	-1.729131000	7.400482000
H	0.183584000	-0.053963000	0.665064000

Conformer-2

C	3.790386000	-4.418305000	0.792769000
---	-------------	--------------	-------------

C	3.240465000	-3.512236000	1.690270000
H	2.306580000	-3.710143000	2.195319000
C	3.978179000	-2.324955000	1.824791000
H	3.683080000	-1.504579000	2.470364000
C	5.117531000	-2.273464000	1.035460000
C	5.907583000	-1.091124000	0.774653000
C	7.240714000	-0.877966000	0.479609000
H	7.974248000	-1.677861000	0.476372000
C	7.560341000	0.471452000	0.203866000
H	8.560376000	0.810342000	-0.039695000
C	6.473198000	1.347489000	0.245117000
C	6.451390000	2.744662000	-0.108457000
C	5.316879000	3.543858000	-0.110136000
C	5.133714000	4.837804000	-0.734799000
H	5.922441000	5.375987000	-1.242015000
C	3.815380000	5.189653000	-0.656170000
H	3.352583000	6.061734000	-1.096118000
C	3.098299000	4.160490000	0.056606000
C	1.752479000	3.981481000	0.346807000
C	1.310840000	2.710415000	0.914201000
C	0.223121000	2.578773000	1.717086000
H	-0.279834000	3.496012000	2.010358000
C	-1.602695000	-2.138673000	1.780649000
C	-0.928667000	-2.900829000	0.882112000
C	-1.348148000	-4.230041000	0.421011000
C	-0.267104000	-5.180157000	0.250316000
C	-0.234359000	-6.522698000	-0.348271000
H	-1.072223000	-7.084003000	-0.738776000
C	1.074112000	-6.896864000	-0.374712000
H	1.489521000	-7.822273000	-0.753004000
C	1.833366000	-5.782585000	0.190094000
C	3.212035000	-5.628300000	0.252018000
C	-2.682253000	-4.454415000	0.073805000
C	-3.451922000	-5.647206000	-0.194728000
H	-3.072731000	-6.655323000	-0.116211000
C	-4.736435000	-5.286998000	-0.495767000
H	-5.556796000	-5.945421000	-0.746219000
C	-4.839765000	-3.842602000	-0.475488000
C	-5.930851000	-3.044163000	-0.802271000
C	-5.861626000	-1.610808000	-0.965760000
C	-6.903389000	-0.684561000	-0.932176000
H	-7.929015000	-0.981644000	-0.745202000
C	-6.505138000	0.656919000	-1.136517000
H	-7.198212000	1.492148000	-1.124344000
C	-5.148292000	0.815367000	-1.357935000
C	-4.306649000	1.970591000	-1.546025000
C	-3.021032000	1.947177000	-2.069293000
H	-2.587787000	1.057335000	-2.512668000
C	-2.336331000	3.164422000	-1.957735000
H	-1.319158000	3.318403000	-2.286809000
C	-3.074004000	4.178436000	-1.363620000
C	-2.600099000	5.490349000	-0.980789000
C	-1.272734000	5.630164000	-0.593339000
C	-0.489935000	6.842125000	-0.373383000
H	-0.843940000	7.859379000	-0.485334000
C	0.767316000	6.426474000	-0.041215000
H	1.614656000	7.047854000	0.222417000
C	0.724265000	4.958341000	-0.018897000
C	7.741823000	3.345895000	-0.592187000
C	8.121011000	3.223155000	-1.946892000
C	9.330336000	3.785913000	-2.368683000
C	10.177600000	4.465019000	-1.488585000
C	9.787926000	4.567956000	-0.150690000
C	8.586080000	4.022680000	0.313605000
C	7.242626000	2.499605000	-2.943048000
H	7.085354000	1.454084000	-2.654438000
H	7.693324000	2.511584000	-3.940303000
H	6.250406000	2.959920000	-3.014525000
C	11.464831000	5.089726000	-1.974986000
H	11.300903000	6.116970000	-2.327878000
H	11.893965000	4.525893000	-2.810342000
H	12.214114000	5.137209000	-1.177504000
C	8.213247000	4.163250000	1.772892000
H	7.311546000	4.773873000	1.901265000
H	9.022272000	4.636733000	2.337894000
H	8.003933000	3.189479000	2.230117000
C	4.119964000	-6.663081000	-0.339761000
C	4.840965000	-7.525818000	0.517528000
C	5.688537000	-8.485008000	-0.040762000
C	5.853310000	-8.611507000	-1.423874000
C	5.141229000	-7.741616000	-2.251373000
C	4.272102000	-6.770597000	-1.739263000
C	4.691949000	-7.437774000	2.019816000
H	5.036942000	-6.471029000	2.404638000
H	5.270710000	-8.223527000	2.514900000
H	3.644400000	-7.543170000	2.325456000

C	6.761183000	-9.672033000	-2.001901000
H	6.264838000	-10.651546000	-2.025358000
H	7.673252000	-9.788016000	-1.405651000
H	7.056068000	-9.430841000	-3.028372000
C	3.532184000	-5.859996000	-2.695998000
H	2.468572000	-6.118030000	-2.758842000
H	3.954754000	-5.936422000	-3.702742000
C	3.586043000	-4.811712000	-2.384538000
C	-7.270274000	-3.695209000	-0.984850000
C	-8.013873000	-4.120113000	0.138163000
C	-9.266247000	-4.714373000	-0.057635000
C	-9.803783000	-4.905142000	-1.332162000
C	-9.054877000	-4.472870000	-2.431325000
C	-7.802832000	-3.870248000	-2.283285000
C	-7.493124000	-3.936650000	1.547471000
H	-6.674782000	-4.631655000	1.772065000
H	-8.287695000	-4.113484000	2.279295000
H	-7.102143000	-2.925754000	1.704970000
C	-11.143666000	-5.577301000	-1.522395000
H	-11.707264000	-5.123883000	-2.345445000
H	-11.756137000	-5.513687000	-0.616937000
H	-11.024577000	-6.642617000	-1.761896000
C	-7.037559000	-3.427629000	-3.509863000
H	-7.534486000	-3.768928000	-4.423290000
H	-6.015091000	-3.821616000	-3.509711000
H	-6.954708000	-2.335398000	-3.559776000
C	-3.542452000	6.649997000	-0.961269000
C	-4.032163000	7.182062000	-2.177568000
C	-4.914432000	8.263529000	-2.138528000
C	-5.340615000	8.829257000	-0.932483000
C	-4.855767000	8.280855000	0.256079000
C	-3.958729000	7.206466000	0.268738000
C	-3.597035000	6.622061000	-3.513384000
H	-3.966910000	5.601657000	-3.665650000
H	-2.504810000	6.578005000	-3.593808000
H	-3.972762000	7.241416000	-4.333547000
C	-6.281803000	10.010967000	-0.921373000
H	-7.054383000	9.915918000	-1.692636000
H	-5.744852000	10.948844000	-1.117128000
H	-6.781133000	10.116483000	0.047250000
C	-3.481269000	6.661127000	1.598547000
H	-3.509157000	5.566850000	1.624559000
H	-4.108814000	7.037207000	2.412855000
H	-2.447044000	6.957516000	1.808907000
N	4.057949000	3.198685000	0.369603000
N	0.959519000	-4.783028000	0.574867000
N	-3.580840000	-3.409340000	-0.100922000
N	-0.479433000	4.519200000	-0.349427000
S	5.313296000	-3.775840000	0.152572000
S	5.027999000	0.423841000	0.658805000
S	-4.358206000	-0.754884000	-1.316317000
S	-4.697205000	3.584565000	-0.971877000
H	-5.279811000	8.675245000	-3.077527000
H	-5.186388000	8.696617000	1.205947000
H	-9.455473000	-4.609854000	-3.434227000
H	-9.837960000	-5.031288000	0.812703000
H	5.265637000	-7.813963000	-3.330127000
H	6.236437000	-9.150590000	0.623833000
H	9.617526000	3.688541000	-3.414128000
H	10.436979000	5.084771000	0.553952000
H	1.887499000	1.821540000	0.655597000
H	-3.312806000	-2.447456000	0.044498000
H	3.898990000	2.503864000	1.082609000
H	-2.497775000	-2.563228000	2.233347000
H	0.038511000	-2.564526000	0.519873000
C	-0.374975000	0.097306000	1.556372000
C	-0.399192000	1.359742000	2.175994000
C	-1.254817000	-0.799559000	2.202182000
C	-1.304278000	1.270176000	3.283952000
C	-1.841666000	-0.102295000	3.301561000
C	-1.596362000	2.296304000	4.173042000
C	-2.743233000	-0.634776000	4.223114000
C	-2.448657000	2.313263000	5.279556000
H	-1.081477000	3.237113000	3.989488000
C	-3.363906000	-0.044265000	5.319119000
H	-3.005344000	-1.680230000	4.074148000
C	-3.234791000	1.272551000	5.793961000
H	-2.506240000	3.259901000	5.816930000
H	-4.039897000	-0.663465000	5.901432000
O	-3.994498000	1.515103000	6.900970000
H	-3.868347000	2.434509000	7.184428000
H	0.174824000	-0.127095000	0.649456000

Conformer-3

C	6.311427000	-1.445401000	0.208999000
---	-------------	--------------	-------------

C	7.411271000	-0.596736000	0.079052000
H	8.378532000	-0.957470000	-0.250627000
C	7.141877000	0.752697000	0.382980000
H	7.878713000	1.546613000	0.320753000
C	5.834181000	0.963670000	0.780187000
C	5.132765000	2.200841000	1.067019000
C	4.165479000	2.429002000	2.021668000
H	3.929533000	1.707572000	2.796859000
C	3.520962000	3.683545000	1.889561000
H	2.775340000	4.043498000	2.591026000
C	3.958365000	4.438969000	0.809908000
C	3.379347000	5.634585000	0.211111000
C	2.003478000	5.749054000	0.134682000
C	1.178252000	6.753653000	-0.509079000
H	1.567690000	7.655129000	-0.961783000
C	-0.123608000	6.341626000	-0.478738000
H	-0.964471000	6.844764000	-0.932599000
C	-0.199979000	5.070353000	0.212128000
C	-1.230474000	4.165680000	0.458013000
C	-0.866532000	2.871597000	1.023215000
C	-1.612959000	2.136201000	1.881236000
H	-2.558305000	2.547468000	2.223584000
C	0.264695000	-2.525194000	1.848835000
C	1.219899000	-2.616985000	0.885365000
C	1.603968000	-3.892259000	0.280393000
C	3.005133000	-4.098568000	-0.013493000
C	3.659349000	-5.241410000	-0.666914000
H	3.186121000	-6.129394000	-1.057538000
C	4.981731000	-4.942654000	-0.731912000
H	5.776981000	-5.541175000	-1.156450000
C	5.124875000	-3.604496000	-0.169208000
C	6.276218000	-2.836260000	-0.161790000
C	0.589116000	-4.793937000	-0.069476000
C	0.599487000	-6.199333000	-0.394198000
H	1.468494000	-6.836518000	-0.353213000
C	-0.676862000	-6.601624000	-0.663293000
H	-1.004166000	-7.597737000	-0.924878000
C	-1.564985000	-5.466105000	-0.549741000
C	-2.936188000	-5.460380000	-0.782530000
C	-3.828372000	-4.333092000	-0.764390000
C	-5.222228000	-4.418096000	-0.820928000
H	-5.736104000	-5.370938000	-0.841115000
C	-5.882282000	-3.184234000	-0.835297000
H	-6.962259000	-3.094784000	-0.854767000
C	-5.045089000	-2.074748000	-0.802579000
C	-5.481970000	-0.702773000	-0.866293000
C	-6.779114000	-0.314947000	-1.200998000
H	-7.556116000	-1.019174000	-1.474139000
C	-6.971912000	1.068538000	-1.183767000
H	-7.914502000	1.545152000	-1.424781000
C	-5.837264000	1.809237000	-0.843494000
C	-5.796887000	3.243513000	-0.771911000
C	-4.681364000	3.989445000	-0.428726000
C	-4.578748000	5.442847000	-0.368612000
H	-5.381315000	6.146000000	-0.548949000
C	-3.288286000	5.713964000	-0.033639000
H	-2.850456000	6.685604000	0.152321000
C	-2.618187000	4.417934000	0.112812000
C	4.267517000	6.635132000	-0.459724000
C	4.360417000	6.701093000	-1.868249000
C	5.215482000	7.646471000	-2.449788000
C	5.980922000	8.526336000	-1.684071000
C	5.884372000	8.437866000	-0.291021000
C	5.048387000	7.510637000	0.333036000
C	3.578469000	5.769974000	-2.771061000
H	3.577550000	4.742464000	-2.394306000
H	4.009102000	5.761568000	-3.777385000
H	2.528902000	6.074536000	-2.864269000
C	6.878431000	9.553468000	-2.334051000
H	6.434273000	10.556893000	-2.288979000
H	7.055159000	9.320374000	-3.389041000
H	7.851554000	9.610933000	-1.832795000
C	4.976065000	7.466227000	1.842586000
H	3.944772000	7.577899000	2.197359000
H	5.577152000	8.266521000	2.285387000
H	5.342647000	6.511473000	2.237953000
C	7.565347000	-3.448293000	-0.634568000
C	8.430312000	-4.057939000	0.298497000
C	9.628671000	-4.619377000	-0.154204000
C	9.994014000	-4.595479000	-1.502927000
C	9.124059000	-3.981301000	-2.407714000
C	7.914976000	-3.406600000	-2.000844000
C	8.080278000	-4.112956000	1.768863000
H	7.927094000	-3.110188000	2.184320000
H	8.876653000	-4.598512000	2.341210000
H	7.151676000	-4.669776000	1.939600000

C	11.279688000	-5.236283000	-1.972103000
H	11.128475000	-6.294684000	-2.224047000
H	12.053952000	-5.195673000	-1.198353000
H	11.670006000	-4.742795000	-2.868645000
C	7.008184000	-2.759901000	-3.024398000
H	6.050628000	-3.287831000	-3.102888000
H	7.475825000	-2.760825000	-4.013788000
H	6.775992000	-1.722281000	-2.759501000
C	-3.574048000	-6.793719000	-1.073723000
C	-3.959192000	-7.644098000	-0.015592000
C	-4.558124000	-8.873786000	-0.313216000
C	-4.782661000	-9.287837000	-1.628341000
C	-4.397951000	-8.428198000	-2.661723000
C	-3.800482000	-7.189154000	-2.410431000
C	-3.738987000	-7.250462000	-1.428650000
H	-2.672236000	-7.229881000	1.682717000
H	-4.228555000	-7.959580000	2.103460000
H	-4.134444000	-6.250788000	1.639479000
C	-5.401174000	-10.633784000	-1.927387000
H	-6.027446000	-10.597210000	-2.825511000
H	-6.021427000	-10.983818000	-1.095504000
H	-4.630245000	-11.396434000	-2.102035000
C	-3.404805000	-6.298938000	-3.566880000
H	-3.616664000	-6.785722000	-4.523830000
H	-2.336711000	-6.054558000	-3.539808000
H	-3.947415000	-5.346680000	-3.544433000
C	-7.069874000	3.973851000	-1.105252000
C	-7.336176000	4.354264000	-2.437550000
C	-8.525127000	5.033725000	-2.723148000
C	-9.455359000	5.348996000	-1.728925000
C	-9.171417000	4.958956000	-0.417489000
C	-7.995243000	4.278209000	-0.085139000
C	-6.360589000	4.043851000	-3.550797000
H	-6.158286000	2.969071000	-3.622214000
H	-5.395210000	4.536021000	-3.385682000
H	-6.751337000	4.380087000	-4.516082000
C	-10.717852000	6.111321000	-2.058554000
H	-11.065787000	5.891626000	-3.073700000
H	-10.555047000	7.195998000	-1.999599000
H	-11.527387000	5.867189000	-1.362340000
C	-7.734072000	3.885333000	1.352048000
H	-7.566824000	2.806678000	1.451285000
H	-8.580548000	4.157686000	1.990026000
H	-6.839450000	4.381611000	1.745889000
N	1.104070000	4.802388000	0.597623000
N	3.897450000	-3.146398000	0.272279000
N	-0.748460000	-4.414794000	-0.177560000
N	-3.466634000	3.414466000	-0.112414000
S	4.911605000	-0.527738000	0.756945000
S	5.270727000	3.585424000	-0.007089000
S	-3.367659000	-2.619100000	-0.746906000
S	-4.485372000	0.707948000	-0.527575000
H	-8.728084000	5.323255000	-3.752583000
H	-9.884299000	5.189215000	0.372181000
H	-4.567983000	-8.728562000	-3.694074000
H	-4.858653000	-9.523029000	0.507101000
H	9.391998000	-3.944917000	-3.462048000
H	10.294177000	-5.086754000	0.569286000
H	5.289545000	7.685841000	-3.534964000
H	6.476290000	9.110705000	0.327122000
H	0.103942000	2.465787000	0.733886000
H	-1.050790000	-3.469750000	0.006220000
H	1.398377000	3.932415000	1.010617000
H	-0.125855000	-3.459795000	2.249736000
H	1.758884000	-1.731185000	0.558576000
C	-0.395587000	-0.080034000	1.682957000
C	-1.253590000	0.815948000	2.342046000
C	-0.354390000	-1.321353000	2.347611000
C	-1.771550000	0.140575000	3.491738000
C	-1.194325000	-1.217905000	3.497854000
C	-2.648056000	0.683224000	4.423318000
C	-1.412040000	-2.216944000	4.444364000
C	-3.201836000	0.114284000	5.571364000
H	-2.953490000	1.711081000	4.237277000
C	-2.206013000	-2.212882000	5.587896000
H	-0.874863000	-3.148311000	4.274760000
C	-3.004897000	-1.173537000	6.093583000
H	-3.874529000	0.756678000	6.139687000
H	-2.223850000	-3.119810000	6.185040000
O	-3.653550000	-1.513698000	7.244794000
H	-4.189281000	-0.763515000	7.547697000
H	0.090416000	0.119872000	0.735119000

Conformer-4

C	4.656485000	-3.707488000	1.071183000
---	-------------	--------------	-------------

C	3.815265000	-2.850801000	1.859831000
H	2.871837000	-3.211981000	2.238927000
C	4.279307000	-1.580334000	2.007439000
H	3.741808000	-0.803510000	2.541150000
C	5.529527000	-1.320967000	1.358736000
C	6.043265000	-0.069598000	1.092143000
C	7.226081000	0.330459000	0.399981000
H	7.996693000	-0.386827000	0.136385000
C	7.273704000	1.653825000	0.054155000
H	8.079789000	2.099889000	-0.515802000
C	6.091136000	2.409339000	0.382601000
C	5.738635000	3.648165000	-0.124497000
C	4.418454000	4.224854000	-0.123156000
C	3.992960000	5.380869000	-0.821479000
H	4.649234000	6.036809000	-1.374632000
C	2.606916000	5.466989000	-0.729276000
H	1.973535000	6.193918000	-1.214337000
C	2.145629000	4.390536000	0.058086000
C	0.826130000	3.963019000	0.422758000
C	0.647016000	2.647849000	0.995978000
C	-0.370195000	2.364605000	1.860625000
H	-0.975809000	3.203500000	2.186629000
C	-1.253951000	-2.571801000	1.908388000
C	-0.320421000	-3.160458000	1.112226000
C	-0.425421000	-4.490713000	0.530807000
C	0.781509000	-5.189601000	0.341534000
C	1.096393000	-6.443920000	-0.318471000
H	0.395621000	-7.126846000	-0.779967000
C	2.460274000	-6.560408000	-0.281417000
H	3.064904000	-7.358813000	-0.692728000
C	2.957189000	-5.358397000	0.382604000
C	4.337581000	-4.918138000	0.483989000
C	-1.722096000	-4.942419000	0.106431000
C	-2.290315000	-6.207701000	-0.120820000
H	-1.801924000	-7.151709000	0.074988000
C	-3.601743000	-6.022527000	-0.564835000
H	-4.320179000	-6.792444000	-0.805946000
C	-3.860395000	-4.631904000	-0.634084000
C	-5.071561000	-3.971375000	-1.046805000
C	-5.320925000	-2.609216000	-1.093127000
C	-6.566873000	-2.014249000	-1.497229000
H	-7.402986000	-2.630219000	-1.803909000
C	-6.601410000	-0.651523000	-1.463448000
H	-7.476428000	-0.079379000	-1.748317000
C	-5.392734000	-0.012033000	-1.043265000
C	-5.190480000	1.356960000	-0.954075000
C	-6.208181000	2.333402000	-1.216097000
H	-7.218633000	2.058332000	-1.493959000
C	-5.797565000	3.624446000	-1.078261000
H	-6.440135000	4.482035000	-1.237941000
C	-4.420141000	3.794991000	-0.709240000
C	-3.796462000	5.021738000	-0.561139000
C	-2.408450000	5.217332000	-0.234203000
C	-1.718388000	6.495361000	-0.184423000
H	-2.167642000	7.471134000	-0.315591000
C	-0.402314000	6.206275000	0.055844000
H	0.405151000	6.908938000	0.211901000
C	-0.318937000	4.766985000	0.181077000
C	6.793920000	4.423592000	-0.869302000
C	6.963280000	4.250475000	-2.259594000
C	7.955094000	4.985715000	-2.918669000
C	8.778643000	5.890115000	-2.243227000
C	8.594231000	6.044103000	-0.866252000
C	7.617603000	5.328477000	-0.166396000
C	6.101979000	3.284342000	-3.042428000
H	6.208501000	2.257379000	-2.674031000
H	6.374815000	3.291575000	-4.102142000
H	5.039225000	3.540802000	-2.965452000
C	9.820722000	6.697066000	-2.982435000
H	9.426109000	7.677296000	-3.282170000
H	10.150351000	6.187420000	-3.893939000
H	10.702445000	6.881259000	-2.358929000
C	7.460622000	5.531814000	1.324186000
H	6.441225000	5.842137000	1.581697000
H	8.149765000	6.300470000	1.687284000
H	7.660471000	4.608874000	1.881099000
C	5.400898000	-5.724809000	-0.200306000
C	6.216805000	-6.590236000	0.560724000
C	7.200851000	-7.342207000	-0.088242000
C	7.403005000	-7.260679000	-1.468638000
C	6.588837000	-6.393464000	-2.201609000
C	5.587807000	-5.626449000	-1.596505000
C	6.038978000	-6.718728000	2.057646000
H	6.279514000	-5.782407000	2.574921000
H	6.690158000	-7.500847000	2.460284000
H	5.004766000	-6.969017000	2.320596000

C	8.454145000	-8.104930000	-2.151291000
H	8.053495000	-9.087491000	-2.435442000
H	9.313312000	-8.283763000	-1.495636000
H	8.819762000	-7.627182000	-3.066520000
C	4.735526000	-4.704737000	-2.439718000
H	3.686122000	-5.022084000	-2.445696000
H	5.088838000	-4.689190000	-3.475495000
H	4.756569000	-3.677748000	-2.058444000
C	-6.185566000	-4.895406000	-1.469154000
C	-7.115565000	-5.363479000	-0.517218000
C	-8.135763000	-6.227537000	-0.929846000
C	-8.259053000	-6.644699000	-2.257881000
C	-7.328772000	-6.166695000	-3.185014000
C	-6.293125000	-5.301540000	-2.816227000
C	-7.029919000	-4.940699000	0.932466000
H	-6.058738000	-5.201570000	1.368774000
H	-7.809507000	-5.427271000	1.526866000
H	-7.147153000	-3.856300000	1.043754000
C	-9.349380000	-7.604549000	-2.674528000
H	-9.661498000	-7.432188000	-3.710255000
H	-10.232870000	-7.510854000	-2.033993000
H	-9.009206000	-8.646843000	-2.608060000
C	-5.314996000	-4.811797000	-3.860493000
H	-5.538765000	-5.247849000	-4.838971000
H	-4.283943000	-5.076929000	-3.599486000
H	-5.345812000	-3.720649000	-3.961491000
C	-4.621193000	6.262371000	-0.784571000
C	-4.725023000	6.822042000	-2.075625000
C	-5.484291000	7.983607000	-2.254112000
C	-6.139995000	8.610354000	-1.190922000
C	-6.024236000	8.038909000	0.079052000
C	-5.274954000	6.878824000	0.302643000
C	-4.033871000	6.185123000	-3.260504000
H	-4.409486000	5.172970000	-3.451109000
H	-2.954798000	6.093801000	-3.092185000
H	-4.187855000	6.778922000	-4.166932000
C	-6.927012000	9.882945000	-1.403556000
H	-7.362596000	9.922392000	-2.407881000
H	-6.288752000	10.770031000	-1.292433000
H	-7.741422000	9.977404000	-0.677116000
C	-5.179615000	6.301736000	1.697550000
H	-5.591056000	5.286463000	1.742846000
H	-5.727012000	6.922021000	2.414402000
H	-4.137320000	6.235316000	2.030771000
N	3.277100000	3.673688000	0.417409000
N	1.939065000	-4.580525000	0.757210000
N	-2.710874000	-4.017944000	-0.206819000
N	-1.566003000	4.201886000	0.008437000
S	6.195100000	-2.844524000	0.722257000
S	5.058315000	1.386941000	1.412508000
S	-4.195040000	-1.278952000	-0.666845000
S	-3.669245000	2.179051000	-0.523320000
H	-5.563498000	8.409399000	-3.252829000
H	-6.529858000	8.507752000	0.921470000
H	-7.409488000	-6.474050000	-4.226082000
H	-8.852753000	-6.583047000	-0.192022000
H	6.735750000	-6.307639000	-3.276695000
H	7.826016000	-8.009078000	0.502790000
H	8.085980000	4.845584000	-3.990022000
H	9.228072000	6.739523000	-0.319046000
H	1.346732000	1.859324000	0.719783000
H	-2.532199000	-3.024424000	-0.217979000
H	3.246058000	2.812963000	0.943172000
H	-2.121025000	-3.154047000	2.213639000
H	0.617605000	-2.647309000	0.930124000
C	-0.464647000	-0.168917000	1.742824000
C	-0.766592000	1.071150000	2.331379000
C	-1.193516000	-1.204378000	2.356952000
C	-1.701245000	0.821818000	3.393634000
C	-1.968577000	-0.619137000	3.408034000
C	-2.240740000	1.784895000	4.240434000
C	-2.808565000	-1.312696000	4.281797000
C	-3.144560000	1.645189000	5.292493000
H	-1.911321000	2.806126000	4.063391000
C	-3.595550000	-0.843526000	5.325699000
H	-2.856891000	-2.388964000	4.130509000
C	-3.749280000	0.477702000	5.782872000
H	-3.417799000	2.568061000	5.803753000
H	-4.179161000	-1.575217000	5.876626000
O	-4.606300000	0.578045000	6.835341000
H	-4.684535000	1.506105000	7.108551000
H	0.158053000	-0.295599000	0.865411000

Conformer-5

C	6.306922000	-1.345880000	0.189101000
---	-------------	--------------	-------------

C	7.467687000	-0.574617000	0.287861000
H	8.449951000	-1.026945000	0.352528000
C	7.250657000	0.805519000	0.281574000
H	8.051362000	1.533034000	0.345797000
C	5.906756000	1.157486000	0.163367000
C	5.417186000	2.503946000	0.037156000
C	6.197097000	3.649589000	-0.071716000
H	7.279694000	3.624525000	-0.022813000
C	5.471762000	4.829697000	-0.282488000
H	5.931668000	5.802703000	-0.406374000
C	4.088701000	4.657292000	-0.345631000
C	3.131303000	5.675357000	-0.679189000
C	1.756635000	5.584479000	-0.522109000
C	0.749514000	6.448221000	-1.088002000
H	0.969869000	7.282935000	-1.738430000
C	-0.484210000	5.980389000	-0.735276000
H	-1.432612000	6.368094000	-1.072874000
C	-0.324812000	4.821334000	0.106326000
C	-1.245386000	3.984027000	0.735567000
C	-0.749926000	2.758968000	1.342248000
C	-1.346127000	2.066034000	2.348080000
H	-2.208902000	2.516901000	2.828469000
C	0.194426000	-2.707634000	2.029054000
C	1.184726000	-2.773979000	1.103813000
C	1.599331000	-3.952904000	0.344620000
C	3.032290000	-4.093988000	0.127893000
C	3.773843000	-5.343607000	-0.065010000
H	3.352820000	-6.339451000	-0.100285000
C	5.090403000	-5.005700000	-0.085699000
H	5.944626000	-5.661476000	-0.189451000
C	5.138665000	-3.557632000	0.075673000
C	6.282160000	-2.777970000	0.105156000
C	0.664021000	-4.808562000	-0.228616000
C	0.817180000	-5.864000000	-1.217427000
H	1.766167000	-6.239559000	-1.569522000
C	-0.413723000	-6.238287000	-1.664257000
H	-0.639052000	-6.980279000	-2.418127000
C	-1.419648000	-5.441499000	-0.985592000
C	-2.777617000	-5.355133000	-1.194969000
C	-3.545392000	-4.463373000	-0.316393000
C	-3.596622000	-4.461508000	1.063525000
H	-3.153035000	-5.255057000	1.655676000
C	-4.264482000	-3.344271000	1.620526000
H	-4.376865000	-3.183469000	2.686918000
C	-4.721828000	-2.444863000	0.676921000
C	-5.143265000	-1.082416000	0.938818000
C	-4.779073000	-0.357778000	2.060762000
H	-4.230036000	-0.793684000	2.886685000
C	-5.058791000	1.017112000	1.957875000
H	-4.787205000	1.746667000	2.709607000
C	-5.660780000	1.385401000	0.771274000
C	-5.841717000	2.741234000	0.273065000
C	-4.782976000	3.621160000	0.417332000
C	-4.738448000	5.059135000	0.166482000
H	-5.586625000	5.691506000	-0.063862000
C	-3.440002000	5.430328000	0.329555000
H	-3.041897000	6.434956000	0.276427000
C	-2.689460000	4.200090000	0.644547000
C	3.677848000	6.945347000	-1.271398000
C	4.067396000	6.984596000	-2.629626000
C	4.572956000	8.175822000	-3.158333000
C	4.711979000	9.330889000	-2.382422000
C	4.330096000	9.268868000	-1.040512000
C	3.812035000	8.099957000	-0.470614000
C	3.939294000	5.767548000	-3.517761000
H	4.623723000	4.969432000	-3.206700000
H	4.167074000	6.019109000	-4.558207000
H	2.928118000	5.347133000	-3.482148000
C	5.237782000	10.612495000	-2.986115000
H	4.440950000	11.167059000	-3.499902000
H	6.021504000	10.415929000	-3.726129000
H	5.653515000	11.275415000	-2.220085000
C	3.415082000	8.097198000	0.989685000
H	2.326164000	8.049872000	1.112114000
H	3.766285000	9.005921000	1.488610000
H	3.831703000	7.234237000	1.520442000
C	7.618417000	-3.467875000	0.034660000
C	8.237877000	-3.921462000	1.217999000
C	9.481574000	-4.556729000	1.130938000
C	10.124811000	-4.760616000	-0.092588000
C	9.492399000	-4.300842000	-1.251122000
C	8.251261000	-3.657044000	-1.212141000
C	7.582278000	-3.734144000	2.568352000
H	7.328469000	-2.684133000	2.752622000
H	8.244840000	-4.069515000	3.372222000
H	6.647258000	-4.301537000	2.641661000

C	11.452180000	-5.479439000	-0.164279000
H	11.312981000	-6.559924000	-0.304685000
H	12.031667000	-5.344578000	0.755313000
H	12.058416000	-5.120212000	-1.002947000
C	7.608299000	-3.183803000	-2.496615000
H	6.632309000	-3.657146000	-2.653839000
H	8.241215000	-3.417343000	-3.358254000
H	7.435827000	-2.101383000	-2.486214000
C	-3.437883000	-6.048425000	-2.343278000
C	-4.347955000	-7.105036000	-2.096273000
C	-4.972735000	-7.737759000	-3.172386000
C	-4.732674000	-7.356292000	-4.496529000
C	-3.842856000	-6.305512000	-4.722017000
C	-3.190201000	-5.642496000	-3.675011000
C	-4.637581000	-7.574512000	-0.688780000
H	-3.712845000	-7.796649000	-0.143348000
H	-5.252503000	-8.479896000	-0.699243000
H	-5.170389000	-6.812293000	-0.108240000
C	-5.405792000	-8.072778000	-5.643853000
H	-5.362873000	-7.482423000	-6.564907000
H	-6.459184000	-8.281320000	-5.424394000
H	-4.923193000	-9.037689000	-5.849855000
C	-2.258287000	-4.496141000	-4.009232000
H	-2.430315000	-4.149746000	-5.033194000
H	-1.203595000	-4.787324000	-3.932970000
H	-2.398402000	-3.644162000	-3.336233000
C	-7.091494000	3.121296000	-0.447565000
C	-7.059937000	3.399084000	-1.833429000
C	-8.254889000	3.732401000	-2.483118000
C	-9.472403000	3.812155000	-1.806605000
C	-9.481261000	3.531337000	-0.435835000
C	-8.320699000	3.179303000	0.254012000
C	-5.784950000	3.317972000	-2.647606000
H	-5.170297000	2.457942000	-2.364849000
H	-5.160613000	4.209281000	-2.514728000
H	-6.019340000	3.232959000	-3.713440000
C	-10.742969000	4.203305000	-2.523998000
H	-10.634666000	4.111000000	-3.609393000
H	-11.017279000	5.244589000	-2.308128000
H	-11.587780000	3.577920000	-2.213401000
C	-8.394492000	2.901135000	1.738836000
H	-8.164505000	1.854514000	1.967769000
H	-9.395634000	3.118570000	2.123556000
H	-7.676293000	3.512137000	2.298239000
N	1.053151000	4.606869000	0.171576000
N	3.856784000	-3.051648000	0.211089000
N	-0.707460000	-4.662647000	-0.077643000
N	-3.508903000	3.165187000	0.739191000
S	4.897047000	-0.281183000	0.102603000
S	3.715479000	2.936651000	-0.116003000
S	-4.380623000	-3.039262000	-0.939790000
S	-5.949601000	-0.045270000	-0.221984000
H	-8.229087000	3.928695000	-3.553198000
H	-10.420104000	3.586471000	0.112251000
H	-3.654946000	-5.980315000	-5.743584000
H	-5.665029000	-8.553515000	-2.971139000
H	9.977342000	-4.445079000	-2.214894000
H	9.958823000	-4.900823000	2.046683000
H	4.866021000	8.201228000	-4.206406000
H	4.439527000	10.153242000	-0.415485000
H	0.158470000	2.342092000	0.907234000
H	-1.115044000	-3.856766000	0.376096000
H	1.477841000	4.012290000	0.868026000
H	-0.285483000	-3.631091000	2.352138000
H	1.783248000	-1.885661000	0.913231000
C	-0.287424000	-0.216134000	2.002082000
C	-0.990979000	0.733840000	2.768375000
C	-0.297059000	-1.477873000	2.623111000
C	-1.444214000	0.066990000	3.950458000
C	-1.004178000	-1.342257000	3.853988000
C	-2.157391000	0.649397000	4.990581000
C	-1.219552000	-2.354790000	4.786207000
C	-2.642474000	0.086525000	6.173854000
H	-2.371355000	1.710694000	4.876393000
C	-1.888397000	-2.324824000	6.007979000
H	-0.793734000	-3.323306000	4.529356000
C	-2.521267000	-1.235582000	6.630205000
H	-3.181484000	0.766244000	6.833864000
H	-1.931489000	-3.249679000	6.575635000
O	-3.077180000	-1.560427000	7.833603000
H	-3.493281000	-0.773909000	8.220557000
H	0.111808000	-0.031561000	1.011736000

