Supporting Information for:

Cyclo[2]carbazole[2]pyrrole: A Preorganized Calix[4]pyrrole Analogue†

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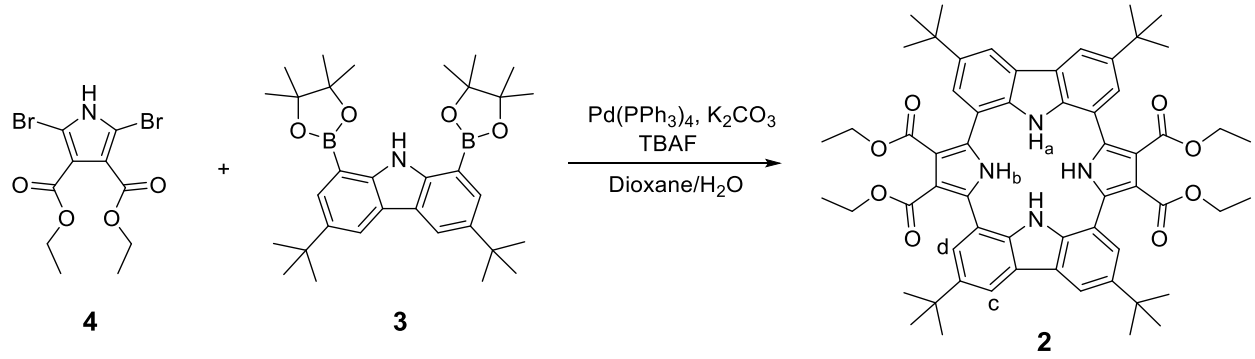
1. General experimental and synthetic details

Solvents and reagents used for the synthetic work were purchased from Aldrich, TCI, or Alfa Aesar and used without further purification. Compounds **3** and **4** were prepared as reported previously.[1,2] NMR spectra were recorded on a Bruker Advance-300 MHz instrument. The NMR spectra were referenced to residual solvent peaks and the spectroscopic solvents were purchased from either Cambridge Isotope Laboratories or Aldrich. Fast atom bombardment (FAB) mass spectra (MS) were recorded on a JMS-700 (JEOL) spectrometer. TLC analyses were carried out using Sorbent Technologies silica gel (200 mm) sheets. Column chromatography was performed on Sorbent silica gel 60 (40–63 mm). The X-ray crystallographic analysis was carried out on a Rigaku Oxford Diffraction HyPix6000E Synergy diffractometer using a μ-focus Cu Kα radiation source (λ = 1.5418 Å) with collimating mirror monochromators. For computations, PCModel[3] was used to locate the lowest energy conformation for the free ligand and various ligand anion complexes. This was done by sampling structures taken from 50 ps molecular dynamics runs using the Merck Force Field 94 model[4] *in vacuo*. The energies for the lowest energy forms of each species were used to compute interaction energies:

$$\Delta E = E_{(complex)} - E_{(host)} - E_{(guest)}$$

Compound 2

3,4-Diethyl 2,5-dibromo-1H-pyrrole-3,4-dicarboxylate (**4**) (500 mg, 1.35 mmol), 3,6-di-tert-butyl-1,8-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole (**3**) (720 mg, 1.35 mmol), $Pd(PPh_3)_4$ (156 mg, 0.135 mmol), K_2CO_3 (excess), and tetrabutylammonium fluoride (TBAF, 210 mg, 0.68 mmol) were dissolved in a mixture of dioxane and water (55ml, 50:5). The reaction mixture was heated to 100 °C and stirred overnight. After the reaction was deemed complete, the volatile solvents were removed *in vacuo*. To the resulting crude product, dichloromethane and water were added. The organic layer was separated off and washed with water three times. The resulting organic layer was dried over anhydrous $MgSO_4$ and evaporated *in vacuo* to give a brownish solid. Column chromatography over silica gel (eluent: ethyl acetate/hexanes = 1/4), followed by recrystallization from dichloromethane and methanol, gave compound **1** (68 mg, 5.16% yield) as a white solid.; ^{1}H NMR (300 MHz, chloroform-*d*) δ 10.15 (s, 2H), 9.51 (s, 2H), 8.08 (d, *J* = 1.8 Hz, 4H), 7.76 (d, *J* = 1.8 Hz, 4H), 4.27 (q, J = 7.2 Hz, 8H), 1.46 (s, 36H), 1.27 (t, J = 7.1 Hz, 12H). ^{13}C NMR (75 MHz, chloroform-*d*) δ 165.2, 142.9, 137.1, 132.5, 126.2, 124.5, 116.6, 115.2, 114.2, 60.6, 34.8, 31.9, 30.9, 14.2. HRMS (FAB) *m/z* 972.5037[M]$^+$ calcd for $C_{60}H_{68}N_4O_8$, found 972.5055.



4 **3** **2**

2. ^{1}H NMR spectral data for titrations with anions

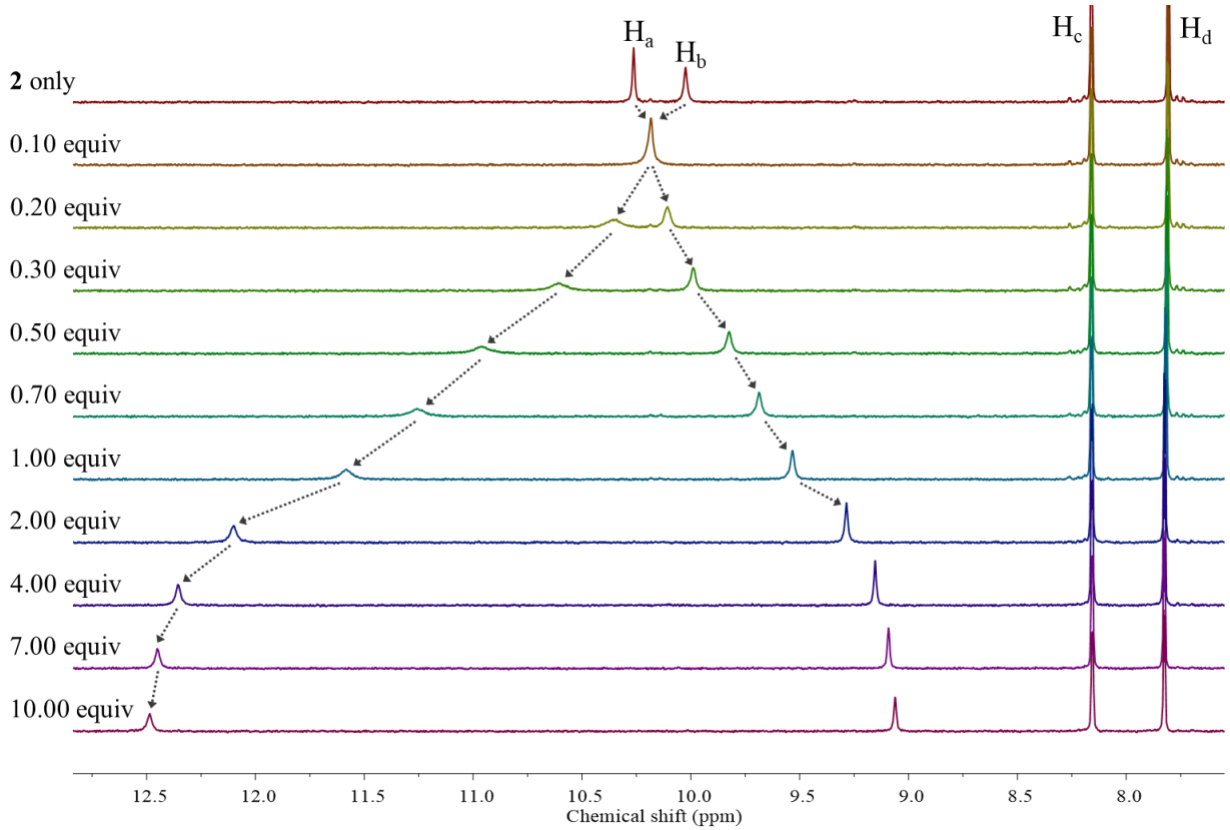


Figure S1. Partial ^{1}H NMR spectra recorded during the titration of receptor **2** (3 mM) with tetrabutylammonium bromide (TBABr) in CD_2Cl_2.

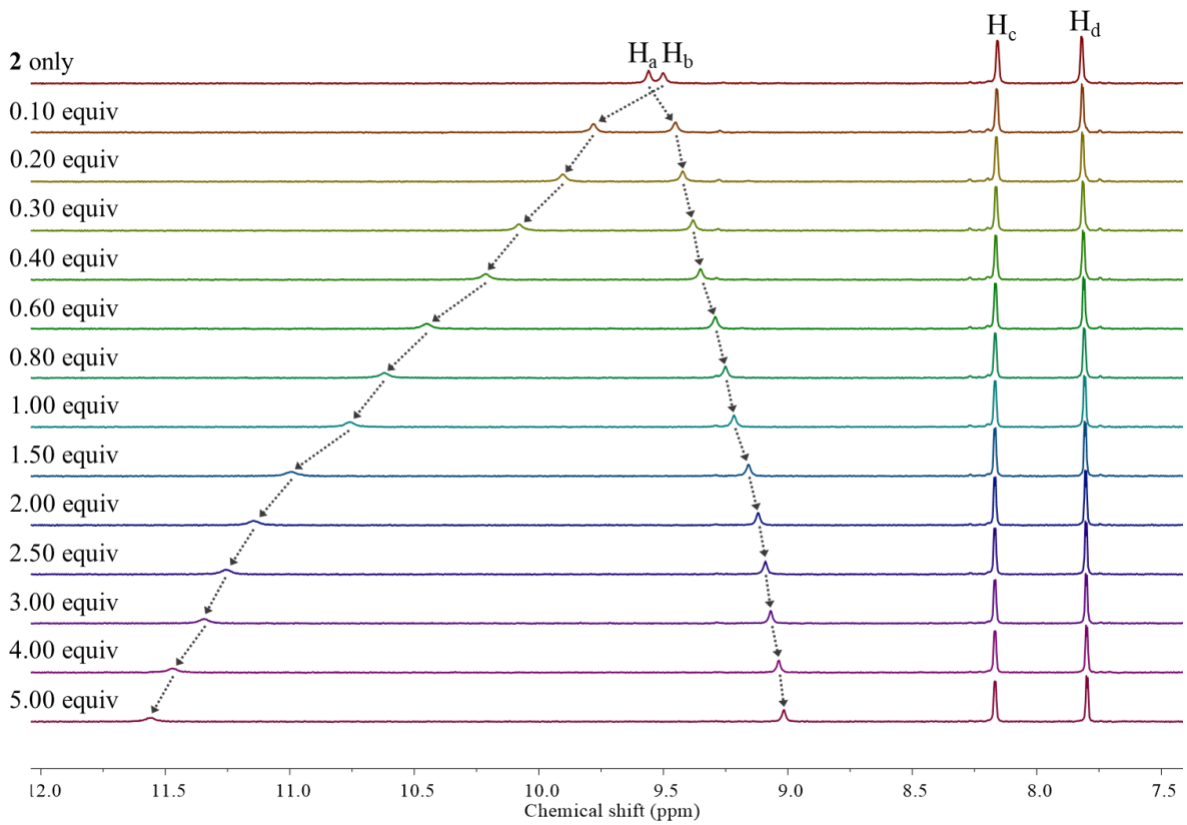


Figure S2. Partial ^{1}H NMR spectra recorded during the titration of receptor **2** (3 mM) with tetrabutylammonium hydrogen sulfate ($TBAHSO_4$) in CD_2Cl_2.

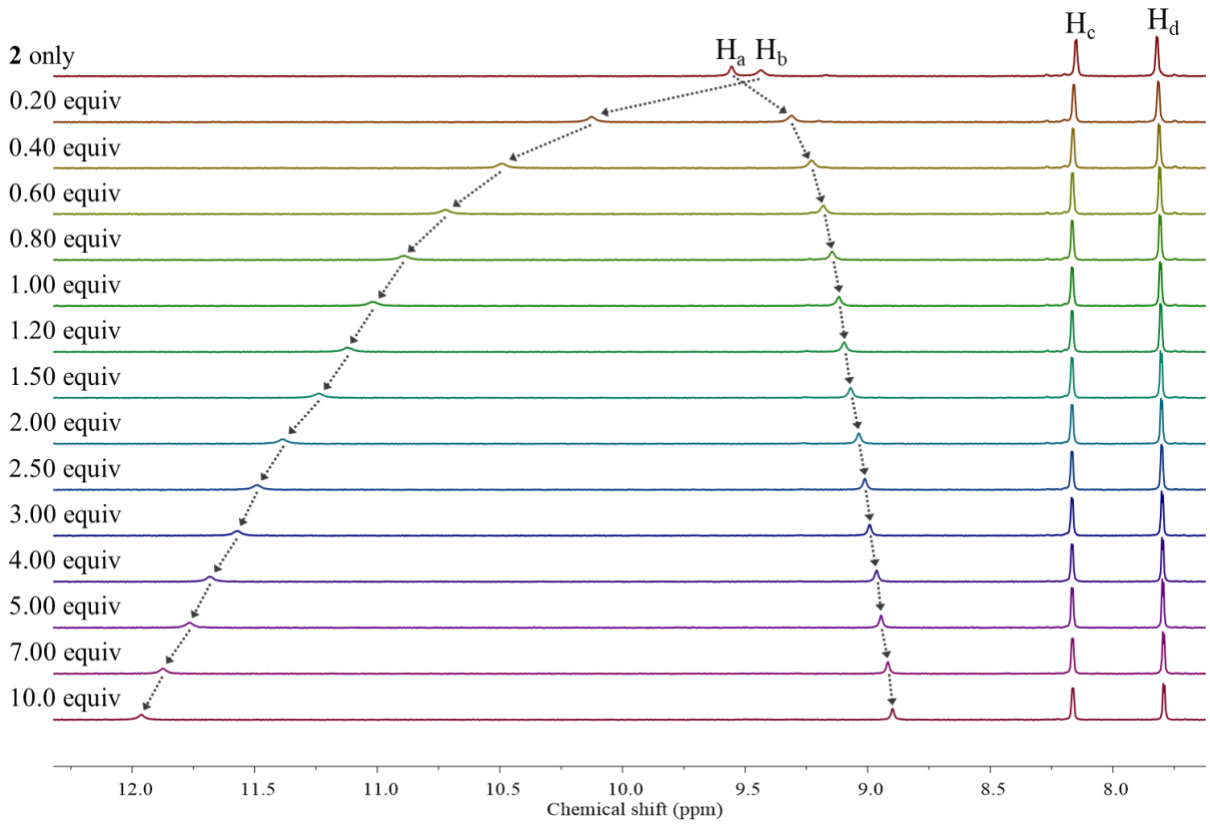


Figure S3. Partial ^{1}H NMR spectra recorded during the titration of receptor **2** (3 mM) with bis(tetrabutylammonium) sulfate ($(TBA)_2 \bullet SO_4$) in CD_2Cl_2

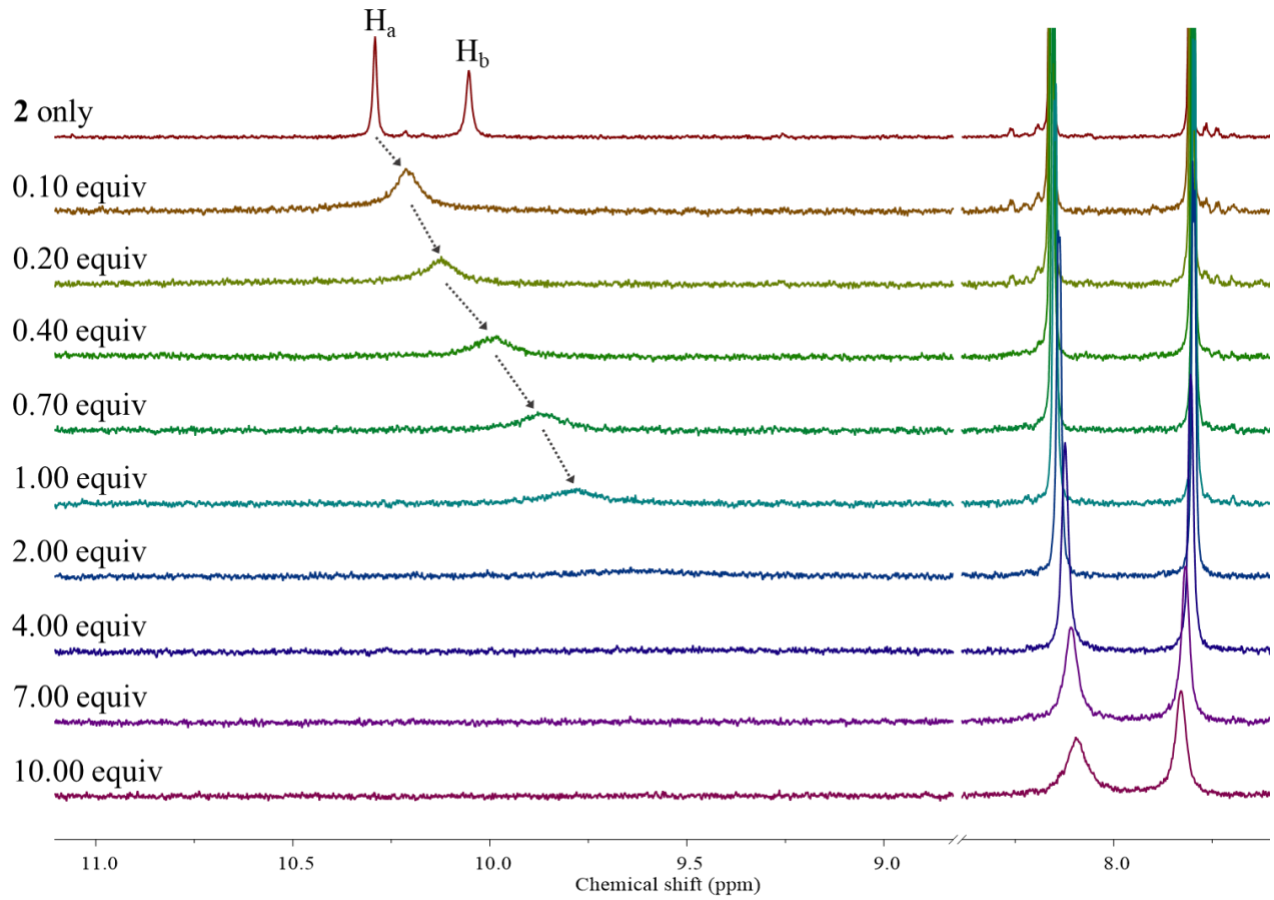


Figure S4. Partial ^{1}H NMR spectra recorded during the titration of receptor **2** (3 mM) with tetrabutylammonium dihydrogen phosphate ($TBAH_2PO_4$) in CD_2Cl_2

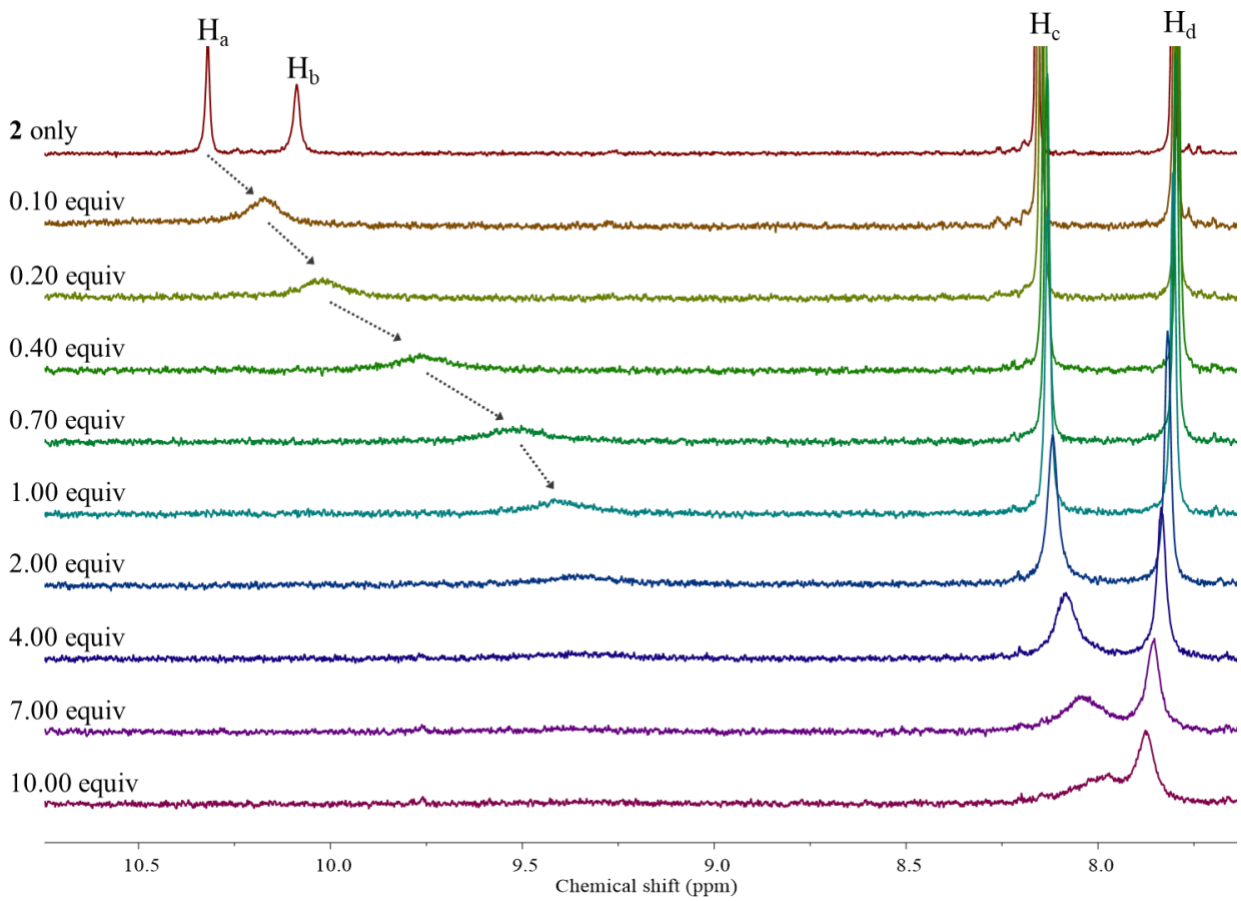


Figure S5. Partial ^{1}H NMR spectra recorded during the titration of receptor **2** (3 mM) with tris(tetrabutylammonium) hydrogen pyrophosphate ($(TBA)_3 \bullet HP_2O_7$) in CD_2Cl_2.

