Electronic Supplementary Material (ESI) for Dalton Transactions

Supplementary Material

Tuning affinity and reversibility for O_2 binding in dinuclear Co(II) complexes

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Table S1 Selected interatomic distances and angles for the crystal structures of **1-5**. The atomic labels corresponds those in Figure 1.

	1	**2**	**3**	**4**	**5**
Co1-O1	1.890	1.897	1.912	1.913	1,901
Co1-O2	1.860	1.859	1.866	1.864	1,865
Co1-O4	1.916	1.913	1.929	1.930	1,922
Co1-N1	1.961	1.965	1.960	1.945	1,957
Co1-N2	1.915	1.919	1.923	1.906	1,915
Co1-N3	2.000	2.002	2.001	1.979	1,988
Co2-O1	1.895	1.899	1.897	1.899	1,892
Co2-O3	1.864	1.866	1.865	1.869	1,865
Co2-O5	1.914	1.933	1.940	1.944	1,934
Co2-N4	2.006	2.005	2.020	1.993	2,022
Co2-N5	1.929	1.914	1.913	1.910	1,918
Co2-N6	1.919	1.895	1.909	1.921	1,920
O2-O3	1.424	1.428	1.411	1.400	1,416
Co1-Co2	3.156	3.164	3.171	3.167	3,160
O1-Co1-O2	84.9	85.6	84.2	85.0	85,100
O1-Co1-O4	91.8	91.1	91.9	91.9	91,3
O1-Co1-N1	96.2	96.3	96.1	96.5	96,5
O1-Co1-N2	174.6	175.0	173.6	173.5	174,6
O1-Co1-N3	86.9	88.9	89.6	87.7	88,6
Co1-O1-Co2	113.0	112.9	112.7	112.3	112,8
O2-Co1-O4	95.6	94.9	94.3	93.7	94,3
O2-Co1-N1	89.9	90.3	90.0	90.1	90,9
O2-Co1-N2	89.9	89.4	89.5	88.6	89,7
O2-Co1-N3	169.2	171.9	171.3	170.8	171,4
Co1-O2-O3	110.2	110.5	110.3	109.3	110,3
O4-Co1-N1	170.7	171.3	171.3	171.1	171,0
O4-Co1-N2	90.0	90.0	89.3	89.6	90,3
O4-Co1-N3	91.8	91.0	92.0	92.1	91,6
N1-Co1-N2	82.5	83.1	83.2	82.5	82,3
N1-Co-N3	83.9	84.5	84.6	85.2	84,0
N2-Co-N3	98.1	96.0	96.6	98.5	96,5
O1-Co2-O3	90.4	90.5	90.4	90.0	90,7
O1-Co2-O5	88.7	88.4	88.0	86.9	87,6
O1-Co2-N4	91.0	92.9	92.5	93.0	92,2
O1-Co2-N5	92.0	93.5	93.5	93.5	92,1
O1-Co2-N6	171.8	172.2	170.7	170.7	172,0
O3-Co2-O5	87.1	87.6	87.5	86.8	87,6
O3-Co2-N4	178.1	176.4	176.7	176.8	177,0
O3-Co2-N5	95.9	95.5	96.1	94.6	95,5
O3-Co2-N6	94.8	93.5	93.8	93.7	94,0
Co2-O3-O4	111.7	112.5	111.6	112.3	111,8

O5-Co2-N4	91.5	91.5	90.9	92.4	91,9
O5-Co2-N5	176.9	176.4	176.1	178.6	176,8
O5-Co2-N6	85.2	85.1	83.8	84.8	86,2
N4-Co2-N5	85,4	85,4	85,4	85,8	86,2
N4-Co2-N6	83,7	83,0	83,2	83,1	83,2
N5-Co2-N6	93,8	92,8	94,3	94,6	94,8

DFT calculations

The density functional theory calculations presented in this work were performed with the Gaussian09 software package and the functional TPSSh by Tao, Perdew, Staroverov and Scuseria.[1, 2] The SDD basis set[3] (Stuttgart/Dresden ECP) were used for cobalt and the basis set TZVP[4] on the peroxido ligand, for all other atoms the split valence basis set by Ahlrich and coworkers[5] was applied with polarisation functions taken from the turbomole basis set libary.[6] All structures were optimised in gas phase and were confirmed to be minima on their potential energy surfaces by calculation of their vibrational frequencies. The thermal correction to the Gibbs free energy was calculated at a temperature of 313.15 K and a pressure equal 1 atm. The effect of the solvent (acetonitrile) were estimated by performing single point calculations on the optimised gas phase structures by invoking a polarised continium model[7] as implemented in Gaussian09. The solvent cavity was constructed with radii taken from the UFF force field scaled by 1.1 with explicit spheres on hydrogen atoms.

Table S2 Selected interatomic distances for the gas face optimised structures of **1**-**4**. The atomic labels corresponds those in Figure S1.

Bond	**1**	**2**	**3**	**4**
Co1-O1	1.935	1.914	1.914	1.915
Co1-O4	1.947	1.933	1.939	1.927
Co1-O2	1.887	1.857	1.857	1.858
Co1-N1	1.927	1.927	1.925	1.923
Co1-N2	1.922	1.926	1.924	1.924
Co1-N3	2.077	2.052	2.050	2.047
Co2-O1	1.951	1.924	1.928	1.923
Co2-O5	1.938	1.914	1.919	1.933
Co2-O3	1.894	1.862	1.861	1.861
Co2-N4	2.025	2.018	2.018	2.024
Co2-N5	1.997	1.981	1.977	1.976
Co2-N6	1.928	1.928	1.929	1.929
O4-O5	2.286	2.268	2.270	2.266
Co1-Co2	3.217	3.175	3.178	3.178
O2-O3	1.373	1.394	1.392	1.392

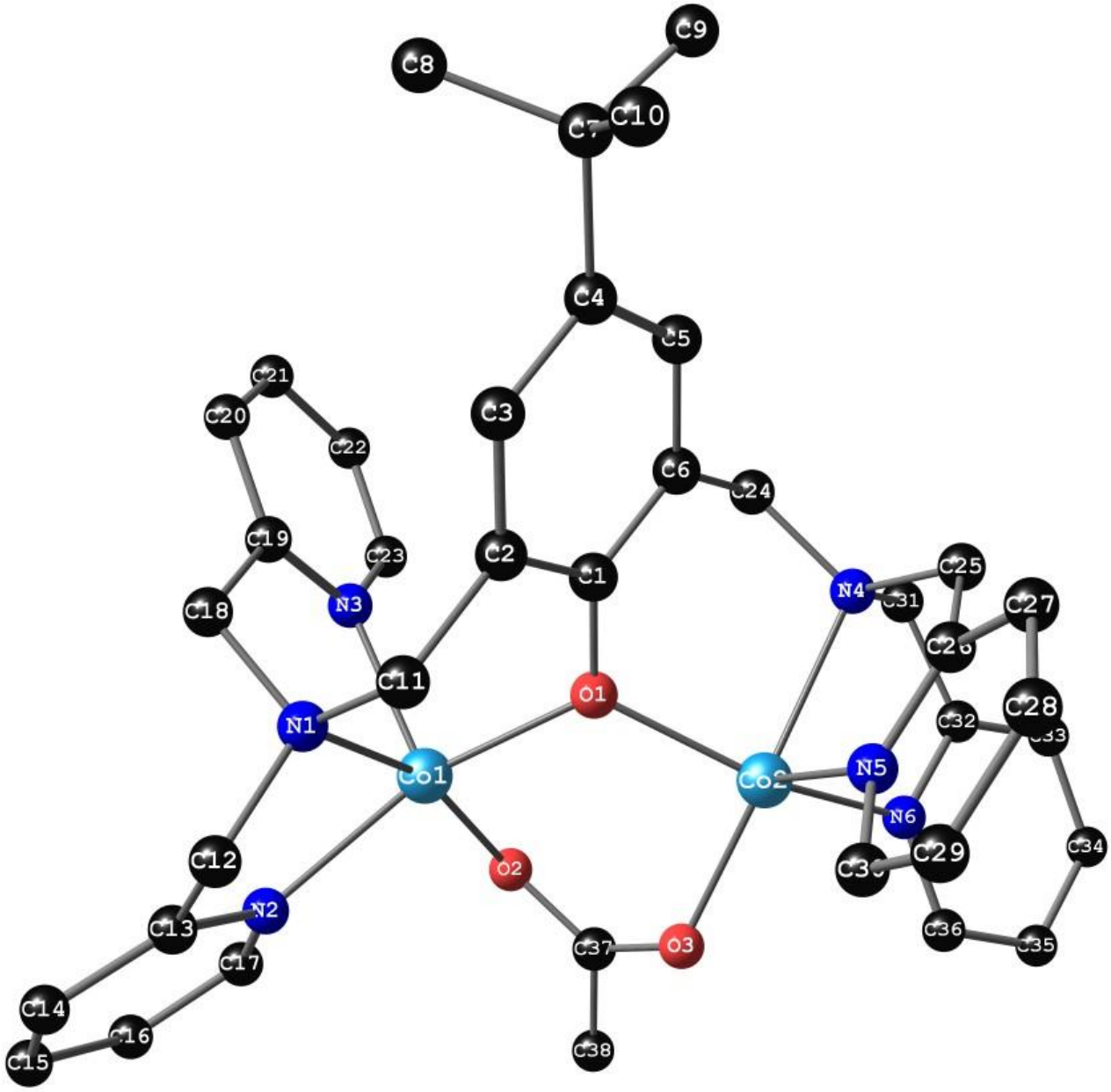

Figure S1 Optimised gas phase structure of high spin $[Co_2(bpbp)(CH_3COO)]^{2+}$, S = 3. Hydrogen atoms omitted for clarity.

Table S3 Selected interatomic distances for the gas face optimised structures of $[Co_2(bpbp)(CH_{(3-n)}Cl_n)]^{2+}$, n = 0-3. The atomic labels corresponds those in Figure S1.

Bond	CH_3	CH_2Cl	$CHCl_2$	CCl_3
Co1-O1	2.039	2.043	2.042	2.032
Co1-O2	2.012	2.033	2.023	2.006
Co1-N1	2.218	2.203	2.224	2.227
Co1-N2	2.121	2.124	2.110	2.091
Co1-N3	2.071	2.074	2.066	2.066
Co2-O1	2.042	2.039	2.040	2.041
Co2-O3	2.014	2.014	2.044	2.035

Co2-N4	2.212	2.213	2.178	2.130
Co2-N5	2.071	2.064	2.080	2.094
Co2-N6	2.123	2.113	2.109	2.139
O2-O3	2.240	2.245	2.247	2.251
Co1-Co2	3.523	3.545	3.579	3.620

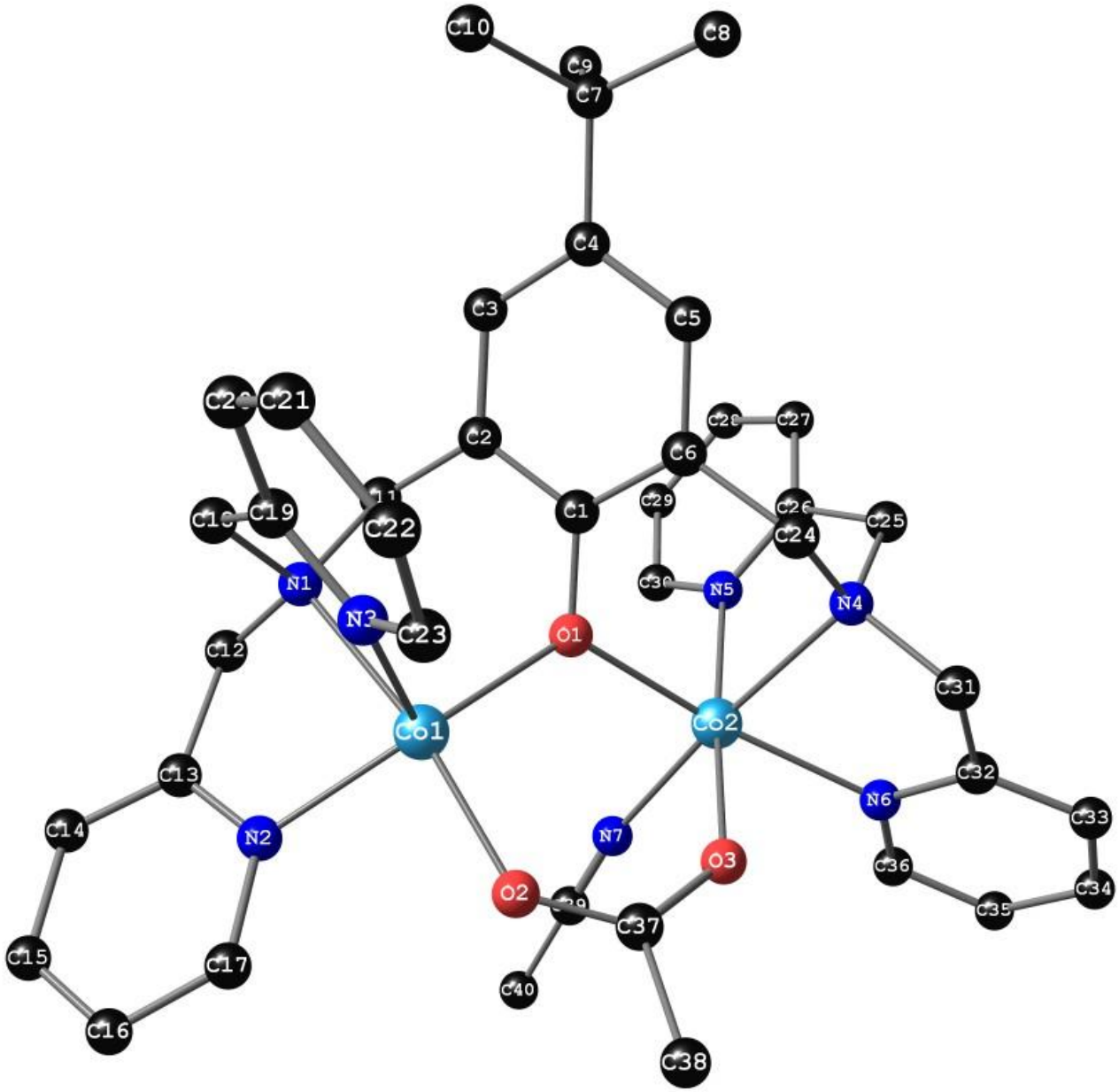

Figure S2 Optimised gas phase structure of high spin $[Co_2(bpbp)(CH_3COO)(MeCN)]^{2+}$, S = 3. Hydrogen atoms omitted for clarity.

Table S4 Selected interatomic distances for the gas face optimised structures of high spin $[Co_2(bpbp)(CH_{(3-n)}Cl_n)(MeCN)]^{2+}$, n = 0-3. The atomic labels corresponds those in Figure S2.