Conformer-6

C	6.429177000	-0.901699000	0.031865000
---	-------------	--------------	-------------

C	7.344097000	0.157460000	-0.294765000
H	8.303489000	-0.057302000	-0.751362000
C	6.884626000	1.420749000	-0.032010000
H	7.440262000	2.325862000	-0.256283000
C	5.601451000	1.446428000	0.587748000
C	4.790852000	2.523781000	0.907054000
C	3.590501000	2.459729000	1.672999000
H	3.326111000	1.574549000	2.242125000
C	2.838129000	3.600425000	1.652454000
H	1.960128000	3.735475000	2.273862000
C	3.352390000	4.648116000	0.813031000
C	2.707099000	5.768285000	0.310784000
C	1.268016000	5.861214000	0.271462000
C	0.420782000	6.890012000	-0.199335000
H	0.753426000	7.871953000	-0.505549000
C	-0.889712000	6.401443000	-0.231387000
H	-1.755473000	6.939336000	-0.586018000
C	-0.881458000	5.068297000	0.236253000
C	-1.857266000	4.020861000	0.409035000
C	-1.307799000	2.726812000	0.833581000
C	-1.816996000	1.962074000	1.827737000
H	-2.722937000	2.320827000	2.307489000
C	0.664693000	-2.445578000	2.104251000
C	1.665669000	-2.556965000	1.185643000
C	2.169858000	-3.839656000	0.707173000
C	3.505860000	-3.926869000	0.303474000
C	4.207794000	-5.017077000	-0.359079000
H	3.785376000	-5.974325000	-0.633029000
C	5.470924000	-4.566226000	-0.603195000
H	6.277391000	-5.087953000	-1.102085000
C	5.513883000	-3.190345000	-0.110313000
C	6.579269000	-2.243011000	-0.290265000
C	1.213487000	-4.923864000	0.559446000
C	1.271054000	-6.326754000	0.598719000
H	2.145850000	-6.906697000	0.857958000
C	-0.014630000	-6.828442000	0.320510000
H	-0.314905000	-7.867122000	0.302541000
C	-0.877255000	-5.737152000	0.109006000
C	-2.283753000	-5.651114000	-0.257854000
C	-2.995542000	-4.500593000	0.028538000
C	-2.626761000	-3.454843000	0.944359000
H	-1.848122000	-3.595898000	1.680112000
C	-3.364637000	-2.316037000	0.848875000
H	-3.202260000	-1.442083000	1.469222000
C	-4.426439000	-2.364290000	-0.104609000
C	-5.198902000	-1.272381000	-0.458251000
C	-6.425178000	-1.179037000	-1.181945000
H	-6.949682000	-2.053765000	-1.553787000
C	-6.892201000	0.102781000	-1.310397000
H	-7.825032000	0.361660000	-1.798709000
C	-6.037033000	1.122635000	-0.762371000
C	-6.233747000	2.494432000	-0.822667000
C	-5.220081000	3.427055000	-0.401618000
C	-5.276588000	4.884792000	-0.464905000
H	-6.138407000	5.478900000	-0.741328000
C	-4.033801000	5.329323000	-0.118106000
H	-3.716643000	6.358828000	-0.025561000
C	-3.233580000	4.145473000	0.159402000
C	3.489711000	6.847798000	-0.375586000
C	3.576329000	6.887415000	-1.785167000
C	4.318106000	7.907410000	-2.389510000
C	4.968703000	8.893196000	-1.642901000
C	4.872596000	8.833079000	-0.250037000
C	4.148599000	7.828286000	0.398715000
C	2.899588000	5.844950000	-2.646963000
H	3.156908000	4.829722000	-2.325411000
H	3.200122000	5.953639000	-3.693575000
H	1.807545000	5.931151000	-2.600391000
C	5.734031000	10.004900000	-2.322183000
H	5.087110000	10.870451000	-2.519420000
H	6.142621000	9.680080000	-3.285022000
H	6.565400000	10.356892000	-1.702028000
C	4.081792000	7.811232000	1.910046000
H	3.047238000	7.762824000	2.268287000
H	4.543984000	8.710617000	2.328601000
H	4.604004000	6.941860000	2.327054000
C	7.855815000	-2.706923000	-0.932076000
C	8.911104000	-3.182250000	-0.124805000
C	10.090438000	-3.621643000	-0.735246000
C	10.253969000	-3.607893000	-2.123098000
C	9.197159000	-3.131958000	-2.903839000
C	7.999771000	-2.683382000	-2.335835000
C	8.784026000	-3.218602000	1.381964000
H	8.635429000	-2.215715000	1.799224000
H	9.682410000	-3.645026000	1.839040000
H	7.923908000	-3.820118000	1.698252000

C	11.525071000	-4.118121000	-2.761775000
H	11.462259000	-5.194900000	-2.969614000
H	12.391523000	-3.964928000	-2.109341000
H	11.725060000	-3.615986000	-3.714472000
C	6.886518000	-2.180637000	-3.228009000
H	5.963449000	-2.752769000	-3.079177000
H	7.167282000	-2.259563000	-4.282876000
H	6.643845000	-1.131846000	-3.020615000
C	-2.886236000	-6.783916000	-1.024506000
C	-3.853276000	-7.614115000	-0.413311000
C	-4.397017000	-8.676085000	-1.143738000
C	-4.018271000	-8.939720000	-2.461781000
C	-3.067154000	-8.101620000	-3.051400000
C	-2.490167000	-7.033950000	-2.359459000
C	-4.306975000	-7.387863000	-1.012348000
H	-3.458510000	-7.244829000	1.690132000
H	-4.889862000	-8.241898000	1.371434000
H	-4.937986000	-6.494891000	1.098386000
C	-4.599909000	-10.108739000	-3.221948000
H	-4.727231000	-9.872677000	-4.284231000
H	-5.575464000	-10.402690000	-2.820705000
H	-3.944271000	-10.988096000	-3.163034000
C	-1.476713000	-6.155327000	-3.057946000
H	-1.437196000	-6.384507000	-4.127320000
H	-0.469804000	-6.296070000	-2.647187000
H	-1.722409000	-5.093113000	-2.948499000
C	-7.506044000	3.031471000	-1.413144000
C	-7.570789000	3.363529000	-2.783632000
C	-8.765895000	3.869656000	-3.305559000
C	-9.897912000	4.063656000	-2.509102000
C	-9.812944000	3.728071000	-1.155355000
C	-8.638814000	3.216412000	-0.592414000
C	-6.374719000	3.173997000	-3.689639000
H	-6.034462000	2.132126000	-3.696766000
H	-5.522630000	3.780242000	-3.360646000
H	-6.615854000	3.459297000	-4.718424000
C	-11.166953000	4.643986000	-3.089465000
H	-11.291492000	4.364725000	-4.141377000
H	-11.160665000	5.741541000	-3.044583000
H	-12.051704000	4.302705000	-2.541282000
C	-8.600077000	2.869284000	0.879494000
H	-8.432647000	1.797270000	1.037238000
H	-9.541297000	3.139456000	1.368643000
H	-7.786316000	3.393262000	1.394129000
N	0.439462000	4.803002000	0.547055000
N	4.348376000	-2.844625000	0.445418000
N	-0.101549000	-4.614953000	0.268275000
N	-4.016230000	3.016034000	0.007358000
S	4.980740000	-0.213416000	0.793004000
S	4.991371000	4.172992000	0.257812000
S	-4.495939000	-4.000102000	-0.823825000
S	-4.606396000	0.361936000	-0.044286000
H	-8.811846000	4.118216000	-4.364391000
H	-10.683813000	3.867233000	-0.517169000
H	-2.768859000	-8.279342000	-4.083044000
H	-5.136785000	-9.315516000	-0.665727000
H	9.304756000	-3.108314000	-3.986781000
H	10.902442000	-3.984204000	-0.107449000
H	4.391613000	7.927872000	-3.475209000
H	5.375749000	9.588226000	0.350970000
H	-0.383122000	2.398828000	0.357513000
H	-0.410191000	-3.679278000	0.050074000
H	0.772898000	3.888303000	0.798143000
H	0.342482000	-3.369292000	2.582157000
H	2.157326000	-1.669063000	0.797219000
C	-0.291695000	-0.101089000	1.722140000
C	-1.257109000	0.727069000	2.328865000
C	-0.072342000	-1.265032000	2.489623000
C	-1.648626000	0.092057000	3.554080000
C	-0.895964000	-1.164496000	3.657365000
C	-2.570614000	0.592395000	4.471560000
C	-0.944402000	-2.092626000	4.698705000
C	-3.009185000	0.061518000	5.682167000
H	-3.024791000	1.545725000	4.212704000
C	-1.699548000	-2.094329000	5.866058000
H	-0.283673000	-2.950448000	4.592630000
C	-2.624055000	-1.134324000	6.310760000
H	-3.750803000	0.656083000	6.215158000
H	-1.573551000	-2.937427000	6.538831000
O	-3.188091000	-1.452803000	7.506884000
H	-3.821230000	-0.764435000	7.766541000
H	0.153378000	0.078153000	0.749964000

Conformer-7

C	3.383114000	-4.568743000	-0.800081000
---	-------------	--------------	--------------

C	2.726398000	-3.390046000	-1.291308000
H	1.712481000	-3.435214000	-1.657665000
C	3.484332000	-2.263814000	-1.274369000
H	3.135280000	-1.302908000	-1.635894000
C	4.810642000	-2.436437000	-0.762067000
C	5.678846000	-1.392348000	-0.514315000
C	7.037171000	-1.337146000	-0.081746000
H	7.621199000	-2.238264000	0.078029000
C	7.532605000	-0.071661000	0.104459000
H	8.543531000	0.138791000	0.434729000
C	6.599919000	0.995729000	-0.147549000
C	6.804965000	2.361868000	-0.069853000
C	5.714510000	3.306635000	-0.212990000
C	5.677485000	4.584466000	-0.807376000
H	6.533975000	5.092053000	-1.228917000
C	4.346711000	5.015088000	-0.834328000
H	3.974627000	5.916178000	-1.298947000
C	3.546746000	4.032120000	-0.216074000
C	2.136700000	3.891508000	0.006943000
C	1.648985000	2.609223000	0.509536000
C	0.572561000	2.519949000	1.340980000
H	0.175434000	3.465103000	1.695422000
C	-1.728566000	-1.991368000	1.378064000
C	-1.110364000	-2.851422000	-0.522029000
C	-1.638831000	-4.136043000	0.075234000
C	-0.688970000	-5.118875000	-0.257607000
C	-0.817911000	-6.468042000	-0.779747000
H	-1.737696000	-6.977469000	-1.035097000
C	0.457567000	-6.950360000	-0.911397000
H	0.762613000	-7.918153000	-1.290117000
C	1.345691000	-5.862311000	-0.520219000
C	2.800451000	-5.803121000	-0.588504000
C	-3.066233000	-4.299202000	-0.522029000
C	-3.940049000	-5.401441000	-0.040790000
H	-3.649581000	-6.421573000	0.166151000
C	-5.241990000	-4.932875000	-0.258714000
H	-6.148537000	-5.521221000	-0.279029000
C	-5.187100000	-3.533043000	-0.443928000
C	-6.258016000	-2.580883000	-0.651468000
C	-6.073563000	-1.259164000	-1.018854000
C	-7.024789000	-0.179143000	-0.944052000
H	-8.048618000	-0.359415000	-0.637169000
C	-6.512719000	1.067956000	-1.193430000
H	-7.095275000	1.980440000	-1.113177000
C	-5.125483000	1.095795000	-1.529962000
C	-4.220868000	2.127887000	-1.677266000
C	-2.831287000	1.947542000	-1.974615000
H	-2.429834000	0.979086000	-2.251617000
C	-2.069468000	3.066653000	-1.862309000
H	-1.002608000	3.097488000	-2.019138000
C	-2.784896000	4.250038000	-1.474871000
C	-2.251332000	5.477397000	-1.129345000
C	-0.829862000	5.582510000	-0.823148000
C	0.023901000	6.761012000	-0.822984000
H	-0.283381000	7.776706000	-1.040929000
C	1.290346000	6.318652000	-0.526448000
H	2.176835000	6.927211000	-0.403011000
C	1.181202000	4.889334000	-0.308962000
C	8.186776000	2.912256000	0.105071000
C	9.122749000	2.840641000	-0.951317000
C	10.402654000	3.375487000	-0.762971000
C	10.785633000	3.979055000	0.436441000
C	9.845153000	4.039666000	1.469744000
C	8.554555000	3.525214000	1.325683000
C	8.773953000	2.213911000	-2.284102000
H	8.739779000	1.119267000	-2.223894000
H	9.517759000	2.480614000	-3.041499000
H	7.791129000	2.539956000	-2.640029000
C	12.164074000	4.574012000	0.606222000
H	12.157576000	5.655251000	0.413055000
H	12.883309000	4.124012000	-0.086001000
H	12.539683000	4.431630000	1.625634000
C	7.583170000	3.614589000	2.481238000
H	6.755779000	4.299530000	2.259593000
H	8.084430000	3.977492000	3.383874000
H	7.137006000	2.639647000	2.708685000
C	3.604590000	-7.041236000	-0.367150000
C	3.614940000	-7.654844000	0.907809000
C	4.371064000	-8.814062000	1.097810000
C	5.105268000	-9.398428000	0.061482000
C	5.076131000	-8.782102000	-1.191340000
C	4.343625000	-7.613943000	-1.427756000
C	2.843234000	-7.069341000	2.069578000
H	3.011914000	-5.991710000	2.166739000
H	3.136531000	-7.548909000	3.008814000
H	1.762667000	-7.207474000	1.944828000

C	5.884394000	-10.673444000	0.285525000
H	5.241562000	-11.557484000	0.176493000
H	6.313195000	-10.709425000	1.293118000
H	6.702643000	-10.775509000	-0.435082000
C	4.348704000	-7.007547000	-2.814308000
H	3.338133000	-6.749273000	-3.148170000
H	4.777875000	-7.707210000	-3.538432000
H	4.942122000	-6.086046000	-2.851666000
C	-7.654370000	-3.068909000	-0.388750000
C	-8.126826000	-3.201959000	0.935728000
C	-9.430716000	-3.658352000	1.151652000
C	-10.280517000	-3.996761000	0.094610000
C	-9.794764000	-3.857115000	-1.207888000
C	-8.499242000	-3.398747000	-1.470889000
C	-7.253749000	-2.846562000	-2.118474000
H	-6.409684000	-3.540205000	2.214734000
H	-7.826709000	-2.883561000	3.050289000
H	-6.830496000	-1.840670000	2.017972000
C	-11.673378000	-4.521916000	0.354444000
H	-12.350759000	-4.290200000	-0.474376000
H	-12.098720000	-4.095738000	1.269559000
H	-11.670922000	-5.613548000	0.476419000
C	-8.029498000	-3.268600000	-2.903176000
H	-8.753750000	-3.716019000	-3.591030000
H	-7.063478000	-3.762047000	-3.056596000
H	-7.897171000	-2.219203000	-3.192424000
C	-3.117438000	6.687910000	-0.978889000
C	-3.628820000	7.342352000	-2.122109000
C	-4.425652000	8.479658000	-1.954419000
C	-4.736496000	8.987220000	-0.690649000
C	-4.225609000	8.322049000	0.427405000
C	-3.417130000	7.188280000	0.308421000
C	-3.323719000	6.847278000	-3.518954000
H	-3.835958000	5.901729000	-3.733124000
H	-2.252265000	6.667571000	-3.659166000
H	-3.647291000	7.578050000	-4.266823000
C	-5.577358000	10.233285000	-0.537174000
H	-6.273540000	10.353084000	-1.374158000
H	-4.951152000	11.135231000	-0.503931000
H	-6.161602000	10.211336000	0.389243000
C	-2.893732000	6.508938000	1.554538000
H	-3.088971000	5.430965000	1.537162000
H	-3.363850000	6.928653000	2.449864000
H	-1.808614000	6.634416000	1.652033000
N	4.4221179000	3.022112000	0.151475000
N	0.644475000	-4.806091000	-0.106020000
N	-3.863331000	-3.194769000	-0.314067000
N	-0.126752000	4.498891000	-0.488863000
S	5.089283000	-4.161299000	-0.419609000
S	5.058753000	0.270977000	-0.676573000
S	-4.537102000	-0.587016000	-1.626748000
S	-4.538739000	3.857014000	-1.388902000
H	-4.812802000	8.982435000	-2.838776000
H	-4.464684000	8.693775000	1.422298000
H	-10.440517000	-4.112629000	-2.046012000
H	-9.792529000	-3.748654000	2.174344000
H	5.637874000	-9.222533000	-2.013022000
H	4.388892000	-9.271430000	2.085470000
H	11.117597000	3.321784000	-1.581909000
H	10.124905000	4.497457000	2.416919000
H	2.161550000	1.701574000	0.193248000
H	-3.497042000	-2.254817000	-0.377799000
H	4.154536000	2.224288000	0.709357000
H	-2.684196000	-2.292564000	1.801525000
H	-0.093870000	-2.640506000	0.210353000
C	-0.247260000	0.092460000	1.164001000
C	-0.155042000	1.356339000	1.776607000
C	-1.235232000	-0.699791000	1.790773000
C	-1.093819000	1.367239000	2.865701000
C	-1.770901000	0.068360000	2.873890000
C	-1.299898000	2.426308000	3.744536000
C	-2.747238000	-0.364063000	3.775377000
C	-2.172298000	2.539351000	4.826325000
H	-0.687287000	3.307913000	3.572409000
C	-3.328975000	0.292787000	4.851552000
H	-3.113172000	-1.376664000	3.622624000
C	-3.077175000	1.592232000	5.327072000
H	-2.144281000	3.491579000	5.355685000
H	-4.081255000	-0.249463000	5.416842000
O	-3.834494000	1.917567000	6.409873000
H	-3.629170000	2.822357000	6.694979000
H	0.304468000	-0.201443000	0.278550000

Conformer-8

C	4.600861000	-4.327266000	0.062582000
---	-------------	--------------	-------------

C	6.024855000	-4.337666000	0.250402000
H	6.581545000	-5.266632000	0.224845000
C	6.593627000	-3.113935000	0.433924000
H	7.659418000	-2.966836000	0.562199000
C	5.667553000	-2.020248000	0.392820000
C	6.036726000	-0.685558000	0.443039000
C	7.370789000	-0.193998000	0.603601000
H	8.207620000	-0.862154000	0.769659000
C	7.507427000	1.160575000	-0.521921000
H	8.452803000	1.680586000	0.617921000
C	6.291111000	1.883688000	0.274562000
C	6.203430000	3.242412000	0.029410000
C	4.985004000	3.979561000	-0.177853000
C	4.792024000	5.181139000	-0.892796000
H	5.578010000	5.732015000	-1.389405000
C	3.426103000	5.466867000	-0.905571000
H	2.941401000	6.274914000	-1.433075000
C	2.758105000	4.472039000	-0.166494000
C	1.376866000	4.231914000	0.123644000
C	1.038838000	2.948721000	0.712736000
C	-0.019272000	2.759698000	1.549518000
H	-0.557418000	3.645078000	1.871721000
C	-1.338462000	-2.082229000	1.493134000
C	-0.507637000	-2.741127000	0.635726000
C	-0.772871000	-4.047316000	0.067553000
C	0.325788000	-4.841522000	-0.291782000
C	0.331449000	-6.146536000	-0.929115000
H	-0.530205000	-6.673177000	-1.314836000
C	1.633877000	-6.545460000	-0.964213000
H	2.037073000	-7.462808000	-1.372503000
C	2.408413000	-5.451573000	-0.384792000
C	3.840857000	-5.441548000	-0.241653000
C	-2.147461000	-4.463147000	-0.133872000
C	-2.804514000	-5.705176000	-0.115598000
H	-2.336624000	-6.652343000	0.111085000
C	-4.166582000	-5.483780000	-0.364642000
H	-4.949870000	-6.227984000	-0.395944000
C	-4.364230000	-4.100530000	-0.557372000
C	-5.591946000	-3.364075000	-0.782174000
C	-5.654393000	-2.035872000	-1.159869000
C	-6.791941000	-1.151437000	-1.100571000
H	-7.767223000	-0.518627000	-0.802410000
C	-6.518411000	0.167375000	-1.350835000
H	-7.260777000	0.956332000	-1.280829000
C	-5.155971000	0.451315000	-1.673945000
C	-4.456236000	1.631102000	-1.810500000
C	-3.053815000	1.708598000	-2.094339000
H	-2.484240000	0.833735000	-2.383916000
C	-2.507921000	2.943073000	-1.951758000
H	-1.463408000	3.165552000	-2.103343000
C	-3.429418000	3.972876000	-1.555761000
C	-3.115764000	5.263337000	-1.176360000
C	-1.732558000	5.560878000	-0.816072000
C	-1.005245000	6.817982000	-0.887166000
H	-1.409652000	7.778397000	-1.183471000
C	0.295663000	6.528370000	-0.549353000
H	1.116065000	7.229628000	-0.464916000
C	0.326969000	5.114960000	-0.231930000
C	7.475609000	4.034507000	-0.100649000
C	8.230689000	3.975801000	-1.292103000
C	9.400869000	4.737406000	-1.392157000
C	9.846069000	5.552638000	-0.348963000
C	9.084755000	5.593250000	0.823117000
C	7.905763000	4.856030000	0.964784000
C	7.802408000	3.112093000	-2.458359000
H	7.931836000	2.044979000	-2.240491000
H	8.393971000	3.344086000	-3.349424000
H	6.745045000	3.258258000	-2.703544000
C	11.097576000	6.387365000	-0.491061000
H	10.860510000	7.405671000	-0.827580000
H	11.787005000	5.955310000	-1.223972000
H	11.629356000	6.478709000	-0.462401000
C	7.120373000	4.939378000	2.254375000
H	6.139541000	5.404005000	2.096472000
H	7.656598000	5.534844000	2.999652000
H	6.937085000	3.946398000	2.680625000
C	4.554910000	-6.751178000	-0.446648000
C	4.638646000	-7.679701000	0.612868000
C	5.295547000	-8.896136000	0.400686000
C	5.862537000	-9.225338000	-0.833711000
C	5.765723000	-8.292666000	-1.869661000
C	5.123031000	-7.061188000	-1.700549000
C	4.039105000	-7.374254000	1.967300000
H	4.449348000	-6.450856000	2.392165000
H	4.233775000	-8.188412000	2.672373000
H	2.953777000	-7.234267000	1.902412000

C	6.535062000	-10.561454000	-1.049101000
H	5.813239000	-11.323222000	-1.373536000
H	7.000772000	-10.929395000	-0.128361000
H	7.310350000	-10.500905000	-1.820448000
C	5.046233000	-6.089896000	-2.857920000
H	4.014487000	-5.775731000	-3.051819000
H	5.440912000	-6.543215000	-3.772580000
H	5.621383000	-5.177551000	-2.659775000
C	-6.875057000	-4.101470000	-0.522929000
C	-7.323537000	-4.310537000	0.800062000
C	-8.521838000	-4.998774000	1.013025000
C	-9.287294000	-5.496236000	-0.045592000
C	-8.827004000	-5.278561000	-1.346562000
C	-7.636940000	-4.590062000	-1.606563000
C	-6.538745000	-3.791991000	1.984356000
H	-5.582940000	-4.319306000	2.090916000
H	-7.101967000	-3.925876000	2.913281000
H	-6.305601000	-2.726568000	1.876962000
C	-10.560578000	-6.268347000	0.211413000
H	-11.263186000	-6.173022000	-0.623319000
H	-11.064170000	-5.920799000	1.120062000
H	-10.356928000	-7.339604000	0.343781000
C	-7.189948000	-4.385546000	-3.037458000
H	-7.810276000	-4.969382000	-3.724693000
H	-6.146333000	-4.686532000	-3.180089000
H	-7.258431000	-3.332864000	-3.336853000
C	-4.155947000	6.327875000	-1.047424000
C	-4.766383000	6.872936000	-2.200256000
C	-5.726353000	7.879282000	-2.049889000
C	-6.105988000	8.360912000	-0.795080000
C	-5.495009000	7.805481000	0.332781000
C	-4.523678000	6.806234000	0.231630000
C	-4.396658000	6.405203000	-3.591048000
H	-4.786317000	5.401103000	-3.797029000
H	-3.310981000	6.359200000	-3.727553000
H	-4.807185000	7.082229000	-4.346877000
C	-7.126203000	9.467387000	-0.660940000
H	-7.823760000	9.474439000	-1.505245000
H	-6.643216000	10.453572000	-0.629997000
H	-7.710126000	9.365050000	0.260372000
C	-3.901506000	6.241709000	1.489700000
H	-3.907140000	5.146271000	1.484579000
H	-4.444784000	6.584964000	2.376237000
H	-2.855096000	6.553022000	1.593267000
N	3.740721000	3.583274000	0.250019000
N	1.617396000	-4.444636000	0.001031000
N	-3.126009000	-3.523333000	-0.404663000
N	-0.933419000	4.582174000	-0.386789000
S	4.012184000	-2.644705000	0.200763000
S	4.942310000	0.699746000	0.207108000
S	-4.262920000	-1.093472000	-1.758467000
S	-5.085729000	3.272696000	-1.511127000
H	-6.188466000	8.298767000	-2.941668000
H	-5.784617000	8.157234000	1.321535000
H	-9.408513000	-5.655504000	-2.185940000
H	-8.867451000	-5.147178000	2.034571000
H	6.201238000	-8.527692000	-2.839201000
H	5.364175000	-9.605393000	1.223621000
H	9.977966000	4.691601000	-2.313838000
H	9.417191000	6.215699000	1.651901000
H	1.657250000	2.091868000	0.449102000
H	-2.940432000	-2.530956000	-0.457411000
H	3.580386000	2.844754000	0.919829000
H	-2.231971000	-2.598460000	1.837159000
H	0.463654000	-2.317928000	0.399842000
C	-0.337963000	0.248244000	1.374259000
C	-0.532842000	1.494685000	1.992251000
C	-1.150849000	-0.737531000	1.966662000
C	-1.484910000	1.302245000	3.049652000
C	-1.872324000	-0.111727000	3.033747000
C	-1.940743000	2.289941000	3.916853000
C	-2.766759000	-0.748615000	3.896366000
C	-2.853989000	2.206623000	4.967089000
H	-1.524844000	3.282719000	3.760210000
C	-3.510986000	-0.235686000	4.951355000
H	-2.905362000	-1.814127000	3.726362000
C	-3.554180000	1.084311000	5.435022000
H	-3.048454000	3.138803000	5.497148000
H	-4.152715000	-0.927171000	5.489429000
O	-4.400070000	1.234666000	6.490735000
H	-4.400640000	2.160360000	6.782471000
H	0.276647000	0.087700000	0.496727000

Conformer-9

C	6.421465000	-1.095785000	-0.035761000
---	-------------	--------------	--------------

C	7.557063000	-0.216493000	0.027892000
H	8.565297000	-0.605015000	-0.052625000
C	7.257594000	1.104496000	0.166284000
H	8.009436000	1.884227000	0.198710000
C	5.851941000	1.390049000	0.212168000
C	5.313711000	2.664816000	0.228260000
C	6.062291000	3.885297000	0.266732000
H	7.141495000	3.887811000	0.364651000
C	5.323327000	5.024637000	0.158332000
H	5.744813000	6.022416000	0.163031000
C	3.907056000	4.824057000	0.010929000
C	2.987019000	5.820262000	-0.252497000
C	1.559455000	5.657483000	-0.360503000
C	0.649638000	6.447521000	-1.089231000
H	0.924970000	7.299913000	-1.693689000
C	-0.622563000	5.888842000	-0.952331000
H	-1.522480000	6.207412000	-1.455790000
C	-0.528047000	4.770857000	-0.103138000
C	-1.504345000	3.827464000	0.371929000
C	-0.990327000	2.598097000	0.936183000
C	-1.607912000	1.858064000	1.897098000
H	-2.541792000	2.236542000	2.301345000
C	0.558415000	-2.668578000	1.964698000
C	1.499716000	-2.726299000	0.982199000
C	1.966618000	-3.965923000	0.378498000
C	3.290081000	-4.017559000	-0.066623000
C	4.005066000	-5.099053000	-0.721566000
H	3.582964000	-6.039737000	-1.048025000
C	5.295070000	-4.676853000	-0.849811000
H	6.126810000	-5.207126000	-1.295085000
C	5.332692000	-3.318561000	-0.311664000
C	6.484255000	-2.453405000	-0.284531000
C	1.002369000	-5.036365000	0.205124000
C	1.051193000	-6.439443000	0.130999000
H	1.934609000	-7.041479000	0.290839000
C	-0.252271000	-6.913993000	-0.102013000
H	-0.560741000	-7.947430000	-0.180922000
C	-1.119470000	-5.806472000	-0.173315000
C	-2.542081000	-5.684633000	-0.488901000
C	-3.215474000	-4.543218000	-0.046440000
C	-2.781400000	-3.576884000	0.923707000
H	-1.984817000	-3.794474000	1.620671000
C	-3.478590000	-2.406927000	0.925061000
H	-3.263016000	-1.579457000	1.591450000
C	-4.568447000	-2.356512000	0.007887000
C	-5.292316000	-1.208269000	-0.272333000
C	-6.540211000	-1.015139000	-0.932870000
H	-7.138809000	-1.842463000	-1.301126000
C	-6.925957000	0.299405000	-1.005475000
H	-7.861256000	0.632554000	-1.441228000
C	-5.977211000	1.243240000	-0.481489000
C	-6.071122000	2.628419000	-0.523090000
C	-4.968504000	3.481053000	-0.170317000
C	-4.910853000	4.932747000	-0.275111000
H	-5.740394000	5.590232000	-0.501870000
C	-3.609537000	5.278735000	-0.040255000
H	-3.195910000	6.276999000	0.006323000
C	-2.894525000	4.039856000	0.220091000
C	3.496785000	7.211249000	-0.518316000
C	4.057285000	7.534307000	-1.773122000
C	4.506381000	8.840674000	-1.999460000
C	4.419778000	9.834172000	-1.021478000
C	3.864695000	9.491227000	0.215190000
C	3.395155000	8.202294000	0.482890000
C	4.180528000	6.503545000	-2.874093000
H	4.954910000	5.760548000	-2.647677000
H	4.444520000	6.980840000	-3.822940000
H	3.245805000	5.951453000	-3.018503000
C	4.885937000	11.244465000	-1.298999000
H	4.055759000	11.878287000	-1.638828000
H	5.652786000	11.267147000	-2.080416000
H	5.302653000	11.713403000	-0.400852000
C	2.800677000	7.887586000	1.837174000
H	1.732983000	7.649357000	1.759263000
H	2.905019000	8.739267000	2.516377000
H	3.287129000	7.021630000	2.300626000
C	7.825821000	-3.076560000	-0.557373000
C	8.520962000	-3.730936000	0.482347000
C	9.761046000	-4.316632000	0.208454000
C	10.329007000	-4.283230000	-1.068321000
C	9.622957000	-3.632898000	-2.083583000
C	8.381883000	-3.028602000	-1.853439000
C	7.949261000	-3.797707000	1.880894000
H	7.748252000	-2.798221000	2.283460000
H	8.640415000	-4.305472000	2.560887000
H	6.996617000	-4.339933000	1.898970000

C	11.653647000	-4.954946000	-1.347720000
H	11.516614000	-6.012669000	-1.610461000
H	12.312463000	-4.922579000	-0.473046000
H	12.176703000	-4.478659000	-2.183889000
C	7.660529000	-2.339938000	-2.991075000
H	6.635656000	-2.711676000	-3.101689000
H	8.184743000	-2.501485000	-3.938187000
H	7.586968000	-1.258075000	-2.828017000
C	-3.205389000	-6.751641000	-1.257742000
C	-4.158672000	-7.603553000	-0.654352000
C	-4.761228000	-8.603871000	-1.424344000
C	-4.454897000	-8.785068000	-2.774801000
C	-3.517411000	-7.926060000	-3.355851000
C	-2.883628000	-6.917650000	-2.625505000
C	-4.535335000	-7.465658000	0.804650000
H	-3.650880000	-7.385856000	1.445845000
H	-5.119450000	-8.330273000	1.135355000
H	-5.140029000	-6.568133000	0.982879000
C	-5.098833000	-9.889797000	-3.579580000
H	-5.267567000	-9.583296000	-4.617814000
H	-6.062518000	-10.187416000	-3.153065000
H	-4.463406000	-10.785427000	-3.606566000
C	-1.890366000	-6.011104000	-3.317499000
H	-1.918676000	-6.161721000	-4.401100000
H	-0.865025000	-6.202234000	-2.979101000
H	-2.102737000	-4.955053000	-3.117109000
C	-7.331658000	3.260648000	-1.040952000
C	-7.455428000	3.591263000	-2.407654000
C	-8.639094000	4.184521000	-2.859375000
C	-9.701796000	4.467023000	-1.996718000
C	-9.558800000	4.131407000	-0.647877000
C	-8.394154000	3.534209000	-0.153844000
C	-6.335292000	3.308946000	-3.383801000
H	-6.076095000	2.244207000	-3.404565000
H	-5.421415000	3.849456000	-3.111224000
H	-6.617061000	3.609351000	-4.397858000
C	-10.956937000	5.139555000	-2.503103000
H	-11.165277000	4.868738000	-3.543906000
H	-10.866418000	6.233662000	-2.465254000
H	-11.829867000	4.866031000	-1.900616000
C	-8.290462000	3.190464000	1.315700000
H	-8.191511000	2.109646000	1.471216000
H	-9.177845000	3.530088000	1.859201000
H	-7.410763000	3.655896000	1.775157000
N	0.819301000	4.648209000	0.215689000
N	4.136995000	-2.945014000	0.146874000
N	-0.326226000	-4.703130000	0.023756000
N	-3.772273000	2.979982000	0.173994000
S	4.929551000	-0.131473000	0.168933000
S	3.580374000	3.059730000	0.086088000
S	-4.727841000	-3.940858000	-0.804801000
S	-4.572576000	0.368651000	0.151523000
H	-8.731498000	4.431803000	-3.915471000
H	-10.375518000	4.338684000	0.041388000
H	-3.275925000	-8.038688000	-4.411250000
H	-5.489752000	-9.260426000	-0.952266000
H	10.047147000	-3.593918000	-3.085312000
H	10.296449000	-4.812867000	1.015991000
H	4.934261000	9.086260000	-2.969654000
H	3.794604000	10.247625000	0.994805000
H	-0.016688000	2.265232000	0.579331000
H	-0.640980000	-3.752568000	-0.102744000
H	1.172590000	4.025526000	0.928203000
H	0.226941000	-3.610982000	2.396963000
H	1.989699000	-1.816935000	0.648174000
C	-0.228273000	-0.267872000	1.741614000
C	-1.128317000	0.596487000	2.391137000
C	-0.095293000	-1.477917000	2.447176000
C	-1.566619000	-0.067065000	3.585858000
C	-0.904674000	-1.377449000	3.624428000
C	-2.452481000	0.455182000	4.524188000
C	-1.020748000	-2.350627000	4.618525000
C	-2.929453000	-0.101091000	5.709756000
H	-2.835558000	1.449713000	4.306880000
C	-1.774109000	-2.351282000	5.786603000
H	-0.425642000	-3.248984000	4.466815000
C	-2.628259000	-1.348744000	6.279291000
H	-3.629199000	0.517073000	6.271717000
H	-1.710245000	-3.231629000	6.419274000
O	-3.212589000	-1.684246000	7.461346000
H	-3.795515000	-0.966335000	7.756139000
H	0.216602000	-0.075632000	0.772701000