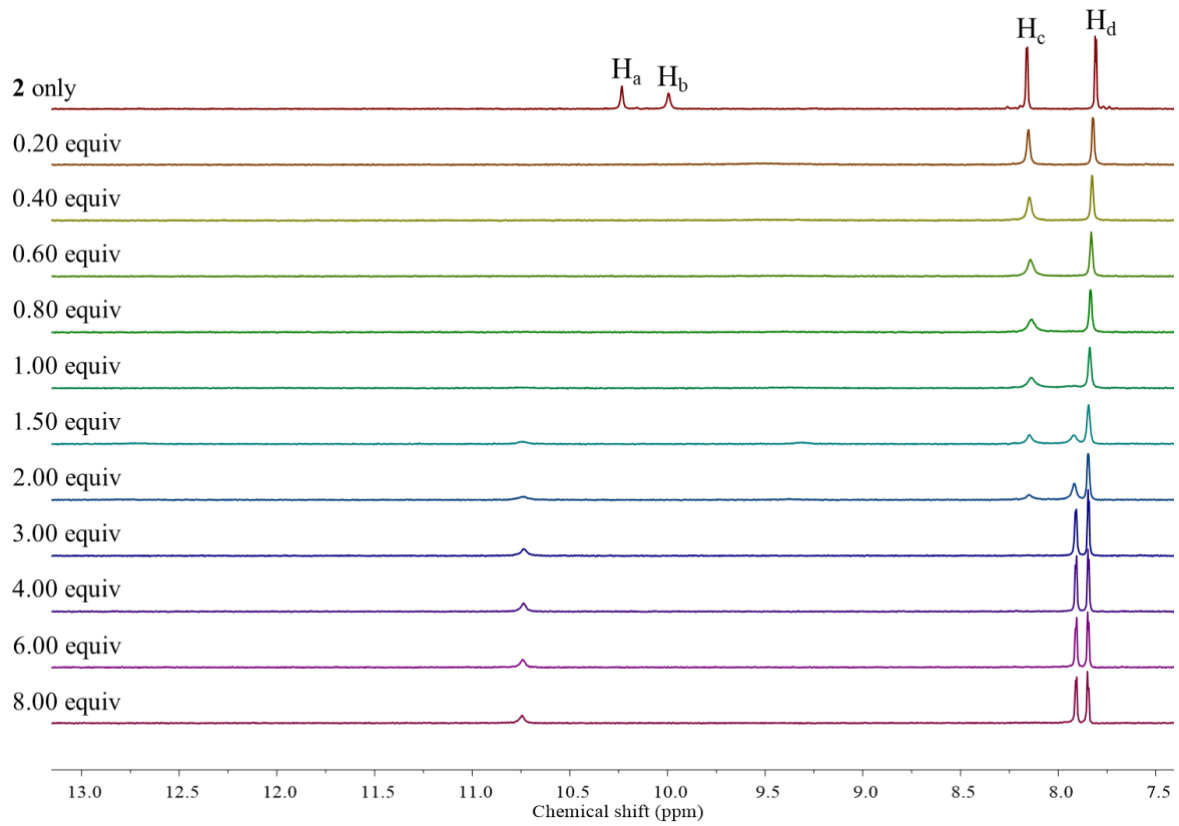


Figure S6. Partial ^{1}H NMR spectra recorded during the titration of receptor **2** (3 mM) with tetraethylammonium bicarbonate ($TEAHCO_3$) in CD_2Cl_2.

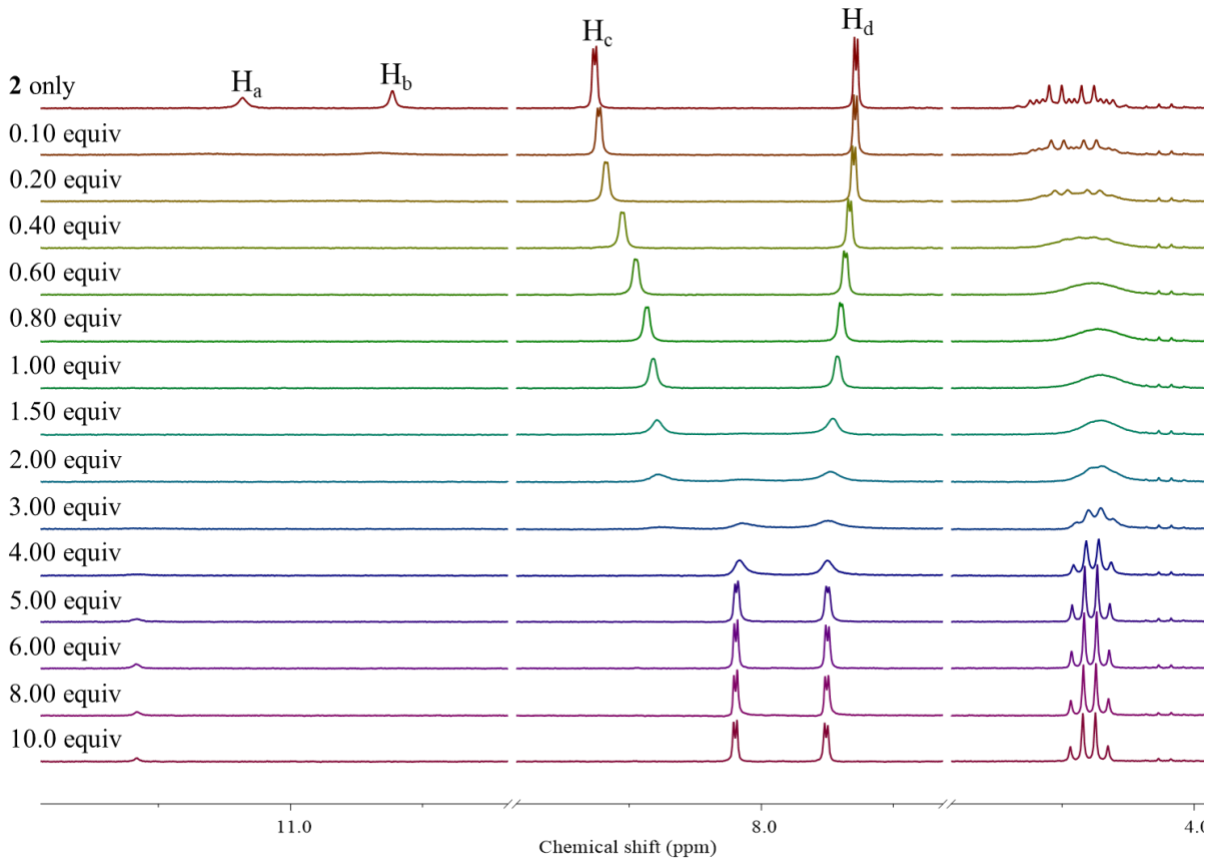


Figure S7. Partial ^{1}H NMR spectra recorded during the titration of receptor **2** (3 mM) with tetrabutylammonium fluoride (TBAF) in acetone-d_6.

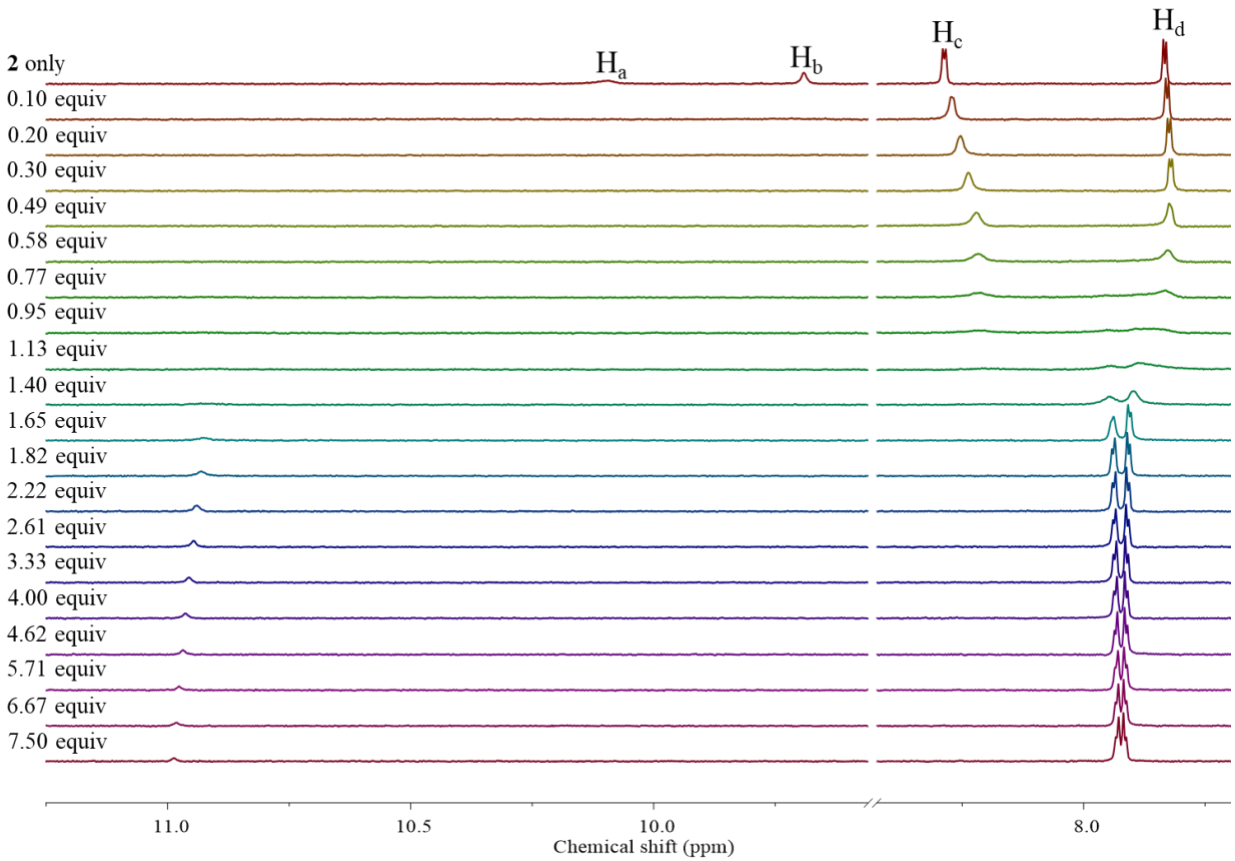


Figure S8. Partial ^{1}H NMR spectra recorded during the titration of receptor **2** (3 mM) with tetrabutylammonium fluoride (TBAF) in CD_3CN.

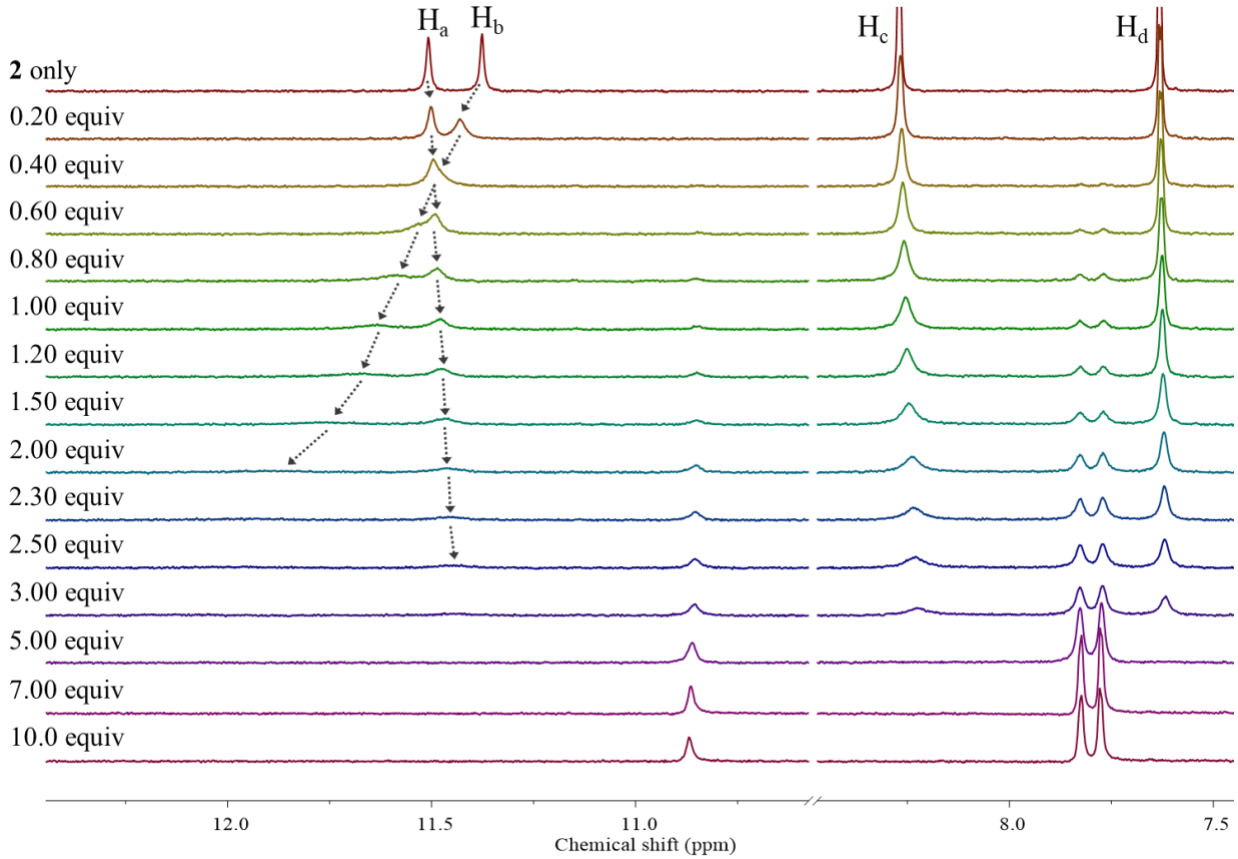


Figure S9. Partial ^{1}H NMR spectra recorded during the titration of receptor **2** (3 mM) with tetrabutylammonium fluoride (TBAF) in DMSO-d_6.

3. UV-vis / Fluorescence spectral data for titrations with anions

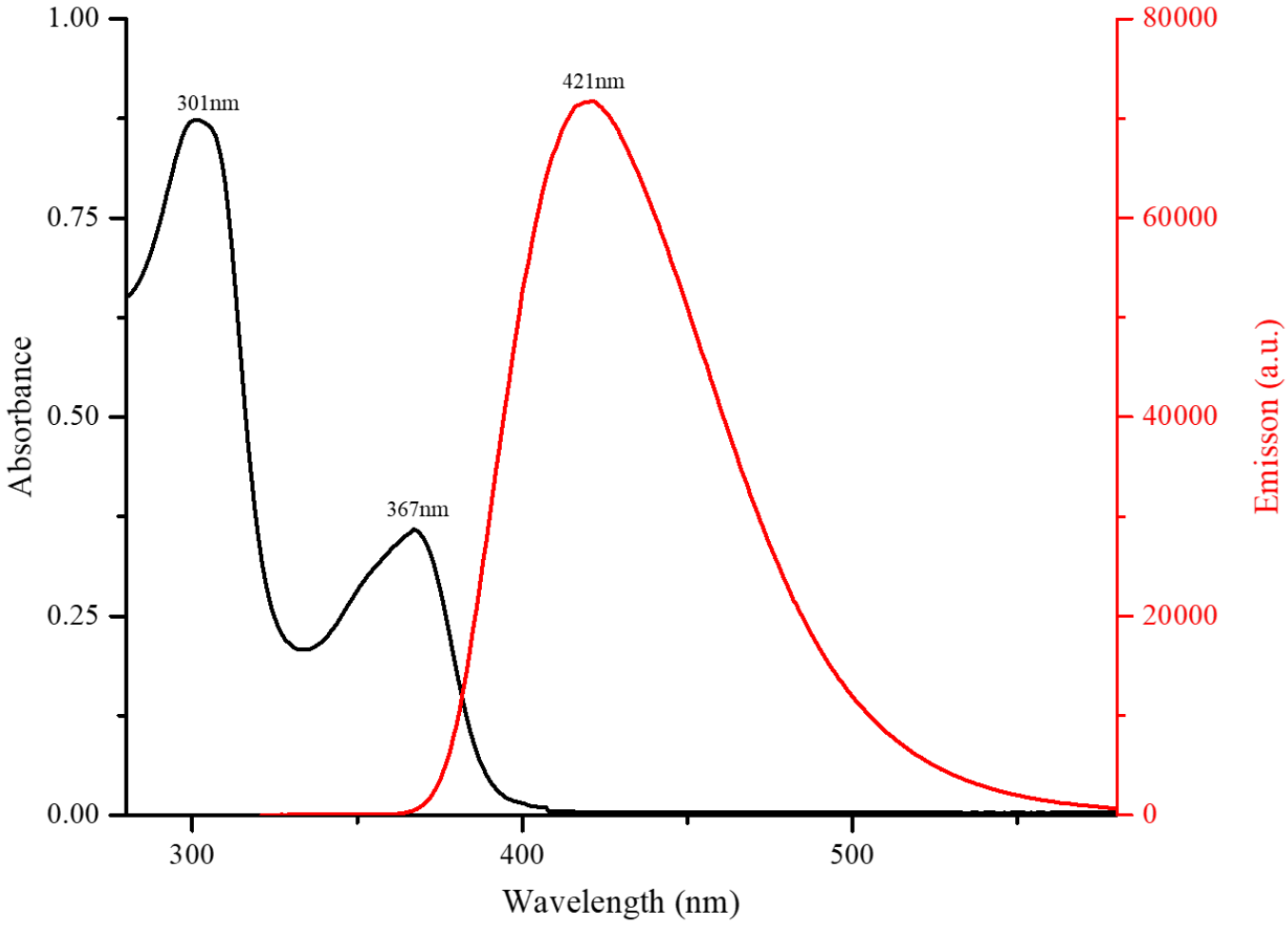


Figure S10. Absorption and emission spectra of receptor **2** (10 μM) in CH_2Cl_2. The excitation wavelength was 301 nm.

