Dicobalt Tetracarboxylate Complexes with Labile Axial Ligands

Supporting Information

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Crystallographic Experimental Section

Complex $[Co_2(\mu\text{-}OH_2)(TPA)_4(THF)_4]$, (1)

Data Collection

A blue crystal with approximate dimensions 0.10 x 0.10 x 0.10 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker SMART APEXII diffractometer with Cu K_α (λ = 1.54178 Å) radiation and a diffractometer to crystal distance of 4.03 cm [1].

The initial cell constants were obtained from three series of θ scans at different starting angles. Each series consisted of 41 frames collected at intervals of 0.6º in a 25º range about θ with the exposure time of 10 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEX3 program. The final cell constants were calculated from a set of 9908 strong reflections from the actual data collection.

The data were collected by using a full sphere data collection routine to survey reciprocal space to the extent of a full sphere to a resolution of 0.81 Å. A total of 118030 data were harvested by collecting 18 sets of frames with 0.5º scans in θ and ϕ with exposure times of 10-45 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements [2].

Structure Solution and Refinement

The systematic absences in the diffraction data were uniquely consistent with the space group $P2_1/n$, yielding chemically reasonable and computationally stable refinement [3-8].

A successful solution by direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located with an alternating series of leastsquares

cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms (except atoms H1A and H1B, bound to atom O1) were included in the structure factor calculation at idealized positions and allowed to ride on their neighboring atoms with relative isotropic displacement coefficients.

The structure consists of one dinuclear Co^{II} complex and one molecule of solvent THF; thus, the structural formula is as follows: $[Co_2(\mu_2\text{-}OOCCPh_3)(OOCCPh_3)_2(\mu_2H_2O)(C_4H_8O)_4] \cdot C_4H_8O$.

Several components of the structure displayed positional disorder which are described below:

Atoms C82 and C84 of the O10 THF ligand are disordered over two positions with the major disorder component occupancy equal to 77.6(7)%. The atoms in the minor component of this disorder were refined isotopically with geometric restraints and atomic displacement parameter constraints.

The O12 THF ligand is disordered over three positions with component occupancy ratios of 44.6(3) : 30.2(3) : 25.2(3)%. All atoms in all disordered components were refined isotopically with geometric restraints and atomic displacement parameter constraints.

All atoms in the O13 THF ligand (atoms O13 and C93-C96) are disordered over two positions with the major disorder component occupancy equal to 58.6(3)%. In addition, atom C93A in the minor component of this disordered THF is further split over two positions. The occupancies of this split atom (C93A and C93B) were constrained to be equal to the occupancy of the minor component of the THF and are as follows: 22.9(3)% and 18.5(3)%. The atoms in the minor disorder component were refined isotopically. All atoms were refined with geometric restraints and atomic displacement parameter constraints.

The solvent molecule of THF in the structure was disordered over two positions, with the major disorder component occupancy equal to 55.9(5)%. Both disorder components were refined with geometric restraints and atomic displacement parameter constraints.

The final least-squares refinement of 1071 parameters against 16286 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0479 and 0.1227, respectively. The final difference Fourier map was featureless.

Summary

Crystal Data for $C_{100}H_{102}Co_2O_{14}$ (*M* =1645.67 g/mol): monoclinic, space group $P2_1/n$ (no. 14), *a* = 14.372(5) Å, *b* = 25.215(9) Å, *c* = 23.014(9) Å, *β* = 92.748(7)°, *V* = 8330(5) $Å^3$, *Z* = 4, *T* = 100.02 K, μ(Cu Kα) = 3.655 mm^{-1}, *Dcalc* = 1.312 g/cm^3, 118030 reflections measured (5.202° ≤ 2Θ ≤ 144.336°), 16286 unique (R_{int} = 0.0674, R_{sigma} = 0.0459) which were used in all calculations. The final R_1 was 0.0479 (I > 2σ(I)) and wR_2 was 0.1227 (all data).

Complex $[Co_2(TPA)_2(MeOH)_4] \cdot TPA \cdot MeOH$

Data Collection

A pink crystal with approximate dimensions 0.21 x 0.20 x 0.075 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker Quazar SMART APEXII diffractometer with Mo K_α (λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 4.96 cm [1].

The initial cell constants were obtained from three series of θ scans at different starting angles. Each series consisted of 12 frames collected at intervals of 0.5º in a 6º range about θ with the exposure time of 10 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEXII program suite. The final cell constants were calculated from a set of 9752 strong reflections from the actual data collection.

The data were collected by using a full sphere data collection routine to survey reciprocal space to a resolution of 0.67 Å. A total of 56968 data were harvested by collecting 6 sets of frames with 0.5º scans in θ and ϕ with exposure times of 17 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [2]

Structure Solution and Refinement

The diffraction data were consistent with the space groups $P\bar{1}$ and $P1$. The *E*statistics strongly suggested the centrosymmetric space group $P\bar{1}$, which yielded chemically reasonable and computationally stable results [3-8].

A successful solution by direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of leastsquares

cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. Most hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. The hydrogen atoms H3, H4, and H6A were allowed to refine freely; these atoms and atom H7A were all involved in hydrogen bonding.

The asymmetric unit contains one-half molecule of $Co(C_{20}H_{16}O_2)_2(C_4H_4O)_4$, one solvent methanol molecule, and one triphenyl acetic acid molecule.

The final least-squares refinement of 471 parameters against 12574 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0323 and 0.0889, respectively. The final difference Fourier map was featureless.

Summary

Crystal Data for $C_{86}H_{86}CoO_{14}$ (*M* =1402.47 g/mol): triclinic, space group P-1 (no. 2), a = 12.130(3) Å, b = 12.137(3) Å, c = 13.833(4) Å, α = 109.773(11)°, β = 98.611(10)°, γ = 104.368(13)°, V = 1794.6(8) Å^3, Z = 1, T = 100.0 K, μ(MoKα) = 0.307 mm^{-1}, *Dcalc* = 1.298 g/cm^3, 56944 reflections measured (3.236° ≤ 2Θ ≤ 64.504°), 12574 unique (R_{int} = 0.0286, R_{sigma} = 0.0215) which were used in all calculations. The final R_1 was 0.0323 (I > 2σ(I)) and wR_2 was
0.0889 (all data).

Complex $[Co_2(TPA)_4(Et_2O)_2]$, (2)

Data Collection

A dichroic crystal with approximate dimensions 0.10 x 0.09 x 0.07 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker D8 VENTURE Photon III four-circle diffractometer with Cu Kα (λ = 1.54178 Å) radiation and the detector to crystal distance of 4.0 cm [1].

The initial cell constants were obtained from a 180° ϕ scan conducted at a 2θ = 50° angle with an exposure time of 1 second per frame. The reflections were successfully indexed by an automated indexing routine built in the APEX3 program. The final cell constants were calculated from a set of 8988 strong reflections from the actual data collection.

The data were collected by using a full sphere data collection routine to survey reciprocal space to a resolution of 0.80 Å. A total of 83395 data were harvested by collecting 27 sets of frames with 0.9º scans in θ and ϕ with exposure times of 4-20 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements [2].

Structure Solution and Refinement

The systematic absences in the diffraction data were consistent for the space groups *C*2/*c* and *Cc*. The *E*-statistics strongly suggested the centrosymmetric space group *C*2/*c,* which yielded chemically reasonable and computationally stable results [3-8].

A successful solution by direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located with an alternating series of leastsquares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic

displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

The structure consists of one bimetallic Co^{II} complex with the following formula: $[Co(\mu\text{-}OOCPh_3)_2(OEt)]_2$. The complex resides on a crystallographic two-fold axis; as such, only one-half of the complex is symmetry-independent.

The final least-squares refinement of 455 parameters against 7493 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0281 and 0.0782, respectively. The final difference Fourier map was featureless.

Summary

Crystal Data for $C_{88}H_{80}Co_2O_{10}$ (M =1415.38 g/mol): monoclinic, space group $C2/c$ (no. 15), a = 20.211(12) Å, b = 16.757(6) Å, c = 21.469(8) Å, β = 90.78(3)°, V = 7270(6) $Å^3$, Z = 4, T = 100.0 K, μ(CuKα) = 4.061 mm^{-1}, *Dcalc* = 1.293 g/cm^3, 83395 reflections measured (6.852° ≤ 2Θ ≤ 150.32°), 7493 unique (R_{int} = 0.0496, R_{sigma} = 0.0250) which were used in all calculations.
The final R_1 was 0.0281 (I > 2σ(I)) and wR_2 was 0.0782 (all data).

Complex $[Co_2(TPA)_4(THF)_2]$, (3)

Data Collection

A violet crystal with approximate dimensions 0.22 x 0.16 x 0.13 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker SMART APEXII diffractometer with Cu K_α (λ = 1.54178 Å) radiation and a diffractometer to crystal distance of 4 cm [1].

The initial cell constants were obtained from three series of θ scans at different starting angles. Each series consisted of 41 frames collected at intervals of 0.6º in a 25º range about θ with the exposure time of 10 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEX3 program.

The data were collected by using a full sphere data collection routine to survey reciprocal space to the extent of a full sphere to a resolution of 0.80 Å. A total of 145922 data were collected with 0.5° scans in θ and ϕ. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements [2].

Structure Solution and Refinement

The systematic absences in the diffraction data were consistent with the space groups *Cc* or *C*2/*c*, with the latter being favored by *E* statistics. Space group *C*2/*c* yielded chemically reasonable and computationally stable refinement [3-8].

A successful solution by direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located with an alternating series of leastsquares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at

idealized positions and allowed to ride on their neighboring atoms with relative isotropic displacement coefficients.

The asymmetric unit consists of one half of the dinuclear Co^{II} complex oriented such that a crystallographic 2-fold axis lies along the Co-Co vector. Several components of this structure displayed positional disorder which is described below:

One of the six phenyl rings in the structure is disordered 674(6):326(6) by a rotation of the C(ipso)–C bond. These disordered carbon atoms were modelled with isotropic thermal displacement parameters.

The carboxylate ligands bind to the Co_2 unit with a helical twist, and we see a disordered superposition of both Δ and Λ stereoisomers. This disorder is manifested in two positions for each of the carboxylate oxygen atoms, with occupancies 71(2):29(2) and 54(4):46(4) for the two independent carboxylate groups.

The C atoms of the axial THF molecules are also disordered over two positions with occupancy ratios of 75(2):25(2) and 53(3):47(3) for the THF molecules at either end of the Co-Co axis.

The final least-squares refinement of 499 parameters (12 restraints) against 7298 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0455 and 0.1221, respectively. The final difference Fourier map was featureless.

Summary

Crystal Data for $C_{88}H_{76}Co_2O_{10}$ (M =1411.35 g/mol): monoclinic, space group C2/C (no. 15), a = 20.931(3) Å, b = 16.880(2) Å, c = 20.205(3) Å, β = 89.668(6)°, V = 7138.9(17) Å^3, Z = 4, T = 100.02 K, μ(Cu Kα) = 4.135 mm^{-1}, *Dcalc* = 1.313 g/cm^3, 145922 reflections measured (6.72° ≤ 2Θ ≤ 151.08°), 7298 unique (R_{int} = 0.0536, R_{sigma} = 0.0186) which were used in all calculations. The final R_1 was 0.0455 (I > 2σ(I)) and wR_2 was 0.1221 (all data).

