Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Surprising Substituent Effect in Corroles on the Electrochemical Activation of Oxygen Reduction

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Experimental

The four cobalt(III) corroles depicted in Scheme 1 were synthesized and characterized according to previously published procedures.[1] Their performance as ORR catalysts was compared using the rotating ring-disk electrode (RRDE) method in both acidic and alkaline solutions. 0.2 mg cobalt(III) corrole was mixed with 1 mL isopropanol (> 99.7%, Daejung) for 10 min. The catalyst solution (5 μL) was applied on a glassy carbon surface of a rotating ring-disk electrode (glassy carbon disk with a surface area of 0.247 cm^2 and a platinum ring) and was left at room temperature to dry. The second setup used for testing the catalytic performance of the same corroles, was to adsorb them onto a high surface area carbon (BP2000, Cabot Corporation) according to previously published procedures.[2]

Electrochemical characterization:

Linear sweep voltammetry (LSV) and rotating ring-disk electrode (RRDE) measurements were all performed with a BioLogic VSP potentiostat. RRDE experiments were conducted with Pine Instruments rotator and electrodes (glassy carbon disk and platinum ring). The collection efficiency of the ring electrode is 37% according to the manufacturer was confirmed in our lab. The electrochemical measurements were conducted either in a 0.1 M aqueous solution of KOH (Acros Organics, 99.98%), or a 0.5 M aqueous solution of H_2SO_4 (Acros Organics, 96%). The counter electrode was a glassy carbon rod (3 mm diameter) and the reference electrode was a homemade hydrogen reference electrode. For the measurement of background currents, Ar gas (99.999% purity) was purged into the cell. When the catalyst-assisted reduction of oxygen was tested, O_2 gas (99.999% purity) was purged in the cell for about 20 min prior to the measurement, to assure the saturation of the solution with dissolved oxygen. Unless stated otherwise, RRDE measurements were performed at selected rotation speeds from 225 to 1600 and a scan rate of 5 mV/s. The disk electrode potential was linearly swept from 1.1 to 0.05 V vs. RHE, whereas the Pt ring's potential was kept constant at 1.2 V vs. RHE.

Computational Methods:

To rationalize the experimental data obtained for ORR catalysis by the cobalt(III) corroles, density functional theory (DFT) theoretical calculations were performed to understand the effect of the various substituents on the electronic structure of the catalysts. Specifically, we used the unrestricted B3LYP (UB3LYP) functional[3] and the 6-31G(d,p) basis set,[4] with the Gaussian 09 program.[5] All calculations were performed using the polarizable continuum model (PCM)[6] and water was used as solvent. For each of these transition metal complexes we evaluated the wavefunction stability with different multiplicities. All complexes were geometry optimized,

followed by frequency calculations to examine the nature of the stationary points. Of the various spin multiplicities (1, 3, and 5) relevant for the neutral corroles, a multiplicity of 3 was determined to correspond to the global electronic minimum for all derivatives. A multiplicity of 2 (rather than 4) appeared to correspond to the global electronic minimum for all reduced corroles (charge -1).

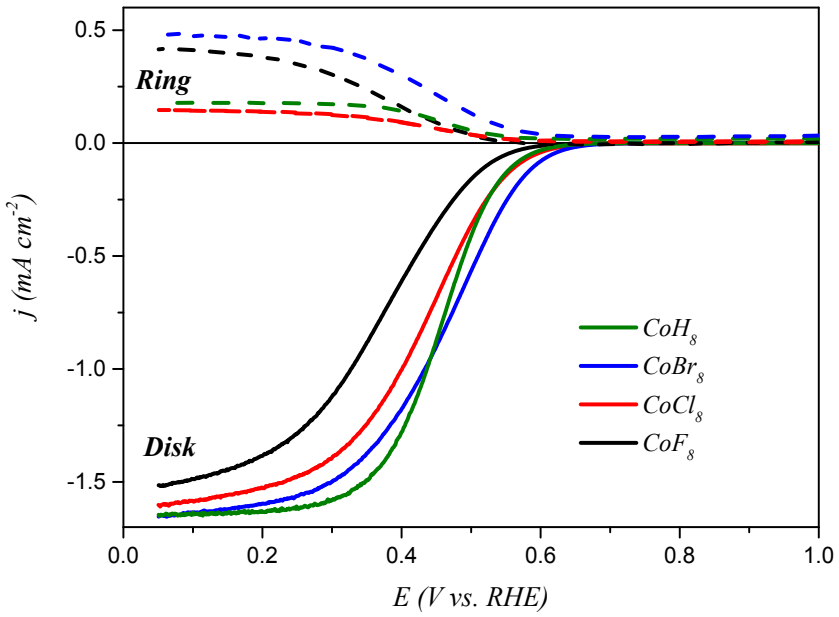
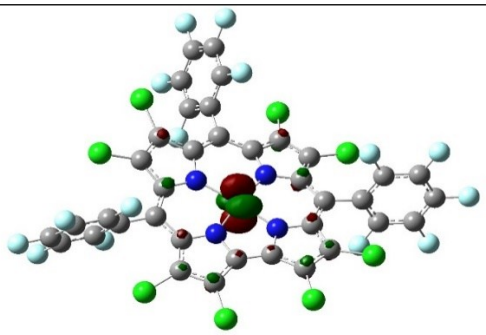


Figure S1. RRDE measurements of Co-X_8 corroles in 0.5 M H_2SO_4, at a rotor speed of 900rpm and a scan rate of 5 mV/s.

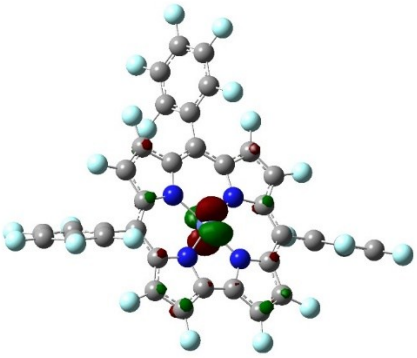
Table S1. Onset potential, half wave potential and limiting currents obtained from the RRDE measurements.