Conformer-10

C	4.328353000	-3.878962000	-0.642983000
---	-------------	--------------	--------------

C	3.414632000	-2.904108000	-1.170370000
H	2.447599000	-3.199721000	-1.546578000
C	3.877938000	-1.627829000	-1.175764000
H	3.312250000	-0.788347000	-1.564741000
C	5.198920000	-1.462607000	-0.649518000
C	5.788689000	-0.234509000	-0.424833000
C	7.091055000	0.153052000	0.009625000
H	7.870731000	-0.579070000	0.195667000
C	7.270605000	1.504582000	0.160389000
H	8.200290000	1.957415000	0.485832000
C	6.114793000	2.313766000	-0.123432000
C	5.994963000	3.692160000	-0.078799000
C	4.723359000	4.364400000	-0.244488000
C	4.415470000	5.615035000	-0.819706000
H	5.146823000	6.308146000	-1.211630000
C	3.023301000	5.742613000	-0.869876000
H	2.467071000	6.549614000	-1.324266000
C	2.449761000	4.594279000	-0.287088000
C	1.100684000	4.143861000	-0.102313000
C	0.898175000	2.777647000	0.372978000
C	-0.131539000	2.456399000	1.205272000
H	-0.731603000	3.292210000	1.548520000
C	-1.266617000	-2.472484000	1.365592000
C	-0.418365000	-3.195504000	0.581575000
C	-0.643820000	-4.566873000	0.136639000
C	0.499893000	-5.334441000	-0.128729000
C	0.682818000	-6.684937000	-0.632403000
H	-0.099099000	-7.387954000	-0.889929000
C	2.035527000	-6.873992000	-0.734028000
H	2.555024000	-7.754153000	-1.092626000
C	2.653879000	-5.609902000	-0.342871000
C	4.056058000	-5.213480000	-0.406120000
C	-2.010055000	-4.989333000	-0.104136000
C	-2.725195000	-6.199570000	-0.065088000
H	-2.316492000	-7.156807000	0.228209000
C	-4.065103000	-5.929583000	-0.407121000
H	-4.876547000	-6.643070000	-0.453918000
C	-4.177163000	-4.556576000	-0.693843000
C	-5.276408000	-3.654109000	-1.037923000
C	-4.965549000	-2.552081000	-1.813139000
C	-3.843639000	-2.430377000	-2.711354000
H	-3.257563000	-3.296137000	-2.995897000
C	-3.612035000	-1.173825000	-3.173014000
H	-2.798561000	-0.932742000	-3.846596000
C	-4.497210000	-0.167622000	-2.657589000
C	-4.194863000	1.179350000	-2.662372000
C	-2.953241000	1.707015000	-3.164450000
H	-2.286970000	1.119892000	-3.784273000
C	-2.646456000	2.950402000	-2.718317000
H	-1.725187000	3.466272000	-2.947033000
C	-3.651582000	3.570048000	-1.897944000
C	-3.520760000	4.758654000	-1.210095000
C	-2.159166000	5.190172000	-0.887074000
C	-1.599176000	6.524030000	-0.743424000
H	-2.132274000	7.460582000	-0.856840000
C	-0.261489000	6.352603000	-0.475581000
H	0.466757000	7.128622000	-0.275696000
C	-0.044459000	4.921258000	-0.399054000
C	7.213807000	4.546892000	0.092917000
C	8.141522000	4.684833000	-0.963760000
C	9.264678000	5.499887000	-0.779890000
C	9.498612000	6.181807000	0.415936000
C	8.569021000	6.031036000	1.449871000
C	7.430401000	5.233947000	1.309903000
C	7.945861000	3.984609000	-2.291190000
H	8.153913000	2.910075000	-2.219877000
H	8.615721000	4.402028000	-3.049487000
H	6.916899000	4.082602000	-2.652712000
C	10.704189000	7.077424000	0.581359000
H	10.449248000	8.127958000	0.387042000
H	11.505830000	6.803222000	-0.112266000
H	11.104815000	7.026754000	1.599927000
C	6.463208000	5.105082000	2.465270000
H	5.499801000	5.577168000	2.237849000
H	6.865183000	5.582183000	3.364401000
H	6.255240000	4.055231000	2.701549000
C	5.127626000	-6.221317000	-0.155427000
C	5.262513000	-6.800255000	1.128931000
C	6.268890000	-7.744300000	1.346532000
C	7.137966000	-8.149542000	0.329104000
C	6.984017000	-7.572408000	-0.933176000
C	5.999108000	-6.614680000	-1.197230000
C	4.355791000	-6.401343000	2.272216000
H	4.255550000	-5.313738000	2.350438000
H	4.744406000	-6.779720000	3.222978000
H	3.343049000	-6.800846000	2.141228000

C	8.193899000	-9.199883000	0.583211000
H	7.778440000	-10.212598000	0.491573000
H	8.610824000	-9.113164000	1.592721000
H	9.018978000	-9.120632000	-0.132394000
C	5.883286000	-6.041988000	-2.593247000
H	4.845488000	-6.031284000	-2.942912000
H	6.474759000	-6.631454000	-3.300873000
H	6.245845000	-5.007955000	-2.638903000
C	-6.619763000	-3.864045000	-0.426493000
C	-6.792763000	-3.824076000	0.978763000
C	-8.063419000	-4.036308000	1.518081000
C	-9.176793000	-4.296427000	0.713888000
C	-8.990372000	-4.327225000	-0.669481000
C	-7.739053000	-4.114455000	-1.256998000
C	-5.641301000	-3.519536000	1.911565000
H	-4.935458000	-4.356947000	1.971130000
H	-6.009955000	-3.318828000	2.922622000
H	-5.076875000	-2.641696000	1.577204000
C	-10.533275000	-4.558195000	1.325006000
H	-11.341576000	-4.300621000	0.632513000
H	-10.677133000	-3.980084000	2.24425000
H	-10.654348000	-5.618102000	1.587148000
C	-7.619761000	-4.173690000	-2.764264000
H	-8.519818000	-4.615596000	-3.203293000
H	-6.756826000	-4.768809000	-3.080476000
H	-7.494730000	-3.175218000	-3.200740000
C	-4.691345000	5.524824000	-0.692768000
C	-5.595726000	6.136281000	-1.593852000
C	-6.676057000	6.864998000	-1.085803000
C	-6.897909000	7.005660000	0.285701000
C	-5.999187000	6.388764000	1.160309000
C	-4.899444000	5.660070000	0.700739000
C	-5.418184000	6.039404000	-3.093654000
H	-5.684450000	5.044434000	-3.470110000
H	-4.381372000	6.225094000	-3.392558000
H	-6.056914000	6.767780000	-3.603365000
C	-8.058013000	7.820119000	0.808599000
H	-8.891763000	7.832497000	0.098553000
H	-7.765195000	8.864263000	0.984391000
H	-8.429264000	7.424317000	1.760324000
C	-3.973861000	5.008957000	1.705028000
H	-3.740147000	3.975900000	1.427747000
H	-4.431874000	5.004482000	2.699953000
H	-3.019075000	5.544454000	1.775442000
N	3.517229000	3.791966000	0.081609000
N	1.729456000	-4.736145000	0.051050000
N	-2.928570000	-4.033666000	-0.483797000
N	-1.229176000	4.261661000	-0.655046000
S	5.879505000	-3.062064000	-0.259108000
S	4.793972000	1.230265000	-0.635605000
S	-5.806614000	-0.968018000	-1.737359000
S	-5.072808000	2.472859000	-1.811262000
H	-7.362974000	7.337565000	-1.785496000
H	-6.161464000	6.471834000	2.233703000
H	-9.843613000	-4.525979000	-1.315281000
H	-8.188843000	-3.987436000	2.598313000
H	7.647697000	-7.876400000	-1.740495000
H	6.378591000	-8.172661000	2.341229000
H	9.973472000	5.606414000	-1.598975000
H	8.736118000	6.546093000	2.394183000
H	1.601331000	2.006937000	0.059958000
H	-2.701147000	-3.057400000	-0.601441000
H	3.421582000	2.950036000	0.630367000
H	-2.158971000	-2.968790000	1.741168000
H	0.550698000	-2.779793000	0.330877000
C	-0.330630000	-0.101938000	1.103541000
C	-0.566492000	1.164925000	1.668836000
C	-1.105300000	-1.091262000	1.748294000
C	-1.497962000	0.979390000	2.748423000
C	-1.835724000	-0.444748000	2.796065000
C	-1.972595000	1.981061000	3.590688000
C	-2.691690000	-1.077734000	3.701046000
C	-2.864143000	1.907569000	4.659766000
H	-1.592671000	2.980944000	3.396530000
C	-3.437599000	-0.552113000	4.747877000
H	-2.792385000	-2.153665000	3.578893000
C	-3.519927000	0.782794000	5.182069000
H	-3.078643000	2.852567000	5.158386000
H	-4.044950000	-1.245223000	5.322468000
O	-4.352971000	0.945207000	6.245351000
H	-4.383829000	1.881436000	6.499571000
H	0.290381000	-0.280290000	0.233276000

Conformer-11

C	6.289089000	-1.285613000	0.099701000
---	-------------	--------------	-------------

C	7.332604000	-0.419453000	-0.225626000
H	8.295473000	-0.783077000	-0.565297000
C	7.020443000	0.947427000	-0.077677000
H	7.715549000	1.753655000	-0.287210000
C	5.738105000	1.156398000	0.396818000
C	5.011766000	2.386323000	0.644263000
C	4.135802000	2.646673000	1.677229000
H	4.009998000	1.972066000	2.517370000
C	3.436534000	3.868171000	1.536221000
H	2.757694000	4.252420000	2.290442000
C	3.736454000	4.565765000	0.373179000
C	3.061740000	5.706493000	-0.226340000
C	1.685213000	5.803959000	-0.135234000
C	0.773883000	6.757934000	-0.735610000
H	1.091191000	7.633045000	-1.285849000
C	-0.507814000	6.338446000	-0.523007000
H	-1.397955000	6.813086000	-0.905146000
C	-0.483267000	5.109567000	0.247028000
C	-1.453793000	4.202336000	0.672004000
C	-0.970027000	2.943919000	1.251586000
C	-1.564427000	2.217805000	2.228238000
H	-2.456454000	2.632389000	2.687352000
C	0.254121000	-2.508824000	2.192475000
C	1.263965000	-2.646971000	1.295285000
C	1.688272000	-3.899232000	0.661451000
C	3.116948000	-4.067446000	0.435499000
C	3.854695000	-5.324235000	0.243247000
H	3.443738000	-6.323531000	0.289288000
C	5.160330000	-4.983125000	0.086077000
H	6.007002000	-5.640451000	-0.062231000
C	5.213192000	-3.528444000	0.180578000
C	6.324114000	-2.724168000	0.012222000
C	0.746230000	-4.790280000	0.147565000
C	0.892680000	-5.923905000	-0.753407000
H	1.836541000	-6.343049000	-1.065651000
C	-0.338509000	-6.308419000	-1.191149000
H	-0.565794000	-7.101344000	-1.890641000
C	-1.337233000	-5.445001000	-0.592325000
C	-2.689637000	-5.347150000	-0.836282000
C	-3.464279000	-4.391934000	-0.042335000
C	-3.488181000	-4.244992000	1.332079000
H	-3.004663000	-4.955166000	1.994560000
C	-4.190862000	-3.104660000	1.783274000
H	-4.284318000	-2.837638000	2.829729000
C	-4.705257000	-2.327906000	0.761046000
C	-5.194574000	-0.970898000	0.893792000
C	-4.958225000	-0.155630000	1.988276000
H	-4.479392000	-0.510634000	2.892849000
C	-5.270149000	1.196877000	1.761239000
H	-5.092243000	1.987363000	2.478818000
C	-5.773349000	1.459526000	0.502705000
C	-5.949685000	2.770246000	-0.107305000
C	-4.929247000	3.690424000	0.056411000
C	-4.901683000	5.107611000	-0.299521000
H	-5.740840000	5.690359000	-0.658236000
C	-3.636427000	5.535708000	-0.048131000
H	-3.269605000	6.547946000	-0.149533000
C	-2.881780000	4.358553000	0.427211000
C	3.837688000	6.669836000	-1.069756000
C	3.758996000	6.631704000	-2.479948000
C	4.513954000	7.544891000	-3.227637000
C	5.342577000	8.492289000	-2.625683000
C	5.415358000	8.507051000	-1.228450000
C	4.684399000	7.615037000	-0.442202000
C	2.896860000	5.623487000	-3.210432000
H	2.972790000	4.625470000	-2.767675000
H	3.197701000	5.551908000	-4.260417000
H	1.835689000	5.900180000	-3.189596000
C	6.129735000	9.482540000	-3.451971000
H	5.671647000	10.480209000	-3.421922000
H	6.180935000	9.176705000	-4.501894000
H	7.155440000	9.589529000	-3.080495000
C	4.794817000	7.681671000	1.064252000
H	3.811258000	7.802553000	1.533148000
H	5.424331000	8.522325000	1.372098000
H	5.230443000	6.765049000	1.479314000
C	7.646291000	-3.357031000	-0.318692000
C	8.564592000	-3.643478000	0.713864000
C	9.790974000	-4.230255000	0.386270000
C	10.135515000	-4.537995000	-0.932940000
C	9.213655000	-4.237811000	-1.939022000
C	7.972809000	-3.655196000	-1.658277000
C	8.239818000	-3.333094000	2.157948000
H	8.065577000	-2.261508000	2.309832000
H	9.058792000	-3.638982000	2.816119000
H	7.330158000	-3.849938000	2.484698000

C	11.455542000	-5.197937000	-1.257950000
H	11.377727000	-6.292262000	-1.203823000
H	12.239532000	-4.894773000	-0.555550000
H	11.791148000	-4.946781000	-2.269800000
C	7.010275000	-3.357444000	-2.786818000
H	6.110137000	-3.979805000	-2.721176000
H	7.479570000	-3.545619000	-3.757407000
H	6.674835000	-2.314539000	-2.767647000
C	-3.333829000	-6.105093000	-1.952819000
C	-4.262905000	-7.132636000	-1.658152000
C	-4.870639000	-7.827040000	-2.705277000
C	-4.596265000	-7.534420000	-4.045589000
C	-3.688792000	-6.510417000	-4.318077000
C	-3.050861000	-5.788496000	-3.301198000
C	-4.590373000	-7.504917000	-0.229922000
H	-3.681994000	-7.710645000	0.348442000
H	-5.224390000	-8.396375000	-0.195949000
H	-5.117990000	-6.696414000	0.289480000
C	-5.255052000	-8.314876000	-5.158947000
H	-5.147728000	-7.806085000	-6.122320000
H	-6.325183000	-8.458402000	-4.969767000
H	-4.810574000	-9.313737000	-5.263047000
C	-2.096603000	-4.676900000	-3.686025000
H	-2.245233000	-4.390677000	-4.731975000
H	-1.047900000	-4.977579000	-3.572821000
H	-2.237051000	-3.784251000	-3.068166000
C	-7.146321000	3.057138000	-0.951223000
C	-7.010475000	3.232522000	-2.347250000
C	-8.157058000	3.480386000	-3.112523000
C	-9.426766000	3.571592000	-2.542099000
C	-9.539106000	3.392766000	-1.158723000
C	-8.429425000	3.129292000	-0.355214000
C	-5.672133000	3.132390000	-3.049994000
H	-5.059555000	2.316848000	-2.653607000
H	-5.084520000	4.051150000	-2.938144000
H	-5.817056000	2.959799000	-4.121208000
C	-10.645576000	3.866010000	-3.384708000
H	-10.433963000	3.742808000	-4.451606000
H	-10.994204000	4.896423000	-3.234404000
H	-11.480727000	3.204339000	-3.126929000
C	-8.615101000	2.960056000	1.136178000
H	-8.377697000	1.941040000	1.461900000
H	-9.649017000	3.173993000	1.424093000
H	-7.959418000	3.632987000	1.701244000
N	0.862419000	4.882927000	0.492587000
N	3.943716000	-3.026729000	0.424207000
N	-0.623611000	-4.611697000	0.265220000
N	-3.678147000	3.304749000	0.522174000
S	4.881909000	-0.358721000	0.607569000
S	4.990652000	3.700640000	-0.521533000
S	-4.374670000	-3.078682000	-0.791672000
S	-5.924581000	-0.046270000	-0.405537000
H	-8.049732000	3.598720000	-4.188991000
H	-10.520167000	3.459359000	-0.691755000
H	-3.474260000	-6.254145000	-5.353855000
H	-5.577470000	-8.620307000	-2.468033000
H	9.464758000	-4.461004000	-2.974324000
H	10.496058000	-4.450751000	1.185653000
H	4.456480000	7.504434000	-4.313739000
H	6.059383000	9.234174000	-0.736888000
H	-0.048688000	2.542703000	0.824969000
H	-1.022504000	-3.763791000	0.644559000
H	1.215308000	4.040941000	0.917352000
H	-0.200519000	-3.416352000	2.589408000
H	1.849606000	-1.773605000	1.014161000
C	-0.367251000	-0.034195000	1.988049000
C	-1.152818000	0.907197000	2.684984000
C	-0.310986000	-1.261746000	2.679729000
C	-1.594648000	0.273879000	3.888898000
C	-1.060618000	-1.104914000	3.882958000
C	-2.371482000	0.862550000	4.879890000
C	-1.234803000	-2.076006000	4.866784000
C	-2.852291000	0.334082000	6.080124000
H	-2.650419000	1.899656000	4.703701000
C	-1.939326000	-2.026195000	6.067608000
H	-0.737141000	-3.025620000	4.678418000
C	-2.659793000	-0.950621000	6.612610000
H	-3.451546000	1.012105000	6.687902000
H	-1.937162000	-2.920275000	6.684124000
O	-3.228052000	-1.246229000	7.817575000
H	-3.705969000	-0.469617000	8.149223000
H	0.053385000	0.125752000	1.001660000

Conformer-12

C	6.306975000	-1.346140000	0.188873000
---	-------------	--------------	-------------

C	7.467778000	-0.574914000	0.287534000
H	8.450023000	-1.027276000	0.352240000
C	7.250794000	0.805220000	0.281130000
H	8.051511000	1.532725000	0.345325000
C	5.906896000	1.157231000	0.162882000
C	5.417403000	2.503681000	0.036428000
C	6.197378000	3.649213000	-0.073247000
H	7.280002000	3.624032000	-0.024995000
C	5.472067000	4.829327000	-0.283972000
H	5.932010000	5.802241000	-0.408421000
C	4.088941000	4.657055000	-0.346281000
C	3.131528000	5.675159000	-0.679555000
C	1.756873000	5.584341000	-0.522298000
C	0.749767000	6.448239000	-1.087990000
H	0.970129000	7.283005000	-1.738345000
C	-0.483960000	5.980467000	-0.735201000
H	-1.432364000	6.368302000	-1.072643000
C	-0.324576000	4.821306000	-0.106253000
C	-1.245151000	3.984003000	0.735498000
C	-0.749713000	2.758860000	1.342042000
C	-1.345798000	2.066021000	2.348005000
H	-2.208411000	2.517033000	2.828554000
C	0.194323000	-2.707759000	2.028939000
C	1.184740000	-2.774139000	1.103817000
C	1.599275000	-3.952968000	0.344483000
C	3.032231000	-4.094099000	0.127703000
C	3.773728000	-5.343766000	-0.065047000
H	3.352669000	-6.339598000	-0.100218000
C	5.090311000	-5.005927000	-0.085694000
H	5.944493000	-5.661773000	-1.679340000
C	5.138633000	-3.557842000	0.075482000
C	6.282159000	-2.778225000	0.105040000
C	0.663930000	-4.808525000	-0.288599000
C	0.817034000	-5.863881000	-1.217767000
H	1.766005000	-6.239430000	-1.569918000
C	-0.413893000	-6.238091000	-1.664602000
H	-0.639257000	-6.980013000	-2.418530000
C	-1.419769000	-5.441327000	-0.985836000
C	-2.777751000	-5.354873000	-1.195168000
C	-3.545425000	-4.463183000	-0.316458000
C	-3.596323000	-4.461268000	1.063485000
H	-3.152550000	-5.254779000	1.655559000
C	-4.264106000	-3.344041000	1.620588000
H	-4.376213000	-3.183204000	2.687006000
C	-4.721740000	-2.444702000	0.677054000
C	-5.143178000	-1.082264000	0.938960000
C	-4.779054000	-0.357684000	2.060958000
H	-4.230051000	-0.793625000	2.886886000
C	-5.058720000	1.017227000	1.958110000
H	-4.787133000	1.746753000	2.709870000
C	-5.660639000	1.385565000	0.771487000
C	-5.841544000	2.741404000	0.273283000
C	-4.782758000	3.621282000	0.417551000
C	-4.738209000	5.059261000	0.166739000
H	-5.586380000	5.691677000	-0.063505000
C	-3.439742000	5.430415000	0.329729000
H	-3.041634000	6.435043000	0.276624000
C	-2.689214000	4.200143000	0.644625000
C	3.678016000	6.945205000	-1.271718000
C	4.066928000	6.984788000	-2.629921000
C	4.572634000	8.176217000	-3.158493000
C	4.712215000	9.330866000	-2.382388000
C	4.331015000	9.268465000	-1.040111000
C	3.812939000	8.099638000	-0.470487000
C	3.938412000	5.768064000	-3.518437000
H	4.622964000	4.969830000	-3.207937000
H	4.165769000	6.019972000	-4.558891000
H	2.927246000	5.347656000	-3.482557000
C	5.237001000	10.613206000	-2.985398000
H	4.431722000	11.187322000	-3.463367000
H	5.992092000	10.415872000	-3.754222000
H	5.688333000	11.258777000	-2.224580000
C	3.416757000	8.096216000	0.990016000
H	2.327958000	8.047723000	1.112988000
H	3.767302000	9.005197000	1.488928000
H	3.834545000	7.233576000	1.520393000
C	7.618399000	-3.468203000	0.034858000
C	8.237707000	-3.921545000	1.218469000
C	9.481361000	-4.556779000	1.131774000
C	10.124820000	-4.760954000	-0.091679000
C	9.492610000	-4.301489000	-1.250350000
C	8.251398000	-3.657645000	-1.211725000
C	7.581828000	-3.733895000	2.568637000
H	7.328360000	-2.683777000	2.752783000
H	8.244048000	-4.069468000	3.372705000
H	6.646572000	-4.300927000	2.641715000

C	11.452190000	-5.479848000	-0.162630000
H	11.312809000	-6.562459000	-0.285380000
H	12.038575000	-5.330763000	0.750426000
H	12.051696000	-5.132864000	-1.011168000
C	7.608710000	-3.184655000	-2.496427000
H	6.632666000	-3.657872000	-2.653682000
H	8.241719000	-3.418520000	-3.357909000
H	7.436419000	-2.102200000	-2.486341000
C	-3.438080000	-6.047877000	-2.343586000
C	-4.348270000	-7.104573000	-2.096721000
C	-4.972918000	-7.737188000	-3.172839000
C	-4.732808000	-7.355523000	-4.497030000
C	-3.842853000	-6.304964000	-4.722349000
C	-3.190245000	-5.641941000	-3.675184000
C	-4.637752000	-7.574267000	-0.689270000
H	-3.712967000	-7.796824000	-0.144084000
H	-5.252966000	-8.479451000	-0.699808000
H	-5.170178000	-6.812007000	-0.108440000
C	-5.407350000	-8.071118000	-5.644078000
H	-5.340697000	-7.492816000	-6.571293000
H	-6.467728000	-8.254119000	-5.435207000
H	-4.943723000	-9.048771000	-5.832505000
C	-2.258165000	-4.495720000	-4.009408000
H	-2.430769000	-4.148720000	-5.033070000
H	-1.203508000	-4.787274000	-3.934032000
H	-2.397563000	-3.644072000	-3.335851000
C	-7.091318000	3.121425000	-0.447326000
C	-7.059869000	3.399611000	-1.832860000
C	-8.255085000	3.733390000	-2.482371000
C	-9.472389000	3.812580000	-1.805962000
C	-9.481035000	3.532002000	-0.434871000
C	-8.320638000	3.179648000	0.254576000
C	-5.785057000	3.319284000	-2.647387000
H	-5.169192000	2.460373000	-2.363922000
H	-5.161842000	4.211567000	-2.515728000
H	-6.019717000	3.232830000	-3.713049000
C	-10.744659000	4.198532000	-2.523184000
H	-10.612828000	4.181016000	-3.609649000
H	-11.066940000	5.210821000	-2.245554000
H	-11.568209000	3.519945000	-2.271691000
C	-8.393887000	2.901993000	1.739524000
H	-8.163525000	1.855517000	1.968729000
H	-9.394973000	3.119276000	2.124478000
H	-7.675674000	3.513378000	2.298499000
N	1.053384000	4.606707000	0.171338000
N	3.856761000	-3.051783000	0.210791000
N	-0.707535000	-4.662555000	-0.077889000
N	-3.508679000	3.165253000	0.739296000
S	4.897139000	-0.281407000	0.102303000
S	3.715663000	2.936522000	-0.116019000
S	-4.380913000	-3.039181000	-0.939722000
S	-5.949458000	-0.045057000	-0.221840000
H	-8.229289000	3.930644000	-3.552245000
H	-10.419670000	3.587899000	0.113562000
H	-3.654648000	-5.979886000	-5.743887000
H	-5.665107000	-8.553077000	-2.971693000
H	9.977696000	-4.445977000	-2.214000000
H	9.958482000	-4.900617000	2.047694000
H	4.865337000	8.201899000	-4.206634000
H	4.441141000	10.152552000	-0.414761000
H	0.158524000	2.341875000	0.906795000
H	-1.115132000	-3.856815000	0.376083000
H	1.478063000	4.012081000	0.867757000
H	-0.285754000	-3.631170000	2.351908000
H	1.783435000	-1.885889000	0.913456000
C	-0.287247000	-0.216222000	2.002035000
C	-0.990776000	0.733798000	2.768278000
C	-0.297075000	-1.477980000	2.623028000
C	-1.444168000	0.066965000	3.950326000
C	-1.004283000	-1.342329000	3.853842000
C	-2.157311000	0.649421000	4.990434000
C	-1.219903000	-2.354892000	4.785980000
C	-2.642546000	0.086558000	6.173661000
H	-2.371124000	1.710754000	4.876301000
C	-1.888867000	-2.324909000	6.007678000
H	-0.794195000	-3.323451000	4.529106000
C	-2.521605000	-1.235592000	6.629932000
H	-3.181472000	0.766335000	6.833680000
H	-1.932173000	-3.249794000	6.575270000
O	-3.077663000	-1.560433000	7.833262000
H	-3.493686000	-0.773881000	8.220231000
H	0.112110000	-0.031682000	1.011733000

Conformer-13

C	5.129097000	-3.106228000	-0.605365000
---	-------------	--------------	--------------

C	4.005907000	-2.390357000	-1.147812000
H	3.133383000	-2.916359000	-1.502873000
C	4.156340000	-1.043258000	-1.201657000
H	3.407683000	-0.373142000	-1.609571000
C	5.408332000	-0.555828000	-0.705372000
C	5.695240000	0.781961000	-0.533229000
C	6.879998000	1.480015000	-0.151670000
H	7.812992000	0.957733000	0.036091000
C	6.741854000	2.840644000	-0.058697000
H	7.545965000	3.512540000	0.219052000
C	5.422114000	3.343755000	-0.338496000
C	4.984359000	4.655203000	-0.346260000
C	3.588094000	5.007909000	-0.495823000
C	2.995725000	6.133037000	-1.102228000
H	3.544457000	6.944391000	-1.559831000
C	1.607892000	5.962252000	-1.079890000
H	0.873422000	6.607297000	-1.538729000
C	1.317855000	4.750543000	-0.419868000
C	0.091161000	4.072141000	-0.105959000
C	0.175307000	2.690311000	0.345357000
C	-0.703679000	2.156080000	1.241331000
H	-1.457140000	2.838811000	1.617926000
C	-0.557640000	-2.898747000	1.544171000
C	0.407012000	-3.418883000	0.736231000
C	0.450390000	-4.796938000	0.240984000
C	1.725180000	-5.324625000	-0.023253000
C	2.178126000	-6.589852000	-0.373495000
H	1.560293000	-7.429403000	-0.864082000
C	3.541839000	-6.498265000	-0.671993000
H	4.2277778000	-7.241668000	-1.059374000
C	3.890056000	-5.150684000	-0.237043000
C	5.172832000	-4.456949000	-0.323636000
C	-0.802396000	-5.434266000	-0.096719000
C	-1.241220000	-6.749525000	-0.350152000
H	-0.650409000	-7.644177000	-0.213270000
C	-2.580928000	-6.695463000	-0.765944000
H	-3.210527000	-7.532865000	-1.033579000
C	-2.978544000	-5.340305000	-0.800021000
C	-4.229851000	-6.679941000	-1.129084000
C	-4.224320000	-3.330218000	-1.449233000
C	-3.105609000	-2.528182000	-1.867375000
H	-2.183758000	-2.976178000	-2.217707000
C	-3.324811000	-1.182089000	-1.853253000
H	-2.579387000	-0.448569000	-2.141147000
C	-4.642509000	-0.789583000	-1.479781000
C	-5.036337000	0.519156000	-1.248771000
C	-6.332549000	1.093881000	-1.096171000
H	-7.243019000	0.509353000	-1.184921000
C	-6.312543000	2.449453000	-0.887588000
H	-7.203813000	3.058847000	-0.786297000
C	-5.003786000	3.036436000	-0.806687000
C	-4.700633000	4.371476000	-0.577884000
C	-3.345693000	4.828375000	-0.413927000
C	-2.867115000	6.196966000	-0.307302000
H	-3.478323000	7.090616000	-0.306560000
C	-1.503207000	6.116944000	-0.210553000
H	-0.810454000	6.934308000	-0.061667000
C	-1.171943000	4.703390000	-0.226625000
C	5.973026000	5.777210000	-0.246353000
C	6.818652000	6.080033000	-1.336880000
C	7.724299000	7.141197000	-1.220520000
C	7.819643000	7.911035000	-0.059548000
C	6.974801000	7.594193000	1.009004000
C	6.050907000	6.548990000	0.936125000
C	6.762252000	5.294881000	-2.629607000
H	7.218498000	4.303004000	-2.524274000
H	7.297677000	5.822887000	-3.424933000
H	5.731027000	5.133264000	-2.960486000
C	8.786139000	9.068756000	0.032911000
H	8.287543000	10.022230000	-0.187721000
H	9.611185000	8.960341000	-0.678763000
H	9.214181000	9.154704000	1.037904000
C	5.166452000	6.250777000	2.125931000
H	4.115590000	6.481819000	1.913414000
H	5.469733000	6.843303000	2.994634000
H	5.209533000	5.191736000	2.404794000
C	6.443292000	-5.192748000	-0.062129000
C	6.703989000	-5.706504000	1.230955000
C	7.896166000	-6.396919000	1.460538000
C	8.834737000	-6.613363000	0.446971000
C	8.555755000	-6.106401000	-0.823773000
C	7.381207000	-5.398296000	-1.100380000
C	5.730547000	-5.502164000	2.370603000
H	5.389573000	-4.463425000	2.431933000
H	6.193442000	-5.769228000	3.325908000
H	4.832380000	-6.119219000	2.248785000

C	10.099246000	-7.395622000	0.714992000
H	9.918558000	-8.477484000	0.655623000
H	10.493249000	-7.189810000	1.716492000
H	10.881329000	-7.155630000	-0.012905000
C	7.141664000	-4.891231000	-2.506042000
H	6.124239000	-5.107856000	-2.848276000
H	7.842745000	-5.355784000	-3.206610000
H	7.276365000	-3.804924000	-2.574071000
C	-5.501512000	-5.453233000	-0.992981000
C	-5.965492000	-5.850680000	0.282828000
C	-7.155773000	-6.576314000	0.379689000
C	-7.900786000	-6.931250000	-0.748414000
C	-7.428586000	-6.527243000	-1.999444000
C	-6.246783000	-5.793846000	-2.145465000
C	-5.214385000	-5.485265000	1.543953000
H	-4.280173000	-6.052502000	1.635701000
H	-5.821716000	-5.695197000	2.430027000
H	-4.948616000	-4.422337000	1.558488000
C	-9.165598000	-7.747505000	-0.619226000
H	-9.853806000	-7.555076000	-1.449105000
H	-9.691569000	-7.526649000	0.315986000
H	-8.946763000	-8.823980000	-0.621063000
C	-5.791228000	-5.391705000	-3.530942000
H	-6.378371000	-5.909736000	-4.295701000
H	-4.734123000	-5.627420000	-3.694140000
H	-5.906400000	-4.313714000	-3.696839000
C	-5.814561000	5.373845000	-0.481233000
C	-6.341139000	5.960340000	-1.651907000
C	-7.370619000	6.900943000	-1.537984000
C	-7.893604000	7.279676000	-0.298794000
C	-7.359491000	6.685407000	0.847863000
C	-6.327712000	5.743642000	0.780186000
C	-5.809840000	5.589216000	-3.018692000
H	-6.011712000	4.538873000	-3.259530000
H	-4.723486000	5.721358000	-3.075885000
H	-6.269633000	6.207270000	-3.796198000
C	-8.984430000	8.320933000	-0.199657000
H	-9.626356000	8.315383000	-1.087178000
H	-8.563902000	9.331767000	-0.110166000
H	-9.618537000	8.155718000	0.678168000
C	-5.783266000	5.131460000	2.051691000
H	-5.871985000	4.038794000	2.042066000
H	-6.320508000	5.509604000	2.927368000
H	-4.718940000	5.361430000	2.180590000
N	2.547693000	4.201194000	-0.093160000
N	2.810154000	-4.498340000	0.188757000
N	-1.892979000	-4.630527000	-0.368564000
N	-2.323867000	3.961857000	-0.350337000
S	6.450823000	-1.936533000	-0.278564000
S	4.378156000	1.963011000	-0.762659000
S	-5.641967000	-2.251868000	-1.235438000
S	-3.781763000	1.765511000	-1.015739000
H	-7.773158000	7.349635000	-2.444390000
H	-7.755812000	6.961168000	1.823593000
H	-7.994313000	-6.791099000	-2.891048000
H	-7.514003000	-6.866400000	1.365821000
H	9.270851000	-6.267540000	-1.628349000
H	8.098609000	-6.773397000	2.461678000
H	8.369827000	7.373128000	-2.065604000
H	7.038438000	8.175202000	1.927351000
H	1.004031000	2.084920000	-0.020292000
H	-1.878833000	-3.628721000	-0.257237000
H	2.659589000	3.392103000	0.500649000
H	-1.306013000	-3.580547000	1.944871000
H	1.257128000	-2.802463000	0.466490000
C	-0.255596000	-0.377141000	1.196251000
C	-0.796545000	0.808513000	1.733448000
C	-0.726982000	-1.507539000	1.897528000
C	-1.619117000	0.426630000	2.850478000
C	-1.570142000	-1.033010000	2.953043000
C	-2.321477000	1.299303000	3.677193000
C	-2.204717000	-1.833808000	3.905910000
C	-3.133368000	1.034603000	4.778708000
H	-2.228533000	2.355462000	3.437916000
C	-3.034575000	-1.483814000	4.962949000
H	-2.019973000	-2.902154000	3.818906000
C	-3.454519000	-0.201715000	5.358880000
H	-3.577929000	1.908270000	5.254947000
H	-3.421558000	-2.289648000	5.579661000
O	-4.272607000	-0.222275000	6.445715000
H	-4.539857000	0.682554000	6.673758000
H	0.370018000	-0.422599000	0.312099000

S	2.199036000	-3.918583000	0.574772000
S	4.916081000	-1.519932000	0.240144000
N	-2.634607000	-4.183833000	-0.054301000
H	-2.391144000	-3.199642000	0.139917000
N	5.105853000	2.653410000	0.308508000
C	-1.686776000	-5.177097000	-0.107848000
C	-3.876260000	-4.697059000	-0.261936000
C	-3.736853000	-6.086791000	-0.461492000
H	-4.544224000	-6.779205000	-0.656607000
C	-2.379334000	-6.385786000	-0.371312000
H	-1.916214000	-7.356100000	-0.461492000
C	-0.270137000	-5.008035000	0.076755000
C	0.413404000	-3.847657000	0.384909000
C	-0.062529000	-2.459102000	0.303554000
C	1.044466000	-1.599579000	0.974619000
H	0.916842000	-0.532275000	1.110327000
C	2.265618000	-2.201037000	0.971467000
C	5.226138000	3.927455000	-0.001538000
C	6.604242000	4.277424000	-0.367499000
H	6.963169000	5.256803000	-0.659718000
C	7.312669000	3.118812000	-0.297609000
H	8.367083000	2.969591000	-0.491172000
C	6.371654000	2.088340000	0.140101000
C	0.538473000	-6.270323000	-0.088112000
C	0.785044000	-7.098111000	1.027403000
C	1.528789000	-8.268233000	0.845353000
H	1.715892000	-8.907765000	1.705747000
C	2.034014000	-8.638109000	-0.403981000
C	1.768783000	-7.804530000	-1.493858000
H	2.145270000	-8.078399000	-2.477497000
C	1.029181000	-6.625159000	-1.362429000
C	3.478133000	-1.452790000	1.236796000
C	5.521421000	-0.025403000	0.948646000
C	4.681371000	0.406908000	1.957392000
H	4.876168000	1.309088000	2.520687000
C	3.538865000	-0.394241000	2.122668000
H	2.746772000	-0.185878000	2.831870000
C	6.596649000	0.739672000	0.336762000
C	7.839574000	0.062002000	-0.133155000
C	8.109182000	-0.058623000	-1.515242000
C	9.274995000	-0.721094000	-1.919377000
H	9.471734000	-0.826745000	-2.984363000
C	10.183418000	-1.253677000	-1.004212000
C	9.895273000	-1.123770000	0.359056000
H	10.589798000	-1.532097000	1.090915000
C	8.740178000	-0.486271000	0.812567000
C	0.261323000	-6.743615000	2.400878000
H	0.517526000	-7.521457000	3.126387000
H	-0.828562000	-6.627572000	2.399354000
H	0.684816000	-5.797835000	2.758678000
C	2.863732000	-9.890168000	-0.567233000
H	2.748216000	-10.320591000	-1.567755000
H	2.585155000	-10.654687000	0.165873000
H	3.932188000	-9.678672000	-0.426164000
C	0.768021000	-5.759291000	-2.574173000
H	1.201538000	-6.208383000	-3.472709000
H	1.202819000	-4.760147000	-2.454355000
H	-0.305654000	-5.623210000	-2.747947000
C	7.168567000	0.477468000	-2.574829000
H	7.380083000	0.010964000	-3.542066000
H	7.272158000	1.561628000	-2.699930000
H	6.119455000	0.286867000	-2.328396000
C	11.447763000	-1.940443000	-1.464266000
H	11.614892000	-2.877938000	-0.921354000
H	12.328845000	-1.308170000	-1.292102000
H	11.412001000	-2.170829000	-2.533721000
C	8.490873000	-0.364754000	2.299322000
H	9.346745000	-0.741814000	2.867252000
H	7.604983000	-0.929952000	2.610550000
H	8.321089000	0.677284000	2.594856000
O	-1.236531000	-2.043150000	0.540790000
S	-2.100072000	4.136223000	0.120731000
S	-3.900248000	0.090171000	0.097948000
N	2.807581000	4.278893000	0.130328000
H	2.552170000	3.296542000	0.295233000
N	-4.973954000	-2.544992000	-0.126177000
C	1.871231000	5.281775000	0.022984000
C	4.064815000	4.783203000	-0.036335000
C	3.946181000	6.168526000	-0.249112000
H	4.768244000	6.853127000	-0.407832000
C	2.588290000	6.481891000	-0.204927000
H	2.140632000	7.456484000	-0.332522000
C	0.438446000	5.139686000	0.068381000
C	-0.318802000	3.992449000	0.202566000
C	0.063136000	2.563832000	0.383901000