Table S1. Table of selected equatorial and axial ligands for papers reporting a single Co_2 complex in references 34-67

Molecular Systems			
Ref #	**Equatorial Ligand**	**Axial Ligand(s)**	**CCDC Deposition Numbers**
34	Valorate	Not Determined	1488002
36	Acetate	Trimethoprim	285445, 285446, 285448
37	Benzoate	4-(Dimethylamino)-Pyridine	636393, 636394
38	Phenylacetate	4-(Dimethylamino)-Pyridine	963437
40	Benzoate	Quinoline	1118447
41	2,6-naphthalenedicarboxylate	trans-1,2-bis(4-pyridyl) ethylene	202099, 202100
42	Isophalate	diazabicyclo[2.2.2]octane and Water	725808
43	Phenylacetate	Quinoline	133572
44	Benzoate	4-Methylquinoline	1118313
45	Pivalate	2,3-cyclododecenopyridine	15785857
47	2,6-di(*p*-tolyl)benzoate	dansyl-piperazine	248959
48	4-(diethylamino)benzoate	*N*,*N*-diethylnicotinamide	807222
51	Tricarboxylatetriphenylamine	tris(4-(pyridinyl)-phenyl)amine	1970534
53	α,α,α′,α′-tetramethyl-1,3-benzenedipropionate	Ethanol	1857630
55	4,4′-sulfonyldibenzoate	1,4-bis[2-(4′-pyridyl)-ethenyl] benzene	1500542, 1500543,1500544,1500545, 1500546, 1500547, 1500548
56	4-methylbenzoate	1,4-bis(imidazol-1-yl)-butane	649460
57	4,4′-oxybis(benzoate)	6-(pyridin-4-yl)-1,3,5-triazine-2,4-diamine	1866805
58	2-(4-bromophenyl)quinoline-4-carboxylate	Methanol	948016
60	4,4′-oxybis(benzoate)	4-bis(pyridin-4-ylmethyl)piperazine	1840168, 1840169, 1840170, 1840171, 1840172, 1840173, 1840175, 1840176, 1840177
61	α,α,α′,α′-tetramethyl-1,3 benzenedipropionate	4-thiomethylpyridine	2077982
62	Acetate	2-benzylidene-6,7-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidin-3-one	239118
63	2,4′-biphenyldicarboxylate	2,4-diamine-6-phenyl-1,3,5-triazine	1050999
65	4,4′,4″-benzene-1,3,5-triyl-benzoate	4,4′-bipyridine	848440
67	10-(4-carboxy-phenyl)-10H-phenoxazine-3,6-dicarboxylate	Water	1412434

Table S2. Table of DOIs for papers from references 34-67 that cannot be adequately described merely in terms of a single axial ligand and equatorial ligand.

Extended MOFs or Surveys		
Ref #	**DOI**	**CCDC Deposition Numbers**
35	10.1002/anie.200502505	1267156
39	10.3390/chemistry2030038	2006795
46	10.1021/acs.inorgchem.8b01130	1833892, 1833893, 1833894, 1833895, 1833899
49	10.1002/chem.201101383	824191
50	10.1016/S0020-1693(03)00246-9	197030
52	10.1021/jacs.9b05872	1944159, 1944160, 1881620, 1944155
54	10.1016/j.poly.2018.12.045	1876447, 1876450
59	10.1021/jacs.6b12353	1567974
64	10.1039/C5DT04062K	1424332
66	10.1021/ja208256u	877431

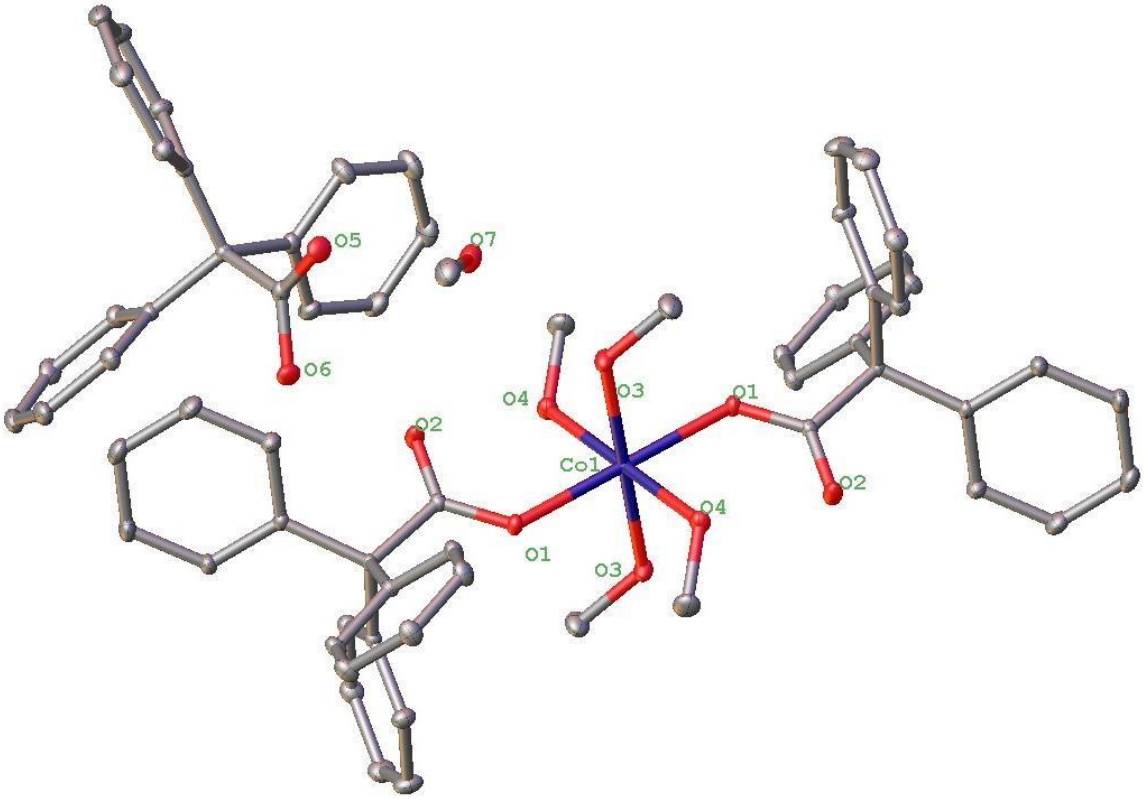


***Figure S1**. Molecular structure of **[Co(TPA)$_2$(MeOH)$_4$] · TPA · MeOH** with hydrogen atoms omitted for clarity. Thermal displacement ellipsoids are drawn at the 50% level.*

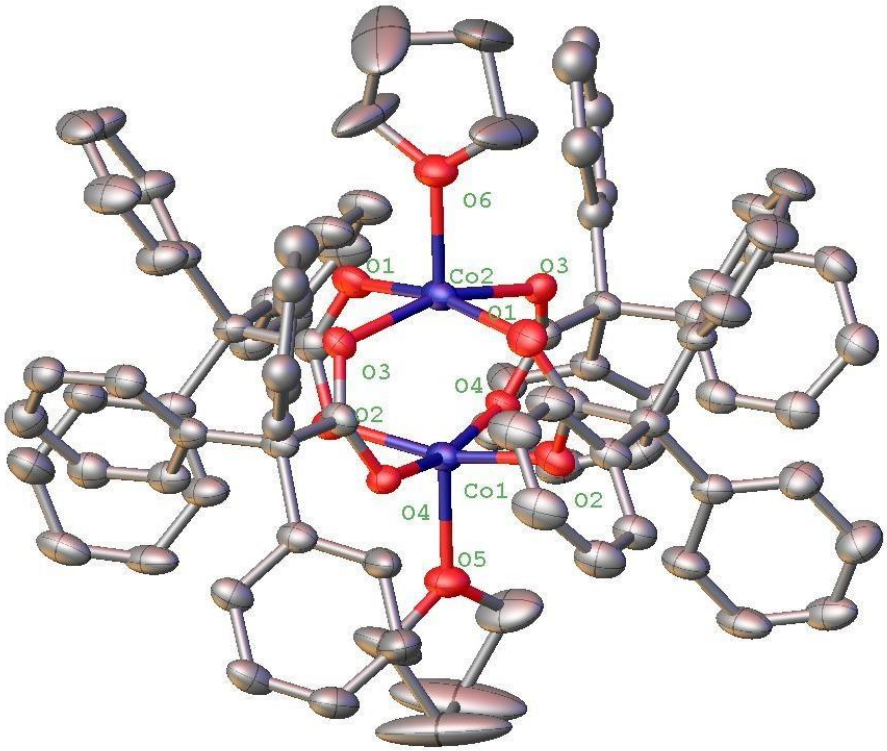


***Figure S2**. Molecular structure of **3** with hydrogen atoms omitted and thermal displacement ellipsoids drawn at the 50% level. The depicted structure represents one orientation of the molecule, which exhibits disorder between the Δ and Λ stereoisomers. . There is also additional positional disorder present within the structure, with the presented configuration being one of the possible conformations.*