Bond	CH_3	CH_2Cl	$CHCl_2$	CCl_3

Co1-O1	1.999	2.004	2.002	2.000
Co1-O2	1.990	1.999	2.012	2.005
Co1-N1	2.264	2.250	2.251	2.238
Co1-N2	2.103	2.099	2.101	2.097
Co1-N3	2.080	2.076	2.075	2.076
Co2-O1	2.083	2.085	2.091	2.090
Co2-O3	2.090	2.101	2.100	2.113
Co2-N4	2.188	2.190	2.186	2.185
Co2-N5	2.137	2.131	2.125	2.123
Co2-N6	2.176	2.179	2.174	2.171
Co2-N7	2.142	2.142	2.140	2.135
O2-O3	2.248	2.255	2.258	2.254
Co1-Co2	3.558	3.597	3.608	3.600

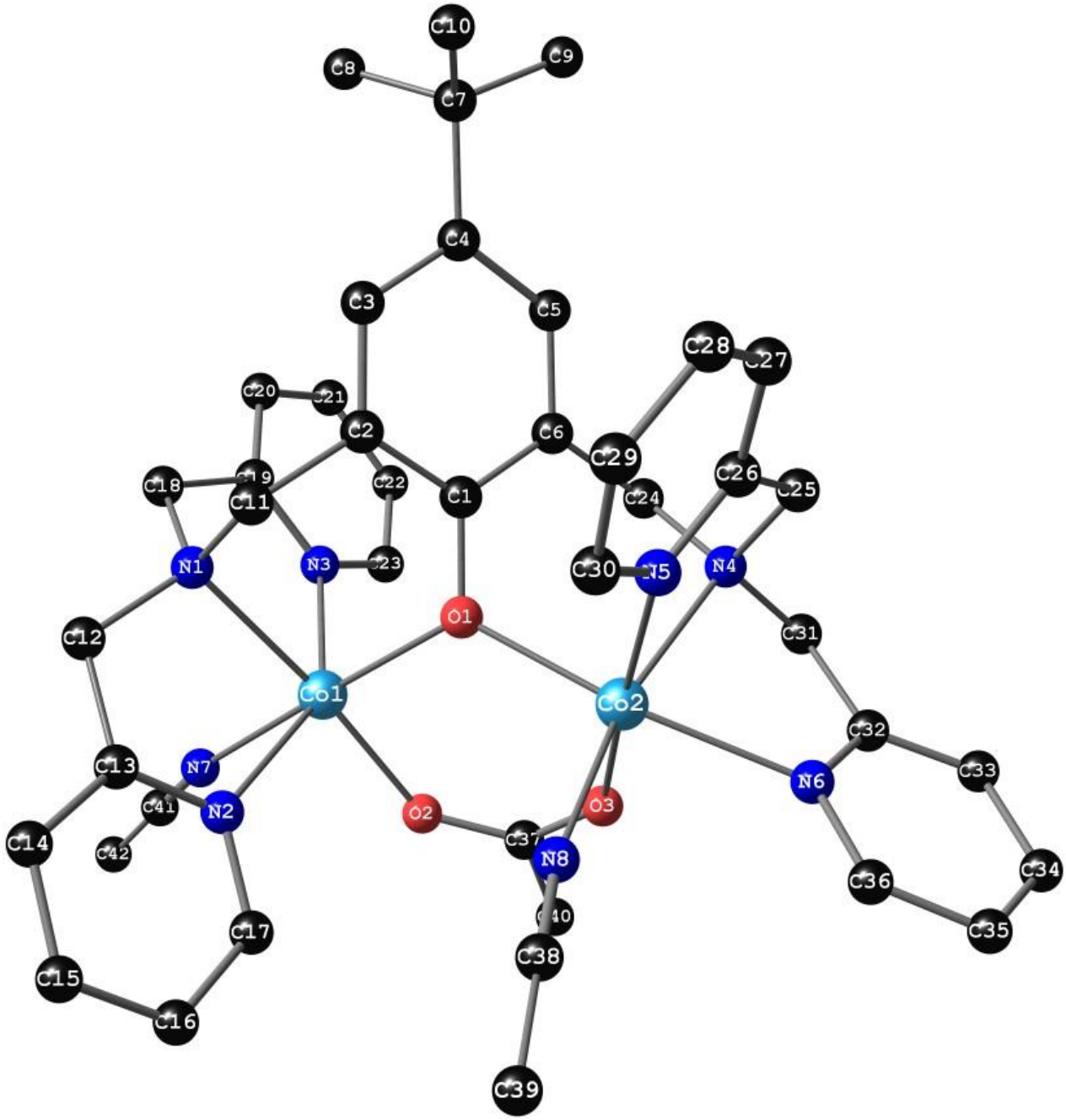

Figure S3 gas phase structure of high spin $[Co_2(bpbp)(CH_3COO)(MeCN)_2]^{2+}$, S = 3. Hydrogen atoms omitted for clarity.

Table S5 Selected interatomic distances for the gas face optimised structures of high spin $[Co_2(bpbp)(CH_{(3-n)}Cl_n)(MeCN)_2]^{2+}$, n = 0-3. The atomic labels corresponds those in Figure S3.

Bond	CH_3	CH_2Cl	$CHCl_2$	CCl_3
Co1-O1	2.082	2.088	2.088	2.096
Co1-O2	2.027	2.043	2.053	2.054
Co1-N1	2.264	2.257	2.250	2.245
Co1-N2	2.151	2.147	2.155	2.150

Co1-N3	2.125	2.120	2.120	2.121
Co2-O1	2.086	2.089	2.097	2.094
Co2-O3	2.065	2.071	2.079	2.092
Co2-N4	2.193	2.191	2.187	2.185
Co2-N5	2.149	2.143	2.130	2.130
Co2-N6	2.224	2.216	2.213	2.217
Co2-N8	2.166	2.162	2.147	2.145
O2-O3	2.257	2.261	2.266	2.261
Co1-Co2	3.718	3.747	3.766	3.765
Co1-N7	2.313	2.302	2.291	2.271

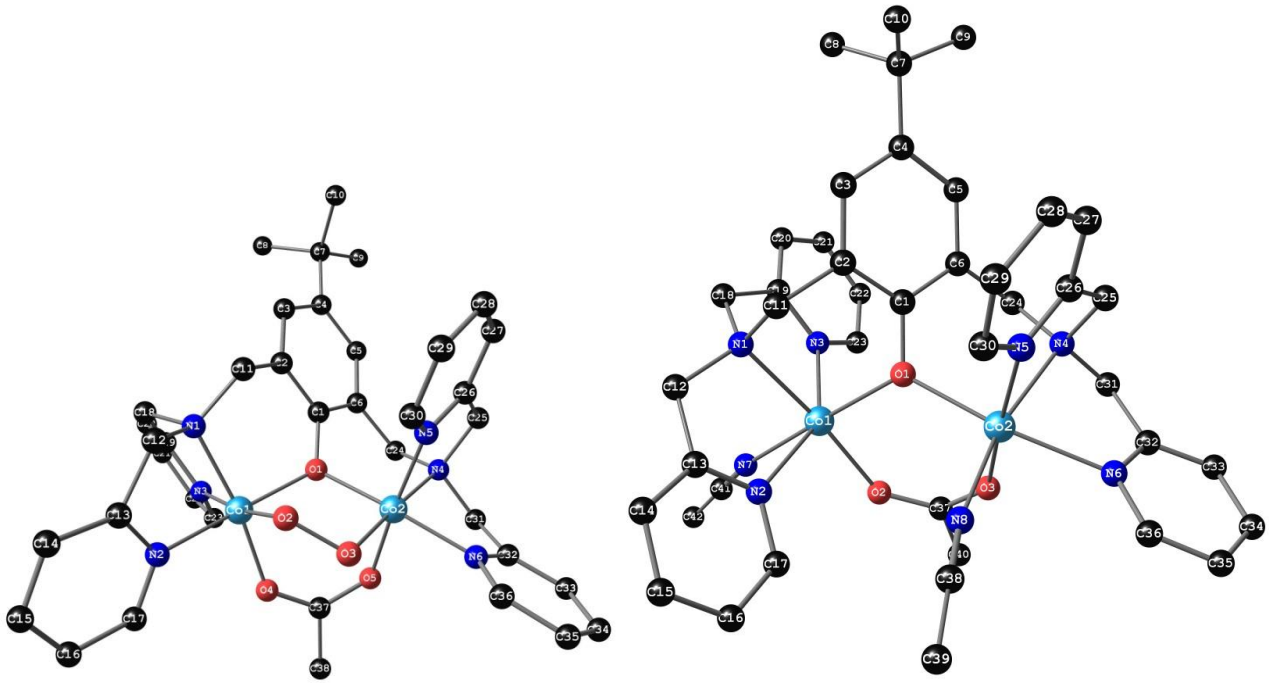

Figure S4 Gas phase structures of (left) $[Co_2(O_2)(bpbp)(CH_3COO)]^{2+}$ S = 0 and high spin $[Co_2(bpbp)(CH_3COO)(MeCN)_2]^{2+}$, S = 3. Hydrogen atoms omitted for clarity. The N2-Co1-N3 angle increase from 95.6° to 148.0° to facilitate the coordination of two acetonitrile molecules.

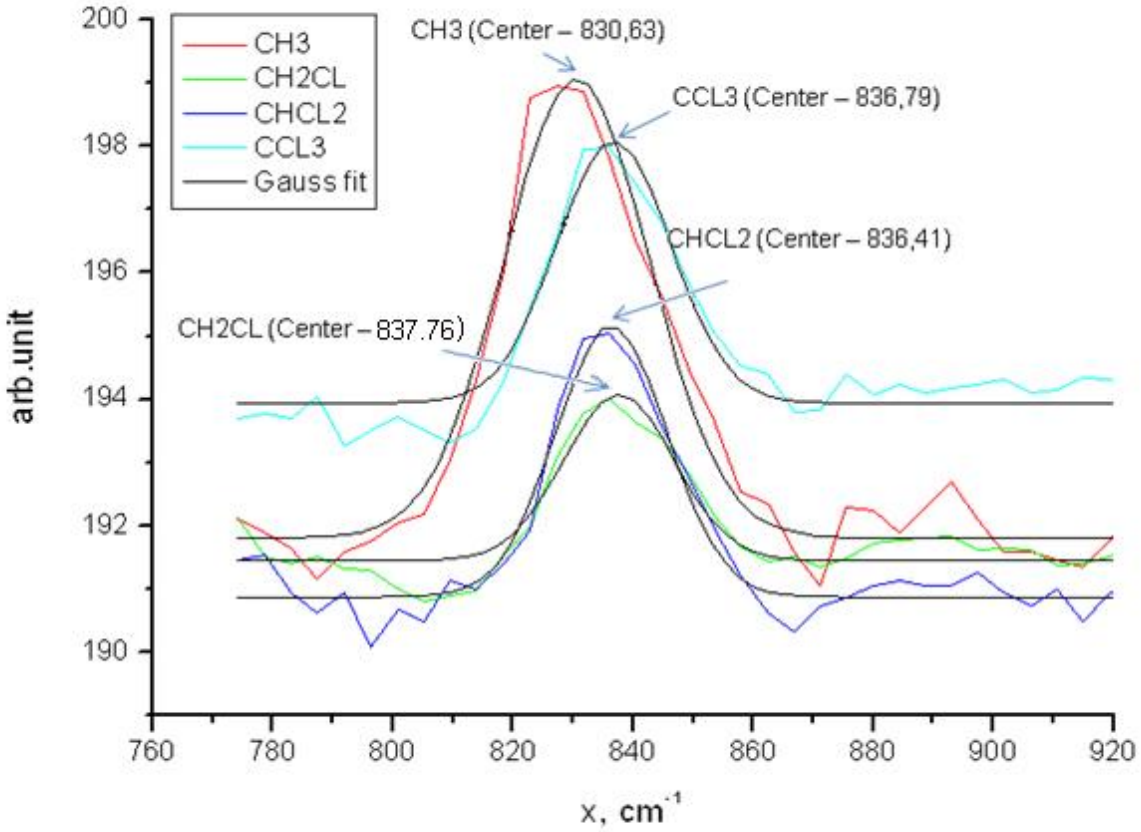

Figure S5 Surface Enhanced Resonance Raman Spectra.

Cartesian coordinate for optimised structures

$[Co_2(\mu\text{-}O_2)(bpbp)(CH_3COO)]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(\mu\text{-}O_2)(bpbp)(CH_3COO)]^{2+}$, S = 0, E = -6479785.44 kJ/mol, G = -6478006.66 kJ/mol, G_{solv} = -6478469.66 kJ/mol.

Co	-1.538292000	-1.118868000	0.059506000
Co	1.617189000	-0.934672000	-0.119211000
O	-0.032040000	0.011910000	-0.319111000
O	-0.436227000	-1.797659000	1.396736000
O	0.751398000	-2.268084000	0.840797000
O	-0.999246000	-2.374087000	-1.287026000
O	1.175759000	-1.904416000	-1.718269000
N	-2.394074000	0.114544000	1.359003000
N	-2.943655000	-2.315478000	0.632460000
N	-2.659661000	-0.136162000	-1.303144000
N	2.654186000	0.483192000	-1.176703000
N	2.195797000	0.043126000	1.441617000
N	3.287022000	-1.890470000	-0.193068000
C	-0.043633000	1.357770000	-0.219556000
C	-0.825883000	2.002121000	0.756701000
C	-0.861931000	3.401495000	0.771796000
H	-1.473303000	3.896326000	1.531779000
C	-0.110079000	4.186210000	-0.126359000
C	0.730045000	3.503669000	-1.024090000
H	1.363253000	4.070702000	-1.709297000
C	0.778530000	2.102690000	-1.080989000
C	-0.213262000	5.720855000	-0.080580000
C	-1.673632000	6.133849000	-0.380993000
H	-2.375946000	5.721157000	0.360676000
H	-1.985361000	5.788053000	-1.379370000
H	-1.769668000	7.230454000	-0.354605000
C	0.705527000	6.391332000	-1.116719000
H	0.452569000	6.091672000	-2.146148000
H	1.767488000	6.160105000	-0.934987000
H	0.593405000	7.484014000	-1.055466000
C	0.184689000	6.224923000	1.326105000
H	-0.472458000	5.819734000	2.111480000
H	0.111443000	7.322678000	1.368299000
H	1.221897000	5.943640000	1.568441000
C	-1.443503000	1.161936000	1.846308000
H	-0.651555000	0.608328000	2.371477000
H	-1.967606000	1.800829000	2.576779000
C	-2.813144000	-0.787231000	2.472935000
H	-1.903166000	-1.073109000	3.021316000
H	-3.499011000	-0.273609000	3.166388000
C	-3.432281000	-2.014446000	1.858098000
C	-4.402421000	-2.809679000	2.465881000
H	-4.788584000	-2.544837000	3.451671000

C	-4.861288000	-3.946649000	1.791904000
H	-5.617415000	-4.588784000	2.248170000
C	-4.344183000	-4.244743000	0.529104000
H	-4.678219000	-5.120751000	-0.028478000
C	-3.380646000	-3.401807000	-0.024027000
H	-2.925285000	-3.583045000	-0.997436000
C	-3.600557000	0.739056000	0.725306000
H	-4.475547000	0.114899000	0.969366000
H	-3.780328000	1.735235000	1.157786000
C	-3.472823000	0.796247000	-0.770495000
C	-4.205603000	1.680563000	-1.565913000
H	-4.850391000	2.429104000	-1.102110000
C	-4.101157000	1.580460000	-2.954477000
H	-4.664917000	2.255908000	-3.601228000
C	-3.267252000	0.600293000	-3.501054000
H	-3.163308000	0.481390000	-4.580496000
C	-2.558233000	-0.235017000	-2.640753000
H	-1.895054000	-1.014538000	-3.012909000
C	1.713850000	1.336424000	-1.983264000
H	1.158614000	0.640250000	-2.629506000
H	2.296062000	2.024010000	-2.619898000
C	3.450572000	1.300795000	-0.213098000
H	3.406569000	2.366714000	-0.484296000
H	4.508538000	0.998746000	-0.283590000
C	3.004376000	1.098007000	1.212012000
C	3.466568000	1.898447000	2.260793000
H	4.112168000	2.752639000	2.048926000
C	3.106671000	1.576332000	3.569792000
H	3.463735000	2.182668000	4.404892000
C	2.294258000	0.460090000	3.794941000
H	2.005223000	0.162965000	4.804094000
C	1.851732000	-0.283882000	2.704120000
H	1.208601000	-1.159140000	2.802354000
C	3.548542000	-0.344318000	-2.030258000
H	4.354618000	0.257886000	-2.481988000
H	2.934400000	-0.766920000	-2.839081000
C	4.099625000	-1.475958000	-1.193244000
C	5.326406000	-2.099841000	-1.421111000
H	5.977672000	-1.748194000	-2.223331000
C	5.698555000	-3.178726000	-0.612206000
H	6.652843000	-3.683775000	-0.775555000
C	4.838183000	-3.600374000	0.405070000
H	5.092495000	-4.440704000	1.052424000
C	3.631225000	-2.926589000	0.589036000
H	2.904058000	-3.208604000	1.353490000
C	0.094171000	-2.540290000	-1.908039000
C	0.115539000	-3.606755000	-2.977650000
H	0.466012000	-4.542179000	-2.511523000
H	0.822249000	-3.341624000	-3.774460000
H	-0.886784000	-3.780840000	-3.388344000

$[Co_2(\mu\text{-}O_2)(bpbp)(CH_2ClCOO)]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(\mu\text{-}O_2)(bpbp)(CH_2ClCOO)]^{2+}$, S = 0, E = -7686103.99 kJ/mol, G = -7684352.43 kJ/mol, G_{solv} = -7684820.02 kJ/mol.