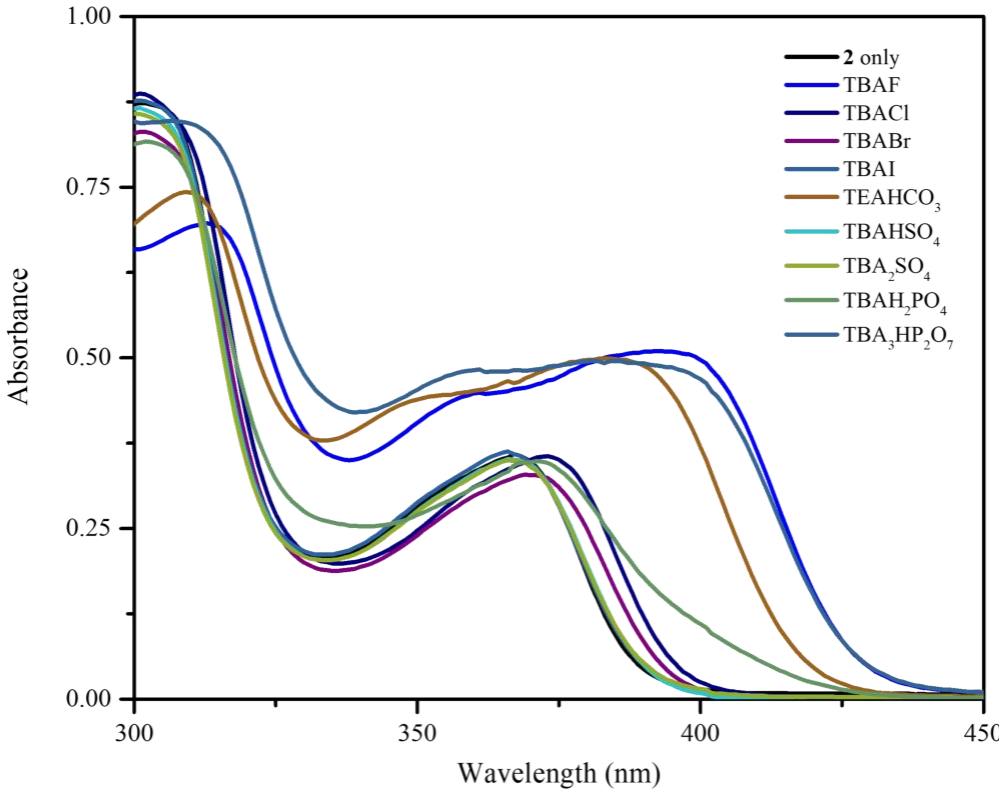


Figure S11. UV-vis spectra of receptor **2 (**10 μM) recorded in the presence of various anion salts in CH_2Cl_2.

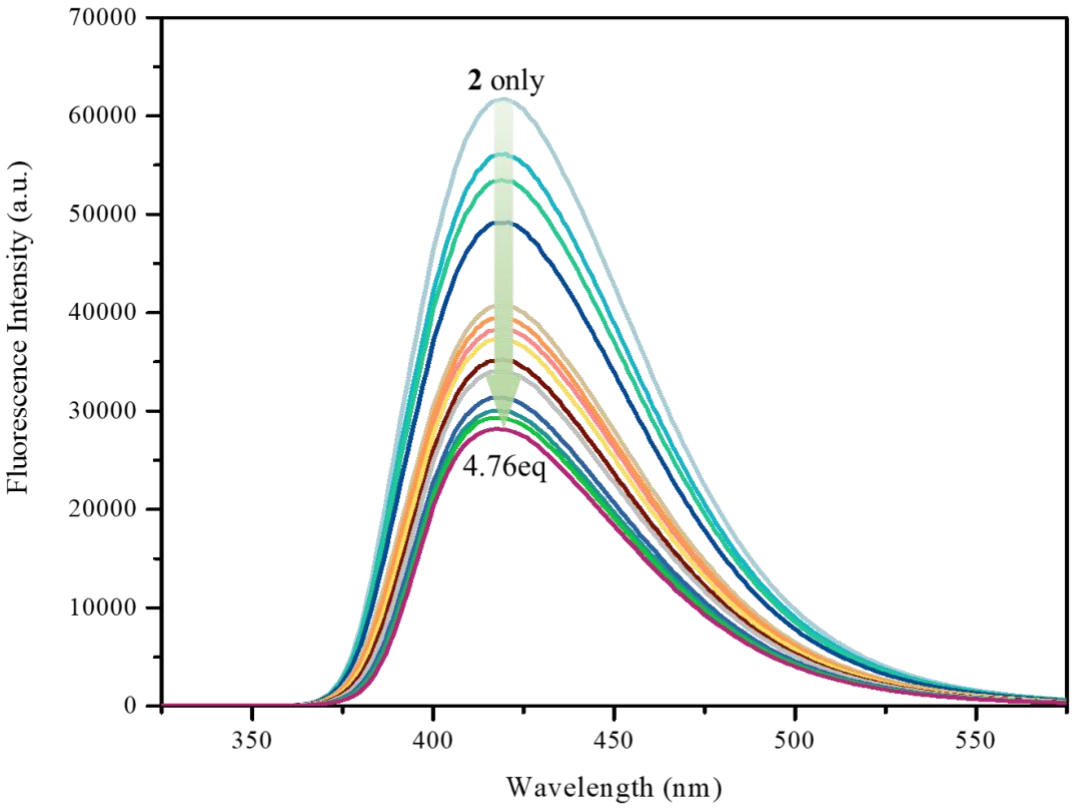


Figure S12. Fluorescence spectra of receptor **2 (**10 μM) recorded during the titration with tetrabutylammonium chloride (TBACl) in CH_2Cl_2. The excitation wavelength was 301 nm.

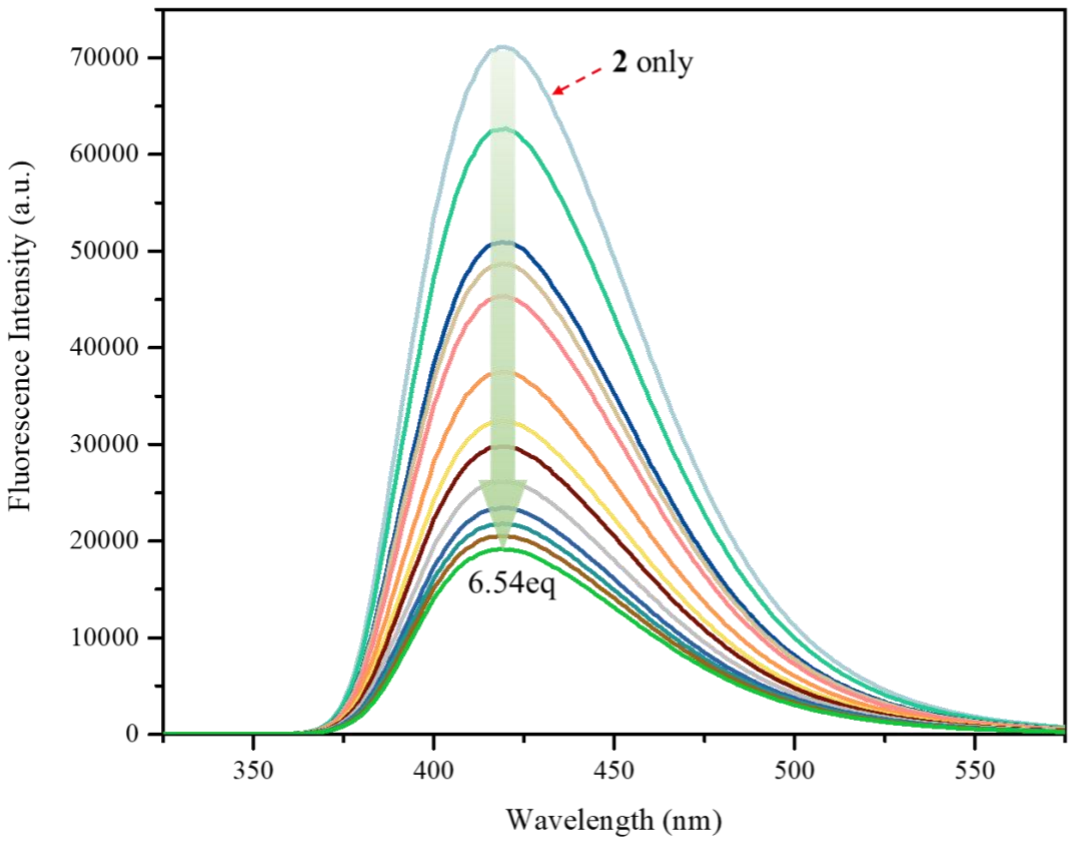


Figure S13. Fluorescence spectra of receptor **2** (10 μM) recorded during the titration with tetrabutylammonium bromide (TBABr) in CH_2Cl_2. The excitation wavelength was 301 nm.

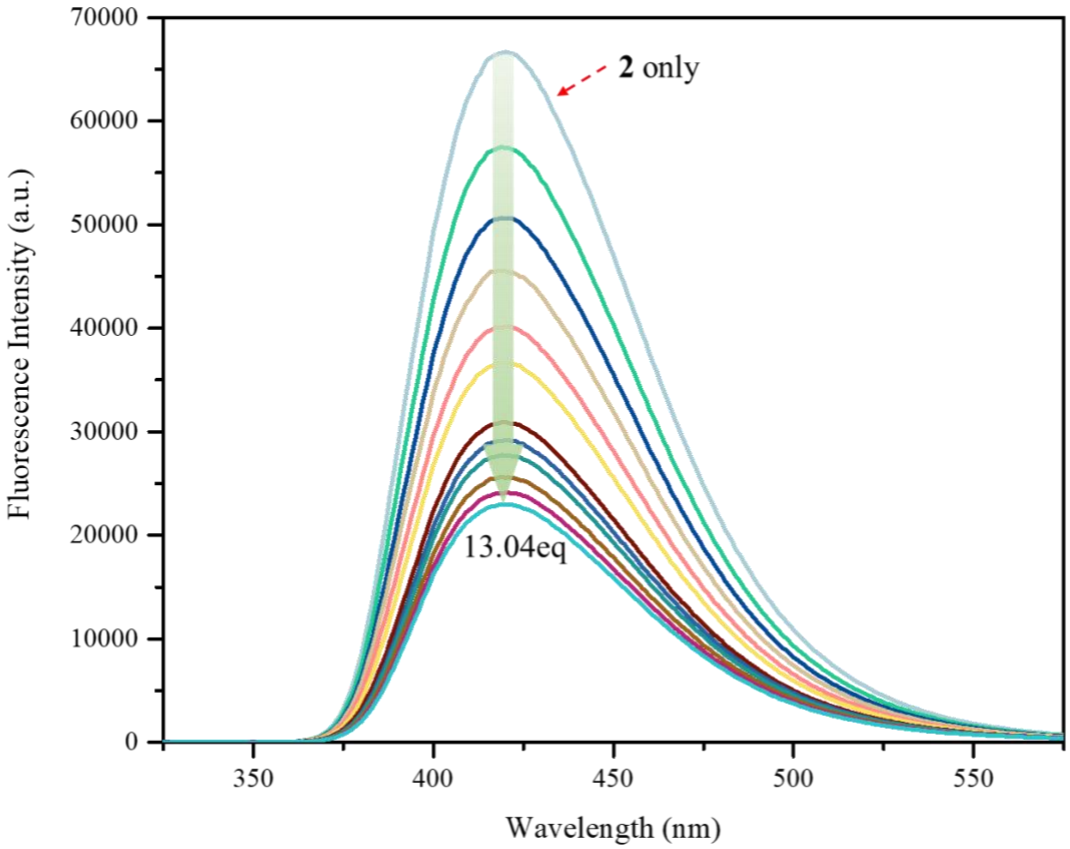


Figure S14. Fluorescence spectra of receptor **2** (10 μM) recorded during a titration with tetrabutylammonium iodide (TBAI) in CH_2Cl_2.

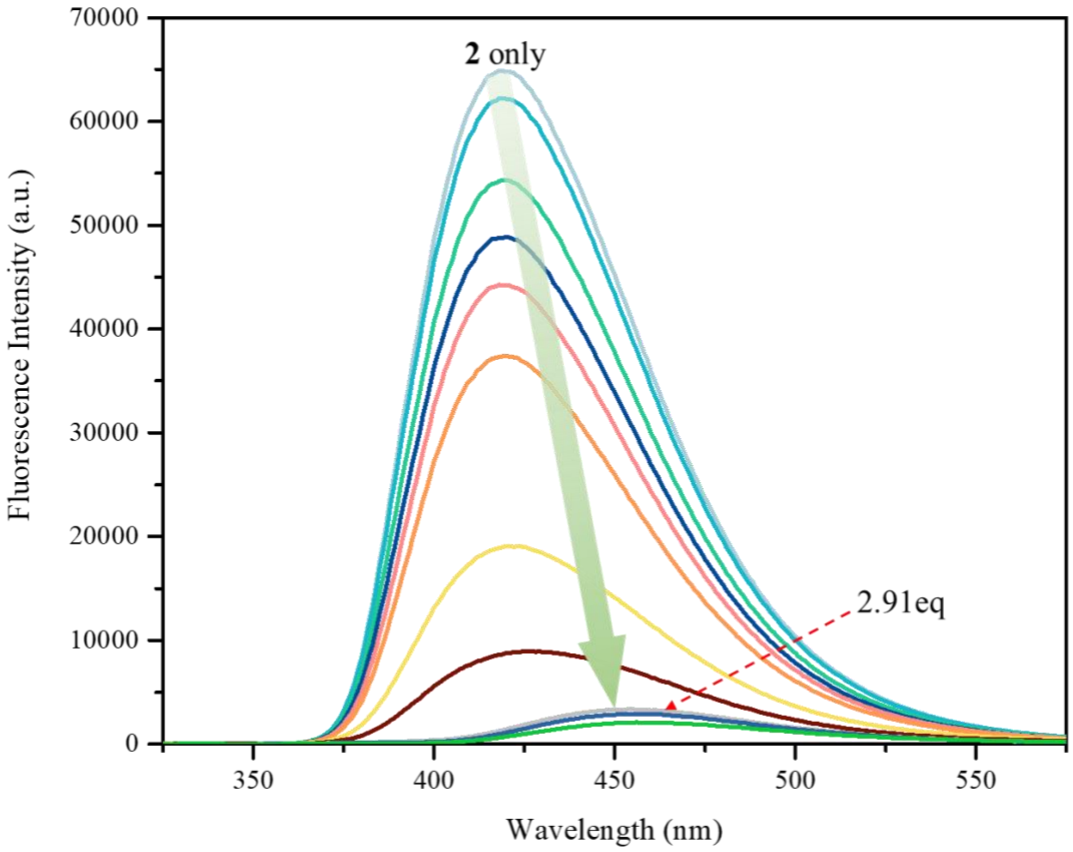


Figure S15. Fluorescence spectra of receptor **2** (10 μM) recorded during a titration with tetraethylammonium bicarbonate ($TEAHCO_3$) in CH_2Cl_2.

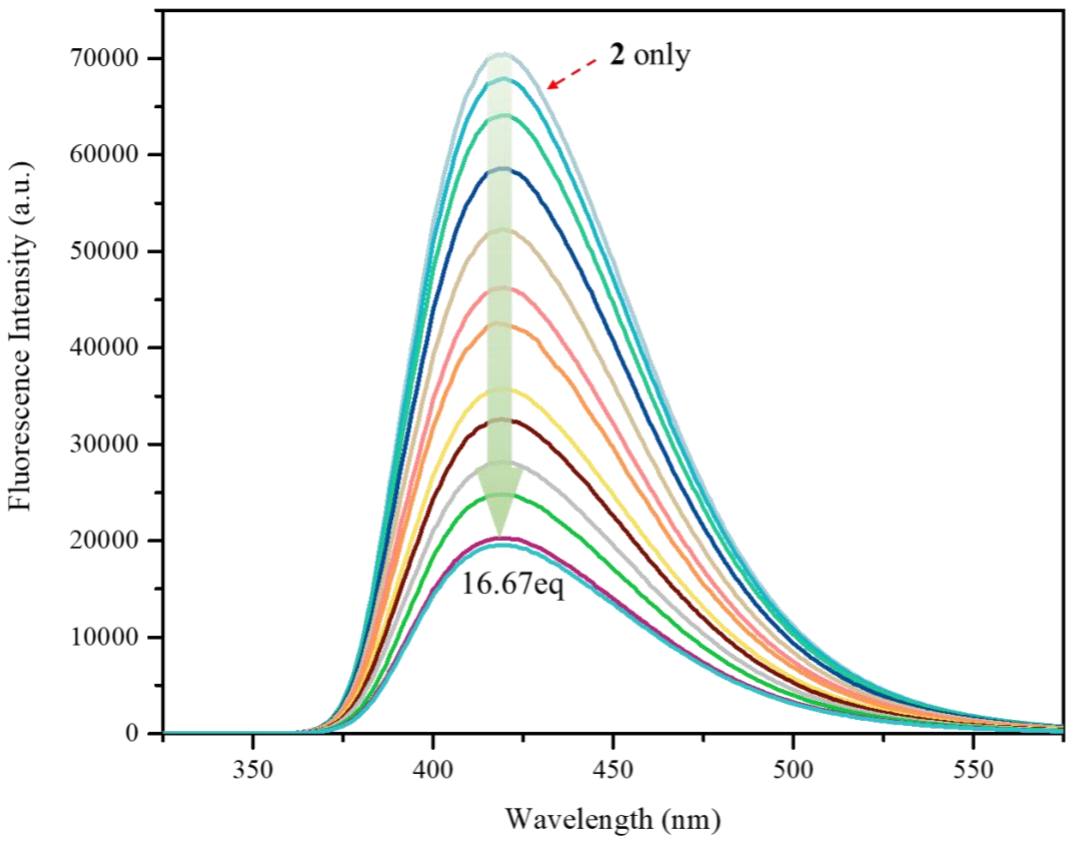


Figure S16. Fluorescence spectra of receptor **2** (10 μM) recorded during a titration with tetrabutylammonium hydrogen sulfate ($TBAHSO_4$) in CH_2Cl_2.

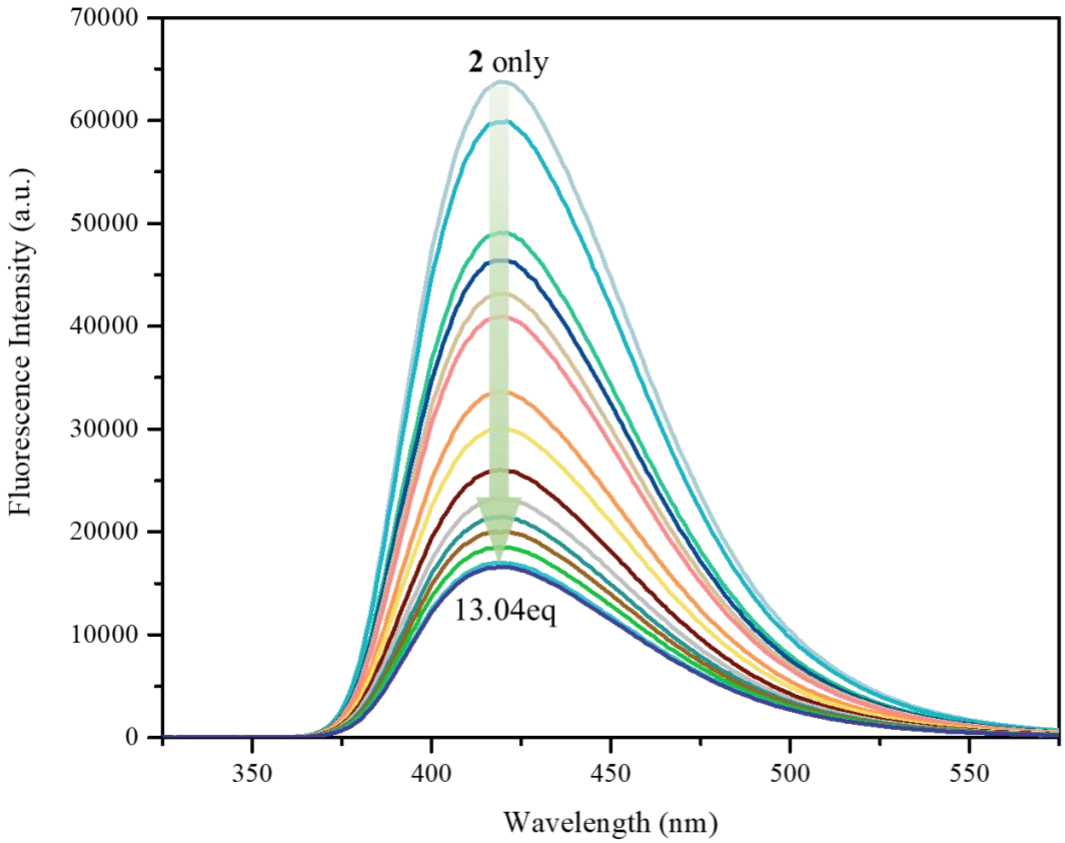


Figure S17. Fluorescence spectra of receptor **2** (10 μM) recorded during a titration with bis(tetrabutylammonium) sulfate ($(TBA)_2 \bullet SO_4$) in CH_2Cl_2.