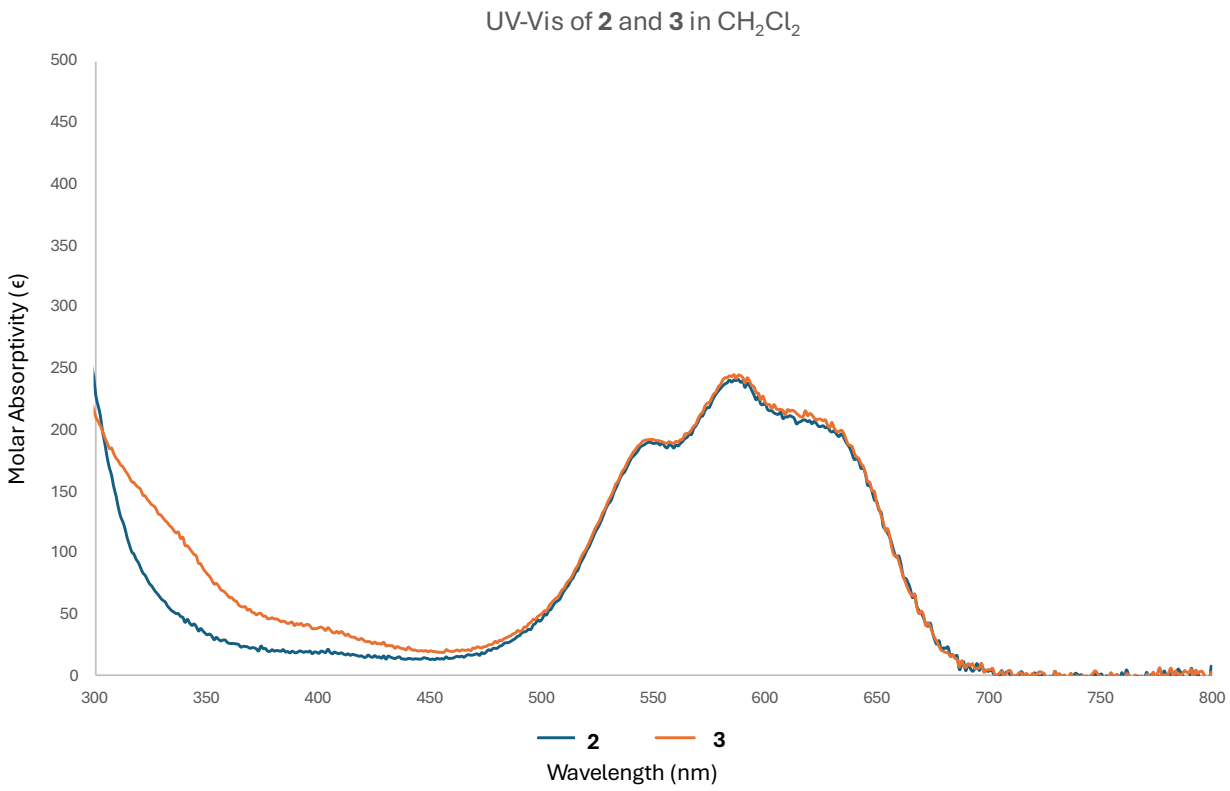


Figure S3. UV-Vis spectra of complexes **2** and **3** in dichloromethane

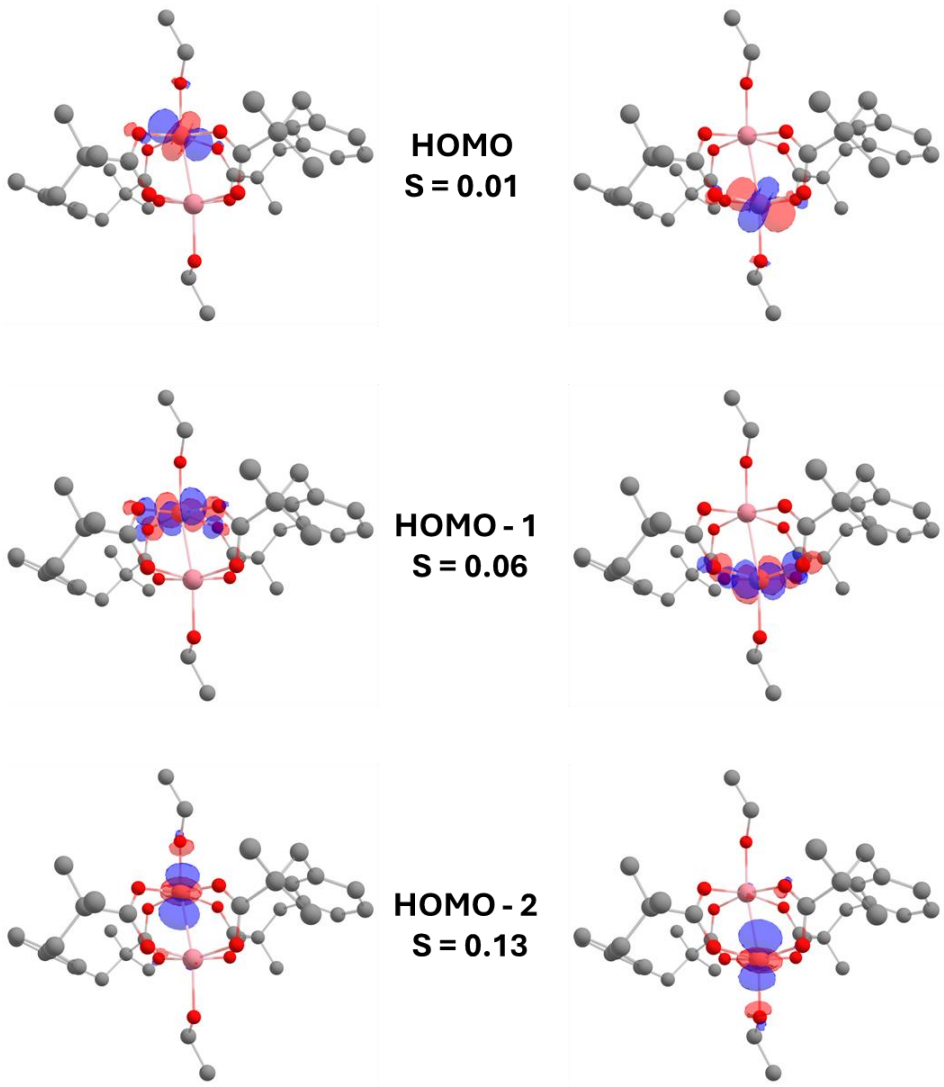


Figure S4. *Calculated magnetic orbitals of $Co_2(esp)_2(EtOH)_2$ of both α (left) and β (right) spin. In between the pairs of orbitals are both the overlap integral S, and the orbital's position relative to the highest occupied molecular orbital (HOMO). Hydrogen atoms omitted for clarity. Grey = carbon, Red = oxygen, Salmon = Cobalt.*

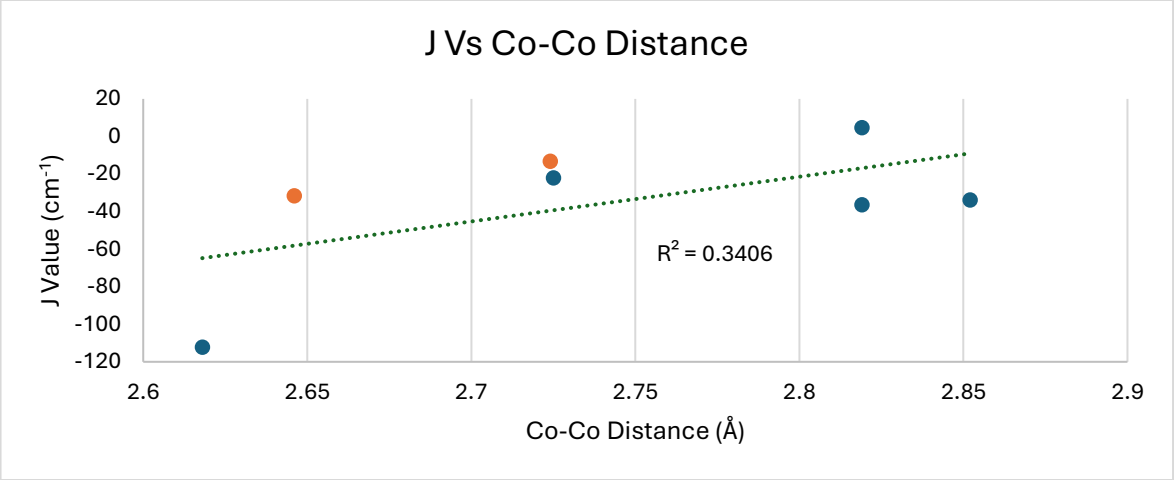


Figure S5. Plot of exchange coupling values for experimental (orange) and calculated (blue) for dicobalt complexes against the Co-Co distance from Table 1 A line of best fit, with the R^2 for the fit, is shown in green.

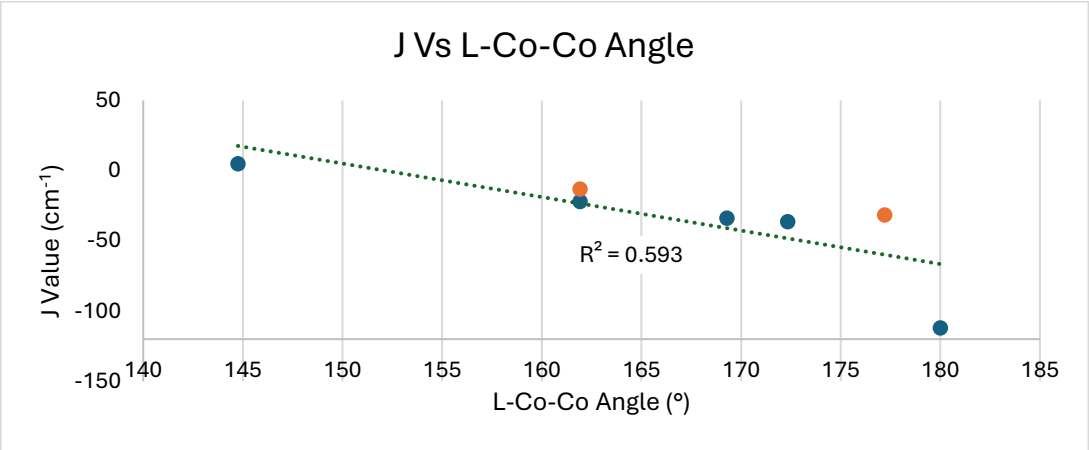
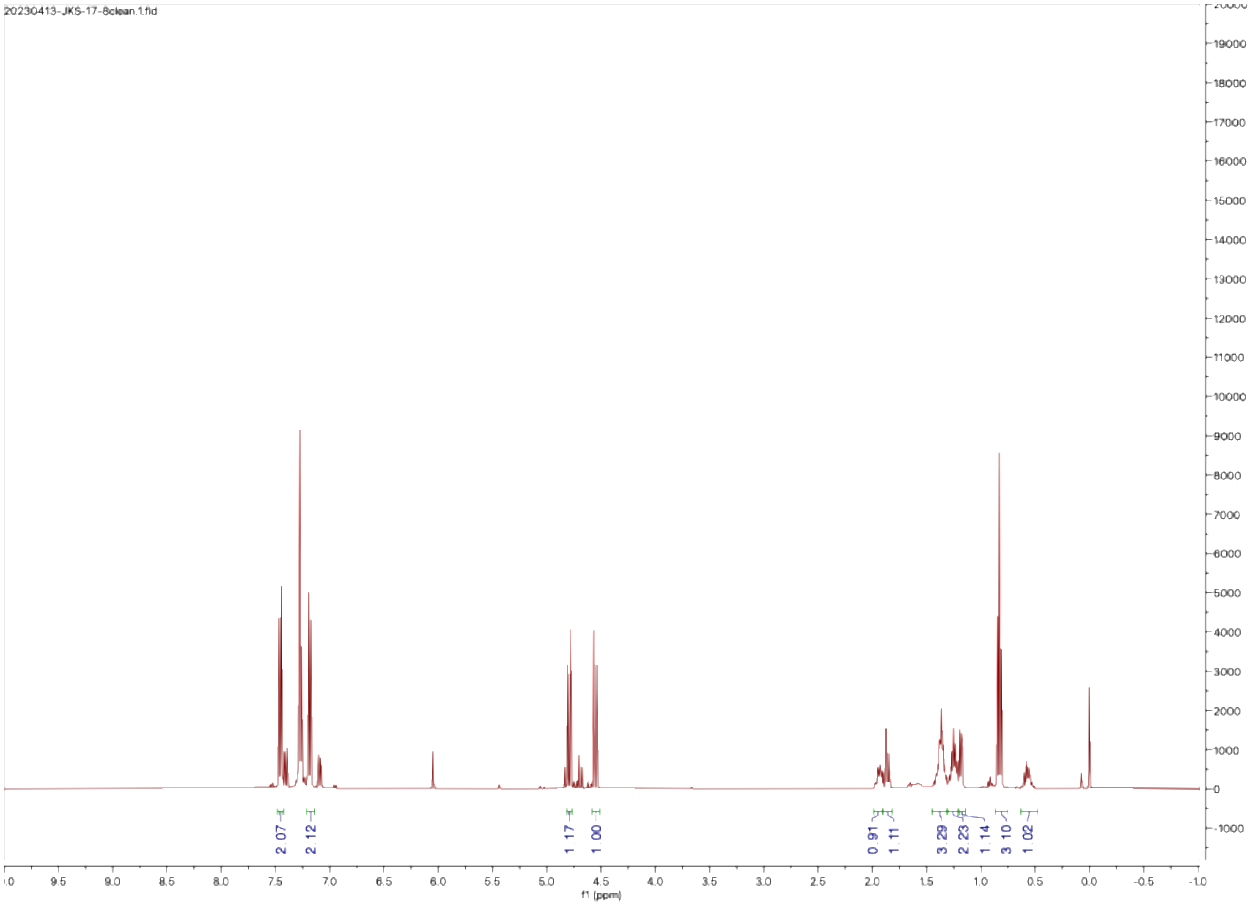