Catalyst material	Onset potential (at j=0.01 mA cm^{-2}) V *vs.* RHE	ORR half wave potential V *vs.* RHE	Limiting current density I mA/cm^2	Limiting current density II mA/cm^2
In 0.1 M KOH				
Co-H_8	0.768	0.606	1.425	2.080
Co-Br_8	0.810	0.644	-	2.26
Co-Cl_8	0.725	0.567	1.71	2.096
Co-F_8	0.630	0.466	1.50	2.161
In 0.5 M H_2SO_4				
Co-H_8	0.636	0.456	1.65	-
Co-Br_8	0.666	0.468	1.65	-
Co-Cl_8	0.647	0.442	1.60	-
Co-F_8	0.607	0.382	1.52	-

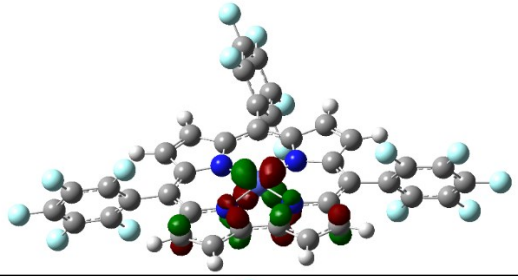
(a) Cl



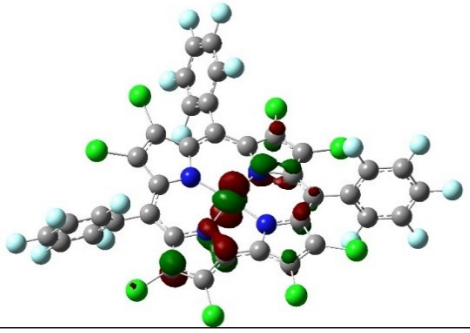
(b) F



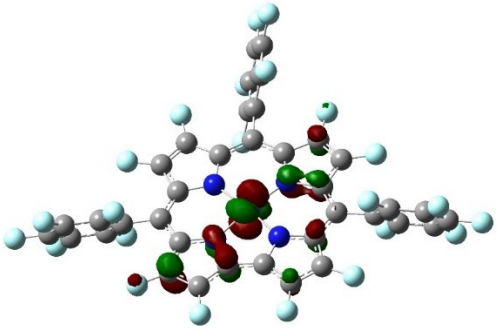
(c) H



(d) Cl



(e) F



(f) H

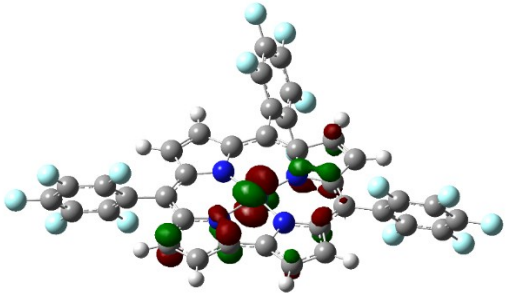
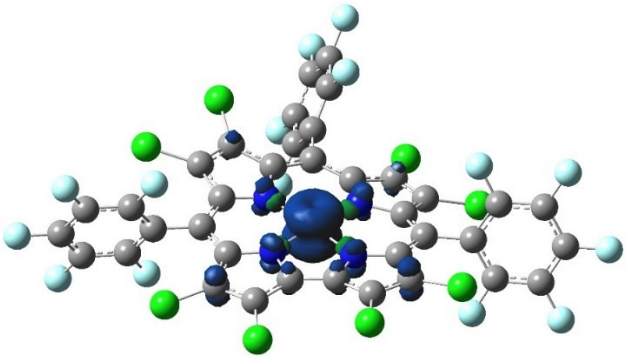
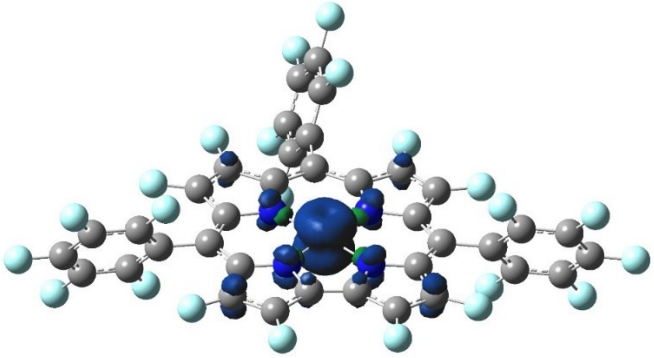


Figure S2: LUMO isovalue surfaces for Co(tpfcX_8)- (a) Cl, (b) F, (c) H and HOMO isovalue surfaces for Co(tpfcX_8) of Co(II) corrole (after vertical electron reduction)- (d) Cl, (e) F, (f) H. Isodensity value: 0.05 e/Å^3.

(a) Cl



(b) F



(c) H

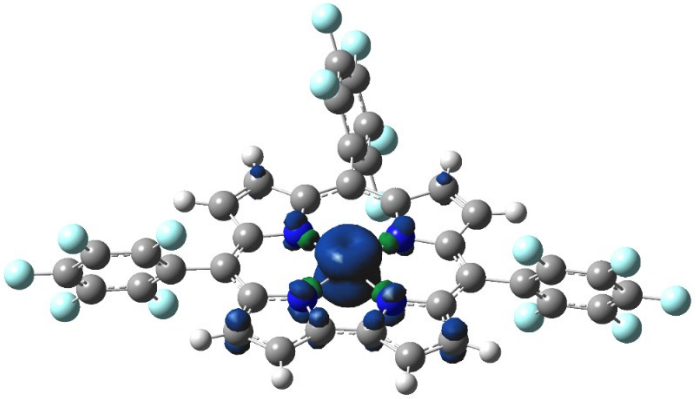
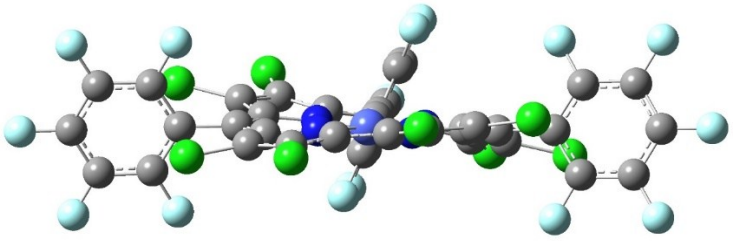


Figure S3: Spin density isovalue surfaces for Co(tpfcX$_8$)- (a) Cl, (b) F, (c) H. Isodensity value: 0.004 e/Å^3.

(a) Cl



(b) H

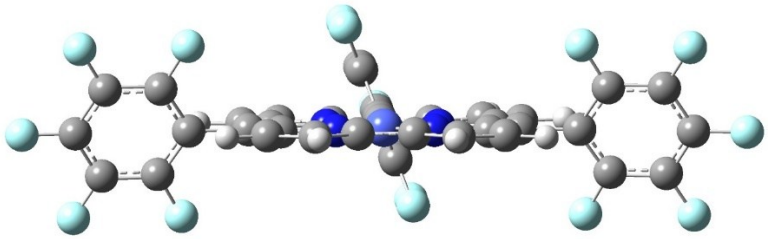


Figure S4: Structures of Co(tpfcX$_8$)- (a) Cl, (b) H.

