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Electronic Supplementary Information
for

Spin-State Modulation by Host-Guest Chemistry with Cucurbiturils

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Contents

1. Materials and methods

All reagents and materials were purchased commercially and were used without further purification. NMR spectra were recorded on a Bruker Advance spectrometer at 400 MHz, using tetramethylsilane (TMS) as the internal standard. The C, H and N elemental analyses were performed on a EUROVECTER EA3000 analyzer. Powder X-ray diffraction (PXRD) data were recorded on a Bruker D8 Advance Diffractometer with Cu Kα radiation (λ = 1.54056 Å). IR spectra were recorded in the range of 4000-400 cm^{-1} on a Thermo IS5 spectrometer with KBr pellets. Thermogravimetric (TG) analyses were performed under a nitrogen atmosphere on a TG-DTA 6200 instrument with a heating rate of 10 °C min^{-1}.The UV-vis spectra were performed on a Hitachi U-3900 spectrophotometer.

Magnetic Susceptibility Measurements

Magnetic measurements Magnetic susceptibilities were determined on a Quantum Design MPMS XL7 magnetometer with a scan rate of 5 K min^{-1}. A field of 5000 Oe was applied in the measured temperature range. Magnetic data were corrected for the sample holder and diamagnetic contributions.

Single-Crystal X-ray Diffraction

Single-crystal X-ray diffraction data were collected on a Rigaku Oxford XtaLAB PRO diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structure was solved by direct methods and further refined by fullmatrix least-squares techniques on F^2 with SHELXL. All hydrogen atoms were generated in the calculated positions with a riding model. The solvent molecules in compound **1** were highly disordered and removed by SQUEEZE embedded in PLATON, and the types and quantities of lattice solvent molecules were then determined by elemental and TG analyses.

Solution Magnetic Susceptibility Measurements

The solution magnetic susceptibility was measured using the Evans method. A solution of specific concentrations of metal complex in D_2O, containing 5% tert-butanol by volume was placed in an NMR coaxial tube with 5% tert-butanol (v/v) in D_2O as reference. The

paramagnetic ^{1}H NMR spectra of the sample were recorded at different temperatures. The difference in the deuterated solvent peaks between the inner and outer tubes was calculated, and the paramagnetic molar magnetic susceptibility at various temperatures was determined using the following equation.

$$\chi_{\mathrm{M}} = \frac{3 \times 10^3 \Delta f}{4\pi m f} + \chi_{\mathrm{M}}^{\mathrm{dia}}$$

Here, m represents the mass of the tested sample (g); Δf denotes the difference in the deuterated solvent peaks between the inner and outer tubes in Hz; f is the frequency of the NMR spectrometer in Hz; and $\chi_{\mathrm{M}}^{\mathrm{dia}}$ is the molar diamagnetic susceptibility: $0.5 \times \mathrm{M} \times 10^{-6}$ $\mathrm{cm^3\ mol^{-1}}$ (where M is the molecular weight of the tested sample).

Since CB[7] is diamagnetic, the magnetic moment of **1**⊂2CB[7] was obtained by subtracting the diamagnetic susceptibility of an equivalent amount of CB[7].

$$\chi'_{\mathrm{M}(\mathbf{1}\subset 2\mathrm{CB}[7])} = \chi_{\mathrm{M}(\mathbf{1}\subset 2\mathrm{CB}[7])} + \chi_{\mathrm{M}(2\mathrm{CB}[7])}^{\mathrm{dia}}$$

$\chi'_{\mathrm{M}(\mathbf{1}\subset 2\mathrm{CB}[7])}$ represents the theoretical molar magnetic susceptibility of **1**⊂2CB[7], $\chi_{\mathrm{M}(\mathbf{1}\subset 2\mathrm{CB}[7])}$ is the experimentally measured molar magnetic susceptibility, and $\chi_{\mathrm{M}(2\mathrm{CB}[7])}^{\mathrm{dia}}$ is the molar diamagnetic susceptibility of an equivalent amount of CB[7].

Fitting of solution magnetic susceptibility data

Thermodynamic parameters for the SCO transitions were obtained from fits of the magnetic susceptibility versus temperature data to eq S1, which reduces to eq S2 upon substitution of realistic values for the maximum $(\chi_{\mathrm{M}}T)_{\mathrm{HS}}$ (= 3.0 $\mathrm{cm^3\ K\ mol^{-1}}$) and minimum $(\chi_{\mathrm{M}}T)_{\mathrm{LS}}$ (= 0.44 $\mathrm{cm^3\ K\ mol^{-1}}$) values taken from the solid-state data.

$$\chi_{\mathrm{M}}T = \frac{(\chi_{\mathrm{M}}T)_{\mathrm{HS}} - (\chi_{\mathrm{M}}T)_{\mathrm{LS}}}{1+\exp\left(\frac{\Delta_{\mathrm{SCO}}H}{RT} - \frac{\Delta_{\mathrm{SCO}}S}{R}\right)} + (\chi_{\mathrm{M}}T)_{\mathrm{LS}} \qquad \text{equation S1}$$

$$\chi_{\mathrm{M}}T = \frac{2.56}{1+\exp\left(\frac{\Delta_{\mathrm{SCO}}H}{RT} - \frac{\Delta_{\mathrm{SCO}}S}{R}\right)} + 0.44 \qquad \text{equation S2}$$

Computational Methods

The DFT calculations were performed using the Gaussian 16 program package[1] with the UTPSSh functional[2-3] and the standard 6-31G(d,p) basis set. The UTPSSh functional was shown to provide a good reproduction of the energetic characteristics and magnetic properties

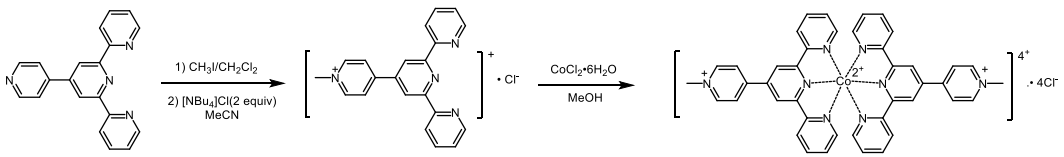
of magnetically bistable cobalt complexes.[4-7] The stationary points on the potential energy surfaces were localized by full geometry optimization with the subsequent confirmation of the stabilities of the DFT wave function. The calculations were performed on the tetracationic structures without inclusion of Cl^- anions. Structural visualizations and orbital analysis were performed using the ChemCraft software.TD-DFT calculations were done using B3LYP functional along with ZORA-def2-TZVP basis set on all atoms.[8] CPCM solvent model (water) and D3BJ dispersion correction were applied. A total of 50 electronic transitions were performed for the LS and HS states. The calculated UV-vis spectra were obtained using ChemCraft program[9] with Gaussian peak broadening and the stick spectra show the absorption wavelengths and oscillator strengths. Orbital transitions with major contributions are reported with an isovalue of 0.05.

Electrochemical Experiments

The cyclic voltammetry (CV) measurements of the complexes were performed with a CH Instruments 660E potentiostat in an aqueous solution containing 0.5 mM target complex and 0.2 M NaCl as supporting electrolyte. A conventional three-electrode system (10 mL capacity) was employed with the following configuration: a glassy carbon electrode (3 mm diameter) as working electrode, an Ag/AgCl (saturated KCl) reference electrode, and a platinum wire counter electrode. Prior to each measurement, the glassy carbon electrode surface was successively polished with 0.05 μm alumina slurry on microcloth pads, followed by ultrasonic cleaning in deionized water and ethanol. Oxygen removal was achieved by purging the solution with nitrogen gas for 30 minutes, and a continuous nitrogen was maintained throughout the experiments to ensure an inert atmosphere.

2. Synthesis

Synthesis of 4′-(1-methyl-1H-pyridin-4-yl)-2,2′:6′,2′′-terpyridine (MPTPY)



PYTPY (4′-(4-pyridyl)-2,2′;6′,2′′-terpyridine (3.605 g, 0.01 mmol)) was dissolved in 100 mL

of dry acetonitrile, an excess of iodomethane (7 mL, 0.11 mmol) was added, and heated for 12 h at 70 °C under N_2 atmosphere. The precipitate was filtered, washed with acetonitrile and dried under vacuum to give [MePyTpy]I as a yellow powder (5.134 g, 98 %). [MePyTpy]I (5.134 g, 10 mmol) was dissolved in 100 ml of acetonitrile and tetrabutyl ammonium chloride (9.4 g, 34 mmol) was added. The white precipitate was filtered, washed with acetonitrile and dried to give 4 g of [MePyTpy]Cl white powder (quantitative yield).^{1}H NMR (400 MHz, DMSO) δ 9.15 (d, 2H), 8.92 (s, 2H), 8.80 (m, 4H), 8.71 (dt, 2H), 8.09 (td, 2H), 7.59 (m, 2H), 4.43 (s, 3H).

Synthesis of 1·3MeOH

The ligand [MePyTpy]Cl (360 mg, 1.0 mmol) and cobalt chloride hexahydrate (119 mg, 0.5 mmol) were dissolved in methanol and stirred for 5 h at RT. The solution was filtered and the filtrate showed a deep red color, and the filtrate was added to a vial encapsulated in a large tube filled with ether. Vapor diffusion of ether after two weeks resulted in deep-red flaky crystals (52 mg, 12%). Elemental analyses (%) calcd for $C_{45}H_{46}CoN_8O_3Cl_4$: C, 77.36; H, 6.59; N, 16.05. Found: C, 77.06; H, 6.90; N, 16.04.

3. Addittional Tables and Figures

Table S1. Crystal parameters for **1**.

CCDC number	2415226
Formula	$C_{168}H_{136}Cl_{16}Co_4N_{32}$
T / K	100
Crystal system	Monoclinic
Space group	$P2_1/n$
a / Å	17.7001(3)
b / Å	29.4982(6)
c / Å	34.4252(6)
α / °	90
β / °	90.631(2)
γ / °	90
V / Å^3	17973.0(6)
Z	16
GOF	1.047
R_1 [$I \geq 2\sigma(I)$]	0.0881
wR_2 (all data)	0.2514

Table S2. Average Co–N distances in four [CoN_6] centers, distortion parameters (Σ and φ), and dihedral angles between the twisted methylpyridinium ring and the terpyridine plane at 100 K.