C	-1.116250000	1.718217000	0.385692000	H	-9.888512000	-0.161474000	-1.827370000
H	-1.037575000	0.640503000	0.485115000	C	-9.420113000	0.209021000	0.238824000
C	-2.302804000	2.379101000	0.258716000	C	-8.438009000	0.066185000	1.222555000
C	-5.047652000	-3.861254000	-0.261740000	H	-8.643213000	0.413069000	2.233385000
C	-6.430227000	-4.322402000	-0.398121000	C	-7.194704000	-0.514070000	0.951699000
H	-6.752828000	-5.348792000	-0.519233000	C	-2.435197000	2.506097000	-1.648773000
C	-7.202212000	-3.206582000	-0.332123000	C	-1.249973000	4.538824000	-0.768172000
H	-8.279984000	-3.136135000	-0.392706000	C	-0.577801000	3.913453000	-1.807504000
C	-6.280998000	-2.083184000	-0.166062000	H	0.380607000	4.265950000	-2.162967000
C	-0.312345000	6.440761000	-0.083102000	C	-1.246588000	2.784794000	-2.307269000
C	-0.659857000	6.910621000	-1.367434000	H	-0.864168000	2.162658000	-3.108493000
C	-1.346502000	8.123934000	-1.477107000	C	-0.801336000	5.638678000	0.058354000
H	-1.611429000	8.486654000	-2.468403000	C	-1.820933000	6.572865000	0.632094000
C	-1.697235000	8.881204000	-0.356074000	C	-2.148094000	6.513893000	2.004781000
C	-1.334293000	8.397611000	0.903775000	C	-3.123471000	7.386248000	2.503081000
H	-1.588871000	8.976131000	1.789735000	H	-3.384454000	7.329018000	3.557866000
C	-0.647611000	7.190026000	1.064206000	C	-3.770966000	8.318736000	1.691381000
C	-3.634065000	1.820592000	0.204694000	C	-3.429168000	8.359582000	0.335217000
C	-5.643550000	0.318817000	0.046351000	H	-3.921550000	9.079157000	-0.316178000
C	-5.956917000	1.678063000	0.119072000	C	-2.473888000	7.501870000	-0.212334000
H	-6.979197000	2.036188000	0.104688000	C	-7.643067000	-1.316343000	-2.780043000
C	-4.835810000	2.516452000	0.204507000	H	-8.540492000	-1.213308000	-3.397299000
H	-4.898021000	3.597580000	0.268757000	H	-7.339167000	-2.369252000	-2.796798000
C	-6.610343000	-0.744820000	-0.076703000	H	-6.839236000	-0.744442000	-2.258458000
C	-8.060029000	-0.348741000	-0.120032000	C	-10.744058000	0.866154000	0.551834000
C	-8.798059000	-0.255570000	1.078649000	H	-11.025571000	0.722181000	1.600387000
C	-10.144804000	0.117252000	1.015671000	H	-11.548685000	0.465821000	-0.074181000
H	-10.711041000	0.191220000	1.942184000	H	-10.701252000	1.948836000	0.372423000
C	-10.779823000	0.397340000	-0.197330000	C	-6.171552000	-0.650820000	2.056913000
C	-10.026173000	0.302280000	-1.370401000	H	-6.539526000	-0.199043000	2.982926000
H	-10.498929000	0.522069000	-2.325765000	H	-5.227790000	-0.159396000	1.794691000
C	-8.676851000	-0.066347000	-1.356986000	H	-5.940496000	-1.702412000	2.262635000
C	-0.302567000	6.131759000	-2.613106000	C	-1.489469000	5.529054000	2.948026000
H	-0.633626000	6.662604000	-3.510761000	H	-2.061992000	5.448364000	3.877130000
H	0.779115000	5.973808000	-2.692377000	H	-0.471265000	5.839282000	3.210896000
H	-0.773473000	5.141907000	-2.614540000	H	-1.412551000	4.528697000	2.510080000
C	-2.467347000	10.173083000	-0.500847000	C	-4.798917000	9.269515000	2.258249000
H	-2.242491000	10.867959000	0.315347000	H	-5.664804000	9.366471000	1.593511000
H	-2.236262000	10.674227000	-1.446978000	H	-4.379511000	10.275875000	2.389233000
H	-3.550771000	9.993312000	-0.485133000	H	-5.158577000	8.934069000	3.236142000
C	-0.275549000	6.712284000	2.449673000	C	-2.136232000	7.599442000	-1.683259000
H	-0.585767000	7.438250000	3.207241000	H	-2.656424000	8.443895000	-2.145086000
H	-0.754233000	5.754517000	2.684963000	H	-2.422698000	6.691731000	-2.227174000
H	0.805991000	6.562613000	2.546413000	H	-1.060169000	7.737220000	-1.840817000
C	-8.160735000	-0.553597000	2.417639000	O	-2.767065000	-2.260137000	-1.918533000
H	-8.869493000	-0.380247000	3.233012000	S	3.410054000	0.135786000	-0.051706000
H	-7.823340000	-1.594814000	2.479093000	S	2.543234000	-4.172788000	0.150243000
H	-7.280166000	0.074410000	2.595308000	N	3.985673000	3.280994000	0.097623000
C	-12.244098000	0.767881000	-0.241430000	H	3.181515000	2.756567000	-0.221003000
H	-12.467199000	1.421027000	-1.091844000	N	-2.075854000	-5.093502000	0.105027000
H	-12.877146000	-0.123990000	-0.342422000	C	5.305114000	2.862381000	0.129961000
H	-12.555152000	1.283567000	0.673382000	C	3.891044000	4.594824000	0.492602000
C	-7.908750000	-0.159535000	-2.656679000	C	5.183151000	5.032409000	0.803818000
H	-8.536093000	0.140248000	-3.501541000	H	5.443405000	6.023729000	1.147544000
H	-7.021377000	0.483753000	-2.649059000	C	6.057690000	3.970351000	0.565448000
H	-7.556851000	-1.180882000	-2.843090000	H	7.128642000	3.967193000	0.698345000
O	1.224819000	2.134308000	0.528419000	C	5.843011000	1.553373000	-0.193436000

Conformer-2

S	-4.791726000	0.995911000	-1.144878000	H	5.093572000	-3.033029000	-0.869755000
S	-2.777387000	3.728713000	-0.446837000	C	3.543624000	-1.627147000	-0.340885000
N	-4.312934000	-3.685402000	-0.401862000	C	-3.236712000	-5.700592000	0.298180000
H	-3.473012000	-3.330048000	-0.883199000	C	-3.063670000	-7.096944000	0.693231000
N	1.514530000	4.825254000	0.063827000	H	-3.852797000	-7.807292000	0.905998000
C	-5.494358000	-2.996718000	-0.370414000	C	-1.718911000	-7.308098000	0.721910000
C	-4.445406000	-4.922628000	0.132307000	H	-1.195887000	-8.222695000	0.968070000
C	-5.798401000	-5.074553000	0.508718000	C	-1.092162000	-6.032597000	0.362771000
H	-6.231290000	-5.946185000	0.980566000	C	7.347745000	1.561745000	-0.328912000
C	-6.450552000	-3.876028000	0.202342000	C	8.154312000	1.275543000	0.788882000
H	-7.486094000	-3.632231000	0.393750000	C	9.543059000	1.379747000	0.661521000
C	-5.603375000	-1.598636000	-0.689156000	H	10.164902000	1.166577000	1.529113000
C	-4.590348000	-0.791213000	-1.182632000	C	10.151735000	1.744308000	-0.541720000
C	-3.256301000	-1.123122000	-1.750115000	C	9.327314000	2.017811000	-1.636374000
C	-2.518352000	0.075756000	-2.050046000	H	9.778608000	2.304892000	-2.584414000
H	-1.486908000	0.004191000	-2.371540000	C	7.935317000	1.932363000	-1.553515000
C	-3.134942000	1.241523000	-1.706268000	C	2.375546000	-2.473016000	-0.224292000
C	2.647817000	5.318413000	0.532779000	C	0.799401000	-4.430783000	0.051042000
C	2.474426000	6.642342000	1.138409000	C	0.161626000	-3.232144000	-0.266926000
H	3.250796000	7.247504000	1.589017000	H	-0.908201000	-3.175476000	-0.406309000
C	1.149866000	6.920028000	1.044501000	C	1.041076000	-2.143349000	-0.404565000
H	0.627578000	7.807086000	1.377426000	H	0.713183000	-1.140942000	-0.659433000
C	0.538539000	5.783274000	0.357749000	C	0.263217000	-5.746616000	0.332499000
C	-6.927092000	-0.961228000	-0.359830000	C	1.241245000	-6.847185000	0.635515000
C	-7.903328000	-0.833326000	-1.370704000	C	1.767838000	-7.624043000	-0.419349000
C	-9.133807000	-0.252990000	-1.048706000	C	2.684009000	-8.636411000	-0.119042000

H	3.092182000	-9.230830000	-0.934132000
C	3.089547000	-8.903621000	1.191571000
C	2.553045000	-8.122186000	2.218080000
H	2.858981000	-8.310410000	3.245304000
C	1.633126000	-7.098779000	1.967869000
C	7.554854000	0.841157000	2.107248000
H	8.315299000	0.829310000	2.894305000
H	6.743651000	1.502796000	2.431019000
H	7.137803000	-0.170704000	2.034481000
C	11.656131000	1.814152000	-0.664180000
H	11.965879000	2.578112000	-1.385841000
H	12.127307000	2.045201000	0.297347000
H	12.071022000	0.856946000	-1.007650000
C	7.090043000	2.200822000	-2.776675000
H	7.709084000	2.543958000	-3.611319000
H	6.570043000	1.290039000	-3.097735000
H	6.324993000	2.963389000	-2.588882000
C	1.350935000	-7.385509000	-1.853431000
H	1.887521000	-8.056662000	-2.530616000
H	0.276461000	-7.553217000	-1.992060000
H	1.553607000	-6.355763000	-2.169670000
C	4.060534000	-10.021802000	1.491140000
H	4.624506000	-9.827541000	2.409453000
H	3.536498000	-10.977534000	1.626663000
H	4.777880000	-10.159140000	0.674962000
C	1.073213000	-6.292858000	3.118915000
H	1.549370000	-6.580270000	4.061102000
H	1.230344000	-5.217652000	2.976617000
H	-0.007255000	-6.444437000	3.226908000
O	6.976026000	-1.096300000	-1.002935000

Conformer-3

S	0.531765000	4.200791000	-1.215388000
S	3.221330000	1.127932000	0.493289000
N	-4.076056000	2.762809000	-1.282405000
H	-3.492993000	1.954806000	-1.014516000
N	4.852275000	-1.004502000	1.358069000
C	-3.547955000	3.918740000	-1.796905000
C	-5.430267000	2.836426000	-1.212553000
C	-5.815561000	4.086375000	-1.743306000
H	-6.830523000	4.449486000	-1.831453000
C	-4.649511000	4.756821000	-2.113099000
H	-4.574264000	5.750216000	-2.531627000
C	-2.149314000	4.253362000	-1.810419000
C	-1.096832000	3.468398000	-1.372141000
C	-1.042871000	2.039700000	-0.959660000
C	0.278630000	1.696453000	-0.490621000
H	0.469883000	0.707681000	-0.090171000
C	1.188271000	2.711390000	-0.513736000
C	5.296116000	-2.234613000	1.578064000
C	6.555097000	-2.238460000	2.323833000
H	7.110887000	-3.114045000	2.634315000
C	6.865697000	-0.932884000	2.533743000
H	7.726463000	-0.526280000	3.047524000
C	5.798134000	-0.152095000	1.911384000
C	-1.833835000	5.648427000	-2.286174000
C	-1.515993000	5.860768000	-3.644473000
C	-1.235646000	7.160967000	-4.075474000
H	-0.996206000	7.323811000	-5.124517000
C	-1.256618000	8.251400000	-3.201560000
C	-1.580263000	8.015166000	-1.862854000
H	-1.610516000	8.851598000	-1.167261000
C	-1.872354000	6.733548000	-1.384996000
C	2.527537000	2.665893000	0.019144000
C	4.650644000	1.916453000	1.145166000
C	4.564940000	3.296387000	0.952116000
H	5.344630000	3.972211000	1.282603000
C	3.383024000	3.715785000	0.316660000
H	3.143653000	4.754193000	0.113883000
C	5.731274000	1.222844000	1.799677000
C	6.836437000	2.063123000	2.374855000
C	6.733015000	2.551368000	3.694621000
C	7.771370000	3.335040000	4.208236000
H	7.688661000	3.711252000	5.226110000
C	8.905473000	3.648679000	3.453977000
C	8.981569000	3.158393000	2.147548000
H	9.852599000	3.396311000	1.539987000
C	7.969386000	2.368756000	1.591729000
C	-1.480117000	4.714715000	-4.630343000
H	-1.279106000	5.079021000	-5.642212000
H	-2.430351000	4.168818000	-4.649133000
H	-0.699965000	3.988616000	-4.373300000
C	-0.915725000	9.641486000	-3.685659000
H	-1.416707000	10.409241000	-3.086462000
H	-1.205815000	9.784316000	-4.732159000

H	0.164142000	9.830899000	-3.619860000
C	-2.224385000	6.536005000	0.072337000
H	-2.170724000	7.484155000	0.615805000
H	-1.541608000	5.829798000	0.558320000
H	-3.238160000	6.135960000	0.189863000
C	5.529263000	2.238176000	4.555231000
H	5.615982000	2.717671000	5.534843000
H	5.419167000	1.159404000	4.715793000
H	4.598899000	2.584951000	4.090700000
C	10.027093000	4.472742000	4.042213000
H	10.556634000	5.039465000	3.269013000
H	10.768379000	3.835148000	4.542492000
H	9.654718000	5.182645000	4.788483000
C	8.106472000	1.857461000	0.174665000
H	9.007048000	2.260307000	-0.298441000
H	7.245479000	2.137921000	-0.442694000
H	8.172289000	0.763429000	0.146975000
O	-1.982956000	1.222569000	-0.993279000
S	0.213868000	-3.297714000	0.424195000
S	-3.677259000	-1.483600000	-0.113648000
N	3.449748000	-3.283460000	0.348872000
H	2.980190000	-2.398198000	0.207076000
N	-5.507564000	0.720898000	-0.095231000
C	3.153666000	-4.472096000	-0.284589000
C	4.635503000	-3.388425000	1.034195000
C	5.079501000	-4.710521000	0.891847000
H	5.983454000	-5.117812000	1.323239000
C	4.174930000	-5.373658000	0.052932000
H	4.226546000	-6.398095000	-0.286836000
C	2.045467000	-4.655786000	-1.207837000
C	0.824245000	-4.057827000	-1.076212000
C	-0.230514000	-4.001926000	-2.150660000
C	-1.455897000	-3.414977000	-1.612809000
H	-2.354175000	-3.356790000	-2.215622000
C	-1.400946000	-3.067536000	-0.303518000
C	-6.155299000	1.785507000	-0.542492000
C	-7.552393000	1.794896000	-0.108523000
H	-8.292161000	2.549534000	-0.345172000
C	-7.705760000	0.691527000	0.673761000
H	-8.598170000	0.357507000	1.186563000
C	-6.409591000	0.016868000	0.686053000
C	2.336951000	-5.602304000	-2.340779000
C	1.878977000	-6.932121000	-2.266554000
C	2.241295000	-7.826005000	-3.280645000
H	1.898247000	-8.856905000	-3.215560000
C	3.022227000	-7.434723000	-4.369426000
C	3.454080000	-6.105702000	-4.423670000
H	4.059320000	-5.776285000	-5.266276000
C	3.128561000	-5.182310000	-3.429204000
C	-2.517886000	-2.620713000	0.513670000
C	-4.733297000	-1.722289000	1.268344000
C	-4.148115000	-2.608163000	2.173122000
H	-4.633509000	-2.893465000	3.099257000
C	-2.889281000	-3.088629000	1.765805000
H	-2.297204000	-3.800011000	2.331121000
C	-6.032612000	-1.101454000	1.404513000
C	-6.981240000	-1.703290000	2.398814000
C	-7.707805000	-2.866931000	2.063258000
C	-8.586575000	-3.409788000	3.004642000
H	-9.150010000	-4.302748000	2.740509000
C	-8.759408000	-2.842136000	4.270758000
C	-8.020797000	-1.698746000	4.583798000
H	-8.131529000	-1.247210000	5.567812000
C	-7.137484000	-1.111959000	3.670440000
C	1.003249000	-7.414637000	-1.130340000
H	0.936386000	-8.507157000	-1.131895000
H	1.380484000	-7.100607000	-0.150920000
H	-0.016783000	-7.021823000	-1.221841000
C	3.369671000	-8.408161000	-5.471448000
H	4.388103000	-8.248068000	-5.843233000
H	3.293014000	-9.445673000	-5.129450000
H	2.692029000	-8.295483000	-6.328314000
C	3.577533000	-3.745853000	-3.555646000
H	4.194896000	-3.606693000	-4.448341000
H	2.711417000	-3.078344000	-3.638617000
H	4.163479000	-3.417953000	-2.688884000
C	-7.560341000	-3.520776000	0.707647000
H	-8.267938000	-4.347711000	0.595372000
H	-7.739907000	-2.807798000	-0.105132000
H	-6.549920000	-3.920235000	0.561129000
C	-9.733979000	-3.436189000	5.260854000
H	-9.466377000	-3.178287000	6.290863000
H	-10.753156000	-3.065888000	5.086294000
H	-9.770004000	-4.528305000	5.182722000
C	-6.368203000	0.129725000	4.066846000
H	-6.470309000	0.321265000	5.139470000

H	-5.300915000	0.038155000	3.837772000
H	-6.730853000	1.015704000	3.532491000
O	-0.072676000	-4.394186000	-3.302699000

Conformer-4

S	-2.702620000	-1.533726000	0.533860000
S	0.285568000	-4.338866000	-1.140597000
N	-4.865308000	0.560893000	1.055530000
H	-4.001936000	0.490711000	0.533583000
N	4.349353000	-2.217264000	-1.428502000
C	-5.552423000	-0.447306000	1.704994000
C	-5.589273000	1.724258000	1.065343000
C	-6.771519000	1.476830000	1.775442000
H	-7.547601000	2.202328000	1.976524000
C	-6.744016000	0.140016000	2.181088000
H	-7.498654000	-0.383743000	2.748138000
C	-5.185507000	-1.845720000	1.790177000
C	-4.044809000	-2.421783000	1.291666000
C	-3.760496000	-3.900608000	1.248788000
C	-2.499121000	-4.148274000	0.548958000
H	-2.134552000	-5.161820000	0.427781000
C	-1.837942000	-3.040657000	0.129898000
C	5.656680000	-2.016727000	-1.500575000
C	6.333173000	-3.062924000	-2.264102000
H	7.394697000	-3.124665000	-2.468134000
C	5.357174000	-3.933462000	-2.638698000
H	5.461774000	-4.839825000	-3.220212000
C	4.101306000	-3.405256000	-2.102734000
C	-6.217433000	-2.698304000	2.486361000
C	-6.128681000	-2.892995000	3.877737000
C	-7.136107000	-3.616870000	4.522857000
H	-7.069190000	-3.760380000	5.599724000
C	-8.219156000	-4.159279000	3.827234000
C	-8.280675000	-3.953619000	2.446410000
H	-9.115975000	-4.366165000	1.883448000
C	-7.297646000	-3.235653000	1.760209000
C	-0.560659000	-2.934943000	-0.531179000
C	1.677290000	-3.365494000	-1.611922000
C	1.435955000	-2.023216000	-1.335986000
H	2.164208000	-1.256956000	-1.557362000
C	0.187601000	-1.785218000	-0.739190000
H	-0.153174000	-0.798434000	-0.444077000
C	2.854623000	-4.002674000	-2.159512000
C	2.710602000	-5.376098000	-2.745674000
C	2.180261000	-5.527775000	-4.047026000
C	2.045461000	-6.813245000	-4.576242000
H	1.640968000	-6.926267000	-5.580222000
C	2.411071000	-7.953615000	-3.853861000
C	2.924823000	-7.779284000	-2.567209000
H	3.204920000	-8.654148000	-1.984004000
C	3.089182000	-6.511620000	-1.997172000
C	-4.963992000	-2.352556000	4.675851000
H	-5.124005000	-2.502953000	5.747920000
H	-4.809755000	-1.280833000	4.505009000
H	-4.030737000	-2.860207000	4.403608000
C	-9.277540000	-4.967585000	4.541093000
H	-10.255599000	-4.865193000	4.058147000
H	-9.381757000	-4.658808000	5.586893000
H	-9.026749000	-6.036909000	4.541510000
C	-7.390085000	-3.079858000	0.260090000
H	-8.345471000	-3.461541000	-0.113141000
H	-6.589629000	-3.640022000	-0.238322000
H	-7.299280000	-2.033323000	-0.052353000
C	1.778457000	-4.327667000	-4.874776000
H	1.451222000	-4.635837000	-5.872183000
H	2.610856000	-3.624216000	-4.993699000
H	0.956432000	-3.770927000	-4.409633000
C	2.272897000	-9.331020000	-4.458813000
H	2.224088000	-10.104948000	-3.686058000
H	3.128054000	-9.568007000	-5.105902000
H	1.370673000	-9.409453000	-5.075239000
C	3.658928000	-6.392061000	-0.599905000
H	3.694655000	-7.371779000	-0.114063000
H	3.061230000	-5.724781000	0.030204000
H	4.678161000	-5.988177000	-0.613112000
O	-4.482580000	-4.774312000	1.719996000
S	3.229580000	2.069138000	-0.143649000
S	-0.904220000	3.358064000	0.172326000
N	5.370370000	-0.082527000	-0.099414000
H	4.377812000	-0.279639000	-0.063943000
N	-3.890270000	2.985504000	-0.108125000
C	6.065474000	0.821212000	0.669093000
C	6.225101000	-0.906835000	-0.780532000
C	7.528959000	-0.488191000	-0.479695000
H	8.438005000	-0.923620000	-0.871470000

C	7.429932000	0.572801000	0.434560000
H	8.242630000	1.126215000	0.883087000
C	5.422707000	1.759456000	1.568541000
C	4.147687000	2.226105000	1.383533000
C	3.313584000	2.940863000	2.410922000
C	2.012437000	3.300670000	1.836999000
H	1.293101000	3.870050000	2.413900000
C	1.850890000	2.969661000	0.532379000
C	-5.131684000	2.882700000	0.346111000
C	-5.983624000	3.982317000	-0.106006000
H	-7.029493000	4.120538000	0.137156000
C	-5.205655000	4.739810000	-0.921470000
H	-5.476380000	5.640317000	-1.456315000
C	-3.880622000	4.123970000	-0.910042000
C	6.260731000	2.198044000	2.736623000
C	6.933366000	3.434257000	2.681001000
C	7.780619000	3.787145000	3.736775000
H	8.310367000	4.736601000	3.686801000
C	7.962322000	2.962091000	4.848505000
C	7.275140000	1.745021000	4.882244000
H	7.398301000	1.087537000	5.740841000
C	6.428491000	1.345431000	3.846538000
C	0.760509000	3.328380000	-0.357509000
C	-1.425335000	4.085739000	-1.342703000
C	-0.340612000	4.230364000	-2.200915000
H	-0.439777000	4.672467000	-3.185291000
C	0.878946000	3.777596000	-1.662559000
H	1.830174000	3.836658000	-2.179846000
C	-2.764670000	4.576208000	-1.582060000
C	-2.912464000	5.647263000	-2.622979000
C	-2.526246000	6.975502000	-2.333432000
C	-2.673126000	7.952382000	-3.321495000
H	-2.383691000	8.976138000	-3.092053000
C	-3.177580000	7.653156000	-4.591118000
C	-3.541350000	6.331453000	-4.857692000
H	-3.926195000	6.074584000	-5.842641000
C	-3.426860000	5.320743000	-3.896194000
C	6.756328000	4.385914000	1.518103000
H	7.500242000	5.187685000	1.558127000
H	6.854977000	3.881598000	0.550352000
H	5.764450000	4.853642000	1.537248000
C	8.852674000	3.382363000	5.994504000
H	9.369540000	2.523968000	6.437886000
H	9.610016000	4.104209000	5.670824000
H	8.270093000	3.857628000	6.795071000
C	5.671413000	0.042444000	3.950266000
H	5.952330000	-0.501134000	4.857404000
H	4.590946000	0.226062000	3.990426000
H	5.860884000	-0.614070000	3.093020000
C	-1.978787000	7.359220000	-0.976854000
H	-1.873718000	8.445056000	-0.893573000
H	-2.633273000	7.018940000	-0.166489000
H	-0.993329000	6.913006000	-0.798054000
C	-3.344948000	8.734052000	-5.633273000
H	-3.361903000	8.316213000	-6.645127000
H	-4.286407000	9.281065000	-5.489907000
H	-2.534332000	9.469269000	-5.582828000
C	-3.845244000	3.908963000	-4.247804000
H	-3.999011000	3.810197000	-5.326753000
H	-3.094911000	3.171741000	-3.942581000
H	-4.782018000	3.630544000	-3.750789000
O	3.671243000	3.180282000	3.560176000

Conformer-5

S	2.763580000	3.483872000	-0.693638000
S	4.696650000	0.626807000	-0.444397000
N	-1.794502000	5.009531000	-0.279516000
H	-1.803133000	4.112625000	-0.784412000
N	4.192036000	-3.732925000	-0.255741000
C	-0.651339000	5.733766000	-0.062611000
C	-2.887402000	5.668148000	0.188737000
C	-2.445764000	6.902047000	0.709195000
H	-3.072491000	7.658461000	1.161864000
C	-1.057725000	6.944574000	0.554857000
H	-0.391979000	7.734556000	0.871962000
C	0.686876000	5.241927000	-0.270369000
C	1.053083000	4.025355000	-0.817083000
C	0.257309000	2.992010000	-1.534294000
C	1.082602000	1.856191000	-1.856663000
H	0.636772000	0.977369000	-2.302898000
C	2.378237000	1.923414000	-1.432619000
C	4.158436000	-4.979877000	0.176723000
C	5.455793000	-5.407903000	0.706420000
H	5.694313000	-6.381616000	1.116510000
C	6.275440000	-4.325916000	0.598829000

H	7.316737000	-4.250070000	0.884074000	H	-2.253916000	0.482527000	-2.897761000
C	5.474145000	-3.260046000	-0.005155000	C	-5.823739000	1.939290000	-0.229814000
C	1.781382000	6.141144000	0.243991000	C	-7.107847000	1.379357000	0.294353000
C	2.398322000	7.054909000	-0.636388000	C	-8.146166000	1.050030000	-0.608571000
C	3.403859000	7.891766000	-0.142902000	C	-9.338197000	0.524608000	-0.107250000
H	3.874498000	8.600376000	-0.821663000	H	-10.137596000	0.281573000	-0.804751000
C	3.817989000	7.844222000	1.190948000	C	-9.531581000	0.300434000	1.260093000
C	3.187381000	6.934085000	2.043472000	C	-8.488586000	0.619059000	2.130980000
H	3.489713000	6.885927000	3.087780000	H	-8.612944000	0.437869000	3.196718000
C	2.172931000	6.080527000	1.598392000	C	-7.279231000	1.160994000	1.679072000
C	3.294164000	0.804409000	-1.481111000	C	-1.519537000	-5.118921000	2.565498000
C	4.890455000	-1.063367000	-0.911796000	H	-1.977052000	-5.195657000	3.556402000
C	3.947624000	-1.405367000	-1.871057000	H	-0.447579000	-5.322103000	2.671183000
H	3.883183000	-2.397791000	-2.291229000	H	-1.618768000	-4.080820000	2.228526000
C	3.067327000	-0.364429000	-2.193258000	C	-4.932281000	-8.733499000	1.691143000
H	2.253958000	-0.482396000	-2.897750000	H	-4.969585000	-9.678841000	1.139265000
C	5.823743000	-1.939327000	-0.229879000	H	-4.813968000	-8.965484000	2.754988000
C	7.107869000	-1.379437000	0.294330000	H	-5.910437000	-8.248631000	1.571213000
C	7.279201000	-1.161103000	1.679063000	C	-1.988192000	-7.144512000	-2.089142000
C	8.488527000	-0.619161000	2.131014000	H	-2.518570000	-7.958316000	-2.592669000
H	8.612854000	-0.437978000	3.196758000	H	-2.211015000	-6.215186000	-3.556402000
C	9.531559000	-0.300525000	1.260155000	H	-0.912181000	-7.324420000	-2.194522000
C	9.338224000	-0.524685000	-0.107186000	C	-7.995972000	1.281254000	-2.095546000
H	10.137643000	-0.281640000	-0.804659000	H	-8.930693000	1.058983000	-2.618986000
C	8.146199000	-1.050113000	-0.608553000	H	-7.722993000	2.319942000	-2.315678000
C	1.988000000	7.144511000	-2.089168000	H	-7.210951000	0.649475000	-2.527119000
H	2.517885000	7.958697000	-2.592600000	C	-10.838685000	-0.254884000	1.775230000
H	0.911883000	7.323765000	-2.194530000	H	-10.733384000	-0.650695000	2.790404000
H	2.211406000	6.215385000	-2.626647000	H	-11.616148000	0.520199000	1.803579000
C	4.932389000	8.733577000	1.690870000	H	-11.212230000	-1.061263000	1.133976000
H	4.813027000	8.967264000	2.754232000	C	-6.190798000	1.476010000	2.683796000
H	4.970976000	9.678047000	1.137601000	H	-6.402996000	0.990986000	3.641616000
H	5.910341000	8.247837000	1.572826000	H	-5.207481000	1.136303000	2.342875000
C	1.519777000	5.118971000	2.565538000	H	-6.107913000	2.553679000	2.867111000
H	1.976535000	5.196612000	3.556721000	O	0.956450000	-3.050328000	-1.820123000
H	1.620204000	4.080783000	2.229157000	Conformer-6			
H	0.447569000	5.321226000	2.670362000	S	-1.784707000	0.181993000	-2.781914000
C	6.190730000	-1.476215000	2.683708000	S	2.421571000	-0.427794000	-2.222628000
H	6.403227000	-0.991837000	3.641790000	N	-4.486780000	0.680780000	-1.479327000
H	6.107376000	-2.553955000	2.866400000	H	-3.646029000	0.409786000	-0.983848000
H	5.207535000	-1.135868000	2.343071000	N	4.720377000	-1.062933000	-0.648782000
C	10.838668000	0.254687000	1.775396000	C	-4.609292000	1.658529000	-2.439363000
H	11.213371000	1.059643000	1.133047000	C	-5.713800000	0.177133000	-1.137663000
H	11.615496000	-0.520962000	1.805774000	C	-6.666323000	0.835581000	-1.925849000
H	10.732842000	0.652337000	2.789801000	H	-7.733446000	0.662191000	-1.900951000
C	7.996017000	-1.281259000	-2.095541000	C	-5.982630000	1.772763000	-2.716476000
H	8.930747000	-1.058981000	-2.618963000	H	-6.409789000	2.457529000	-3.435061000
H	7.211018000	-0.649420000	-2.527081000	C	-3.488665000	2.393663000	-2.998769000
H	7.723003000	-2.319919000	-2.315740000	C	-2.215952000	1.894164000	-3.071253000
O	-0.956483000	3.050247000	-1.819865000	C	-0.977104000	2.688344000	-3.384890000
S	-2.763562000	-3.483777000	-0.693669000	C	0.202478000	1.818433000	-3.322676000
S	-4.696571000	-0.626789000	-0.444429000	H	1.189580000	2.208295000	-3.541843000
N	1.794460000	-5.009502000	-0.279603000	C	-0.060994000	0.514175000	-3.066243000
H	1.803100000	-4.112619000	-0.784548000	C	5.787482000	-0.814054000	0.095492000
N	-4.192046000	3.732906000	-0.255662000	C	6.906636000	-1.690753000	-0.242259000
C	0.651291000	-5.733734000	-0.062711000	H	7.885188000	-1.686084000	0.221161000
C	2.887352000	-5.668138000	0.188642000	C	6.446691000	-2.518936000	-1.219304000
C	2.445702000	-6.902035000	0.709096000	H	6.981268000	-3.310388000	-1.727740000
H	3.072420000	-7.658450000	1.161772000	C	5.068168000	-2.114066000	-1.484780000
C	1.057661000	-6.944534000	0.554781000	C	-3.830105000	3.761848000	-3.519123000
H	0.391910000	-7.734512000	0.871887000	C	-4.035869000	3.951110000	-4.899671000
C	-0.686912000	-5.241889000	-0.270483000	C	-4.444027000	5.209826000	-5.352686000
C	-1.053114000	-4.025326000	-0.817229000	H	-4.615812000	5.351381000	-6.418120000
C	-0.257342000	-2.992053000	-1.534549000	C	-4.631765000	6.285751000	-4.482442000
C	-1.082627000	-1.856228000	-1.856940000	C	-4.410723000	6.073189000	-3.118684000
H	-0.636817000	-0.977455000	-2.303289000	H	-4.547517000	6.898076000	-2.421914000
C	-2.378229000	-1.923379000	-1.432762000	C	-4.015679000	4.830608000	-2.618729000
C	-4.158470000	4.979862000	0.176803000	C	0.876404000	-0.596362000	-3.016964000
C	-5.455851000	5.407882000	0.706448000	C	2.895872000	-2.058598000	-2.687480000
H	-5.694405000	6.381605000	1.116496000	C	1.863634000	-2.669311000	-3.394573000
C	-6.275479000	4.325883000	0.598856000	H	1.950175000	-3.677054000	-3.783672000
H	-7.316783000	4.250033000	0.884072000	C	0.719861000	-1.861817000	-3.554877000
C	-5.474144000	3.260004000	-0.005062000	H	-0.174254000	-2.173274000	-4.083716000
C	-1.781417000	-6.141055000	0.243967000	C	4.191708000	-2.639348000	-2.411339000
C	-2.172846000	-6.080413000	1.598391000	C	4.569747000	-3.872688000	-3.178076000
C	-3.187261000	-6.933970000	2.043580000	C	5.053601000	-3.760764000	-4.500109000
H	-3.489519000	-6.885773000	3.087907000	C	5.399167000	-4.924130000	-5.193345000
C	-3.817926000	-7.844132000	1.191140000	H	5.776915000	-4.834512000	-6.210079000
C	-3.403916000	-7.891698000	-0.142756000	C	5.272258000	-6.193511000	-4.620857000
H	-3.874619000	-8.600317000	-0.821464000	C	4.781922000	-6.278927000	-3.315704000
C	-2.398441000	-7.054843000	-0.636346000	H	4.665653000	-7.257738000	-2.854475000
C	-3.294120000	-0.804340000	-1.481183000	C	4.432254000	-5.142231000	-2.578042000
C	-4.890435000	1.063387000	-0.911799000	C	-3.815594000	2.836088000	-5.897941000
C	-3.947603000	1.405446000	-1.871029000	H	-4.220337000	3.108543000	-6.877710000
H	-3.883175000	2.397895000	-2.291145000				
C	-3.067285000	0.364530000	-2.193275000				