Equation S1: $j_L=0.2nFD^{2/3}\omega^{1/2}\nu^{-1/6}C(O_2)$

jL- Exchange current density (A/cm^2)
n- number of electrons transferred
F- Faraday constant (C/mol)
D- Oxygen diffusion coefficient (cm^2/s)
ω- rotation speed (rpm)
ν- kinematic viscosity of the solution (cm^2/s)
C(O_2)- bulk concentration of oxygen in solution (mol/cm^3)

Table S2:

Parameter	**Symbol**	**0.5M H_2SO_4**	**0.1M KOH**
oxygen diffusion coefficient	D	1.5×10^{-5}	1.9×10^{-5}
bulk concentration of oxygen	$C(O_2)$	1.3×10^{-6}	1.2×10^{-6}
kinematic viscosity of the solution	ν	0.01	0.01

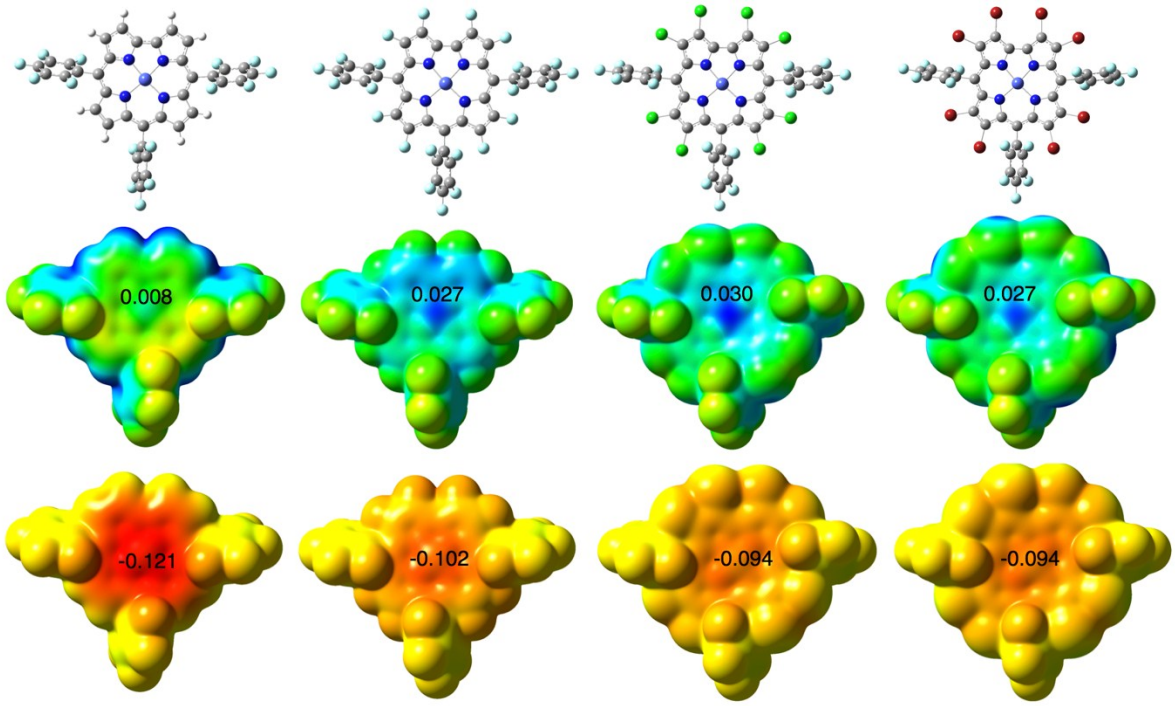
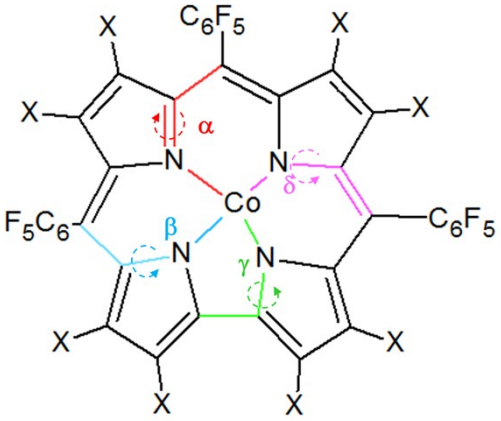


Figure S5. Molecular electrostatic potentials (MEP) for various β-corrole complexes. Top row (left to right): β-H, F, Cl, Br-corroles; middle row – neutral Co(III) complexes; bottom row – anionic Co(II) complexes. The extrema values near the Co atom are marked (a.u.). Color code: Blue – positive MEP, red – negative MEP.

Table S3. Co(III)corrole complexes: dihedral angles of Co-N-C-C and average Co-N distance (Å) according to Scheme 1S.

Corrole	Dihedral angles				Average Co-N distance (Å)
	α	β	γ	δ	
Co-H_8	-0.3	-1.1	-1.0	2.1	1.857
Co-Br_8	13.3	-11.2	6.1	-11.0	1.871
Co-Cl_8	17.2	-13.4	6.6	-14.3	1.870
Co-F_8	3.4	-3.5	-0.7	0.2	1.861



Scheme S1. The chemical structure of the cobalt(III) metallocorrole with the four dihedral angels (Table 3)

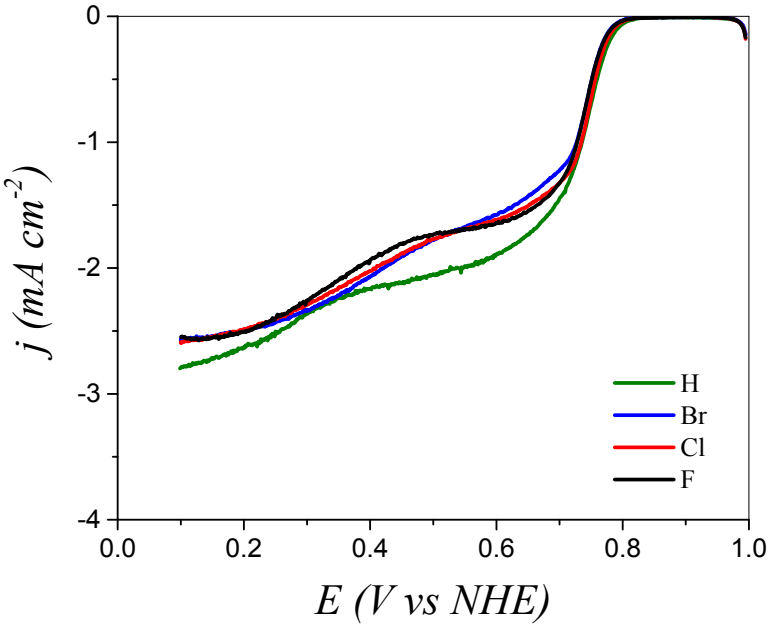


Figure S6. RDE measurements of the halogenated Co corroles that were adsorbed on BP2000 carbon in 0.5M H_2SO_4, at a rotor speed of 900 rpm and a scan rate of 5 mV/s.