Co	0.618205000	1.746465000	0.041859000
Co	-1.700124000	-0.392868000	0.396882000
Cl	-4.006048000	1.704447000	-3.118392000
O	0.108195000	-0.084195000	-0.181893000
O	-0.824331000	2.015223000	1.180027000
O	-1.255159000	0.815012000	1.742392000
O	-0.560222000	2.176829000	-1.429193000
O	-2.356057000	0.933849000	-0.816728000
N	2.225046000	1.533591000	-1.215765000
N	1.885240000	1.413896000	1.454531000
N	1.106728000	3.609318000	-0.005766000
N	-1.276598000	-1.918169000	1.587731000
N	-1.972752000	-1.814153000	-1.009560000
N	-3.462033000	-0.585087000	1.155059000
C	1.059251000	-1.040028000	-0.234512000
C	2.056210000	-0.939022000	-1.223080000
C	3.011445000	-1.955343000	-1.322643000
H	3.775318000	-1.876458000	-2.101373000
C	3.013979000	-3.072963000	-0.461819000
C	2.047186000	-3.097947000	0.558220000
H	2.054412000	-3.910272000	1.287560000
C	1.082975000	-2.086615000	0.700022000
C	4.061504000	-4.184945000	-0.645357000
C	3.887632000	-4.810995000	-2.049173000
H	4.630025000	-5.609844000	-2.201271000
H	4.028182000	-4.068801000	-2.850621000
H	2.884462000	-5.251214000	-2.163872000
C	3.912449000	-5.296812000	0.407665000
H	4.673162000	-6.072468000	0.234419000
H	2.926759000	-5.786081000	0.351805000
H	4.058257000	-4.917132000	1.431709000
C	5.480653000	-3.582625000	-0.521770000
H	6.237966000	-4.371370000	-0.650463000
H	5.631598000	-3.125015000	0.469099000
H	5.670943000	-2.815688000	-1.289042000
C	2.066178000	0.306556000	-2.073020000
H	1.109501000	0.433388000	-2.601405000
H	2.880781000	0.269292000	-2.815963000
C	3.468024000	1.472804000	-0.388289000
H	4.011012000	2.426353000	-0.492815000
H	4.138448000	0.683744000	-0.761640000
C	3.170091000	1.260550000	1.074217000
C	4.176048000	0.997883000	2.009053000
H	5.207312000	0.869260000	1.675374000

C	3.842884000	0.920771000	3.361668000
H	4.614060000	0.724360000	4.109473000
C	2.510514000	1.110203000	3.743401000
H	2.209968000	1.075083000	4.791575000
C	1.553962000	1.351875000	2.760978000
H	0.496939000	1.499723000	2.984341000
C	2.181117000	2.791273000	-2.008800000
H	1.365435000	2.692380000	-2.739847000
H	3.121589000	2.960399000	-2.559588000
C	1.866628000	3.938861000	-1.076897000
C	2.271760000	5.257305000	-1.285816000
H	2.893395000	5.507887000	-2.147298000
C	1.864562000	6.243110000	-0.380483000
H	2.168181000	7.281793000	-0.526765000
C	1.068363000	5.883942000	0.710536000
H	0.728074000	6.625776000	1.434298000
C	0.706530000	4.546501000	0.869198000
H	0.076340000	4.195691000	1.689345000
C	0.184464000	-1.985252000	1.907949000
H	0.401421000	-1.052588000	2.449335000
H	0.356903000	-2.835018000	2.589406000
C	-1.741222000	-3.190574000	0.946183000
H	-2.759632000	-3.402894000	1.310581000
H	-1.100649000	-4.027541000	1.263274000
C	-1.802338000	-3.069312000	-0.550020000
C	-1.793604000	-4.174812000	-1.403306000
H	-1.645118000	-5.177786000	-0.999226000
C	-1.991466000	-3.970453000	-2.770406000
H	-1.993900000	-4.816374000	-3.460898000
C	-2.197491000	-2.668768000	-3.236206000
H	-2.376598000	-2.464834000	-4.292792000
C	-2.176017000	-1.614699000	-2.324952000
H	-2.354234000	-0.586235000	-2.637548000
C	-2.086256000	-1.633890000	2.811266000
H	-1.595069000	-0.803408000	3.340096000
H	-2.121289000	-2.509686000	3.479634000
C	-3.456396000	-1.199711000	2.360391000
C	-4.631942000	-1.371613000	3.088818000
H	-4.608665000	-1.876192000	4.056214000
C	-5.830334000	-0.881905000	2.557836000
H	-6.764667000	-0.999336000	3.110566000
C	-5.816999000	-0.248696000	1.312903000
H	-6.731503000	0.142505000	0.865148000
C	-4.606864000	-0.116162000	0.631548000
H	-4.524920000	0.376080000	-0.338827000
C	-1.776412000	1.828714000	-1.481887000
C	-2.618437000	2.627708000	-2.470840000
H	-1.996256000	2.957938000	-3.310836000
H	-3.013946000	3.512862000	-1.950413000

$[Co_2(\mu\text{-}O_2)(bpbp)(CHCl_2COO)]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(\mu\text{-}O_2)(bpbp)(CHCl_2COO)]^{2+}$, S = 0, E = -8892413.05 kJ/mol, G = -8890692.39 kJ/mol, G_{solv} = -8891162.88 kJ/mol.

Co	-0.313346000	1.727012000	0.144761000
Co	-0.951178000	-1.369527000	0.467668000
Cl	-4.982184000	1.195563000	-1.057786000
Cl	-4.087902000	-0.817841000	-3.036637000
O	0.314530000	-0.055713000	-0.155675000
O	-1.582368000	1.080517000	1.336252000
O	-1.210460000	-0.156280000	1.855091000
O	-1.609809000	1.429167000	-1.266169000
O	-2.320525000	-0.640778000	-0.662549000
N	1.047572000	2.518175000	-1.168057000
N	0.982078000	2.159410000	1.502059000
N	-1.006028000	3.521881000	0.170689000
N	0.334470000	-2.388856000	1.570242000
N	-2.237626000	-2.559921000	1.274378000
N	-0.417394000	-2.651287000	-0.996704000
C	1.640610000	-0.279277000	-0.276488000
C	2.348689000	0.409979000	-1.279511000
C	3.711428000	0.142967000	-1.445789000
H	4.252192000	0.673269000	-2.234737000
C	4.400415000	-0.787928000	-0.640460000
C	3.673986000	-1.399095000	0.396119000
H	4.184460000	-2.073844000	1.085938000
C	2.309700000	-1.140826000	0.606517000
C	5.891099000	-1.071932000	-0.895298000
C	6.061555000	-1.624970000	-2.329598000
H	7.124589000	-1.828914000	-2.531381000
H	5.709616000	-0.910866000	-3.090510000
H	5.502942000	-2.565342000	-2.459701000
C	6.459705000	-2.102117000	0.096042000
H	6.398175000	-1.749438000	1.138091000
H	7.522124000	-2.279779000	-0.127415000
H	5.941813000	-3.071933000	0.022438000
C	6.695789000	0.241074000	-0.750018000
H	6.588700000	0.660858000	0.263028000
H	6.373190000	1.004178000	-1.475891000
H	7.765603000	0.050217000	-0.927079000
C	1.595448000	1.448235000	-2.073773000
H	2.247339000	1.910133000	-2.834328000
H	0.723757000	1.004647000	-2.577485000
C	2.131022000	3.178047000	-0.379562000
H	3.115661000	2.956396000	-0.818758000
H	1.995444000	4.270536000	-0.438116000
C	2.098937000	2.783794000	1.074327000
C	3.124465000	3.123331000	1.961598000
H	4.022497000	3.619304000	1.588965000
C	2.970701000	2.837543000	3.318583000
H	3.755153000	3.102367000	4.030640000
C	1.792645000	2.219976000	3.751834000
H	1.623725000	1.996005000	4.806121000
C	0.818356000	1.889164000	2.813697000
H	-0.118171000	1.398130000	3.079119000
C	0.239003000	3.529982000	-1.900383000
H	-0.398054000	2.988805000	-2.615431000

H	0.875921000	4.230297000	-2.466384000
C	-0.642886000	4.254874000	-0.908190000
C	-1.106499000	5.560170000	-1.072057000
H	-0.797189000	6.145263000	-1.940018000
C	-1.973992000	6.096392000	-0.114058000
H	-2.352227000	7.114711000	-0.225244000
C	-2.349860000	5.316326000	0.982630000
H	-3.029766000	5.698119000	1.745389000
C	-1.841215000	4.022873000	1.095426000
H	-2.103112000	3.351187000	1.915650000
C	1.579073000	-1.604102000	1.842011000
H	2.243871000	-2.209700000	2.480373000
H	1.243901000	-0.727970000	2.416020000
C	-0.420864000	-2.650800000	2.832586000
H	0.094092000	-3.399702000	3.456168000
H	-0.470168000	-1.701512000	3.386612000
C	-1.812907000	-3.079239000	2.450002000
C	-2.632582000	-3.909094000	3.212284000
H	-2.268549000	-4.324138000	4.153678000
C	-3.922825000	-4.189865000	2.749505000
H	-4.587346000	-4.832898000	3.330190000
C	-4.346232000	-3.642698000	1.536250000
H	-5.343817000	-3.839809000	1.141560000
C	-3.472348000	-2.826779000	0.817615000
H	-3.745766000	-2.361269000	-0.129617000
C	0.656205000	-3.684158000	0.887108000
H	1.676677000	-4.003139000	1.148465000
H	-0.035208000	-4.451892000	1.270979000
C	0.464679000	-3.589235000	-0.599770000
C	1.069210000	-4.465487000	-1.503609000
H	1.784623000	-5.210159000	-1.150233000
C	0.730878000	-4.376013000	-2.855338000
H	1.184799000	-5.050684000	-3.584133000
C	-0.203600000	-3.417057000	-3.256433000
H	-0.510011000	-3.323713000	-4.299246000
C	-0.752748000	-2.568100000	-2.297401000
H	-1.498113000	-1.817399000	-2.559413000
C	-2.410286000	0.453122000	-1.269065000
C	-3.661370000	0.663456000	-2.137362000
H	-3.492495000	1.459977000	-2.868376000

$[Co_2(\mu\text{-}O_2)(bpbp)(CCl_3COO)]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(\mu\text{-}O_2)(bpbp)(CCl_3COO)]^{2+}$, S = 0, E = -10098715.22 kJ/mol, G = -10097027.50 kJ/mol, G_{solv} = -10097494.08 kJ/mol.

Cl	-4.518885000	-1.557826000	-1.811988000
Cl	-3.030076000	0.286623000	-3.504523000
Cl	-4.778693000	1.304109000	-1.371416000
Co	-0.530783000	-1.575584000	0.628228000
Co	-0.479535000	1.595969000	0.429644000
O	0.407558000	-0.035001000	-0.039494000
O	-0.838622000	-0.486837000	2.106084000
O	-1.475909000	0.683522000	1.704968000
O	-2.125672000	-1.063752000	-0.336966000
O	-1.836699000	1.123951000	-0.853936000
N	1.026064000	-2.393879000	1.529299000

N	-1.494443000	-3.002405000	1.497616000
N	0.058241000	-2.674490000	-0.966071000
N	0.551715000	2.665836000	-0.977779000
N	0.870048000	2.200883000	1.658075000
N	-1.468911000	3.234142000	0.628343000
C	1.728845000	-0.010361000	-0.318577000
C	2.635829000	-0.775199000	0.436838000
C	3.986531000	-0.769833000	0.068923000
H	4.688135000	-1.366380000	0.658814000
C	4.473324000	0.005086000	-1.003527000
C	3.547757000	0.823558000	-1.675183000
H	3.888003000	1.472482000	-2.484375000
C	2.183916000	0.832277000	-1.345881000
C	5.966826000	-0.043493000	-1.370764000
C	6.296584000	0.865819000	-2.567447000
H	5.742764000	0.571657000	-3.473195000
H	7.369503000	0.793024000	-2.799594000
H	6.080038000	1.924481000	-2.351794000
C	6.808567000	0.417463000	-0.157939000
H	6.650701000	-0.225353000	0.722315000
H	6.560476000	1.452783000	0.125348000
H	7.880480000	0.380515000	-0.406819000
C	6.348282000	-1.496308000	-1.740484000
H	5.761974000	-1.851281000	-2.602818000
H	6.181236000	-2.190418000	-0.901468000
H	7.414967000	-1.550159000	-2.008047000
C	2.143746000	-1.414252000	1.711545000
H	1.736843000	-0.636607000	2.374332000
H	2.972327000	-1.921088000	2.233725000
C	0.476564000	-2.832755000	2.847951000
H	0.331906000	-1.928721000	3.458095000
H	1.179387000	-3.503726000	3.368205000
C	-0.857335000	-3.483049000	2.590866000
C	-1.433290000	-4.470502000	3.387871000
H	-0.899400000	-4.850651000	4.260485000
C	-2.702617000	-4.953086000	3.050018000
H	-3.178550000	-5.722987000	3.660763000
C	-3.348471000	-4.441142000	1.922436000
H	-4.338135000	-4.792022000	1.627058000
C	-2.711588000	-3.460610000	1.161910000
H	-3.167416000	-3.012129000	0.278575000
C	1.477991000	-3.587515000	0.742652000
H	0.961153000	-4.474033000	1.144787000
H	2.557526000	-3.745731000	0.887567000
C	1.122138000	-3.461394000	-0.710966000
C	1.773924000	-4.176278000	-1.718179000
H	2.637273000	-4.798989000	-1.477299000
C	1.293782000	-4.084995000	-3.026095000
H	1.780463000	-4.636177000	-3.833377000
C	0.179477000	-3.280995000	-3.281709000
H	-0.236180000	-3.187105000	-4.285903000
C	-0.407057000	-2.586283000	-2.225929000
H	-1.276306000	-1.949581000	-2.382562000
C	1.174829000	1.747738000	-1.994965000
H	0.342595000	1.176648000	-2.432692000
H	1.645870000	2.350026000	-2.789921000
C	1.580373000	3.489452000	-0.274073000
H	2.529392000	3.479375000	-0.831593000

H	1.236958000	4.536720000	-0.249169000
C	1.796012000	3.039464000	1.148028000
C	2.842229000	3.526605000	1.936677000
H	3.584897000	4.196797000	1.500046000
C	2.906647000	3.160435000	3.281471000
H	3.710580000	3.537073000	3.917368000
C	1.920813000	2.316286000	3.803195000
H	1.924097000	2.020894000	4.853414000
C	0.916197000	1.849401000	2.959584000
H	0.122510000	1.180241000	3.293327000
C	-0.505786000	3.533391000	-1.566732000
H	-1.115903000	2.907658000	-2.234988000
H	-0.073141000	4.356034000	-2.160350000
C	-1.379188000	4.052173000	-0.446902000
C	-2.089898000	5.251660000	-0.489835000
H	-2.002100000	5.907602000	-1.357744000
C	-2.915595000	5.589013000	0.587936000
H	-3.483837000	6.521383000	0.572391000
C	-3.005366000	4.722418000	1.680640000
H	-3.643740000	4.949624000	2.535445000
C	-2.261081000	3.543793000	1.667643000
H	-2.293286000	2.811902000	2.477416000
C	-2.422403000	0.016547000	-0.894816000
C	-3.668110000	-0.001070000	-1.840376000

$[Co_2(bpbp)(CH_3COO)]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CH_3COO)]^{2+}$, S = 3, E = -6084936.15 kJ/mol, G = -6083219.50 kJ/mol, G_{solv} = -6083687.72 kJ/mol.

Co	-1.699365000	-1.251169000	-0.167629000
Co	1.807375000	-1.119022000	0.148641000
O	0.012265000	-0.156540000	0.002591000
O	-0.769181000	-2.937601000	-0.749246000
O	0.997985000	-2.900230000	0.626693000
N	-2.807782000	0.204856000	1.085137000
N	-3.321483000	-2.412672000	0.552740000
N	-2.512498000	-0.077044000	-1.668013000
N	2.799803000	0.440114000	-1.067013000
N	2.510879000	0.086858000	1.677909000
N	3.542440000	-2.125599000	-0.546620000
C	-0.043596000	1.201613000	-0.001195000
C	-0.965502000	1.889656000	0.820276000
C	-1.010663000	3.289155000	0.795808000
H	-1.728876000	3.786147000	1.454830000
C	-0.169618000	4.066483000	-0.019930000
C	0.737277000	3.360111000	-0.821780000
H	1.409557000	3.906059000	-1.487030000
C	0.814391000	1.957421000	-0.826163000
C	-0.266139000	5.601205000	-0.004705000
C	-1.697963000	6.027192000	-0.403900000
H	-2.452285000	5.632335000	0.294967000
H	-1.946816000	5.672338000	-1.416846000

H	-1.783219000	7.125011000	-0.396547000
C	0.725661000	6.249242000	-0.986383000
H	0.536887000	5.938361000	-2.026391000
H	1.770632000	6.008088000	-0.733393000
H	0.623143000	7.343890000	-0.945958000
C	0.044961000	6.116034000	1.420170000
H	-0.664365000	5.720016000	2.163853000
H	-0.021173000	7.214874000	1.449955000
H	1.061686000	5.827383000	1.731156000
C	-1.843853000	1.119350000	1.764779000
H	-1.225160000	0.478308000	2.414006000
H	-2.396534000	1.819931000	2.416622000
C	-3.549738000	-0.578321000	2.099965000
H	-2.835860000	-0.846412000	2.896559000
H	-4.349868000	0.016657000	2.574354000
C	-4.098017000	-1.851851000	1.502775000
C	-5.285893000	-2.450543000	1.926938000
H	-5.897392000	-1.972696000	2.694816000
C	-5.671901000	-3.666997000	1.354245000
H	-6.597551000	-4.154401000	1.667693000
C	-4.859650000	-4.244805000	0.374690000
H	-5.126122000	-5.191256000	-0.098037000
C	-3.690286000	-3.583774000	-0.000104000
H	-3.014778000	-3.984744000	-0.758825000
C	-3.743673000	0.920156000	0.183425000
H	-4.709941000	0.388501000	0.212622000
H	-3.934822000	1.945855000	0.541982000
C	-3.298250000	0.940289000	-1.262407000
C	-3.760601000	1.905224000	-2.163228000
H	-4.387150000	2.726405000	-1.810224000
C	-3.418068000	1.795070000	-3.512180000
H	-3.774843000	2.533572000	-4.233307000
C	-2.616394000	0.726164000	-3.926821000
H	-2.334498000	0.598683000	-4.972955000
C	-2.176827000	-0.183254000	-2.968566000
H	-1.540173000	-1.031168000	-3.234488000
C	1.760196000	1.258299000	-1.759884000
H	1.205080000	0.556191000	-2.403741000
H	2.251554000	1.998246000	-2.417293000
C	3.646331000	1.239356000	-0.146893000
H	3.719209000	2.286885000	-0.484771000
H	4.667726000	0.823887000	-0.182224000
C	3.197981000	1.182366000	1.297506000
C	3.565277000	2.166280000	2.221610000
H	4.113973000	3.049591000	1.889626000
C	3.230468000	1.995284000	3.566031000
H	3.514458000	2.748063000	4.304533000
C	2.530563000	0.847447000	3.953761000
H	2.258292000	0.671701000	4.995445000
C	2.182190000	-0.078265000	2.974203000

H	1.626632000	-0.987433000	3.218817000
C	3.628552000	-0.262535000	-2.073493000
H	4.377577000	0.408432000	-2.529127000
H	2.956142000	-0.588406000	-2.884566000
C	4.281190000	-1.485800000	-1.476512000
C	5.526036000	-1.968496000	-1.884494000
H	6.104750000	-1.428636000	-2.636515000
C	6.011143000	-3.150939000	-1.316442000
H	6.982552000	-3.548951000	-1.617431000
C	5.238268000	-3.811263000	-0.357412000
H	5.581895000	-4.734776000	0.110876000
C	4.006704000	-3.264360000	0.001780000
H	3.356979000	-3.734142000	0.743443000
C	0.142189000	-3.520938000	-0.080341000
C	0.185705000	-5.029281000	-0.101183000
H	-0.409187000	-5.405087000	0.747914000
H	1.212011000	-5.396592000	0.023064000
H	-0.255149000	-5.418023000	-1.027715000

$[Co_2(bpbp)(CH_2ClCOO)]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CH_2ClCOO)]^{2+}$, S = 3, E = -7291250.51 kJ/mol, G = -7289556.28 kJ/mol, G_{solv} = -7290035.18 kJ/mol.