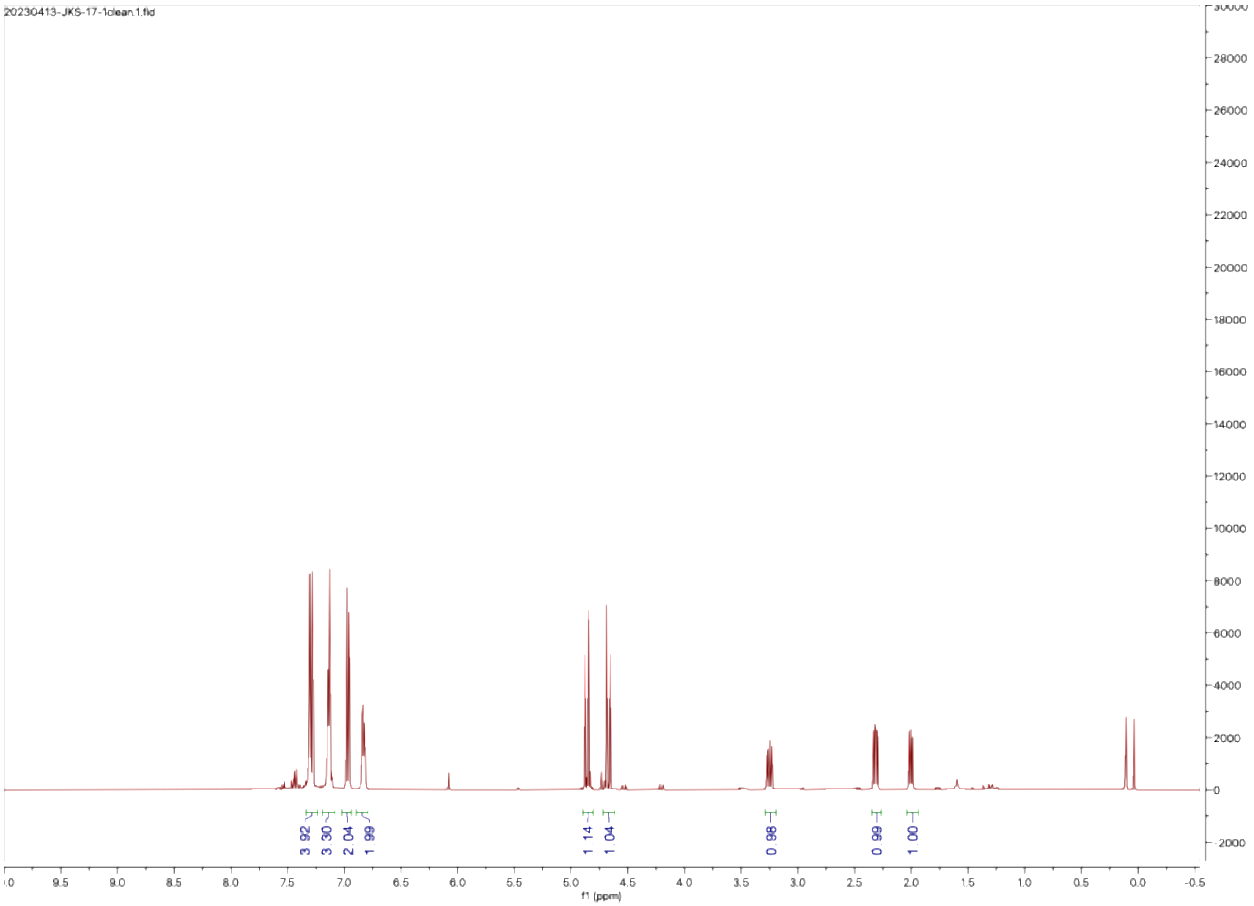
Figure S6. Plot of exchange coupling values for experimental (orange) and calculated (blue) for dicobalt complexes against the L-Co-Co angle from Table 1. A line of best fit, with the R^2 for the fit, is shown in green.

^{1}H NMR Data for compounds **4a**, **5a**, and **8a**, and crude reaction mixtures of **6a**, **7a**, **9a**, **10a**, and **11a**.

Product **4a**



Product **5a**


20230413-JKS-17-1clean.1.fid
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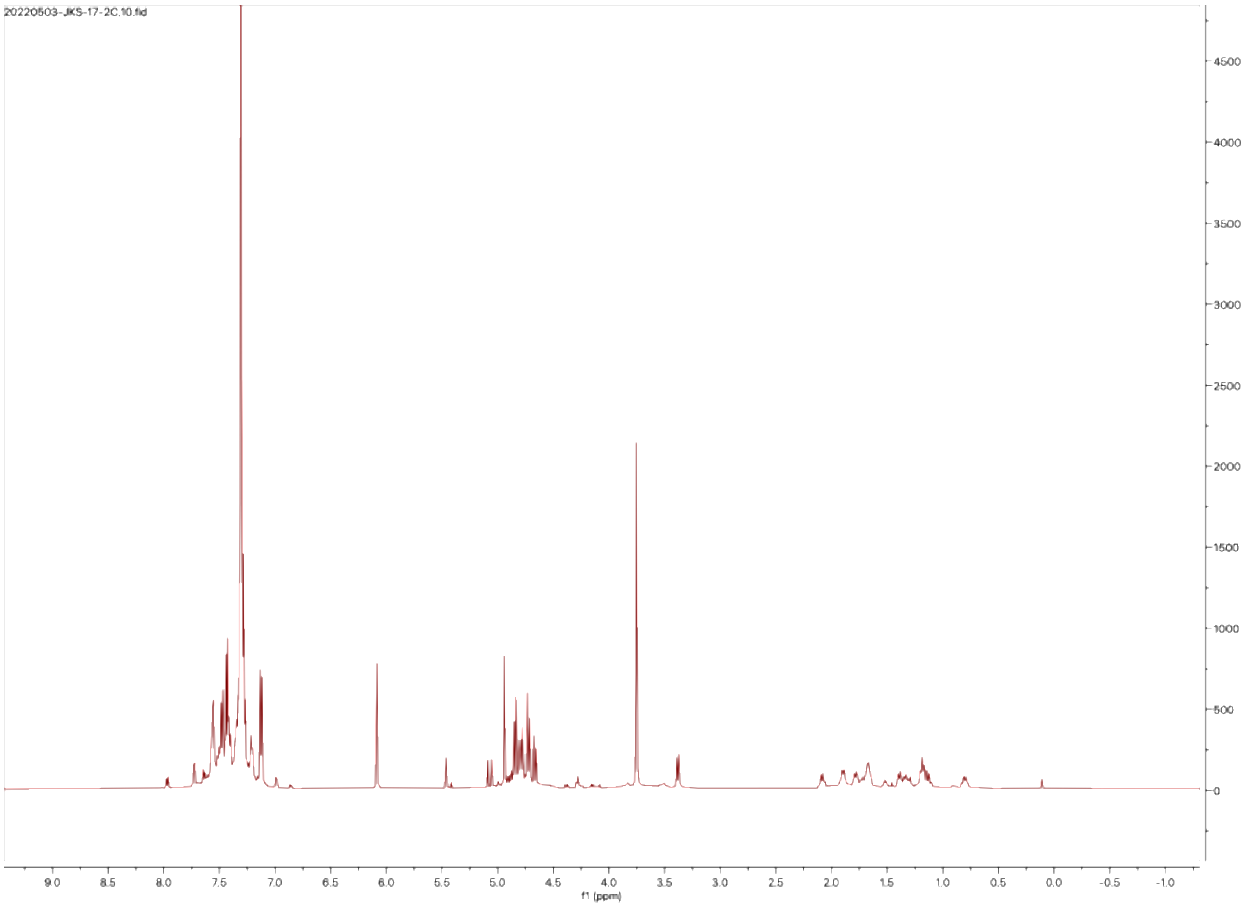
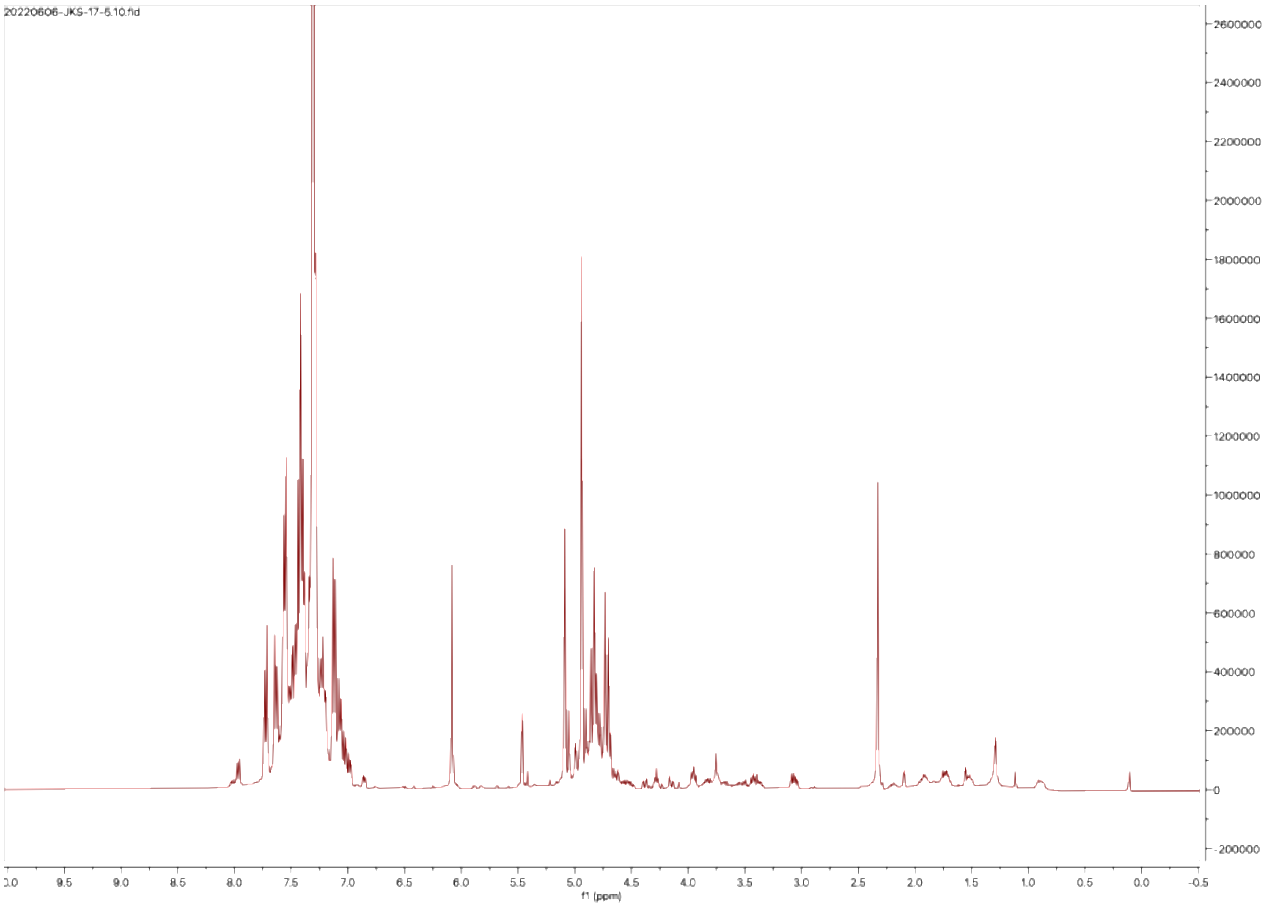
3.30
2.04
1.99
1.14
1.04
0.98
0.99
1.00
f1 (ppm)