Table S4. Onset potential, half wave potential and limiting currents obtained from the RRDE measurements.

Catalyst material	Onset potential (at j=0.01 mA cm^{-2}) V *vs.* RHE	Half wave potential V *vs.* RHE	Limiting current density I mA/cm^2	Limiting current density II mA/cm^2
In 0.1 M KOH				
Co-H_8/BP2000	0.847	0.784	3.571	3.772
Co-Br_8/BP2000	0.849	0.790	3.15	3.57
Co-Cl_8/BP2000	0.844	0.783	3.00	3.54
Co-F_8/BP2000	0.845	0.791	2.318	3.008
In 0.5 M H_2SO_4				
Co-H_8/BP2000	0.784	0.738	1.53	2.18
Co-Br_8/BP2000	0.781	0.743	1.69	2.57
Co-Cl_8/BP2000	0.785	0.746	1.67	2.60
Co-F_8/BP2000	0.781	0.738	1.69	2.57

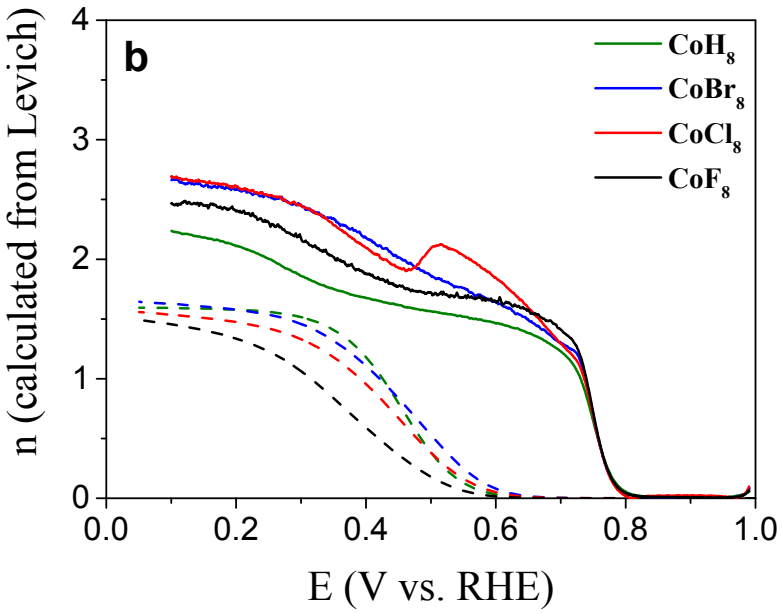


Figure S7. The calculated number of electrons (using the Levich equation) transferred during the ORR on the Co-X_8 corroles in 0.5M H_2SO_4, at a rotation speed of 900 rpm and a scan rate of 5 mV/s. Dashed line- corrole on glassy carbon (GC), solid line- corrole adsorbed on BP2000.

Co-Br_8 –No solvent (charge=0, multiplicity=3)

```
0 3
 C                -1.22974700    2.18569800    0.14071800
 C                -2.52357900    2.77514800    0.37310900
 C                -3.45936000    1.77376700    0.33534100
 C                -2.78169700    0.52991800    0.10234300
 N                -1.40225300    0.81296600    0.01885700
 C                -0.69942500   -3.13403400   -0.05571400
 C                -1.77076100   -4.03551100   -0.22854400
 C                -2.93745600   -3.27932900   -0.28015800
 C                -2.58503400   -1.89856400   -0.12469100
 N                -1.22165900   -1.84465800   -0.01276100
 C                 0.69938500   -3.13404300    0.05569400
 C                 1.77070800   -4.03553400    0.22853000
 C                 2.93741200   -3.27936800    0.28015300
 C                 2.58501100   -1.89859800    0.12468200
 N                 1.22163600   -1.84467400    0.01274300
 C                 1.22977500    2.18568200   -0.14072600
 C                 2.52361500    2.77511500   -0.37312000
 C                 3.45938200    1.77372100   -0.33535300
 C                 2.78170300    0.52988100   -0.10235000
 N                 1.40226400    0.81294800   -0.01886400
 C                 0.00001900    2.84727500   -0.00000400
 C                 3.36657400   -0.73426500    0.03160500
 C                -3.36658300   -0.73422200   -0.03160800
 Co               -0.00000300   -0.45028300   -0.00000600
 C                 4.84767700   -0.89150600    0.05126700
```

C	5.57391600	-0.74090500	1.23243500
C	5.55067700	-1.24288100	-1.10159300
C	6.95211600	-0.92052500	1.27083700
C	6.92822300	-1.42514600	-1.09089500
C	7.62961800	-1.26362400	0.10258400
C	-4.84768700	-0.89145200	-0.05125300
C	-5.57393500	-0.74089000	-1.23242200
C	-5.55067900	-1.24279100	1.10162300
C	-6.95213400	-0.92051000	-1.27080800
C	-6.92822500	-1.42505600	1.09094000
C	-7.62962900	-1.26357200	-0.10254000
C	0.00002900	4.33796400	-0.00000400
C	-0.31735000	5.05989400	-1.15054400
C	0.31741600	5.05988900	1.15053700
C	-0.31960700	6.44944000	-1.16464000
C	0.31969100	6.44943500	1.16463500
C	0.00004600	7.14479100	-0.00000200
F	0.62675900	4.41020800	2.27982800
F	0.62436600	7.12076900	2.28024900
F	0.00005400	8.47936300	-0.00000100
F	-0.62427400	7.12078000	-2.28025300
F	-0.62670200	4.41021900	-2.27983500
F	-4.94148600	-0.41323000	-2.36604500
F	-7.62806300	-0.76908500	-2.41426300
F	-8.95238300	-1.43758600	-0.12627200
F	-7.58167200	-1.75498400	2.20977200
F	-4.89395900	-1.40379000	2.25723900
F	4.94146100	-0.41320300	2.36604300
F	7.62803600	-0.76906100	2.41429200
F	8.95237200	-1.43763800	0.12633200
F	7.58167700	-1.75511000	-2.20971200
F	4.89396500	-1.40391500	-2.25720900
Br	-5.28669900	2.09858500	0.60848400
Br	-2.99263800	4.55299700	0.74929400
Br	2.99269700	4.55295700	-0.74930900
Br	5.28672400	2.09851000	-0.60851300
Br	4.62194400	-4.04251700	0.56538700
Br	1.71358100	-5.89081800	0.42449400
Br	-1.71366000	-5.89079500	-0.42450700
Br	-4.62200100	-4.04245600	-0.56537400