Co	0.313512000	2.015232000	0.271005000
Co	-1.787783000	-0.824204000	-0.024982000
Cl	-5.119718000	2.387281000	-1.162311000
O	0.077030000	-0.005180000	0.078176000
O	-1.645232000	2.360863000	0.693270000
O	-2.647579000	0.881228000	-0.665052000
N	2.074560000	1.996896000	-1.052345000
N	1.795350000	1.844766000	1.711736000
N	0.446592000	4.046322000	-0.336473000
N	-1.141680000	-2.575156000	1.165040000
N	-1.395797000	-2.135583000	-1.569243000
N	-3.610953000	-1.461199000	0.832257000
C	1.170055000	-0.811588000	-0.005154000
C	2.230111000	-0.501159000	-0.886881000
C	3.343171000	-1.347852000	-0.961776000
H	4.136634000	-1.084176000	-1.667172000
C	3.467527000	-2.516023000	-0.189826000
C	2.402496000	-2.800945000	0.676086000
H	2.445592000	-3.687530000	1.312188000
C	1.268526000	-1.978165000	0.780417000
C	4.712640000	-3.408653000	-0.323700000
C	4.805978000	-3.931665000	-1.776192000
H	5.695122000	-4.570641000	-1.893360000
H	4.888900000	-3.109010000	-2.503648000
H	3.918546000	-4.529783000	-2.037647000
C	4.660172000	-4.615896000	0.628838000

H	5.568554000	-5.223865000	0.503869000
H	3.797412000	-5.267681000	0.417206000
H	4.613460000	-4.305084000	1.684829000
C	5.975794000	-2.579710000	0.006144000
H	6.876274000	-3.205912000	-0.091427000
H	5.938087000	-2.195906000	1.038219000
H	6.093984000	-1.723119000	-0.676206000
C	2.127806000	0.697500000	-1.786769000
H	1.199560000	0.646144000	-2.379498000
H	2.976829000	0.708679000	-2.493753000
C	3.265402000	2.224322000	-0.196864000
H	3.481797000	3.306124000	-0.201313000
H	4.154364000	1.721203000	-0.613205000
C	3.061016000	1.822247000	1.247047000
C	4.140056000	1.538652000	2.090776000
H	5.155018000	1.516013000	1.689745000
C	3.899798000	1.297199000	3.444458000
H	4.729292000	1.081915000	4.121425000
C	2.584943000	1.337127000	3.921032000
H	2.355339000	1.162800000	4.973158000
C	1.560885000	1.605382000	3.017138000
H	0.515473000	1.638124000	3.335281000
C	1.899212000	3.108538000	-2.015871000
H	1.192750000	2.766717000	-2.790758000
H	2.843515000	3.357138000	-2.531113000
C	1.313505000	4.321087000	-1.332890000
C	1.589149000	5.632836000	-1.724636000
H	2.296817000	5.827314000	-2.532887000
C	0.942246000	6.684125000	-1.067254000
H	1.141561000	7.718928000	-1.353819000
C	0.042174000	6.391830000	-0.038625000
H	-0.481048000	7.183426000	0.499793000
C	-0.179096000	5.056516000	0.296669000
H	-0.876645000	4.767625000	1.085827000
C	0.191445000	-2.298244000	1.777279000
H	0.039292000	-1.439848000	2.451960000
H	0.498204000	-3.159890000	2.397557000
C	-1.122677000	-3.740278000	0.245409000
H	-2.088794000	-4.263260000	0.345141000
H	-0.340198000	-4.461010000	0.537556000
C	-0.975167000	-3.365527000	-1.213272000
C	-0.522918000	-4.281850000	-2.168135000
H	-0.178481000	-5.269983000	-1.857417000
C	-0.530589000	-3.917769000	-3.515923000
H	-0.188215000	-4.621156000	-4.278000000
C	-0.986659000	-2.645376000	-3.877057000
H	-1.019169000	-2.327498000	-4.920100000
C	-1.403639000	-1.780151000	-2.869256000
H	-1.764248000	-0.772264000	-3.090865000
C	-2.146209000	-2.765876000	2.237418000

H	-1.903210000	-2.057168000	3.046559000
H	-2.092566000	-3.778311000	2.674294000
C	-3.537801000	-2.456590000	1.741838000
C	-4.680890000	-3.093477000	2.226764000
H	-4.591389000	-3.899527000	2.957681000
C	-5.934195000	-2.677320000	1.764902000
H	-6.843564000	-3.160377000	2.128775000
C	-6.003259000	-1.638640000	0.833600000
H	-6.959669000	-1.280148000	0.450361000
C	-4.817060000	-1.055700000	0.387284000
H	-4.815784000	-0.235337000	-0.334868000
C	-2.607986000	1.972833000	-0.039527000
C	-3.778371000	2.943849000	-0.126931000
H	-3.417658000	3.903843000	-0.521398000
H	-4.167028000	3.119833000	0.886365000

$[Co_2(bpbp)(CHCl_2COO)]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CHCl_2COO)]^{2+}$, S = 3, E = -8497563.11 kJ/mol, G = -8495896.97 kJ/mol, G_{solv} = -8496375.84 kJ/mol.

Co	-0.289478000	2.037898000	-0.005179000
Co	1.535503000	-1.004732000	0.466165000
Cl	5.250536000	1.906492000	-0.057170000
O	-0.205646000	0.002183000	0.127046000
O	1.527878000	2.265608000	-0.864861000
O	2.535023000	0.778487000	0.485119000
N	-2.163406000	2.058817000	1.193100000
N	-1.666688000	2.168890000	-1.539844000
N	-0.193988000	3.924838000	0.933824000
N	0.969937000	-2.636869000	-0.859844000
N	0.675379000	-2.264949000	1.879441000
N	3.398862000	-1.929420000	0.118647000
C	-1.350501000	-0.715888000	-0.036628000
C	-2.516941000	-0.380845000	0.686990000
C	-3.691586000	-1.117161000	0.491838000
H	-4.572362000	-0.837055000	1.077074000
C	-3.772560000	-2.200004000	-0.401864000
C	-2.595110000	-2.524613000	-1.090039000
H	-2.595132000	-3.355826000	-1.798151000
C	-1.395571000	-1.812043000	-0.921843000
C	-5.094866000	-2.963977000	-0.584287000
C	-5.538785000	-3.551803000	0.775297000
H	-6.485967000	-4.101208000	0.658984000
H	-5.701241000	-2.766504000	1.530229000
H	-4.784656000	-4.252387000	1.167974000
C	-4.958999000	-4.117062000	-1.593819000
H	-5.924469000	-4.635064000	-1.694370000
H	-4.217861000	-4.863847000	-1.266390000
H	-4.672965000	-3.756303000	-2.594706000

C	-6.177217000	-1.986649000	-1.099618000
H	-7.132575000	-2.516426000	-1.238319000
H	-5.885210000	-1.549945000	-2.068031000
H	-6.354486000	-1.163348000	-0.389603000
C	-2.454531000	0.698676000	1.730441000
H	-1.640905000	0.474693000	2.439291000
H	-3.399192000	0.722127000	2.303793000
C	-3.227769000	2.553578000	0.284870000
H	-3.273744000	3.650910000	0.390155000
H	-4.216217000	2.163932000	0.583048000
C	-2.960855000	2.262228000	-1.175483000
C	-3.988191000	2.196091000	-2.121245000
H	-5.030154000	2.264034000	-1.803119000
C	-3.659187000	2.052206000	-3.470969000
H	-4.445822000	2.005139000	-4.227094000
C	-2.312569000	1.973274000	-3.840949000
H	-2.014646000	1.870188000	-4.885289000
C	-1.345235000	2.027862000	-2.840732000
H	-0.278241000	1.964068000	-3.068796000
C	-1.948300000	3.000135000	2.314792000
H	-1.392505000	2.458800000	3.098365000
H	-2.900805000	3.326576000	2.768157000
C	-1.119665000	4.185352000	1.881485000
C	-1.246157000	5.452469000	2.454055000
H	-2.007730000	5.636684000	3.214275000
C	-0.382989000	6.471942000	2.040773000
H	-0.462398000	7.471133000	2.474290000
C	0.576226000	6.194534000	1.063131000
H	1.266739000	6.961982000	0.710549000
C	0.635632000	4.907386000	0.531310000
H	1.357580000	4.636163000	-0.241523000
C	-0.173696000	-2.190120000	-1.713548000
H	0.195116000	-1.323917000	-2.287019000
H	-0.426282000	-2.987079000	-2.435438000
C	0.634622000	-3.806345000	-0.010031000
H	1.543218000	-4.424972000	0.083212000
H	-0.131873000	-4.437977000	-0.489534000
C	0.210383000	-3.433637000	1.393257000
C	-0.541950000	-4.304062000	2.189123000
H	-0.915732000	-5.240180000	1.770336000
C	-0.794743000	-3.963778000	3.518725000
H	-1.373190000	-4.633491000	4.158706000
C	-0.294071000	-2.757321000	4.020298000
H	-0.459655000	-2.459209000	5.056546000
C	0.428116000	-1.933028000	3.162230000
H	0.832402000	-0.975888000	3.502575000
C	2.158762000	-2.918693000	-1.699008000
H	2.204153000	-2.141408000	-2.479765000
H	2.074314000	-3.891668000	-2.213754000
C	3.424203000	-2.838888000	-0.877443000

C	4.569335000	-3.586293000	-1.157613000
H	4.563223000	-4.319019000	-1.966887000
C	5.719196000	-3.371510000	-0.390759000
H	6.628251000	-3.943016000	-0.589684000
C	5.689472000	-2.415997000	0.628227000
H	6.567551000	-2.213198000	1.242811000
C	4.506691000	-1.711763000	0.849601000
H	4.436458000	-0.941150000	1.619954000
C	2.536106000	1.643111000	-0.428543000
C	3.855551000	1.969825000	-1.143608000
H	3.821182000	2.959866000	-1.608496000
Cl	3.993637000	0.783260000	-2.502663000

$[Co_2(bpbp)(CCl_3COO)]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CCl_3COO)]^{2+}$, S = 3, E = -9703864.05 kJ/mol, G = -9702231.18 kJ/mol, G_{solv} = -9702714.61 kJ/mol.

Cl	4.239623000	2.892255000	-1.616023000
Cl	3.302026000	0.481071000	-2.991562000
Cl	5.281525000	0.297693000	-0.831125000
Co	-0.045419000	1.961684000	0.368749000
Co	1.142020000	-1.438265000	0.731277000
O	-0.321297000	-0.050383000	0.419337000
O	1.777524000	1.889503000	-0.465962000
O	2.581352000	-0.116187000	0.163317000
N	-1.982585000	2.264085000	1.424622000
N	0.370401000	3.641990000	1.540881000
N	-1.228629000	2.494233000	-1.239504000
N	0.478738000	-2.763836000	-0.798843000
N	-0.129111000	-2.621189000	1.902199000
N	2.758569000	-2.837172000	0.666035000
C	-1.541412000	-0.502083000	0.012262000
C	-2.718261000	-0.000486000	0.611316000
C	-3.967400000	-0.449420000	0.167698000
H	-4.858889000	-0.050416000	0.660195000
C	-4.112908000	-1.395385000	-0.863172000
C	-2.927765000	-1.885374000	-1.430038000
H	-2.980127000	-2.616671000	-2.239303000
C	-1.652805000	-1.461684000	-1.015908000
C	-5.512028000	-1.845581000	-1.316195000
C	-5.443572000	-2.877341000	-2.455473000
H	-4.944143000	-2.471227000	-3.349567000
H	-6.462313000	-3.168658000	-2.751633000
H	-4.916702000	-3.794715000	-2.146952000
C	-6.255969000	-2.483904000	-0.120393000
H	-6.380297000	-1.774901000	0.713074000
H	-5.712053000	-3.364164000	0.257728000
H	-7.260647000	-2.811279000	-0.430136000
C	-6.304554000	-0.615597000	-1.817848000

H	-5.796679000	-0.139683000	-2.671933000
H	-6.430722000	0.141514000	-1.027396000
H	-7.310200000	-0.921025000	-2.146403000
C	-2.601701000	0.950920000	1.770749000
H	-1.953223000	0.506628000	2.542540000
H	-3.595205000	1.117931000	2.224897000
C	-1.685774000	3.027527000	2.658022000
H	-1.354992000	2.305333000	3.422730000
H	-2.583907000	3.527135000	3.061919000
C	-0.568623000	4.020582000	2.434624000
C	-0.461479000	5.218726000	3.142848000
H	-1.238280000	5.506250000	3.854077000
C	0.654154000	6.035013000	2.928618000
H	0.759566000	6.976628000	3.471699000
C	1.626264000	5.631182000	2.009556000
H	2.510380000	6.239274000	1.813072000
C	1.445714000	4.427337000	1.330039000
H	2.166139000	4.066673000	0.592376000
C	-2.824719000	3.063937000	0.501943000
H	-2.634213000	4.129554000	0.715464000
H	-3.897933000	2.888775000	0.691391000
C	-2.498984000	2.844856000	-0.958626000
C	-3.424596000	3.097692000	-1.974833000
H	-4.450861000	3.373141000	-1.724928000
C	-3.011693000	3.003284000	-3.306033000
H	-3.716320000	3.203781000	-4.116001000
C	-1.686689000	2.654854000	-3.587150000
H	-1.323316000	2.580975000	-4.613050000
C	-0.825888000	2.400713000	-2.522302000
H	0.218960000	2.122126000	-2.680743000
C	-0.421917000	-1.990943000	-1.707482000
H	0.185524000	-1.161209000	-2.105238000
H	-0.719142000	-2.626495000	-2.560484000
C	-0.199306000	-3.920727000	-0.162784000
H	-1.006461000	-4.307635000	-0.806607000
H	0.540774000	-4.731942000	-0.058979000
C	-0.728010000	-3.620376000	1.222806000
C	-1.728376000	-4.402944000	1.810323000
H	-2.206414000	-5.198216000	1.235414000
C	-2.093667000	-4.158717000	3.134661000
H	-2.866026000	-4.763817000	3.614255000
C	-1.455540000	-3.131247000	3.838535000
H	-1.704423000	-2.913647000	4.878154000
C	-0.487066000	-2.380672000	3.178931000
H	0.029898000	-1.559755000	3.683348000
C	1.719439000	-3.181761000	-1.494621000
H	2.066188000	-2.324838000	-2.095702000
H	1.535652000	-4.019364000	-2.190208000
C	2.795421000	-3.532816000	-0.489599000
C	3.799475000	-4.468695000	-0.750462000

H	3.802298000	-5.022570000	-1.691219000
C	4.797169000	-4.674073000	0.206630000
H	5.594259000	-5.398173000	0.025351000
C	4.758509000	-3.942089000	1.396368000
H	5.518520000	-4.071195000	2.168243000
C	3.719769000	-3.031814000	1.585103000
H	3.653575000	-2.435712000	2.498747000
C	2.627593000	0.968060000	-0.459473000
C	3.855072000	1.174328000	-1.402323000

$[Co_2(bpbp)(CH_3COO)(MeCN)]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CH_3COO)(MeCN)]^{2+}$, S = 3, E = -6433324.26 kJ/mol, G = -6431502.98 kJ/mol, G_{solv} = -6431955.66 kJ/mol.