	Co–N(ave.) (Å)	Σ (°)	φ (°)	Dihedral angles (°)
Co_1	2.008(4)	87.7(1)	177.92(16)	5.2 and 27.0
Co_2	2.011(4)	84.9(6)	177.08(15)	24.7 and 19.7
Co_3	2.011(4)	85.6(7)	176.29(17)	39.7 and 15.1
Co_4	2.009(4)	84.6(1)	175.07(17)	11.0 and 28.6

Table S3. Thermodynamic parameters ($\Delta_{SCO}H$ / kJ mol^{-1}; $\Delta_{SCO}S$ / J K^{-1} mol^{-1}) and $T_{1/2}$ / K of **1** and **1**⊂2CB[7] in D_2O determined by fitting Eq. 2.

	1	**1**⊂2CB[7]
$\Delta_{SCO}H$	6.97 ± 0.48	6.94 ± 0.34
$\Delta_{SCO}S$	21.08 ± 1.51	17.02 ± 1.03
$T_{1/2}$	330.6	407.7

Table S4. Spin states (S), total energies (E), relative energies (ΔE), spin density at the metal center (q_s^M) and expectation values of the spin-squared operator ($\hat{S}^2$) of the LS and HS states of the compounds **1** and **1**⊂2CB[7] calculated by the DFT UTPSSh/6-31G(d,p) method.

Structure	S	E, a.u.	ΔE, kcal mol^{-1}	q_s^M	$\hat{S}^2$
1 LS-Co(II)	1/2	−3440.793069	0.0	0.764	0.98
1 HS-Co(II)	3/2	−3440.785420	4.8	3.764	2.78
1⊂2CB[7] LS-Co(II)	1/2	−11866.230871	0.0	0.763	0.97
1⊂2CB[7] HS-Co(II)	3/2	−11866.221209	6.1	3.767	2.75

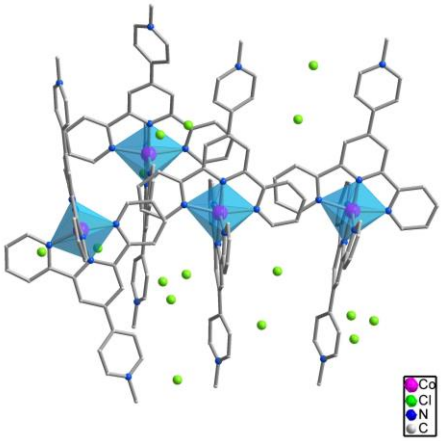


Figure S1. Illustration of asymmetric unit in the crystal structure of **1·3CH$_3$OH**. Hydrogen atoms and solvent molecules are omitted for clarity.

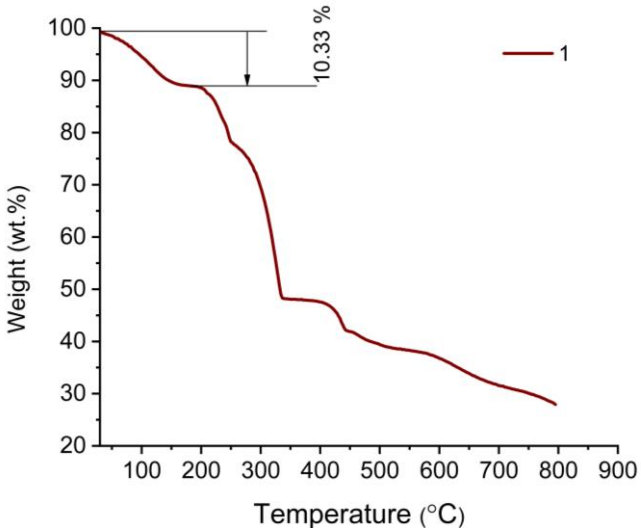


Figure S2. Thermogravimetric data of **1·3CH$_3$OH**.

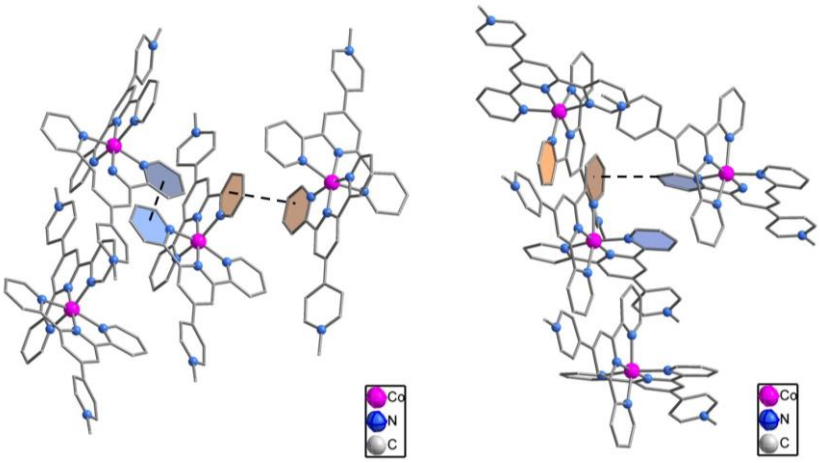


Figure S3. Major intermolecular interactions within the crystal structure of **1·3CH$_3$OH**.

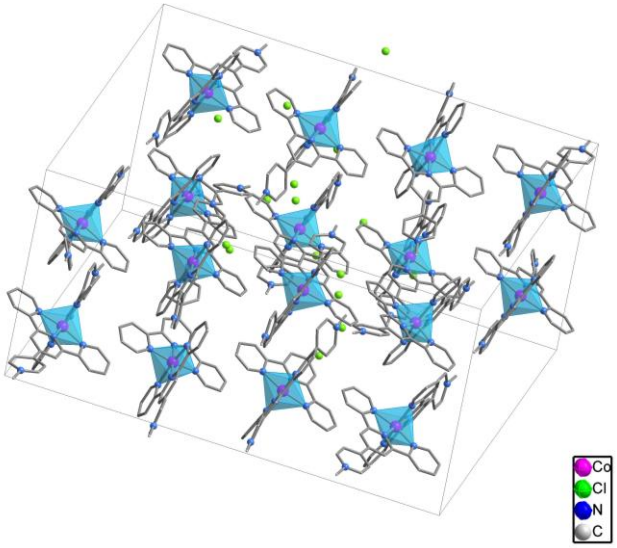


Figure S4. The packing of **1** in one unit cell at 100 K.

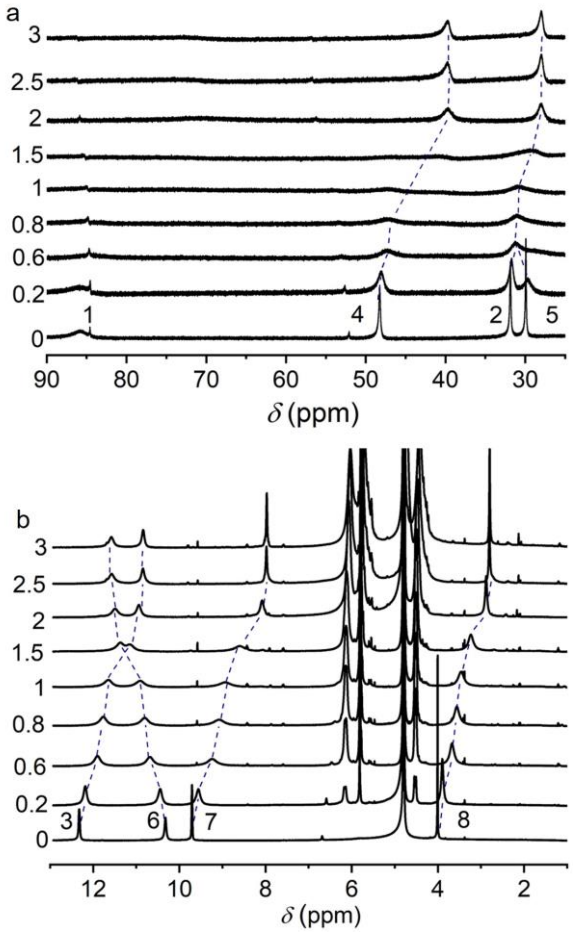


Figure S5. ^{1}H NMR spectra of **1** (4.0 mM) in D_2O with increasing equivalents of CB[7] (0, 0.2, 0.6, 0.8, 1, 1.5, 2, 2.5, and 3 eq); a, b: paramagnetic and diamagnetic region, respectively.

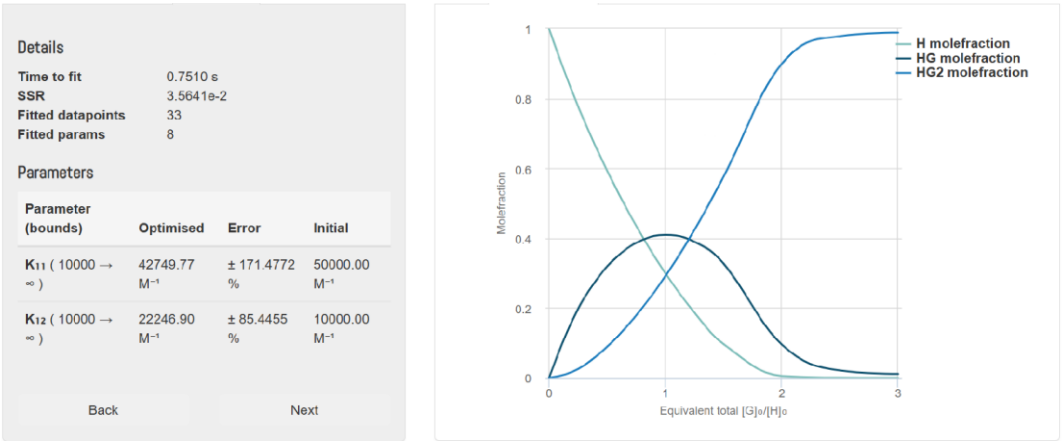


Figure S6. Binding isotherm (1:2 system) using Bindfit to calculate the binding constant of **1** and CB[7].