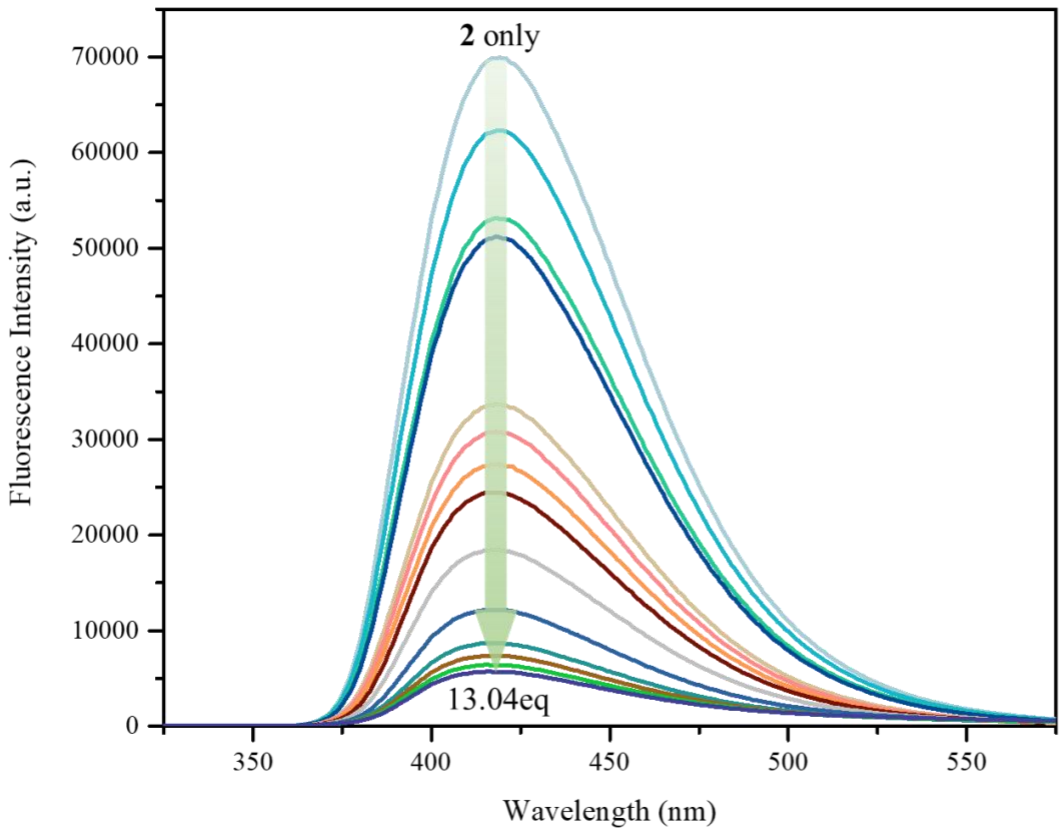


Figure S18. Fluorescence spectra of receptor **2** (10 μM) recorded during a titration with tris(tetraethylammonium) hydrogen pyrophosphate ($(TBA)_3 \bullet HP_2O_7$)) in CH_2Cl_2.

4. Single crystal X-ray diffraction data

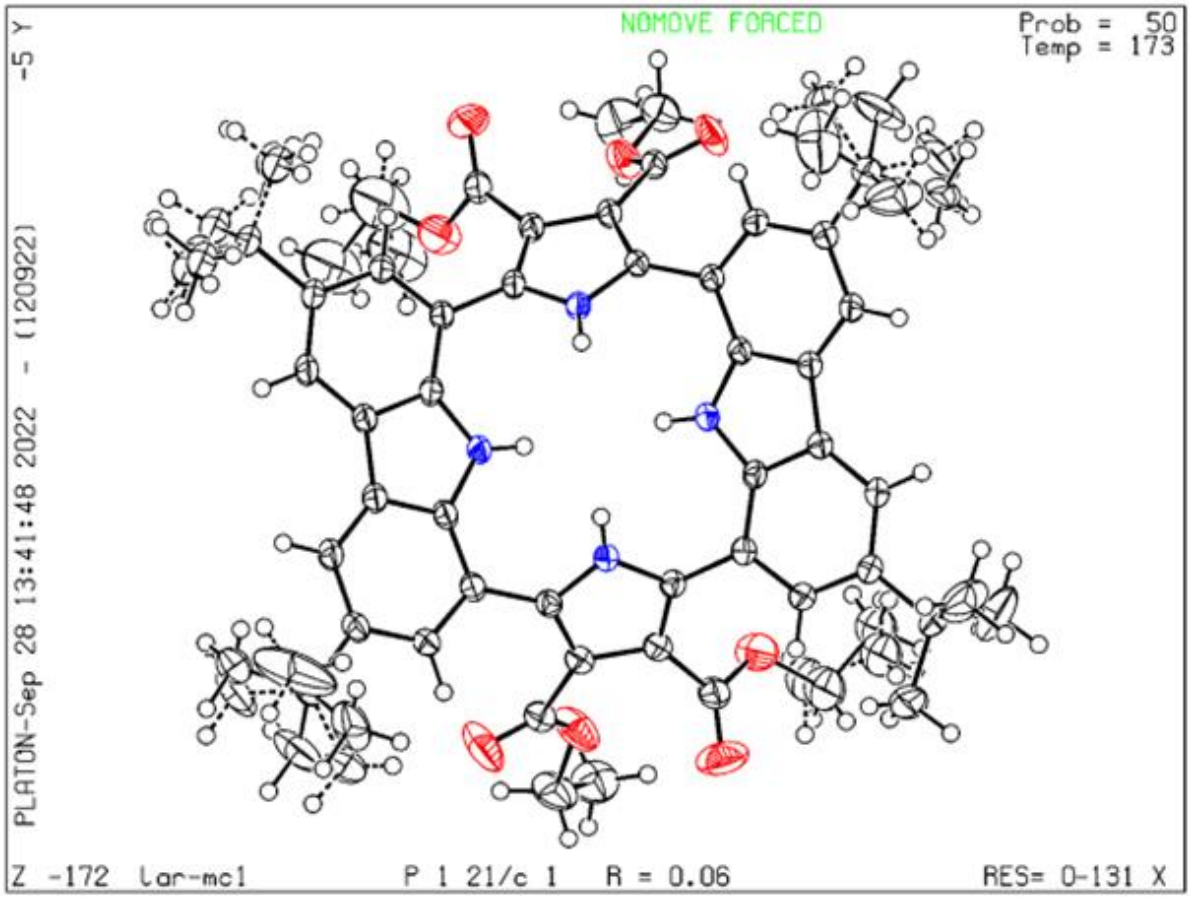


Figure S19. Single crystal X-ray diffraction structure of receptor **2**. Solvent molecules have been omitted for clarity. Displacement ellipsoids are scaled to the 50% probability level.

Table S1. Crystal data and structure refinement for **2**.

Empirical formula	C60 H68 N4 O8	
Formula weight	973.18	
Temperature	173.15 K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 15.9159(3) Å	α = 90°.
	b = 21.2730(4) Å	β = 107.1160(10) °.
	c = 18.6760(3) Å	γ = 90°.
Volume	6043.25(19) $Å^3$	
Z	4	
Density (calculated)	1.070 Mg/m^3	
Absorption coefficient	0.071 mm^{-1}	
F(000)	2080	
Crystal size	0.412 x 0.327 x 0.289 mm^3	
Theta range for data collection	2.22 to 26.34°.	
Index ranges	-21<=h<=21, -28<=k<=28, -24<=l<=21	
Reflections collected	14976	
Independent reflections	9703 [R(int) = 0.0423]	
Completeness to theta = 56.6°	99.4 %	
Absorption correction	Multi-scan	
Max. and min. transmission	0.7457 and 0.7114	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14976 / 12 / 729	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0631, wR2 = 0.1663	
R indices (all data)	R1 = 0.0894, wR2 = 0.1846	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.583 and -0.604 $e.Å^{-3}$	
ccdc number	2219418	

X-ray experimental for [**2**-2H]$^{2-}$•2(TBA^{+}): Crystals grew as clusters of colorless prisms by slow evaporation from acetone and diethyl ether. The data crystal was cut from a larger crystal and had approximate dimensions; 0.22 x 0.12 x 0.061 mm. The data were collected on a Rigaku Oxford Diffraction HyPix6000E Synergy diffractometer using a μ-focus Cu Kα radiation source (λ = 1.5418 Å) with collimating mirror monochromators. A total of 2154 frames of data were collected using ω-scans with a scan range of 0.5° and a counting time of 8 seconds per frame for frames collected with a detector offset of +/- 47.8° and 31 seconds per frame with frames collected with a detector offset of +/- 104.5°. The data were collected at 100 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table S2. Data collection, unit cell refinement and data reduction were performed using Rigaku Oxford Diffraction's CrysAlisPro V 1.171.41.123a.[5] The structure was solved by direct methods using SHELXT[2] and refined by full-matrix least-squares on F[6] with anisotropic displacement parameters for the non-H atoms using SHELXL-2018/3.[7] tructure analysis was aided by use of the programs PLATON[8] and OLEX2.[9] The hydrogen atoms on the carbon atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The hydrogen atoms on the nitrogen atoms were observed in a ΔF map and refined with isotropic displacement parameters. The data crystal was twinned. The twin law and twin fractions were determined using CrysAlisPro.

The function, $\Sigma w(|F_O|^2 - |F_C|^2)^2$, was minimized, where $w = 1/[(\sigma(F_O))^2 + (0.0631*P)^2 + (1.6026*P)]$ and $P = (|F_O|^2 + 2|F_C|^2)/3$. $R_W(F^2)$ refined to 0.112, with R(F) equal to 0.0422 and a goodness of fit, S, = 1.04. Definitions used for calculating R(F), $R_W(F^2)$ and the goodness of fit, S, are given below.[10] The data were checked for secondary extinction effects but no correction was necessary. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[11] All figures were generated using SHELXTL/PC.[12] Tables of positional and thermal parameters, bond lengths and angles, torsion angles and figures may be obtained from the Cambridge Crystallographic Centre by referencing CCDC number 2219688.

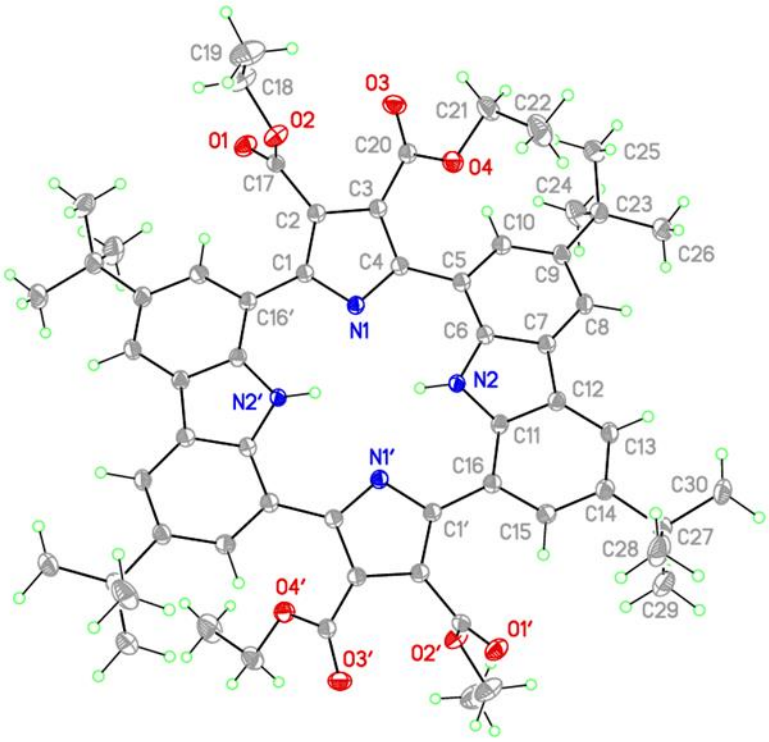


Figure S20. View of macrocycle 1 in [**2**-2H]$^{2-}$•2(TBA^{+}) showing the atom labeling scheme. Solvent molecules and two tetrabutylammonium cations have been omitted for clarity. Displacement ellipsoids are scaled to the 50% probability level. The macrocycle resides around a crystallographic inversion center at ½, ½, ½. Atoms related by 1-x, 1-y, 1-z have labels appended by α ‘.

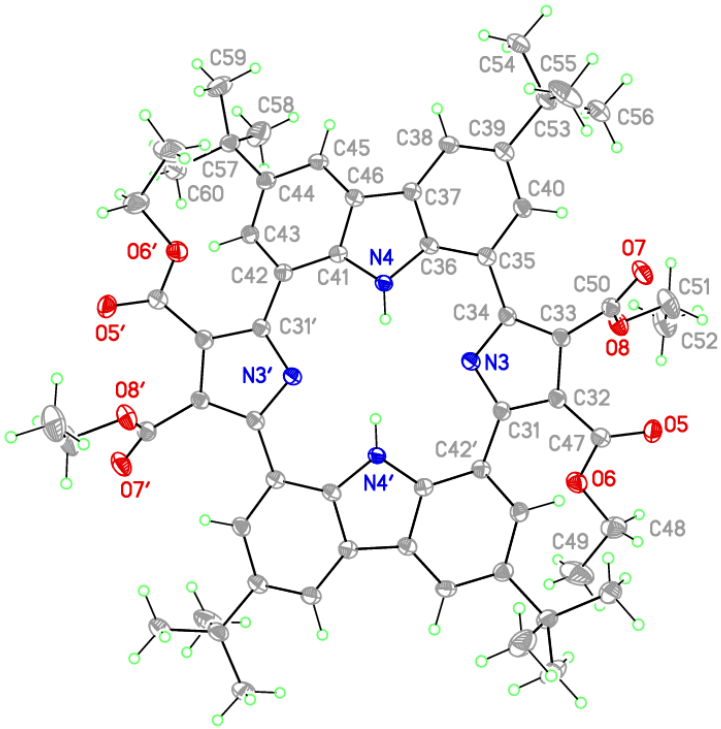


Figure S21. View of macrocycle 2 in [**2**-2H]$^{2-}$•2(TBA^{+}) showing the atom labeling scheme. Solvent molecules and two tetrabutylammonium cations have been omitted for clarity. Displacement ellipsoids are scaled to the 50% probability level. The macrocycle resides around a crystallographic inversion center at ½, 1, ½. Atoms related by 1-x, 2-y, 1-z have labels appended by α ‘.

Table S2. Crystal data and structure refinement for [**2**-2H]$^{2-}$•2(TBA^{+}).

Empirical formula	C96 H148 N6 O9	
Formula weight	1530.20	
Temperature	100.0(6) K	
Wavelength	1.54184 Å	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 17.4296(3) Å	a= 90°.
	b = 29.0372(5) Å	b= 91.2569(12)°.
	c = 18.0368(2) Å	g = 90°.
Volume	9126.4(2) Å^3	
Z	4	
Density (calculated)	1.114 Mg/m^3	
Absorption coefficient	0.548 mm^{-1}	
F(000)	3352	
Crystal size	0.22 x 0.12 x 0.061 mm^3	
Theta range for data collection	2.885 to 76.479°.	
Index ranges	-21<=h<=21, -35<=k<=35, -22<=l<=22	
Reflections collected	30978	
Independent reflections	30978 [R(int) = ?]	
Completeness to theta = 67.684°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.80527	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	30978 / 16 / 1055	
Goodness-of-fit on F2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0422, wR2 = 0.1080	
R indices (all data)	R1 = 0.0496, wR2 = 0.1120	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.290 and -0.410 e.Å^{-3}	
ccdc number	2219688	

5. NMR and HRMS Spectra

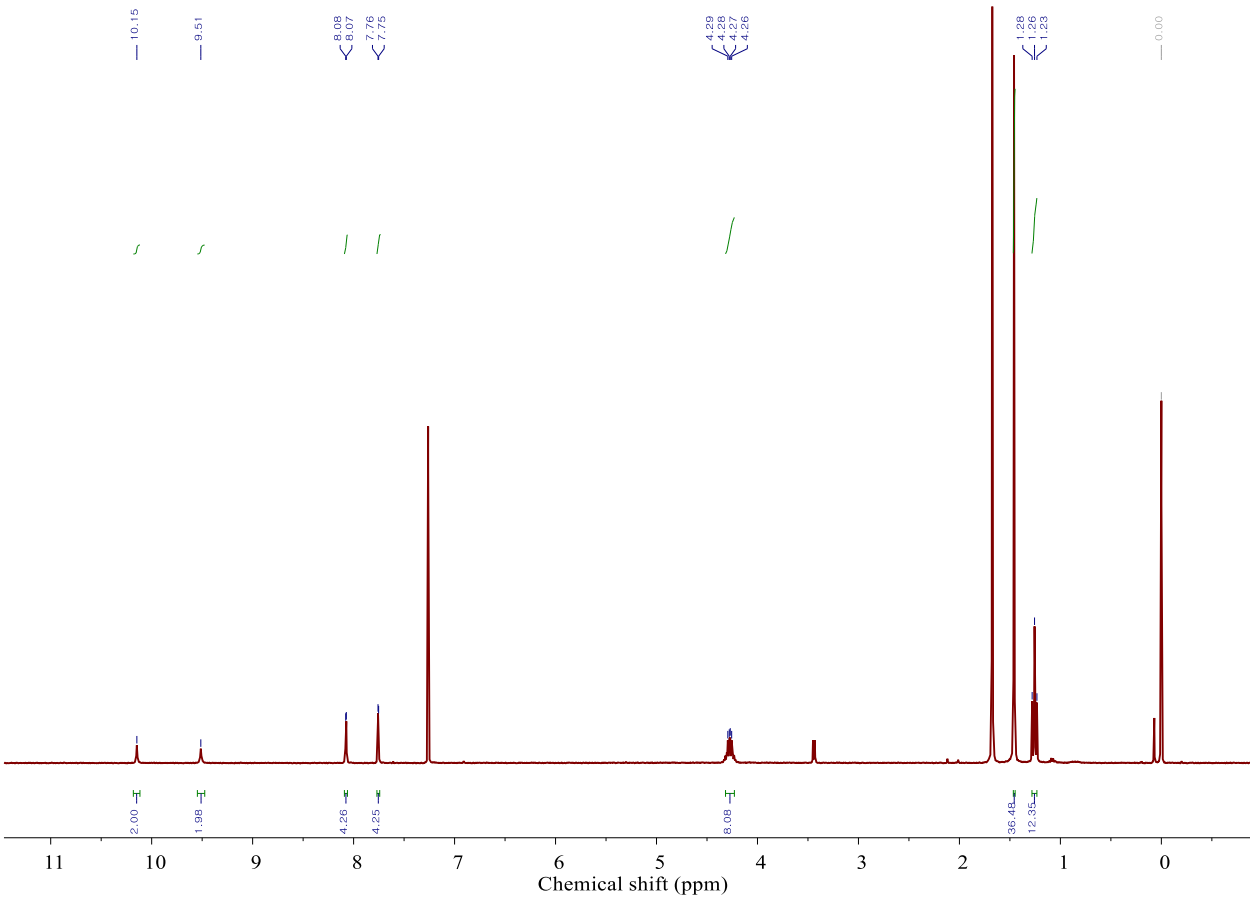


Figure S21. ^{1}H NMR spectrum of receptor **2** recorded in $CDCl_3$.

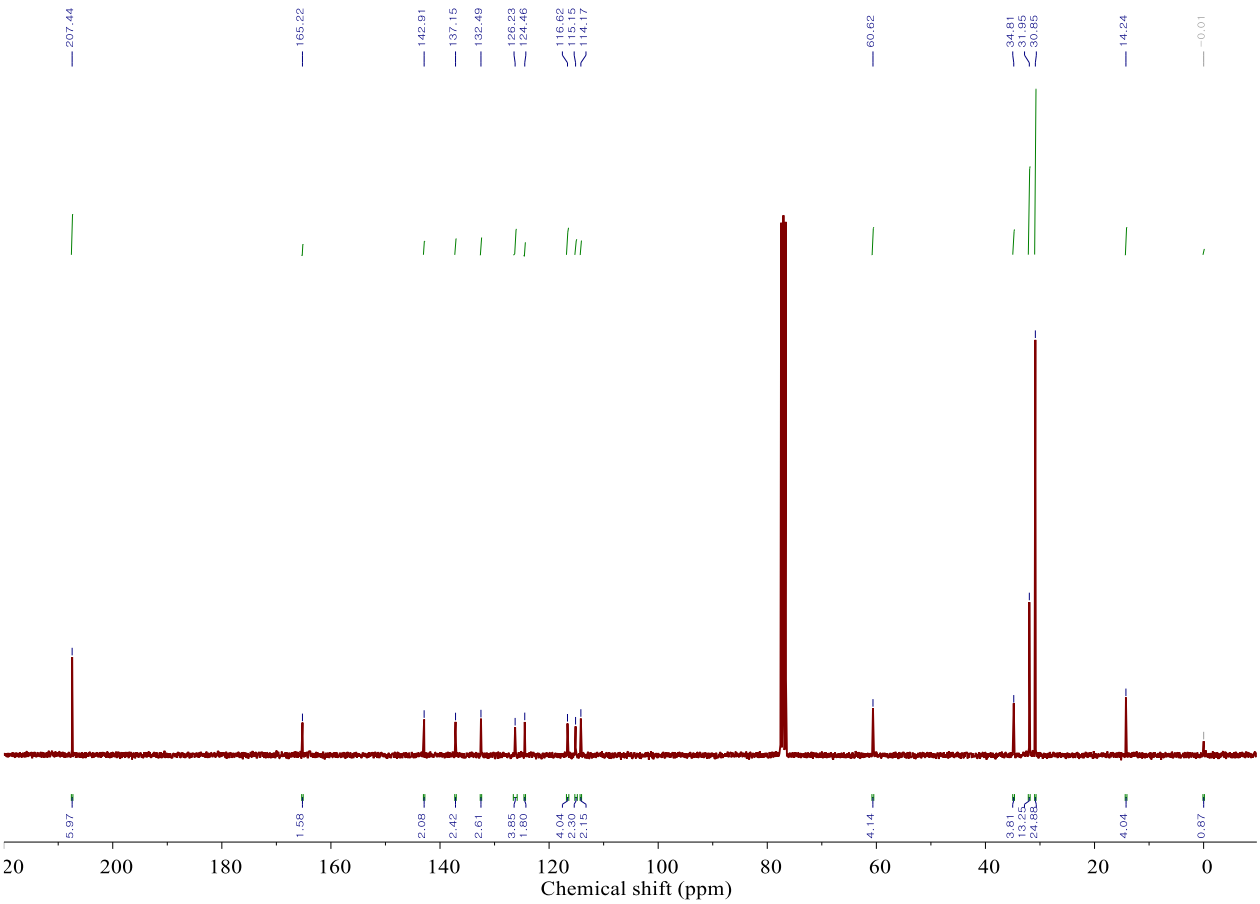


Figure S22. ^{13}C NMR spectrum of receptor **2** recorded in $CDCl_3$.