H	-0.698797000	-4.236602000	-3.265640000
H	-1.098580000	-2.746342000	-4.150765000
H	-2.374004000	-3.562378000	-3.222680000
Co	1.360157000	-1.543624000	-0.305836000
Co	-2.002196000	-0.448990000	0.091347000
O	0.049368000	-0.088668000	0.095015000
O	0.239973000	-2.602724000	-1.563882000
O	-1.799057000	-1.656714000	-1.602259000
N	2.745907000	-0.645392000	1.243035000
N	2.317877000	-3.237771000	0.492400000
N	2.714846000	-0.556671000	-1.537080000
N	-2.394342000	1.351265000	-1.088880000
N	-2.213095000	0.996396000	1.651105000
N	-4.126890000	-0.609883000	-0.349832000
C	0.512287000	1.183022000	0.087684000
C	1.573090000	1.554829000	0.943328000
C	2.055062000	2.868301000	0.923947000
H	2.867169000	3.127541000	1.609982000
C	1.525947000	3.855952000	0.072688000
C	0.476926000	3.457974000	-0.769706000
H	0.038639000	4.179187000	-1.462788000
C	-0.037205000	2.150314000	-0.779548000
C	2.093797000	5.285736000	0.093166000
C	1.381802000	6.203069000	-0.916099000
H	1.496618000	5.842832000	-1.950880000
H	1.816396000	7.212878000	-0.868233000
H	0.306120000	6.297327000	-0.696766000
C	1.918780000	5.884967000	1.507900000
H	2.443662000	5.291360000	2.272796000
H	0.853919000	5.934277000	1.786207000
H	2.327486000	6.907068000	1.541079000
C	3.597931000	5.243511000	-0.263441000
H	3.752522000	4.817226000	-1.267613000
H	4.172448000	4.641335000	0.458295000
H	4.019867000	6.260824000	-0.256178000
C	2.107766000	0.530721000	1.905687000
H	1.276308000	0.123352000	2.502279000
H	2.826555000	0.999240000	2.602660000
C	3.011462000	-1.708618000	2.233176000
H	2.156673000	-1.730349000	2.929591000
H	3.910459000	-1.499935000	2.840605000

C	3.114703000	-3.061866000	1.567748000
C	3.929872000	-4.089291000	2.048628000
H	4.573302000	-3.918160000	2.913946000
C	3.908187000	-5.330271000	1.403694000
H	4.540476000	-6.146883000	1.758925000
C	3.074817000	-5.505862000	0.295408000
H	3.033885000	-6.455996000	-0.239365000
C	2.296092000	-4.431036000	-0.132777000
H	1.633656000	-4.496891000	-0.999143000
C	3.983705000	-0.279634000	0.517073000
H	4.656626000	-1.154062000	0.535576000
H	4.516820000	0.541780000	1.027047000
C	3.750615000	0.062173000	-0.937315000
C	4.619553000	0.889579000	-1.655011000
H	5.445823000	1.388076000	-1.144863000
C	4.417007000	1.059815000	-3.026157000
H	5.086090000	1.698483000	-3.606772000
C	3.350674000	0.398976000	-3.644222000
H	3.164207000	0.497203000	-4.714554000
C	2.518867000	-0.395684000	-2.859597000
H	1.669553000	-0.934539000	-3.285748000
C	-1.122531000	1.759722000	-1.750057000
H	-0.803642000	0.889602000	-2.346430000
H	-1.318059000	2.596550000	-2.445498000
C	-2.938876000	2.401711000	-0.201399000
H	-2.683795000	3.409742000	-0.570544000
H	-4.039226000	2.327328000	-0.221478000
C	-2.508594000	2.244164000	1.239947000
C	-2.505687000	3.327436000	2.126854000
H	-2.739669000	4.329942000	1.763747000
C	-2.206827000	3.104808000	3.471148000
H	-2.205101000	3.934248000	4.181584000
C	-1.909714000	1.804383000	3.893396000
H	-1.675794000	1.584962000	4.936232000
C	-1.916190000	0.784131000	2.945824000
H	-1.679972000	-0.246954000	3.220129000
C	-3.394546000	0.915893000	-2.086342000
H	-2.877050000	0.256463000	-2.800171000
H	-3.812117000	1.768676000	-2.651519000
C	-4.495952000	0.122624000	-1.420424000
C	-5.810641000	0.116017000	-1.896891000
H	-6.081737000	0.725302000	-2.761356000
C	-6.763178000	-0.676223000	-1.251378000
H	-7.795977000	-0.697702000	-1.605516000
C	-6.374719000	-1.430452000	-0.140951000
H	-7.087584000	-2.055680000	0.398721000
C	-5.045338000	-1.364426000	0.274554000
H	-4.698204000	-1.932318000	1.141037000
C	-0.938270000	-2.466126000	-2.037209000
C	-1.303168000	-3.321322000	-3.232194000
N	-1.871211000	-2.213233000	1.299307000
C	-1.917182000	-3.255741000	1.806777000
C	-1.982826000	-4.569117000	2.431338000
H	-2.252864000	-4.468782000	3.493090000
H	-2.741179000	-5.183431000	1.923096000
H	-1.005797000	-5.068338000	2.352220000

$[Co_2(bpbp)(CH_2ClCOO)(MeCN)]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CH_2ClCOO)(MeCN)]^{2+}$, S = 3, E = -7639646.27 kJ/mol, G = -7637846.97 kJ/mol, G_{solv} = -7638301.99 kJ/mol.

H	0.721382000	-3.878897000	3.297107000
Cl	1.101827000	-1.774919000	4.336448000
H	2.431577000	-3.311262000	3.106336000
Co	-1.343476000	-1.567259000	0.064147000
Co	1.988877000	-0.293232000	-0.395829000
O	-0.079947000	-0.052981000	-0.289185000
O	-0.151593000	-2.615104000	1.280114000
O	1.896701000	-1.677436000	1.181675000
N	-2.803488000	-0.650206000	-1.382203000
N	-2.259637000	-3.256864000	-0.779855000
N	-2.673140000	-0.687719000	1.393701000
N	2.311316000	1.408523000	0.945119000
N	2.095252000	1.292750000	-1.814458000
N	4.125110000	-0.388083000	0.022047000
C	-0.603991000	1.193150000	-0.186175000
C	-1.702241000	1.569182000	-0.990786000
C	-2.244595000	2.853697000	-0.871122000
H	-3.085303000	3.117816000	-1.519712000
C	-1.742613000	3.805507000	0.035430000
C	-0.657529000	3.401574000	0.827819000
H	-0.238366000	4.093218000	1.561650000
C	-0.082512000	2.122863000	0.736450000
C	-2.378446000	5.203401000	0.129239000
C	-1.677677000	6.085561000	1.177165000
H	-1.740586000	5.651720000	2.187860000
H	-2.161550000	7.073234000	1.211589000
H	-0.615621000	6.247876000	0.932629000
C	-2.279138000	5.903438000	-1.245762000
H	-2.800617000	5.337073000	-2.033252000
H	-1.227605000	6.023357000	-1.551844000
H	-2.736646000	6.904110000	-1.197067000
C	-3.866165000	5.063295000	0.527519000
H	-3.966108000	4.571524000	1.508347000
H	-4.434109000	4.475988000	-0.211453000
H	-4.336937000	6.056733000	0.593980000
C	-2.225377000	0.582141000	-1.997476000
H	-1.398191000	0.237425000	-2.637805000
H	-2.980068000	1.061644000	-2.647288000
C	-3.063909000	-1.669470000	-2.418955000
H	-2.234225000	-1.621666000	-3.143896000
H	-3.990848000	-1.464711000	-2.984086000
C	-3.094424000	-3.058349000	-1.822293000
C	-3.884519000	-4.091457000	-2.331746000
H	-4.559318000	-3.902616000	-3.169013000
C	-3.798141000	-5.360870000	-1.750854000

H	-4.409833000	-6.182692000	-2.129357000
C	-2.927102000	-5.558909000	-0.675812000
H	-2.835562000	-6.531937000	-0.190866000
C	-2.176135000	-4.477604000	-0.216175000
H	-1.487814000	-4.563352000	0.627820000
C	-4.028891000	-0.368055000	-0.598877000
H	-4.671391000	-1.264093000	-0.643550000
H	-4.605945000	0.458530000	-1.048948000
C	-3.758994000	-0.091383000	0.863153000
C	-4.637836000	0.656290000	1.651693000
H	-5.505912000	1.137550000	1.197441000
C	-4.390166000	0.770227000	3.021544000
H	-5.066352000	1.345919000	3.657226000
C	-3.268647000	0.137158000	3.565755000
H	-3.042063000	0.195900000	4.631204000
C	-2.429392000	-0.577829000	2.714472000
H	-1.534276000	-1.082636000	3.085745000
C	1.038279000	1.716072000	1.657734000
H	0.769112000	0.800143000	2.207440000
H	1.216015000	2.513940000	2.401914000
C	2.800129000	2.553659000	0.145390000
H	2.516966000	3.514038000	0.609030000
H	3.902690000	2.518289000	0.138549000
C	2.345567000	2.510177000	-1.296014000
C	2.276984000	3.667781000	-2.080182000
H	2.475143000	4.642879000	-1.631271000
C	1.960036000	3.554198000	-3.433965000
H	1.906594000	4.443721000	-4.065310000
C	1.712520000	2.285236000	-3.968589000
H	1.467180000	2.150893000	-5.023137000
C	1.783345000	1.184640000	-3.118730000
H	1.588144000	0.172877000	-3.482253000
C	3.342383000	0.939835000	1.895958000
H	2.863887000	0.208339000	2.565984000
H	3.729550000	1.765166000	2.520430000
C	4.469121000	0.255838000	1.156511000
C	5.785979000	0.259179000	1.627573000
H	6.036205000	0.794937000	2.545349000
C	6.767145000	-0.427171000	0.908372000
H	7.801985000	-0.438076000	1.257030000
C	6.404581000	-1.088483000	-0.268317000
H	7.140160000	-1.628303000	-0.866518000
C	5.071179000	-1.040615000	-0.672643000
H	4.742981000	-1.538847000	-1.587883000
C	1.020941000	-2.394160000	1.718681000
C	1.373161000	-3.031757000	3.059058000
N	1.944795000	-1.935825000	-1.770455000
C	2.055545000	-2.910501000	-2.390216000
C	2.205403000	-4.136884000	-3.160253000
H	2.596073000	-3.905647000	-4.162443000

H	2.905743000	-4.813119000	-2.647414000
H	1.231089000	-4.637588000	-3.260056000

$[Co_2(bpbp)(CHCl_2COO)(MeCN)]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CHCl_2COO)(MeCN)]^{2+}$, S = 3, E = -8845961.74 kJ/mol, G = -8844195.76 kJ/mol, G_{solv} = -8844655.47 kJ/mol.

H	-2.618832000	3.266099000	2.657762000
Cl	-2.191432000	1.324865000	3.936304000
Cl	-4.558023000	1.979180000	2.272346000
Co	0.638773000	1.935280000	-0.088030000
Co	-1.663542000	-0.786626000	-0.643496000
O	0.258082000	-0.009491000	-0.369916000
O	-1.021972000	2.397082000	0.950560000
O	-2.358964000	0.585311000	0.785582000
N	2.493838000	1.718690000	-1.345096000
N	0.755741000	3.803953000	-1.041275000
N	2.081479000	1.868914000	1.402412000
N	-1.307272000	-2.337000000	0.855990000
N	-0.868364000	-2.320442000	-1.880359000
N	-3.634681000	-1.657895000	-0.359416000
C	1.282763000	-0.860009000	-0.111471000
C	2.505821000	-0.729570000	-0.805571000
C	3.560275000	-1.606474000	-0.526715000
H	4.489354000	-1.488756000	-1.092362000
C	3.461004000	-2.627306000	0.436364000
C	2.238496000	-2.727026000	1.117521000
H	2.111513000	-3.489352000	1.888974000
C	1.155032000	-1.868625000	0.865145000
C	4.652867000	-3.563574000	0.700977000
C	4.338873000	-4.603151000	1.791236000
H	4.102675000	-4.128367000	2.756907000
H	5.215218000	-5.249886000	1.948141000
H	3.496619000	-5.254411000	1.507339000
C	5.011102000	-4.314219000	-0.602713000
H	5.289375000	-3.620956000	-1.411887000
H	4.162325000	-4.923158000	-0.952733000
H	5.866318000	-4.986705000	-0.431740000
C	5.868909000	-2.726613000	1.161390000
H	5.644392000	-2.186314000	2.094948000
H	6.169136000	-1.988691000	0.400456000
H	6.733788000	-3.382813000	1.346381000
C	2.617047000	0.325569000	-1.870149000
H	1.796127000	0.203541000	-2.594586000
H	3.570820000	0.219012000	-2.418554000
C	2.357828000	2.676647000	-2.461343000
H	1.718539000	2.203155000	-3.225070000
H	3.326158000	2.892935000	-2.947137000
C	1.687554000	3.952800000	-2.007158000
C	1.960226000	5.200285000	-2.573067000
H	2.726042000	5.295141000	-3.345456000
C	1.241356000	6.316417000	-2.133398000
H	1.440246000	7.302501000	-2.558729000
C	0.274204000	6.152809000	-1.137701000
H	-0.303482000	6.998857000	-0.762460000
C	0.063902000	4.878056000	-0.613325000

H	-0.667141000	4.687027000	0.175387000
C	3.624616000	2.092358000	-0.462893000
H	3.781452000	3.180304000	-0.560085000
H	4.560746000	1.607092000	-0.789713000
C	3.366772000	1.814025000	1.001318000
C	4.406662000	1.615550000	1.914007000
H	5.439330000	1.565884000	1.563803000
C	4.103140000	1.490000000	3.271671000
H	4.900647000	1.339623000	4.002484000
C	2.767947000	1.561348000	3.680284000
H	2.488505000	1.474521000	4.731168000
C	1.784786000	1.744383000	2.711005000
H	0.726028000	1.798530000	2.975056000
C	-0.113505000	-1.972699000	1.671184000
H	-0.349588000	-1.002940000	2.137782000
H	0.019067000	-2.712473000	2.481776000
C	-1.138985000	-3.629941000	0.155422000
H	-0.504494000	-4.319778000	0.737792000
H	-2.131583000	-4.104384000	0.075611000
C	-0.601393000	-3.480459000	-1.249898000
C	0.063412000	-4.528442000	-1.897278000
H	0.275115000	-5.454374000	-1.359291000
C	0.442878000	-4.372466000	-3.230538000
H	0.957784000	-5.179366000	-3.756347000
C	0.153508000	-3.168568000	-3.882056000
H	0.427701000	-3.007002000	-4.925604000
C	-0.496511000	-2.168052000	-3.164371000
H	-0.737684000	-1.205653000	-3.622337000
C	-2.528258000	-2.334981000	1.691329000
H	-2.504671000	-1.424294000	2.310125000
H	-2.558481000	-3.203607000	2.373666000
C	-3.763694000	-2.295023000	0.822573000
C	-4.979900000	-2.854610000	1.226321000
H	-5.052163000	-3.368433000	2.186858000
C	-6.090206000	-2.745272000	0.386562000
H	-7.050684000	-3.173114000	0.681449000
C	-5.948434000	-2.089427000	-0.839583000
H	-6.786567000	-1.989862000	-1.530866000
C	-4.701283000	-1.561883000	-1.170020000
H	-4.543286000	-1.044397000	-2.118977000
C	-2.008734000	1.670839000	1.282182000
C	-2.812771000	2.204126000	2.480896000
N	-2.249813000	0.601021000	-2.163117000
C	-2.766308000	1.369874000	-2.862084000
C	-3.429296000	2.331916000	-3.730244000
H	-3.587436000	1.892271000	-4.726325000
H	-4.402947000	2.608788000	-3.298607000
H	-2.810402000	3.235799000	-3.829520000

[Co_2 (bpbp)(CCl_3COO)(MeCN)]$^{2+}$

Cartesian Coordinates for the optimised structure of [Co_2(bpbp)(CCl_3COO)(MeCN)]$^{2+}$, S = 3, E = -10052265.38 kJ/mol, G = -10050530.23 kJ/mol, G_{solv} = -10050990.81 kJ/mol.