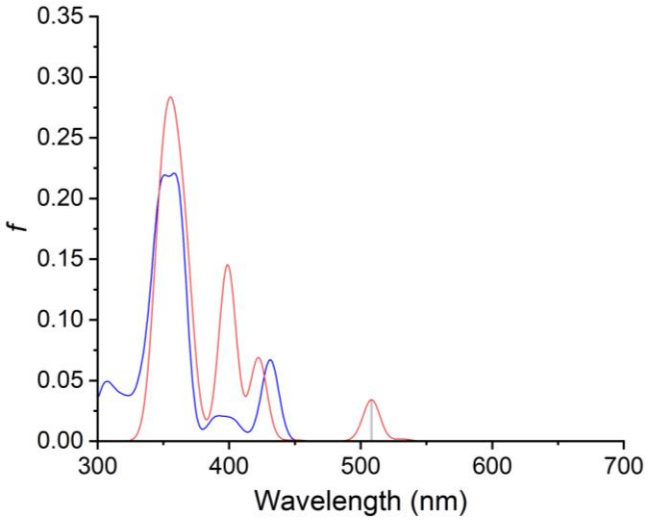


Figure S7. TD-DFT calculated UV-vis spectra of **1** in the LS state (red) and HS state (blue). 508 nm band hightighted with stick corresponds to MLCT transitions.

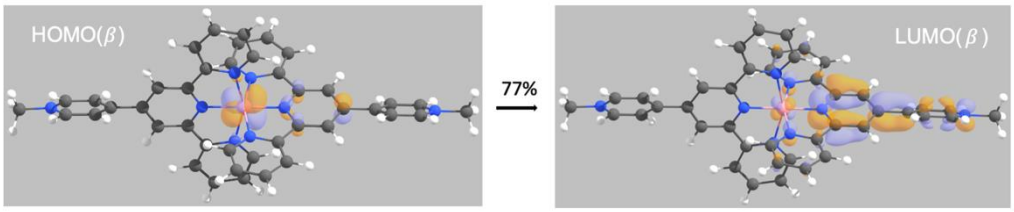


Figure S8. Dominant natural transition orbital contributions (77%) for the 508 nm transition of **1** in the LS state, corresponding to a MLCT transition. Left picture corresponds to the HOMO orbital with dominant d orbital feature; right picture corresponds to LUMO orbital with dominant ligand π* orbital contribution. Isovalue = 0.05 a.u.

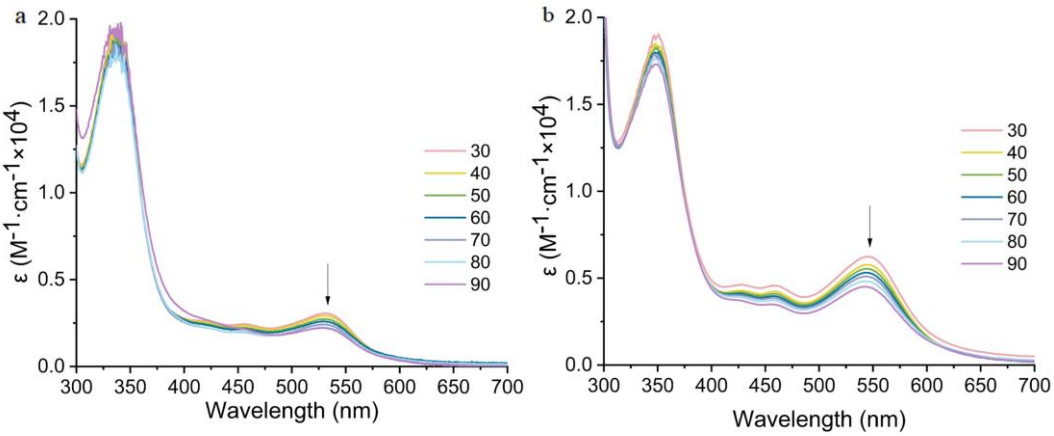


Figure S9. Variable temperature UV spectra of (a) 0.33 mM **1** in water (b) 0.33 mM **1** and 2 eq CB [7] in water within 303-363 K.

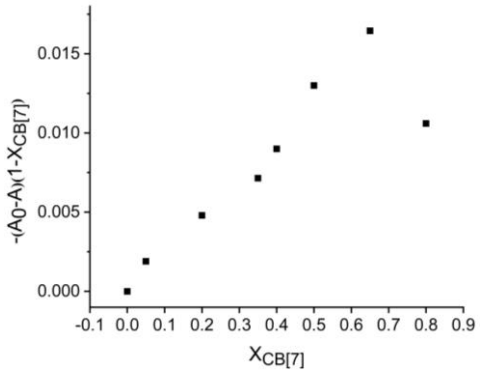


Figure S10. UV-vis Job's plot at 546 nm for **1** (10 μM, 2.5 mL) in water titrated with CB[7] (1.0 mM) at specified molar ratios (X). The plot indicates a 2:1 complex stoichiometry.

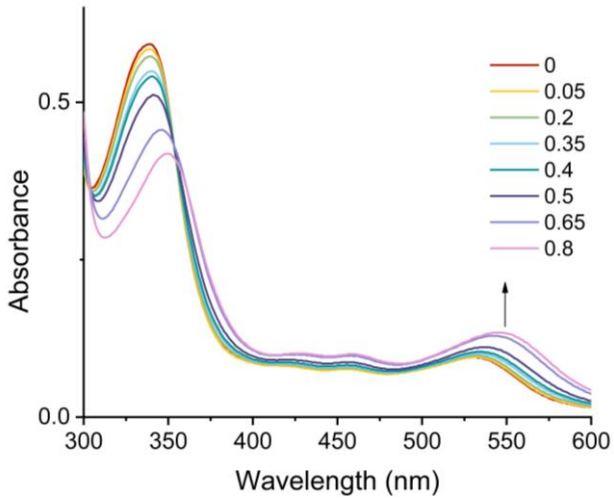


Figure S11. UV-vis spectra of **1** (20 μM, 2.5 mL) in water titrated with CB[7] (0.5mM) to specified molar ratios (X).

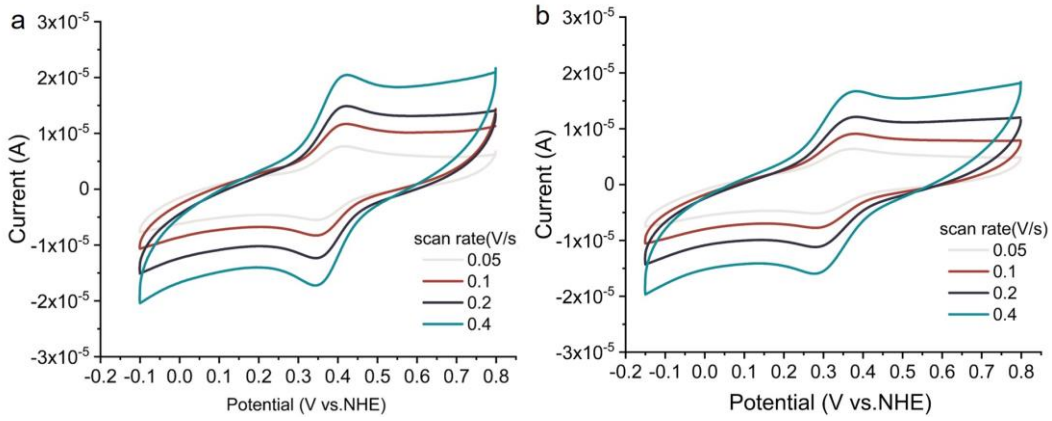


Figure S12. Cyclic voltammetry curves on glassy carbon electrodes:(a) with 0.5 mM **1**, (b) with 2 eq CB[7] and 0.5 mM **1**; in a 0.2 M NaCl aqueous system with potential scan rates of 50, 100, 200, 400 mVs^{-1}.

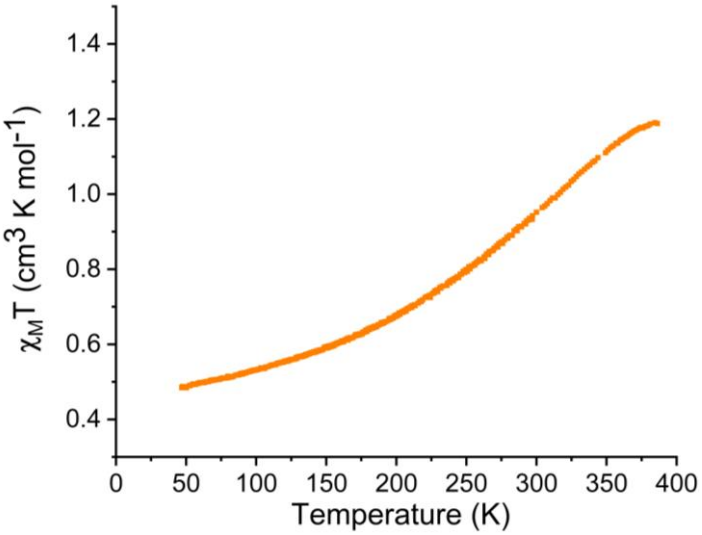


Figure S13. $\chi_M T$ versus T plots for **1·3CH₃OH** between 50-390 K.

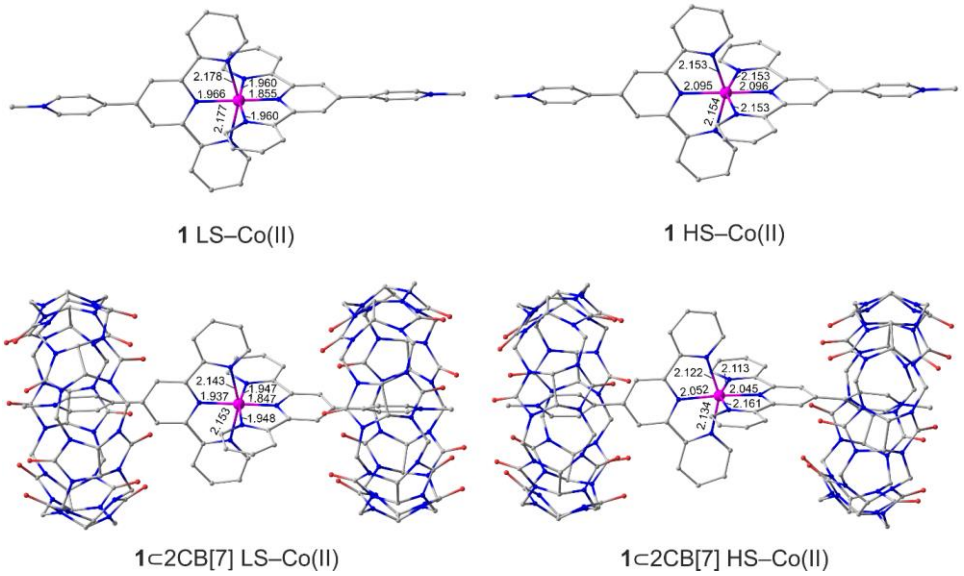


Figure S14. Optimized geometries of the LS and HS states of **1** and **1**⊂2CB[7] calculated by the DFT UTPSSh/6-31G(d,p) method. Here and in Figures S15-16 hydrogen atoms are omitted for clarity.