Co-Cl_8 –No solvent (charge=0, multiplicity=3)

0 3

C	1.21840700	1.94585300	-0.19957600
C	2.49635500	2.52480300	-0.52383100
C	3.43597300	1.52556500	-0.49473900
C	2.77440200	0.29058100	-0.17866500
N	1.40011000	0.57737700	-0.04480600
C	0.69946500	-3.36055400	0.04373200
C	1.76688300	-4.26666400	0.21794600
C	2.93730300	-3.51372400	0.26361700
C	2.58968700	-2.13045300	0.09481300
N	1.22537100	-2.07565200	-0.01598400
C	-0.69967400	-3.36051600	-0.04369400
C	-1.76715000	-4.26657300	-0.21782900
C	-2.93752700	-3.51356700	-0.26350900
C	-2.58982300	-2.13030600	-0.09480100
N	-1.22550200	-2.07558000	0.01595700
C	-1.21830800	1.94593400	0.19945600
C	-2.49623600	2.52496900	0.52364800
C	-3.43591100	1.52578600	0.49454400
C	-2.77439900	0.29075200	0.17854900
N	-1.40008800	0.57746300	0.04471500
C	0.00007200	2.61392500	-0.00005200
C	-3.37123600	-0.96716700	0.02096100
C	3.37117200	-0.96736500	-0.02100700
Co	-0.00002600	-0.68344900	-0.00003000
C	-4.85516800	-1.10377200	-0.01557800
C	-5.57432800	-0.82012800	-1.17798600
C	-5.57302500	-1.54856100	1.09618600

C	-6.95689700	-0.96459800	-1.23690400
C	-6.95486000	-1.69668000	1.06423500
C	-7.64774100	-1.40329300	-0.10923800
C	4.85509600	-1.10403600	0.01557500
C	5.57427200	-0.82003000	1.17788400
C	5.57294500	-1.54916800	-1.09605900
C	6.95684100	-0.96448400	1.23683700
C	6.95478100	-1.69727700	-1.06407400
C	7.64767400	-1.40353000	0.10930100
C	0.00013400	4.10593500	-0.00001200
C	0.45545100	4.82973100	1.10339200
C	-0.45511500	4.82984500	-1.10336800
C	0.45837600	6.22003700	1.11724100
C	-0.45791300	6.22015100	-1.11712600
C	0.00026400	6.91614700	0.00008000
F	-0.90698900	4.18045000	-2.18487800
F	-0.89756200	6.89051100	-2.18691800
F	0.00032500	8.25024800	0.00012300
F	0.89808600	6.89028700	2.18707600
F	0.90726300	4.18022500	2.18486100
F	4.93095900	-0.39041500	2.27169700
F	7.62286800	-0.68510800	2.36139500
F	8.97341400	-1.54416100	0.15272300
F	7.61987900	-2.12031600	-2.14360300
F	4.92473000	-1.84170700	-2.23134200
F	-4.93100200	-0.39090600	-2.27194600
F	-7.62291600	-0.68558000	-2.36155600
F	-8.97348200	-1.54392700	-0.15262700
F	-7.61997100	-2.11936700	2.14389400
F	-4.92482000	-1.84072300	2.23157300
Cl	5.09430700	1.79732700	-0.87843300
Cl	2.88063000	4.14049000	-0.98472800
Cl	-2.88044000	4.14069400	0.98446900
Cl	-5.09425700	1.79765700	0.87811200
Cl	-4.48720100	-4.20708000	-0.54193700
Cl	-1.68125900	-5.97153100	-0.40297500
Cl	1.68088600	-5.97160600	0.40319000
Cl	4.48691900	-4.20731200	0.54216500

Co-F_8 –No solvent (charge=0, multiplicity=3)

0 3

C	-1.23070400	1.79396000	0.09862600
C	-2.53109200	2.38466200	0.17345600
C	-3.45722700	1.38556600	0.14531300
C	-2.77570500	0.13436600	0.05035100
N	-1.39371900	0.41710200	0.02975600
C	-0.68433200	-3.50603200	-0.03447800
C	-1.75375100	-4.41808600	-0.09492500
C	-2.92189600	-3.67373200	-0.09170400
C	-2.58222500	-2.28724400	-0.02383300
N	-1.21577800	-2.22055900	0.01287400
C	0.71001500	-3.50153800	-0.03845600
C	1.78528800	-4.40695700	-0.09521100
C	2.94852500	-3.65489700	-0.10104000
C	2.59972100	-2.27014300	-0.04387700
N	1.23310400	-2.21229900	-0.00375400
C	1.22305500	1.80340700	0.06177200
C	2.52053900	2.40504700	0.05736900
C	3.45293000	1.41187600	0.02925800
C	2.77843300	0.15348300	0.00094600
N	1.39435600	0.42616800	0.02656000
C	-0.00606600	2.47036500	0.10190600
C	3.38496600	-1.10603300	-0.04050200
C	-3.37515000	-1.12848200	0.00204400
Co	0.00428400	-0.83309900	0.01758900
C	4.86764100	-1.23970300	-0.09540600
C	5.58022100	-1.83357300	0.95049100
C	5.60429100	-0.80780800	-1.20262500
C	6.96197200	-1.98984700	0.90680700
C	6.98625300	-0.94912300	-1.26890200