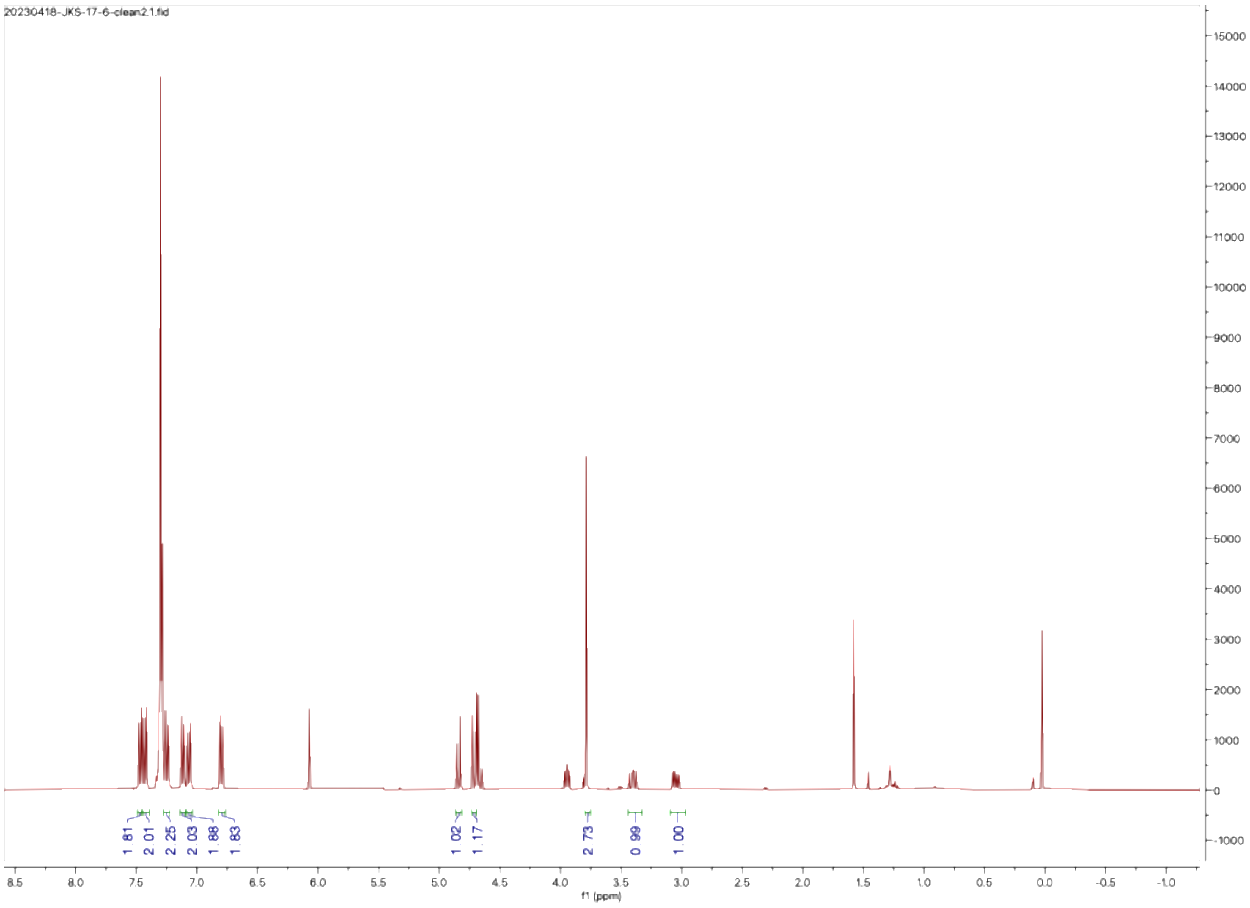
Crude Mixture Product **6a**



Crude Mixture Reaction **7a**



Product **8a**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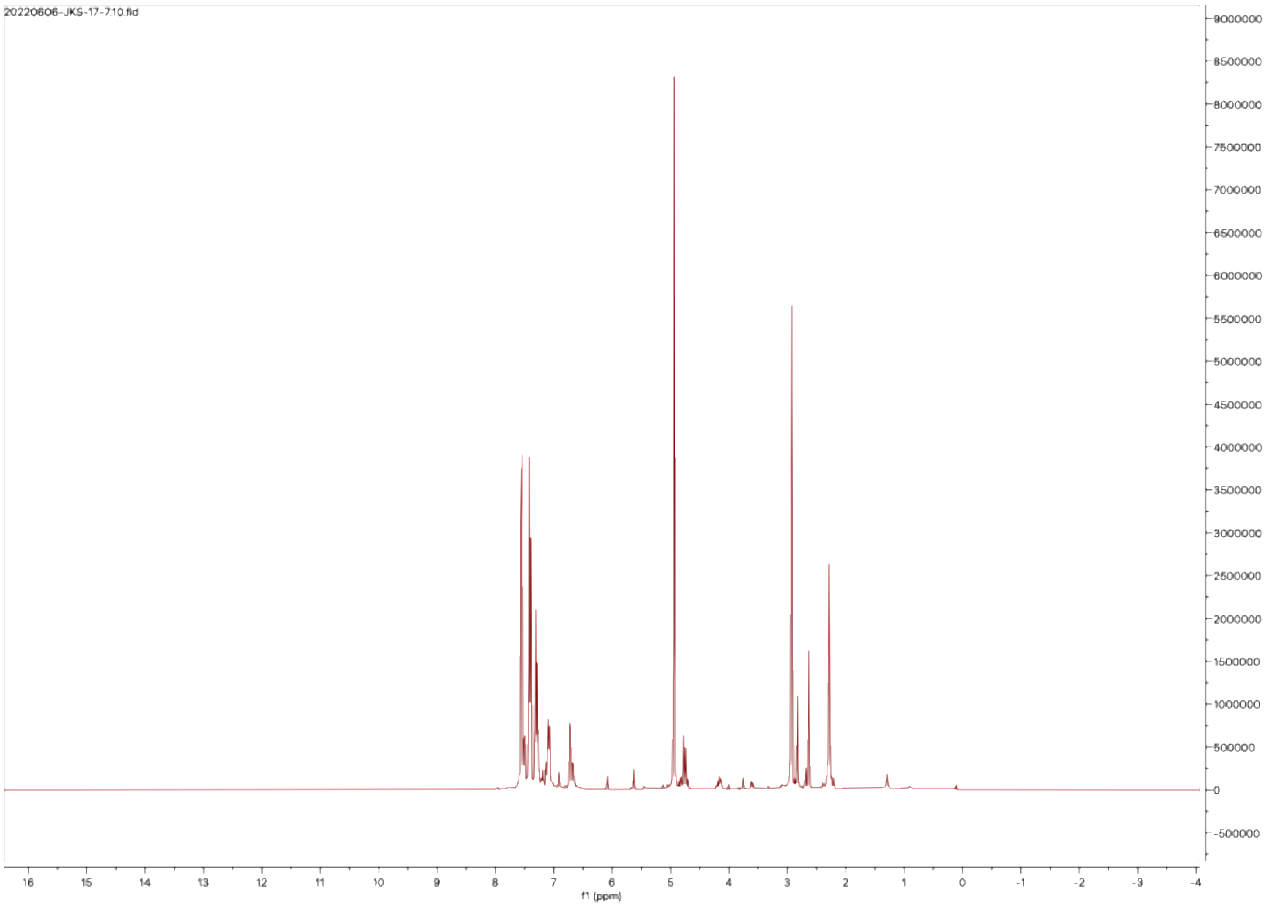
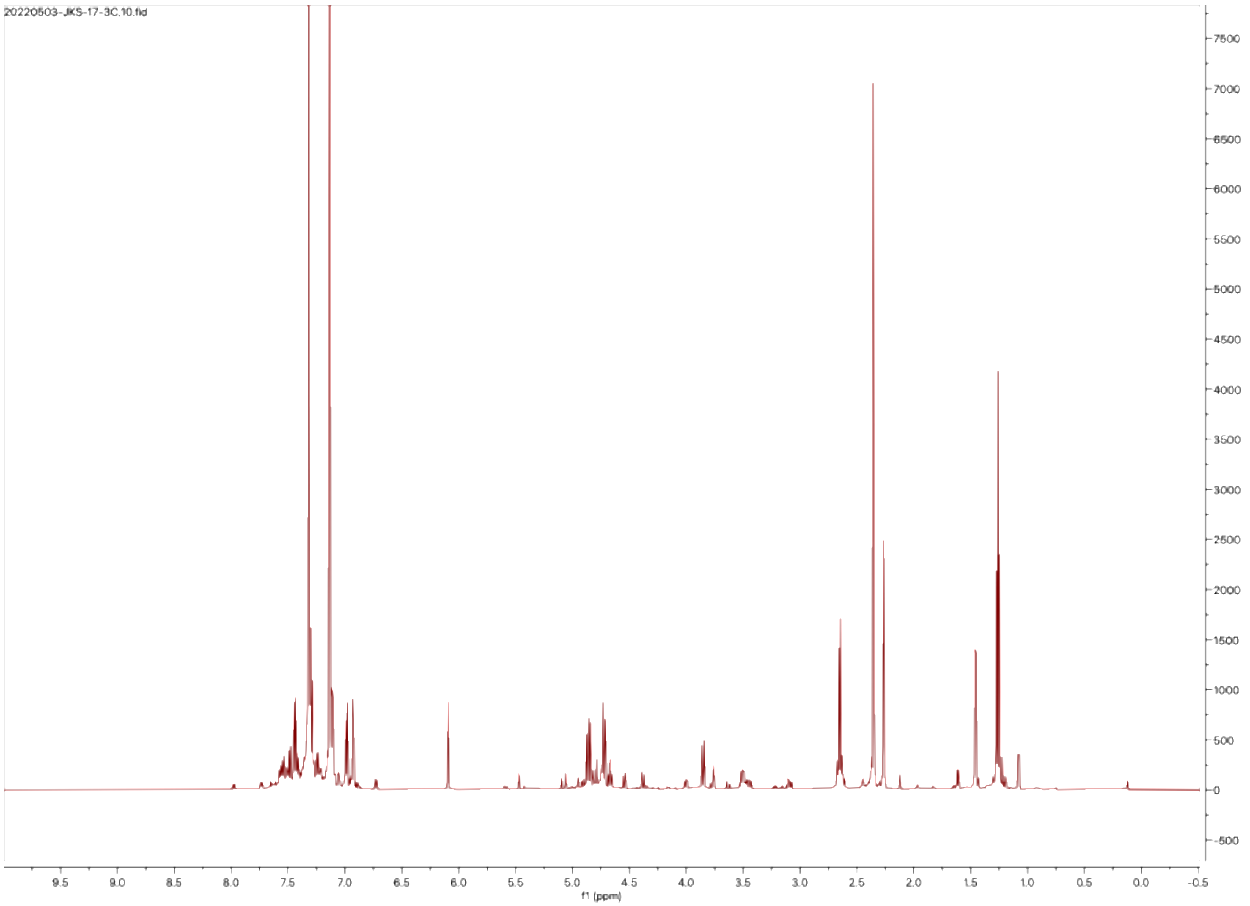
2.01
2.25
2.03
1.88
1.83
1.02
1.17
2.73
0.99
1.00
f1 (ppm)