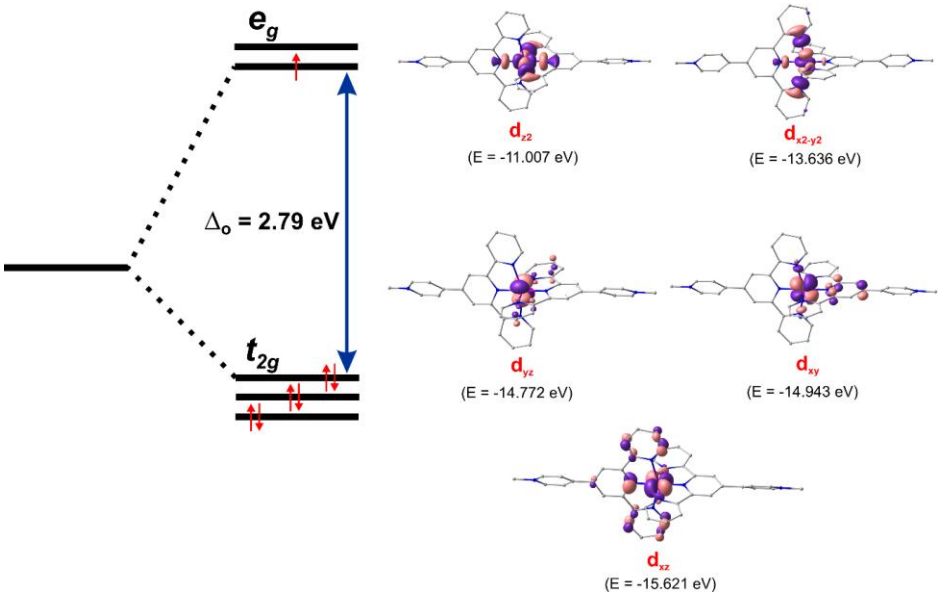


Figure S15. Energy level diagram and α spin molecular 3d-orbitals for LS state of **1** calculated by the DFT UTPSSh/6-31G(d,p) method (contour value = 0.04 e $Å^{-3}$).

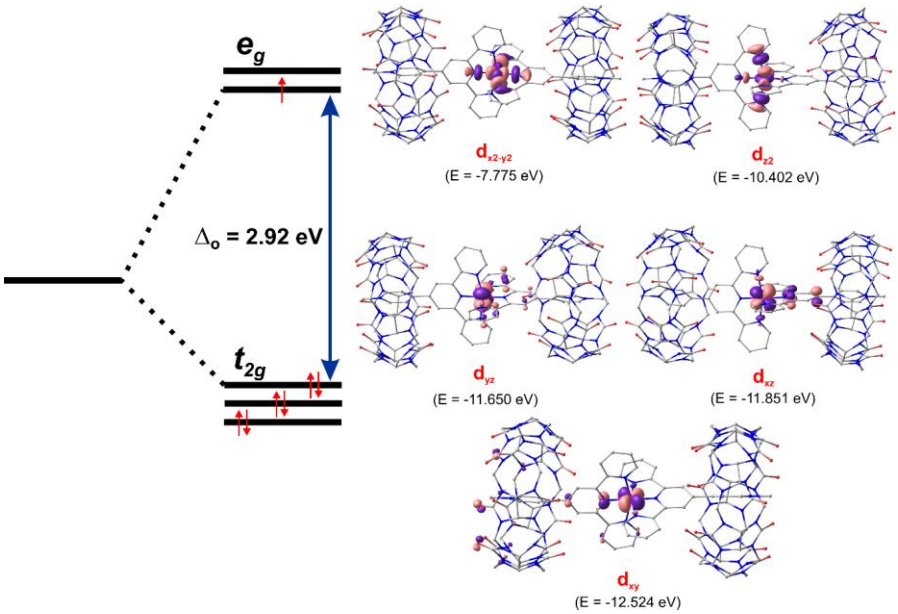


Figure S16. Energy level diagram and α spin molecular 3d-orbitals for LS state of **1**⊂2CB[7] calculated by the DFT UTPSSh/6-31G(d,p) method (contour value = 0.04 e Å^{-3}).

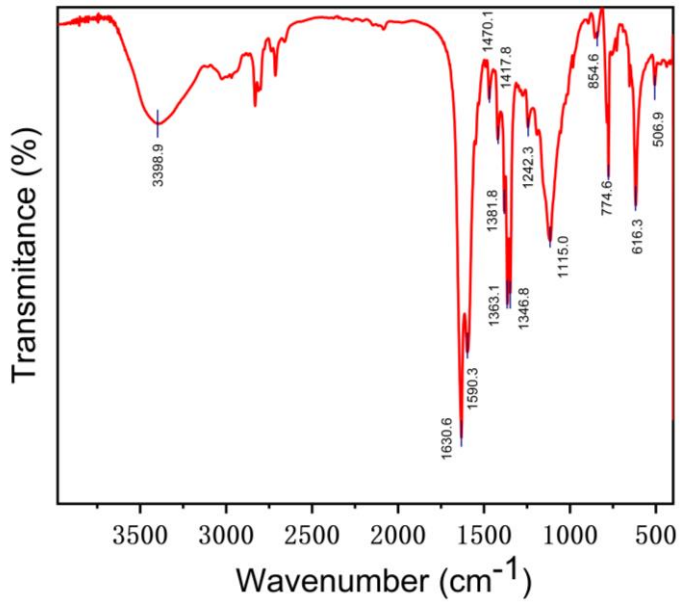


Figure S17. IR spectrum of **1**·3CH_3OH (KBr pellet, cm^{-1}).

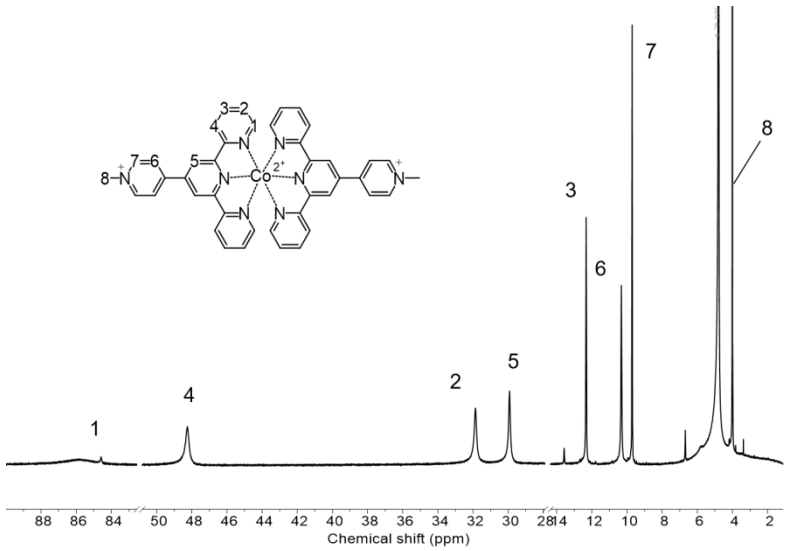


Figure S18. ^{1}H NMR (400Hz, D_2O) spectrum of **1**.

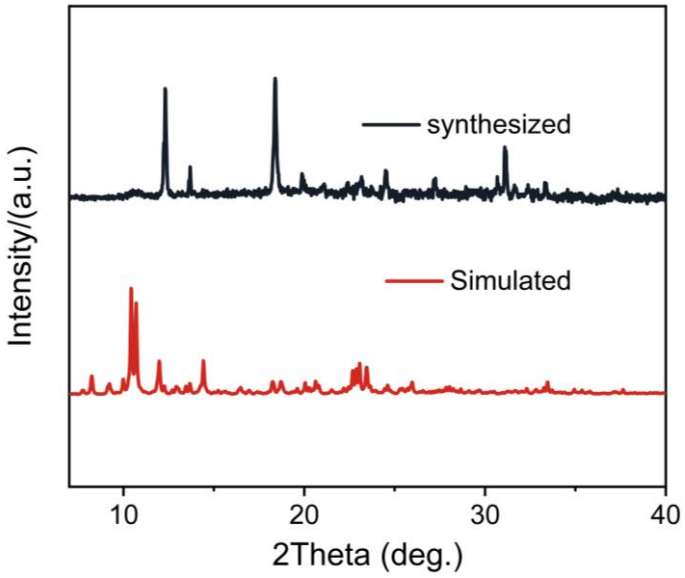


Figure S19. PXRD pattern of **1·3CH$_3$OH** at room temperature. (The observed mismatch between the theoretical and experimental PXRD patterns arise from the rapid loss of lattice solvent in **1·3CH$_3$OH** upon air exposure, as well as temperature differences between the 100 K SCXRD data and the 298 K PXRD measurements.).

Table S5. Cartesian Coordinates of the optimized structure of **1**-LS.