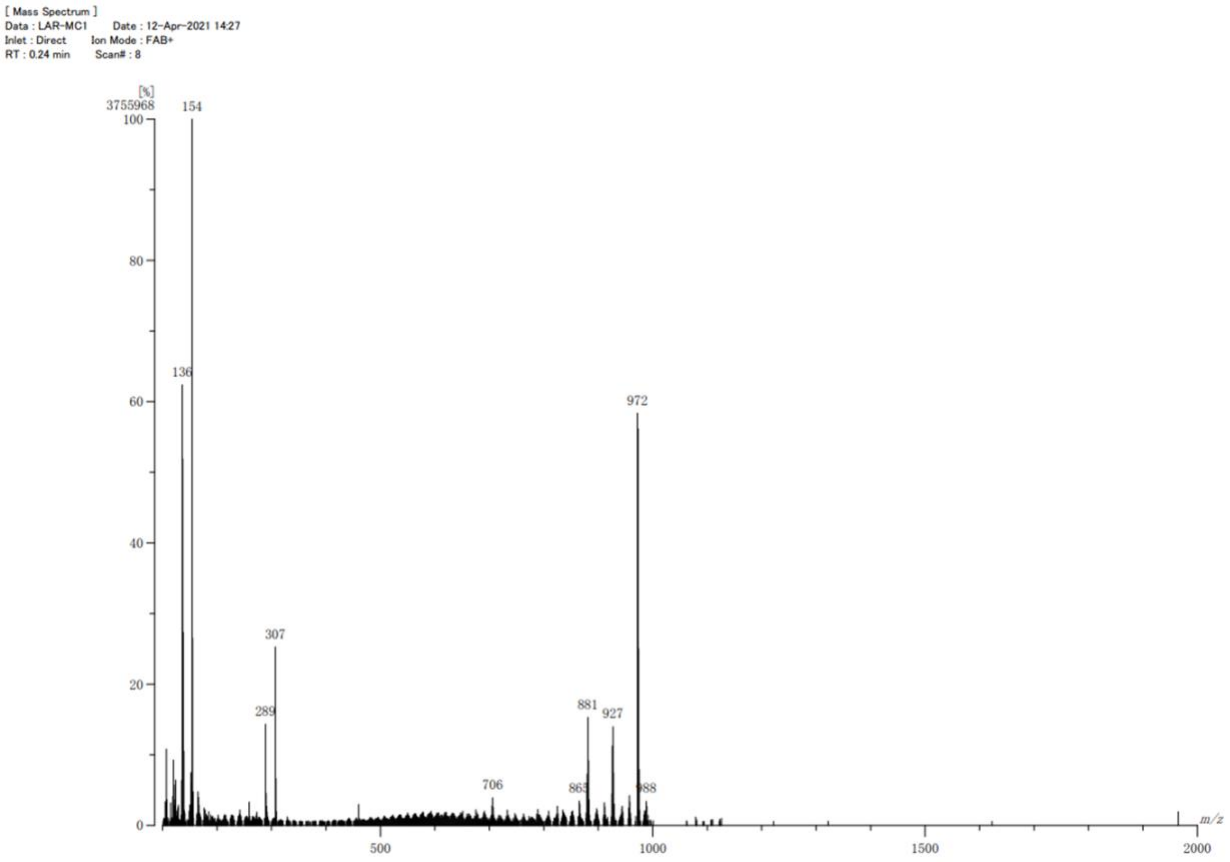


Figure S12. FAB mass spectrum of receptor **2**.

Data : LAR-MC1_HR Date : 12-Apr-2021 16:09
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : FAB+
RT : 0.27 min Scan# : 9
Elements : C 100/1, H 100/1, N 10/1, O 10/1
Mass Tolerance : 1000ppm, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 30.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	972.5055	100.00	+1.8 / +1.8	29.0	C60 H68 N4 O8
2			+0.5 / +0.4	28.5	C62 H70 N O9

Figure S24. HR FAB mass spectral data for receptor **2**.

6. References

1) Brewster, J. T.; Zafar, H.; McVeigh, M.; Wight, C. D.; Anguera, G.; Steinbrück, A.; Lynch, V. M.; Sessler, J. L. *J. Org. Chem.* **2018**, *83*, 9568-9570.

2) Arnold, L.; Baumgarten, M.; Müllen, K. *Chem. Commun.* **2012**, *48*, 9640-9642.

3) Conformational searches performed with PCModel, Version 9.3; Serena Software: Bloomington, IN, 2012.

4) T. A. Halgren, *J. Comp. Chem.* **1996**, *17*, 490-519.

5) CrysAlisPro. Rigaku Oxford Diffraction, HyPix6000E System, CrysAlisPro Software System, 1.171.41.123a.

6) Sheldrick. G. M. SHELXT. A program for crystal structure solution. *Acta Cryst. A* **2015**, *71*, 3-8.

7) Sheldrick, G. M. SHELXL-2018/3. Program for the Refinement of Crystal Structures. *Acta Cryst. C* **2015**, *71*, 9-18.

8) Spek, A. L. PLATON, A Multipurpose Crystallographic Tool. Utrecht University, The Netherlands. *Acta Cryst. D* **2009**, *65*, 148-155.

9) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2: A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Cryst.* **2009**, *42*, 339-341.

10) $R_W(F^2) = \{\Sigma w(|F_O|^2 - |F_C|^2)^2/\Sigma w(|F_O|)^4\}^{1/2}$ where w is the weight given each reflection.

$R(F) = \Sigma (|F_O| - |F_C|)/\Sigma|F_O|\}$ for reflections with $F_O > 4(\Sigma(F_O))$.

$S = [\Sigma w(|F_O|^2 - |F_C|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

11) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

12) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

HEADER MMFF94 OPTIMIZED HOST

COMPND LOWEST ENERGY FORM BY SAMPLING IN VACUO MD RUN

AUTHOR GENERATED BY PCMODEL V 9.30

HETATM 1 N -0.082 2.528 2.003
HETATM 2 O -1.379 -4.000 -2.013
HETATM 3 N -2.230 -0.037 1.639
HETATM 4 N -0.082 -2.528 2.004
HETATM 5 O -2.800 -4.828 -0.419
HETATM 6 N 2.026 0.038 1.456
HETATM 7 O 0.865 4.000 -2.110
HETATM 8 O -2.985 3.538 -0.855
HETATM 9 O 2.417 4.828 -0.644
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HETATM 12 C 1.016 2.913 1.273
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HETATM 17 C -2.539 -2.523 1.905
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HETATM 19 C 2.721 -1.098 1.792
HETATM 20 C -2.537 2.447 1.903
HETATM 21 C -3.475 -3.469 2.349
HETATM 22 C -5.012 -1.737 3.036
HETATM 23 C -4.095 0.682 2.598
HETATM 24 C -3.469 3.397 2.352
HETATM 25 C -4.718 -3.110 2.909
HETATM 26 C 3.966 -0.681 2.251
HETATM 27 C -0.865 -3.622 0.234
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HETATM 30 C 2.355 -2.447 1.693
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HEADER MMFF94 OPTIMIZED HOST

COMPND USING COORDINATES FROM XRAY STRUCTURE

AUTHOR GENERATED BY PCMODEL V 9.30

HETATM 1 N 0.078 2.505 0.800
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HETATM 3 N -2.096 -0.023 0.333
HETATM 4 N 0.000 -2.546 0.776
HETATM 5 O -2.671 -4.800 -1.740
HETATM 6 N 2.167 -0.023 0.333
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HETATM 9 O 2.741 4.742 -1.737
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HETATM 11 C -2.791 -1.148 0.705
HETATM 12 C 1.213 2.870 0.118
HETATM 13 C -1.139 -2.915 0.102
HETATM 14 C -2.753 1.124 0.708
HETATM 15 C 2.528 2.456 0.596
HETATM 16 C -4.002 -0.709 1.230
HETATM 17 C -2.451 -2.503 0.588
HETATM 18 C 2.868 1.100 0.702
HETATM 19 C 2.830 -1.172 0.687
HETATM 20 C -2.371 2.467 0.594
HETATM 21 C -3.417 -3.434 1.000
HETATM 22 C -4.948 -1.678 1.639
HETATM 23 C -3.977 0.725 1.235
HETATM 24 C -3.297 3.436 1.019
HETATM 25 C -4.672 -3.056 1.520
HETATM 26 C 4.062 -0.777 1.198
HETATM 27 C -0.735 -3.638 -1.014
HETATM 28 C 1.127 -2.885 0.069
HETATM 29 C 3.497 3.385 1.005
HETATM 30 C 2.448 -2.514 0.563
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HETATM 33 C -4.557 3.100 1.542
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HETATM 35 C -1.622 -4.230 -2.011
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HETATM 46 C 5.645 -4.264 1.856
HETATM 47 C -1.500 4.214 -2.004
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END

HEADER MMFF94 OPTIMIZED HOST:FLOURIDE COMPLEX

COMPND LOWEST ENERGY PYRROLE-BOUND FORM BY SAMPLING IN VACUO MD RUN

AUTHOR GENERATED BY PCMODEL V 9.30

HETATM 1 N -0.233 0.595 -3.011
HETATM 2 O -1.851 -3.288 3.637
HETATM 3 N -2.530 0.263 -0.697
HETATM 4 N -0.575 0.567 1.850
HETATM 5 O -3.264 -1.684 4.457
HETATM 6 N 1.725 0.283 -0.467
HETATM 7 O 1.081 -3.227 -4.840
HETATM 8 O -2.771 -2.411 -4.503
HETATM 9 O 2.478 -1.600 -5.642
HETATM 10 C -1.337 -0.049 -3.541
HETATM 11 C -3.361 0.400 0.390
HETATM 12 C 0.945 0.014 -3.455
HETATM 13 C -1.747 -0.031 2.288
HETATM 14 C -3.200 0.394 -1.889
HETATM 15 C 2.265 0.395 -2.926
HETATM 16 C -4.625 0.669 -0.126
HETATM 17 C -3.071 0.342 1.763
HETATM 18 C 2.555 0.440 -1.552
HETATM 19 C 2.394 0.407 0.727
HETATM 20 C -2.718 0.329 -3.205
HETATM 21 C -4.153 0.609 2.623
HETATM 22 C -5.683 0.905 0.780
HETATM 23 C -4.523 0.664 -1.562
HETATM 24 C -3.666 0.584 -4.217
HETATM 25 C -5.461 0.887 2.170
HETATM 26 C 3.715 0.694 0.402
HETATM 27 C -1.373 -1.053 3.157
HETATM 28 C 0.536 -0.072 2.373
HETATM 29 C 3.345 0.681 -3.783
HETATM 30 C 1.913 0.323 2.042
HETATM 31 C -0.856 -1.050 -4.380
HETATM 32 C -5.442 0.893 -2.612
HETATM 33 C -5.024 0.865 -3.958
HETATM 34 C 4.214 0.874 2.800
HETATM 35 C -2.266 -1.997 3.818
HETATM 36 C 4.650 0.967 -3.327
HETATM 37 O -1.316 -2.398 -6.268
HETATM 38 C 3.816 0.716 -1.033
HETATM 39 C 0.582 -1.002 -4.336

HETATM 40 C 2.858 0.577 3.056
HETATM 41 C 4.631 0.921 1.455
HETATM 42 C 0.064 -1.087 3.200
HETATM 43 C 4.872 0.973 -1.937
HETATM 44 C 1.483 -1.931 -5.006
HETATM 45 C -5.988 1.135 -5.126
HETATM 46 C 5.175 1.141 3.971
HETATM 47 C -1.647 -2.000 -5.156
HETATM 48 C -2.664 -4.262 4.294
HETATM 49 C 1.904 -4.186 -5.507
HETATM 50 C 1.306 -5.560 -5.276
HETATM 51 C -6.026 -0.090 -6.066
HETATM 52 C -7.443 1.415 -4.685
HETATM 53 C -2.053 -5.627 4.048
HETATM 54 C -5.507 2.369 -5.920
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HETATM 56 C -6.582 1.156 3.189
HETATM 57 C 0.865 -2.036 3.966
HETATM 58 C -6.751 -0.068 4.115
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HETATM 62 C 7.143 1.540 -3.694
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HETATM 65 C -4.760 -3.713 -4.349
HETATM 66 C 5.225 -0.094 4.897
HETATM 67 C 6.626 1.440 3.533
HETATM 68 C 4.681 2.361 4.779
HETATM 69 O 1.993 -2.429 3.310
HETATM 70 C 2.813 -3.355 4.023
HETATM 71 C 3.994 -3.711 3.141
HETATM 72 O 0.538 -2.451 5.074
HETATM 73 H -0.281 1.347 -2.313
HETATM 74 H -1.523 0.326 -0.628
HETATM 75 H -0.534 1.327 1.160
HETATM 76 H 0.717 0.337 -0.536
HETATM 78 H -3.956 0.596 3.694
HETATM 79 H -6.659 1.120 0.361
HETATM 80 H -3.315 0.561 -5.247
HETATM 81 H 3.148 0.678 -4.854
HETATM 82 H -6.467 1.111 -2.337
HETATM 83 H 2.508 0.539 4.086
HETATM 84 H 5.653 1.152 1.182

HETATM 85 H 5.846 1.193 -1.516
HETATM 86 H -3.680 -4.232 3.885
HETATM 87 H -2.692 -4.060 5.371
HETATM 88 H 1.930 -3.972 -6.582
HETATM 89 H 2.920 -4.150 -5.098
HETATM 90 H 1.255 -5.783 -4.205
HETATM 91 H 0.281 -5.604 -5.659
HETATM 92 H 1.902 -6.333 -5.770
HETATM 93 H -6.346 -0.990 -5.527
HETATM 94 H -6.728 0.069 -6.893
HETATM 95 H -5.049 -0.304 -6.512
HETATM 96 H -7.868 0.566 -4.137
HETATM 97 H -7.507 2.302 -4.045
HETATM 98 H -8.090 1.596 -5.551
HETATM 99 H -1.027 -5.665 4.431
HETATM 100 H -2.641 -6.411 4.533
HETATM 101 H -2.000 -5.838 2.975
HETATM 102 H -4.520 2.214 -6.369
HETATM 103 H -6.197 2.606 -6.738
HETATM 104 H -5.439 3.252 -5.274
HETATM 105 H -6.968 -0.974 3.537
HETATM 106 H -5.854 -0.264 4.712
HETATM 107 H -7.576 0.082 4.822
HETATM 108 H -8.300 0.579 1.943
HETATM 109 H -8.725 1.614 3.307
HETATM 110 H -7.934 2.316 1.897
HETATM 111 H -5.311 2.243 4.627
HETATM 112 H -6.068 3.276 3.409
HETATM 113 H -7.025 2.629 4.751
HETATM 114 H 4.486 2.349 -5.769
HETATM 115 H 5.233 3.375 -4.540
HETATM 116 H 6.196 2.753 -5.889
HETATM 117 H 7.906 1.739 -4.456
HETATM 118 H 7.108 2.418 -3.038
HETATM 119 H 7.493 0.685 -3.103
HETATM 120 H 5.054 -0.152 -5.881
HETATM 121 H 6.773 0.212 -5.987
HETATM 122 H 6.175 -0.863 -4.714
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HETATM 124 H -3.942 -2.869 -6.150
HETATM 125 H -4.414 -4.177 -3.419
HETATM 126 H -5.424 -4.411 -4.866
HETATM 127 H -5.331 -2.823 -4.065
HETATM 128 H 5.554 -0.984 4.349

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HETATM  132  H            7.272   1.618   4.400
HETATM  133  H            6.682   2.335   2.903
HETATM  134  H            5.369   2.596   5.600
HETATM  135  H            3.696   2.192   5.226
HETATM  136  H            4.605   3.250   4.142
HETATM  137  H            3.168  -2.894   4.951
HETATM  138  H            2.240  -4.260   4.256
HETATM  139  H            4.666  -4.408   3.650
HETATM  140  H            3.653  -4.167   2.207
HETATM  141  H            4.557  -2.812   2.867
HETATM   77  F           -0.411   2.056  -0.572
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CONECT    2   35   48
CONECT    3   11   14   74
CONECT    4   13   28   75
CONECT    5   35
CONECT    6   18   19   76
CONECT    7   44   49
CONECT    8   47   64
CONECT    9   44
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CONECT   11    3   16   17
CONECT   12    1   15   39
CONECT   13    4   17   27
CONECT   14    3   20   23
CONECT   15   12   18   29
CONECT   16   11   22   23
CONECT   17   11   13   21
CONECT   18    6   15   38
CONECT   19    6   26   30
CONECT   20   10   14   24
CONECT   21   17   25   78
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CONECT   29   15   36   81
CONECT   30   19   28   40
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CONECT 71 70 139 140 141
CONECT 72 57
CONECT 73 1
CONECT 74 3

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CONECT 116  61
CONECT 117  62
CONECT 118  62
CONECT 119  62
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CONECT  135   68
CONECT  136   68
CONECT  137   70
CONECT  138   70
CONECT  139   71
CONECT  140   71
CONECT  141   71
END
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HEADER MMFF94 OPTIMIZED HOST:FLOURIDE COMPLEX

COMPND LOWEST ENERGY CARBZOLE-BOUND FORM BY SAMPLING IN VACUO MD RUN

AUTHOR GENERATED BY PCMODEL V 9.30

HETATM	1	N	2.846	1.134	1.035
HETATM	2	O	-4.100	-2.397	-0.868
HETATM	3	N	0.702	0.741	-1.400
HETATM	4	N	-1.862	1.170	0.522
HETATM	5	O	-4.468	-0.724	-2.385
HETATM	6	N	0.276	0.709	2.949
HETATM	7	O	5.038	-2.484	2.367
HETATM	8	O	4.849	-1.484	-1.547
HETATM	9	O	5.425	-0.841	3.911
HETATM	10	C	3.511	0.610	-0.048
HETATM	11	C	-0.356	1.200	-2.161
HETATM	12	C	3.312	0.628	2.226
HETATM	13	C	-2.335	0.690	-0.677
HETATM	14	C	1.910	1.174	-1.915
HETATM	15	C	2.729	1.071	3.494
HETATM	16	C	0.202	1.749	-3.313
HETATM	17	C	-1.745	1.145	-1.938
HETATM	18	C	1.340	1.143	3.718
HETATM	19	C	-0.926	1.151	3.472
HETATM	20	C	3.215	1.084	-1.400
HETATM	21	C	-2.561	1.642	-2.973
HETATM	22	C	-0.660	2.221	-4.330
HETATM	23	C	1.627	1.730	-3.159
HETATM	24	C	4.251	1.552	-2.234
HETATM	25	C	-2.057	2.165	-4.179
HETATM	26	C	-0.636	1.683	4.724
HETATM	27	C	-3.309	-0.254	-0.364
HETATM	28	C	-2.534	0.638	1.596
HETATM	29	C	3.551	1.541	4.537
HETATM	30	C	-2.232	1.087	2.956
HETATM	31	C	4.410	-0.325	0.456
HETATM	32	C	2.700	2.176	-3.965
HETATM	33	C	4.032	2.085	-3.519
HETATM	34	C	-3.036	2.064	5.090
HETATM	35	C	-4.010	-1.109	-1.313
HETATM	36	C	3.054	2.051	5.752
HETATM	37	O	6.433	-1.497	0.100
HETATM	38	C	0.790	1.679	4.879
HETATM	39	C	4.274	-0.323	1.897