C	7.66704600	-1.54400400	-0.20867600
C	-4.85740700	-1.26888500	-0.02901200
C	-5.61662800	-0.80635500	-1.10859000
C	-5.54875000	-1.89587000	1.01208800
C	-6.99903400	-0.95172500	-1.15347400
C	-6.93038400	-2.05667300	0.98928100
C	-7.65779300	-1.58089900	-0.09918300
C	-0.01262700	3.96370400	0.15387500
C	-0.37928100	4.72783500	-0.95604600
C	0.34386300	4.65349400	1.31454300
C	-0.39366700	6.11857300	-0.92072500
C	0.34079900	6.04323900	1.37583100
C	-0.03088200	6.77761600	0.25178100
F	0.71537400	3.96982100	2.40661500
F	0.69042200	6.67497800	2.50128900
F	-0.03904000	8.11114400	0.29839000
F	-0.75195700	6.82222100	-1.99976600
F	-0.74381400	4.11721500	-2.09254000
F	-5.01075500	-0.19469300	-2.13554300
F	-7.69589000	-0.49650400	-2.19941700
F	-8.98314700	-1.72725300	-0.13254000
F	-7.56033000	-2.65875500	2.00295900
F	-4.87442800	-2.36611100	2.07107700
F	4.92683400	-2.27630100	2.03406500
F	7.61303900	-2.55981100	1.92567600
F	8.99222700	-1.68621800	-0.26230500
F	7.66170800	-0.52267500	-2.34076000
F	4.97622300	-0.22981200	-2.23583300
F	-2.80621900	3.68339500	0.27643400
F	-4.77557800	1.55945700	0.22115300
F	-4.15196400	-4.17708300	-0.15119900
F	-1.65539200	-5.74245800	-0.15274400
F	1.69558900	-5.73238900	-0.14162900
F	4.18190500	-4.15057700	-0.15695000
F	4.77166200	1.59824800	0.03873300
F	2.78940700	3.70896800	0.07512600

Co-H_8 –No solvent (charge=0, multiplicity=3)

0 3

C	-1.23290800	1.60312500	0.07512300
C	-2.52768600	2.21577700	0.08053000
C	-3.46069000	1.21848600	0.03030000
C	-2.76850500	-0.03288800	-0.01639000
N	-1.38789000	0.22928000	0.01565100
H	-2.71099900	3.27958700	0.11382600
H	-4.53473200	1.33122400	0.03017600
C	-0.70841300	-3.69734400	-0.13846900
C	-1.78657400	-4.60792800	-0.20905900
C	-2.95190200	-3.85300300	-0.19557000
C	-2.58679800	-2.47336800	-0.11376200
N	-1.22355700	-2.40774800	-0.07977700
H	-1.70972900	-5.68465600	-0.26558000
H	-3.96391400	-4.22953800	-0.24202800
C	0.69661300	-3.69975300	-0.12701000
C	1.77257100	-4.61376600	-0.18599100
C	2.94012300	-3.86295700	-0.15261100
C	2.57861600	-2.48246200	-0.06946900
N	1.21520500	-2.41226300	-0.05392800
H	1.69287900	-5.68992200	-0.24907900
H	3.95137400	-4.24270800	-0.18799900
C	1.23540200	1.59779100	0.10963000
C	2.53116300	2.20346700	0.18653900
C	3.46155700	1.20318000	0.14642200
C	2.76662700	-0.04330100	0.04436700
N	1.38697600	0.22474700	0.02891300
H	2.71631500	3.26388400	0.27416800
H	4.53513100	1.30982000	0.19608000
C	0.00224400	2.26346800	0.12380400
C	3.35756000	-1.31030000	-0.01576000
C	-3.36232800	-1.29820800	-0.08135100

Co	-0.00224800	-1.02810000	-0.01893400
C	4.84025600	-1.43311700	-0.02541500
C	5.52755600	-2.05921300	1.02194000
C	5.61507100	-0.95017900	-1.08751400
C	6.91287800	-2.20089300	1.01960400
C	7.00218400	-1.07258600	-1.10759300
C	7.65308400	-1.70309100	-0.04995900
C	-4.84507300	-1.41721600	-0.12280600
C	-5.59530500	-0.94890700	-1.20860000
C	-5.55631500	-2.02637000	0.91839900
C	-6.98202500	-1.06786100	-1.25672600
C	-6.94169700	-2.16458600	0.88839600
C	-7.65733900	-1.68076300	-0.20405500
C	0.00543300	3.75334900	0.19241300
C	-0.42551200	4.43742400	1.33486200
C	0.44016200	4.53507100	-0.88426400
C	-0.43176100	5.82834600	1.40748700
C	0.45230000	5.92687400	-0.83231900
C	0.01171000	6.57541200	0.31884100
F	0.86410600	3.94635400	-2.01066500
F	0.87458000	6.64207700	-1.88099400
F	0.01432400	7.90932300	0.37872100
F	-0.85102300	6.44890200	2.51606100
F	-0.85259700	3.75203700	2.40449600
F	-4.98134500	-0.36513500	-2.24687700
F	-7.66606900	-0.60863900	-2.31038200
F	-8.98606100	-1.80377700	-0.24221400
F	-7.58752500	-2.74807700	1.90401500
F	-4.90361700	-2.49527500	1.99097700
F	4.85110200	-2.54094400	2.07404200
F	7.53529400	-2.80069300	2.04040000
F	8.98197100	-1.82951400	-0.06141000
F	7.70993900	-0.59999100	-2.13937900
F	5.02531700	-0.34968600	-2.12991800

Co-Br_8 – Solvent= water (charge=0, multiplicity=3)

0 3

C	-1.22974700	2.18569800	0.14071800
C	-2.52357900	2.77514800	0.37310900
C	-3.45936000	1.77376700	0.33534100
C	-2.78169700	0.52991800	0.10234300
N	-1.40225300	0.81296600	0.01885700
C	-0.69942500	-3.13403400	-0.05571400
C	-1.77076100	-4.03551100	-0.22854400
C	-2.93745600	-3.27932900	-0.28015800
C	-2.58503400	-1.89856400	-0.12469100
N	-1.22165900	-1.84465800	-0.01276100
C	0.69938500	-3.13404300	0.05569400
C	1.77070800	-4.03553400	0.22853000
C	2.93741200	-3.27936800	0.28015300
C	2.58501100	-1.89859800	0.12468200
N	1.22163600	-1.84467400	0.01274300
C	1.22977500	2.18568200	-0.14072600
C	2.52361500	2.77511500	-0.37312000
C	3.45938200	1.77372100	-0.33535300
C	2.78170300	0.52988100	-0.10235000
N	1.40226400	0.81294800	-0.01886400
C	0.00001900	2.84727500	-0.00000400
C	3.36657400	-0.73426500	0.03160500
C	-3.36658300	-0.73422200	-0.03160800
Co	-0.00000300	-0.45028300	-0.00000600
C	4.84767700	-0.89150600	0.05126700
C	5.57391600	-0.74090500	1.23243500
C	5.55067700	-1.24288100	-1.10159300
C	6.95211600	-0.92052500	1.27083700
C	6.92822300	-1.42514600	-1.09089500
C	7.62961800	-1.26362400	0.10258400
C	-4.84768700	-0.89145200	-0.05125300
C	-5.57393500	-0.74089000	-1.23242200
C	-5.55067900	-1.24279100	1.10162300