Atom number	Element	X	Y	Z
1	Co	0.095035	-0.00184	0.000518
2	N	1.950421	-0.00121	0.0008
3	N	0.377438	0.605549	1.842581
4	N	0.378539	-0.6102	-1.84112
5	N	9.016931	0.010781	-0.00269
6	N	-1.87119	-0.00052	-0.00032
7	N	-0.36457	2.014448	-0.68229
8	N	-0.36705	-2.01727	0.681666
9	N	-8.95372	0.002207	0.009297
10	C	2.618575	0.375836	1.1218
11	C	4.015252	0.393011	1.145392
12	H	4.537385	0.674573	2.052586
13	C	4.734072	0.002161	0.000538
14	C	4.016004	-0.39053	-1.14415
15	H	4.538513	-0.67086	-2.05151
16	C	2.619266	-0.37656	-1.12034
17	C	1.694195	0.725152	2.207174
18	C	2.072647	1.136205	3.485348
19	H	3.121135	1.219079	3.747635
20	C	1.088302	1.437684	4.427073
21	H	1.362091	1.758059	5.426404
22	C	-0.25063	1.31725	4.055609
23	H	-1.04941	1.540404	4.753549
24	C	-0.5608	0.900544	2.761996
25	H	-1.59071	0.796796	2.444285
26	C	1.695489	-0.72813	-2.20552
27	C	2.074616	-1.14036	-3.48312
28	H	3.123237	-1.22186	-3.74531
29	C	1.090765	-1.44508	-4.42431
30	H	1.365082	-1.76644	-5.42318
31	C	-0.24837	-1.32679	-4.05288
32	H	-1.04676	-1.55273	-4.75037
33	C	-0.55923	-0.90863	-2.7599
34	H	-1.5893	-0.8063	-2.44226
35	C	8.340849	0.997675	0.631682
36	H	8.937892	1.764218	1.110452
37	C	6.954189	1.014956	0.649
38	H	6.462435	1.842604	1.146857
39	C	6.22252	0.004479	0.000513
40	C	6.957826	-1.00487	-0.65004
41	H	6.46762	-1.83286	-1.14889

42	C	8.342217	-0.9811	-0.63594
43	H	8.945011	-1.74373	-1.115
44	C	10.5111	-0.01	0.002076
45	H	10.86127	-0.1463	-1.02121
46	H	10.84601	-0.8332	0.635444
47	H	10.87339	0.937678	0.39506
48	C	-2.54887	1.115103	-0.37885
49	C	-3.94898	1.14289	-0.37904
50	H	-4.47097	2.035484	-0.70175
51	C	-4.67068	0.00131	-0.00006
52	C	-3.95042	-1.14132	0.378535
53	H	-4.47351	-2.03317	0.701504
54	C	-2.55028	-1.1154	0.37801
55	C	-1.69544	2.255976	-0.77966
56	C	-2.19437	3.484515	-1.22511
57	H	-3.26002	3.664371	-1.30425
58	C	-1.29758	4.494375	-1.57762
59	H	-1.6628	5.454342	-1.92639
60	C	0.070591	4.245685	-1.47407
61	H	0.801358	5.002075	-1.73707
62	C	0.488088	2.992155	-1.02291
63	H	1.544399	2.760006	-0.93067
64	C	-1.69824	-2.25747	0.778342
65	C	-2.19861	-3.48588	1.222519
66	H	-3.26448	-3.66467	1.301146
67	C	-1.30301	-4.49701	1.574421
68	H	-1.66938	-5.4569	1.922209
69	C	0.065459	-4.24969	1.471575
70	H	0.795346	-5.00708	1.734116
71	C	0.48447	-2.99618	1.021755
72	H	1.541053	-2.76501	0.930215
73	C	-8.27788	1.097585	0.432273
74	H	-8.87657	1.935411	0.768935
75	C	-6.89163	1.122767	0.434647
76	H	-6.39879	2.012839	0.808385
77	C	-6.16085	0.002589	0.000516
78	C	-6.8942	-1.11757	-0.43098
79	H	-6.40317	-2.00929	-0.80317
80	C	-8.27983	-1.09293	-0.41936
81	H	-8.88132	-1.93045	-0.75225
82	C	-10.4481	0.010495	-0.01996
83	H	-10.8073	-0.99187	0.208614
84	H	-10.7751	0.316163	-1.01574
85	H	-10.8084	0.712296	0.730167

Table S6. Cartesian Coordinates of the optimized structure of **1**⊂2CB[7]-LS.

1	O	-11.2828	-1.74398	-3.68789
2	O	-5.21864	-1.51467	-3.49537
3	N	-9.38472	-0.96284	-4.79467
4	N	-9.46951	-3.11987	-4.19012
5	N	-6.94313	-0.97351	-4.96651
6	N	-7.04653	-2.91986	-3.86243
7	C	-10.1749	-1.92092	-4.1553
8	C	-8.20144	-1.54391	-5.40033
9	H	-8.26877	-1.52856	-6.49625
10	C	-8.17049	-2.98475	-4.79467
11	H	-8.00239	-3.77279	-5.54044
12	C	-6.28656	-1.76611	-4.03699
13	C	-10.0369	-4.34684	-3.66973
14	H	-11.1082	-4.16633	-3.55836
15	H	-9.85971	-5.1571	-4.38441
16	C	-6.4459	-4.10259	-3.27772
17	H	-6.41909	-4.9039	-4.03092
18	H	-5.43068	-3.83111	-2.97887
19	O	-11.2107	-3.73353	-1.10779
20	O	-5.29806	-4.25474	-0.65681
21	N	-9.54711	-4.76864	-2.36978
22	N	-9.47288	-4.94896	-0.13245
23	N	-7.11278	-4.59234	-2.08346
24	N	-7.11113	-5.60154	-0.08327
25	C	-10.197	-4.39837	-1.19892
26	C	-8.30511	-5.44659	-2.10793
27	H	-8.16541	-6.29305	-2.79121
28	C	-8.43453	-5.85658	-0.60859
29	H	-8.71681	-6.90568	-0.45813
30	C	-6.38753	-4.75731	-0.90973
31	C	-10.146	-5.10461	1.149616
32	H	-10.2951	-6.16975	1.368076
33	H	-11.1111	-4.60158	1.051045
34	C	-6.65618	-5.94289	1.250004
35	H	-7.00646	-6.95632	1.476142
36	H	-5.56509	-5.91432	1.236142
37	O	-10.6726	-2.51641	2.298419
38	O	-4.93149	-4.24133	2.766825
39	N	-9.4567	-4.4993	2.266652
40	N	-9.06882	-3.02937	3.911581
41	N	-7.0695	-5.03574	2.308363
42	N	-6.75378	-3.79329	4.141852

43	C	-9.82259	-3.25727	2.766295
44	C	-8.35966	-5.09349	2.987474
45	H	-8.59437	-6.12552	3.276308
46	C	-8.16591	-4.12483	4.205688
47	H	-8.40865	-4.58104	5.173623
48	C	-6.12335	-4.33207	3.036761
49	C	-9.50911	-2.06399	4.903667
50	H	-9.63054	-2.58189	5.866059
51	H	-10.4699	-1.6625	4.571207
52	C	-6.02281	-3.025	5.131283
53	H	-6.25148	-3.41781	6.128246
54	H	-4.9655	-3.1695	4.903709
55	O	-10.2531	0.672	4.566641
56	O	-4.48246	-0.93828	3.809384
57	N	-8.62593	-0.92729	5.056648
58	N	-8.20312	1.219526	5.53522
59	N	-6.27382	-1.5981	5.146148
60	N	-5.93524	0.591005	4.81041
61	C	-9.15712	0.363276	4.988534
62	C	-7.38735	-0.96275	5.815654
63	H	-7.53509	-1.40101	6.811392
64	C	-6.97729	0.540012	5.844525
65	H	-6.57587	0.872875	6.81038
66	C	-5.46201	-0.68057	4.498901
67	C	-8.43259	2.643825	5.647829
68	H	-7.99506	2.993471	6.589658
69	H	-9.51451	2.795125	5.652382
70	C	-5.07667	1.742957	4.607797
71	H	-4.78451	2.154854	5.58577
72	H	-4.19494	1.385117	4.071374
73	O	-9.98889	3.92818	3.600536
74	O	-4.14391	2.648306	2.040386
75	N	-7.91912	3.442863	4.552829
76	N	-7.9895	4.790034	2.762204
77	N	-5.66063	2.804496	3.808104
78	N	-5.61083	4.440723	2.280421
79	C	-8.78056	4.026186	3.628755
80	C	-6.5467	3.827116	4.365519
81	H	-6.12058	4.21816	5.299533
82	C	-6.62069	4.890941	3.219817
83	H	-6.39171	5.911719	3.555405
84	C	-5.04783	3.225763	2.637433
85	C	-8.62869	5.768938	1.906816
86	H	-8.29992	6.781743	2.169019

87	H	-9.70256	5.665703	2.078922
88	C	-5.1658	5.197393	1.1321
89	H	-4.2055	4.779898	0.821403
90	H	-5.04619	6.247001	1.431296
91	O	-10.1366	4.07067	0.126741
92	O	-4.43669	4.133365	-1.41175
93	N	-8.39589	5.58036	0.487511
94	N	-8.69602	4.750968	-1.57355
95	N	-6.03684	5.125767	-0.03691
96	N	-6.37483	5.112987	-2.25552
97	C	-9.1846	4.724221	-0.26683
98	C	-7.21566	5.982142	-0.23025
99	H	-6.97085	7.032253	-0.03179
100	C	-7.5905	5.68664	-1.71617
101	H	-7.88568	6.576396	-2.28548
102	C	-5.5016	4.718442	-1.25584
103	C	-9.5802	4.380109	-2.66548
104	H	-9.76444	5.259618	-3.29897
105	H	-10.516	4.038925	-2.2151
106	C	-6.13824	4.803133	-3.65505
107	H	-6.47632	5.654555	-4.25399
108	H	-5.06154	4.66982	-3.76678
109	O	-10.7516	1.771499	-2.89742
110	O	-4.89569	2.21553	-4.02064
111	N	-9.08311	3.291692	-3.47973
112	N	-9.38146	1.480242	-4.76092
113	N	-6.76126	3.600095	-4.17484
114	N	-6.92903	1.478976	-4.87794
115	C	-9.84063	2.128681	-3.62341
116	C	-8.14876	3.476184	-4.57464
117	H	-8.44136	4.318609	-5.21397
118	C	-8.19375	2.090552	-5.29576
119	H	-8.24627	2.15947	-6.38927
120	C	-6.07173	2.408111	-4.31229
121	C	-10.0012	0.268044	-5.25315
122	H	-11.0278	0.250923	-4.87984
123	H	-9.99852	0.305951	-6.34985
124	C	-6.3834	0.260769	-5.46483
125	H	-5.31899	0.258048	-5.22143
126	H	-6.52385	0.288776	-6.5533
127	O	11.052	-3.91155	1.238294
128	O	5.147411	-4.18135	0.499751
129	N	9.282304	-4.87419	2.409691
130	N	9.321244	-5.05828	0.172813