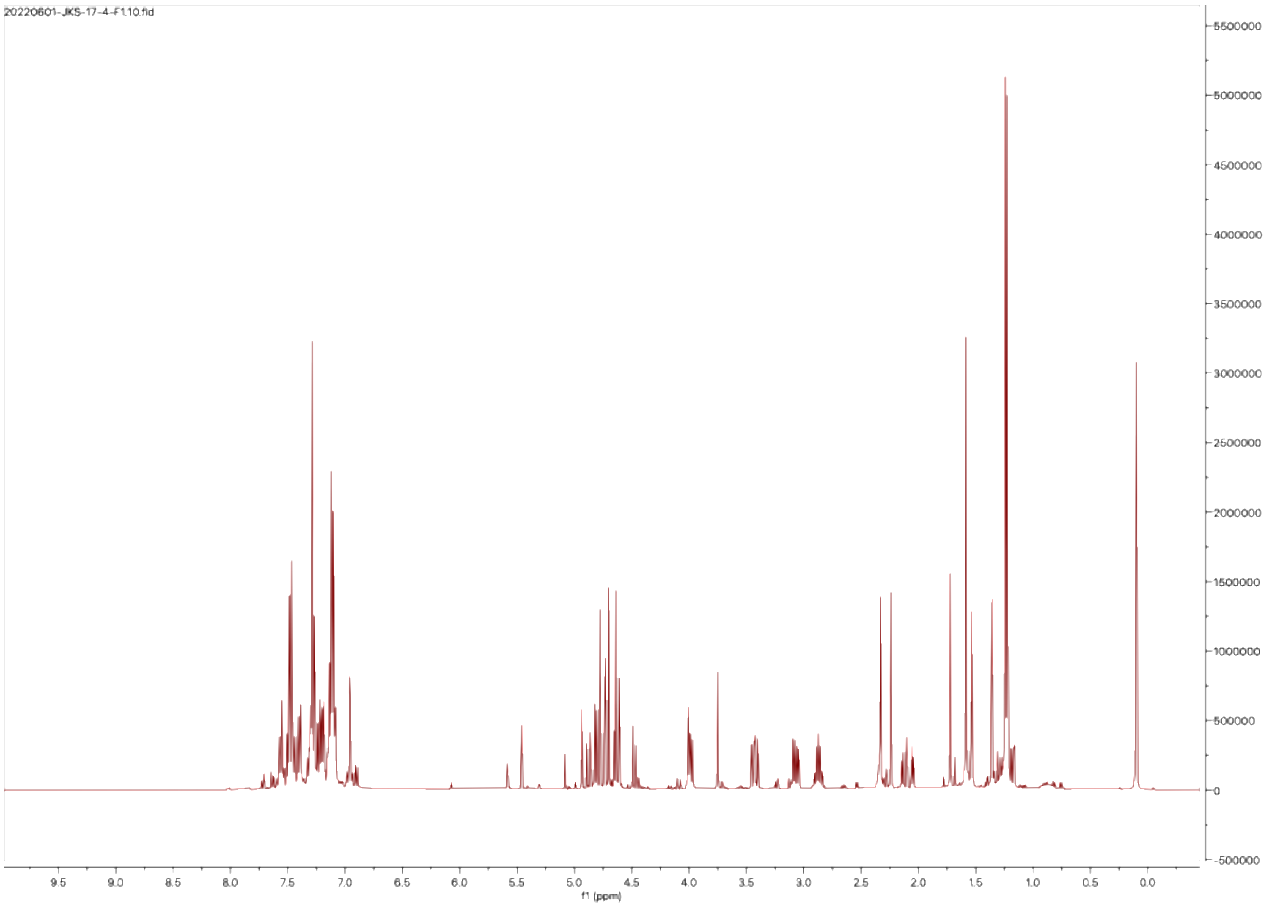
Crude Reaction Mixture Product **9a**



Crude Reaction Mixture Product **10a**



Crude Reaction Mixture **11a**



.xyz files from DFT Calculations

$Co_2(esp)_2(EtOH)_2$, Single Point

C	13.51167	-7.59985	4.650997
C	13.42265	-7.05438	5.921345
C	13.12977	-7.4656	2.147572
C	13.09702	-6.87737	3.540156
C	12.89172	-5.78793	6.104336
C	12.75074	-3.44783	-2.0212
C	12.59709	-5.58637	3.735904
C	12.4672	-5.03333	5.00664
C	12.21157	-4.24806	-0.89477
C	11.94698	-8.64068	0.269226
C	11.82855	-8.21058	1.745366
C	11.82672	-3.67996	5.187111
C	11.60341	-9.43862	2.618407
C	10.65106	-7.23813	1.819381
C	10.28066	-3.70845	5.189305
C	9.771633	-4.2649	3.843537
C	9.766704	-2.25859	5.306067
C	9.752028	-4.55192	6.347244
C	8.17256	-5.88805	-3.17972
C	8.157884	-8.18138	-2.13854
C	8.152955	-6.17507	-0.67601
C	7.643924	-6.73152	-2.02178
C	7.273528	-3.20184	1.348143
C	6.321178	-1.00135	0.549117
C	6.097869	-6.76	-2.01959
C	6.096039	-2.22938	1.422158
C	5.977612	-1.79929	2.898298
C	5.713015	-6.1919	4.06229
C	5.457384	-5.40663	-1.83912
C	5.327498	-4.8536	-0.56838
C	5.173849	-6.99214	5.188724
C	5.03287	-4.65204	-2.93681
C	4.827568	-3.56259	-0.37263
C	4.794814	-2.97436	1.019952
C	4.501939	-3.38558	-2.75382
C	4.412913	-2.84012	-1.48347
Co	9.749191	-4.31804	0.933388
Co	8.175397	-6.12192	2.234136
H	13.88976	-8.09841	2.086556
H	13.85898	-8.4764	4.539482
H	13.72704	-7.55233	6.671189

H	13.36235	-3.99955	-2.55236
H	13.29347	-6.73609	1.498004
H	13.23374	-2.67024	-1.66876
H	12.95952	-4.54634	-0.31833
H	12.81505	-5.43052	6.980964
H	12.70384	-9.25542	0.168419
H	12.33807	-10.0732	2.484972
H	12.33767	-5.07232	2.980447
H	12.13926	-3.29288	6.043542
H	12.13324	-3.08323	4.459493
H	12.09279	-7.84992	-0.29063
H	12.01185	-3.14094	-2.58804
H	11.76317	-5.05442	-1.25288
H	11.59931	-2.70671	0.051048
H	11.57012	-9.16859	3.559902
H	11.12183	-9.08974	-0.00749
H	10.75567	-9.86394	2.370896
H	10.11238	-4.20956	7.191638
H	10.10941	-1.7309	4.555712
H	10.07909	-1.87079	6.149575
H	10.03257	-5.48414	6.226921
H	9.151155	-5.93551	-3.19777
H	9.136584	-8.18254	-2.11984
H	8.788004	-2.25742	5.287362
H	8.773433	-4.50446	6.365293
H	7.892016	-4.95582	-3.0594
H	7.845498	-8.56917	-2.98205
H	7.815181	-8.70906	-1.38819
H	7.81221	-6.23041	-4.02411
H	7.168923	-0.57603	0.796628
H	6.802763	-1.35023	3.175015
H	6.354466	-1.27137	-0.39238
H	6.325276	-7.73326	3.116477
H	6.161414	-5.38554	4.420407
H	5.91274	-7.29902	5.755564
H	5.8318	-2.59004	3.45815
H	5.791352	-7.35673	-1.29197
H	5.785326	-7.14709	-2.87602
H	5.586913	-5.36765	0.187077
H	5.586516	-0.36678	0.682552
H	5.220744	-1.18455	2.999105
H	5.109538	-5.00944	-3.81344
H	4.96507	-5.89363	3.48585
H	4.690846	-7.76973	4.836288

H	4.631115	-3.70388	1.66952
H	4.562236	-6.44041	5.719882
H	4.197546	-2.88763	-3.50367
H	4.065609	-1.96357	-1.37196
H	4.034824	-2.34155	1.080968
O	11.27638	-3.49797	-0.10675
O	10.77351	-6.1313	1.245334
O	10.20616	-3.70692	2.790694
O	9.584641	-7.58917	2.424564
O	8.962294	-5.21998	3.86544
O	8.962294	-5.21998	-0.69792
O	8.339946	-2.8508	0.74296
O	7.718432	-6.73304	0.376831
O	7.151078	-4.30866	1.922191
O	6.648209	-6.942	3.2742732

$Co_2(esp)_2(EtOH)_2$, Geometry Optimization

C	4.66977	-3.56748	-0.09590
C	4.21963	-2.92661	-1.24868
C	4.19523	-3.59977	-2.46357
C	4.63575	-4.91449	-2.54737
C	5.09425	-5.57797	-1.41047
C	5.08019	-4.89445	-0.19735
C	5.62992	-6.98495	-1.47477
C	7.16319	-7.08990	-1.70681
C	7.57721	-8.56644	-1.58596
C	7.54276	-6.55913	-3.08920
C	7.90122	-6.32093	-0.60279
C	7.20434	-3.33599	1.53180
C	6.14563	-2.22746	1.53786
C	6.11181	-1.63770	2.95750
C	6.49206	-1.13440	0.52768
C	4.75573	-2.85127	1.22679
C	5.40490	-6.81624	3.48349
C	4.27560	-7.73245	3.06434
C	12.51396	-3.62356	-0.32162
C	13.64206	-2.70145	0.08757
C	10.71645	-7.10773	1.64335
C	11.77598	-8.21531	1.63482
C	11.80680	-8.80480	0.21495
C	11.43268	-9.30882	2.64558
C	13.16624	-7.59063	1.94261
C	13.25470	-6.87384	3.26485
C	13.70563	-7.51473	4.41732

C	13.73216	-6.84116	5.63194
C	13.29305	-5.52597	5.71575
C	12.83406	-4.86240	4.57911
C	12.84595	-5.54634	3.36620
C	12.29989	-3.45485	4.64354
C	10.76653	-3.34850	4.87440
C	10.35437	-1.87130	4.75548
C	10.38525	-3.88089	6.25568
C	10.02887	-4.11515	3.76838
Co	8.23673	-5.90215	2.58286
Co	9.68763	-4.53881	0.58721
H	3.88236	-1.89854	-1.19447
H	3.83281	-3.09592	-3.35111
H	4.61890	-5.42926	-3.50032
H	5.14272	-7.53352	-2.28472
H	7.05781	-9.16287	-2.33923
H	8.65115	-8.68120	-1.74575
H	7.01131	-7.12254	-3.85996
H	8.61328	-6.66426	-3.26047
H	7.29332	-5.50499	-3.19571
H	13.44368	-1.67618	-0.22859
H	5.42930	-5.40040	0.68935
H	5.39109	-7.50613	-0.54637
H	7.33407	-8.96136	-0.59964
H	5.35157	-0.85593	3.01843
H	7.07507	-1.19197	3.21416
H	7.45640	-0.68467	0.76121
H	5.72931	-0.35260	0.55521
H	6.54785	-1.52944	-0.48494
H	4.02253	-2.04156	1.25927
H	6.56671	-7.45094	1.98821
H	5.88366	-2.40762	3.69412
H	4.51041	-3.54378	2.03290
H	5.22491	-5.78832	3.16395
H	5.54253	-6.82042	4.56440
H	3.33932	-7.40617	3.52150
H	4.13900	-7.71009	1.97994
H	11.35403	-2.98306	1.17205
H	12.03247	-8.03452	-0.52208
H	13.40940	-6.89821	1.13578
H	12.69692	-4.64858	0.00574
H	12.37392	-3.62849	-1.40220
H	14.57854	-3.03025	-0.36732
H	13.77978	-2.71324	1.17201
H	12.56757	-9.58585	0.15199

H	10.84329	-9.25134	-0.03938
H	10.46820	-9.75934	2.41416
H	12.19606	-10.08993	2.61625
H	11.37880	-8.91396	3.65838
H	13.89973	-8.40001	1.90881
H	12.49639	-5.04023	2.47974
H	12.53994	-2.93361	3.71548
H	10.59904	-1.47507	3.77008
H	4.47155	-8.76102	3.37118
H	14.04182	-8.54315	4.36311
H	14.09509	-7.34505	6.51925
H	13.31139	-5.01090	6.66851
H	12.78702	-2.90717	5.45413
H	10.87354	-1.27670	5.51033
H	9.28035	-1.75557	4.91414
H	10.91647	-3.31905	7.02774
H	9.31467	-3.77503	6.42613
H	10.63370	-4.93538	6.36094
O	8.77037	-5.47552	-0.94174
O	7.60797	-6.59672	0.59503
O	8.21614	-3.19846	0.80218
O	6.99955	-4.33097	2.28244
O	6.66571	-7.26416	2.94011
O	10.92045	-6.11104	0.89469
O	11.25339	-3.17406	0.22111
O	9.70449	-7.24759	2.37236
O	10.32204	-3.83624	2.57140
O	9.16037	-4.96197	4.10577