C	-6.95213400	-0.92051000	-1.27080800
C	-6.92822500	-1.42505600	1.09094000
C	-7.62962900	-1.26357200	-0.10254000
C	0.00002900	4.33796400	-0.00000400
C	-0.31735000	5.05989400	-1.15054400
C	0.31741600	5.05988900	1.15053700
C	-0.31960700	6.44944000	-1.16464000
C	0.31969100	6.44943500	1.16463500
C	0.00004600	7.14479100	-0.00000200
F	0.62675900	4.41020800	2.27982800
F	0.62436600	7.12076900	2.28024900
F	0.00005400	8.47936300	-0.00000100
F	-0.62427400	7.12078000	-2.28025300
F	-0.62670200	4.41021900	-2.27983500
F	-4.94148600	-0.41323000	-2.36604500
F	-7.62806300	-0.76908500	-2.41426300
F	-8.95238300	-1.43758600	-0.12627200
F	-7.58167200	-1.75498400	2.20977200
F	-4.89395900	-1.40379000	2.25723900
F	4.94146100	-0.41320300	2.36604300
F	7.62803600	-0.76906100	2.41429200
F	8.95237200	-1.43763800	0.12633200
F	7.58167700	-1.75511000	-2.20971200
F	4.89396500	-1.40391500	-2.25720900
Br	-5.28669900	2.09858500	0.60848400
Br	-2.99263800	4.55299700	0.74929400
Br	2.99269700	4.55295700	-0.74930900
Br	5.28672400	2.09851000	-0.60851300
Br	4.62194400	-4.04251700	0.56538700
Br	1.71358100	-5.89081800	0.42449400
Br	-1.71366000	-5.89079500	-0.42450700
Br	-4.62200100	-4.04245600	-0.56537400

Co-Cl_8 – Solvent= water (charge=0, multiplicity=3)

0 3

C	1.21840700	1.94585300	-0.19957600
C	2.49635500	2.52480300	-0.52383100
C	3.43597300	1.52556500	-0.49473900
C	2.77440200	0.29058100	-0.17866500
N	1.40011000	0.57737700	-0.04480600
C	0.69946500	-3.36055400	0.04373200
C	1.76688300	-4.26666400	0.21794600
C	2.93730300	-3.51372400	0.26361700
C	2.58968700	-2.13045300	0.09481300
N	1.22537100	-2.07565200	-0.01598400
C	-0.69967400	-3.36051600	-0.04369400
C	-1.76715000	-4.26657300	-0.21782900
C	-2.93752700	-3.51356700	-0.26350900
C	-2.58982300	-2.13030600	-0.09480100
N	-1.22550200	-2.07558000	0.01595700
C	-1.21830800	1.94593400	0.19945600
C	-2.49623600	2.52496900	0.52364800
C	-3.43591100	1.52578600	0.49454400
C	-2.77439900	0.29075200	0.17854900
N	-1.40008800	0.57746300	0.04471500
C	0.00007200	2.61392500	-0.00005200
C	-3.37123600	-0.96716700	0.02096100
C	3.37117200	-0.96736500	-0.02100700
Co	-0.00002600	-0.68344900	-0.00003000
C	-4.85516800	-1.10377200	-0.01557800
C	-5.57432800	-0.82012800	-1.17798600
C	-5.57302500	-1.54856100	1.09618600
C	-6.95689700	-0.96459800	-1.23690400
C	-6.95486000	-1.69668000	1.06423500
C	-7.64774100	-1.40329300	-0.10923800
C	4.85509600	-1.10403600	0.01557500
C	5.57427200	-0.82003000	1.17788400
C	5.57294500	-1.54916800	-1.09605900
C	6.95684100	-0.96448400	1.23683700
C	6.95478100	-1.69727700	-1.06407400

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 C                  7.64767400   -1.40353000    0.10930100
 C                  0.00013400    4.10593500   -0.00001200
 C                  0.45545100    4.82973100    1.10339200
 C                 -0.45511500    4.82984500   -1.10336800
 C                  0.45837600    6.22003700    1.11724100
 C                 -0.45791300    6.22015100   -1.11712600
 C                  0.00026400    6.91614700    0.00008000
 F                 -0.90698900    4.18045000   -2.18487800
 F                 -0.89756200    6.89051100   -2.18691800
 F                  0.00032500    8.25024800    0.00012300
 F                  0.89808600    6.89028700    2.18707600
 F                  0.90726300    4.18022500    2.18486100
 F                  4.93095900   -0.39041500    2.27169700
 F                  7.62286800   -0.68510800    2.36139500
 F                  8.97341400   -1.54416100    0.15272300
 F                  7.61987900   -2.12031600   -2.14360300
 F                  4.92473000   -1.84170700   -2.23134200
 F                 -4.93100200   -0.39090600   -2.27194600
 F                 -7.62291600   -0.68558000   -2.36155600
 F                 -8.97348200   -1.54392700   -0.15262700
 F                 -7.61997100   -2.11936700    2.14389400
 F                 -4.92482000   -1.84072300    2.23157300
 Cl                 5.09430700    1.79732700   -0.87843300
 Cl                 2.88063000    4.14049000   -0.98472800
 Cl                -2.88044000    4.14069400    0.98446900
 Cl                -5.09425700    1.79765700    0.87811200
 Cl                -4.48720100   -4.20708000   -0.54193700
 Cl                -1.68125900   -5.97153100   -0.40297500
 Cl                 1.68088600   -5.97160600    0.40319000
 Cl                 4.48691900   -4.20731200    0.54216500
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Co-F_8 – Solvent= water (charge=0, multiplicity=3)