131	N	6.87127	-4.60676	2.013816
132	N	6.936281	-5.5875	-0.00066
133	C	10.00815	-4.53394	1.274978
134	C	8.029486	-5.5039	2.085146
135	H	7.827257	-6.34853	2.755102
136	C	8.21564	-5.91205	0.590421
137	H	8.451469	-6.97362	0.447004
138	C	6.202625	-4.72755	0.800802
139	C	10.05002	-5.24069	-1.07417
140	H	11.03444	-4.79208	-0.9204
141	H	10.15222	-6.31017	-1.29683
142	C	6.53751	-5.89642	-1.35898
143	H	6.853765	-6.92251	-1.57853
144	H	5.449562	-5.81852	-1.40208
145	O	10.71492	-2.63867	-2.11217
146	O	4.967797	-4.12282	-2.95395
147	N	9.454334	-4.5906	-2.21995
148	N	9.187259	-3.05187	-3.82522
149	N	7.046258	-4.99858	-2.38462
150	N	6.874996	-3.74836	-4.23281
151	C	9.874498	-3.34084	-2.65266
152	C	8.364426	-5.11443	-3.00259
153	H	8.55905	-6.15213	-3.30021
154	C	8.278776	-4.1163	-4.20835
155	H	8.575739	-4.55785	-5.16779
156	C	6.167706	-4.26044	-3.16227
157	C	9.705566	-2.06504	-4.7568
158	H	9.880099	-2.55484	-5.72577
159	H	10.64956	-1.69291	-4.35041
160	C	6.229535	-2.94708	-5.25574
161	H	6.524056	-3.32586	-6.24048
162	H	5.156236	-3.07687	-5.10926
163	O	10.46249	0.643559	-4.26224
164	O	4.631015	-0.86165	-4.00327
165	N	8.852627	-0.90838	-4.93064
166	N	8.512773	1.258672	-5.38497
167	N	6.502358	-1.52458	-5.2241
168	N	6.185426	0.661344	-4.84837
169	C	9.400177	0.369423	-4.7835
170	C	7.677541	-0.89644	-5.78608
171	H	7.895526	-1.31102	-6.77897
172	C	7.300321	0.614763	-5.80406
173	H	6.979364	0.981644	-6.78738
174	C	5.664056	-0.60675	-4.61121

175	C	8.780112	2.67948	-5.4488
176	H	8.42101	3.055898	-6.41351
177	H	9.862103	2.808382	-5.37041
178	C	5.337216	1.827246	-4.67523
179	H	5.118815	2.266771	-5.66015
180	H	4.415282	1.474712	-4.20743
181	O	10.21899	3.955983	-3.31653
182	O	4.289018	2.663486	-2.12448
183	N	8.203348	3.465019	-4.37646
184	N	8.18025	4.838003	-2.60645
185	N	5.885955	2.85881	-3.8155
186	N	5.791113	4.440183	-2.23296
187	C	9.014364	4.058902	-3.41434
188	C	6.826489	3.873407	-4.28645
189	H	6.479176	4.285538	-5.24385
190	C	6.83284	4.921129	-3.12219
191	H	6.600842	5.943075	-3.45235
192	C	5.225956	3.247559	-2.65889
193	C	8.766152	5.803105	-1.70115
194	H	8.446063	6.81856	-1.96296
195	H	9.848273	5.707986	-1.81662
196	C	5.27169	5.186871	-1.10987
197	H	5.155115	6.236872	-1.40999
198	H	4.301081	4.755758	-0.85459
199	O	10.18522	4.080825	0.130717
200	O	4.407131	4.124773	1.390867
201	N	8.458491	5.588767	-0.29899
202	N	8.652242	4.72816	1.761429
203	N	6.077712	5.119903	0.10534
204	N	6.302533	5.093126	2.337986
205	C	9.209994	4.724025	0.482417
206	C	7.24263	5.978382	0.364036
207	H	7.003844	7.02977	0.165214
208	C	7.544627	5.666847	1.862769
209	H	7.815777	6.549387	2.4548
210	C	5.48055	4.707172	1.292331
211	C	9.474084	4.329834	2.891188
212	H	9.627886	5.193611	3.553477
213	H	10.43114	3.993617	2.483873
214	C	5.999852	4.767753	3.72125
215	H	4.9174	4.651008	3.785793
216	H	6.325793	5.605088	4.34614
217	O	10.57792	1.686387	3.077866
218	O	4.692172	2.203842	4.008612

219	N	8.928243	3.228081	3.654291
220	N	9.130769	1.365051	4.876956
221	N	6.579438	3.546184	4.249038
222	N	6.677268	1.412776	4.927782
223	C	9.648712	2.041617	3.782455
224	C	7.945884	3.393244	4.708542
225	H	8.218081	4.214713	5.383126
226	C	7.941055	1.987791	5.394429
227	H	7.964925	2.028014	6.490388
228	C	5.860616	2.367381	4.345187
229	C	9.714959	0.132104	5.360074
230	H	9.682753	0.146998	6.457042
231	H	10.75111	0.103802	5.014891
232	C	6.089927	0.192007	5.467068
233	H	6.193894	0.193046	6.559982
234	H	5.034534	0.215122	5.187958
235	O	11.00638	-1.88025	3.802543
236	O	4.949058	-1.52993	3.434732
237	N	9.089116	-1.07729	4.85966
238	N	9.151757	-3.22697	4.227326
239	N	6.643401	-1.04145	4.959006
240	N	6.746201	-2.96909	3.823103
241	C	9.880396	-2.04177	4.231992
242	C	7.876442	-1.6437	5.420237
243	H	7.911673	-1.64698	6.517824
244	C	7.836482	-3.07347	4.790648
245	H	7.627619	-3.86965	5.517339
246	C	5.998997	-1.80733	3.998055
247	C	9.718853	-4.46446	3.7313
248	H	10.79769	-4.30674	3.668603
249	H	9.492295	-5.2707	4.436689
250	C	6.153074	-4.1257	3.18232
251	H	5.161229	-3.82362	2.837839
252	H	6.069229	-4.94256	3.914543
253	Co	0.129312	-0.07871	-0.11964
254	N	1.973327	-0.06212	-0.02442
255	N	0.31213	1.287146	1.257175
256	N	0.473655	-1.43771	-1.47129
257	N	9.017204	-0.06783	0.19322
258	N	-1.80558	-0.10008	-0.20422
259	N	-0.23849	1.421005	-1.60583
260	N	-0.33402	-1.59082	1.341883
261	N	-8.86468	-0.03547	-0.11901
262	C	2.587992	0.778714	0.844314

263	C	3.980563	0.811763	0.935973
264	H	4.451706	1.472127	1.654122
265	C	4.737593	-0.04735	0.118407
266	C	4.075417	-0.91701	-0.76621
267	H	4.626215	-1.57174	-1.42933
268	C	2.682689	-0.89782	-0.8216
269	C	1.608283	1.573575	1.599583
270	C	1.92159	2.528474	2.566308
271	H	2.955391	2.732414	2.815256
272	C	0.881279	3.21094	3.196947
273	H	1.102952	3.957207	3.952495
274	C	-0.43605	2.923472	2.843482
275	H	-1.27779	3.431139	3.299726
276	C	-0.6806	1.95659	1.871719
277	H	-1.69475	1.715131	1.578903
278	C	1.802151	-1.70485	-1.6755
279	C	2.231323	-2.65605	-2.59989
280	H	3.286412	-2.8511	-2.74846
281	C	1.275085	-3.35712	-3.33377
282	H	1.589127	-4.10643	-4.0523
283	C	-0.07697	-3.08406	-3.12959
284	H	-0.85157	-3.60513	-3.68035
285	C	-0.43596	-2.11838	-2.19279
286	H	-1.47567	-1.87732	-2.0076
287	C	8.352523	1.104492	0.320943
288	H	8.970516	1.991502	0.40547
289	C	6.964639	1.139359	0.313773
290	H	6.46887	2.099554	0.385093
291	C	6.222557	-0.04586	0.167811
292	C	6.948269	-1.24581	0.039859
293	H	6.42962	-2.19421	-0.0453
294	C	8.33221	-1.23013	0.056017
295	H	8.939185	-2.12145	-0.04031
296	C	10.51056	-0.10289	0.220921
297	H	10.84687	-0.73633	-0.60056
298	H	10.8264	-0.50992	1.183158
299	H	10.87704	0.914968	0.107308
300	C	-2.45489	0.75634	-1.03367
301	C	-3.85243	0.798283	-1.07682
302	H	-4.34909	1.475916	-1.76104
303	C	-4.58766	-0.06486	-0.2499
304	C	-3.89847	-0.95292	0.588093
305	H	-4.43367	-1.60709	1.264115
306	C	-2.50164	-0.94677	0.594224

307	C	-1.55898	1.609467	-1.85002
308	C	-2.01209	2.535057	-2.79476
309	H	-3.06914	2.673502	-2.98189
310	C	-1.06692	3.282184	-3.49827
311	H	-1.39338	4.004958	-4.23879
312	C	0.289841	3.09182	-3.24096
313	H	1.05266	3.657575	-3.76401
314	C	0.661784	2.147872	-2.28382
315	H	1.708186	1.97214	-2.05222
316	C	-1.66529	-1.82429	1.44322
317	C	-2.18266	-2.81951	2.276746
318	H	-3.24599	-3.00826	2.351707
319	C	-1.29202	-3.5896	3.024528
320	H	-1.67349	-4.37276	3.671041
321	C	0.077024	-3.34337	2.927989
322	H	0.798716	-3.91872	3.496845
323	C	0.511849	-2.3318	2.071704
324	H	1.568554	-2.10462	1.964646
325	C	-8.19065	1.134638	-0.21452
326	H	-8.80058	2.030856	-0.21842
327	C	-6.80341	1.154449	-0.27479
328	H	-6.29468	2.109556	-0.31821
329	C	-6.0745	-0.04579	-0.23284
330	C	-6.80628	-1.24396	-0.13632
331	H	-6.29656	-2.20201	-0.1297
332	C	-8.18931	-1.21106	-0.08126
333	H	-8.80027	-2.10146	-0.00309
334	C	-10.3589	-0.0498	-0.06876
335	H	-10.6633	-0.70373	0.749653
336	H	-10.7332	-0.42104	-1.0244
337	H	-10.7034	0.969146	0.094331

Table S7. Cartesian Coordinates of the optimized structure of **1**-HS.