H	-4.288743000	1.898644000	-5.585365000
H	-2.746046000	2.630449000	-6.027208000
C	-5.034548000	7.646663000	-5.000524000
H	-5.687027000	8.169538000	-4.292401000
H	-5.562689000	7.572079000	-5.957095000
H	-4.155621000	8.285079000	-5.162261000
C	-3.749374000	4.662758000	-1.141057000
H	-3.976333000	5.584240000	-0.596538000
H	-2.695449000	4.419053000	-0.960462000
H	-4.350318000	3.857206000	-0.703194000
C	5.215077000	-2.412580000	-5.165949000
H	5.676351000	-2.518532000	-6.152333000
H	5.842801000	-1.741319000	-4.568724000
H	4.249965000	-1.909643000	-5.298376000
C	5.676464000	-7.432903000	-5.384616000
H	5.151366000	-8.320201000	-5.015937000
H	6.753015000	-7.626588000	-5.285983000
H	5.463619000	-7.332324000	-6.454466000
C	3.911265000	-5.297910000	-1.165649000
H	3.708867000	-6.349830000	-0.942156000
H	2.985692000	-4.733134000	-1.008577000
H	4.633946000	-4.931913000	-0.426912000
O	-0.958257000	3.887744000	-3.643279000
S	1.784560000	0.182007000	2.782021000
S	-2.421690000	-0.427592000	2.222761000
N	4.486770000	0.680590000	1.479319000
H	3.645999000	0.409560000	0.983901000
N	-4.720527000	-1.062568000	0.648907000
C	4.609323000	1.658265000	2.439405000
C	5.713768000	0.176835000	1.137676000
C	6.666317000	0.835244000	1.925870000
H	7.733437000	0.661844000	1.900948000
C	5.982660000	1.772395000	2.716563000
H	6.409841000	2.457128000	3.435163000
C	3.488752000	2.393517000	2.998812000
C	2.215998000	1.894128000	3.071297000
C	0.977219000	2.688424000	3.384930000
C	-0.202459000	1.818619000	3.322785000
H	-1.189469000	2.208682000	3.541974000
C	0.060881000	0.514342000	3.066357000
C	-5.787571000	-0.813761000	-0.095465000
C	-6.906620000	-1.690715000	0.241969000
H	-7.885083000	-1.686181000	-0.221645000
C	-6.446753000	-2.518829000	1.219103000
H	-6.981300000	-3.310403000	1.727379000
C	-5.068347000	-2.113746000	1.484867000
C	3.830343000	3.761680000	3.519108000
C	4.016391000	4.830299000	2.618604000
C	4.411578000	6.072840000	3.118483000
H	4.548695000	6.897616000	2.421640000
C	4.632356000	6.285530000	4.482285000
C	4.444139000	5.209782000	5.352611000
H	4.615649000	5.351455000	6.418072000
C	4.035799000	3.951080000	4.899665000
C	-0.876560000	-0.596189000	3.017168000
C	-2.896073000	-2.058371000	2.687646000
C	-1.863903000	-2.669077000	3.394824000
H	-1.950500000	-3.676777000	3.784027000
C	-0.720102000	-1.861612000	3.555160000
H	0.173946000	-2.173154000	4.084046000
C	-4.191933000	-2.639063000	2.411417000
C	-4.570002000	-3.872466000	3.178082000
C	-4.431622000	-5.142031000	2.578316000
C	-4.781292000	-6.278761000	3.315927000
H	-4.664322000	-7.257596000	2.854925000
C	-5.272494000	-6.193341000	4.620755000
C	-5.400299000	-4.923926000	5.192967000
H	-5.778733000	-4.834307000	6.209445000
C	-5.054767000	-3.760524000	4.499770000
C	3.750511000	4.662273000	1.140871000
H	3.976723000	5.583995000	0.596451000
H	4.352330000	3.857315000	0.703094000
H	2.696870000	4.417570000	0.960012000
C	5.035489000	7.646412000	5.000175000
H	5.559913000	7.572120000	5.958800000
H	5.691543000	8.167291000	4.293861000
H	4.157065000	8.286549000	5.157743000
C	3.815023000	2.836272000	5.898057000
H	4.219524000	3.108826000	6.877899000
H	2.745401000	2.630846000	6.027047000
H	4.288103000	1.898692000	5.585783000
C	-3.909749000	-5.297637000	1.166248000
H	-3.707428000	-6.349566000	0.942726000
H	-4.631894000	-4.931368000	0.427114000
H	-2.983956000	-4.733038000	1.009841000
C	-5.676667000	-7.432783000	5.384452000

H	-5.464477000	-7.331977000	6.454411000
H	-6.753087000	-7.626891000	5.285228000
H	-5.151020000	-8.319931000	5.016199000
C	-5.217316000	-2.412270000	5.165198000
H	-5.677568000	-2.518371000	6.152042000
H	-4.252718000	-1.908058000	5.296511000
H	-5.846441000	-1.742057000	4.568259000
O	0.958478000	3.887793000	3.643462000

Conformer-7

S	3.874939000	-0.559496000	0.165058000
S	1.854627000	-4.476964000	0.044366000
N	5.081417000	2.269790000	0.117728000
H	4.173895000	1.884420000	-0.106485000
N	-2.884770000	-4.124930000	0.333397000
C	6.303593000	1.628680000	0.050951000
C	5.252540000	3.605003000	0.381011000
C	6.629152000	3.832264000	0.511914000
H	7.090047000	4.783779000	0.737240000
C	7.279079000	2.613435000	0.303063000
H	8.341957000	2.426999000	0.333910000
C	6.540240000	0.227875000	-0.230832000
C	5.594546000	-0.762163000	-0.266645000
C	5.855142000	-2.194378000	-0.652490000
C	4.615661000	-2.964971000	-0.583752000
H	4.612241000	-4.015153000	-0.851634000
C	3.517419000	-2.271164000	-0.193625000
C	-4.146079000	-4.516272000	0.457342000
C	-4.269920000	-5.961249000	0.646375000
H	-5.192285000	-6.513910000	0.769650000
C	-3.003325000	-6.443490000	0.620069000
H	-2.678050000	-7.469421000	0.725081000
C	-2.123223000	-5.288570000	0.428249000
C	7.991189000	-0.096632000	-0.485154000
C	8.534038000	0.086875000	-1.771461000
C	9.898743000	-0.140915000	-1.966460000
H	10.316116000	0.001815000	-2.961529000
C	10.737432000	-0.546766000	-0.925076000
C	10.173113000	-0.720637000	0.340945000
H	10.808067000	-1.032011000	1.168355000
C	8.811848000	-0.510313000	0.581347000
C	2.171017000	-2.761606000	-0.021439000
C	0.123816000	-4.211857000	0.226120000
C	-0.153535000	-2.847058000	0.240693000
H	-1.166834000	-2.484020000	0.345420000
C	0.991572000	-2.041353000	0.107444000
H	0.964455000	-0.956709000	0.088607000
C	-0.744176000	-5.357536000	0.358107000
C	-0.086983000	-6.709671000	0.423541000
C	0.340023000	-7.225480000	1.666722000
C	0.961743000	-8.477160000	1.699992000
H	1.292983000	-8.871234000	2.658731000
C	1.171056000	-9.231512000	0.541972000
C	0.738927000	-8.700048000	-0.675851000
H	0.896105000	-9.268888000	-1.590084000
C	0.109301000	-7.453925000	-0.759675000
C	7.663109000	0.487686000	-2.939354000
H	8.266937000	0.656793000	-3.836149000
H	7.098113000	1.404888000	-2.736036000
H	6.934521000	-0.298894000	-3.170549000
C	12.204280000	-0.815985000	-1.167655000
H	12.798385000	-0.650113000	-0.262451000
H	12.605472000	-0.173552000	-1.959202000
H	12.370151000	-1.856055000	-1.479144000
C	8.249782000	-0.748499000	1.964530000
H	9.054494000	-0.912225000	2.687941000
H	7.605243000	-1.635837000	1.978369000
H	7.645841000	0.095475000	2.316634000
C	0.124198000	-6.457694000	2.951632000
H	0.546804000	-6.999158000	3.803115000
H	-0.942287000	-6.297346000	3.149029000
H	0.593035000	-5.467486000	2.917217000
C	1.822674000	-10.592933000	0.609303000
H	2.335663000	-10.838392000	-0.326430000
H	1.078769000	-11.380667000	0.789266000
H	2.554635000	-10.647164000	1.422155000
C	-0.353814000	-6.934969000	-2.102971000
H	-0.036273000	-7.604802000	-2.907574000
H	0.049326000	-5.938428000	-2.316112000
H	-1.446209000	-6.851360000	-2.145959000
O	6.944045000	-2.646795000	-0.993209000
S	-3.874815000	0.559495000	0.164254000
S	-1.854653000	4.476966000	0.044180000
N	-5.081373000	-2.269783000	0.117621000
H	-4.173859000	-1.884478000	-0.106734000

N	2.884790000	4.124926000	0.333293000	C	-1.558010000	3.086416000	-0.606005000
C	-6.303554000	-1.628687000	0.050643000	C	5.401262000	2.438023000	-0.155850000
C	-5.252526000	-3.605008000	0.380814000	C	6.336066000	3.445470000	0.345661000
C	-6.629151000	-3.832284000	0.511542000	H	7.405614000	3.463060000	0.179219000
H	-7.090070000	-4.783806000	0.736784000	C	5.590087000	4.302654000	1.087901000
C	-7.279061000	-2.613460000	0.302610000	H	5.920018000	5.178532000	1.630213000
H	-8.341945000	-2.427044000	0.333332000	C	4.209375000	3.833086000	0.991455000
C	-6.540184000	-0.227891000	-0.231154000	C	-5.963801000	2.516530000	-2.876871000
C	-5.594450000	0.762108000	-0.267309000	C	-6.167294000	1.625646000	-3.950113000
C	-5.855104000	2.194318000	-0.653159000	C	-6.962627000	2.032494000	-5.023015000
C	-4.615655000	2.964970000	-0.584415000	H	-7.113391000	1.344863000	-5.853140000
H	-4.612263000	4.015140000	-0.852333000	C	-7.564303000	3.293881000	-5.061702000
C	-3.517365000	2.271171000	-0.194413000	C	-7.348937000	4.156426000	-3.984987000
C	4.146088000	4.516268000	0.457407000	H	-7.812480000	5.141166000	-3.991346000
C	4.269899000	5.961241000	0.646462000	C	-6.550186000	3.796995000	-2.894181000
H	5.192248000	6.513905000	0.769845000	C	-0.466644000	3.408236000	0.296672000
C	3.003297000	6.443465000	0.620130000	C	1.743546000	4.031376000	1.320729000
H	2.678008000	7.469392000	0.725142000	C	0.648661000	4.305219000	2.133352000
C	2.123232000	5.288551000	0.428112000	H	0.754393000	4.781734000	3.100728000
C	-7.991183000	0.096681000	-0.485129000	C	-0.587130000	3.928072000	1.574571000
C	-8.811536000	0.510232000	-0.581644000	H	-1.545429000	4.086856000	2.056537000
C	-10.172874000	0.720641000	0.341633000	C	3.112408000	4.404942000	1.599685000
H	-10.807591000	1.031936000	1.169254000	C	3.316655000	5.484966000	2.622566000
C	-10.737535000	0.546945000	-0.924241000	C	3.725268000	5.145570000	3.930068000
C	-9.899125000	0.141211000	-1.965919000	C	3.893937000	6.167677000	4.871420000
H	-10.316769000	-0.001367000	-2.960898000	H	4.197346000	5.902351000	5.882261000
C	-8.534388000	-0.086625000	-1.771325000	C	3.684894000	7.511194000	4.552629000
C	-2.170959000	2.761612000	-0.022276000	C	3.282380000	7.822360000	3.249900000
C	-0.123777000	4.211862000	0.225545000	H	3.113365000	8.863024000	2.979763000
C	0.153631000	2.847070000	0.239463000	C	3.087279000	6.836324000	2.279352000
H	1.166961000	2.484027000	0.343869000	C	-5.500565000	0.270446000	-3.975823000
C	-0.991458000	2.041364000	0.106066000	H	-5.802328000	-0.296287000	-4.861863000
H	-0.964276000	0.956731000	0.086663000	H	-5.750204000	-0.328961000	-3.092557000
C	0.744186000	5.357518000	0.357840000	H	-4.409405000	0.377522000	-4.001903000
C	0.086967000	6.709627000	0.423537000	C	-8.399317000	3.719126000	-6.246857000
C	-0.109392000	7.454075000	-0.759534000	H	-9.112301000	4.504606000	-5.974663000
C	-0.739035000	8.700183000	-0.675461000	H	-8.964062000	2.877665000	-6.663502000
H	-0.896257000	9.269186000	-1.589584000	H	-7.768728000	4.116229000	-7.053617000
C	-1.171119000	9.231424000	0.542465000	C	-6.331541000	4.788375000	-1.772258000
C	-0.961737000	8.476870000	1.700352000	H	-7.015487000	5.637448000	-1.867939000
H	-1.292943000	8.870764000	2.659177000	H	-5.308725000	5.184025000	-1.787837000
C	-0.339991000	7.225220000	1.666834000	H	-6.487049000	4.338941000	-7.850944000
C	-8.249114000	0.748187000	1.964725000	C	3.975250000	3.709279000	4.337653000
H	-9.053635000	0.912042000	2.688319000	H	4.067234000	3.627525000	5.425021000
H	-7.645302000	-0.095958000	2.316637000	H	4.899404000	3.319791000	3.894552000
H	-7.604354000	1.635368000	1.978518000	H	3.166235000	3.045500000	4.014197000
C	-12.204442000	0.816175000	-1.166452000	C	3.908739000	8.600055000	5.575769000
H	-12.606330000	0.172341000	-1.956517000	H	3.183156000	9.412961000	5.462128000
H	-12.798042000	0.652234000	-0.260572000	H	4.908449000	9.042706000	5.471974000
H	-12.370166000	1.855683000	-1.479881000	H	3.828211000	8.213374000	6.596915000
C	-7.663746000	-0.487267000	-2.939487000	C	2.654468000	7.231823000	0.885317000
H	-8.267788000	-0.656254000	-3.836160000	H	2.654903000	8.320051000	0.772370000
H	-6.935233000	0.299364000	-3.170732000	H	1.643695000	6.872057000	0.659181000
H	-7.098692000	-1.404492000	-2.736428000	H	3.319128000	6.811485000	0.122122000
C	0.353673000	6.935369000	-2.102942000	O	-3.294621000	3.279265000	-3.683303000
H	0.036064000	7.605326000	-2.907415000	S	2.729797000	-1.796197000	-0.142069000
H	1.446072000	6.851814000	-2.146002000	S	-0.635112000	-4.283968000	1.239287000
H	-0.049434000	5.938849000	-2.316231000	N	4.913478000	0.173583000	-0.944372000
C	-1.822783000	10.592807000	0.610106000	H	3.952852000	0.249905000	-0.637181000
H	-2.556365000	10.646123000	1.421566000	N	-4.470249000	-1.842687000	1.513210000
H	-1.079197000	11.380275000	0.792527000	C	5.531872000	-0.904529000	-1.547771000
H	-2.333892000	10.839402000	-0.326349000	C	5.781243000	1.229208000	-0.834564000
C	-0.124123000	6.457190000	2.951594000	C	7.000129000	0.829813000	-1.397962000
H	-0.546459000	6.998623000	3.803231000	H	7.890721000	1.439034000	-1.466022000
H	-0.593211000	5.467101000	2.917105000	C	6.842157000	-0.482040000	-1.853107000
H	0.942354000	6.296555000	3.148784000	H	7.586885000	-1.099920000	-2.331746000
O	-6.944006000	2.646668000	-0.993966000	C	4.988681000	-2.234497000	-1.739913000

Conformer-8

S	-3.009520000	2.315117000	0.076398000	C	3.820376000	-2.715744000	-1.208815000
S	1.210233000	3.280895000	-0.178831000	C	3.278999000	-4.108228000	-1.405132000
N	-5.296056000	0.315817000	0.081113000	C	2.006508000	-4.256553000	-0.697242000
H	-4.320485000	0.043959000	0.076239000	H	1.447664000	-5.182498000	-0.767070000
N	4.149459000	2.686119000	0.203425000	C	1.579755000	-3.153479000	-0.034233000
C	-5.907857000	1.231935000	-0.742517000	C	-5.757409000	-1.534631000	1.550019000
C	-6.223190000	-0.411936000	0.777464000	C	-6.533810000	-2.499055000	2.327124000
C	-7.486113000	0.087406000	0.429827000	H	-7.600560000	-2.466446000	2.509756000
H	-8.432353000	-0.262597000	0.819185000	C	-5.642102000	-3.437674000	2.743988000
C	-7.290960000	1.095502000	-0.527782000	H	-5.833010000	-4.315847000	3.346511000
H	-8.051419000	1.685841000	-1.018833000	C	-4.336616000	-3.030887000	2.221250000
C	-5.182246000	2.077904000	-1.670277000	C	5.862134000	-3.124532000	-2.588538000
C	-3.881669000	2.463054000	-1.477719000	C	6.835668000	-3.942841000	-1.984004000
C	-2.978491000	3.069627000	-2.516195000	C	7.688344000	-4.690660000	-2.800759000
C	-1.667579000	3.365860000	-1.927846000	H	8.445085000	-5.317067000	-2.331901000
H	-0.898079000	3.856574000	-2.512261000	C	7.593566000	-4.661384000	-4.194643000
				C	6.615424000	-3.845475000	-4.767886000
				H	6.524000000	-3.804646000	-5.851709000
				C	5.745224000	-3.075377000	-3.990709000

C	0.344252000	-2.946912000	0.683820000
C	-1.913153000	-3.196511000	1.775817000
C	-1.536877000	-1.875240000	1.563918000
H	-2.181031000	-1.049132000	1.828653000
C	-0.273106000	-1.737211000	0.963843000
H	0.164577000	-0.779771000	0.702186000
C	-3.148564000	-3.732573000	2.307368000
C	-3.129826000	-5.110379000	2.898530000
C	-3.623282000	-6.208235000	2.160763000
C	-3.572961000	-7.483456000	2.736186000
H	-3.941131000	-8.330447000	2.160866000
C	-3.063052000	-7.700274000	4.017499000
C	-2.581740000	-6.596453000	4.729377000
H	-2.178282000	-6.742903000	5.729493000
C	-2.599219000	-5.306890000	4.194393000
C	6.954918000	-4.046699000	-0.480953000
H	7.857437000	-4.598095000	-0.199374000
H	6.995745000	-3.062918000	0.000000000
H	6.094161000	-4.580000000	-0.059558000
C	8.503188000	-5.508202000	-5.054049000
H	8.665021000	-5.053556000	-6.037441000
H	9.481300000	-5.653551000	-4.582438000
H	8.073811000	-6.504808000	-5.223660000
C	4.685181000	-2.231727000	-4.660839000
H	4.794078000	-2.261476000	-5.749263000
H	3.679824000	-2.595174000	-4.415703000
H	4.735190000	-1.182752000	-4.346102000
C	-4.193321000	-6.044910000	0.767761000
H	-4.301285000	-7.018760000	0.280709000
H	-5.181793000	-5.570966000	0.788773000
H	-3.555219000	-5.419708000	0.134402000
C	-3.046813000	-9.081762000	4.628589000
H	-2.122265000	-9.261471000	5.188496000
H	-3.880339000	-9.215044000	5.331071000
H	-3.136108000	-9.859368000	3.863327000
C	-2.074508000	-4.147408000	5.011217000
H	-1.779946000	-4.479027000	6.011293000
H	-1.199637000	-3.683042000	4.541121000
H	-2.829331000	-3.360389000	5.123897000
O	3.814760000	-4.986413000	-2.074651000

Conformer-9

S	0.213346000	-3.297829000	0.424274000
S	-3.677685000	-1.483436000	-0.113842000
N	3.449365000	-3.283685000	0.348970000
H	2.979998000	-2.398360000	0.206980000
N	-5.507738000	0.721366000	-0.095251000
C	3.153104000	-4.472347000	-0.284357000
C	4.635038000	-3.388793000	1.034407000
C	5.078744000	-4.711014000	0.892342000
H	5.982541000	-5.118457000	1.323905000
C	4.174100000	-5.374094000	0.053456000
H	4.225553000	-6.398589000	-0.286149000
C	2.044956000	-4.655925000	-1.207737000
C	0.823741000	-4.057968000	-1.076149000
C	-0.231015000	-4.002018000	-2.150618000
C	-1.456313000	-3.414915000	-1.612839000
H	-2.354587000	-3.356655000	-2.215658000
C	-1.401392000	-3.067501000	-0.303528000
C	-6.155346000	1.786089000	-0.542432000
C	-7.552469000	1.795542000	-0.108556000
H	-8.292157000	2.550267000	-0.345167000
C	-7.706000000	0.692068000	0.673543000
H	-8.598486000	0.358049000	1.186201000
C	-6.409871000	0.017325000	0.685891000
C	2.336641000	-5.602289000	-2.340771000
C	3.128432000	-5.182051000	-3.429046000
C	3.454156000	-6.105233000	-4.423564000
H	4.059471000	-5.775645000	-5.266056000
C	3.022422000	-7.434363000	-4.369546000
C	2.241305000	-7.825824000	-3.281036000
H	1.898262000	-8.856730000	-3.216189000
C	1.878727000	-6.932078000	-2.266840000
C	-2.518394000	-2.620572000	0.513508000
C	-4.733737000	-1.722023000	1.268117000
C	-4.148597000	-2.607838000	2.172989000
H	-4.634021000	-2.893020000	3.099139000
C	-2.889781000	-3.088370000	1.765705000
H	-2.297698000	-3.799738000	2.331035000
C	-6.033033000	-1.101112000	1.404251000
C	-6.981758000	-1.703006000	2.398410000
C	-7.138388000	-1.111670000	3.669862000
C	-8.021976000	-1.698544000	4.583068000
H	-8.133074000	-1.246939000	5.566991000
C	-8.760293000	-2.841961000	4.269955000

C	-8.587120000	-3.409672000	3.003786000
H	-9.150464000	-4.302659000	2.739506000
C	-7.708212000	-2.866820000	2.062692000
C	3.577360000	-3.745550000	-3.555127000
H	4.194427000	-3.606085000	-4.447978000
H	4.163621000	-3.417990000	-2.688444000
H	2.711257000	-3.077963000	-3.637561000
C	3.370692000	-8.407567000	-5.471515000
H	3.282151000	-9.445320000	-5.133254000
H	4.393634000	-8.255329000	-5.834215000
H	2.701459000	-8.286351000	-6.333803000
C	1.002687000	-7.414790000	-1.130950000
H	0.935601000	-8.507293000	-1.132871000
H	-0.017240000	-7.021736000	-1.222547000
H	1.379791000	-7.101158000	-0.151348000
C	-6.369475000	0.130162000	4.066530000
H	-6.470764000	0.320825000	5.139387000
H	-6.733149000	1.016346000	3.533201000
H	-5.302347000	0.039425000	3.836445000
C	-9.734683000	-3.436834000	5.259742000
H	-9.752328000	-4.530522000	5.197864000
H	-10.758016000	-3.086165000	5.069797000
H	-9.481118000	-3.159281000	6.288130000
C	-7.560449000	-3.520560000	0.707063000
H	-8.267842000	-4.347651000	0.594682000
H	-6.549925000	-3.919772000	0.560616000
H	-7.740112000	-2.807582000	-0.105692000
O	-0.073213000	-4.394474000	-3.302598000
S	0.532109000	4.200920000	-1.215004000
S	3.221536000	1.127817000	0.493450000
N	-4.075943000	2.763357000	-1.281891000
H	-3.492944000	1.955390000	-1.013678000
N	4.852292000	-1.004874000	1.358024000
C	-3.547689000	3.919230000	-1.796353000
C	-5.430165000	2.837032000	-1.212307000
C	-5.815298000	4.086979000	-1.743184000
H	-6.830227000	4.450114000	-1.831595000
C	-4.649148000	4.757364000	-2.112763000
H	-4.573774000	5.750723000	-2.531344000
C	-2.149008000	4.253709000	-1.809819000
C	-1.096608000	3.468719000	-1.371374000
C	-1.042792000	2.040125000	-0.958536000
C	0.278734000	1.696779000	-0.489672000
H	0.469900000	0.708064000	-0.089048000
C	1.188537000	2.711562000	-0.513187000
C	5.295888000	-2.235050000	1.578127000
C	6.554862000	-2.239068000	2.323929000
H	7.110495000	-3.114715000	2.634501000
C	6.865726000	-0.933535000	2.533684000
H	7.726571000	-0.527053000	3.047422000
C	5.798315000	-0.152595000	1.911248000
C	-1.833374000	5.648659000	-2.285803000
C	-1.871490000	6.733885000	-1.384744000
C	-1.579233000	8.015395000	-1.862806000
H	-1.609197000	8.851908000	-1.167305000
C	-1.255809000	8.251412000	-3.201597000
C	-1.235241000	7.160872000	-4.075400000
H	-0.995990000	7.323554000	-5.124508000
C	-1.515770000	5.860788000	-3.644199000
C	2.527906000	2.665889000	0.019416000
C	4.651073000	1.916113000	1.145092000
C	4.565569000	3.296059000	0.952028000
H	5.345420000	3.971758000	1.282383000
C	3.383614000	3.715644000	0.316765000
H	3.144369000	4.754086000	0.114020000
C	5.731664000	1.222351000	1.799507000
C	6.836977000	2.062480000	2.374612000
C	7.969976000	2.367842000	1.591459000
C	8.982290000	3.157381000	2.147187000
H	9.853353000	3.395085000	1.539598000
C	8.906270000	3.647821000	3.453556000
C	7.772116000	3.334442000	4.207855000
H	7.689484000	3.710772000	5.225688000
C	6.733633000	2.550888000	3.694333000
C	-2.223171000	6.536556000	0.072703000
H	-2.170365000	7.484960000	0.615805000
H	-3.236521000	6.135545000	0.190507000
H	-1.539617000	5.831216000	0.558868000
C	-0.914737000	9.641367000	-3.685943000
H	-1.205541000	9.784321000	-4.732224000
H	-1.414961000	10.409315000	-3.086373000
H	0.165261000	9.830337000	-3.620951000
C	-1.480365000	4.714608000	-4.629939000
H	-1.278977000	5.078685000	-5.641813000
H	-0.700678000	3.988095000	-4.372676000
H	-2.430912000	4.169255000	-4.648833000

C	8.106963000	1.856350000	0.174455000
H	9.007639000	2.258922000	-0.298685000
H	8.172507000	0.762303000	0.146896000
H	7.246042000	2.136950000	-0.442946000
C	10.028010000	4.471774000	4.041720000
H	9.655672000	5.182127000	4.787579000
H	10.768950000	3.834160000	4.542478000
H	10.557934000	5.037982000	3.268410000
C	5.529795000	2.238049000	4.554949000
H	5.616908000	2.717085000	5.534748000
H	4.599595000	2.585596000	4.090663000
H	5.419055000	1.159283000	4.715059000
O	-1.982984000	1.223096000	-0.991755000

Conformer-10

S	-3.410174000	-0.135747000	0.051518000
S	-2.543229000	4.172877000	-0.150136000
N	-3.985840000	-3.280883000	-0.097604000
H	-3.181643000	-2.756422000	0.220872000
N	2.075962000	5.093226000	-0.105260000
C	-5.305286000	-2.862284000	-0.129838000
C	-3.891219000	-4.594702000	-0.492605000
C	-5.183353000	-5.032340000	-0.803627000
H	-5.443627000	-6.023687000	-1.147268000
C	-6.057893000	-3.970293000	-0.565175000
H	-7.128865000	-3.967174000	-0.697927000
C	-5.843140000	-1.553278000	0.193606000
C	-5.156597000	-0.377061000	0.342965000
C	-5.797560000	0.941855000	0.696682000
C	-4.807921000	2.013430000	0.639606000
H	-5.093485000	3.033074000	0.869984000
C	-3.543661000	1.627184000	0.340746000
C	3.236860000	5.700246000	-0.298366000
C	3.063914000	7.096588000	-0.693506000
H	3.853095000	7.806886000	-0.906244000
C	1.719170000	7.307831000	-0.722221000
H	1.196209000	8.222442000	-0.968470000
C	1.092332000	6.032369000	-0.363103000
C	-7.347868000	-1.561562000	0.329106000
C	-8.154407000	-1.275188000	-0.788706000
C	-9.543134000	-1.379376000	-0.661410000
H	-10.164946000	-1.166060000	-1.528995000
C	-10.151867000	-1.744104000	0.541786000
C	-9.327503000	-2.017761000	1.636407000
H	-9.778839000	-2.304948000	2.584392000
C	-7.935475000	-1.932313000	1.553612000
C	-2.375568000	2.472968000	0.223827000
C	-0.799317000	4.430606000	-0.051759000
C	-0.161522000	3.231766000	0.265397000
H	0.908383000	3.174982000	0.404100000
C	-1.041034000	2.143049000	0.403201000
H	-0.713123000	1.140511000	0.657535000
C	-0.263057000	5.746462000	-0.332938000
C	-1.241015000	6.847156000	-0.635746000
C	-1.767115000	7.624251000	0.419240000
C	-2.683163000	8.636740000	0.119150000
H	-3.090961000	9.231308000	0.934331000
C	-3.089078000	8.903915000	-1.191400000
C	-2.553065000	8.122303000	-2.217974000
H	-2.859266000	8.310521000	-3.245117000
C	-1.633261000	7.098689000	-1.967955000
C	-7.554847000	-0.840818000	-2.107030000
H	-8.315542000	-0.827610000	-2.893821000
H	-6.744597000	-1.503344000	-2.431420000
H	-7.136448000	0.170453000	-2.033912000
C	-11.656281000	-1.813865000	0.664060000
H	-11.965955000	-2.573550000	1.390225000
H	-12.127000000	-2.050970000	-0.296239000
H	-12.071747000	-0.854744000	1.001444000
C	-7.090239000	-2.201008000	2.776745000
H	-7.709382000	-2.543727000	3.611485000
H	-6.569763000	-1.290442000	3.097635000
H	-6.325584000	-2.963988000	2.588989000
C	-1.349695000	7.385818000	1.853191000
H	-1.886927000	8.056190000	2.530642000
H	-0.275386000	7.554761000	1.991671000
H	-1.551086000	6.355760000	2.169210000
C	-4.060052000	10.022220000	-1.490539000
H	-4.617496000	9.832678000	-2.413781000
H	-3.536882000	10.979742000	-1.616407000
H	-4.783134000	10.153194000	-0.678344000
C	-1.073841000	6.292614000	-3.119129000
H	-1.550307000	6.579984000	-4.061174000
H	-1.231017000	5.217434000	-2.976687000
H	0.006605000	6.444093000	-3.227525000

O	-6.975905000	1.096309000	1.003632000
S	4.791672000	-0.996099000	1.145305000
S	2.777286000	-3.728660000	0.447201000
N	4.313077000	3.685172000	0.402134000
H	3.473239000	3.329930000	0.883730000
N	-1.514702000	-4.825086000	-0.063855000
C	5.494487000	2.996432000	0.370648000
C	4.445530000	4.922275000	-0.132326000
C	5.798480000	5.074083000	-0.508925000
H	6.231340000	5.945626000	-0.980967000
C	6.450623000	3.875587000	-0.202424000
H	7.486137000	3.631729000	-0.393910000
C	5.603498000	1.598380000	0.689546000
C	4.590479000	0.791038000	1.183160000
C	3.256517000	1.123043000	1.750780000
C	2.518459000	-0.075767000	2.050682000
H	1.487065000	-0.004084000	2.372294000
C	3.134893000	-1.241571000	1.706751000
C	-2.647967000	-5.318244000	-0.532866000
C	-2.474533000	-6.642119000	-1.138581000
H	-3.250880000	-7.247258000	-1.589269000
C	-1.149951000	-6.919746000	-1.044726000
H	-0.627636000	-7.806765000	-1.377715000
C	-0.538671000	-5.783040000	-0.357864000
C	6.927126000	0.960877000	0.360054000
C	7.903430000	0.832813000	1.370818000
C	9.133842000	0.252391000	1.048656000
H	9.888604000	0.160733000	1.827248000
C	9.419996000	-0.209523000	-0.238927000
C	8.437802000	-0.066525000	-1.222567000
H	8.642886000	-0.413341000	-2.233449000
C	7.194578000	0.513798000	-0.951547000
C	2.435031000	-2.506057000	1.649098000
C	1.249811000	-4.538725000	0.768324000
C	0.577557000	-3.913331000	1.807606000
H	-0.380892000	-4.265813000	2.162973000
C	1.246335000	-2.784721000	2.307469000
H	0.863817000	-2.162605000	3.108658000
C	0.801199000	-5.638458000	-0.058381000
C	1.820806000	-6.572591000	-0.632192000
C	2.147988000	-6.513457000	-2.004941000
C	3.123374000	-7.385644000	-2.503318000
H	3.384451000	-7.328176000	-3.558080000
C	3.770882000	-8.318295000	-1.691685000
C	3.429226000	-8.359167000	-0.335644000
H	3.921792000	-9.078654000	0.315775000
C	2.473837000	-7.501534000	0.212117000
C	7.643346000	1.315709000	2.780320000
H	8.540926000	1.212865000	3.397295000
H	7.339188000	2.368541000	2.797103000
H	6.839759000	0.743583000	3.258793000
C	10.743851000	-0.866716000	-0.552186000
H	11.026551000	-0.720321000	-1.600095000
H	11.548074000	-0.468434000	0.075645000
H	10.700172000	-1.949818000	-0.375551000
C	6.171362000	0.650776000	-2.056673000
H	6.538901000	0.198353000	-2.982548000
H	5.227293000	0.160132000	-1.794119000
H	5.941014000	1.702445000	-2.262820000
C	1.489419000	-5.528394000	-2.947944000
H	2.061924000	-5.447598000	-3.877103000
H	0.471173000	-5.838473000	-3.210889000
H	1.412608000	-4.528108000	-2.509868000
C	4.797951000	-9.269610000	-2.259237000
H	5.654234000	-9.383919000	-1.585015000
H	4.371500000	-10.270173000	-2.410676000
H	5.172943000	-8.923197000	-3.227543000
C	2.136445000	-7.599188000	1.683095000
H	2.656619000	-8.443753000	2.144743000
H	2.423150000	-6.691572000	2.227048000
H	1.060398000	-7.736844000	1.840858000
O	2.767448000	2.260112000	1.919331000

Conformer-11

S	2.100125000	4.136176000	-0.120896000
S	3.900302000	0.090215000	-0.098092000
N	-2.807540000	4.278903000	-0.130654000
H	-2.552131000	3.296588000	-0.295725000
N	4.973943000	-2.544921000	0.126215000
C	-1.871166000	5.281708000	-0.022798000
C	-4.064761000	4.783189000	0.036225000
C	-3.946098000	6.168403000	0.249609000
H	-4.768137000	6.852990000	0.408500000
C	-2.588184000	6.481739000	0.205642000
H	-2.140520000	7.456276000	0.333607000