2, Single Point

C	21.24843	20.57004	-2.51259
C	21.1241	21.77619	-1.858
C	20.34438	19.53926	-2.27784
C	20.09745	21.94685	-0.94231
C	19.57004	15.17388	-2.34901
C	19.55695	17.94372	2.498677
C	19.50503	18.38501	1.181902
C	19.29672	19.69814	-1.37443
C	19.24398	16.23241	-1.5103
C	19.20985	15.19715	-3.68033
C	19.20033	20.91609	-0.69518
C	19.03612	22.42102	-4.8399
C	18.97202	23.30724	-5.90839
C	18.85721	25.80432	-0.65768

C	18.76099	25.36793	0.64702
C	18.56624	17.34866	-1.98522
C	18.53736	16.3016	-4.16943
C	18.50219	17.24047	3.043014
C	18.38995	18.12851	0.401586
C	18.29504	18.5523	-1.06806
C	18.23865	17.37167	-3.34265
C	18.15504	22.54229	-3.78046
C	18.07152	25.23656	-1.64724
C	18.02369	24.3117	-5.89144
C	17.8864	24.33323	0.940867
C	17.38461	16.96912	2.26703
C	17.332	17.40724	0.958861
C	17.17777	23.53795	-3.76425
C	17.15393	24.22235	-1.36566
C	17.12921	24.42085	-4.83353
C	17.08841	23.77112	-0.04773
C	16.85559	19.13071	-1.26631
C	16.47153	20.59347	3.01418
C	16.27658	23.69123	-2.52546
C	16.09313	13.888	0.120999
C	15.97384	14.6436	-1.03472
C	15.90292	20.44469	-6.30107
C	15.58925	22.34502	-2.19362
C	15.13734	14.00478	1.112621
C	15.08809	24.62928	-2.82183
C	15.05623	20.21414	2.692997
C	14.94329	25.8834	-2.24756
C	14.8968	15.49625	-1.18975
C	14.50416	20.13105	-5.83968
C	14.50416	17.7945	-5.15798
C	14.11151	24.2026	-3.72985
C	14.06503	14.87621	0.963809
C	13.95209	22.31275	2.080722
C	13.92023	15.62477	-0.19474
C	13.87097	26.69814	-2.5907
C	13.41906	17.88848	-0.89341
C	13.1054	17.28196	-5.37833
C	13.03447	25.00484	-4.05764
C	12.91519	26.26337	-3.48955
C	12.73173	16.57503	-0.44929
C	12.53679	22.16565	2.555492
C	12.15273	21.09716	-1.84003
C	11.9199	17.84003	1.682681

C	11.87911	14.71875	-2.00292
C	11.85439	16.7509	0.814155
C	11.83054	16.03812	-1.57616
C	11.67632	23.74679	-0.89072
C	11.62371	24.81962	-0.02337
C	11.12191	17.89771	2.818447
C	10.98463	14.2419	-2.95355
C	10.93679	15.74439	1.122121
C	10.85328	16.86886	-2.12522
C	10.76966	21.46372	-4.53651
C	10.71328	21.69143	-1.98391
C	10.61837	22.83902	-0.97272
C	10.50613	25.00811	0.776785
C	10.47096	21.92132	-5.809
C	10.44208	22.21305	-3.40442
C	10.24732	16.86732	3.127094
C	10.15111	15.79782	2.261745
C	10.03629	15.07966	-3.50798
C	9.972198	16.40141	-3.08366
C	9.80799	19.89899	-0.39844
C	9.79847	23.1155	-5.99053
C	9.764335	23.40956	-3.60426
C	9.711591	20.56061	-1.62606
C	9.503285	23.04236	-0.17689
C	9.451363	24.12249	0.696006
C	9.438273	23.85102	-4.88058
C	8.91086	18.89705	-0.05253
C	8.66393	20.20877	-2.47317
C	7.884215	18.54854	-0.91632
C	7.759884	19.21347	-2.11681
Co	14.50416	20.47902	-0.30181
Co	14.50416	19.74594	-2.8145
H	21.95851	20.4411	-3.13039
H	21.7351	22.48266	-2.03211
H	20.44301	18.71533	-2.74046
H	20.32437	18.12748	3.027716
H	20.23816	18.8653	0.815026
H	20.04492	14.42753	-2.00263
H	20.00704	22.77285	-0.48176
H	19.6874	21.72927	-4.83711
H	19.57198	23.22376	-6.64037
H	19.48961	16.19232	-0.59353
H	19.46658	26.49871	-0.87933
H	19.42015	14.46738	-4.251

H	19.28381	25.76891	1.33142
H	18.54101	16.94339	3.944586
H	18.51003	21.04073	-0.05454
H	18.27714	16.32655	-5.08274
H	18.21635	21.93683	-3.05091
H	18.15921	25.54543	-2.5414
H	17.98275	24.93295	-6.60894
H	17.8321	24.00394	1.830278
H	17.80373	18.13451	-3.70515
H	17.02433	20.50372	2.20993
H	16.8265	13.29437	0.230916
H	16.81687	20.00275	3.715637
H	16.65651	16.48248	2.635411
H	16.62993	14.57571	-1.71836
H	16.5659	17.21559	0.430781
H	16.49797	21.52203	3.326652
H	16.48931	23.06914	0.177515
H	16.47514	25.10968	-4.84261
H	16.42631	20.78809	-5.5471
H	16.32335	19.62969	-6.6465
H	15.86925	21.1206	-7.01005
H	15.58233	26.1881	-1.61419
H	15.21426	13.48421	1.903548
H	15.02964	19.26946	2.397951
H	15.02759	17.68636	-5.99132
H	14.94189	17.25766	-4.45061
H	14.81772	16.00547	-1.9878
H	14.5057	22.68418	2.812513
H	14.50261	20.29449	3.509711
H	14.1906	23.34412	-4.12887
H	14.06643	20.96405	-5.53196
H	13.98072	19.77411	-6.60043
H	13.97868	22.95057	1.323979
H	13.79405	27.56235	-2.20378
H	13.42599	14.9599	1.661671
H	13.13907	16.33085	-5.61262
H	12.68497	17.78335	-6.10782
H	12.58201	17.39787	-4.55799
H	12.53317	14.13311	-1.64016
H	12.51901	18.553	1.49511
H	12.51035	21.55079	3.318263
H	12.44242	23.62441	-1.43901
H	12.37839	24.69447	-4.67053
H	12.35181	25.42801	0.025528

H	12.19144	23.04089	2.829254
H	12.18182	26.82297	-3.71609
H	11.98399	21.80884	1.829158
H	11.20459	20.62563	-4.43194
H	11.17621	18.6536	3.391254
H	11.02557	13.33229	-3.22442
H	10.84911	15.00316	0.534336
H	10.79197	17.77163	-1.8357
H	10.73117	21.40916	-6.56561
H	10.49829	20.1384	0.208713
H	10.46731	25.74339	1.377163
H	9.724506	16.89728	3.919742
H	9.588166	23.42391	-6.86409
H	9.541732	15.09318	2.448262
H	9.518709	23.93633	-2.85287
H	9.436336	14.75644	-4.17001
H	9.320918	16.98614	-3.45328
H	9.001272	18.44829	0.779939
H	8.963395	24.66654	-4.98989
H	8.770151	22.44013	-0.22794
H	8.683947	24.25204	1.24086
H	8.565303	20.65467	-3.30627
H	7.273214	17.85928	-0.68323
H	7.049803	18.98997	-2.70702
O	16.45523	19.93183	-0.3855
O	16.18268	18.78621	-2.26585
O	15.60639	21.43656	-3.06075
O	14.97491	22.26861	-1.09851
O	14.50416	21.05122	1.659435
O	14.50416	19.17421	-4.77414
O	14.0334	18.54178	-0.0112
O	13.40192	18.18813	-2.11301
O	12.82564	20.85012	-2.86801

2, Geometry Optimization

C	14.01000	20.26793	-5.79008
C	15.21136	20.97445	-6.38395
C	15.73055	22.35513	-2.03622
C	16.24540	23.72338	-2.59215
C	17.25477	23.43877	-3.71309
C	18.17685	22.40017	-3.58020
C	19.11685	22.14794	-4.56727
C	19.15662	22.93549	-5.71287
C	18.25242	23.97902	-5.85091

C	17.31039	24.22753	-4.85776
C	15.01283	24.44959	-3.18485
C	14.13624	23.76960	-4.03372
C	13.05446	24.40952	-4.61758
C	12.82633	25.75799	-4.37573
C	13.70314	26.45426	-3.55665
C	14.78608	25.80766	-2.96921
C	16.88097	24.53276	-1.45997
C	18.21732	24.91568	-1.48118
C	18.77518	25.63367	-0.42587
C	18.00212	25.98412	0.66952
C	16.65836	25.62000	0.69575
C	16.10810	24.90670	-0.35581
C	12.29368	21.30369	-1.88361
C	10.82959	21.84776	-1.89629
C	10.36983	22.12885	-3.33041
C	10.44196	21.12845	-4.30689
C	10.04472	21.37330	-5.61175
C	9.54805	22.62190	-5.97535
C	9.44390	23.61188	-5.01126
C	9.85087	23.36505	-3.70308
C	9.97098	20.74382	-1.23203
C	8.77371	20.30810	-1.79516
C	10.35318	20.19629	-0.00240
C	10.79681	23.12655	-1.04875
C	9.77354	23.38773	-0.14497
C	9.75049	24.57465	0.58251
C	10.75054	25.52069	0.41210
C	11.77374	25.27253	-0.49740
C	11.79306	24.08932	-1.21720
C	14.55094	22.55198	2.15836
C	13.11740	23.02284	2.27882
C	7.99921	19.33656	-1.16822
C	8.40583	18.78214	0.03579
C	9.58626	19.22416	0.62000
C	14.58797	17.93255	-5.28746
C	13.28163	17.16720	-5.22954
C	16.81678	18.86894	-1.29942
C	18.23545	18.35021	-0.92236
C	18.69542	17.24557	-1.88103
C	18.67795	17.44821	-3.26544
C	19.08348	16.45140	-4.13913
C	19.53406	15.22766	-3.65293
C	19.58353	15.02460	-2.28299
C	19.16794	16.02428	-1.40877

C	19.15800	19.59332	-0.99492
C	20.36076	19.57632	-1.69697
C	21.19246	20.69213	-1.71713
C	20.83925	21.84513	-1.03270
C	19.64974	21.86890	-0.31506
C	18.82265	20.75691	-0.29465
C	18.17440	17.81925	0.51649
C	19.20499	18.04087	1.42303
C	19.15807	17.49429	2.70209
C	18.07746	16.71626	3.09201
C	17.04417	16.48469	2.19006
C	17.09617	17.02951	0.91725
C	14.81310	20.22519	2.90260
C	16.28946	20.03139	3.17698
C	13.30256	17.96805	-0.72688
C	12.74041	16.52522	-0.53983
C	11.78766	16.22064	-1.70394
C	10.87758	17.18637	-2.13517
C	11.76401	14.97148	-2.31511
C	13.97654	15.59643	-0.62041
C	14.85476	15.70089	-1.70356
C	15.95538	14.86788	-1.82029
C	16.20035	13.89521	-0.85894
C	15.32328	13.76160	0.20646
C	14.22085	14.60314	0.32413
C	12.01840	16.39600	0.80588
C	12.03628	16.60597	3.22213
C	12.67992	16.70521	1.99937
C	9.98667	16.91922	-3.16236
C	9.98111	15.67188	-3.77758
C	10.86915	14.69763	-3.34470
C	10.70149	15.95449	0.88876
C	10.05285	15.84824	2.11576
C	10.71229	16.18161	3.28797
Co	14.62301	19.71368	-2.82396
Co	14.49678	20.46900	-0.11123
H	13.41084	19.76615	-6.55349
H	15.85202	20.27836	-6.92884
H	14.88080	21.74839	-7.08011
H	10.11725	20.58228	-6.34828
H	9.23879	22.81319	-6.99528
H	18.16819	21.77931	-2.69724
H	19.81828	21.33471	-4.43400
H	19.88589	22.73691	-6.48833
H	18.27306	24.60404	-6.73506