1	Co	-5.4E-05	0.001071	0.000207
2	N	-2.09546	0.000454	0.00066
3	N	-0.54345	-1.51184	1.433615
4	N	-0.54382	1.51393	-1.4312
5	N	-9.1566	-0.00445	-0.01116
6	N	2.095553	0.001711	-0.00139
7	N	0.543267	-1.51224	-1.43227
8	N	0.543954	1.513238	1.43257
9	N	9.156594	-0.00441	0.011617
10	C	-2.75757	-0.85396	0.808308

11	C	-4.1582	-0.88447	0.824497
12	H	-4.6865	-1.55964	1.487039
13	C	-4.87351	-0.00125	-0.0007
14	C	-4.15847	0.88291	-0.82517
15	H	-4.68693	1.557073	-1.48859
16	C	-2.75786	0.854205	-0.80744
17	C	-1.87388	-1.71439	1.632138
18	C	-2.34702	-2.66424	2.541082
19	H	-3.40999	-2.81108	2.69186
20	C	-1.43359	-3.4307	3.2675
21	H	-1.7825	-4.17069	3.979682
22	C	-0.0706	-3.22458	3.060973
23	H	0.674017	-3.79525	3.604009
24	C	0.325225	-2.2559	2.137725
25	H	1.376815	-2.06288	1.953304
26	C	-1.87434	1.715917	-1.63008
27	C	-2.34762	2.666741	-2.53791
28	H	-3.41061	2.813457	-2.68865
29	C	-1.43436	3.434547	-3.26309
30	H	-1.78341	4.175303	-3.97441
31	C	-0.07131	3.228863	-3.05638
32	H	0.673136	3.800598	-3.59852
33	C	0.324709	2.259367	-2.13414
34	H	1.37631	2.066738	-1.94942
35	C	-8.48126	-1.17823	0.035612
36	H	-9.08073	-2.08037	0.058466
37	C	-7.09519	-1.20278	0.044608
38	H	-6.60168	-2.16771	0.055728
39	C	-6.36452	-0.0023	-0.00149
40	C	-7.09679	1.197319	-0.0507
41	H	-6.60452	2.162866	-0.06345
42	C	-8.48259	1.170621	-0.05189
43	H	-9.08368	2.071644	-0.07886
44	C	-10.6507	-0.00252	0.019757
45	H	-11.0108	0.853947	-0.54808
46	H	-10.9775	0.063895	1.05936
47	H	-11.0108	-0.92437	-0.43395
48	C	2.757613	-0.85245	-0.80934
49	C	4.15821	-0.88341	-0.8252
50	H	4.686512	-1.55884	-1.48747
51	C	4.873532	-0.0005	0.000335
52	C	4.158591	0.883505	0.825032
53	H	4.687126	1.557454	1.488612
54	C	2.757977	0.854829	0.807371

55	C	1.873756	-1.71218	-1.63368
56	C	2.346785	-2.65894	-2.54584
57	H	3.409708	-2.80343	-2.69921
58	C	1.433313	-3.42523	-3.27243
59	H	1.782238	-4.16274	-3.98719
60	C	0.070397	-3.22217	-3.06265
61	H	-0.67429	-3.79296	-3.60545
62	C	-0.32535	-2.25634	-2.13636
63	H	-1.37694	-2.06596	-1.94922
64	C	1.874451	1.715835	1.630788
65	C	2.347795	2.66633	2.538924
66	H	3.41078	2.813441	2.689318
67	C	1.434498	3.433342	3.264944
68	H	1.783597	4.173863	3.976499
69	C	0.071461	3.227139	3.058831
70	H	-0.67299	3.798259	3.601616
71	C	-0.32457	2.257846	2.136332
72	H	-1.37619	2.064719	1.95224
73	C	8.480901	-1.17831	-0.03487
74	H	9.080597	-2.08037	-0.05722
75	C	7.095069	-1.20264	-0.04421
76	H	6.601249	-2.16742	-0.05516
77	C	6.364572	-0.00178	0.001345
78	C	7.096934	1.197517	0.050224
79	H	6.604911	2.163194	0.062518
80	C	8.482976	1.17059	0.051684
81	H	9.083864	2.07169	0.078361
82	C	10.65075	-0.00622	-0.01842
83	H	11.01187	0.881382	0.498316
84	H	10.97821	-0.00068	-1.05989
85	H	11.0091	-0.90063	0.488891

Table S8. Cartesian Coordinates of the optimized structure of **1**⊂2CB[7]-HS.

1	O	-11.1943	1.947526	3.736994
2	O	-5.13893	1.602087	3.440207
3	N	-9.2704	1.148791	4.78783
4	N	-9.35767	3.309506	4.193299
5	N	-6.82894	1.145365	4.978814
6	N	-6.95424	3.032334	3.778833
7	C	-10.0731	2.115187	4.173041
8	C	-8.08465	1.732899	5.39095
9	H	-8.15949	1.744846	6.486518
10	C	-8.04117	3.155492	4.750422

11	H	-7.82421	3.956963	5.468902
12	C	-6.19243	1.885522	3.992658
13	C	-9.92169	4.544044	3.687784
14	H	-11.0016	4.391831	3.629877
15	H	-9.6879	5.354716	4.385692
16	C	-6.35979	4.178841	3.121545
17	H	-6.26881	5.005414	3.84218
18	H	-5.37089	3.867819	2.776493
19	O	-11.3167	4.049084	1.218574
20	O	-5.38403	4.171215	0.426321
21	N	-9.49016	4.938246	2.359274
22	N	-9.56227	5.132141	0.124304
23	N	-7.08303	4.648128	1.952156
24	N	-7.16339	5.585449	-0.08139
25	C	-10.2485	4.628231	1.237013
26	C	-8.23402	5.553604	2.019802
27	H	-8.01999	6.402439	2.680973
28	C	-8.42664	5.952259	0.522102
29	H	-8.63101	7.019453	0.371384
30	C	-6.43023	4.734841	0.729588
31	C	-10.2993	5.328014	-1.11461
32	H	-10.3518	6.39593	-1.35856
33	H	-11.3021	4.931802	-0.93804
34	C	-6.78388	5.846082	-1.4544
35	H	-7.08613	6.870336	-1.70117
36	H	-5.69837	5.747395	-1.51416
37	O	-10.9926	2.675262	-1.98426
38	O	-5.26878	4.015745	-3.03394
39	N	-9.75481	4.627697	-2.25742
40	N	-9.48653	2.969192	-3.73947
41	N	-7.32796	4.924456	-2.44205
42	N	-7.19924	3.652868	-4.28099
43	C	-10.1674	3.344048	-2.58523
44	C	-8.64587	5.070469	-3.06099
45	H	-8.79709	6.100839	-3.40488
46	C	-8.60208	4.016715	-4.21854
47	H	-8.94069	4.409033	-5.18556
48	C	-6.4696	4.167002	-3.22582
49	C	-10.0297	1.925912	-4.58987
50	H	-10.2667	2.355864	-5.57421
51	H	-10.9418	1.559734	-4.11191
52	C	-6.58419	2.827534	-5.30407
53	H	-6.91673	3.181377	-6.28592
54	H	-5.50687	2.964262	-5.19957

55	O	-10.6584	-0.77278	-3.86418
56	O	-4.87334	0.780354	-4.14743
57	N	-9.15878	0.780075	-4.7527
58	N	-8.82946	-1.39542	-5.17022
59	N	-6.84225	1.403408	-5.2268
60	N	-6.47378	-0.77318	-4.83649
61	C	-9.66194	-0.49992	-4.50714
62	C	-8.04803	0.753774	-5.69064
63	H	-8.3419	1.143956	-6.6737
64	C	-7.6598	-0.75484	-5.70238
65	H	-7.41683	-1.14501	-6.69884
66	C	-5.94835	0.504536	-4.66603
67	C	-9.08603	-2.81885	-5.1832
68	H	-8.79746	-3.20859	-6.16709
69	H	-10.157	-2.96087	-5.02018
70	C	-5.5974	-1.92733	-4.71167
71	H	-5.44225	-2.37521	-5.70391
72	H	-4.65113	-1.55349	-4.3144
73	O	-10.3791	-4.24496	-3.07253
74	O	-4.47965	-2.60646	-2.13391
75	N	-8.41974	-3.568	-4.13725
76	N	-8.28431	-5.09297	-2.50469
77	N	-6.06315	-2.96003	-3.80903
78	N	-5.96351	-4.4044	-2.10045
79	C	-9.17461	-4.28507	-3.21097
80	C	-7.03661	-3.97929	-4.17322
81	H	-6.78059	-4.40467	-5.15348
82	C	-6.93425	-5.01388	-2.99987
83	H	-6.57674	-6.0026	-3.31891
84	C	-5.4059	-3.24381	-2.62284
85	C	-8.77015	-6.04942	-1.53661
86	H	-8.36946	-7.04553	-1.75381
87	H	-9.85786	-6.05058	-1.63638
88	C	-5.34695	-5.11036	-0.99713
89	H	-4.40558	-4.60336	-0.77237
90	H	-5.15702	-6.1493	-1.30079
91	O	-10.2699	-4.31109	0.220249
92	O	-4.51955	-3.94981	1.478609
93	N	-8.46258	-5.73902	-0.15076
94	N	-8.69373	-4.7917	1.867853
95	N	-6.11973	-5.10256	0.236804
96	N	-6.33222	-5.03185	2.466678
97	C	-9.25907	-4.87922	0.594108
98	C	-7.22635	-6.02605	0.524633

99	H	-6.91978	-7.06639	0.364782
100	C	-7.5465	-5.67667	2.010473
101	H	-7.78009	-6.5487	2.63323
102	C	-5.54691	-4.61395	1.404799
103	C	-9.52578	-4.35913	2.975942
104	H	-9.66259	-5.19154	3.680839
105	H	-10.4886	-4.06617	2.549145
106	C	-6.04038	-4.6579	3.839695
107	H	-6.33674	-5.49032	4.485814
108	H	-4.96299	-4.49921	3.901965
109	O	-10.6669	-1.72127	3.013872
110	O	-4.78069	-2.07736	4.155599
111	N	-9.0065	-3.21044	3.688533
112	N	-9.25497	-1.29335	4.817502
113	N	-6.65964	-3.44166	4.331541
114	N	-6.80902	-1.30707	4.991308
115	C	-9.7433	-2.02925	3.749202
116	C	-8.03795	-3.31296	4.76258
117	H	-8.29993	-4.12214	5.456062
118	C	-8.08408	-1.88858	5.408624
119	H	-8.16257	-1.89997	6.502933
120	C	-5.95885	-2.2535	4.446506
121	C	-9.89066	-0.07208	5.266694
122	H	-10.9108	-0.06847	4.875313
123	H	-9.90846	-0.08278	6.364607
124	C	-6.26504	-0.06581	5.525698
125	H	-5.20133	-0.07254	5.279535
126	H	-6.40277	-0.04793	6.614575
127	O	11.43563	3.846082	-1.0165
128	O	5.495273	4.188208	-0.87099
129	N	9.800017	4.740931	-2.41519
130	N	9.619289	5.063999	-0.20108
131	N	7.359383	4.509659	-2.23644
132	N	7.23643	5.624747	-0.29643
133	C	10.40639	4.4684	-1.19556
134	C	8.528209	5.395917	-2.25416
135	H	8.399758	6.195493	-2.99381
136	C	8.572956	5.899188	-0.77778
137	H	8.809428	6.965656	-0.67947
138	C	6.578411	4.712989	-1.10585
139	C	10.22094	5.316427	1.099921
140	H	11.21377	4.861094	1.070291
141	H	10.30496	6.396436	1.27294
142	C	6.714244	6.009848	0.99911