C	-0.438379000	5.139595000	-0.068144000
C	0.318844000	3.992413000	-0.202768000
C	-0.063088000	2.563805000	-0.384275000
C	1.116309000	1.718192000	-0.386117000
H	1.037669000	0.640495000	-0.485729000
C	2.302848000	2.379098000	-0.259126000
C	5.047594000	-3.861147000	0.262082000
C	6.430149000	-4.322320000	0.398576000
H	6.752694000	-5.348700000	0.519896000
C	7.202180000	-3.206547000	0.332296000
H	8.279956000	-3.136120000	0.392812000
C	6.281000000	-2.083147000	0.166007000
C	0.312417000	6.440615000	0.083780000
C	0.647661000	7.190350000	-1.063399000
C	1.334209000	8.397805000	-0.902625000
H	1.588681000	8.976655000	-1.788419000
C	1.697174000	8.881041000	0.357513000
C	1.346518000	8.123459000	1.478181000
H	1.611433000	8.485889000	2.469564000
C	0.659875000	6.910017000	1.368135000
C	3.634126000	1.820613000	-0.205210000
C	5.643616000	0.318838000	-0.046844000
C	5.956993000	1.678050000	-0.120026000
H	6.979277000	2.036167000	-0.105924000
C	4.835884000	2.516444000	-0.205477000
H	4.898121000	3.597548000	-0.270069000
C	6.610385000	-0.744818000	0.076396000
C	8.060089000	-0.348786000	0.119577000
C	8.676962000	-0.065998000	1.356436000
C	10.026288000	0.302533000	1.369717000
H	10.499043000	0.522676000	2.325000000
C	10.779951000	0.397097000	0.196589000
C	10.144907000	0.116623000	-1.016285000
H	10.711156000	0.190184000	-1.942819000
C	8.798107000	-0.256106000	-1.079125000
C	0.275456000	6.712976000	-2.448958000
H	0.586065000	7.438899000	-3.206406000
H	-0.806154000	6.563850000	-2.545763000
H	0.753671000	5.755006000	-2.684343000
C	2.467332000	10.172924000	0.502008000
H	2.258845000	10.659308000	1.460898000
H	2.220230000	10.879156000	-0.297959000
H	3.550466000	9.996673000	0.455858000
C	0.302703000	6.130828000	2.613633000
H	0.633390000	6.661682000	3.511419000
H	0.774052000	5.141185000	2.615004000
H	-0.778918000	5.972385000	2.692720000
C	7.908882000	-0.158836000	2.656170000
H	8.535977000	0.141979000	3.500848000
H	7.557783000	-1.180348000	2.843266000
H	7.021016000	0.483739000	2.648099000
C	12.244252000	0.767546000	0.240640000
H	12.556459000	1.278861000	-0.676211000
H	12.876994000	-0.123959000	0.346637000
H	12.466511000	1.424638000	1.088244000
C	8.160783000	-0.554580000	-2.418018000
H	8.869304000	-0.380756000	-3.233495000
H	7.279759000	0.072817000	-2.595561000
H	7.824093000	-1.596025000	-2.479425000
O	-1.224777000	2.134263000	-0.528673000
S	-2.199127000	-3.918505000	-0.574698000
S	-4.916129000	-1.519927000	-0.240308000
N	2.634541000	-4.183660000	0.054657000
H	2.391173000	-3.199558000	-0.139893000
N	-5.105883000	2.653489000	-0.309035000
C	1.686682000	-5.176888000	0.108315000
C	3.876183000	-4.696913000	0.262420000
C	3.736704000	-6.086583000	0.462257000
H	4.544028000	-6.778993000	0.657566000
C	2.379172000	-6.385544000	0.372068000
H	1.916020000	-7.355819000	0.477272000
C	0.270040000	-5.007835000	-0.076385000
C	-0.413478000	-3.847519000	-0.384759000
C	0.062470000	-2.459003000	-0.633790000
C	-1.044561000	-1.599546000	-0.974985000
H	-0.916983000	-0.532256000	-1.110812000
C	-2.265696000	-2.201026000	-0.971658000
C	-5.226090000	3.927468000	0.001235000
C	-6.604164000	4.277466000	0.367343000
H	-6.963015000	5.256822000	0.659720000
C	-7.312649000	3.118916000	0.297316000
H	-8.367045000	2.969697000	0.490985000
C	-6.371712000	2.088426000	-0.140553000
C	-0.538576000	-6.270098000	0.088705000
C	-1.029027000	-6.624896000	1.362996000
C	-1.768636000	-7.804378000	1.494546000

H	-2.144966000	-8.078257000	2.478223000
C	-2.034001000	-8.637915000	0.404812000
C	-1.528906000	-8.268047000	-0.844701000
H	-1.716045000	-8.907637000	-1.705061000
C	-0.785292000	-7.097984000	-1.026848000
C	-3.478243000	-1.452849000	-1.237077000
C	-5.521478000	-0.025408000	-0.948866000
C	-4.681512000	0.406794000	-1.957717000
H	-4.876311000	1.308984000	-2.521021000
C	-3.538984000	-0.394372000	-2.123015000
H	-2.746891000	-0.186080000	-2.832235000
C	-6.596696000	0.739762000	-0.337061000
C	-7.839666000	0.062098000	0.132834000
C	-8.740321000	-0.485973000	-0.812922000
C	-9.895380000	-1.123584000	-0.359471000
H	-10.589960000	-1.531718000	-1.091387000
C	-10.183400000	-1.253794000	1.003794000
C	-9.274947000	-0.721324000	1.918995000
H	-9.471660000	-0.827152000	2.983964000
C	-8.109163000	-0.058743000	1.514910000
C	-0.767580000	-5.759158000	2.574773000
H	-1.201561000	-6.207954000	3.473231000
H	0.306154000	-5.623776000	2.748764000
H	-1.201698000	-4.759739000	2.454850000
C	-2.863844000	-9.889947000	0.567613000
H	-2.568219000	-10.663516000	-0.149247000
H	-2.768153000	-10.306542000	1.575963000
H	-3.929591000	-9.683354000	0.401066000
C	-0.261763000	-6.743413000	-2.400379000
H	-0.517953000	-7.521281000	-3.125863000
H	-0.685424000	-5.797685000	-2.758109000
H	0.828105000	-6.627225000	-2.398980000
C	-8.491008000	-0.364261000	-2.299661000
H	-9.347206000	-0.740488000	-2.867655000
H	-8.320361000	0.677693000	-2.594940000
H	-7.605598000	-0.930144000	-2.611065000
C	-11.447573000	-1.940949000	1.463753000
H	-11.414063000	-2.166423000	2.534314000
H	-12.329466000	-1.311278000	1.286377000
H	-11.611450000	-2.881269000	0.924705000
C	-7.168540000	0.477268000	2.574515000
H	-7.380248000	0.010955000	3.541799000
H	-6.119455000	0.286405000	2.328211000
H	-7.271902000	1.561480000	2.699474000
O	1.236489000	-2.043115000	-0.541243000

Conformer-12

S	-0.270173000	4.210783000	-1.559302000
S	2.684160000	3.463283000	0.357489000
N	-4.509061000	1.983021000	-1.474590000
H	-3.765847000	1.270749000	-1.474853000
N	5.022197000	-0.016379000	1.308779000
C	-4.283617000	3.290216000	-1.824387000
C	-5.828509000	1.760900000	-1.252912000
C	-6.512068000	2.969387000	-1.511026000
H	-7.578163000	3.124533000	-1.416464000
C	-5.553930000	3.920401000	-1.862554000
H	-5.723146000	4.963640000	-2.088181000
C	-2.984044000	3.899013000	-1.900642000
C	-1.765440000	3.250279000	-1.811440000
C	-1.424570000	1.805870000	-1.913260000
C	0.003046000	1.616033000	-1.783980000
H	0.420466000	0.617371000	-1.748272000
C	0.712599000	2.745662000	-1.515768000
C	5.711919000	-1.000596000	1.856247000
C	6.693728000	-0.509023000	2.823755000
H	7.377483000	-1.112150000	3.408394000
C	6.541648000	0.843876000	2.851354000
H	7.097854000	1.563557000	3.437936000
C	5.500357000	1.162821000	1.875301000
C	-2.982564000	5.402186000	-1.999313000
C	-2.876545000	6.012767000	-3.267020000
C	-2.888875000	7.408581000	-3.345314000
H	-2.814611000	7.878078000	-4.324291000
C	-2.993533000	8.213066000	-2.207263000
C	-3.100721000	7.583588000	-0.964368000
H	-3.189855000	8.191475000	-0.066132000
C	-3.101431000	6.190957000	-0.835289000
C	2.106114000	2.703067000	-1.110551000
C	4.144129000	2.477863000	0.344111000
C	4.186354000	1.697135000	-0.799111000
H	5.012109000	1.031608000	-1.008793000
C	3.046249000	1.824186000	-1.614089000
H	2.884944000	1.264976000	-2.528953000
C	5.026493000	2.405094000	1.495964000

C	5.339323000	3.637991000	2.277594000
C	4.818642000	3.807414000	3.580534000
C	5.115807000	4.984966000	4.277194000
H	4.700094000	5.120155000	5.273637000
C	5.918758000	5.988429000	3.733396000
C	6.422703000	5.799159000	2.441928000
H	7.050932000	6.569077000	1.997976000
C	6.143531000	4.650472000	1.700434000
C	-2.756171000	5.187674000	-4.528650000
H	-2.778554000	5.828616000	-5.415079000
H	-3.570807000	4.459746000	-4.615732000
H	-1.817928000	4.620642000	-4.548163000
C	-2.966237000	9.719775000	-2.315967000
H	-3.521524000	10.191315000	-1.498184000
H	-3.399079000	10.061753000	-3.262212000
H	-1.937376000	10.101671000	-2.273013000
C	-3.231260000	5.562534000	0.534179000
H	-3.239548000	6.330671000	1.313286000
H	-2.401408000	4.878541000	0.744312000
H	-4.156838000	4.981724000	0.622799000
C	3.929736000	2.771960000	4.238089000
H	3.395378000	3.212232000	5.085621000
H	4.507740000	1.920847000	4.616549000
H	3.187386000	2.366493000	3.543415000
C	6.249986000	7.236465000	4.517207000
H	6.191816000	8.132062000	3.888282000
H	7.270238000	7.192520000	4.921001000
H	5.568025000	7.371312000	5.362736000
C	6.729317000	4.497500000	0.314444000
H	7.420674000	5.316440000	0.094382000
H	5.951874000	4.498200000	-0.458172000
H	7.278156000	3.554201000	0.211031000
O	-2.220651000	0.858541000	-2.055765000
S	1.183106000	-3.169549000	0.522083000
S	-2.970952000	-2.183072000	-0.313295000
N	4.321472000	-2.566802000	0.652317000
H	3.721789000	-1.801528000	0.368425000
N	-5.356936000	-0.393248000	-0.302468000
C	4.320759000	-3.848991000	0.151077000
C	5.421577000	-2.353277000	1.442646000
C	6.122451000	-3.563670000	1.509263000
H	7.036932000	-3.732668000	2.061398000
C	5.453532000	-4.484199000	0.684377000
H	5.736269000	-5.508482000	0.486417000
C	3.354196000	-4.315239000	-0.830155000
C	2.046059000	-3.914808000	-0.858496000
C	1.102858000	-4.092499000	-2.018016000
C	-0.249516000	-3.687196000	-1.628684000
H	-1.085329000	-3.823927000	-2.304581000
C	-0.374389000	-3.268916000	-0.344779000
C	-6.251793000	0.513337000	-0.667090000
C	-7.604140000	0.156238000	-0.238796000
H	-8.506433000	0.724933000	-0.426097000
C	-7.478295000	-1.008519000	0.450735000
H	-8.256339000	-1.586769000	0.931099000
C	-6.055306000	-1.345420000	0.426082000
C	3.895376000	-5.300544000	-1.829045000
C	3.651100000	-6.674982000	-1.642676000
C	4.239315000	-7.588809000	-2.524829000
H	4.060889000	-8.651548000	-2.371900000
C	5.041118000	-7.178578000	-3.590998000
C	5.258622000	-5.807200000	-3.759297000
H	5.875426000	-5.463457000	-4.587713000
C	4.702909000	-4.860712000	-2.897780000
C	-1.613170000	-3.032997000	0.384210000
C	-4.012762000	-2.655095000	1.024934000
C	-3.286287000	-3.383929000	1.963594000
H	-3.738837000	-3.774053000	2.867568000
C	-1.933970000	-3.567464000	1.621991000
H	-1.226270000	-4.130428000	2.220330000
C	-5.428099000	-2.364604000	1.113662000
C	-6.231090000	-3.217997000	2.053240000
C	-6.644609000	-4.506865000	1.649915000
C	-7.391774000	-5.285518000	2.537718000
H	-7.714734000	-6.275514000	2.221152000
C	-7.731842000	-4.831788000	3.815993000
C	-7.300690000	-3.559117000	4.196713000
H	-7.544543000	-3.190677000	5.191304000
C	-6.560617000	-2.737628000	3.338254000
C	2.769985000	-7.185939000	-0.522986000
H	2.874538000	-8.270027000	-0.413971000
H	3.012733000	-6.724442000	0.440503000
H	1.712130000	-6.974671000	-0.721389000
C	5.636379000	-8.180981000	-4.552048000
H	6.652325000	-7.898006000	-4.850321000
H	5.679385000	-9.182603000	-4.111537000

H	5.038891000	-8.252880000	-5.470703000
C	4.922363000	-3.387941000	-3.149350000
H	5.595969000	-3.232276000	-3.997657000
H	3.970078000	-2.895254000	-3.380102000
H	5.354986000	-2.880979000	-2.278801000
C	-6.304917000	-5.046757000	0.278813000
H	-6.786750000	-6.014670000	0.111301000
H	-6.629422000	-4.364238000	-0.514910000
H	-5.223984000	-5.183653000	0.156492000
C	-8.560233000	-5.685947000	4.747184000
H	-8.405769000	-5.403868000	5.793850000
H	-9.632664000	-5.579746000	4.535351000
H	-8.314823000	-6.748482000	4.642192000
C	-6.127084000	-1.365524000	3.807714000
H	-6.291780000	-1.255934000	4.884066000
H	-5.066351000	-1.181651000	3.605550000
H	-6.687541000	-0.571082000	3.300877000
O	1.429792000	-4.514576000	-3.123538000

Conformer-13

S	-1.183324000	3.169655000	0.522126000
S	2.970734000	2.183190000	-0.313302000
N	-4.321681000	2.566537000	0.652345000
H	-3.721881000	1.801343000	0.368497000
N	5.356865000	0.393574000	-0.302393000
C	-4.321025000	3.848764000	0.151211000
C	-5.421690000	2.352919000	1.442762000
C	-6.122633000	3.563275000	1.509477000
H	-7.037088000	3.732201000	2.061673000
C	-5.453816000	4.483877000	0.684598000
H	-5.736636000	5.508148000	0.486708000
C	-3.354563000	4.315065000	-0.830103000
C	-2.046391000	3.914720000	-0.858480000
C	-1.103294000	4.092325000	-2.018079000
C	0.249146000	3.687096000	-1.628796000
H	1.084905000	3.823746000	-2.304780000
C	0.374113000	3.268980000	-0.344848000
C	6.251772000	-0.512983000	-0.666952000
C	7.604091000	-0.155819000	-0.238605000
H	8.506410000	-0.724482000	-0.425858000
C	7.478163000	1.008933000	0.450913000
H	8.256154000	1.587220000	0.931315000
C	6.055169000	1.345796000	0.426167000
C	-3.895837000	5.300254000	-1.829033000
C	-4.703630000	4.860316000	-2.897529000
C	-5.259406000	5.806700000	-3.759128000
H	-5.876403000	5.462852000	-4.587353000
C	-5.041713000	7.178082000	-3.591139000
C	-4.239671000	7.588426000	-2.525188000
H	-4.061117000	8.651176000	-2.372498000
C	-3.651381000	6.674711000	-1.642979000
C	1.612941000	3.033176000	0.384109000
C	4.012548000	2.655426000	1.024882000
C	3.286058000	3.384376000	1.963431000
H	3.738607000	3.774660000	2.867332000
C	1.933735000	3.567829000	1.621813000
H	1.226002000	4.130834000	2.220079000
C	5.427890000	2.364993000	1.113658000
C	6.230826000	3.218482000	2.053198000
C	6.560412000	2.738157000	3.338254000
H	7.300378000	3.559711000	4.196681000
H	7.544246000	3.191326000	5.191292000
C	7.731426000	4.832449000	3.815914000
C	7.391301000	5.286113000	2.537675000
H	7.714139000	6.276139000	2.221104000
C	6.644198000	4.507344000	1.649858000
C	-4.923336000	3.387530000	-3.148808000
H	-5.596986000	3.231826000	-3.997071000
H	-5.356027000	2.880798000	-2.278161000
H	-3.971150000	2.894614000	-3.379487000
C	-5.636965000	8.180356000	-4.552329000
H	-5.679368000	9.182158000	-4.112177000
H	-6.653146000	7.897682000	-4.850085000
H	-5.039834000	8.251654000	-5.471265000
C	-2.770032000	7.185807000	-0.523537000
H	-2.874666000	8.269891000	-0.414550000
H	-1.712206000	6.974645000	-0.722203000
H	-3.012490000	6.724331000	0.440033000
C	6.126990000	1.366014000	3.807699000
H	6.291889000	1.256352000	4.884012000
H	6.687360000	0.571617000	3.300695000
H	5.066222000	1.182140000	3.605722000
C	8.559917000	5.686481000	4.747134000
H	8.320522000	6.749763000	4.636270000
H	9.632762000	5.573676000	4.540846000

H	8.399192000	5.409864000	5.794335000
C	6.304376000	5.047233000	0.278787000
H	6.786284000	6.015094000	0.111184000
H	5.223440000	5.184237000	0.156611000
H	6.628700000	4.364659000	-0.514962000
O	-1.430307000	4.514272000	-3.123623000
S	0.270426000	-4.210754000	-1.559340000
S	-2.683895000	-3.463447000	0.357382000
N	4.509158000	-1.982769000	-1.474550000
H	3.765916000	-1.270547000	-1.474939000
N	-5.022114000	0.016054000	1.308868000
C	4.283819000	-3.289987000	-1.824335000
C	5.828581000	-1.760570000	-1.252786000
C	6.512219000	-2.969039000	-1.510765000
H	7.578309000	-3.124131000	-1.416088000
C	5.554165000	-3.920100000	-1.862404000
H	5.723455000	-4.963335000	-2.087987000
C	2.984287000	-3.898869000	-1.900652000
C	1.765650000	-3.250205000	-1.811490000
C	1.424736000	-1.805814000	-1.913426000
C	-0.002890000	-1.616016000	-1.784143000
H	-0.420346000	-0.617368000	-1.748478000
C	-0.712403000	-2.745659000	-1.515867000
C	-5.711901000	1.000211000	1.856368000
C	-6.693622000	0.508546000	2.823918000
H	-7.377427000	1.111610000	3.408561000
C	-6.541393000	-0.844334000	2.851536000
H	-7.097494000	-1.564068000	3.438149000
C	-5.500168000	-1.163188000	1.875378000
C	2.982898000	-5.402045000	-1.999330000
C	3.101708000	-6.190807000	-0.835360000
C	3.101061000	-7.583489000	-0.964482000
H	3.190132000	-8.191376000	-0.066250000
C	2.994000000	-8.212917000	-2.207350000
C	2.889371000	-7.408379000	-3.345435000
H	2.815179000	-7.877872000	-4.324425000
C	2.876982000	-6.012623000	-3.267109000
C	-2.105910000	-2.703117000	-1.110614000
C	-4.143905000	-2.478086000	0.344108000
C	-4.186185000	-1.697288000	-0.799065000
H	-5.011969000	-1.031776000	-1.008674000
C	-3.046100000	-1.824253000	-1.614086000
H	-2.884819000	-1.264993000	-2.528926000
C	-5.026233000	-2.405422000	1.495998000
C	-5.338924000	-3.638352000	2.277624000
C	-6.143014000	-4.650868000	1.700544000
C	-6.421991000	-5.799659000	2.442082000
H	-7.050064000	-6.569691000	1.998137000
C	-5.918011000	-5.988855000	3.733467000
C	-5.114953000	-4.985332000	4.277186000
H	-4.698972000	-5.120573000	5.273517000
C	-4.818024000	-3.807788000	3.580555000
C	3.231412000	-5.562425000	0.534139000
H	3.239718000	-6.330587000	1.313218000
H	4.156934000	-4.981537000	0.622823000
H	2.401484000	-4.878508000	0.744252000
C	2.966867000	-9.719609000	-2.316353000
H	3.408666000	-10.061821000	-3.258400000
H	3.513958000	-10.191472000	-1.493284000
H	1.937417000	-10.100908000	-2.283538000
C	2.756676000	-5.187448000	-4.528688000
H	2.778970000	-5.828340000	-5.415156000
H	1.818507000	-4.620298000	-4.548152000
H	3.571401000	-4.459614000	-4.615737000
C	-6.728863000	-4.498067000	0.314560000
H	-7.420231000	-5.317035000	0.094635000
H	-7.277712000	-3.554785000	0.211057000
H	-5.951460000	-4.498866000	-0.458096000
C	-6.249706000	-7.236331000	4.517965000
H	-5.556343000	-7.380957000	5.352576000
H	-7.263072000	-7.183383000	4.937806000
H	-6.210337000	-8.130178000	3.885229000
C	-3.928987000	-2.772308000	4.237900000
H	-3.394750000	-3.212457000	5.085571000
H	-3.186528000	-2.367144000	3.543161000
H	-4.506868000	-1.920998000	4.616098000
O	2.220802000	-0.858493000	-2.056042000

Conformer-14

S	0.140881000	-3.309121000	0.315747000
S	-4.281664000	-2.942625000	-0.009923000
N	3.402520000	-3.481478000	0.303586000
H	2.814081000	-2.741119000	-0.055252000
N	-5.546465000	1.526148000	0.275183000
C	3.092964000	-4.834182000	0.331070000

C	4.719478000	-3.289165000	0.666564000
C	5.246307000	-4.549234000	0.984430000
H	6.251990000	-4.738548000	1.329662000
C	4.251242000	-5.498721000	0.769609000
H	4.328120000	-6.566020000	0.908267000
C	1.862382000	-5.498090000	-0.066977000
C	0.613968000	-4.953937000	-0.184951000
C	-0.593856000	-5.703275000	-0.694914000
C	-1.785224000	-4.875985000	-0.565381000
H	-2.750980000	-5.260387000	-0.872135000
C	-1.582019000	-3.629688000	-0.070147000
C	-6.248047000	2.646571000	-0.223848000
C	-7.687664000	2.389417000	0.231013000
H	-8.474650000	3.132423000	0.195631000
C	-7.819782000	1.035025000	0.279509000
H	-8.734682000	0.457625000	0.300668000
C	-6.460809000	0.487630000	0.304301000
C	2.061090000	-6.972208000	-0.332315000
C	2.559187000	-7.398581000	-1.578654000
C	2.816007000	-8.757325000	-1.774717000
H	3.199080000	-9.083841000	-2.739864000
C	2.593024000	-9.704631000	-0.771520000
C	2.100095000	-9.255233000	0.455502000
H	1.923796000	-9.974278000	1.253448000
C	1.820518000	-7.905497000	0.693870000
C	-2.570110000	-2.606714000	0.164286000
C	-4.703779000	-1.267533000	0.352544000
C	-3.550915000	-0.533172000	0.619633000
H	-3.575615000	0.517109000	0.857841000
C	-2.368134000	-1.281447000	0.514829000
H	-1.385739000	-0.850256000	0.672890000
C	-6.087619000	-0.846977000	0.311513000
C	-7.147863000	-1.907494000	0.237266000
C	-7.586050000	-2.543109000	1.420096000
C	-8.568210000	-3.533070000	1.330533000
H	-8.904295000	-4.020740000	2.243571000
C	-9.125988000	-3.914256000	0.106504000
C	-8.673745000	-3.273986000	-1.049564000
H	-9.088868000	-3.561446000	-2.013522000
C	-7.697589000	-2.272369000	-1.010369000
C	2.776589000	-6.419623000	-2.708315000
H	3.221020000	-6.916747000	-3.576012000
H	3.438228000	-5.595009000	-2.417780000
H	1.824618000	-5.977513000	-3.026403000
C	2.851655000	-11.172856000	-1.017330000
H	3.070096000	-11.704005000	-0.084624000
H	3.695768000	-11.323946000	-1.699360000
H	1.977684000	-11.658931000	-1.471472000
C	1.256203000	-7.486031000	2.032994000
H	1.316777000	-8.307691000	2.753509000
H	0.200542000	-7.201525000	1.944493000
H	1.787266000	-6.626047000	2.456009000
C	-7.023032000	-2.159850000	2.770239000
H	-7.500085000	-2.736611000	3.568200000
H	-7.177798000	-1.095477000	2.982371000
H	-5.943100000	-2.340322000	2.824979000
C	-10.203468000	-4.971390000	0.040856000
H	-10.231197000	-5.454749000	-0.941218000
H	-11.196796000	-4.538121000	0.219627000
H	-10.049280000	-5.748522000	0.797305000
C	-7.254992000	-1.606941000	-2.295224000
H	-7.684495000	-2.117527000	-3.162426000
H	-6.164871000	-1.615953000	-2.404179000
H	-7.569131000	-0.557245000	-2.333632000
O	-0.573587000	-6.836975000	-1.164817000
S	0.497446000	5.046775000	-0.216083000
S	3.238583000	1.574636000	0.169519000
N	-4.174266000	3.843430000	0.124911000
H	-3.601680000	2.990739000	0.227227000
N	4.976913000	-0.841885000	0.377876000
C	-3.630737000	5.092076000	-0.007924000
C	-5.529770000	3.895487000	0.130386000
C	-5.900611000	5.251833000	0.001967000
H	-6.912998000	5.631272000	-0.028036000
C	-4.722904000	5.996960000	-0.085549000
H	-4.637272000	7.068176000	-0.199661000
C	-2.222512000	5.364809000	-0.089292000
C	-1.181360000	4.452635000	-0.010485000
C	-1.157941000	2.986192000	0.238851000
C	0.193783000	2.486933000	0.228987000
H	0.386049000	1.433392000	0.395201000
C	1.161345000	3.418763000	0.002758000
C	5.457296000	-2.053167000	0.632424000
C	6.912942000	-2.043828000	0.827373000
H	7.535722000	-2.901373000	1.042265000
C	7.304046000	-0.761516000	0.653147000

H	8.303891000	-0.354288000	0.710785000
C	6.088969000	0.004087000	0.381864000
C	-1.871087000	6.814952000	-0.302229000
C	-1.651844000	7.652568000	0.811836000
C	-1.341362000	8.997983000	0.591239000
H	-1.176526000	9.644198000	1.451199000
C	-1.241123000	9.533731000	-0.695666000
C	-1.470894000	8.684564000	-1.781563000
H	-1.407354000	9.083589000	-2.792017000
C	-1.785839000	7.332686000	-1.612030000
C	2.581761000	3.188610000	-0.050897000
C	4.881396000	2.174420000	0.024625000
C	4.875004000	3.551493000	-0.201917000
H	5.789341000	4.119666000	-0.318811000
C	3.591223000	4.117168000	-0.246200000
H	3.403795000	5.173811000	-0.404842000
C	6.065160000	1.369665000	0.183398000
C	7.375153000	2.111497000	0.146529000
C	8.067377000	2.249471000	-1.074772000
C	9.276746000	2.952729000	-1.090579000
H	9.806388000	3.061423000	-2.035069000
C	9.820559000	3.517119000	0.066322000
C	9.114287000	3.369207000	1.263446000
H	9.516988000	3.804839000	2.175869000
C	7.900127000	2.677844000	1.327481000
C	-1.751075000	7.122723000	2.224562000
H	-1.589657000	7.923914000	2.951906000
H	-2.734609000	6.680464000	2.420657000
H	-1.004955000	6.341930000	2.413232000
C	-0.872167000	10.983514000	-0.907277000
H	-1.306930000	11.377346000	-1.832137000
H	-1.214898000	11.610100000	-0.076946000
H	0.216453000	11.109133000	-0.980978000
C	-2.030370000	6.457829000	-2.820879000
H	-1.930582000	7.035608000	-3.744563000
H	-1.317426000	5.626327000	-2.865540000
H	-3.034639000	6.018986000	-2.803199000
C	7.528707000	1.651558000	-2.355713000
H	8.155265000	1.930509000	-3.208214000
H	7.496473000	0.556867000	-2.305581000
H	6.506526000	1.988593000	-2.562558000
C	11.144745000	4.243949000	0.029556000
H	11.189142000	5.035502000	0.785251000
H	11.979703000	3.558672000	0.228348000
H	11.325462000	4.699113000	-0.949994000
C	7.180854000	2.541999000	2.651028000
H	7.727974000	3.057868000	3.445758000
H	6.170398000	2.964661000	2.607807000
H	7.071911000	1.491117000	2.943386000
O	-2.140722000	2.244151000	0.445690000

15'

Conformer-1

S	-2.202477000	-3.875294000	0.590584000
S	-4.698399000	-1.482563000	0.531481000
N	2.465059000	-4.492660000	0.129652000
N	-4.931733000	2.899651000	0.248879000
C	1.524610000	-5.477854000	-0.034848000
C	3.666479000	-5.011776000	-0.197424000
C	3.521948000	-6.390489000	-0.581753000
H	4.316926000	-7.049376000	-0.906844000
C	2.181542000	-6.679612000	-0.488945000
H	1.692990000	-7.617150000	-0.717363000
C	0.139566000	-5.272861000	0.168217000
C	-0.432847000	-4.088403000	0.672673000
C	0.148917000	-2.934678000	1.311032000
C	-0.801891000	-1.978743000	1.684426000
H	-0.501711000	-1.037423000	2.127037000
C	-2.113767000	-2.290506000	1.338455000
C	-5.069634000	4.229948000	-0.032428000
C	-6.461682000	4.454214000	-0.222267000
H	-6.910562000	5.412688000	-0.444935000
C	-7.116868000	3.240680000	-0.082464000
H	-8.180473000	3.060119000	-0.155647000
C	-6.148881000	2.237148000	0.224634000
C	-0.787231000	-6.390190000	-0.227330000
C	-1.197694000	-6.525696000	-1.570980000
C	-2.056668000	-7.575649000	-1.912129000
H	-2.373490000	-7.676549000	-2.948415000
C	-2.514735000	-8.495306000	-0.965374000
C	-2.085226000	-8.347579000	0.356485000
H	-2.421192000	-9.059573000	1.107983000
C	-1.232890000	-7.310308000	0.746286000
C	-3.198625000	-1.382395000	1.451831000

C	-5.173540000	0.155138000	1.017708000
C	-4.228099000	0.661635000	1.929163000
H	-4.357810000	1.619133000	2.419392000
C	-3.149995000	-0.176590000	2.163871000
H	-2.334308000	0.072169000	2.831676000
C	-6.268787000	0.847774000	0.433030000
C	-7.479053000	0.121138000	-0.050678000
C	-8.353472000	-0.486512000	0.883228000
C	-9.484779000	-1.159658000	0.417256000
H	-10.157465000	-1.616301000	1.140825000
C	-9.777344000	-1.262492000	-0.946251000
C	-8.895409000	-0.669913000	-1.852265000
H	-9.093654000	-0.755804000	-2.918880000
C	-7.754423000	0.023732000	-1.435098000
C	-0.723425000	-5.565878000	-2.639472000
H	-1.213853000	-5.776291000	-3.594770000
H	0.359690000	-5.638844000	-2.792300000
H	-0.938137000	-4.525265000	-2.371684000
C	-3.466561000	-9.602711000	-1.353523000
H	-3.318259000	-10.494589000	-0.735080000
H	-3.339739000	-9.891708000	-1.402282000
H	-4.511818000	-9.290232000	-1.226436000
C	-0.795381000	-7.197382000	2.189326000
H	-1.184069000	-8.032633000	2.779787000
H	-1.154119000	-6.267435000	2.646052000
H	0.296824000	-7.195960000	2.280184000
C	-8.101744000	-0.405163000	2.372650000
H	-8.972689000	-0.762157000	2.930867000
H	-7.890143000	0.621404000	2.691526000
H	-7.241469000	-1.014979000	2.673169000
C	-11.020788000	-1.976895000	-1.420862000
H	-10.916611000	-2.317657000	-2.456151000
H	-11.897821000	-1.316833000	-1.380825000
H	-11.245194000	-2.849097000	-0.797060000
C	-6.834610000	0.617968000	-2.480477000
H	-7.052337000	0.195209000	-3.466161000
H	-5.781526000	0.421808000	-2.253792000
H	-6.947985000	1.706079000	-2.553413000
S	2.106562000	4.259485000	0.045283000
S	3.669860000	0.107785000	0.125415000
N	-2.681231000	4.554312000	0.018045000
N	4.757554000	-2.835723000	-0.020421000
C	-1.790073000	5.580077000	-0.118025000
C	-3.929789000	5.070299000	-0.120726000
C	-3.852676000	6.484014000	-0.349653000
H	-4.691127000	7.154220000	-0.490534000
C	-2.515759000	6.807119000	-0.339287000
H	-2.074566000	7.784703000	-0.476298000
C	-0.374674000	5.423161000	-0.074360000
C	0.327039000	4.215952000	0.060836000
C	-0.105763000	2.837201000	0.181343000
C	0.954019000	1.925329000	0.223291000
H	0.780177000	0.857686000	0.301244000
C	2.227383000	2.498932000	0.160264000
C	4.831629000	-4.198267000	-0.202601000
C	6.196201000	-4.512610000	-0.388034000
H	6.587777000	-5.507646000	-0.548839000
C	6.918894000	-3.332980000	-0.308030000
H	7.988536000	-3.216405000	-0.403417000
C	6.012382000	-2.253596000	-0.089868000
C	0.438763000	6.684444000	-0.206091000
C	0.793254000	7.414856000	0.948303000
C	1.539472000	8.588799000	0.804050000
H	1.808698000	9.151095000	1.696185000
C	1.943513000	9.059479000	-0.448103000
C	1.572705000	8.324701000	-1.577594000
H	1.868350000	8.678914000	-2.563348000
C	0.828036000	7.144856000	-1.482430000
C	3.484239000	1.867939000	0.154704000
C	5.443757000	0.208397000	0.080475000
C	5.815789000	1.579977000	0.112694000
H	6.855467000	1.882374000	0.101166000
C	4.759582000	2.467683000	0.145611000
H	4.886373000	3.545178000	0.165200000
C	6.332669000	-0.875472000	-0.012928000
C	7.801814000	-0.541786000	-0.070403000
C	8.421494000	-0.281210000	-1.311082000
C	9.786147000	0.026342000	-1.336583000
H	10.259851000	0.228480000	-2.295449000
C	10.554186000	0.082412000	-0.170342000
C	9.918239000	-0.174081000	1.047414000
H	10.495739000	-0.128879000	1.968889000
C	8.556675000	-0.487046000	1.120475000
C	0.373688000	6.953766000	2.325997000
H	0.733803000	7.645229000	3.093867000
H	-0.717155000	6.889009000	2.412580000

H	0.771943000	5.958477000	2.555154000
C	2.777011000	10.313340000	-0.575785000
H	2.581678000	10.830574000	-1.521354000
H	2.576343000	11.013665000	0.242084000
H	3.850297000	10.081458000	-0.548719000
C	0.447082000	6.391907000	-2.737163000
H	0.833869000	6.898396000	-3.626711000
H	0.847105000	5.371389000	-2.729758000
H	-0.640920000	6.308210000	-2.840825000
C	7.637829000	-0.325662000	-2.603984000
H	8.289115000	-0.127149000	-3.460668000
H	7.167688000	-1.304029000	-2.755573000
H	6.832367000	0.417898000	-2.613023000
C	12.033358000	0.386395000	-0.226658000
H	12.374681000	0.888647000	0.684881000
H	12.624975000	-0.533142000	-0.331144000
H	12.278966000	1.027833000	-1.079797000
C	7.918390000	-0.754599000	2.465275000
H	8.650943000	-0.650954000	3.271543000
H	7.093934000	-0.060642000	2.665689000
H	7.499853000	-1.766425000	2.517128000
O	-1.359967000	2.429717000	0.248411000
H	-2.009458000	3.263228000	0.169352000
O	1.429084000	-2.728291000	1.562976000
H	1.995253000	-3.425532000	1.007562000
H	3.876964000	-2.359968000	0.116900000
H	-4.037859000	2.435065000	0.320966000