Cl	4.015201000	2.665742000	-2.135897000
Cl	2.828034000	0.426120000	-3.589472000
Cl	5.013474000	-0.025526000	-1.680617000

Co	0.025653000	1.918878000	0.304203000
Co	1.002462000	-1.523931000	0.693732000
O	-0.427057000	-0.026977000	0.404995000
O	1.828429000	1.701031000	-0.546655000
O	2.297103000	-0.501901000	-0.627438000
N	-1.847150000	2.406902000	1.427936000
N	0.603381000	3.611042000	1.399938000
N	-1.179041000	2.535340000	-1.270323000
N	0.147978000	-2.727940000	-0.916945000
N	-0.410428000	-2.660548000	1.798288000
N	2.463816000	-3.110288000	0.446395000
C	-1.686021000	-0.372332000	0.037412000
C	-2.799887000	0.206868000	0.685568000
C	-4.094824000	-0.151689000	0.294571000
H	-4.935944000	0.304894000	0.824516000
C	-4.346768000	-1.079073000	-0.732879000
C	-3.222734000	-1.631082000	-1.365170000
H	-3.358591000	-2.342295000	-2.182534000
C	-1.906651000	-1.295514000	-1.004796000
C	-5.792730000	-1.442443000	-1.112995000
C	-5.847618000	-2.474045000	-2.253241000
H	-5.374685000	-2.096385000	-3.173763000
H	-6.896770000	-2.704190000	-2.492584000
H	-5.358835000	-3.421000000	-1.973106000
C	-6.509061000	-2.038339000	0.121192000
H	-6.545197000	-1.325075000	0.959572000
H	-5.998186000	-2.949616000	0.470722000
H	-7.546731000	-2.305267000	-0.133428000
C	-6.536676000	-0.166714000	-1.571537000
H	-6.049345000	0.279268000	-2.453285000
H	-6.569857000	0.594391000	-0.775831000
H	-7.576276000	-0.409108000	-1.842387000
C	-2.557576000	1.154915000	1.827032000
H	-1.912335000	0.668632000	2.576010000
H	-3.513087000	1.411488000	2.319868000
C	-1.433250000	3.165999000	2.626909000
H	-1.109840000	2.433352000	3.385068000
H	-2.270395000	3.733377000	3.071135000
C	-0.267807000	4.078738000	2.319725000
C	-0.060039000	5.297550000	2.969031000
H	-0.784639000	5.658759000	3.701535000
C	1.083668000	6.042095000	2.662445000
H	1.264899000	7.000464000	3.153923000
C	1.983129000	5.547778000	1.713960000
H	2.883111000	6.101314000	1.442031000
C	1.705488000	4.326914000	1.099552000
H	2.363053000	3.895216000	0.341027000
C	-2.657768000	3.253738000	0.521334000
H	-2.375466000	4.304903000	0.702681000
H	-3.733405000	3.169203000	0.754524000

C	-2.408941000	2.980591000	-0.945029000
C	-3.359677000	3.276040000	-1.925988000
H	-4.352234000	3.626784000	-1.637390000
C	-3.016268000	3.124246000	-3.271193000
H	-3.741926000	3.354705000	-4.054143000
C	-1.732521000	2.678436000	-3.600185000
H	-1.420877000	2.555776000	-4.638344000
C	-0.844601000	2.387417000	-2.567327000
H	0.168513000	2.032354000	-2.770000000
C	-0.733977000	-1.868916000	-1.757802000
H	-0.092001000	-1.059379000	-2.140508000
H	-1.096427000	-2.450264000	-2.625174000
C	-0.582320000	-3.865398000	-0.312702000
H	-1.409370000	-4.198749000	-0.962508000
H	0.116966000	-4.714642000	-0.231264000
C	-1.093633000	-3.573287000	1.080719000
C	-2.167602000	-4.281411000	1.632553000
H	-2.709959000	-5.008823000	1.025700000
C	-2.525348000	-4.048369000	2.960746000
H	-3.356010000	-4.594648000	3.412726000
C	-1.804546000	-3.106214000	3.702772000
H	-2.047536000	-2.897865000	4.745752000
C	-0.760585000	-2.430568000	3.076800000
H	-0.171731000	-1.678349000	3.607567000
C	1.320748000	-3.190421000	-1.691140000
H	1.717530000	-2.320903000	-2.238324000
H	1.044184000	-3.960276000	-2.433775000
C	2.396902000	-3.704143000	-0.762919000
C	3.293319000	-4.709650000	-1.137401000
H	3.211170000	-5.175945000	-2.121126000
C	4.287175000	-5.103425000	-0.238259000
H	4.999090000	-5.885935000	-0.509155000
C	4.348187000	-4.487014000	1.014627000
H	5.101967000	-4.769708000	1.750958000
C	3.415004000	-3.495257000	1.312892000
H	3.423016000	-2.988676000	2.280793000
C	2.463435000	0.689412000	-0.943234000
C	3.568582000	0.951327000	-2.020884000
N	1.996640000	-0.531312000	2.301021000
C	2.726768000	-0.037741000	3.055887000
C	3.655641000	0.575040000	3.994020000
H	3.527208000	0.133173000	4.993349000
H	4.688474000	0.406187000	3.654013000
H	3.469421000	1.657650000	4.050907000

$[Co_2(bpbp)(CH_3COO)(MeCN)_2]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CH_3COO)(MeCN)_2]^{2+}$, S = 3, E = -6781655.02 kJ/mol, G = -6779734.62 kJ/mol, G_{solv} = -6780178.57 kJ/mol.

Co	-1.585130000	-1.454671000	-0.349650000
Co	1.966707000	-0.397972000	-0.050210000
N	-3.194061000	-2.930128000	-1.113626000
N	2.176659000	-1.989944000	1.403117000
N	-1.616402000	-2.807619000	1.321893000
N	-2.916214000	-0.389869000	1.140882000
N	-2.659455000	-0.122647000	-1.609781000
N	2.310565000	1.348592000	-1.330341000
N	2.309678000	1.127657000	1.423646000
N	4.083792000	-0.592715000	-0.701952000
O	-0.089124000	-0.049667000	0.002485000
C	-0.836943000	-3.898735000	1.404674000
H	-0.164652000	-4.063316000	0.559827000
C	-0.900889000	-4.778644000	2.484596000
H	-0.274191000	-5.672272000	2.502506000
C	-1.795067000	-4.498672000	3.523917000
H	-1.869637000	-5.161063000	4.389289000
C	-2.607009000	-3.366938000	3.431129000
H	-3.328309000	-3.128015000	4.215282000
C	-2.505894000	-2.551196000	2.297598000
C	-3.474921000	-1.419959000	2.035949000
H	-4.352852000	-1.863675000	1.538827000
H	-3.830080000	-0.987104000	2.989252000
C	-3.972635000	0.325018000	0.392351000
H	-4.312244000	1.228514000	0.927344000
H	-4.843856000	-0.345877000	0.317964000
C	-3.568306000	0.676786000	-1.023946000
C	-4.191794000	1.712687000	-1.729241000
H	-4.917573000	2.355601000	-1.227714000
C	-3.874864000	1.903802000	-3.074898000
H	-4.350878000	2.704247000	-3.645430000
C	-2.944719000	1.053216000	-3.681663000
H	-2.677987000	1.160540000	-4.734158000
C	-2.356614000	0.055236000	-2.907708000
H	-1.621664000	-0.637123000	-3.325919000
C	-2.052600000	0.547146000	1.926054000
H	-1.270050000	-0.072830000	2.392486000
H	-2.656600000	1.003681000	2.732412000
C	-1.438908000	1.616697000	1.068059000
C	-1.818626000	2.958841000	1.185615000
H	-2.552071000	3.219416000	1.955000000
C	-1.296227000	3.970064000	0.358578000
C	-0.370887000	3.562803000	-0.614673000
H	0.044819000	4.299163000	-1.306011000
C	0.044754000	2.228816000	-0.753936000
C	-0.477283000	1.236140000	0.105490000
C	0.997066000	1.822784000	-1.846756000
H	0.576481000	0.979141000	-2.416677000
H	1.154576000	2.665547000	-2.545288000
C	3.009729000	2.384526000	-0.540832000
H	2.805374000	3.394120000	-0.937806000
H	4.094986000	2.217685000	-0.643356000
C	2.680516000	2.325341000	0.933756000
C	2.828735000	3.443342000	1.763075000
H	3.125901000	4.403071000	1.336087000
C	2.593292000	3.310810000	3.131547000
H	2.707495000	4.168700000	3.797653000
C	2.203153000	2.065018000	3.633711000

H	2.004046000	1.917657000	4.696219000
C	2.067423000	1.005385000	2.740719000
H	1.753165000	0.015595000	3.079205000
C	3.160672000	0.840660000	-2.424983000
H	3.524983000	1.655372000	-3.077388000
H	2.537816000	0.169285000	-3.036777000
C	4.317694000	0.045692000	-1.865817000
C	5.548341000	-0.045605000	-2.524096000
H	5.707382000	0.491135000	-3.461500000
C	6.561759000	-0.826477000	-1.964054000
H	7.530867000	-0.914448000	-2.459694000
C	6.316878000	-1.481009000	-0.754142000
H	7.082491000	-2.092298000	-0.273945000
C	5.063506000	-1.332834000	-0.161065000
H	4.831515000	-1.824230000	0.785982000
C	0.786117000	-2.520671000	-2.000841000
O	-0.402683000	-2.575157000	-1.555631000
O	1.697402000	-1.749807000	-1.587827000
C	-1.749423000	5.430191000	0.535500000
C	-3.280704000	5.521750000	0.341429000
H	-3.569033000	5.188501000	-0.668425000
H	-3.823804000	4.905739000	1.075570000
H	-3.619478000	6.562200000	0.467141000
C	-1.077326000	6.370558000	-0.480140000
H	0.019384000	6.373607000	-0.373704000
H	-1.325276000	6.098651000	-1.518634000
H	-1.426297000	7.401438000	-0.316748000
C	-1.385729000	5.908394000	1.960195000
H	-1.872254000	5.294775000	2.734588000
H	-0.297250000	5.863414000	2.124562000
H	-1.710433000	6.950583000	2.107478000
C	2.505693000	-2.828981000	2.133598000
C	2.930262000	-3.878229000	3.049508000
H	2.067865000	-4.237583000	3.629699000
H	3.361907000	-4.717122000	2.483347000
H	3.688601000	-3.483932000	3.742441000
C	1.136140000	-3.493644000	-3.111433000
H	2.093694000	-3.236575000	-3.580167000
H	1.212944000	-4.506217000	-2.683177000
H	0.333924000	-3.521775000	-3.862276000
C	-3.848160000	-3.705128000	-1.677169000
C	-4.659737000	-4.680451000	-2.393522000
H	-5.042193000	-4.237043000	-3.324674000
H	-4.049711000	-5.562005000	-2.639834000
H	-5.509929000	-4.994916000	-1.770551000

$[Co_2(bpbp)(CH_2ClCOO)(MeCN)_2]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CH_2ClCOO)(MeCN)_2]^{2+}$, S = 3, E = -7987978.42 kJ/mol, G = -7986084.00 kJ/mol, G_{solv} = -7986533.89 kJ/mol.

Co	0.824483000	2.011130000	-0.197006000
Co	-1.779073000	-0.636969000	0.302686000
N	1.477989000	4.103526000	-0.898397000
N	-2.547085000	0.566674000	1.926298000
N	0.340174000	3.108011000	1.584161000
N	2.621163000	1.629763000	1.115418000

N	2.272125000	1.408383000	-1.623601000
N	-1.411373000	-2.230625000	-1.155917000
N	-1.193453000	-2.238463000	1.599890000
N	-3.796320000	-1.410713000	-0.188654000
O	0.186470000	0.050783000	0.136452000
C	-0.854928000	3.678113000	1.811008000
H	-1.601322000	3.543944000	1.024981000
C	-1.121962000	4.413088000	2.965407000
H	-2.095464000	4.888104000	3.100619000
C	-0.112615000	4.538958000	3.926610000
H	-0.285435000	5.102939000	4.846000000
C	1.128462000	3.946339000	3.686072000
H	1.943297000	4.038155000	4.407038000
C	1.327995000	3.253435000	2.485938000
C	2.693187000	2.750925000	2.071047000
H	3.200612000	3.591545000	1.570243000
H	3.296787000	2.494992000	2.961120000
C	3.819393000	1.559985000	0.250472000
H	4.597641000	0.908112000	0.683221000
H	4.251409000	2.572247000	0.192224000
C	3.506532000	1.130890000	-1.167919000
C	4.482858000	0.572701000	-2.001043000
H	5.474609000	0.346080000	-1.605166000
C	4.169663000	0.318364000	-3.337337000
H	4.917014000	-0.114315000	-4.005964000
C	2.889387000	0.629379000	-3.807154000
H	2.607263000	0.455942000	-4.846709000
C	1.969281000	1.169210000	-2.911661000
H	0.953793000	1.430628000	-3.218738000
C	2.389608000	0.347616000	1.853034000
H	1.460634000	0.485549000	2.429414000
H	3.218342000	0.189456000	2.568002000
C	2.266856000	-0.830644000	0.929688000
C	3.241664000	-1.834350000	0.880766000
H	4.092112000	-1.759962000	1.565462000
C	3.164428000	-2.922831000	-0.007044000
C	2.055579000	-2.949259000	-0.867291000
H	1.958901000	-3.754785000	-1.598377000
C	1.052596000	-1.967135000	-0.840565000
C	1.140583000	-0.899740000	0.079902000
C	-0.096128000	-1.996974000	-1.813356000
H	-0.182150000	-1.024142000	-2.322527000
H	0.076635000	-2.770747000	-2.584136000
C	-1.456427000	-3.527692000	-0.447205000
H	-0.864507000	-4.293744000	-0.977696000
H	-2.501847000	-3.879096000	-0.446943000
C	-1.015736000	-3.428116000	0.994988000
C	-0.522930000	-4.538492000	1.690164000
H	-0.383734000	-5.488474000	1.170717000
C	-0.217334000	-4.412002000	3.045245000
H	0.164579000	-5.266431000	3.608105000
C	-0.403473000	-3.173419000	3.668085000
H	-0.174829000	-3.028674000	4.724979000
C	-0.886781000	-2.114736000	2.903624000
H	-1.038519000	-1.124759000	3.339557000
C	-2.519381000	-2.112130000	-2.126246000
H	-2.535649000	-2.959027000	-2.836278000
H	-2.363305000	-1.187833000	-2.704679000

C	-3.839563000	-1.995764000	-1.402203000
C	-5.039465000	-2.442077000	-1.965063000
H	-5.037328000	-2.915835000	-2.948606000
C	-6.228270000	-2.271937000	-1.253410000
H	-7.178068000	-2.610252000	-1.672792000
C	-6.177993000	-1.671917000	0.007550000
H	-7.079731000	-1.528695000	0.604799000
C	-4.940044000	-1.258874000	0.497327000
H	-4.855917000	-0.790613000	1.479944000
C	-1.870400000	1.830287000	-1.630138000
O	-0.815572000	2.466993000	-1.327316000
O	-2.323737000	0.800426000	-1.085692000
C	4.264843000	-3.999001000	-0.013261000
C	5.618452000	-3.346832000	-0.379087000
H	5.576944000	-2.891622000	-1.381628000
H	5.903029000	-2.564730000	0.342909000
H	6.419025000	-4.103392000	-0.381124000
C	3.974909000	-5.115883000	-1.030930000
H	3.029858000	-5.637313000	-0.808935000
H	3.926239000	-4.731551000	-2.062230000
H	4.780568000	-5.864655000	-0.996511000
C	4.367809000	-4.634974000	1.392316000
H	4.622336000	-3.890012000	2.162536000
H	3.416511000	-5.110394000	1.680020000
H	5.153122000	-5.407193000	1.404377000
C	-3.157837000	1.084698000	2.765786000
C	-3.935559000	1.726077000	3.816318000
H	-3.289241000	2.393185000	4.405092000
H	-4.753326000	2.312124000	3.370786000
H	-4.362835000	0.961900000	4.482830000
C	-2.654528000	2.462845000	-2.783617000
Cl	-3.870403000	1.375245000	-3.519766000
H	-3.183469000	3.351593000	-2.409630000
H	-1.960164000	2.784292000	-3.569771000
C	1.647502000	5.127680000	-1.416648000
C	1.851376000	6.411215000	-2.075236000
H	2.648472000	6.324393000	-2.828244000
H	0.921061000	6.724547000	-2.571670000
H	2.137345000	7.173358000	-1.335498000

$[Co_2(bpbp)(CHCl_2COO)(MeCN)_2]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CHCl_2COO)(MeCN)_2]^{2+}$, S = 3, E = -9194300.63 kJ/mol, G = -9192434.21 kJ/mol, G_{solv} = -9192880.740388 kJ/mol.