143	H	7.030052	7.040265	1.197516
144	H	5.625822	5.953235	0.939053
145	O	10.73211	2.749783	2.296896
146	O	4.958848	4.340621	2.514425
147	N	9.511432	4.72943	2.214713
148	N	9.04768	3.248383	3.829888
149	N	7.100899	5.156622	2.112589
150	N	6.723611	4.000068	3.991271
151	C	9.858633	3.486657	2.724867
152	C	8.351085	5.290374	2.857099
153	H	8.523612	6.338314	3.131321
154	C	8.130744	4.342986	4.08634
155	H	8.345338	4.817595	5.052062
156	C	6.135244	4.470454	2.832589
157	C	9.461863	2.294865	4.842493
158	H	9.566321	2.821058	5.802659
159	H	10.42718	1.886478	4.532656
160	C	5.965211	3.259907	4.982002
161	H	6.163972	3.686875	5.971158
162	H	4.914389	3.391563	4.719615
163	O	10.17636	-0.45599	4.512238
164	O	4.439858	1.124565	3.719872
165	N	8.568117	1.165379	4.994277
166	N	8.148678	-0.96335	5.548389
167	N	6.216004	1.834086	5.051848
168	N	5.888666	-0.36653	4.783033
169	C	9.091299	-0.12916	4.953147
170	C	7.326594	1.223916	5.748445
171	H	7.471251	1.69618	6.728837
172	C	6.919084	-0.27697	5.826132
173	H	6.511064	-0.57874	6.799212
174	C	5.413222	0.892682	4.426734
175	C	8.385072	-2.37798	5.740939
176	H	7.93896	-2.67337	6.697634
177	H	9.467013	-2.52719	5.765674
178	C	5.039451	-1.53092	4.604045
179	H	4.719434	-1.90244	5.589289
180	H	4.173134	-1.19848	4.027557
181	O	9.981637	-3.85534	3.875247
182	O	4.224599	-2.51913	2.023675
183	N	7.888055	-3.23531	4.685292
184	N	7.996027	-4.74099	3.031096
185	N	5.648657	-2.62481	3.869659
186	N	5.667182	-4.30995	2.394238

187	C	8.770729	-3.9223	3.857285
188	C	6.515273	-3.62172	4.495592
189	H	6.069897	-3.95739	5.442297
190	C	6.602684	-4.75129	3.413378
191	H	6.306674	-5.74037	3.789178
192	C	5.092626	-3.08195	2.683569
193	C	8.638353	-5.77771	2.250841
194	H	8.251974	-6.76426	2.532005
195	H	9.704385	-5.71129	2.480006
196	C	5.255661	-5.11237	1.264036
197	H	5.090168	-6.14229	1.607194
198	H	4.324587	-4.68449	0.885649
199	O	10.28383	-4.16928	0.514996
200	O	4.69276	-4.13747	-1.35575
201	N	8.494493	-5.63559	0.814394
202	N	8.924007	-4.86281	-1.24521
203	N	6.185151	-5.12249	0.13978
204	N	6.641137	-5.20676	-2.05524
205	C	9.341476	-4.81191	0.084888
206	C	7.344441	-6.02209	0.042716
207	H	7.053428	-7.05714	0.256839
208	C	7.811847	-5.78353	-1.42662
209	H	8.122078	-6.69668	-1.94883
210	C	5.729323	-4.74719	-1.12067
211	C	9.867494	-4.51707	-2.29344
212	H	10.08315	-5.40825	-2.89995
213	H	10.77786	-4.17116	-1.79699
214	C	6.490892	-4.94742	-3.477
215	H	5.424043	-4.81452	-3.66076
216	H	6.860289	-5.82237	-4.02112
217	O	11.02505	-1.89501	-2.47978
218	O	5.268679	-2.39302	-4.06079
219	N	9.421066	-3.44458	-3.15715
220	N	9.787014	-1.6457	-4.43806
221	N	7.149343	-3.76509	-3.9991
222	N	7.359627	-1.67939	-4.7876
223	C	10.17037	-2.2737	-3.26323
224	C	8.561602	-3.65443	-4.30668
225	H	8.893799	-4.51557	-4.90016
226	C	8.661052	-2.28959	-5.06317
227	H	8.818987	-2.39079	-6.14406
228	C	6.465156	-2.58775	-4.24812
229	C	10.45509	-0.45872	-4.93032
230	H	10.55579	-0.5533	-6.01945

231	H	11.44256	-0.4198	-4.46425
232	C	6.861658	-0.48694	-5.4614
233	H	7.085957	-0.55599	-6.53376
234	H	5.781667	-0.47864	-5.30127
235	O	11.6321	1.668923	-3.44406
236	O	5.565071	1.342555	-3.62889
237	N	9.801164	0.79166	-4.59355
238	N	9.837373	2.986331	-4.13503
239	N	7.381836	0.766642	-4.96963
240	N	7.403007	2.751316	-3.93131
241	C	10.54999	1.800214	-3.9796
242	C	8.66738	1.325977	-5.32703
243	H	8.826126	1.255329	-6.41136
244	C	8.577488	2.794082	-4.80164
245	H	8.437535	3.538879	-5.5962
246	C	6.662616	1.585173	-4.11094
247	C	10.36026	4.250968	-3.66238
248	H	11.42708	4.096249	-3.48729
249	H	10.20754	5.013925	-4.43263
250	C	6.755715	3.948823	-3.43379
251	H	5.73252	3.671528	-3.16925
252	H	6.749516	4.713381	-4.22488
253	Co	0.0032	0.033398	-0.39979
254	N	2.046808	0.101427	-0.4072
255	N	0.538119	-1.46591	-1.78857
256	N	0.43991	1.670783	0.941185
257	N	9.070871	0.066846	0.12119
258	N	-2.03588	0.091009	-0.17905
259	N	-0.38511	-1.44385	1.089779
260	N	-0.63602	1.276544	-1.99564
261	N	-9.07922	0.030456	0.092577
262	C	2.737068	-0.78311	-1.15584
263	C	4.135866	-0.8262	-1.11506
264	H	4.677435	-1.53277	-1.73239
265	C	4.810459	0.077642	-0.27991
266	C	4.070962	1.003984	0.47477
267	H	4.567585	1.692504	1.146084
268	C	2.676824	0.985779	0.390739
269	C	1.869936	-1.66072	-1.97883
270	C	2.354191	-2.60739	-2.88603
271	H	3.417803	-2.74675	-3.03252
272	C	1.435746	-3.36948	-3.60767
273	H	1.78868	-4.10655	-4.32137
274	C	0.069741	-3.1741	-3.40534

275	H	-0.6713	-3.75064	-3.94736
276	C	-0.3362	-2.20989	-2.48489
277	H	-1.38903	-2.02364	-2.29418
278	C	1.767146	1.894784	1.135469
279	C	2.224238	2.919623	1.966204
280	H	3.280702	3.099491	2.11956
281	C	1.287996	3.732141	2.60718
282	H	1.628989	4.537988	3.248515
283	C	-0.07198	3.499922	2.410979
284	H	-0.82927	4.108736	2.891424
285	C	-0.44975	2.455268	1.568744
286	H	-1.49581	2.233962	1.384191
287	C	8.402907	-1.11065	0.045942
288	H	9.014044	-2.00356	0.125168
289	C	7.023734	-1.13715	-0.09957
290	H	6.51835	-2.09461	-0.13033
291	C	6.293964	0.063658	-0.166
292	C	7.018203	1.265527	-0.08781
293	H	6.509788	2.22105	-0.16767
294	C	8.397069	1.239412	0.053655
295	H	9.001312	2.134819	0.120315
296	C	10.55394	0.057511	0.308938
297	H	10.94172	1.040474	0.048573
298	H	10.97025	-0.7048	-0.34946
299	H	10.76055	-0.15959	1.358614
300	C	-2.63126	-0.70554	0.732051
301	C	-4.02412	-0.74336	0.859422
302	H	-4.48482	-1.38557	1.600115
303	C	-4.80098	0.066287	0.014213
304	C	-4.162	0.88446	-0.93081
305	H	-4.73419	1.48077	-1.63037
306	C	-2.76703	0.860597	-1.01018
307	C	-1.67259	-1.51701	1.521809
308	C	-2.03548	-2.30414	2.617294
309	H	-3.06289	-2.35309	2.956112
310	C	-1.04227	-3.02873	3.277298
311	H	-1.30322	-3.64113	4.134246
312	C	0.276023	-2.95628	2.829352
313	H	1.075691	-3.50597	3.312476
314	C	0.561437	-2.15028	1.72922
315	H	1.574649	-2.0652	1.34996
316	C	-1.95319	1.611547	-1.99312
317	C	-2.46938	2.574437	-2.86368
318	H	-3.51881	2.841686	-2.85244

319	C	-1.60067	3.200329	-3.75758
320	H	-1.98118	3.956093	-4.43656
321	C	-0.25122	2.84684	-3.76895
322	H	0.450518	3.306735	-4.4554
323	C	0.187532	1.878624	-2.86862
324	H	1.226886	1.567111	-2.83666
325	C	-8.39786	-1.13358	0.23056
326	H	-9.00662	-2.0265	0.322113
327	C	-7.01101	-1.14992	0.227252
328	H	-6.49796	-2.09987	0.311693
329	C	-6.28727	0.046645	0.073407
330	C	-7.02541	1.23538	-0.05998
331	H	-6.5181	2.190716	-0.1455
332	C	-8.41118	1.200108	-0.04559
333	H	-9.02755	2.084135	-0.14627
334	C	-10.5735	0.007035	0.062793
335	H	-10.9383	1.01749	0.236908
336	H	-10.9142	-0.66537	0.850164
337	H	-10.8852	-0.33857	-0.92485

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