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0 3
 C                 -1.23070400    1.79396000    0.09862600
 C                 -2.53109200    2.38466200    0.17345600
 C                 -3.45722700    1.38556600    0.14531300
 C                 -2.77570500    0.13436600    0.05035100
 N                 -1.39371900    0.41710200    0.02975600
 C                 -0.68433200   -3.50603200   -0.03447800
 C                 -1.75375100   -4.41808600   -0.09492500
 C                 -2.92189600   -3.67373200   -0.09170400
 C                 -2.58222500   -2.28724400   -0.02383300
 N                 -1.21577800   -2.22055900    0.01287400
 C                  0.71001500   -3.50153800   -0.03845600
 C                  1.78528800   -4.40695700   -0.09521100
 C                  2.94852500   -3.65489700   -0.10104000
 C                  2.59972100   -2.27014300   -0.04387700
 N                  1.23310400   -2.21229900   -0.00375400
 C                  1.22305500    1.80340700    0.06177200
 C                  2.52053900    2.40504700    0.05736900
 C                  3.45293000    1.41187600    0.02925800
 C                  2.77843300    0.15348300    0.00094600
 N                  1.39435600    0.42616800    0.02656000
 C                 -0.00606600    2.47036500    0.10190600
 C                  3.38496600   -1.10603300   -0.04050200
 C                 -3.37515000   -1.12848200    0.00204400
 Co                 0.00428400   -0.83309900    0.01758900
 C                  4.86764100   -1.23970300   -0.09540600
 C                  5.58022100   -1.83357300    0.95049100
 C                  5.60429100   -0.80780800   -1.20262500
 C                  6.96197200   -1.98984700    0.90680700
 C                  6.98625300   -0.94912300   -1.26890200
 C                  7.66704600   -1.54400400   -0.20867600
 C                 -4.85740700   -1.26888500   -0.02901200
 C                 -5.61662800   -0.80635500   -1.10859000
 C                 -5.54875000   -1.89587000    1.01208800
 C                 -6.99903400   -0.95172500   -1.15347400
 C                 -6.93038400   -2.05667300    0.98928100
 C                 -7.65779300   -1.58089900   -0.09918300
 C                 -0.01262700    3.96370400    0.15387500
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C	-0.37928100	4.72783500	-0.95604600
C	0.34386300	4.65349400	1.31454300
C	-0.39366700	6.11857300	-0.92072500
C	0.34079900	6.04323900	1.37583100
C	-0.03088200	6.77761600	0.25178100
F	0.71537400	3.96982100	2.40661500
F	0.69042200	6.67497800	2.50128900
F	-0.03904000	8.11114400	0.29839000
F	-0.75195700	6.82222100	-1.99976600
F	-0.74381400	4.11721500	-2.09254000
F	-5.01075500	-0.19469300	-2.13554300
F	-7.69589000	-0.49650400	-2.19941700
F	-8.98314700	-1.72725300	-0.13254000
F	-7.56033000	-2.65875500	2.00295900
F	-4.87442800	-2.36611100	2.07107700
F	4.92683400	-2.27630100	2.03406500
F	7.61303900	-2.55981100	1.92567600
F	8.99222700	-1.68621800	-0.26230500
F	7.66170800	-0.52267500	-2.34076000
F	4.97622300	-0.22981200	-2.23583300
F	-2.80621900	3.68339500	0.27643400
F	-4.77557800	1.55945700	0.22115300
F	-4.15196400	-4.17708300	-0.15119900
F	-1.65539200	-5.74245800	-0.15274400
F	1.69558900	-5.73238900	-0.14162900
F	4.18190500	-4.15057700	-0.15695000
F	4.77166200	1.59824800	0.03873300
F	2.78940700	3.70896800	0.07512600

Co-H_8 – Solvent= water (charge=0, multiplicity=3)

0 3

C	-1.23290800	1.60312500	0.07512300
C	-2.52768600	2.21577700	0.08053000
C	-3.46069000	1.21848600	0.03030000
C	-2.76850500	-0.03288800	-0.01639000
N	-1.38789000	0.22928000	0.01565100
H	-2.71099900	3.27958700	0.11382600
H	-4.53473200	1.33122400	0.03017600
C	-0.70841300	-3.69734400	-0.13846900
C	-1.78657400	-4.60792800	-0.20905900
C	-2.95190200	-3.85300300	-0.19557000
C	-2.58679800	-2.47336800	-0.11376200
N	-1.22355700	-2.40774800	-0.07977700
H	-1.70972900	-5.68465600	-0.26558000
H	-3.96391400	-4.22953800	-0.24202800
C	0.69661300	-3.69975300	-0.12701000
C	1.77257100	-4.61376600	-0.18599100
C	2.94012300	-3.86295700	-0.15261100
C	2.57861600	-2.48246200	-0.06946900
N	1.21520500	-2.41226300	-0.05392800
H	1.69287900	-5.68992200	-0.24907900
H	3.95137400	-4.24270800	-0.18799900
C	1.23540200	1.59779100	0.10963000
C	2.53116300	2.20346700	0.18653900
C	3.46155700	1.20318000	0.14642200
C	2.76662700	-0.04330100	0.04436700
N	1.38697600	0.22474700	0.02891300
H	2.71631500	3.26388400	0.27416800
H	4.53513100	1.30982000	0.19608000
C	0.00224400	2.26346800	0.12380400
C	3.35756000	-1.31030000	-0.01576000
C	-3.36232800	-1.29820800	-0.08135100
Co	-0.00224800	-1.02810000	-0.01893400
C	4.84025600	-1.43311700	-0.02541500
C	5.52755600	-2.05921300	1.02194000
C	5.61507100	-0.95017900	-1.08751400
C	6.91287800	-2.20089300	1.01960400
C	7.00218400	-1.07258600	-1.10759300
C	7.65308400	-1.70309100	-0.04995900
C	-4.84507300	-1.41721600	-0.12280600

C	-5.59530500	-0.94890700	-1.20860000
C	-5.55631500	-2.02637000	0.91839900
C	-6.98202500	-1.06786100	-1.25672600
C	-6.94169700	-2.16458600	0.88839600
C	-7.65733900	-1.68076300	-0.20405500
C	0.00543300	3.75334900	0.19241300
C	-0.42551200	4.43742400	1.33486200
C	0.44016200	4.53507100	-0.88426400
C	-0.43176100	5.82834600	1.40748700
C	0.45230000	5.92687400	-0.83231900
C	0.01171000	6.57541200	0.31884100
F	0.86410600	3.94635400	-2.01066500
F	0.87458000	6.64207700	-1.88099400
F	0.01432400	7.90932300	0.37872100
F	-0.85102300	6.44890200	2.51606100
F	-0.85259700	3.75203700	2.40449600
F	-4.98134500	-0.36513500	-2.24687700
F	-7.66606900	-0.60863900	-2.31038200
F	-8.98606100	-1.80377700	-0.24221400
F	-7.58752500	-2.74807700	1.90401500
F	-4.90361700	-2.49527500	1.99097700
F	4.85110200	-2.54094400	2.07404200
F	7.53529400	-2.80069300	2.04040000
F	8.98197100	-1.82951400	-0.06141000
F	7.70993900	-0.59999100	-2.13937900
F	5.02531700	-0.34968600	-2.12991800

All calculations were performed with the Gaussian 09 program, Revision B.01,
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