Co	-0.106164000	2.101715000	-0.170562000
Co	-0.970909000	-1.531058000	0.319758000
N	-0.633672000	4.202630000	-0.915346000
N	-2.253628000	-0.831837000	1.892490000
N	-0.999401000	2.866983000	1.635213000
N	1.691725000	2.687878000	1.049115000
N	1.377609000	2.272732000	-1.674507000
N	0.131819000	-2.711018000	-1.154540000
N	0.365453000	-2.589189000	1.597403000
N	-2.305672000	-3.239264000	-0.125645000

O	0.350126000	0.086951000	0.135534000
C	-2.310147000	2.789082000	1.923917000
H	-2.938933000	2.307107000	1.171854000
C	-2.845189000	3.316417000	3.098844000
H	-3.919280000	3.259413000	3.284498000
C	-1.982057000	3.928731000	4.013804000
H	-2.363836000	4.345734000	4.948376000
C	-0.623255000	4.016413000	3.705401000
H	0.076353000	4.505038000	4.386561000
C	-0.168598000	3.492282000	2.489734000
C	1.244643000	3.721009000	2.002173000
H	1.245650000	4.690253000	1.477101000
H	1.937714000	3.817294000	2.857920000
C	2.733433000	3.194251000	0.128540000
H	3.748648000	3.010703000	0.519816000
H	2.614218000	4.287534000	0.055511000
C	2.608066000	2.642407000	-1.276523000
C	3.696312000	2.619449000	-2.156310000
H	4.688079000	2.911973000	-1.806461000
C	3.491095000	2.225267000	-3.479427000
H	4.325201000	2.204069000	-4.184151000
C	2.203624000	1.863282000	-3.889570000
H	1.998105000	1.559856000	-4.917211000
C	1.176059000	1.896638000	-2.949673000
H	0.151211000	1.621437000	-3.211345000
C	2.144916000	1.472336000	1.797631000
H	1.282176000	1.138089000	2.395959000
H	2.956169000	1.759099000	2.492157000
C	2.609199000	0.381732000	0.876155000
C	3.956995000	0.011765000	0.798599000
H	4.663697000	0.506242000	1.472280000
C	4.425910000	-0.958069000	-0.106201000
C	3.465920000	-1.536796000	-0.950674000
H	3.776195000	-2.272079000	-1.696582000
C	2.102881000	-1.204859000	-0.889862000
C	1.654206000	-0.245364000	0.045271000
C	1.111312000	-1.822982000	-1.838825000
H	0.512893000	-1.037931000	-2.327034000
H	1.641895000	-2.389895000	-2.626072000
C	0.788569000	-3.834391000	-0.452021000
H	1.688122000	-4.173137000	-0.994505000
H	0.087193000	-4.685258000	-0.439547000
C	1.130474000	-3.513063000	0.985673000
C	2.135901000	-4.202274000	1.672982000
H	2.745244000	-4.942065000	1.150406000
C	2.341785000	-3.932460000	3.026208000
H	3.117823000	-4.461984000	3.583067000
C	1.542028000	-2.973226000	3.655875000
H	1.669207000	-2.731814000	4.712157000
C	0.571158000	-2.321658000	2.899420000

H	-0.073845000	-1.557081000	3.339046000
C	-0.900999000	-3.188792000	-2.096767000
H	-0.494955000	-3.920359000	-2.819055000
H	-1.257422000	-2.315395000	-2.665764000
C	-2.069409000	-3.775069000	-1.339452000
C	-2.873218000	-4.789870000	-1.868211000
H	-2.649930000	-5.206668000	-2.852295000
C	-3.956107000	-5.256418000	-1.119998000
H	-4.599990000	-6.046614000	-1.511762000
C	-4.192396000	-4.703189000	0.141060000
H	-5.019461000	-5.045143000	0.765036000
C	-3.339782000	-3.698332000	0.595972000
H	-3.484473000	-3.243387000	1.577879000
C	-2.533153000	0.596295000	-1.310335000
O	-1.881319000	1.656329000	-1.100148000
O	-2.224330000	-0.582457000	-1.040243000
C	5.918345000	-1.331644000	-0.144702000
C	6.762545000	-0.067972000	-0.429072000
H	6.487189000	0.378710000	-1.398016000
H	6.633147000	0.697030000	0.352824000
H	7.832848000	-0.325050000	-0.464632000
C	6.223381000	-2.372261000	-1.236259000
H	5.677087000	-3.314421000	-1.068864000
H	5.971967000	-1.998506000	-2.241729000
H	7.297698000	-2.610447000	-1.231273000
C	6.329069000	-1.922714000	1.223981000
H	6.165588000	-1.205940000	2.044046000
H	5.751896000	-2.833991000	1.448461000
H	7.398055000	-2.188376000	1.220293000
C	-3.154524000	-0.612466000	2.589519000
C	-4.299876000	-0.347727000	3.447112000
H	-4.043124000	0.419106000	4.192244000
H	-5.141125000	0.004327000	2.831391000
H	-4.596506000	-1.269259000	3.969906000
C	-3.915603000	0.836593000	-1.951167000
Cl	-4.386688000	-0.453949000	-3.070060000
Cl	-5.098214000	0.996018000	-0.583491000
H	-3.949024000	1.789042000	-2.487761000
C	-1.019006000	5.181895000	-1.403816000
C	-1.509659000	6.405951000	-2.023237000
H	-1.042175000	6.539587000	-3.009933000
H	-2.601116000	6.347936000	-2.147308000
H	-1.266333000	7.272127000	-1.390450000

$[Co_2(bpbp)(CCl_3COO)(MeCN)_2]^{2+}$

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CCl_3COO)(MeCN)_2]^{2+}$, S = 3, E = -10400604.87 kJ/mol, G = -10398771.57 kJ/mol, G_{solv} = -10399217.32 kJ/mol.

27	0.427568000	-1.990798000	0.114566000

27	0.436627000	1.761915000	0.418198000
7	1.576316000	-3.855428000	-0.486510000
7	1.690153000	1.387587000	2.117491000
7	1.217417000	-2.512086000	2.045401000
7	-1.346144000	-2.916847000	1.132188000
7	-0.764495000	-2.541966000	-1.550533000
7	-0.755254000	2.625617000	-1.196247000
7	-1.203603000	2.538428000	1.532664000
7	1.394480000	3.722080000	0.022720000
8	-0.485560000	-0.106306000	0.206611000
6	2.436360000	-2.151492000	2.483192000
1	3.033239000	-1.557171000	1.787624000
6	2.921757000	-2.539370000	3.731382000
1	3.928085000	-2.252398000	4.041893000
6	2.102053000	-3.314534000	4.558979000
1	2.446236000	-3.630801000	5.546161000
6	0.842033000	-3.696530000	4.095759000
1	0.184514000	-4.318987000	4.705918000
6	0.439868000	-3.293430000	2.816936000
6	-0.819937000	-3.822370000	2.170913000
1	-0.550236000	-4.774581000	1.685450000
1	-1.581463000	-4.053971000	2.938053000
6	-2.152390000	-3.641836000	0.124384000
1	-3.226031000	-3.629461000	0.377126000
1	-1.836793000	-4.697772000	0.135633000
6	-1.942781000	-3.134272000	-1.287228000
6	-2.882871000	-3.369061000	-2.297509000
1	-3.836802000	-3.842257000	-2.057252000
6	-2.577509000	-2.997959000	-3.607640000
1	-3.294448000	-3.175075000	-4.412278000
6	-1.339419000	-2.404236000	-3.875685000
1	-1.055640000	-2.112298000	-4.887911000
6	-0.463712000	-2.190477000	-2.813749000
1	0.517640000	-1.733471000	-2.965133000
6	-2.112365000	-1.800235000	1.770989000
1	-1.401790000	-1.273204000	2.427865000
1	-2.914558000	-2.226688000	2.401118000
6	-2.695040000	-0.864475000	0.751389000
6	-4.075531000	-0.800549000	0.526705000
1	-4.726375000	-1.414433000	1.156756000
6	-4.646029000	0.009975000	-0.471386000
6	-3.750080000	0.753795000	-1.254138000
1	-4.130906000	1.377889000	-2.065523000
6	-2.361502000	0.728571000	-1.047790000
6	-1.815239000	-0.073291000	-0.021241000
6	-1.435117000	1.521717000	-1.929258000
1	-0.631640000	0.876065000	-2.317478000
1	-1.990457000	1.934776000	-2.791337000
6	-1.718216000	3.582943000	-0.607682000
1	-2.622264000	3.673411000	-1.234123000
1	-1.244170000	4.578570000	-0.591849000
6	-2.099034000	3.244068000	0.816261000
6	-3.287590000	3.712497000	1.387982000
1	-3.999202000	4.276087000	0.781637000
6	-3.543196000	3.452709000	2.734557000
1	-4.462150000	3.813018000	3.201920000
6	-2.606959000	2.722241000	3.473760000
1	-2.766857000	2.496661000	4.529106000

6	-1.455625000	2.278941000	2.828396000
1	-0.698450000	1.694497000	3.356347000
6	0.228414000	3.310745000	-2.060020000
1	-0.261363000	3.911425000	-2.847830000
1	0.832064000	2.533018000	-2.554201000
6	1.147138000	4.170671000	-1.224316000
6	1.725447000	5.345489000	-1.715018000
1	1.498041000	5.684694000	-2.727536000
6	2.589606000	6.071534000	-0.892518000
1	3.054565000	6.991593000	-1.252812000
6	2.838123000	5.605995000	0.401225000
1	3.497482000	6.146097000	1.082321000
6	2.217278000	4.427749000	0.814102000
1	2.380250000	4.032430000	1.818820000
6	2.546329000	-0.004703000	-0.944468000
8	2.168996000	-1.134686000	-0.558534000
8	1.993042000	1.104292000	-0.815679000
6	-6.171453000	0.041922000	-0.672092000
6	-6.678299000	-1.381339000	-1.002134000
1	-6.216045000	-1.759065000	-1.928365000
1	-6.456317000	-2.093018000	-0.191107000
1	-7.770198000	-1.373240000	-1.145759000
6	-6.582143000	0.980275000	-1.820259000
1	-6.274358000	2.020862000	-1.628818000
1	-6.154393000	0.662624000	-2.784550000
1	-7.677237000	0.975623000	-1.928116000
6	-6.846892000	0.535572000	0.628354000
1	-6.623133000	-0.123057000	1.482200000
1	-6.509907000	1.552549000	0.885316000
1	-7.941082000	0.560102000	0.504516000
6	2.498212000	1.382931000	2.949781000
6	3.523791000	1.388338000	3.982561000
1	3.322183000	0.593695000	4.715580000
1	4.509886000	1.221890000	3.523334000
1	3.527587000	2.359507000	4.499727000
6	3.946517000	-0.009154000	-1.654403000
17	4.329665000	1.540028000	-2.423789000
17	5.165396000	-0.355440000	-0.367733000
17	3.991593000	-1.306380000	-2.889564000
6	2.382758000	-4.545348000	-0.954567000
6	3.409794000	-5.387056000	-1.551587000
1	2.967605000	-6.031693000	-2.325277000
1	4.178377000	-4.746243000	-2.009147000
1	3.876906000	-6.017767000	-0.781102000

Higher energy local minima of $[Co_2(bpbp)(CH_{(3-n)}\ Cl_nCOO)(MeCN)_2]^{2+}$

The following structures of $[Co_2(bpbp)(CH_{(3-n)}\ Cl_nCOO)(MeCN)_2]^{2+}$ were optimised with both acetonitrile ligands coordinating in the cavity left by the desorption of oxygen.

$[Co_2(bpbp)(CH_3COO)(MeCN)_2]^{2+}$ higher energy conformation

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CH_3COO)(MeCN)_2]^{2+}$, S = 3, E = -6781650.35 kJ/mol, G = -6779725.90 kJ/mol, G_{solv} = -6780172.70 kJ/mol.

Co	-1.738439000	-1.081543000	-0.187506000
Co	1.882001000	-0.839883000	0.053001000
O	-0.033118000	0.027345000	0.150248000
O	-0.874188000	-2.492965000	-1.354572000
O	1.319529000	-2.017850000	-1.551448000
N	-2.986111000	0.381616000	0.929371000
N	-3.653878000	-2.065034000	-0.042560000
N	-2.316739000	0.244859000	-1.769826000
N	2.661672000	0.814113000	-1.136621000
N	2.519152000	0.473453000	1.600002000
N	3.974326000	-1.470798000	-0.517392000
C	-0.155837000	1.368758000	0.175550000
C	-1.104951000	1.995072000	1.021754000
C	-1.185814000	3.391952000	1.070731000
H	-1.917615000	3.836046000	1.752374000
C	-0.377122000	4.232723000	0.285714000
C	0.506706000	3.591647000	-0.593921000
H	1.124541000	4.188219000	-1.268887000
C	0.625139000	2.194132000	-0.666865000
C	-0.500206000	5.761965000	0.400161000
C	-1.946863000	6.191916000	0.063587000
H	-2.678960000	5.740030000	0.751520000
H	-2.215286000	5.901176000	-0.964756000
H	-2.048244000	7.285550000	0.145154000
C	0.457229000	6.489912000	-0.559291000
H	0.246684000	6.246706000	-1.613023000
H	1.511051000	6.245821000	-0.349393000
H	0.341886000	7.578122000	-0.442718000
C	-0.163892000	6.190964000	1.847291000
H	-0.848041000	5.732974000	2.578859000
H	-0.248298000	7.284307000	1.950400000
H	0.864586000	5.900862000	2.115460000
C	-2.060617000	1.149713000	1.818646000
H	-1.520805000	0.400818000	2.420748000
H	-2.645411000	1.789191000	2.504996000
C	-3.946566000	-0.422043000	1.710168000
H	-3.399718000	-0.852618000	2.563714000
H	-4.760572000	0.197200000	2.128685000
C	-4.507782000	-1.545184000	0.861692000
C	-5.805330000	-2.042811000	1.012138000
H	-6.483446000	-1.597698000	1.743283000
C	-6.217296000	-3.110423000	0.207634000
H	-7.227652000	-3.514095000	0.302813000
C	-5.322959000	-3.644302000	-0.724042000
H	-5.608444000	-4.473061000	-1.373802000
C	-4.045625000	-3.089185000	-0.817726000
H	-3.299941000	-3.460292000	-1.525385000
C	-3.704507000	1.246286000	-0.036083000
H	-4.714746000	0.826072000	-0.177776000
H	-3.840035000	2.263834000	0.366729000

C	-3.062361000	1.303243000	-1.404357000
C	-3.323238000	2.357902000	-2.287314000
H	-3.917718000	3.211894000	-1.957319000
C	-2.823197000	2.292221000	-3.588202000
H	-3.019841000	3.099652000	-4.296847000
C	-2.075251000	1.173994000	-3.971122000
H	-1.679924000	1.073800000	-4.983107000
C	-1.839282000	0.178992000	-3.025200000
H	-1.257328000	-0.712574000	-3.266912000
C	1.511878000	1.564708000	-1.706618000
H	0.938147000	0.832329000	-2.296557000
H	1.884726000	2.342862000	-2.398317000
C	3.514596000	1.662028000	-0.275070000
H	3.529205000	2.706324000	-0.631172000
H	4.549804000	1.288135000	-0.344889000
C	3.112756000	1.607336000	1.182013000
C	3.416575000	2.644720000	2.071253000
H	3.890205000	3.557134000	1.704182000
C	3.107444000	2.492356000	3.423109000
H	3.338585000	3.287404000	4.135291000
C	2.495968000	1.308807000	3.850671000
H	2.240072000	1.148833000	4.899098000
C	2.213866000	0.329813000	2.901451000
H	1.726047000	-0.608401000	3.177055000
C	3.439033000	0.169751000	-2.214475000
H	3.983403000	0.910721000	-2.828041000
H	2.719187000	-0.348591000	-2.867636000
C	4.392065000	-0.848426000	-1.637313000
C	5.627394000	-1.135229000	-2.228094000
H	5.935350000	-0.608383000	-3.133437000
C	6.455450000	-2.093036000	-1.639118000
H	7.424767000	-2.334515000	-2.080329000
C	6.028263000	-2.720689000	-0.465962000
H	6.650734000	-3.459351000	0.041516000
C	4.781863000	-2.375806000	0.056480000
H	4.417177000	-2.833712000	0.978414000
C	0.272677000	-2.649766000	-1.875950000
C	0.400778000	-3.706492000	-2.956503000
H	0.597800000	-4.677772000	-2.473255000
H	1.243497000	-3.486082000	-3.623994000
H	-0.532266000	-3.802796000	-3.527350000
N	-1.386199000	-2.352132000	1.675428000
N	1.746479000	-2.646603000	1.248655000
C	1.866892000	-3.761164000	1.546921000
C	-1.536886000	-3.071714000	2.573576000
C	-1.745114000	-3.976111000	3.698004000
H	-1.914442000	-4.999208000	3.330437000
H	-0.868995000	-3.968197000	4.363064000
H	-2.627290000	-3.659309000	4.274350000
C	2.027414000	-5.165662000	1.897600000

H	1.098707000	-5.714340000	1.681571000
H	2.841421000	-5.604435000	1.300985000
H	2.272803000	-5.267849000	2.965127000

$[Co_2(bpbp)(CH_2ClCOO)(MeCN)_2]^{2+}$ higher energy conformation

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CH_2ClCOO)(MeCN)_2]^{2+}$, S = 3, E = -7987977.55 kJ/mol, G = -7986074.62 kJ/mol, G_{solv} = -7986519.94 kJ/mol.