Conformer-2

S	-4.723696000	1.265051000	0.930016000
S	-2.495097000	3.825593000	0.524247000
N	-4.695604000	-3.279221000	0.250453000
N	1.990514000	4.656426000	-0.012005000
C	-5.869778000	-2.573493000	0.203871000
C	-4.914241000	-4.490926000	-0.294325000
C	-6.294348000	-4.614051000	-0.686545000
H	-6.752108000	-5.472222000	-1.162002000
C	-6.891787000	-3.412716000	-0.377377000
H	-7.919984000	-3.126467000	-0.555595000
C	-5.918464000	-1.205611000	0.549784000
C	-4.810553000	-0.509728000	1.089418000
C	-3.626838000	-0.972168000	1.756337000
C	-2.728360000	0.052188000	2.067434000
H	-1.763616000	-0.168924000	2.506302000
C	-3.114846000	1.315177000	1.630481000
C	3.239566000	5.102577000	-0.349877000
C	3.100369000	6.477285000	-0.698443000
H	3.912960000	7.123011000	-1.001122000
C	1.766524000	6.812316000	-0.595532000
H	1.314662000	7.776727000	-0.780906000
C	1.042636000	5.662693000	-0.147833000
C	-7.166075000	-0.432440000	0.231085000
C	-7.424391000	-0.006900000	-1.090016000
C	-8.598208000	0.708287000	-1.351781000
H	-8.792342000	1.039538000	-2.370132000
C	-9.523428000	1.007177000	-0.349103000
C	-9.250813000	0.567185000	0.949546000
H	-9.963327000	0.780266000	1.744244000
C	-8.087436000	-0.141297000	1.261607000
C	-2.241051000	2.433666000	1.568867000
C	-0.847109000	4.410553000	0.799520000
C	-0.200062000	3.570931000	1.725172000
H	0.790058000	3.784496000	2.110319000
C	-0.966319000	2.493342000	2.148358000
H	-0.615626000	1.755661000	2.860810000
C	-0.332795000	5.532094000	0.100945000
C	-1.265794000	6.569970000	-0.442384000
C	-1.899745000	7.476704000	0.439100000
C	-2.768244000	8.437739000	-0.084384000
H	-3.248128000	9.137121000	0.597609000
C	-3.037231000	8.525753000	-1.453556000
C	-2.409381000	7.614503000	-2.305708000
H	-2.616866000	7.655992000	-3.373223000
C	-1.524482000	6.640955000	-1.830183000
C	-6.464869000	-0.306078000	-2.221132000
H	-6.746375000	0.247184000	-3.122402000
H	-6.456628000	-1.373692000	-2.470208000
H	-5.436591000	-0.031061000	-1.962819000
C	-10.769933000	1.805465000	-0.652182000
H	-11.610828000	1.490172000	-0.024778000
H	-11.069625000	1.699175000	-1.700108000
H	-10.610702000	2.876080000	-0.465735000
C	-7.842243000	-0.594827000	2.683293000
H	-8.706280000	-0.371709000	3.316607000
H	-6.968636000	-0.096060000	3.119442000

H	-7.650832000	-1.672599000	2.735793000
C	-1.644709000	7.435931000	1.929346000
H	-2.089968000	8.305687000	2.422024000
H	-0.572610000	7.428332000	2.155510000
H	-2.073115000	6.537176000	2.388790000
C	-3.962286000	9.589978000	-1.995809000
H	-4.408990000	9.285313000	-2.947980000
H	-3.424229000	10.530786000	-2.174351000
H	-4.774535000	9.810657000	-1.294761000
C	-0.885210000	5.680385000	-2.809612000
H	-1.381409000	5.736913000	-3.783333000
H	-0.944632000	4.644358000	-2.459532000
H	0.177019000	5.904996000	-2.963496000
S	3.469851000	0.078708000	-0.002446000
S	2.189507000	-4.193513000	0.060999000
N	4.334739000	2.943756000	-0.076569000
N	-2.528650000	-4.843986000	-0.250909000
C	5.631780000	2.525099000	-0.092231000
C	4.384465000	4.275604000	-0.337216000
C	5.739981000	4.735281000	-0.541246000
H	6.050160000	5.749174000	-0.760434000
C	6.530560000	3.637677000	-0.368624000
H	7.608530000	3.585421000	-0.434912000
C	6.064856000	1.187558000	0.113352000
C	5.238403000	0.060738000	0.212021000
C	5.659287000	-1.299630000	0.424741000
C	4.642467000	-2.235364000	0.368427000
H	4.832327000	-3.295112000	0.491499000
C	3.373235000	-1.692152000	0.122359000
C	-3.788792000	-5.341328000	-0.499929000
C	-3.615200000	-6.659200000	-0.971370000
H	-4.413348000	-7.324795000	-1.270844000
C	-2.250298000	-6.935014000	-0.975778000
H	-1.771469000	-7.850724000	-1.292295000
C	-1.554193000	-5.775988000	-0.533705000
C	7.563585000	1.009049000	0.198105000
C	8.228775000	1.205079000	1.431901000
C	9.623480000	1.096246000	1.476537000
H	10.129484000	1.246251000	2.428023000
C	10.380905000	0.809013000	0.337675000
C	9.705486000	0.629061000	-0.873547000
H	10.277238000	0.412294000	-1.773623000
C	8.313229000	0.721662000	-0.968066000
C	2.185454000	-2.424524000	-0.035883000
C	0.454947000	-4.302413000	-0.310247000
C	-0.055490000	-2.983010000	-0.481864000
H	-1.074996000	-2.781519000	-0.786308000
C	0.880083000	-1.976642000	-0.334549000
H	0.646571000	-0.924850000	-0.466764000
C	-0.151583000	-5.561682000	-0.432247000
C	0.715622000	-6.788715000	-0.467622000
C	1.346285000	-7.176392000	-1.670228000
C	2.141944000	-8.326234000	-1.678289000
H	2.624694000	-8.622642000	-2.607652000
C	2.334779000	-9.101147000	-0.531355000
C	1.704389000	-8.697291000	0.648537000
H	1.847518000	-9.282201000	1.555157000
C	0.892722000	-7.559862000	0.702429000
C	7.456453000	1.528027000	2.690862000
H	8.128737000	1.607508000	3.550294000
H	6.914019000	2.474806000	2.590870000
H	6.709401000	0.757950000	2.914508000
C	11.882866000	0.668921000	0.416897000
H	12.364724000	0.990996000	-0.512372000
H	12.297888000	1.261384000	1.238874000
H	12.174338000	-0.375888000	0.588393000
C	7.632523000	0.515230000	-2.301824000
H	8.370750000	0.391362000	-3.099712000
H	6.994929000	-0.376572000	-2.292932000
H	6.988808000	1.363919000	-2.556791000
C	1.172845000	-6.376119000	-2.941608000
H	1.634631000	-6.890713000	-3.789888000
H	0.114676000	-6.215449000	-3.176499000
H	1.636012000	-5.385715000	-2.858431000
C	3.178591000	-10.353938000	-0.572518000
H	3.644893000	-10.555090000	0.397858000
H	2.573063000	-11.233438000	-0.830276000
H	3.973814000	-10.277479000	-1.321767000
C	0.229423000	-7.172640000	2.005365000
H	0.565847000	-7.821062000	2.820120000
H	0.455775000	-6.136797000	2.282055000
H	-0.862086000	-7.254397000	1.939762000
O	6.922214000	-1.715574000	0.657048000
H	7.525205000	-0.948251000	0.638868000
O	-3.338079000	-2.227877000	2.082309000
H	-3.861635000	-2.825425000	1.411281000

H	-2.382097000	-3.951346000	0.197137000
H	1.804162000	3.681403000	0.177105000

Conformer-4

S	3.480806000	-1.056882000	-0.246873000
S	0.990368000	-4.649659000	0.454204000
N	4.971978000	1.268419000	-0.264548000
N	-3.424089000	-3.397383000	1.330248000
C	6.093505000	0.632230000	-0.699830000
C	5.396449000	2.450671000	0.242086000
C	6.834615000	2.593932000	0.120568000
H	7.424821000	3.447024000	0.430150000
C	7.270217000	1.462505000	-0.505806000
H	8.284998000	1.205045000	-0.778405000
C	6.102494000	-0.715263000	-1.145997000
C	5.002158000	-1.565267000	-1.001890000
C	4.934024000	-2.972744000	-1.293959000
C	3.769162000	-3.593062000	-0.872709000
H	3.594886000	-4.654532000	-1.006060000
C	2.855475000	-2.712599000	-0.274385000
C	-4.773098000	-3.367680000	1.571459000
C	-5.091735000	-4.551802000	2.273490000
H	-6.075536000	-4.815414000	2.636720000
C	-3.926037000	-5.297910000	2.399293000
H	-3.810132000	-6.256120000	2.885955000
C	-2.866492000	-4.578970000	1.785325000
C	7.395769000	-1.232624000	-1.722654000
C	7.670452000	-1.047344000	-3.098457000
C	8.896786000	-1.484176000	-3.611775000
H	9.102338000	-1.339304000	-4.670430000
C	9.863141000	-2.091065000	-2.804903000
C	9.576769000	-2.256423000	-1.446298000
H	10.318731000	-2.720250000	-0.799416000
C	8.363554000	-1.841439000	-0.887414000
C	1.602179000	-3.001679000	0.277092000
C	-0.526566000	-4.078449000	1.177109000
C	-0.496706000	-2.659535000	1.268312000
H	-1.283754000	-2.091265000	1.748811000
C	0.659844000	-2.083244000	0.790110000
H	0.846355000	-1.014664000	0.808248000
C	-1.522233000	-4.978650000	1.572869000
C	-1.197558000	-6.435195000	1.725002000
C	-0.514728000	-6.887910000	2.876390000
C	-0.224576000	-8.249698000	3.001766000
H	0.297657000	-8.594228000	3.892403000
C	-0.583391000	-9.176653000	2.019236000
C	-1.250868000	-8.706891000	0.885238000
H	-1.528939000	-9.410266000	0.102571000
C	-1.571305000	-7.355625000	0.720533000
C	6.663169000	-0.383984000	-4.010279000
H	7.036059000	-0.342295000	-5.038016000
H	6.444689000	0.638612000	-3.682700000
H	5.708340000	-0.922095000	-4.017017000
C	11.168321000	-2.579616000	-3.387936000
H	11.982508000	-2.513734000	-2.658388000
H	11.454867000	-1.999347000	-4.271227000
H	11.094822000	-3.630530000	-3.698196000
C	8.100730000	-2.052502000	0.586239000
H	8.991313000	-2.443285000	1.087478000
H	7.284660000	-2.766545000	0.748306000
H	7.809773000	-1.118567000	1.078558000
C	-0.100975000	-5.931473000	3.972466000
H	0.277111000	-6.478441000	4.841722000
H	-0.938745000	-5.306588000	4.301253000
H	0.690680000	-5.251801000	3.635141000
C	-0.280271000	-10.646986000	2.190422000
H	-0.161295000	-11.146905000	1.223267000
H	-1.090988000	-11.161043000	2.724420000
H	0.637195000	-10.802845000	2.768101000
C	-2.295975000	-6.907419000	-0.529383000
H	-2.348060000	-7.721019000	-1.259461000
H	-1.794053000	-6.057640000	-1.004984000
H	-3.321760000	-6.589938000	-0.307025000
S	-3.467078000	1.225075000	-0.260588000
S	-0.256397000	3.075220000	0.244907000
N	-5.085160000	-1.300561000	0.346658000
N	3.180288000	3.508336000	0.652802000
C	-6.169754000	-0.656682000	-0.195630000
C	-5.595127000	-2.344525000	1.026286000
C	-7.043268000	-2.376917000	0.976086000
H	-7.686031000	-3.110600000	1.446029000
C	-7.406119000	-1.327183000	0.187305000
H	-8.406357000	-1.026662000	-0.093559000
C	-6.103568000	0.478486000	-1.017449000
C	-4.966241000	1.296339000	-1.229344000

C	-4.889031000	2.415941000	-2.102859000
C	-3.751360000	3.203203000	-1.931567000
H	-3.571256000	4.089139000	-2.527114000
C	-2.882226000	2.743719000	-0.946471000
C	4.551666000	3.444205000	0.779552000
C	4.951502000	4.588336000	1.525585000
H	5.967814000	4.798029000	1.827466000
C	3.831900000	5.326326000	1.810947000
H	3.781393000	6.246670000	2.373096000
C	2.691176000	4.686320000	1.218422000
C	-7.400418000	0.871743000	-1.685649000
C	-8.230414000	1.861261000	-1.105691000
C	-9.450114000	2.165133000	-1.716537000
H	-10.088290000	2.920470000	-1.262149000
C	-9.873538000	1.529384000	-2.888638000
C	-9.041982000	0.554132000	-3.443908000
H	-9.354783000	0.041759000	-4.351354000
C	-7.816284000	0.204816000	-2.862427000
C	-1.803806000	3.557650000	-0.468815000
C	0.223039000	4.767466000	0.535063000
C	-0.811442000	5.608357000	0.094991000
H	-0.749336000	6.684294000	0.192076000
C	-1.894540000	4.952076000	-0.470915000
H	-2.780921000	5.463444000	-0.826255000
C	1.419845000	5.263674000	1.129262000
C	1.317518000	6.675176000	1.658073000
C	1.766849000	7.767765000	0.885281000
C	1.643365000	9.062111000	1.403708000
H	1.981331000	9.902318000	0.799944000
C	1.099002000	9.305599000	2.667120000
C	0.658162000	8.208891000	3.413618000
H	0.226396000	8.375332000	4.398800000
C	0.751300000	6.899478000	2.932136000
C	-7.821718000	2.583012000	0.157973000
H	-8.644164000	3.196668000	0.537620000
H	-7.526380000	1.878698000	0.942757000
H	-6.963998000	3.243379000	-0.016510000
C	-11.180366000	1.906660000	-3.545697000
H	-11.554954000	1.100802000	-4.185050000
H	-11.950698000	2.136646000	-2.801565000
H	-11.063848000	2.797926000	-4.176552000
C	-6.966573000	-0.876301000	-3.493074000
H	-7.367566000	-1.165554000	-4.469134000
H	-5.930043000	-0.550421000	-3.632394000
H	-6.932531000	-1.770263000	-2.859939000
C	2.368497000	7.572093000	-0.489351000
H	2.459797000	8.529509000	-1.011664000
H	3.369216000	7.127300000	-0.430752000
H	1.759643000	6.903919000	-1.107762000
C	1.009527000	10.708848000	3.220296000
H	0.128914000	10.832792000	3.859930000
H	1.889509000	10.952739000	3.830697000
H	0.954316000	11.453095000	2.418840000
C	0.252966000	5.752182000	3.781994000
H	-0.057958000	6.105987000	4.769725000
H	-0.605475000	5.251682000	3.318555000
H	1.026476000	4.988756000	3.922508000
O	-5.785455000	2.776302000	-3.047612000
H	-6.552798000	2.174720000	-3.013323000
O	5.900340000	-3.694648000	-1.902028000
H	6.655014000	-3.111834000	-2.110447000
H	2.660876000	2.866199000	0.069219000
H	-2.993530000	-2.739350000	0.695046000

Conformer-5

S	2.903875000	3.414141000	-0.537846000
S	4.685921000	0.458110000	-0.494425000
N	-1.438692000	5.204755000	-0.339242000
N	3.906361000	-4.012079000	-0.337664000
C	-0.310080000	5.920412000	-0.048071000
C	-2.509130000	5.934520000	0.052270000
C	-2.072695000	7.191838000	0.594359000
H	-2.708205000	7.971063000	0.995624000
C	-0.697315000	7.183313000	0.534459000
H	-0.020787000	7.955763000	0.874731000
C	0.997879000	5.390673000	-0.206027000
C	1.287573000	4.136284000	-0.776875000
C	0.489925000	3.233310000	-1.569599000
C	1.162158000	2.061150000	-1.912322000
H	0.666357000	1.277692000	-2.470460000
C	2.458394000	1.948745000	-1.402580000
C	3.799302000	-5.336707000	0.004110000
C	5.107673000	-5.772576000	0.331552000
H	5.375014000	-6.780875000	0.617375000
C	5.963602000	-4.684212000	0.215879000

H	7.031357000	-4.673610000	0.385432000
C	5.202529000	-3.549977000	-0.193383000
C	2.140546000	6.194619000	0.351075000
C	2.894924000	7.023928000	-0.507105000
C	3.946405000	7.773757000	0.028148000
H	4.520720000	8.418071000	-0.634838000
C	4.278236000	7.719482000	1.384709000
C	3.515595000	6.894669000	2.215449000
H	3.753640000	6.842045000	3.276137000
C	2.449664000	6.131855000	1.727142000
C	3.233159000	0.765413000	-1.448708000
C	4.691406000	-1.264603000	-0.936962000
C	3.645506000	-1.507367000	-1.855346000
H	3.494917000	-2.468418000	-2.330608000
C	2.859309000	-0.405638000	-2.132592000
H	2.017030000	-0.443597000	-2.812273000
C	5.575177000	-2.192532000	-0.340283000
C	6.872672000	-1.733294000	0.247848000
C	7.032264000	-1.640949000	1.649590000
C	8.255790000	-1.200835000	2.164771000
H	8.369081000	-1.117197000	3.243964000
C	9.328891000	-0.859076000	1.338239000
C	9.149075000	-0.954273000	-0.044653000
H	9.971143000	-0.689696000	-0.706992000
C	7.942401000	-1.379216000	-0.606865000
C	2.576420000	7.120777000	-1.982226000
H	3.212261000	7.866559000	-2.468947000
H	1.530941000	7.402885000	-2.151381000
H	2.733517000	6.162260000	-2.490873000
C	5.443922000	8.509960000	1.931758000
H	5.291813000	8.773448000	2.983933000
H	5.600081000	9.436417000	1.368692000
H	6.376825000	7.933272000	1.872867000
C	1.651923000	5.264637000	2.675686000
H	2.105846000	5.261020000	3.671382000
H	1.597205000	4.227855000	2.325722000
H	0.620680000	5.622967000	2.776095000
C	5.907803000	-1.982916000	2.602987000
H	6.138325000	-1.628836000	3.612481000
H	5.738719000	-3.064844000	2.659188000
H	4.961369000	-1.527050000	2.293101000
C	10.651767000	-0.420698000	1.921519000
H	11.168003000	0.283641000	1.260449000
H	11.323357000	-1.276932000	2.071230000
H	10.519943000	0.062051000	2.895643000
C	7.810810000	-1.463927000	-2.111352000
H	8.780599000	-1.308143000	-2.593825000
H	7.119741000	-0.706482000	-2.500045000
H	7.425002000	-2.438900000	-2.429274000
S	-2.903868000	-3.413991000	-0.537695000
S	-4.686141000	-0.458249000	-0.494732000
N	1.438746000	-5.204438000	-0.339360000
N	-3.906200000	4.012011000	-0.337018000
C	0.310151000	-5.920167000	-0.048338000
C	2.509135000	-5.934353000	0.052013000
C	2.072708000	-7.191825000	0.593843000
H	2.708209000	-7.971146000	0.994937000
C	0.697363000	-7.183241000	0.533962000
H	0.020803000	-7.955742000	0.874060000
C	-0.997872000	-5.390585000	-0.206247000
C	-1.287766000	-4.136311000	-0.777308000
C	-0.490484000	-3.233613000	-1.570595000
C	-1.162698000	-2.061508000	-1.913351000
H	-0.667102000	-1.278321000	-2.472056000
C	-2.458724000	-1.948840000	-1.403035000
C	-3.799265000	5.336726000	0.004481000
C	-5.107715000	5.772654000	0.331398000
H	-5.375151000	6.781010000	0.616931000
C	-5.963617000	4.684245000	0.215661000
H	-7.031427000	4.673669000	0.384868000
C	-5.202420000	3.549953000	-0.193108000
C	-2.140414000	-6.194476000	0.351170000
C	-2.448923000	-6.131966000	1.727367000
C	-3.514758000	-6.894743000	2.215992000
H	-3.752347000	-6.842284000	3.276789000
C	-4.277860000	-7.719276000	1.385430000
C	-3.946634000	-7.773307000	0.028692000
H	-4.521324000	-8.417416000	-0.634173000
C	-2.895313000	-7.023507000	-0.506864000
C	-3.233394000	-0.765526000	-1.449059000
C	-4.691362000	1.264578000	-0.936800000
C	-3.645471000	1.507396000	-1.855221000
H	-3.494714000	2.468523000	-2.330268000
C	-2.859410000	0.405657000	-2.132704000
H	-2.017110000	0.443698000	-2.812355000
C	-5.575063000	2.192466000	-0.340028000

C	-6.872571000	1.733226000	0.248016000
C	-7.942291000	1.379158000	-0.606802000
C	-9.148962000	0.954221000	-0.044701000
H	-9.970980000	0.689639000	-0.707111000
C	-9.328876000	0.858993000	1.338228000
C	-8.255868000	1.200743000	2.164803000
H	-8.369246000	1.117130000	3.243982000
C	-7.032262000	1.640866000	1.649697000
C	-1.650630000	-5.265113000	2.675787000
H	-2.104980000	-5.260455000	3.671284000
H	-0.619835000	-5.624570000	2.776858000
H	-1.594552000	-4.228594000	2.325286000
C	-5.443416000	-8.509758000	1.932751000
H	-5.597655000	-9.437820000	1.371781000
H	-5.292541000	-8.770422000	2.985795000
H	-6.376924000	-7.934352000	1.870981000
C	-2.577495000	-7.120079000	-1.982151000
H	-3.213227000	-7.866121000	-2.468616000
H	-2.735320000	-6.161594000	-2.490639000
H	-1.531967000	-7.401659000	-2.151860000
C	-7.810591000	1.464009000	-2.111272000
H	-8.780252000	1.307745000	-2.593846000
H	-7.425285000	2.439223000	-2.429088000
H	-7.119067000	0.706982000	-2.499955000
C	-10.651849000	0.420488000	1.921182000
H	-10.521263000	-0.052742000	2.900099000
H	-11.327546000	1.275223000	2.060612000
H	-11.162987000	-0.292059000	1.264910000
C	-5.907858000	1.982749000	2.603196000
H	-6.138544000	1.628785000	3.612693000
H	-4.961468000	1.526691000	2.293446000
H	-5.738590000	3.064650000	2.659327000
O	0.751869000	-3.442114000	-1.987470000
H	1.172525000	-4.185917000	-1.378788000
O	-0.752593000	3.441497000	-1.985773000
H	-1.173125000	4.186092000	-1.377183000
H	-3.093673000	3.421508000	-0.447239000
H	3.093811000	-3.421626000	-0.448017000

Conformer-6

S	2.664472000	-2.141251000	-0.526312000
S	-0.556075000	-3.152358000	0.385279000
N	4.686939000	-0.109858000	0.174610000
N	-3.639666000	-2.425622000	1.297941000
C	5.634841000	-0.931948000	-0.367436000
C	5.352210000	0.663575000	1.060177000
C	6.759242000	0.320655000	1.128308000
H	7.506628000	0.792376000	1.753486000
C	6.946520000	-0.654988000	0.193895000
H	7.869422000	-1.156956000	-0.063852000
C	5.364060000	-1.963978000	-1.294055000
C	4.093160000	-2.515263000	-1.521804000
C	3.776592000	-3.605528000	-2.393602000
C	2.526984000	-4.167602000	-2.176880000
H	2.169777000	-5.017008000	-2.745659000
C	1.791042000	-3.533752000	-1.168214000
C	-4.805868000	-1.810532000	1.687796000
C	-5.403494000	-2.641297000	2.670982000
H	-6.313344000	-2.406980000	3.205610000
C	-4.622197000	-3.768848000	2.808958000
H	-4.790657000	-4.607378000	3.469049000
C	-3.522311000	-3.672726000	1.904224000
C	6.561089000	-2.548912000	-2.002967000
C	7.091248000	-1.889450000	-3.137067000
C	8.228427000	-2.417352000	-3.760789000
H	8.629294000	-1.908361000	-4.634974000
C	8.865279000	-3.567139000	-3.287550000
C	8.334245000	-4.194920000	-2.155988000
H	8.821456000	-5.086290000	-1.765631000
C	7.193902000	-3.713938000	-1.506000000
C	0.583688000	-4.040050000	-0.632193000
C	-1.498340000	-4.621191000	0.731315000
C	-0.908900000	-5.713107000	0.058958000
H	-1.314389000	-6.713917000	0.142410000
C	0.198090000	-5.390504000	-0.704012000
H	0.778123000	-6.122420000	-1.253897000
C	-2.631254000	-4.707543000	1.567895000
C	-2.972805000	-6.078613000	2.088896000
C	-2.255145000	-6.607772000	3.184555000
C	-2.582528000	-7.881373000	3.659932000
H	-2.031369000	-8.281346000	4.509048000
C	-3.591463000	-8.652990000	3.076262000
C	-4.279081000	-8.116482000	1.984743000
H	-5.059273000	-8.705808000	1.506454000
C	-3.994699000	-6.841712000	1.482520000

C	6.454530000	-0.627585000	-3.675597000
H	6.929625000	-0.321375000	-4.612445000
H	6.546660000	0.197274000	-2.959932000
H	5.383295000	-0.760603000	-3.863353000
C	10.076933000	-4.132402000	-3.990708000
H	10.778623000	-4.582357000	-3.280053000
H	10.610997000	-3.359527000	-4.553004000
H	9.791045000	-4.916895000	-4.704077000
C	6.658150000	-4.439036000	-0.292568000
H	7.360660000	-5.209024000	0.040398000
H	5.702419000	-4.930685000	-0.510023000
H	6.480785000	-3.750470000	0.540048000
C	-1.149472000	-5.821763000	3.853500000
H	-0.810236000	-6.326028000	4.763601000
H	-1.478757000	-4.812919000	4.125737000
H	-0.282673000	-5.703559000	3.192499000
C	-3.942721000	-10.016496000	3.624538000
H	-4.371168000	-10.661874000	2.850366000
H	-4.683560000	-9.941782000	4.432060000
H	-3.063347000	-10.521319000	4.039002000
C	-4.776410000	-6.318095000	0.297592000
H	-5.366422000	-7.117757000	-0.161004000
H	-4.117026000	-5.898611000	-0.469900000
H	-5.467871000	-5.520046000	0.593444000
S	-2.664444000	2.141166000	-0.526464000
S	0.555988000	3.152322000	0.385467000
N	-4.687048000	0.109693000	0.174284000
N	3.639568000	2.425411000	1.298269000
C	-5.634894000	0.931920000	-0.367535000
C	-5.352333000	-0.663814000	1.059848000
C	-6.759321000	-0.320793000	1.128096000
H	-7.506718000	-0.792530000	1.753250000
C	-6.946569000	0.654984000	0.193808000
H	-7.869450000	1.157045000	-0.063831000
C	-5.364093000	1.964130000	-1.294057000
C	-4.093259000	2.515461000	-1.521692000
C	-3.776756000	3.606026000	-2.393244000
C	-2.527234000	4.168109000	-2.176392000
H	-2.170129000	5.017718000	-2.744929000
C	-1.791120000	3.533968000	-1.167959000
C	4.805685000	1.810247000	1.688265000
C	5.403214000	2.640917000	2.671526000
H	6.313004000	2.406573000	3.206245000
C	4.621907000	3.768515000	2.809466000
H	4.790343000	4.607025000	3.469587000
C	3.522171000	3.672457000	1.904612000
C	-6.561186000	2.549068000	-2.002870000
C	-7.194205000	3.713855000	-1.505610000
C	-8.334645000	4.194795000	-2.155470000
H	-8.822010000	5.085981000	-1.764888000
C	-8.865574000	3.567191000	-3.287176000
C	-8.228514000	2.417635000	-3.760709000
H	-8.629299000	1.908793000	-4.635019000
C	-7.091234000	1.889790000	-3.137134000
C	-0.583769000	4.040123000	-0.631976000
C	1.498330000	4.621117000	0.731592000
C	0.908885000	5.713121000	0.059260000
H	1.314411000	6.713910000	0.142775000
C	-0.198046000	5.390605000	-0.703734000
H	-0.778006000	6.122576000	-1.253618000
C	2.631221000	4.707398000	1.568087000
C	2.973033000	6.078480000	2.088905000
C	3.994984000	6.841353000	1.482338000
C	4.279583000	8.116150000	1.984358000
H	5.059820000	8.705301000	1.505928000
C	3.592135000	8.652901000	3.075871000
C	2.583161000	7.881498000	3.659743000
H	2.032144000	8.281652000	4.508866000
C	2.255559000	6.607872000	3.184563000
C	-6.658566000	4.438747000	-0.292003000
H	-7.361162000	5.208595000	0.041107000
H	-6.481164000	3.750015000	0.540468000
H	-5.702874000	4.930536000	-0.509317000
C	-10.077338000	4.132400000	-3.990188000
H	-10.611245000	3.359570000	-4.552694000
H	-10.779122000	4.582024000	-3.279416000
H	-9.791602000	4.917142000	-4.703344000
C	-6.454241000	0.628209000	-3.675995000
H	-6.929566000	0.321885000	-4.612689000
H	-5.383128000	0.761662000	-3.864150000
H	-6.545777000	-0.196735000	-2.960351000
C	4.776458000	6.317468000	0.297376000
H	5.367378000	7.116736000	-0.160735000
H	5.467023000	5.518581000	0.593032000
H	4.116820000	5.899004000	-0.470465000
C	3.943641000	10.016432000	3.623928000

H	3.064396000	10.521399000	4.038492000
H	4.684619000	9.941731000	4.431323000
H	4.372018000	10.661674000	2.849603000
C	1.149809000	5.822135000	3.853704000
H	0.810937000	6.326431000	4.763925000
H	0.282817000	5.704266000	3.192893000
H	1.478839000	4.813167000	4.125774000
O	-4.579824000	4.121634000	-3.350569000
H	-5.439860000	3.661475000	-3.331562000
O	4.579593000	-4.120997000	-3.351061000
H	5.439586000	-3.660756000	-3.332131000
H	3.106229000	2.098410000	0.502625000
H	-3.106303000	-2.098621000	0.502313000

Conformer-7

S	-3.950782000	0.280527000	0.111836000
S	-1.956507000	4.231938000	-0.079717000
N	-5.132862000	-2.314256000	0.005992000
N	2.886336000	4.123701000	0.075224000
C	-6.397007000	-1.796959000	0.018536000
C	-5.289716000	-3.654158000	-0.047084000
C	-6.688019000	-4.032670000	-0.059650000
H	-7.081392000	-5.040688000	-0.096385000
C	-7.387751000	-2.862549000	-0.017194000
H	-8.461756000	-2.734102000	-0.013657000
C	-6.680293000	-0.415000000	0.032579000
C	-5.700983000	0.593340000	0.053266000
C	-5.915457000	2.008791000	0.019175000
C	-4.754506000	2.770463000	0.037418000
H	-4.777620000	3.853834000	0.026998000
C	-3.583137000	2.010674000	0.103403000
C	4.193630000	4.546227000	0.102006000
C	4.168129000	5.959688000	0.194549000
H	5.042320000	6.593016000	0.252432000
C	2.846269000	6.360427000	0.205060000
H	2.469119000	7.370067000	0.277942000
C	2.015976000	5.200743000	0.127870000
C	-8.141238000	-0.036158000	0.012714000
C	-8.823682000	0.097511000	-1.220217000
C	-10.191730000	0.390608000	-1.209757000
H	-10.711985000	0.491536000	-2.160061000
C	-10.906460000	0.551585000	-0.019131000
C	-10.215455000	0.408550000	1.187707000
H	-10.754617000	0.522775000	2.125898000
C	-8.847806000	0.116992000	1.229545000
C	-2.265933000	2.512574000	0.150769000
C	-0.212263000	4.035239000	0.170980000
C	0.063031000	2.667368000	0.420364000
H	1.045587000	2.296654000	0.686833000
C	-1.054063000	1.843316000	0.401605000
H	-1.011220000	0.778789000	0.610277000
C	0.605768000	5.179945000	0.111543000
C	-0.071789000	6.521310000	0.008705000
C	-0.509774000	7.181446000	1.178013000
C	-1.137952000	8.424802000	1.059497000
H	-1.474542000	8.929912000	1.962921000
C	-1.346558000	9.033407000	-0.181506000
C	-0.907556000	8.361462000	-1.325010000
H	-1.065777000	8.814601000	-2.301781000
C	-0.269318000	7.118642000	-1.254958000
C	-8.097032000	-0.070297000	-2.535200000
H	-8.781197000	0.065996000	-3.377937000
H	-7.646223000	-1.065510000	-2.616019000
H	-7.282605000	0.655739000	-2.640090000
C	-12.376653000	0.898226000	-0.036262000
H	-12.890776000	0.507258000	0.848043000
H	-12.873089000	0.494835000	-0.925076000
H	-12.526748000	1.986079000	-0.045368000
C	-8.147512000	-0.031681000	2.561036000
H	-8.853435000	0.090702000	3.387816000
H	-7.352464000	0.713093000	2.682811000
H	-7.675718000	-1.015982000	2.654528000
C	-0.307777000	6.569194000	2.545750000
H	-0.657370000	7.247135000	3.330351000
H	0.748518000	6.346683000	2.735531000
H	-0.856210000	5.625439000	2.648291000
C	-2.004379000	10.390154000	-0.280143000
H	-2.503087000	10.524448000	-1.245792000
H	-1.267195000	11.198214000	-0.179338000
H	-2.749997000	10.532677000	0.509523000
C	0.193511000	6.440767000	-2.525288000
H	-0.121139000	7.009603000	-3.405521000
H	-0.214914000	5.427837000	-2.614340000
H	1.285760000	6.349552000	-2.556352000
S	3.950762000	-0.280506000	-0.111968000

S	1.956530000	-4.231848000	0.079989000
N	5.132867000	2.314223000	-0.005999000
N	-2.886393000	-4.123728000	-0.074436000
C	6.397019000	1.796971000	-0.018857000
C	5.289678000	3.654112000	0.047621000
C	6.687972000	4.032655000	0.060212000
H	7.081321000	5.040669000	0.097295000
C	7.387740000	2.862574000	0.017218000
H	8.461750000	2.734182000	0.013559000
C	6.680309000	0.415012000	-0.033441000
C	5.700994000	-0.593322000	-0.054193000
C	5.915491000	-2.008791000	-0.020762000
C	4.754544000	-2.770467000	-0.038780000
H	4.777634000	-3.853842000	-0.028898000
C	3.583146000	-2.010646000	-0.104012000
C	-4.193668000	-4.546304000	-0.101076000
C	-4.168120000	-5.959800000	-0.193044000
H	-5.042289000	-6.593186000	-0.250645000
C	-2.846244000	-6.360489000	-0.203463000
H	-2.469061000	-7.370144000	-0.275952000
C	-2.015989000	-5.200740000	-0.126742000
C	8.141244000	0.036131000	-0.013992000
C	8.823749000	-0.098766000	1.218772000
C	10.191785000	-0.391898000	1.207950000
H	10.712094000	-0.493736000	2.158127000
C	10.906437000	-0.551778000	0.017130000
C	10.215368000	-0.407565000	-1.189531000
H	10.754466000	-0.520945000	-2.127861000
C	8.847734000	-0.115876000	-1.231010000
C	2.265926000	-2.512547000	-0.150950000
C	0.212245000	-4.035199000	-0.170470000
C	-0.063068000	-2.667393000	-0.420205000
H	-1.045645000	-2.296733000	-0.686674000
C	1.054025000	-1.843340000	-0.401796000
H	1.011168000	-0.778858000	-0.610692000
C	-0.605781000	-5.179894000	-0.110570000
C	0.071813000	-6.521220000	-0.007388000
C	0.509588000	-7.181770000	-1.176539000
C	1.137784000	-8.425081000	-1.057700000
H	1.474226000	-8.930503000	-1.961004000
C	1.346599000	-9.033259000	0.183481000
C	0.907800000	-8.360914000	1.326825000
H	1.066184000	-8.813713000	2.303727000
C	0.269562000	-7.118109000	1.256451000
C	8.097119000	0.067543000	2.533955000
H	8.781794000	-0.067383000	3.376499000
H	7.644218000	1.061775000	2.614943000
H	7.284283000	-0.660268000	2.639048000
C	12.376612000	-0.898514000	0.033837000
H	12.890756000	-0.506495000	-0.849991000
H	12.873068000	-0.496232000	0.923142000
H	12.526652000	-1.986385000	0.041614000
C	8.147419000	0.034357000	-2.562315000
H	8.852901000	-0.089279000	-3.389283000
H	7.350800000	-0.708726000	-2.684022000
H	7.677619000	1.019654000	-2.655519000
C	0.307295000	-6.570006000	-2.544450000
H	0.657079000	-7.248059000	-3.328869000
H	-0.749102000	-6.347949000	-2.734226000
H	0.855362000	-5.626078000	-2.647318000
C	2.004431000	-10.389974000	0.282468000
H	2.503322000	-10.523935000	1.248070000
H	1.267223000	-11.198066000	0.182085000
H	2.749898000	-10.532777000	-0.507289000
C	-0.193051000	-6.439808000	2.526634000
H	0.121997000	-7.008200000	3.407012000
H	0.215149000	-5.426742000	2.615139000
H	-1.285315000	-6.348847000	2.557991000
O	7.112312000	-2.632764000	0.022229000
H	7.825092000	-1.965837000	0.021988000
O	-7.112253000	2.632758000	-0.024641000
H	-7.825034000	1.965830000	-0.024702000
H	-2.652372000	-3.156720000	0.092412000
H	2.652246000	3.156833000	-0.092339000