HETATM 40 C -3.262 1.556 3.797
HETATM 41 C -1.704 2.131 5.538
HETATM 42 C -3.445 -0.277 1.078
HETATM 43 C 1.658 2.124 5.903
HETATM 44 C 4.963 -1.202 2.833
HETATM 45 C 5.224 2.556 -4.369
HETATM 46 C -4.222 2.538 5.947
HETATM 47 C 5.330 -1.153 -0.316
HETATM 48 C -4.781 -3.283 -1.756
HETATM 49 C 5.706 -3.394 3.241
HETATM 50 C 5.735 -4.754 2.572
HETATM 51 C 4.825 3.095 -5.761
HETATM 52 C 5.969 3.692 -3.635
HETATM 53 C -4.826 -4.654 -1.110
HETATM 54 C 6.196 1.378 -4.600
HETATM 55 C 4.031 2.519 6.844
HETATM 56 C -3.028 2.663 -5.264
HETATM 57 C -4.376 -1.105 1.836
HETATM 58 C -2.325 3.173 -6.543
HETATM 59 C -3.871 3.831 -4.709
HETATM 60 C -3.968 1.515 -5.691
HETATM 61 C 4.956 1.351 7.253
HETATM 62 C 4.890 3.684 6.308
HETATM 63 C 3.335 3.018 8.131
HETATM 64 C 5.712 -2.307 -2.331
HETATM 65 C 5.010 -2.613 -3.639
HETATM 66 C -4.950 3.696 5.232
HETATM 67 C -5.209 1.370 6.161
HETATM 68 C -3.815 3.050 7.348
HETATM 69 O -3.900 -1.461 3.063
HETATM 70 C -4.774 -2.286 3.833
HETATM 71 C -4.076 -2.621 5.136
HETATM 72 O -5.484 -1.428 1.416
HETATM 73 H 2.084 1.791 0.962
HETATM 74 H 0.608 0.139 -0.571
HETATM 75 H -1.091 1.816 0.605
HETATM 76 H 0.363 0.119 2.111
HETATM 78 H -3.639 1.622 -2.814
HETATM 79 H -0.200 2.634 -5.220
HETATM 80 H 5.267 1.500 -1.845
HETATM 81 H 4.628 1.508 4.377
HETATM 82 H 2.453 2.598 -4.932
HETATM 83 H -4.278 1.524 3.408
HETATM 84 H -1.450 2.534 6.511

HETATM 85 H 1.204 2.528 6.800
HETATM 86 H -4.242 -3.341 -2.708
HETATM 87 H -5.802 -2.926 -1.931
HETATM 88 H 6.731 -3.052 3.422
HETATM 89 H 5.165 -3.460 4.191
HETATM 90 H 6.240 -5.489 3.204
HETATM 91 H 4.718 -5.104 2.365
HETATM 92 H 6.254 -4.700 1.609
HETATM 93 H 4.167 3.969 -5.682
HETATM 94 H 5.707 3.408 -6.332
HETATM 95 H 4.309 2.332 -6.357
HETATM 96 H 5.297 4.533 -3.427
HETATM 97 H 6.389 3.363 -2.679
HETATM 98 H 6.803 4.071 -4.237
HETATM 99 H -3.813 -5.020 -0.911
HETATM 100 H -5.344 -4.609 -0.146
HETATM 101 H -5.341 -5.373 -1.754
HETATM 102 H 5.691 0.544 -5.103
HETATM 103 H 7.042 1.681 -5.228
HETATM 104 H 6.615 0.993 -3.665
HETATM 105 H -1.672 4.028 -6.332
HETATM 106 H -1.720 2.388 -7.011
HETATM 107 H -3.056 3.505 -7.290
HETATM 108 H -3.230 4.654 -4.370
HETATM 109 H -4.548 4.229 -5.474
HETATM 110 H -4.491 3.528 -3.859
HETATM 111 H -3.398 0.653 -6.056
HETATM 112 H -4.600 1.166 -4.866
HETATM 113 H -4.642 1.834 -6.495
HETATM 114 H 5.582 1.006 6.423
HETATM 115 H 5.633 1.648 8.061
HETATM 116 H 4.373 0.491 7.604
HETATM 117 H 5.507 3.385 5.453
HETATM 118 H 4.261 4.521 5.982
HETATM 119 H 5.572 4.060 7.079
HETATM 120 H 2.719 2.233 8.586
HETATM 121 H 4.071 3.327 8.883
HETATM 122 H 2.694 3.884 7.934
HETATM 123 H 5.924 -3.241 -1.797
HETATM 124 H 6.649 -1.775 -2.530
HETATM 125 H 4.065 -3.136 -3.456
HETATM 126 H 5.638 -3.235 -4.283
HETATM 127 H 4.763 -1.688 -4.170
HETATM 128 H -5.375 3.387 4.270

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HETATM  130  H           -5.779   4.077   5.840
HETATM  131  H           -5.633   1.005   5.219
HETATM  132  H           -6.051   1.675   6.793
HETATM  133  H           -4.716   0.522   6.650
HETATM  134  H           -3.145   3.916   7.283
HETATM  135  H           -3.310   2.271   7.931
HETATM  136  H           -4.693   3.366   7.924
HETATM  137  H           -4.997  -3.208   3.285
HETATM  138  H           -5.704  -1.744   4.040
HETATM  139  H           -3.138  -3.153   4.945
HETATM  140  H           -4.712  -3.245   5.771
HETATM  141  H           -3.817  -1.708   5.682
HETATM   77  F            0.477  -0.990   0.761
CONECT    1   10   12   73
CONECT    2   35   48
CONECT    3   11   14   74
CONECT    4   13   28   75
CONECT    5   35
CONECT    6   18   19   76
CONECT    7   44   49
CONECT    8   47   64
CONECT    9   44
CONECT   10    1   20   31
CONECT   11    3   16   17
CONECT   12    1   15   39
CONECT   13    4   17   27
CONECT   14    3   20   23
CONECT   15   12   18   29
CONECT   16   11   22   23
CONECT   17   11   13   21
CONECT   18    6   15   38
CONECT   19    6   26   30
CONECT   20   10   14   24
CONECT   21   17   25   78
CONECT   22   16   25   79
CONECT   23   14   16   32
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CONECT   27   13   35   42
CONECT   28    4   30   42
CONECT   29   15   36   81
CONECT   30   19   28   40
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CONECT  39  12  31  44
CONECT  40  30  34  83
CONECT  41  26  34  84
CONECT  42  27  28  57
CONECT  43  36  38  85
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CONECT  47   8  31  37
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CONECT  51  45  93  94  95
CONECT  52  45  96  97  98
CONECT  53  48  99 100 101
CONECT  54  45 102 103 104
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CONECT  56  25  58  59  60
CONECT  57  42  69  72
CONECT  58  56 105 106 107
CONECT  59  56 108 109 110
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CONECT  64   8  65 123 124
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CONECT  71  70 139 140 141
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CONECT  74   3
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CONECT 78 21
CONECT 79 22
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CONECT 81 29
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CONECT 141 71
END

HEADER MMFF94 OPTIMIZED HOST:CHLORIDE COMPLEX

COMPND LOWEST ENERGY PYRROLE-BOUND FORM BY SAMPLING IN VACUO MD RUN

AUTHOR GENERATED BY PCMODEL V 9.30

HETATM	1	N	0.082	2.064	-2.428
HETATM	2	O	-1.629	-1.920	4.071
HETATM	3	N	-2.265	1.632	-0.124
HETATM	4	N	-0.356	2.041	2.482
HETATM	5	O	-3.106	-0.356	4.856
HETATM	6	N	1.993	1.646	0.174
HETATM	7	O	1.382	-1.874	-4.053
HETATM	8	O	-2.507	-0.937	-3.846
HETATM	9	O	2.848	-0.293	-4.823
HETATM	10	C	-1.017	1.388	-2.924
HETATM	11	C	-3.094	1.865	0.946
HETATM	12	C	1.254	1.431	-2.800
HETATM	13	C	-1.524	1.396	2.849
HETATM	14	C	-2.891	1.869	-1.322
HETATM	15	C	2.558	1.839	-2.271
HETATM	16	C	-4.328	2.224	0.414
HETATM	17	C	-2.831	1.800	2.323
HETATM	18	C	2.820	1.894	-0.894
HETATM	19	C	2.617	1.877	1.374
HETATM	20	C	-2.389	1.808	-2.629
HETATM	21	C	-3.905	2.116	3.172
HETATM	22	C	-5.382	2.522	1.306
HETATM	23	C	-4.200	2.227	-1.018
HETATM	24	C	-3.293	2.131	-3.658
HETATM	25	C	-5.187	2.472	2.700
HETATM	26	C	3.923	2.247	1.073
HETATM	27	C	-1.163	0.332	3.670
HETATM	28	C	0.747	1.368	2.972
HETATM	29	C	3.630	2.171	-3.118
HETATM	30	C	2.116	1.800	2.680
HETATM	31	C	-0.537	0.341	-3.706
HETATM	32	C	-5.078	2.531	-2.084
HETATM	33	C	-4.636	2.488	-3.422
HETATM	34	C	4.358	2.489	3.480
HETATM	35	C	-2.070	-0.641	4.265
HETATM	36	C	4.909	2.531	-2.643
HETATM	37	O	-0.968	-1.104	-5.529
HETATM	38	C	4.051	2.257	-0.358
HETATM	39	C	0.900	0.372	-3.632

HETATM 40 C 3.018 2.120 3.713
HETATM 41 C 4.800 2.547 2.142
HETATM 42 C 0.274 0.311 3.745
HETATM 43 C 5.104 2.571 -1.248
HETATM 44 C 1.814 -0.590 -4.235
HETATM 45 C -5.558 2.827 -4.606
HETATM 46 C 5.278 2.824 4.667
HETATM 47 C -1.332 -0.622 -4.461
HETATM 48 C -2.457 -2.922 4.666
HETATM 49 C 2.217 -2.864 -4.656
HETATM 50 C 1.584 -4.221 -4.420
HETATM 51 C -7.003 3.187 -4.190
HETATM 52 C -4.990 4.039 -5.376
HETATM 53 C -1.814 -4.272 4.418
HETATM 54 C -5.649 1.615 -5.559
HETATM 55 C 6.027 2.874 -3.643
HETATM 56 C -6.307 2.798 3.704
HETATM 57 C 1.076 -0.653 4.491
HETATM 58 C -6.557 1.579 4.619
HETATM 59 C -7.657 3.151 3.039
HETATM 60 C -5.894 4.008 4.569
HETATM 61 C 7.374 3.230 -2.975
HETATM 62 C 6.285 1.665 -4.569
HETATM 63 C 5.606 4.089 -4.498
HETATM 64 C -3.336 -1.852 -4.564
HETATM 65 C -4.584 -2.100 -3.739
HETATM 66 C 6.720 3.197 4.254
HETATM 67 C 4.700 4.025 5.447
HETATM 68 C 5.377 1.605 5.609
HETATM 69 O 2.253 -0.955 3.874
HETATM 70 C 3.089 -1.870 4.583
HETATM 71 C 4.338 -2.100 3.756
HETATM 72 O 0.716 -1.147 5.555
HETATM 73 H 0.032 2.888 -1.820
HETATM 74 H -1.278 1.453 -0.037
HETATM 75 H -0.313 2.871 1.881
HETATM 76 H 1.007 1.461 0.086
HETATM 78 H -3.723 2.082 4.246
HETATM 79 H -6.335 2.807 0.875
HETATM 80 H -2.919 2.103 -4.680
HETATM 81 H 3.448 2.145 -4.191
HETATM 82 H -6.091 2.816 -1.826
HETATM 83 H 2.643 2.080 4.734
HETATM 84 H 5.810 2.841 1.887

HETATM 85 H 6.054 2.858 -0.814
HETATM 86 H -3.453 -2.897 4.210
HETATM 87 H -2.540 -2.746 5.744
HETATM 88 H 2.300 -2.678 -5.733
HETATM 89 H 3.213 -2.836 -4.200
HETATM 90 H 1.478 -4.416 -3.347
HETATM 91 H 0.578 -4.257 -4.851
HETATM 92 H 2.188 -5.017 -4.865
HETATM 93 H -7.029 4.071 -3.542
HETATM 94 H -7.622 3.413 -5.067
HETATM 95 H -7.488 2.359 -3.659
HETATM 96 H -4.884 4.909 -4.718
HETATM 97 H -4.005 3.831 -5.808
HETATM 98 H -5.649 4.325 -6.204
HETATM 99 H -0.808 -4.305 4.848
HETATM 100 H -2.413 -5.076 4.856
HETATM 101 H -1.707 -4.456 3.344
HETATM 102 H -6.031 0.731 -5.037
HETATM 103 H -6.323 1.823 -6.400
HETATM 104 H -4.676 1.349 -5.988
HETATM 105 H -6.817 0.691 4.031
HETATM 106 H -5.680 1.327 5.225
HETATM 107 H -7.382 1.771 5.316
HETATM 108 H -8.033 2.324 2.425
HETATM 109 H -8.424 3.367 3.793
HETATM 110 H -7.574 4.039 2.402
HETATM 111 H -5.000 3.804 5.167
HETATM 112 H -5.681 4.884 3.945
HETATM 113 H -6.692 4.283 5.269
HETATM 114 H 7.285 4.112 -2.330
HETATM 115 H 7.756 2.400 -2.369
HETATM 116 H 8.140 3.459 -3.727
HETATM 117 H 7.109 1.869 -5.264
HETATM 118 H 6.551 0.774 -3.989
HETATM 119 H 5.410 1.413 -5.178
HETATM 120 H 5.386 4.958 -3.866
HETATM 121 H 6.400 4.376 -5.195
HETATM 122 H 4.712 3.884 -5.098
HETATM 123 H -2.802 -2.796 -4.720
HETATM 124 H -3.612 -1.419 -5.532
HETATM 125 H -4.323 -2.524 -2.764
HETATM 126 H -5.262 -2.786 -4.253
HETATM 127 H -5.111 -1.160 -3.544
HETATM 128 H 6.740 4.087 3.614

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HETATM  131  H            4.589   4.900   4.797
HETATM  132  H            5.358   4.308   6.278
HETATM  133  H            3.718   3.806   5.877
HETATM  134  H            6.049   1.809   6.451
HETATM  135  H            5.765   0.727   5.079
HETATM  136  H            4.407   1.328   6.036
HETATM  137  H            3.362  -1.444   5.555
HETATM  138  H            2.562  -2.819   4.730
HETATM  139  H            5.021  -2.788   4.264
HETATM  140  H            4.080  -2.519   2.777
HETATM  141  H            4.859  -1.156   3.570
HETATM   77 Cl           -0.145   4.285   0.037
CONECT    1   10   12   73
CONECT    2   35   48
CONECT    3   11   14   74
CONECT    4   13   28   75
CONECT    5   35
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CONECT    7   44   49
CONECT    8   47   64
CONECT    9   44
CONECT   10    1   20   31
CONECT   11    3   16   17
CONECT   12    1   15   39
CONECT   13    4   17   27
CONECT   14    3   20   23
CONECT   15   12   18   29
CONECT   16   11   22   23
CONECT   17   11   13   21
CONECT   18    6   15   38
CONECT   19    6   26   30
CONECT   20   10   14   24
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CONECT   30   19   28   40
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CONECT  135   68
CONECT  136   68
CONECT  137   70
CONECT  138   70
CONECT  139   71
CONECT  140   71
CONECT  141   71
END
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HEADER MMFF94 OPTIMIZED HOST:CHLORIDE COMPLEX

COMPND LOWEST ENERGY CARBAZOLE-BOUND FORM BY SAMPLING IN VACUO MD RUN

AUTHOR GENERATED BY PCMODEL V 9.30

HETATM	1	Cl	0.028	-2.350	0.000
HETATM	2	O	-4.604	-3.232	-0.477
HETATM	3	N	-0.324	0.076	-2.165
HETATM	4	N	-2.379	0.538	0.326
HETATM	5	O	-5.391	-1.625	-1.903
HETATM	6	N	0.323	0.075	2.165
HETATM	7	O	4.649	-3.168	0.469
HETATM	8	O	3.537	-2.138	-3.296
HETATM	9	O	5.413	-1.555	1.900
HETATM	10	C	2.709	-0.004	-1.524
HETATM	11	C	-1.540	0.526	-2.641
HETATM	12	C	3.069	0.022	0.723
HETATM	13	C	-3.070	-0.019	-0.723
HETATM	14	C	0.713	0.541	-2.949
HETATM	15	C	2.823	0.477	2.090
HETATM	16	C	-1.289	1.089	-3.889
HETATM	17	C	-2.830	0.443	-2.089
HETATM	18	C	1.532	0.541	2.642
HETATM	19	C	-0.721	0.523	2.951
HETATM	20	C	2.103	0.471	-2.766
HETATM	21	C	-3.886	0.915	-2.888
HETATM	22	C	-2.383	1.545	-4.661
HETATM	23	C	0.131	1.097	-4.084
HETATM	24	C	2.905	0.951	-3.819
HETATM	25	C	-3.700	1.452	-4.178
HETATM	26	C	-0.147	1.085	4.086
HETATM	27	C	-3.860	-1.031	-0.187
HETATM	28	C	-2.709	-0.045	1.524
HETATM	29	C	3.873	0.962	2.891
HETATM	30	C	-2.110	0.435	2.767
HETATM	31	C	3.657	-0.983	-1.246
HETATM	32	C	0.974	1.562	-5.121
HETATM	33	C	2.375	1.483	-5.010
HETATM	34	C	-2.395	1.437	5.014
HETATM	35	C	-4.692	-1.955	-0.949
HETATM	36	C	3.680	1.493	4.181
HETATM	37	O	5.466	-2.263	-2.076
HETATM	38	C	1.273	1.098	3.892
HETATM	39	C	3.874	-0.978	0.185

HETATM 40 C -2.918 0.900 3.822
HETATM 41 C -0.995 1.535 5.125
HETATM 42 C -3.643 -1.037 1.244
HETATM 43 C 2.361 1.566 4.665
HETATM 44 C 4.719 -1.891 0.944
HETATM 45 C 3.321 1.964 -6.124
HETATM 46 C -3.348 1.903 6.128
HETATM 47 C 4.315 -1.856 -2.213
HETATM 48 C -5.377 -4.188 -1.200
HETATM 49 C 5.435 -4.116 1.191
HETATM 50 C 5.258 -5.472 0.535
HETATM 51 C 4.217 3.102 -5.589
HETATM 52 C 4.212 0.792 -6.591
HETATM 53 C -5.181 -5.543 -0.548
HETATM 54 C 2.591 2.506 -7.373
HETATM 55 C 4.890 1.978 5.000
HETATM 56 C -4.918 1.921 -4.994
HETATM 57 C -4.289 -1.921 2.208
HETATM 58 C -4.558 2.457 -6.400
HETATM 59 C -5.638 3.061 -4.242
HETATM 60 C -5.897 0.744 -5.194
HETATM 61 C 5.886 0.814 5.196
HETATM 62 C 5.595 3.129 4.250
HETATM 63 C 4.523 2.504 6.405
HETATM 64 C 4.131 -3.013 -4.253
HETATM 65 C 3.125 -3.244 -5.365
HETATM 66 C -4.260 3.029 5.596
HETATM 67 C -4.223 0.717 6.593
HETATM 68 C -2.626 2.452 7.380
HETATM 69 O -3.507 -2.195 3.291
HETATM 70 C -4.088 -3.081 4.246
HETATM 71 C -3.080 -3.300 5.357
HETATM 72 O -5.434 -2.344 2.071
HETATM 73 N 2.371 0.572 -0.325
HETATM 74 H -0.210 -0.556 -1.368
HETATM 75 H -1.702 1.280 0.225
HETATM 76 H 0.217 -0.557 1.367
HETATM 77 H -4.892 0.858 -2.474
HETATM 78 H -2.163 1.969 -5.634
HETATM 79 H 3.985 0.904 -3.688
HETATM 80 H 4.880 0.920 2.476
HETATM 81 H 0.496 1.981 -6.000
HETATM 82 H -3.997 0.840 3.690
HETATM 83 H -0.523 1.959 6.004