Co	0.640049000	1.881281000	-0.129201000
Co	-1.758253000	-0.926292000	0.142469000
O	0.167984000	-0.108182000	0.180676000
O	-0.942022000	2.335434000	-1.346309000
O	-2.364753000	0.589126000	-1.154435000
N	2.487352000	1.676791000	1.078399000
N	1.360818000	3.923901000	0.054575000
N	2.040597000	1.396517000	-1.647510000
N	-1.140363000	-2.471016000	-1.291655000
N	-1.171484000	-2.502446000	1.463714000
N	-3.667779000	-1.847664000	-0.574955000
C	1.210134000	-0.965324000	0.174190000
C	2.297283000	-0.785791000	1.062385000
C	3.344080000	-1.715206000	1.081051000
H	4.156942000	-1.554406000	1.795884000
C	3.390956000	-2.827602000	0.221184000
C	2.339796000	-2.943460000	-0.700382000
H	2.347999000	-3.755563000	-1.430747000
C	1.266407000	-2.039100000	-0.741908000
C	4.560236000	-3.824873000	0.297296000
C	5.888260000	-3.085746000	0.012299000
H	6.073181000	-2.281508000	0.741858000
H	5.882588000	-2.641565000	-0.996083000
H	6.735439000	-3.787160000	0.070366000
C	4.411649000	-4.965669000	-0.724497000
H	4.405645000	-4.591853000	-1.760828000
H	3.489962000	-5.546394000	-0.558419000
H	5.260017000	-5.660391000	-0.630581000
C	4.611817000	-4.441810000	1.714218000
H	4.758889000	-3.674495000	2.490401000
H	5.447031000	-5.155976000	1.788757000
H	3.679049000	-4.981969000	1.942235000
C	2.340291000	0.449223000	1.919796000
H	1.402986000	0.573167000	2.485741000
H	3.175743000	0.386237000	2.640857000
C	2.537514000	2.900755000	1.903058000
H	1.753965000	2.811467000	2.673247000
H	3.503428000	3.008344000	2.429215000
C	2.253936000	4.116867000	1.045902000
C	2.844713000	5.364691000	1.265363000
H	3.572751000	5.494207000	2.068806000
C	2.491393000	6.434832000	0.436957000
H	2.942514000	7.418436000	0.584804000
C	1.562752000	6.224769000	-0.586382000
H	1.266422000	7.032071000	-1.257983000
C	1.019458000	4.948392000	-0.742982000
H	0.287222000	4.722607000	-1.522264000
C	3.654949000	1.608067000	0.166645000

H	4.090098000	2.619255000	0.095770000
H	4.442753000	0.956017000	0.578287000
C	3.305532000	1.182618000	-1.243893000
C	4.278041000	0.687667000	-2.120775000
H	5.294379000	0.507874000	-1.765283000
C	3.929760000	0.440486000	-3.449501000
H	4.673929000	0.060750000	-4.152938000
C	2.618823000	0.692901000	-3.867516000
H	2.310232000	0.528070000	-4.900979000
C	1.703598000	1.162663000	-2.928475000
H	0.663418000	1.372909000	-3.188847000
C	0.213219000	-2.140271000	-1.812360000
H	0.109977000	-1.169234000	-2.321512000
H	0.513234000	-2.891183000	-2.566609000
C	-1.163920000	-3.779997000	-0.603870000
H	-0.476696000	-4.495461000	-1.088275000
H	-2.178824000	-4.200060000	-0.700295000
C	-0.856336000	-3.669432000	0.871532000
C	-0.340937000	-4.746676000	1.600780000
H	-0.088999000	-5.679227000	1.092311000
C	-0.156149000	-4.608398000	2.976829000
H	0.241415000	-5.436983000	3.566846000
C	-0.482032000	-3.391981000	3.585491000
H	-0.349754000	-3.239647000	4.657642000
C	-0.980350000	-2.365071000	2.787679000
H	-1.241653000	-1.392419000	3.210916000
C	-2.144388000	-2.408535000	-2.370758000
H	-2.021838000	-3.231520000	-3.098767000
H	-1.985250000	-1.460922000	-2.910018000
C	-3.538946000	-2.412293000	-1.791862000
C	-4.631495000	-2.948866000	-2.480578000
H	-4.488328000	-3.405984000	-3.461754000
C	-5.897105000	-2.893645000	-1.892775000
H	-6.766784000	-3.304726000	-2.409687000
C	-6.025625000	-2.315965000	-0.627232000
H	-6.991781000	-2.262276000	-0.123156000
C	-4.883471000	-1.808168000	-0.008514000
H	-4.940403000	-1.354047000	0.982147000
C	-2.066749000	1.769341000	-1.467260000
C	-3.195223000	2.626223000	-2.042273000
Cl	-4.195534000	3.257723000	-0.663152000
H	-3.873461000	2.033393000	-2.665942000
H	-2.813724000	3.500073000	-2.580503000
N	-0.700299000	2.649660000	1.502931000
N	-2.824675000	0.112577000	1.708596000
C	-3.617871000	0.629536000	2.377722000
C	-1.360363000	3.490113000	1.956057000
C	-2.182225000	4.572519000	2.478815000
H	-3.042538000	4.722855000	1.809473000
H	-2.536166000	4.337369000	3.493164000
H	-1.591807000	5.500186000	2.517393000
C	-4.630830000	1.278543000	3.197460000
H	-5.152107000	2.039889000	2.597978000
H	-5.362280000	0.534458000	3.546712000
H	-4.165555000	1.752094000	4.074407000

$[Co_2(bpbp)(CHCl_2COO)(MeCN)_2]^{2+}$ higher energy conformation

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CHCl_2COO)(MeCN)_2]^{2+}$, S = 3, E = -9194295.11 kJ/mol, G = -9192421.03 kJ/mol, G_{solv} = -9192872.36 kJ/mol.

Co	1.010371000	-1.583637000	0.193494000
Co	0.134117000	1.972858000	0.304754000
O	-0.392958000	-0.063682000	0.288105000
O	2.451297000	-0.447538000	-0.684344000
O	1.639559000	1.618227000	-1.120616000
N	-0.393593000	-3.057230000	1.039233000
N	2.256270000	-3.320165000	0.487132000
N	0.122011000	-2.339645000	-1.601572000
N	-1.410972000	2.484563000	-1.143161000
N	-1.488790000	2.355452000	1.613472000
N	0.518148000	4.122902000	-0.189462000
C	-1.684758000	-0.406062000	0.103952000
C	-2.274711000	-1.454590000	0.854078000
C	-3.629712000	-1.762729000	0.682036000
H	-4.050176000	-2.566932000	1.293433000
C	-4.456754000	-1.092796000	-0.236415000
C	-3.837264000	-0.105877000	-1.015507000
H	-4.411867000	0.413827000	-1.785378000
C	-2.483965000	0.239603000	-0.868492000
C	-5.942502000	-1.469167000	-0.366978000
C	-6.062816000	-2.954683000	-0.780006000
H	-5.606404000	-3.624752000	-0.034167000
H	-5.573005000	-3.134720000	-1.750459000
H	-7.122434000	-3.239399000	-0.875789000
C	-6.663067000	-0.612334000	-1.422381000
H	-6.231807000	-0.747295000	-2.427163000
H	-6.630858000	0.459964000	-1.170496000
H	-7.722107000	-0.906191000	-1.477203000
C	-6.642656000	-1.259114000	0.995522000
H	-6.196729000	-1.883279000	1.785781000
H	-7.708429000	-1.526758000	0.921514000
H	-6.576108000	-0.206792000	1.314857000
C	-1.426511000	-2.275737000	1.786825000
H	-0.875452000	-1.633920000	2.493172000
H	-2.066657000	-2.962087000	2.370343000
C	0.412505000	-3.901632000	1.944722000
H	0.607745000	-3.315047000	2.856508000
H	-0.134367000	-4.809524000	2.256815000
C	1.731938000	-4.265244000	1.293369000
C	2.390769000	-5.475885000	1.524251000
H	1.942187000	-6.231913000	2.172097000
C	3.626037000	-5.700554000	0.907070000
H	4.159133000	-6.640112000	1.068019000
C	4.161259000	-4.713311000	0.075501000
H	5.118517000	-4.853941000	-0.428842000
C	3.440797000	-3.532021000	-0.110285000

H	3.805041000	-2.725012000	-0.751549000
C	-0.969370000	-3.876039000	-0.054598000
H	-0.401184000	-4.820421000	-0.103650000
H	-2.015102000	-4.148595000	0.163235000
C	-0.865321000	-3.236151000	-1.421594000
C	-1.686381000	-3.645969000	-2.478626000
H	-2.491117000	-4.361476000	-2.299375000
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H	-2.072725000	-3.449942000	-4.598239000
C	-0.396847000	-2.237532000	-3.944189000
H	-0.161482000	-1.834647000	-4.930434000
C	0.358011000	-1.859101000	-2.836071000
H	1.195421000	-1.164825000	-2.929807000
C	-1.855866000	1.231294000	-1.809312000
H	-0.953250000	0.796112000	-2.267283000
H	-2.565852000	1.475982000	-2.620759000
C	-2.515195000	3.171125000	-0.436115000
H	-3.477605000	3.016185000	-0.953046000
H	-2.313130000	4.255109000	-0.459829000
C	-2.624305000	2.764552000	1.016425000
C	-3.822384000	2.886282000	1.729542000
H	-4.730631000	3.212385000	1.219360000
C	-3.834319000	2.587749000	3.092388000
H	-4.756988000	2.679411000	3.669450000
C	-2.649372000	2.167427000	3.706287000
H	-2.615719000	1.925979000	4.769673000
C	-1.501987000	2.058502000	2.924842000
H	-0.552093000	1.722865000	3.348236000
C	-0.746459000	3.378573000	-2.113095000
H	-1.464504000	3.811954000	-2.832752000
H	-0.028273000	2.766164000	-2.681198000
C	0.007906000	4.467550000	-1.388626000
C	0.179005000	5.747705000	-1.925777000
H	-0.252188000	5.994858000	-2.897939000
C	0.899675000	6.697710000	-1.198541000
H	1.047119000	7.704233000	-1.595693000
C	1.412333000	6.341405000	0.051582000
H	1.965435000	7.056154000	0.662932000
C	1.195418000	5.043725000	0.514316000
H	1.569813000	4.727872000	1.490261000
C	2.488043000	0.693384000	-1.203455000
C	3.741246000	1.043124000	-2.028302000
Cl	5.061787000	1.461457000	-0.871143000
H	3.577444000	1.930496000	-2.646286000
Cl	4.216434000	-0.294800000	-3.103870000
N	1.882359000	-1.078820000	2.215303000
N	1.755838000	2.055018000	1.715426000
C	2.815480000	2.286114000	2.127397000
C	2.473913000	-1.115911000	3.213032000
C	3.224182000	-1.180229000	4.461100000

H	4.303807000	-1.160336000	4.249850000
H	2.963513000	-0.329958000	5.108433000
H	2.986779000	-2.114108000	4.992388000
C	4.151422000	2.583245000	2.622735000
H	4.804036000	1.711485000	2.469249000
H	4.569094000	3.432265000	2.061254000
H	4.115547000	2.839746000	3.691846000

$[Co_2(bpbp)(CCl_3COO)(MeCN)_2]^{2+}$ higher energy conformation

Cartesian Coordinates for the optimised structure of $[Co_2(bpbp)(CCl_3COO)(MeCN)_2]^{2+}$, S = 3, E = -10400598.61 kJ/mol, G = -10398760.59 kJ/mol, G_{solv} = -10399212.60 kJ/mol.

Co	-0.213779000	1.888670000	0.288400000
Co	-0.665022000	-1.756489000	0.528044000
O	0.541081000	-0.037329000	0.364953000
O	-2.025399000	1.343945000	-0.486081000
O	-2.046876000	-0.893635000	-0.793912000
N	1.679541000	2.766688000	0.986454000
N	-0.731624000	3.959603000	0.597417000
N	0.767369000	2.229250000	-1.587592000
N	0.451903000	-2.800834000	-1.023557000
N	0.817947000	-2.690341000	1.712221000
N	-1.837558000	-3.620345000	0.149466000
C	1.850631000	-0.188168000	0.075240000
C	2.836841000	0.587185000	0.735680000
C	4.193369000	0.380541000	0.455668000
H	4.922859000	0.985362000	1.003268000
C	4.645423000	-0.556040000	-0.490254000
C	3.650330000	-1.261621000	-1.181470000
H	3.933880000	-1.964715000	-1.967852000
C	2.280297000	-1.092827000	-0.923441000
C	6.150337000	-0.751840000	-0.740151000
C	6.778485000	0.586689000	-1.192372000
H	6.662483000	1.372704000	-0.429431000
H	6.315761000	0.942425000	-2.126936000
H	7.857363000	0.459717000	-1.373680000
C	6.419910000	-1.805453000	-1.828416000
H	5.986322000	-1.514426000	-2.798546000
H	6.019341000	-2.793505000	-1.550001000
H	7.504734000	-1.919206000	-1.973105000
C	6.825033000	-1.217744000	0.570964000
H	6.702824000	-0.479300000	1.378885000
H	7.905299000	-1.363824000	0.413291000
H	6.397725000	-2.172968000	0.915746000
C	2.419416000	1.672879000	1.690435000
H	1.734529000	1.284704000	2.461697000
H	3.308593000	2.089848000	2.197273000
C	1.298872000	3.852550000	1.912346000
H	0.972295000	3.385176000	2.854713000

H	2.155660000	4.505885000	2.157291000
C	0.153587000	4.660400000	1.335101000
C	-0.009881000	6.028801000	1.566795000
H	0.725934000	6.578352000	2.157590000
C	-1.124833000	6.677364000	1.025022000
H	-1.272716000	7.747133000	1.188068000
C	-2.038350000	5.940808000	0.266482000
H	-2.917170000	6.411275000	-0.177161000
C	-1.803533000	4.578026000	0.074567000
H	-2.480638000	3.951240000	-0.511558000
C	2.427097000	3.314494000	-0.170360000
H	2.216984000	4.396069000	-0.225473000
H	3.514993000	3.211924000	-0.023288000
C	2.015879000	2.724352000	-1.500634000
C	2.858141000	2.794594000	-2.616331000
H	3.871699000	3.186169000	-2.511296000
C	2.378518000	2.370438000	-3.855966000
H	3.015210000	2.422431000	-4.741802000
C	1.068477000	1.889503000	-3.946592000
H	0.644841000	1.567172000	-4.898957000
C	0.301848000	1.828845000	-2.784906000
H	-0.727807000	1.467009000	-2.805025000
C	1.260466000	-1.802500000	-1.771950000
H	0.539315000	-1.076328000	-2.179350000
H	1.763072000	-2.296547000	-2.623977000
C	1.287516000	-3.840135000	-0.381965000
H	2.192432000	-4.049111000	-0.977787000
H	0.704314000	-4.775631000	-0.351927000
C	1.661781000	-3.499147000	1.043476000
C	2.780775000	-4.063219000	1.667109000
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C	3.016745000	-3.790339000	3.014866000
H	3.881068000	-4.223626000	3.522723000
C	2.132324000	-2.953142000	3.703620000
H	2.279640000	-2.716504000	4.758370000
C	1.049986000	-2.419645000	3.009002000
H	0.334208000	-1.751075000	3.493742000
C	-0.577635000	-3.394766000	-1.902504000
H	-0.132878000	-4.065708000	-2.659776000
H	-1.073876000	-2.567378000	-2.434249000
C	-1.608846000	-4.126465000	-1.078471000
C	-2.293495000	-5.248849000	-1.555970000
H	-2.080038000	-5.634575000	-2.554820000
C	-3.241848000	-5.864464000	-0.736567000
H	-3.790291000	-6.741562000	-1.086453000
C	-3.461754000	-5.348508000	0.543472000
H	-4.177829000	-5.809164000	1.225780000
C	-2.735693000	-4.226858000	0.942024000
H	-2.869177000	-3.799835000	1.938203000
C	-2.482582000	0.267214000	-0.933547000

C	-3.823790000	0.403600000	-1.737191000
Cl	-5.141384000	0.423861000	-0.497043000
Cl	-4.077078000	-0.959308000	-2.845953000
Cl	-3.861802000	1.928646000	-2.661299000
N	-1.068688000	1.748589000	2.371777000
N	-2.094178000	-1.232757000	2.046757000
C	-3.144536000	-1.081905000	2.515967000
C	-1.529997000	1.996663000	3.407275000
C	-2.109618000	2.326616000	4.703277000
H	-3.123871000	2.730905000	4.567331000
H	-2.156367000	1.431260000	5.340540000
H	-1.492425000	3.085985000	5.206429000
C	-4.474856000	-0.898683000	3.077459000
H	-4.814252000	0.131416000	2.894954000
H	-5.176788000	-1.588869000	2.585746000
H	-4.467220000	-1.102322000	4.158414000

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