Conformer-8

S	-3.467175000	1.224891000	-0.260584000
S	-0.256722000	3.075149000	0.244875000
N	-5.085092000	-1.300892000	0.346804000
N	3.180058000	3.508391000	0.653067000
C	-6.169776000	-0.656975000	-0.195251000
C	-5.594954000	-2.344880000	1.026483000
C	-7.043104000	-2.377238000	0.976559000
H	-7.685797000	-3.110915000	1.446608000
C	-7.406082000	-1.327460000	0.187895000

H	-8.406368000	-1.026890000	-0.092749000
C	-6.103715000	0.478176000	-1.017112000
C	-4.966414000	1.295999000	-1.229213000
C	-4.889299000	2.415494000	-2.102886000
C	-3.751644000	3.202808000	-1.931777000
H	-3.571634000	4.088674000	-2.527451000
C	-2.882433000	2.743494000	-0.946654000
C	4.551426000	3.444346000	0.780029000
C	4.951076000	4.588497000	1.526112000
H	5.967319000	4.798242000	1.828189000
C	3.831391000	5.326471000	1.811223000
H	3.780759000	6.246817000	2.373353000
C	2.690810000	4.686404000	1.218508000
C	-7.400659000	0.871446000	-1.685106000
C	-7.816870000	0.204329000	-2.861665000
C	-9.042637000	0.553685000	-3.442961000
H	-9.355699000	0.041160000	-4.350233000
C	-9.873950000	1.529169000	-2.887719000
C	-9.450200000	2.165089000	-1.715836000
H	-10.088181000	2.920601000	-1.261466000
C	-8.230408000	1.861181000	-1.105179000
C	-1.804015000	3.557508000	-0.469167000
C	0.222782000	4.767440000	0.534716000
C	-0.811590000	5.608286000	0.094278000
H	-0.749450000	6.684242000	0.191126000
C	-1.894644000	4.951945000	-0.471624000
H	-2.780921000	5.463317000	-0.827213000
C	1.419481000	5.263737000	1.129028000
C	1.317046000	6.675315000	1.657621000
C	0.750455000	6.899813000	2.931485000
C	0.657192000	8.209298000	3.412744000
H	0.225146000	8.375890000	4.397778000
C	1.098256000	9.305892000	2.666211000
C	1.642987000	9.062211000	1.402994000
H	1.981142000	9.902324000	0.799204000
C	1.766613000	7.767786000	0.884801000
C	-6.967441000	-0.877042000	-3.492263000
H	-7.368580000	-1.166317000	-4.468257000
H	-6.933536000	-1.770945000	-2.859036000
H	-5.930852000	-0.551402000	-3.631704000
C	-11.180846000	1.906489000	-3.544617000
H	-11.950715000	2.137739000	-2.800402000
H	-11.556181000	1.100149000	-4.182928000
H	-11.064082000	2.796985000	-4.176515000
C	-7.821367000	2.583167000	0.158239000
H	-8.643859000	3.196545000	0.538237000
H	-6.963987000	3.243855000	-0.016717000
H	-7.525380000	1.879026000	0.942930000
C	0.251818000	5.752652000	3.781347000
H	-0.059005000	6.106537000	4.769082000
H	1.025109000	4.989006000	3.921842000
H	-0.606774000	5.252404000	3.317909000
C	1.008637000	10.709225000	3.219149000
H	0.953278000	11.453327000	2.417567000
H	1.888631000	10.953339000	3.829445000
H	0.128051000	10.833166000	3.858819000
C	2.368640000	7.571899000	-0.489635000
H	2.460299000	8.529260000	-1.011986000
H	1.759827000	6.903814000	-1.108188000
H	3.369246000	7.126898000	-0.430711000
S	3.480942000	-1.056723000	-0.246854000
S	0.990656000	-4.649664000	0.453775000
N	4.972003000	1.268644000	-0.264146000
N	-3.423859000	-3.397719000	1.330067000
C	6.093631000	0.632540000	-0.699307000
C	5.396339000	2.450860000	0.242667000
C	6.834524000	2.594189000	0.121408000
H	7.424641000	3.447272000	0.431183000
C	7.270276000	1.462838000	-0.505003000
H	8.285114000	1.205421000	-0.777428000
C	6.102723000	-0.714897000	-1.145634000
C	5.002391000	-1.564963000	-1.001767000
C	4.934339000	-2.972400000	-1.294024000
C	3.769443000	-3.592813000	-0.872977000
H	3.595210000	-4.654268000	-1.006507000
C	2.855677000	-2.712460000	-0.274637000
C	-4.772836000	-3.368068000	1.571446000
C	-5.091355000	-4.552259000	2.273426000
H	-6.075113000	-4.815939000	2.636724000
C	-3.925626000	-5.298338000	2.399036000
H	-3.809637000	-6.256590000	2.885596000
C	-2.866166000	-4.579316000	1.785009000
C	7.396100000	-1.232137000	-1.722158000
C	8.363715000	-1.8411131000	-0.886862000
C	9.577044000	-2.255999000	-1.445603000
H	10.318873000	-2.719978000	-0.798678000

C	9.863687000	-2.090338000	-2.804108000
C	8.897490000	-1.483259000	-3.611039000
H	9.103256000	-1.338144000	-4.669620000
C	7.671059000	-1.046547000	-3.097868000
C	1.602359000	-3.001648000	0.276779000
C	-0.526307000	-4.078604000	1.176713000
C	-0.496553000	-2.659697000	1.267994000
H	-1.283631000	-2.091496000	1.748524000
C	0.659965000	-2.083299000	0.789830000
H	0.846394000	-1.014705000	0.808015000
C	-1.521899000	-4.978903000	1.572450000
C	-1.197140000	-6.435441000	1.724449000
C	-1.570840000	-7.355804000	0.719854000
C	-1.250352000	-8.707042000	0.884408000
H	-1.528373000	-9.410343000	0.101651000
C	-0.582855000	-9.176905000	2.018397000
C	-0.224095000	-8.250056000	3.000997000
H	0.298150000	-8.594655000	3.891596000
C	-0.514309000	-6.888233000	2.875763000
C	8.100630000	-2.052481000	0.586704000
H	8.991129000	-2.443357000	1.088022000
H	7.809596000	-1.118632000	1.079143000
H	7.284531000	-2.766548000	0.748509000
C	11.168964000	-2.578774000	-3.387017000
H	11.456231000	-1.997600000	-4.269482000
H	11.982791000	-2.514099000	-2.656964000
H	11.095166000	-3.629287000	-3.698561000
C	6.663976000	-0.382932000	-4.009725000
H	7.036799000	-0.341579000	-5.037500000
H	5.708914000	-0.920624000	-4.016272000
H	6.445973000	0.639823000	-3.682313000
C	-2.295501000	-6.907460000	-0.530017000
H	-2.347744000	-7.721035000	-1.260112000
H	-3.321224000	-6.589821000	-0.307604000
H	-1.793468000	-6.057747000	-1.005624000
C	-0.279781000	-10.647278000	2.189305000
H	0.633745000	-10.803363000	2.773095000
H	-1.093857000	-11.162859000	2.716687000
H	-0.153686000	-11.145544000	1.222176000
C	-0.100600000	-5.931911000	3.971957000
H	0.277714000	-6.478959000	4.841062000
H	0.690865000	-5.252009000	3.634653000
H	-0.938458000	-5.307263000	4.300975000
O	5.900731000	-3.694197000	-1.902096000
H	6.655456000	-3.111358000	-2.110263000
O	-5.785797000	2.775699000	-3.047631000
H	-6.553134000	2.174117000	-3.013180000
H	-2.993372000	-2.739572000	0.694936000
H	2.660807000	2.866324000	0.069265000

Conformer-10

S	-3.469724000	0.078905000	-0.002993000
S	-2.189632000	-4.193419000	0.060959000
N	-4.334554000	2.944079000	-0.076709000
N	2.528393000	-4.844185000	-0.251378000
C	-5.631570000	2.525450000	-0.092396000
C	-4.384253000	4.275960000	-0.337346000
C	-5.739755000	4.735648000	-0.541354000
H	-6.049914000	5.749554000	-0.760515000
C	-6.530350000	3.638042000	-0.368805000
H	-7.608319000	3.585800000	-0.435099000
C	-6.064659000	1.187877000	0.113184000
C	-5.238249000	0.061052000	0.211778000
C	-5.659183000	-1.299315000	0.424621000
C	-4.642429000	-2.235087000	0.368242000
H	-4.832344000	-3.294824000	0.491326000
C	-3.373179000	-1.691966000	0.121982000
C	3.788510000	-5.341671000	-0.500290000
C	3.614833000	-6.659582000	-0.971539000
H	4.412910000	-7.325247000	-1.271054000
C	2.249907000	-6.935350000	-0.975800000
H	1.771026000	-7.851061000	-1.292240000
C	1.553894000	-5.776230000	-0.533884000
C	-7.563386000	1.009339000	0.197878000
C	-8.228564000	1.204722000	1.431789000
C	-9.623264000	1.095890000	1.476373000
H	-10.129270000	1.245446000	2.427928000
C	-10.380695000	0.809204000	0.337373000
C	-9.705288000	0.629825000	-0.873936000
H	-10.277045000	0.413481000	-1.774110000
C	-8.313031000	0.722510000	-0.968425000
C	-2.185496000	-2.424437000	-0.036310000
C	-0.455130000	-4.302480000	-0.310547000
C	0.055362000	-2.983121000	-0.482536000
H	1.074842000	-2.781801000	-0.787182000

C	-0.880128000	-1.976689000	-0.335270000
H	-0.646578000	-0.924934000	-0.467715000
C	0.151288000	-5.561806000	-0.432288000
C	-0.715972000	-6.788803000	-0.466868000
C	-1.346980000	-7.176665000	-1.669594000
C	-2.142678000	-8.326488000	-1.677241000
H	-2.625692000	-8.623040000	-2.606420000
C	-2.335212000	-9.101211000	-0.530133000
C	-1.704478000	-8.697180000	0.649520000
H	-1.847373000	-9.281934000	1.556279000
C	-0.892770000	-7.559766000	0.702996000
C	-7.456158000	1.526586000	2.690971000
H	-8.128766000	1.608605000	3.549908000
H	-6.910909000	2.471683000	2.590609000
H	-6.711513000	0.754468000	2.915719000
C	-11.882658000	0.669101000	0.416548000
H	-12.364492000	0.991167000	-0.512734000
H	-12.297708000	1.261567000	1.238511000
H	-12.174131000	-0.375707000	0.588054000
C	-7.632321000	0.516880000	-2.302308000
H	-8.370538000	0.391971000	-3.100042000
H	-6.993478000	-0.374018000	-2.293486000
H	-6.989819000	1.366442000	-2.557465000
C	-1.173914000	-6.376613000	-2.941165000
H	-1.635323000	-6.891708000	-3.789347000
H	-0.115831000	-6.215345000	-3.176007000
H	-1.637712000	-5.386475000	-2.858285000
C	-3.179065000	-10.353989000	-0.570835000
H	-3.645755000	-10.554509000	0.399489000
H	-2.573474000	-11.233682000	-0.827787000
H	-3.973992000	-10.277967000	-1.320440000
C	-0.229076000	-7.172375000	2.005682000
H	-0.565884000	-7.820158000	2.820787000
H	-0.454642000	-6.136233000	2.281876000
H	0.862372000	-7.254965000	1.940017000
S	4.723552000	1.264682000	0.929400000
S	2.495138000	3.825545000	0.524108000
N	4.695267000	-3.279475000	0.249735000
N	-1.990321000	4.656681000	-0.012056000
C	5.869528000	-2.573860000	0.203325000
C	4.913968000	-4.491242000	-0.294817000
C	6.294185000	-4.614587000	-0.686661000
H	6.751987000	-5.472889000	-1.161843000
C	6.891642000	-3.413268000	-0.377527000
H	7.919913000	-3.127127000	-0.555496000
C	5.918292000	-1.206019000	0.549251000
C	4.810396000	-0.510088000	1.088967000
C	3.626679000	-0.972427000	1.755849000
C	2.728181000	0.051950000	2.066829000
H	1.763414000	-0.169117000	2.505667000
C	3.114749000	1.314907000	1.629878000
C	-3.239344000	5.102882000	-0.349896000
C	-3.100109000	6.477653000	-0.698331000
H	-3.912689000	7.123388000	-1.001017000
C	-1.766298000	6.812664000	-0.595269000
H	-1.314414000	7.777094000	-0.780494000
C	-1.042414000	5.662968000	-0.147666000
C	7.165955000	-0.432879000	0.230737000
C	7.424482000	-0.007389000	-1.090349000
C	8.598339000	0.707780000	-1.351965000
H	8.792632000	1.038980000	-2.370303000
C	9.523405000	1.006725000	-0.349158000
C	9.250578000	0.566809000	0.949470000
H	9.962957000	0.779945000	1.744273000
C	8.087156000	-0.141664000	1.261384000
C	2.240973000	2.433438000	1.568404000
C	0.847220000	4.410582000	0.799512000
C	0.200097000	3.570816000	1.724956000
H	-0.789992000	3.784432000	2.110168000
C	0.966264000	2.493059000	2.147919000
H	0.615531000	1.755231000	2.860197000
C	0.332962000	5.532336000	0.101174000
C	1.266049000	6.570329000	-0.441768000
C	1.900203000	7.476588000	0.440073000
C	2.768833000	8.437698000	-0.083039000
H	3.248871000	9.136702000	0.599235000
C	3.037743000	8.526280000	-1.452198000
C	2.409686000	7.615513000	-2.304699000
H	2.617093000	7.657458000	-3.372210000
C	1.524675000	6.641868000	-1.829544000
C	6.465081000	-0.306485000	-2.221594000
H	6.746724000	0.246806000	-3.122802000
H	6.456782000	-1.374081000	-2.470731000
H	5.436791000	-0.031413000	-1.963378000
C	10.769952000	1.805002000	-0.652093000
H	11.610628000	1.490058000	-0.024224000

H	11.070061000	1.698286000	-1.699857000
H	10.610546000	2.875684000	-0.466178000
C	7.841799000	-0.595178000	2.683050000
H	8.705778000	-0.372074000	3.316449000
H	6.968158000	-0.096408000	3.119121000
H	7.650375000	-1.672949000	2.735522000
C	1.645279000	7.435244000	1.930323000
H	2.089957000	8.305190000	2.423193000
H	0.573209000	7.426808000	2.156556000
H	2.074381000	6.536689000	2.389522000
C	3.962965000	5.950590000	-1.993999000
H	4.407884000	9.287200000	-2.947406000
H	3.425540000	10.532241000	-2.169974000
H	4.776530000	9.809232000	-1.293829000
C	0.885333000	5.681772000	-2.809394000
H	1.381753000	5.738478000	-3.782991000
H	0.944430000	4.645625000	-2.459614000
H	-0.176811000	5.906666000	-2.963451000
O	3.337850000	-2.228141000	2.081942000
H	3.861306000	-2.825620000	1.411107000
O	-6.922087000	-1.715128000	0.657277000
H	-7.525137000	-0.947861000	0.638388000
H	-1.804024000	3.681684000	0.177234000
H	2.381911000	-3.951634000	0.196881000

Conformer-11

S	2.106663000	4.259535000	0.045180000
S	3.669883000	0.107804000	0.125377000
N	-2.681158000	4.554349000	0.018320000
N	4.757483000	-2.835791000	-0.020688000
C	-1.790012000	5.580121000	-0.117778000
C	-3.929734000	5.070340000	-0.120338000
C	-3.852629000	6.484044000	-0.349338000
H	-4.691092000	7.154233000	-0.490229000
C	-2.515717000	6.807168000	-0.338965000
H	-2.074532000	7.784752000	-0.476003000
C	-0.374606000	5.423228000	-0.074237000
C	0.327137000	4.216018000	0.060882000
C	-0.105653000	2.837273000	0.181397000
C	0.954121000	1.925391000	0.223309000
H	0.780276000	0.857750000	0.301294000
C	2.227480000	2.498979000	0.160201000
C	4.831573000	-4.198363000	-0.202647000
C	6.196165000	-4.512736000	-0.387891000
H	6.587748000	-5.507789000	-0.548572000
C	6.918859000	-3.333107000	-0.307890000
H	7.988516000	-3.216558000	-0.403147000
C	6.012331000	-2.253684000	-0.089973000
C	0.438805000	6.684522000	-0.206039000
C	0.828009000	7.144904000	-1.482422000
C	1.572649000	8.324750000	-1.577661000
H	1.868244000	8.678933000	-2.563443000
C	1.943497000	9.059578000	-0.448203000
C	1.539520000	8.588940000	0.803975000
H	1.808776000	9.151272000	1.696076000
C	0.793323000	7.414981000	0.948305000
C	3.484323000	1.867957000	0.154591000
C	5.443778000	0.208349000	0.080307000
C	5.815858000	1.579915000	0.112477000
H	6.855546000	1.882276000	0.100886000
C	4.759684000	2.467663000	0.145446000
H	4.886514000	3.545154000	0.165015000
C	6.332646000	-0.875564000	-0.013085000
C	7.801802000	-0.541926000	-0.070547000
C	8.556620000	-0.487055000	1.120335000
C	9.918210000	-0.174145000	1.047270000
H	10.495689000	-0.128852000	1.968752000
C	10.554194000	0.082176000	-0.170487000
C	9.786179000	0.025986000	-1.336756000
H	10.259913000	0.228003000	-2.295635000
C	8.421531000	-0.281526000	-1.311254000
C	0.447002000	6.391903000	-2.737109000
H	0.833803000	6.898325000	-3.626689000
H	-0.641006000	6.308259000	-2.840750000
H	0.846970000	5.371365000	-2.729652000
C	2.776959000	10.313450000	-0.576012000
H	2.577816000	11.012938000	0.242936000
H	2.580062000	10.831713000	-1.520701000
H	3.850255000	10.081377000	-0.551094000
C	0.373806000	6.953952000	2.326034000
H	0.733996000	7.645418000	3.093867000
H	0.772020000	5.958649000	2.555199000
H	-0.717037000	6.889255000	2.412675000
C	7.918300000	-0.754438000	2.465151000
H	8.650831000	-0.650686000	3.271426000

H	7.499769000	-1.766262000	2.517124000
H	7.093833000	-0.060463000	2.665455000
C	12.033374000	0.386109000	-0.226863000
H	12.278569000	1.029818000	-1.078419000
H	12.624800000	-0.533218000	-0.334237000
H	12.375301000	0.885850000	0.685820000
C	7.637890000	-0.326114000	-2.604164000
H	8.289170000	-0.127583000	-3.460848000
H	6.832354000	0.417365000	-2.613252000
H	7.167847000	-1.304536000	-2.755711000
S	-2.202631000	-3.875439000	0.591008000
S	-4.698526000	-1.482669000	0.531726000
N	2.465017000	-4.492640000	0.129721000
N	-4.931709000	2.899715000	0.249470000
C	1.524513000	-5.477779000	-0.034747000
C	3.666390000	-5.011838000	-0.197403000
C	3.521768000	-6.390539000	-0.581753000
H	4.316691000	-7.049461000	-0.906908000
C	2.181357000	-6.679593000	-0.488867000
H	1.692751000	-7.617105000	-0.717269000
C	0.139481000	-5.272788000	0.168396000
C	-0.432966000	-4.088388000	0.672969000
C	0.148690000	-2.934663000	1.311358000
C	-0.802157000	-1.978822000	1.684847000
H	-0.501992000	-1.037485000	2.127426000
C	-2.114028000	-2.290666000	1.338920000
C	-5.069582000	4.229999000	-0.032021000
C	-6.461595000	4.454218000	-0.222131000
H	-6.910459000	5.412675000	-0.444910000
C	-7.116775000	3.240661000	-0.082497000
H	-8.180361000	3.060076000	-0.155905000
C	-6.148833000	2.237166000	0.224850000
C	-0.787329000	-6.390084000	-0.227228000
C	-1.232896000	-7.310350000	0.746294000
C	-2.085240000	-8.347581000	0.356409000
H	-2.421129000	-9.059692000	1.107831000
C	-2.514853000	-8.495125000	-0.965439000
C	-2.056883000	-7.575319000	-1.912093000
H	-2.373790000	-7.676069000	-2.948368000
C	-1.197901000	-6.525396000	-1.570858000
C	-3.198876000	-1.382562000	1.452276000
C	-5.173600000	0.155083000	1.017901000
C	-4.228244000	0.661542000	1.929448000
H	-4.357932000	1.619063000	2.419639000
C	-3.150204000	-0.176732000	2.164264000
H	-2.334554000	0.071959000	2.832141000
C	-6.268728000	0.847775000	0.433086000
C	-7.478917000	0.121172000	-0.050917000
C	-7.753928000	0.023703000	-1.435422000
C	-8.894762000	-0.669988000	-1.852849000
H	-9.092699000	-0.755982000	-2.919516000
C	-9.776953000	-1.262509000	-0.947011000
C	-9.484760000	-1.159593000	0.416544000
H	-10.157651000	-1.616173000	1.139958000
C	-8.353546000	-0.486426000	0.882781000
C	-0.795280000	-7.197625000	2.189317000
H	-1.183880000	-8.032987000	2.779678000
H	0.296931000	-7.196160000	2.280090000
H	-1.154034000	-6.267767000	2.646213000
C	-3.466679000	-9.602504000	-1.353661000
H	-3.340458000	-9.890829000	-2.402675000
H	-3.317784000	-10.494729000	-0.735859000
H	-4.511924000	-9.290341000	-1.225705000
C	-0.723747000	-5.565403000	-2.639242000
H	-1.214189000	-5.775734000	-3.594551000
H	-0.938538000	-4.524842000	-2.371314000
H	0.359369000	-5.638258000	-2.792113000
C	-6.833895000	0.618015000	-2.480562000
H	-7.051233000	0.195140000	-3.466284000
H	-6.947528000	1.706096000	-2.553603000
H	-5.780836000	0.422122000	-2.253558000
C	-11.020309000	-1.976816000	-1.422002000
H	-11.247741000	-2.846144000	-0.795320000
H	-11.896366000	-1.315166000	-1.386968000
H	-10.914000000	-2.321862000	-2.455665000
C	-8.102108000	-0.405160000	2.372253000
H	-8.973473000	-0.761397000	2.930303000
H	-7.242420000	-1.015722000	2.672968000
H	-7.889687000	0.621227000	2.691131000
O	1.428874000	-2.728062000	1.563246000
H	1.995066000	-3.425159000	1.008048000
O	-1.359855000	2.429782000	0.248492000
H	-2.009324000	3.263290000	0.169527000
H	-4.037822000	2.435082000	0.321130000
H	3.876864000	-2.360063000	0.116540000

Conformer-12

S	3.987406000	2.631748000	1.238809000
S	4.797492000	-0.580150000	0.851465000
N	0.281422000	5.074965000	-0.120325000
N	2.623167000	-4.227349000	-0.387453000
C	1.564161000	5.578244000	-0.151750000
C	-0.486657000	5.872714000	-0.876415000
C	0.295207000	6.958720000	-1.414840000
H	-0.066571000	7.744394000	-2.065511000
C	1.575536000	6.777407000	-0.955384000
H	2.444599000	7.385174000	-1.168736000
C	2.657894000	4.899356000	0.409150000
C	2.547302000	3.670279000	1.105276000
C	1.428441000	2.999762000	1.693287000
C	1.741760000	1.709575000	2.158647000
H	0.968335000	1.047860000	2.528518000
C	3.046508000	1.315528000	1.909580000
C	2.096450000	-5.251194000	-1.122962000
C	3.207095000	-5.960398000	-1.688216000
H	3.122134000	-6.836173000	-2.316402000
C	4.361548000	-5.335389000	-1.289916000
H	5.378230000	-5.615363000	-1.528100000
C	4.013144000	-4.214539000	-0.457809000
C	4.034395000	5.453969000	0.168676000
C	4.690770000	5.231362000	-1.061214000
C	5.970916000	5.764403000	-1.248362000
H	6.476713000	5.588238000	-2.195768000
C	6.614718000	6.512698000	-0.260161000
C	5.940718000	6.727640000	0.945483000
H	6.419590000	7.316608000	1.725462000
C	4.664934000	6.208646000	1.182376000
C	3.489152000	-0.045129000	1.894864000
C	4.294001000	-2.264242000	0.987831000
C	3.231635000	-2.369273000	1.889318000
H	2.803653000	-3.323968000	2.175121000
C	2.792138000	-1.141787000	2.397466000
H	1.959968000	-1.040975000	3.085060000
C	4.845671000	-3.257047000	0.112767000
C	6.282078000	-3.176630000	-0.298144000
C	7.292745000	-3.501353000	0.638731000
C	8.631397000	-3.419528000	0.251700000
H	9.402904000	-3.678556000	0.974453000
C	9.007180000	-3.014793000	-1.033654000
C	7.996905000	-2.684201000	-1.938027000
H	8.268317000	-2.348935000	-2.937118000
C	6.640172000	-2.758845000	-1.600171000
C	4.042513000	4.437365000	-2.174126000
H	4.761644000	4.236976000	-2.974295000
H	3.193677000	4.976026000	-2.611236000
H	3.659434000	3.476063000	-1.815338000
C	8.009376000	7.052111000	-0.476695000
H	8.158135000	8.002187000	0.047950000
H	8.215952000	7.215263000	-1.539748000
H	8.768239000	6.352496000	-0.101173000
C	3.978263000	6.473835000	2.503389000
H	4.581750000	7.139032000	3.128407000
H	3.810902000	5.546241000	3.063346000
H	2.996320000	6.939212000	2.360418000
C	6.948459000	-3.951980000	2.040768000
H	7.845186000	-4.285775000	2.571699000
H	6.229878000	-4.779542000	2.032874000
H	6.494317000	-3.144043000	2.626564000
C	10.463381000	-2.953886000	-1.431014000
H	10.609744000	-2.335938000	-2.322710000
H	10.856084000	-3.954377000	-1.656736000
H	11.081669000	-2.540054000	-0.626445000
C	5.605013000	-2.367062000	-2.633540000
H	6.070695000	-1.798270000	-3.444292000
H	4.810339000	-1.750465000	-2.201673000
H	5.121296000	-3.244131000	-3.080082000
S	-2.433449000	-2.341094000	0.017291000
S	-3.322311000	1.179467000	-0.110890000
N	-0.222247000	-4.781660000	-0.546618000
N	-2.489808000	4.468453000	-0.585411000
C	-1.378255000	-5.470563000	-0.704762000
C	0.719777000	-5.514799000	-1.213049000
C	0.145295000	-6.669373000	-1.863589000
H	0.670248000	-7.399528000	-2.466562000
C	-1.176203000	-6.655536000	-1.528514000
H	-1.937406000	-7.366973000	-1.818027000
C	-2.625535000	-5.180887000	-0.058380000
C	-3.073498000	-3.961635000	0.444344000
C	-4.239511000	-3.773928000	1.276520000
C	-4.622546000	-2.467515000	1.444544000
H	-5.489846000	-2.214573000	2.038366000

C	-3.816964000	-1.514436000	0.775581000
C	-1.870164000	5.598079000	-1.080857000
C	-2.861568000	6.368931000	-1.712503000
H	-2.689589000	7.311201000	-2.214288000
C	-4.077849000	5.715946000	-1.547986000
H	-5.045600000	6.040340000	-1.901254000
C	-3.850975000	4.517053000	-0.827820000
C	-3.543496000	-6.377650000	0.052883000
C	-3.260536000	-7.406126000	0.984934000
C	-4.098730000	-8.526586000	1.037542000
H	-3.881843000	-9.308225000	1.762822000
C	-5.194345000	-8.672365000	0.183206000
C	-5.445222000	-7.655027000	-0.743257000
H	-6.286501000	-7.755439000	-1.426273000
C	-4.648896000	-6.509007000	-0.823078000
C	-4.186602000	-0.166440000	0.677876000
C	-4.704526000	2.304216000	0.110164000
C	-5.738614000	1.605880000	0.801171000
H	-6.672192000	2.093789000	1.050476000
C	-5.455881000	0.307543000	1.116060000
H	-6.165152000	-0.334405000	1.621703000
C	-4.847340000	3.609623000	-0.358874000
C	-6.247504000	4.172021000	-0.358233000
C	-7.151281000	3.810230000	-1.380796000
C	-8.440665000	4.353596000	-1.371346000
H	-9.131744000	4.076278000	-2.165252000
C	-8.864869000	5.236959000	-0.375349000
C	-7.957109000	5.573730000	0.632871000
H	-8.269892000	6.251523000	1.425088000
C	-6.654454000	5.065378000	0.657086000
C	-2.076979000	-7.313115000	1.922361000
H	-2.133312000	-8.085214000	2.695794000
H	-1.133724000	-7.443218000	1.379448000
H	-2.024522000	-6.336496000	2.415164000
C	-6.097868000	-9.879523000	0.272991000
H	-6.477904000	-10.169305000	-0.712635000
H	-5.575534000	-10.740376000	0.702914000
H	-6.969707000	-9.675204000	0.908767000
C	-4.973804000	-5.444654000	-1.847082000
H	-5.719018000	-5.810108000	-2.560217000
H	-5.379140000	-4.541359000	-1.375794000
H	-4.083238000	-5.138966000	-2.405846000
C	-6.753596000	2.853309000	-2.483100000
H	-7.513314000	2.832207000	-3.270676000
H	-5.798231000	3.135644000	-2.938412000
H	-6.634571000	1.830625000	-2.105511000
C	-10.254177000	5.830641000	-0.400669000
H	-10.625982000	6.024682000	0.611277000
H	-10.268336000	6.787613000	-0.939700000
H	-10.965716000	5.165888000	-0.901986000
C	-5.716102000	5.469078000	1.772417000
H	-6.250819000	6.026750000	2.547522000
H	-5.246778000	4.597795000	2.242417000
H	-4.904095000	6.105798000	1.401272000
O	-4.940688000	-4.751298000	1.894861000
H	-4.619922000	-5.621564000	1.593501000
O	0.193270000	3.464184000	1.799373000
H	0.074929000	4.187342000	1.046938000
H	-2.016054000	3.777179000	-0.018211000
H	2.040828000	-3.532690000	0.059359000

Conformer-13

S	-2.434455000	2.340135000	0.017400000
S	-3.321793000	-1.180821000	-0.110921000
N	-0.224327000	4.781663000	-0.546490000
N	-2.487830000	-4.469448000	-0.585411000
C	-1.380624000	5.470098000	-0.704558000
C	0.717372000	5.515228000	-1.212915000
C	0.142392000	6.669606000	-1.863361000
H	0.667026000	7.400028000	-2.466289000
C	-1.179090000	6.655201000	-1.528248000
H	-1.940591000	7.366347000	-1.817692000
C	-2.627781000	5.179851000	-0.058197000
C	-3.075206000	3.960387000	0.444499000
C	-4.241144000	3.772142000	1.276660000
C	-4.623643000	2.465560000	1.444593000
H	-5.490852000	2.212224000	2.038380000
C	-3.817648000	1.512858000	0.775593000
C	-1.867688000	-5.598852000	-1.080749000
C	-2.858735000	-6.370157000	-1.712406000
H	-2.686325000	-7.312365000	-2.214157000
C	-4.075298000	-5.717684000	-1.547981000
H	-5.042889000	-6.042497000	-1.901305000
C	-3.848975000	-4.518664000	-0.827849000
C	-3.546249000	6.376225000	0.053086000

1	-7.597743000	1.133085000	-1.550689000
6	-6.384031000	2.878822000	-1.198076000
1	-7.097549000	3.641779000	-1.482591000
6	-5.056496000	3.235835000	-0.776026000
6	-4.564710000	4.530307000	-0.721967000
6	-3.224015000	4.931511000	-0.393531000
6	-2.713162000	6.253670000	-0.316226000
1	-3.308580000	7.146351000	-0.439065000
6	-1.351174000	6.186082000	-0.042339000
1	-0.683664000	7.019905000	0.123510000
6	-0.996976000	4.826275000	0.079259000
6	6.111992000	5.575833000	-0.448437000
6	6.807937000	5.637261000	-1.676803000
6	7.704151000	6.690189000	-1.888248000
6	7.937174000	7.674133000	-0.923149000
6	7.239437000	7.586387000	0.286521000
6	6.324299000	6.562472000	0.541501000
6	6.603644000	4.607113000	-2.767216000
1	7.068795000	3.646234000	-2.514169000s
1	7.049083000	4.947691000	-3.705959000
1	5.542102000	4.408536000	-2.952325000
6	8.893655000	8.812053000	-1.185694000
1	8.360535000	9.691845000	-1.569065000
1	9.648702000	8.539025000	-1.929195000
1	9.410391000	9.120509000	-0.271159000
6	5.602270000	6.519809000	1.870563000
1	4.526156000	6.700553000	1.754427000
1	5.991432000	7.285482000	2.547139000
1	5.714729000	5.548228000	2.366129000
6	6.097691000	-5.590838000	-0.448691000
6	6.304095000	-6.578401000	0.541406000
6	7.216700000	-7.605246000	0.288431000
6	7.917249000	-7.694877000	-0.919305000
6	7.690013000	-6.709729000	-1.884781000
6	6.796745000	-5.654092000	-1.675373000
6	5.578752000	-6.533978000	1.868598000
1	5.692557000	-5.562812000	2.364659000
1	5.964036000	-7.300816000	2.546059000
1	4.502466000	-6.711825000	1.749667000
6	8.870404000	-8.835847000	-1.180649000
1	8.340030000	-9.701986000	-1.597517000
1	9.359772000	-9.168580000	-0.259730000
1	9.647358000	-8.554125000	-1.898007000
6	6.598519000	-4.622941000	-2.765984000
1	5.538095000	-4.420661000	-2.953478000
1	7.044902000	-4.964862000	-3.703789000
1	7.066416000	-3.663722000	-2.511698000
6	-5.527164000	-5.637565000	-1.064166000
6	-6.322506000	-6.212334000	-0.049810000
6	-7.189143000	-7.257536000	-0.384771000
6	-7.290300000	-7.747925000	-1.690329000
6	-6.494573000	-7.157069000	-2.677117000
6	-5.611016000	-6.111763000	-2.391237000
6	-6.259975000	-5.719320000	1.379472000
1	-5.240042000	-5.762621000	1.780478000
1	-6.898056000	-6.327026000	2.026908000
1	-6.594236000	-4.678169000	1.466259000
6	-8.213116000	-8.896326000	-2.020898000
1	-8.590436000	-8.825605000	-3.045995000
1	-9.071571000	-8.929733000	-1.342782000
1	-7.690749000	-9.857890000	-1.932703000
6	-4.778878000	-5.508095000	-3.501258000
1	-4.981548000	-6.007101000	-4.452763000
1	-3.704559000	-5.599801000	-3.300226000
1	-4.989236000	-4.440024000	-3.634321000
6	-5.509310000	5.653499000	-1.064439000
6	-5.587949000	6.127802000	-2.391751000
6	-6.467787000	7.175553000	-2.680415000
6	-7.264879000	7.768758000	-1.696224000
6	-7.168994000	7.278253000	-0.390261000
6	-6.306223000	6.230761000	-0.052752000
6	-4.754272000	5.521662000	-3.499235000
1	-4.967827000	4.454346000	-3.633168000
1	-3.680334000	5.609708000	-3.294639000
1	-4.952210000	6.021554000	-4.451267000
6	-8.183617000	8.919619000	-2.029587000
1	-8.551459000	8.854380000	-3.058448000
1	-7.661357000	9.880294000	-1.931572000
1	-9.048347000	8.950362000	-1.359315000
6	-6.249471000	5.737461000	1.376695000
1	-6.587657000	4.697445000	1.462214000
1	-6.887346000	6.347497000	2.022218000
1	-5.230383000	5.777181000	1.780301000
7	2.694529000	4.103479000	0.217217000
7	2.683119000	-4.108925000	0.209966000
7	-2.179543000	-4.093428000	-0.121578000