HETATM 84 H 2.136 1.985 5.639
HETATM 85 H -5.039 -4.227 -2.242
HETATM 86 H -6.437 -3.913 -1.166
HETATM 87 H 6.491 -3.826 1.157
HETATM 88 H 5.098 -4.162 2.232
HETATM 89 H 5.844 -6.235 1.053
HETATM 90 H 4.204 -5.769 0.542
HETATM 91 H 5.571 -5.436 -0.514
HETATM 92 H 4.860 2.772 -4.766
HETATM 93 H 4.877 3.488 -6.375
HETATM 94 H 3.613 3.939 -5.219
HETATM 95 H 4.849 0.407 -5.787
HETATM 96 H 3.603 -0.044 -6.956
HETATM 97 H 4.877 1.100 -7.406
HETATM 98 H -4.123 -5.825 -0.557
HETATM 99 H -5.494 -5.514 0.500
HETATM 100 H -5.757 -6.314 -1.068
HETATM 101 H 1.967 3.375 -7.132
HETATM 102 H 3.306 2.828 -8.140
HETATM 103 H 1.951 1.742 -7.830
HETATM 104 H -3.898 3.330 -6.341
HETATM 105 H -4.060 1.691 -7.006
HETATM 106 H -5.456 2.768 -6.945
HETATM 107 H -4.961 3.903 -4.058
HETATM 108 H -6.490 3.438 -4.819
HETATM 109 H -6.029 2.735 -3.271
HETATM 110 H -5.405 -0.098 -5.695
HETATM 111 H -6.300 0.373 -4.246
HETATM 112 H -6.754 1.044 -5.809
HETATM 113 H 6.294 0.450 4.247
HETATM 114 H 6.739 1.124 5.812
HETATM 115 H 5.406 -0.036 5.695
HETATM 116 H 5.990 2.811 3.278
HETATM 117 H 4.906 3.962 4.068
HETATM 118 H 6.442 3.517 4.828
HETATM 119 H 4.036 1.731 7.010
HETATM 120 H 5.417 2.827 6.952
HETATM 121 H 3.851 3.369 6.350
HETATM 122 H 4.385 -3.968 -3.779
HETATM 123 H 5.036 -2.552 -4.665
HETATM 124 H 2.208 -3.691 -4.967
HETATM 125 H 3.537 -3.905 -6.132
HETATM 126 H 2.840 -2.295 -5.830
HETATM 127 H -4.900 2.692 4.772

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HETATM  128  H           -3.668   3.875   5.229
HETATM  129  H           -4.925   3.404   6.383
HETATM  130  H           -4.854   0.325   5.788
HETATM  131  H           -4.892   1.015   7.408
HETATM  132  H           -3.602  -0.111   6.956
HETATM  133  H           -2.014   3.329   7.140
HETATM  134  H           -1.975   1.695   7.834
HETATM  135  H           -3.345   2.761   8.147
HETATM  136  H           -4.329  -4.038   3.770
HETATM  137  H           -5.000  -2.634   4.659
HETATM  138  H           -2.156  -3.733   4.958
HETATM  139  H           -3.482  -3.969   6.123
HETATM  140  H           -2.808  -2.349   5.824
HETATM  141  H            1.684   1.304  -0.222
CONECT    2   35   48
CONECT    3   11   14   74
CONECT    4   13   28   75
CONECT    5   35
CONECT    6   18   19   76
CONECT    7   44   49
CONECT    8   47   64
CONECT    9   44
CONECT   10   20   31   73
CONECT   11    3   16   17
CONECT   12   15   39   73
CONECT   13    4   17   27
CONECT   14    3   20   23
CONECT   15   12   18   29
CONECT   16   11   22   23
CONECT   17   11   13   21
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CONECT   19    6   26   30
CONECT   20   10   14   24
CONECT   21   17   25   77
CONECT   22   16   25   78
CONECT   23   14   16   32
CONECT   24   20   33   79
CONECT   25   21   22   56
CONECT   26   19   38   41
CONECT   27   13   35   42
CONECT   28    4   30   42
CONECT   29   15   36   80
CONECT   30   19   28   40
CONECT   31   10   39   47
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CONECT  123   64
CONECT  124   65
CONECT  125   65
CONECT  126   65
CONECT  127   66
CONECT  128   66
CONECT  129   66
CONECT  130   67
CONECT  131   67
CONECT  132   67
CONECT  133   68
CONECT  134   68
CONECT  135   68
CONECT  136   70
CONECT  137   70
CONECT  138   71
CONECT  139   71
CONECT  140   71
CONECT  141   73
END
```

HEADER MMFF94 OPTIMIZED HOST:HYDROGEN SULFATE COMPLEX

COMPND LOWEST ENERGY PYRROLE-BOUND FORM BY SAMPLING IN VACUO MD RUN

AUTHOR GENERATED BY PCMODEL V 9.30

HETATM 1 S 0.187 4.572 0.365
HETATM 2 O 0.093 3.402 -0.500
HETATM 3 O -0.535 5.751 -0.070
HETATM 4 O 1.732 4.982 0.237
HETATM 5 O 0.096 4.235 1.779
HETATM 6 H 2.196 4.396 0.865
HETATM 7 O 1.687 -2.243 -4.083
HETATM 8 O -2.220 -1.400 -3.914
HETATM 9 O 3.165 -0.630 -4.755
HETATM 10 C -0.803 0.965 -2.988
HETATM 11 C -2.853 1.431 0.886
HETATM 12 C 1.464 1.065 -2.822
HETATM 13 C -1.295 0.854 2.743
HETATM 14 C -2.663 1.460 -1.380
HETATM 15 C 2.736 1.543 -2.275
HETATM 16 C -4.096 1.774 0.368
HETATM 17 C -2.600 1.295 2.256
HETATM 18 C 2.973 1.639 -0.893
HETATM 19 C 2.767 1.608 1.376
HETATM 20 C -2.180 1.366 -2.693
HETATM 21 C -3.673 1.544 3.125
HETATM 22 C -5.154 2.016 1.274
HETATM 23 C -3.976 1.792 -1.065
HETATM 24 C -3.102 1.648 -3.717
HETATM 25 C -4.957 1.908 2.668
HETATM 26 C 4.040 2.080 1.076
HETATM 27 C -0.896 -0.317 3.382
HETATM 28 C 0.956 0.948 2.969
HETATM 29 C 3.792 1.938 -3.115
HETATM 30 C 2.291 1.468 2.689
HETATM 31 C -0.284 -0.075 -3.753
HETATM 32 C -4.871 2.061 -2.126
HETATM 33 C -4.446 1.997 -3.469
HETATM 34 C 4.472 2.316 3.484
HETATM 35 C -1.758 -1.414 3.811
HETATM 36 C 5.033 2.400 -2.633
HETATM 37 O -0.653 -1.538 -5.575
HETATM 38 C 4.171 2.097 -0.354
HETATM 39 C 1.154 -0.010 -3.649

HETATM 40 C 3.170 1.830 3.721
HETATM 41 C 4.894 2.437 2.145
HETATM 42 C 0.537 -0.255 3.525
HETATM 43 C 5.207 2.476 -1.237
HETATM 44 C 2.108 -0.950 -4.225
HETATM 45 C -5.388 2.300 -4.648
HETATM 46 C 5.376 2.690 4.672
HETATM 47 C -1.044 -1.060 -4.514
HETATM 48 C -3.742 -2.617 3.409
HETATM 49 C 2.562 -3.212 -4.663
HETATM 50 C 1.936 -4.581 -4.479
HETATM 51 C -4.839 3.494 -5.458
HETATM 52 C -5.485 1.062 -5.567
HETATM 53 C -4.885 -2.660 2.413
HETATM 54 C -6.828 2.662 -4.219
HETATM 55 C 6.135 2.809 -3.626
HETATM 56 C -6.083 2.173 3.682
HETATM 57 C 1.413 -1.290 4.058
HETATM 58 C -6.335 0.900 4.521
HETATM 59 C -7.430 2.565 3.033
HETATM 60 C -5.677 3.329 4.621
HETATM 61 C 7.444 3.276 -2.949
HETATM 62 C 6.495 1.608 -4.528
HETATM 63 C 5.635 3.975 -4.506
HETATM 64 C -3.014 -2.341 -4.636
HETATM 65 C -4.260 -2.626 -3.820
HETATM 66 C 5.595 1.451 5.568
HETATM 67 C 6.772 3.205 4.257
HETATM 68 C 4.707 3.806 5.503
HETATM 69 O 1.048 -2.532 3.624
HETATM 70 C 1.854 -3.594 4.140
HETATM 71 C 1.297 -4.904 3.617
HETATM 72 O 2.374 -1.072 4.786
HETATM 73 N 0.271 1.672 -2.491
HETATM 74 O -2.849 -1.576 3.010
HETATM 75 N -2.012 1.275 -0.186
HETATM 76 N -0.176 1.647 2.613
HETATM 77 O -1.516 -2.117 4.787
HETATM 78 N 2.156 1.343 0.173
HETATM 79 H -3.487 1.451 4.194
HETATM 80 H -6.114 2.294 0.855
HETATM 81 H -2.742 1.600 -4.743
HETATM 82 H 3.625 1.882 -4.190
HETATM 83 H -5.888 2.329 -1.863

HETATM 84 H 2.814 1.719 4.744
HETATM 85 H 5.881 2.807 1.892
HETATM 86 H 6.131 2.834 -0.800
HETATM 87 H -4.132 -2.406 4.411
HETATM 88 H -3.216 -3.578 3.411
HETATM 89 H 2.691 -3.007 -5.732
HETATM 90 H 3.535 -3.179 -4.160
HETATM 91 H 0.952 -4.621 -4.957
HETATM 92 H 2.571 -5.361 -4.909
HETATM 93 H 1.783 -4.795 -3.416
HETATM 94 H -3.860 3.280 -5.900
HETATM 95 H -5.513 3.754 -6.283
HETATM 96 H -4.728 4.382 -4.825
HETATM 97 H -4.518 0.790 -6.002
HETATM 98 H -5.856 0.190 -5.016
HETATM 99 H -6.172 1.244 -6.402
HETATM 100 H -5.402 -1.695 2.377
HETATM 101 H -4.508 -2.855 1.403
HETATM 102 H -5.605 -3.438 2.678
HETATM 103 H -6.849 3.561 -3.592
HETATM 104 H -7.461 2.865 -5.092
HETATM 105 H -7.302 1.845 -3.663
HETATM 106 H -6.606 0.054 3.881
HETATM 107 H -5.455 0.605 5.102
HETATM 108 H -7.154 1.054 5.234
HETATM 109 H -7.806 1.773 2.375
HETATM 110 H -8.200 2.742 3.795
HETATM 111 H -7.342 3.486 2.445
HETATM 112 H -4.787 3.090 5.213
HETATM 113 H -5.458 4.241 4.052
HETATM 114 H -6.479 3.563 5.331
HETATM 115 H 7.880 2.487 -2.325
HETATM 116 H 8.200 3.550 -3.696
HETATM 117 H 7.280 4.159 -2.320
HETATM 118 H 6.820 0.749 -3.930
HETATM 119 H 5.648 1.280 -5.141
HETATM 120 H 7.308 1.861 -5.218
HETATM 121 H 5.343 4.835 -3.892
HETATM 122 H 6.415 4.309 -5.200
HETATM 123 H 4.767 3.694 -5.112
HETATM 124 H -2.451 -3.268 -4.787
HETATM 125 H -3.297 -1.918 -5.607
HETATM 126 H -3.992 -3.042 -2.842
HETATM 127 H -4.913 -3.334 -4.337

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HETATM  129  H            6.040   0.627   4.998
HETATM  130  H            4.660   1.082   6.003
HETATM  131  H            6.268   1.681   6.402
HETATM  132  H            7.329   2.450   3.689
HETATM  133  H            7.378   3.458   5.136
HETATM  134  H            6.702   4.112   3.644
HETATM  135  H            3.753   3.486   5.937
HETATM  136  H            4.508   4.691   4.887
HETATM  137  H            5.348   4.117   6.336
HETATM  138  H            1.820  -3.590   5.235
HETATM  139  H            2.889  -3.470   3.800
HETATM  140  H            0.255  -5.031   3.929
HETATM  141  H            1.882  -5.751   3.986
HETATM  142  H            1.306  -4.917   2.522
HETATM  143  H            0.190   2.496  -1.887
HETATM  144  H           -1.021   1.114  -0.107
HETATM  145  H           -0.177   2.603   2.250
HETATM  146  H            1.200   1.043   0.080
CONECT    1    2    3    4    5
CONECT    2    1
CONECT    3    1
CONECT    4    1    6
CONECT    5    1
CONECT    6    4
CONECT    7   44   49
CONECT    8   47   64
CONECT    9   44
CONECT   10   20   31   73
CONECT   11   16   17   75
CONECT   12   15   39   73
CONECT   13   17   27   76
CONECT   14   20   23   75
CONECT   15   12   18   29
CONECT   16   11   22   23
CONECT   17   11   13   21
CONECT   18   15   38   78
CONECT   19   26   30   78
CONECT   20   10   14   24
CONECT   21   17   25   79
CONECT   22   16   25   80
CONECT   23   14   16   32
CONECT   24   20   33   81
CONECT   25   21   22   56
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CONECT  28  30  42  76
CONECT  29  15  36  82
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CONECT  32  23  33  83
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CONECT  35  27  74  77
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CONECT  37  47
CONECT  38  18  26  43
CONECT  39  12  31  44
CONECT  40  30  34  84
CONECT  41  26  34  85
CONECT  42  27  28  57
CONECT  43  36  38  86
CONECT  44   7   9  39
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CONECT  46  34  66  67  68
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CONECT  68  46 135 136 137
CONECT  69  57  70
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CONECT 71 70 140 141 142
CONECT 72 57
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CONECT 75 11 14 144
CONECT 76 13 28 145
CONECT 77 35
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CONECT 104 54
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CONECT 106 58
CONECT 107 58
CONECT 108 58
CONECT 109 59
CONECT 110 59
CONECT 111 59
CONECT 112 60
CONECT 113 60

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CONECT  114   60
CONECT  115   61
CONECT  116   61
CONECT  117   61
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CONECT  119   62
CONECT  120   62
CONECT  121   63
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CONECT  131   66
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CONECT  133   67
CONECT  134   67
CONECT  135   68
CONECT  136   68
CONECT  137   68
CONECT  138   70
CONECT  139   70
CONECT  140   71
CONECT  141   71
CONECT  142   71
CONECT  143   73
CONECT  144   75
CONECT  145   76
CONECT  146   78
END
```

HEADER MMFF94 OPTIMIZED HOST:HYDROGEN SULFATE COMPLEX

COMPND LOWEST ENERGY CARBAZOLE-BOUND FORM BY SAMPLING IN VACUO MD RUN

AUTHOR GENERATED BY PCMODEL V 9.30

HETATM 1 O 1.040 -4.129 -1.714
HETATM 2 S 0.414 -4.036 -0.244
HETATM 3 O 1.508 -4.571 0.548
HETATM 4 O -0.775 -4.865 -0.325
HETATM 5 O 0.171 -2.604 -0.080
HETATM 6 H 1.945 -4.468 -1.546
HETATM 7 N -0.053 -0.902 -2.233
HETATM 8 O -4.381 -2.991 -2.409
HETATM 9 O -4.041 -3.829 2.465
HETATM 10 O -5.549 -3.514 -0.521
HETATM 11 C -2.643 -0.976 1.364
HETATM 12 C 1.582 -0.538 2.600
HETATM 13 C -2.859 -1.056 -0.902
HETATM 14 C 3.144 -1.123 0.729
HETATM 15 C -0.678 -0.475 2.845
HETATM 16 C -2.566 -0.600 -2.265
HETATM 17 C 1.312 -0.008 3.857
HETATM 18 C 2.882 -0.661 2.090
HETATM 19 C -1.258 -0.500 -2.770
HETATM 20 C 1.006 -0.479 -3.010
HETATM 21 C -2.065 -0.522 2.627
HETATM 22 C 3.934 -0.253 2.930
HETATM 23 C 2.398 0.386 4.674
HETATM 24 C -0.113 0.030 4.013
HETATM 25 C -2.882 -0.067 3.679
HETATM 26 C 3.727 0.261 4.225
HETATM 27 C 0.456 0.049 -4.173
HETATM 28 C 3.871 -2.192 0.212
HETATM 29 C 2.948 -1.037 -1.532
HETATM 30 C -3.603 -0.142 -3.105
HETATM 31 C 2.391 -0.561 -2.793
HETATM 32 C -3.655 -1.879 1.070
HETATM 33 C -0.972 0.473 5.045
HETATM 34 C -2.371 0.421 4.898
HETATM 35 C 2.726 0.390 -5.051
HETATM 36 C 4.582 -3.232 0.953
HETATM 37 C -3.378 0.375 -4.392
HETATM 38 O -5.452 -2.071 2.561
HETATM 39 C -0.970 0.041 -4.019

HETATM 40 C -3.760 -1.976 -0.367
HETATM 41 C 3.223 -0.125 -3.837
HETATM 42 C 1.328 0.483 -5.198
HETATM 43 C 3.772 -2.111 -1.226
HETATM 44 C -2.041 0.471 -4.832
HETATM 45 C -4.651 -2.890 -1.078
HETATM 46 C -3.337 0.881 6.004
HETATM 47 C 3.705 0.830 -6.154
HETATM 48 C -4.455 -2.589 2.063
HETATM 49 C 4.748 -4.433 2.966
HETATM 50 C -5.166 -3.957 -3.109
HETATM 51 C -4.729 -3.955 -4.561
HETATM 52 C -4.195 2.056 5.488
HETATM 53 C -4.264 -0.288 6.405
HETATM 54 C 4.108 -4.473 4.340
HETATM 55 C -2.629 1.361 7.291
HETATM 56 C -4.522 0.852 -5.304
HETATM 57 C 4.933 0.670 5.089
HETATM 58 C 4.328 -3.041 -2.194
HETATM 59 C 5.847 -0.553 5.317
HETATM 60 C 4.547 1.216 6.483
HETATM 61 C 5.735 1.778 4.373
HETATM 62 C -5.933 0.586 -4.731
HETATM 63 C -4.394 2.373 -5.529
HETATM 64 C -4.448 0.130 -6.668
HETATM 65 C -2.878 -4.442 1.878
HETATM 66 C -2.630 -5.752 2.600
HETATM 67 C 3.011 1.354 -7.432
HETATM 68 C 4.606 1.967 -5.625
HETATM 69 C 4.588 -0.365 -6.574
HETATM 70 O 3.870 -4.311 -1.985
HETATM 71 C 4.420 -5.284 -2.876
HETATM 72 C 3.873 -6.643 -2.483
HETATM 73 O 5.089 -2.711 -3.096
HETATM 74 N -2.192 -0.493 0.162
HETATM 75 O 4.209 -3.316 2.260
HETATM 76 N 0.370 -0.916 2.063
HETATM 77 N 2.603 -0.451 -0.341
HETATM 78 O 5.444 -3.941 0.442
HETATM 79 H 0.040 -1.465 -1.387
HETATM 80 H 4.948 -0.345 2.544
HETATM 81 H 2.164 0.788 5.653
HETATM 82 H -3.961 -0.090 3.528
HETATM 83 H -4.614 -0.198 -2.709

HETATM 84 H -0.510 0.854 5.948
HETATM 85 H 4.300 -0.194 -3.685
HETATM 86 H 0.877 0.883 -6.100
HETATM 87 H -1.807 0.889 -5.806
HETATM 88 H 5.833 -4.314 3.066
HETATM 89 H 4.527 -5.363 2.430
HETATM 90 H -6.227 -3.692 -3.043
HETATM 91 H -5.005 -4.951 -2.676
HETATM 92 H -3.662 -4.189 -4.643
HETATM 93 H -4.871 -2.964 -5.003
HETATM 94 H -5.298 -4.686 -5.141
HETATM 95 H -4.821 1.770 4.635
HETATM 96 H -3.564 2.893 5.166
HETATM 97 H -4.868 2.427 6.269
HETATM 98 H -4.896 -0.622 5.575
HETATM 99 H -4.936 0.003 7.221
HETATM 100 H -3.683 -1.154 6.744
HETATM 101 H 4.300 -3.542 4.883
HETATM 102 H 4.493 -5.311 4.927
HETATM 103 H 3.020 -4.571 4.254
HETATM 104 H -1.983 2.225 7.098
HETATM 105 H -2.016 0.568 7.734
HETATM 106 H -3.358 1.669 8.051
HETATM 107 H 5.300 -1.366 5.811
HETATM 108 H 6.703 -0.294 5.951
HETATM 109 H 6.252 -0.951 4.380
HETATM 110 H 3.998 0.470 7.070
HETATM 111 H 3.925 2.115 6.406
HETATM 112 H 5.438 1.489 7.061
HETATM 113 H 6.150 1.439 3.418
HETATM 114 H 6.579 2.115 4.986
HETATM 115 H 5.104 2.651 4.166
HETATM 116 H -6.712 0.917 -5.429
HETATM 117 H -6.097 1.126 -3.792
HETATM 118 H -6.097 -0.482 -4.545
HETATM 119 H -4.425 2.917 -4.577
HETATM 120 H -5.210 2.751 -6.156
HETATM 121 H -3.455 2.638 -6.028
HETATM 122 H -4.489 -0.958 -6.542
HETATM 123 H -3.528 0.364 -7.215
HETATM 124 H -5.284 0.422 -7.316
HETATM 125 H -3.078 -4.642 0.822
HETATM 126 H -2.007 -3.792 1.998
HETATM 127 H -2.467 -5.577 3.670

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HETATM  128  H           -3.500  -6.411   2.516
HETATM  129  H           -1.756  -6.266   2.191
HETATM  130  H            2.394   2.236  -7.224
HETATM  131  H            3.748   1.649  -8.189
HETATM  132  H            2.371   0.589  -7.886
HETATM  133  H            4.006   2.822  -5.290
HETATM  134  H            5.224   1.647  -4.779
HETATM  135  H            5.290   2.324  -6.404
HETATM  136  H            3.975  -1.205  -6.923
HETATM  137  H            5.268  -0.088  -7.387
HETATM  138  H            5.209  -0.733  -5.750
HETATM  139  H            4.126  -5.050  -3.905
HETATM  140  H            5.512  -5.289  -2.795
HETATM  141  H            4.132  -6.877  -1.446
HETATM  142  H            2.780  -6.652  -2.548
HETATM  143  H            4.271  -7.427  -3.134
HETATM  144  H           -1.467   0.203   0.068
HETATM  145  H            0.268  -1.470   1.212
HETATM  146  H            1.995   0.352  -0.257
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CONECT    3    2
CONECT    4    2
CONECT    5    2
CONECT    6    1
CONECT    7   19   20   79
CONECT    8   45   50
CONECT    9   48   65
CONECT   10   45
CONECT   11   21   32   74
CONECT   12   17   18   76
CONECT   13   16   40   74
CONECT   14   18   28   77
CONECT   15   21   24   76
CONECT   16   13   19   30
CONECT   17   12   23   24
CONECT   18   12   14   22
CONECT   19    7   16   39
CONECT   20    7   27   31
CONECT   21   11   15   25
CONECT   22   18   26   80
CONECT   23   17   26   81
CONECT   24   15   17   33
CONECT   25   21   34   82
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CONECT 28 14 36 43
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CONECT 32 11 40 48
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CONECT 62 56 116 117 118
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CONECT 64 56 122 123 124
CONECT 65 9 66 125 126
CONECT 66 65 127 128 129
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CONECT 68 47 133 134 135
CONECT 69 47 136 137 138

CONECT 70 58 71
CONECT 71 70 72 139 140
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CONECT 75 36 49
CONECT 76 12 15 145
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CONECT 97 52
CONECT 98 53
CONECT 99 53
CONECT 100 53
CONECT 101 54
CONECT 102 54
CONECT 103 54
CONECT 104 55
CONECT 105 55
CONECT 106 55
CONECT 107 59
CONECT 108 59
CONECT 109 59
CONECT 110 60
CONECT 111 60
CONECT 112 60
CONECT 113 61

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CONECT  114   61
CONECT  115   61
CONECT  116   62
CONECT  117   62
CONECT  118   62
CONECT  119   63
CONECT  120   63
CONECT  121   63
CONECT  122   64
CONECT  123   64
CONECT  124   64
CONECT  125   65
CONECT  126   65
CONECT  127   66
CONECT  128   66
CONECT  129   66
CONECT  130   67
CONECT  131   67
CONECT  132   67
CONECT  133   68
CONECT  134   68
CONECT  135   68
CONECT  136   69
CONECT  137   69
CONECT  138   69
CONECT  139   71
CONECT  140   71
CONECT  141   72
CONECT  142   72
CONECT  143   72
CONECT  144   74
CONECT  145   76
CONECT  146   77
END
```

HEADER MMFF94 OPTIMIZED CALIX[4]PYRROLE:CHLORIDE COMPLEX

COMPND LOWEST ENERGY COMPLEX BY SAMPLING IN VACUO MD RUN

AUTHOR GENERATED BY PCMODEL V 9.30

HETATM 1 Cl 0.000 0.000 2.529
HETATM 2 N 2.391 0.000 0.187
HETATM 4 N 0.000 2.437 0.170
HETATM 6 N -2.391 0.000 0.188
HETATM 8 N 0.000 -2.437 0.170
HETATM 10 C 2.758 -1.139 -0.511
HETATM 11 C 3.269 -0.705 -1.721
HETATM 13 C 3.269 0.704 -1.721
HETATM 15 C 2.758 1.139 -0.511
HETATM 16 C 3.605 3.497 -0.617
HETATM 20 C 2.541 2.556 0.015
HETATM 21 C 2.787 2.648 1.538
HETATM 25 C 1.139 3.045 -0.329
HETATM 26 C 0.705 4.080 -1.138
HETATM 28 C -0.706 4.080 -1.138
HETATM 30 C -1.139 3.045 -0.329
HETATM 31 C -3.605 3.498 -0.615
HETATM 35 C -2.540 2.556 0.016
HETATM 36 C -2.786 2.648 1.539
HETATM 40 C -2.758 1.139 -0.510
HETATM 41 C -3.270 0.705 -1.720
HETATM 43 C -3.270 -0.705 -1.719
HETATM 45 C -2.758 -1.139 -0.510
HETATM 46 C -3.605 -3.497 -0.615
HETATM 50 C -2.540 -2.556 0.016
HETATM 51 C -2.786 -2.648 1.539
HETATM 55 C -1.139 -3.045 -0.329
HETATM 56 C -0.706 -4.080 -1.138
HETATM 58 C 0.705 -4.080 -1.138
HETATM 60 C 1.139 -3.045 -0.329
HETATM 61 C 3.605 -3.498 -0.617
HETATM 65 C 2.541 -2.556 0.015
HETATM 66 C 2.787 -2.648 1.538
HETATM 3 H 1.885 0.000 1.074
HETATM 5 H 0.000 1.640 0.809
HETATM 7 H -1.884 0.000 1.075
HETATM 9 H 0.000 -1.640 0.809
HETATM 12 H 3.603 -1.340 -2.529
HETATM 14 H 3.603 1.340 -2.529

```
HETATM   17  H            4.623   3.150  -0.400
HETATM   18  H            3.516   4.520  -0.230
HETATM   19  H            3.509   3.559  -1.707
HETATM   22  H            2.072   2.064   2.118
HETATM   23  H            2.700   3.683   1.891
HETATM   24  H            3.788   2.288   1.800
HETATM   27  H            1.339   4.759  -1.691
HETATM   29  H           -1.340   4.759  -1.690
HETATM   32  H           -3.516   4.520  -0.228
HETATM   33  H           -4.623   3.150  -0.396
HETATM   34  H           -3.510   3.559  -1.706
HETATM   37  H           -2.071   2.064   2.119
HETATM   38  H           -3.787   2.288   1.803
HETATM   39  H           -2.698   3.683   1.892
HETATM   42  H           -3.604   1.340  -2.527
HETATM   44  H           -3.604  -1.340  -2.527
HETATM   47  H           -4.623  -3.150  -0.396
HETATM   48  H           -3.516  -4.520  -0.228
HETATM   49  H           -3.510  -3.559  -1.706
HETATM   52  H           -2.071  -2.064   2.119
HETATM   53  H           -2.698  -3.683   1.892
HETATM   54  H           -3.787  -2.288   1.803
HETATM   57  H           -1.340  -4.759  -1.690
HETATM   59  H            1.339  -4.759  -1.691
HETATM   62  H            3.516  -4.520  -0.230
HETATM   63  H            4.623  -3.150  -0.400
HETATM   64  H            3.509  -3.559  -1.707
HETATM   67  H            2.072  -2.064   2.118
HETATM   68  H            3.788  -2.288   1.800
HETATM   69  H            2.700  -3.683   1.891
CONECT    2   10   15    3
CONECT    4   25   30    5
CONECT    6   40   45    7
CONECT    8   55   60    9
CONECT   10    2   11   65
CONECT   11   10   13   12
CONECT   13   11   15   14
CONECT   15    2   13   20
CONECT   16   20   17   18   19
CONECT   20   15   16   21   25
CONECT   21   20   22   23   24
CONECT   25    4   20   26
CONECT   26   25   28   27
CONECT   28   26   30   29
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CONECT  30   4  28  35
CONECT  31  35  32  33  34
CONECT  35  30  31  36  40
CONECT  36  35  37  38  39
CONECT  40   6  35  41
CONECT  41  40  43  42
CONECT  43  41  45  44
CONECT  45   6  43  50
CONECT  46  50  47  48  49
CONECT  50  45  46  51  55
CONECT  51  50  52  53  54
CONECT  55   8  50  56
CONECT  56  55  58  57
CONECT  58  56  60  59
CONECT  60   8  58  65
CONECT  61  65  62  63  64
CONECT  65  10  60  61  66
CONECT  66  65  67  68  69
CONECT   3   2
CONECT   5   4
CONECT   7   6
CONECT   9   8
CONECT  12  11
CONECT  14  13
CONECT  17  16
CONECT  18  16
CONECT  19  16
CONECT  22  21
CONECT  23  21
CONECT  24  21
CONECT  27  26
CONECT  29  28
CONECT  32  31
CONECT  33  31
CONECT  34  31
CONECT  37  36
CONECT  38  36
CONECT  39  36
CONECT  42  41
CONECT  44  43
CONECT  47  46
CONECT  48  46
CONECT  49  46
CONECT  52  51
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CONECT  53  51
CONECT  54  51
CONECT  57  56
CONECT  59  58
CONECT  62  61
CONECT  63  61
CONECT  64  61
CONECT  67  66
CONECT  68  66
CONECT  69  66
END
```

HEADER MMFF94 OPTIMIZED CALIX[4]PYRROLE HOST

COMPND LOWEST ENERGY 1,3-ALTERNATE CONFORMER BY SAMPLING IN VACUO MD RUN

AUTHOR GENERATED BY PCMODEL V 9.30

HETATM 1 C -1.135 2.679 -0.605
HETATM 2 C -0.707 3.104 -1.849
HETATM 3 C 0.707 3.104 -1.849
HETATM 4 C 1.135 2.679 -0.605
HETATM 5 C 2.520 2.520 0.000
HETATM 6 C 2.679 1.135 0.605
HETATM 7 C 3.105 0.707 1.849
HETATM 8 C 3.105 -0.707 1.849
HETATM 9 C 2.679 -1.135 0.605
HETATM 10 C 2.520 -2.520 0.000
HETATM 11 C 1.135 -2.679 -0.605
HETATM 12 C 0.707 -3.104 -1.850
HETATM 13 C -0.707 -3.104 -1.850
HETATM 14 C -1.135 -2.679 -0.605
HETATM 15 C -2.520 -2.520 0.000
HETATM 16 C -2.679 -1.135 0.605
HETATM 17 C -3.104 -0.707 1.850
HETATM 18 C -3.104 0.707 1.850
HETATM 19 C -2.679 1.135 0.605
HETATM 20 C -2.520 2.520 0.000
HETATM 21 C 2.716 3.622 1.067
HETATM 22 C 2.716 -3.622 1.066
HETATM 23 C 3.622 -2.716 -1.067
HETATM 24 C -2.716 -3.622 1.067
HETATM 25 C -2.716 3.622 1.067
HETATM 26 C -3.622 2.716 -1.067
HETATM 27 C 3.621 2.716 -1.067
HETATM 28 C -3.622 -2.716 -1.067
HETATM 29 N 0.000 2.397 0.125
HETATM 30 N 2.397 0.000 -0.125
HETATM 31 N 0.000 -2.397 0.124
HETATM 32 N -2.397 0.000 -0.124
HETATM 37 H -1.343 3.407 -2.672
HETATM 38 H 1.343 3.407 -2.672
HETATM 39 H 3.407 1.343 2.672
HETATM 40 H 3.407 -1.343 2.671
HETATM 41 H 1.343 -3.407 -2.672
HETATM 42 H -1.343 -3.407 -2.672
HETATM 43 H -3.406 -1.343 2.672

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HETATM   44  H           -3.406   1.343   2.672
HETATM   45  H            2.000   3.521   1.892
HETATM   46  H            3.723   3.588   1.500
HETATM   47  H            2.576   4.621   0.636
HETATM   48  H            2.000  -3.521   1.892
HETATM   49  H            2.576  -4.621   0.636
HETATM   50  H            3.723  -3.588   1.500
HETATM   51  H            3.521  -2.000  -1.892
HETATM   52  H            4.621  -2.576  -0.637
HETATM   53  H            3.588  -3.722  -1.500
HETATM   54  H           -2.000  -3.522   1.892
HETATM   55  H           -3.722  -3.588   1.500
HETATM   56  H           -2.575  -4.621   0.636
HETATM   57  H           -2.000   3.521   1.892
HETATM   58  H           -2.576   4.621   0.636
HETATM   59  H           -3.722   3.588   1.500
HETATM   60  H           -3.522   2.000  -1.892
HETATM   61  H           -4.621   2.576  -0.636
HETATM   62  H           -3.588   3.723  -1.500
HETATM   63  H            3.521   2.000  -1.892
HETATM   64  H            3.588   3.723  -1.500
HETATM   65  H            4.621   2.576  -0.636
HETATM   66  H           -3.521  -2.000  -1.892
HETATM   67  H           -3.588  -3.723  -1.500
HETATM   68  H           -4.621  -2.576  -0.636
HETATM   33  H            0.000   2.035   1.071
HETATM   34  H            2.035   0.000  -1.071
HETATM   35  H            0.000  -2.035   1.071
HETATM   36  H           -2.035   0.000  -1.071
CONECT    1   2  20  29
CONECT    2   1   3  37
CONECT    3   2   4  38
CONECT    4   3   5  29
CONECT    5   4   6  21  27
CONECT    6   5   7  30
CONECT    7   6   8  39
CONECT    8   7   9  40
CONECT    9   8  10  30
CONECT   10   9  11  22  23
CONECT   11  10  12  31
CONECT   12  11  13  41
CONECT   13  12  14  42
CONECT   14  13  15  31
CONECT   15  14  16  24  28
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CONECT 16 15 17 32
CONECT 17 16 18 43
CONECT 18 17 19 44
CONECT 19 18 20 32
CONECT 20 1 19 25 26
CONECT 21 5 45 46 47
CONECT 22 10 48 49 50
CONECT 23 10 51 52 53
CONECT 24 15 54 55 56
CONECT 25 20 57 58 59
CONECT 26 20 60 61 62
CONECT 27 5 63 64 65
CONECT 28 15 66 67 68
CONECT 29 1 4 33
CONECT 30 6 9 34
CONECT 31 11 14 35
CONECT 32 16 19 36
CONECT 37 2
CONECT 38 3
CONECT 39 7
CONECT 40 8
CONECT 41 12
CONECT 42 13
CONECT 43 17
CONECT 44 18
CONECT 45 21
CONECT 46 21
CONECT 47 21
CONECT 48 22
CONECT 49 22
CONECT 50 22
CONECT 51 23
CONECT 52 23
CONECT 53 23
CONECT 54 24
CONECT 55 24
CONECT 56 24
CONECT 57 25
CONECT 58 25
CONECT 59 25
CONECT 60 26
CONECT 61 26
CONECT 62 26
CONECT 63 27

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CONECT  64  27
CONECT  65  27
CONECT  66  28
CONECT  67  28
CONECT  68  28
CONECT  33  29
CONECT  34  30
CONECT  35  31
CONECT  36  32
END
```

HEADER MMFF94 OPTIMIZED CALIX[4]PYRROLE HOST

COMPND 1,2-ALTERNATE CONFORMER

AUTHOR GENERATED BY PCMODEL V 9.30

HETATM	1	N	0.138	2.412	-0.037
HETATM	2	N	-2.508	-0.174	0.283
HETATM	3	C	1.218	2.973	-0.686
HETATM	4	C	0.700	3.777	-1.684
HETATM	5	C	-0.710	3.688	-1.628
HETATM	6	C	-1.049	2.839	-0.589
HETATM	7	C	-2.397	2.360	-0.070
HETATM	8	C	-2.630	0.928	-0.535
HETATM	9	C	-2.961	0.446	-1.790
HETATM	10	C	-3.055	-0.961	-1.715
HETATM	11	C	-2.759	-1.337	-0.418
HETATM	12	C	2.649	2.705	-0.245
HETATM	13	C	-2.446	2.486	1.473
HETATM	14	C	-3.541	3.259	-0.602
HETATM	15	C	3.070	3.826	0.731
HETATM	16	C	3.613	2.756	-1.453
HETATM	35	C	-2.649	-2.705	0.245
HETATM	36	C	-1.218	-2.973	0.686
HETATM	37	N	-0.138	-2.412	0.037
HETATM	38	C	1.049	-2.839	0.589
HETATM	39	C	0.710	-3.688	1.628
HETATM	40	C	-0.700	-3.777	1.684
HETATM	43	C	2.397	-2.360	0.070
HETATM	44	C	2.630	-0.928	0.535
HETATM	45	N	2.508	0.174	-0.283
HETATM	46	C	2.759	1.337	0.418
HETATM	47	C	3.055	0.961	1.714
HETATM	48	C	2.961	-0.446	1.790
HETATM	52	C	2.446	-2.486	-1.473
HETATM	56	C	3.541	-3.259	0.602
HETATM	61	C	-3.070	-3.826	-0.731
HETATM	65	C	-3.613	-2.756	1.453
HETATM	17	H	0.219	1.762	0.736
HETATM	18	H	-2.242	-0.155	1.259
HETATM	19	H	1.275	4.375	-2.379
HETATM	20	H	-1.405	4.197	-2.283
HETATM	21	H	-3.115	1.052	-2.674
HETATM	22	H	-3.296	-1.628	-2.533
HETATM	23	H	-1.676	1.886	1.971

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HETATM   24  H           -2.292   3.525   1.789
HETATM   25  H           -3.416   2.159   1.868
HETATM   26  H           -3.411   4.300  -0.284
HETATM   27  H           -4.516   2.917  -0.234
HETATM   28  H           -3.595   3.261  -1.697
HETATM   29  H            2.420   3.857   1.615
HETATM   30  H            3.011   4.812   0.255
HETATM   31  H            4.100   3.689   1.081
HETATM   32  H            3.317   2.053  -2.241
HETATM   33  H            4.637   2.502  -1.153
HETATM   34  H            3.643   3.754  -1.905
HETATM   60  H           -0.219  -1.762  -0.736
HETATM   42  H            1.405  -4.197   2.283
HETATM   41  H           -1.275  -4.375   2.379
HETATM   51  H            2.242   0.155  -1.259
HETATM   50  H            3.296   1.627   2.533
HETATM   49  H            3.115  -1.052   2.674
HETATM   53  H            1.676  -1.886  -1.971
HETATM   54  H            2.292  -3.525  -1.789
HETATM   55  H            3.416  -2.159  -1.868
HETATM   57  H            3.411  -4.300   0.284
HETATM   58  H            4.516  -2.917   0.234
HETATM   59  H            3.595  -3.261   1.697
HETATM   62  H           -2.420  -3.857  -1.615
HETATM   63  H           -3.011  -4.812  -0.255
HETATM   64  H           -4.100  -3.689  -1.081
HETATM   66  H           -3.317  -2.053   2.241
HETATM   67  H           -4.637  -2.502   1.153
HETATM   68  H           -3.643  -3.754   1.905
CONECT    1   3   6  17
CONECT    2   8  11  18
CONECT    3   1   4  12
CONECT    4   3   5  19
CONECT    5   4   6  20
CONECT    6   1   5   7
CONECT    7   6   8  13  14
CONECT    8   2   7   9
CONECT    9   8  10  21
CONECT   10   9  11  22
CONECT   11   2  10  35
CONECT   12   3  15  16  46
CONECT   13   7  23  24  25
CONECT   14   7  26  27  28
CONECT   15  12  29  30  31
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CONECT  16  12  32  33  34
CONECT  35  11  36  61  65
CONECT  36  35  37  40
CONECT  37  36  38  60
CONECT  38  37  39  43
CONECT  39  38  40  42
CONECT  40  36  39  41
CONECT  43  38  44  52  56
CONECT  44  43  45  48
CONECT  45  44  46  51
CONECT  46  12  45  47
CONECT  47  46  48  50
CONECT  48  44  47  49
CONECT  52  43  53  54  55
CONECT  56  43  57  58  59
CONECT  61  35  62  63  64
CONECT  65  35  66  67  68
CONECT  17   1
CONECT  18   2
CONECT  19   4
CONECT  20   5
CONECT  21   9
CONECT  22  10
CONECT  23  13
CONECT  24  13
CONECT  25  13
CONECT  26  14
CONECT  27  14
CONECT  28  14
CONECT  29  15
CONECT  30  15
CONECT  31  15
CONECT  32  16
CONECT  33  16
CONECT  34  16
CONECT  60  37
CONECT  42  39
CONECT  41  40
CONECT  51  45
CONECT  50  47
CONECT  49  48
CONECT  53  52
CONECT  54  52
CONECT  55  52
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CONECT  57  56
CONECT  58  56
CONECT  59  56
CONECT  62  61
CONECT  63  61
CONECT  64  61
CONECT  66  65
CONECT  67  65
CONECT  68  65
END
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