H	16.60986	25.04020	-4.98633
H	14.29904	22.72433	-4.22535
H	12.37527	23.84509	-5.24240
H	11.97340	26.25684	-4.81762
H	13.54776	27.50882	-3.36527
H	15.45732	26.37441	-2.34171
H	18.84039	24.64923	-2.32158
H	19.81993	25.91570	-0.46808
H	18.43454	26.54152	1.49095
H	16.03683	25.89558	1.53906
H	15.06278	24.63830	-0.32782
H	13.35603	20.95166	-5.25330
H	15.80296	21.44737	-5.60072
H	10.81580	20.15182	-4.04310
H	9.04978	24.58659	-5.27067
H	9.76965	24.15606	-2.97335
H	8.43400	20.72614	-2.73072
H	11.26431	20.52815	0.46663
H	8.98697	22.66167	0.00306
H	8.94524	24.75404	1.28403
H	10.73457	26.44243	0.98020
H	12.56035	25.99939	-0.65319
H	12.59352	23.91760	-1.92076
H	15.11006	22.69313	3.08589
H	15.07839	23.06753	1.36093
H	12.58770	22.87093	1.33963
H	12.58898	22.49012	3.07222
H	13.09483	24.08958	2.51166
H	7.07703	19.01159	-1.63376
H	7.81458	18.01184	0.51391
H	9.92442	18.79664	1.55424
H	19.05261	16.63365	-5.20634
H	19.84932	14.44891	-4.33597
H	15.00040	17.96646	-6.29926
H	12.53019	17.61124	-5.88470
H	13.44070	16.13520	-5.54882
H	18.34127	18.39299	-3.66161
H	19.94043	14.08356	-1.88336
H	19.20490	15.83522	-0.34706
H	20.66235	18.68829	-2.23127
H	22.11939	20.65275	-2.27574
H	21.47954	22.71756	-1.06066
H	19.34908	22.76295	0.21421
H	17.89951	20.79958	0.25984
H	20.05371	18.64440	1.13445

H	19.97153	17.68107	3.39200
H	18.03963	16.29300	4.08800
H	16.19676	15.87258	2.47039
H	16.28898	16.83020	0.22875
H	14.27610	20.60020	3.77783
H	14.34287	19.29379	2.59132
H	16.78898	19.63118	2.29658
H	16.76962	20.97045	3.45852
H	16.42649	19.32071	3.99393
H	10.86063	18.15956	-1.66884
H	12.45224	14.20267	-1.99418
H	14.68097	16.45173	-2.45558
H	16.63371	14.99412	-2.65309
H	17.06941	13.25563	-0.94073
H	15.49361	13.00230	0.95955
H	13.54953	14.47414	1.15934
H	12.57176	16.85753	4.12943
H	13.70936	17.02503	1.96710
H	15.34078	17.48775	-4.63624
H	12.88842	17.15594	-4.21449
H	9.29587	17.69054	-3.47655
H	9.28932	15.46243	-4.58385
H	10.87295	13.71904	-3.80843
H	10.16198	15.69995	-0.01036
H	9.02547	15.50741	2.14594
H	10.20802	16.10570	4.24310
O	15.51693	21.47705	-2.91770
O	15.52903	22.20772	-0.81523
O	12.78451	20.78658	-2.90542
O	12.87815	21.39780	-0.76879
O	16.35973	18.69807	-2.45339
O	16.21887	19.49819	-0.38911
O	14.42746	19.28497	-4.81951
O	14.59684	21.14779	1.81618
O	13.52234	18.31499	-1.91635
O	13.54383	18.68666	0.27042

3, Geometry Optimization

C	13.95697	20.25632	-5.71853
C	15.94012	22.34216	-2.01122
C	16.50341	23.67484	-2.59292
C	17.38952	23.33295	-3.79784
C	18.29837	22.27817	-3.71137
C	19.15134	21.98510	-4.76309

C	19.11804	22.74861	-5.92560
C	18.22728	23.80867	-6.01675
C	17.37021	24.09746	-4.95893
C	15.25087	24.45886	-3.05697
C	14.33728	23.85001	-3.92331
C	13.22243	24.52981	-4.38533
C	12.99413	25.84434	-3.99652
C	13.90191	26.46748	-3.15382
C	15.02070	25.78172	-2.68868
C	17.30641	24.45525	-1.54418
C	18.59320	24.91502	-1.81309
C	19.32053	25.62241	-0.86105
C	18.77350	25.88681	0.38465
C	17.48071	25.45302	0.66033
C	16.75649	24.75523	-0.29344
C	12.42548	21.25652	-1.83792
C	10.96147	21.80480	-1.81266
C	10.48755	22.12218	-3.23231
C	10.49876	21.12566	-4.21432
C	10.08807	21.39235	-5.50997
C	9.64622	22.66541	-5.86007
C	9.61142	23.65645	-4.89222
C	10.02731	23.38469	-3.59142
C	10.10187	20.69506	-1.15860
C	8.88503	20.29056	-1.70265
C	10.50146	20.11473	0.05011
C	10.94087	23.06060	-0.93176
C	9.87565	23.33525	-0.08029
C	9.85423	24.49742	0.68449
C	10.90178	25.40423	0.60819
C	11.96532	25.14499	-0.25003
C	11.98023	23.98792	-1.01288
C	14.03188	22.58777	1.96834
C	8.10881	19.31870	-1.07777
C	8.53107	18.73521	0.10706
C	9.73172	19.14566	0.67282
C	13.63467	17.97283	-5.07743
C	16.96983	18.85538	-1.23385
C	18.41671	18.38836	-0.89259
C	18.89693	17.29830	-1.86010
C	18.83790	17.48748	-3.24528
C	19.26172	16.49984	-4.12124
C	19.77180	15.29905	-3.63809
C	19.86218	15.10954	-2.26804
C	19.42986	16.09970	-1.39147

C	19.27164	19.67608	-1.00250
C	20.43435	19.73413	-1.76590
C	21.19500	20.89889	-1.81906
C	20.80723	22.02576	-1.11075
C	19.65841	21.97460	-0.33086
C	18.90552	20.81298	-0.27426
C	18.43479	17.86607	0.54973
C	19.49819	18.13129	1.40561
C	19.53435	17.59025	2.68711
C	18.50420	16.77317	3.13072
C	17.44068	16.49510	2.27818
C	17.41020	17.03447	1.00222
C	13.64406	20.38907	2.80156
C	13.45969	17.99292	-0.72912
C	12.90306	16.54373	-0.54369
C	11.99728	16.23891	-1.74606
C	11.04687	17.18086	-2.14651
C	12.06665	15.03789	-2.44164
C	14.15420	15.63343	-0.56797
C	15.06969	15.73420	-1.62078
C	16.18533	14.91488	-1.68431
C	16.41272	13.96554	-0.69570
C	15.50397	13.84103	0.34398
C	14.38428	14.66570	0.40630
C	12.12958	16.41061	0.77135
C	12.01617	16.69075	3.17773
C	12.71428	16.79135	1.98422
C	10.21076	16.94122	-3.22393
C	10.30277	15.74362	-3.92759
C	11.22831	14.79164	-3.52655
C	10.84138	15.88410	0.80820
C	10.14197	15.77134	2.00587
C	10.71945	16.18576	3.19579
C	12.72870	21.37109	3.53096
C	12.63891	22.55585	2.56236
C	13.22611	19.53040	-6.83633
C	12.57213	18.36072	-6.09302
Co	14.77116	19.69140	-2.81735
Co	14.75065	20.55919	-0.10110
H	13.29993	20.94132	-5.18464
H	10.10385	20.60179	-6.25017
H	9.32553	22.87486	-6.87279
H	18.35064	21.68043	-2.81342
H	19.84520	21.16006	-4.66765
H	19.78250	22.51988	-6.74946

H	18.19409	24.41718	-6.91198
H	16.68311	24.92711	-5.04651
H	14.50227	22.83062	-4.23043
H	12.52054	24.02445	-5.03473
H	12.11637	26.37309	-4.34542
H	13.74436	27.49446	-2.84840
H	15.71699	26.29119	-2.03990
H	19.04839	24.71179	-2.76990
H	20.32151	25.95952	-1.09979
H	19.34069	26.42919	1.13060
H	17.03179	25.66152	1.62369
H	15.75394	24.43462	-0.06452
H	14.86123	20.77528	-6.03281
H	10.83254	20.13338	-3.95463
H	9.26313	24.65072	-5.14269
H	9.99877	24.17537	-2.85725
H	8.52987	20.73387	-2.62069
H	11.43617	20.41270	0.49270
H	9.05511	22.63597	-0.00348
H	9.01568	24.68778	1.34274
H	10.88942	26.30630	1.20709
H	12.78572	25.84566	-0.33530
H	12.81135	23.81075	-1.67927
H	14.75574	23.07981	2.62397
H	14.07704	23.02844	0.97749
H	7.17147	19.01793	-1.52909
H	7.93805	17.96538	0.58343
H	10.08433	18.69150	1.58911
H	19.19545	16.67172	-5.18852
H	20.10019	14.52737	-4.32304
H	14.35502	17.26011	-5.48411
H	18.45098	18.41242	-3.64107
H	20.26542	14.18669	-1.86996
H	19.50116	15.92078	-0.32990
H	20.75964	18.86844	-2.32257
H	22.09225	20.91929	-2.42512
H	21.38729	22.93769	-1.16732
H	19.33459	22.84637	0.22114
H	18.01925	20.78964	0.33876
H	20.30913	18.76435	1.07441
H	20.37219	17.81153	3.33658
H	18.52950	16.35427	4.12900
H	16.63192	15.85177	2.60042
H	16.58183	16.79639	0.35271
H	13.09643	19.64388	2.23253

H	14.35507	19.88539	3.45640
H	10.96061	18.11534	-1.61301
H	12.78498	14.28627	-2.14762
H	14.91570	16.46789	-2.39456
H	16.88881	15.03535	-2.49669
H	17.29407	13.33877	-0.73477
H	15.66217	13.10217	1.11975
H	13.68909	14.54427	1.22309
H	12.49109	17.00056	4.10071
H	13.72395	17.16924	1.98941
H	13.22921	17.59351	-4.14352
H	9.48573	17.69278	-3.50908
H	9.65428	15.55461	-4.77397
H	11.30530	13.85021	-4.05623
H	10.36452	15.56476	-0.10575
H	9.13933	15.36227	1.99978
H	10.17444	16.10754	4.12811
H	12.37469	23.49224	3.05147
H	11.91135	22.36674	1.77447
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H	11.66856	18.69017	-5.57978
H	12.50571	20.17953	-7.33254
H	13.93093	19.16298	-7.58540
O	15.65293	21.46603	-2.86698
O	15.74666	22.22216	-0.77927
O	12.90967	20.79001	-2.88467
O	13.00984	21.29302	-0.72066
O	16.52898	18.74280	-2.40202
O	16.33743	19.38805	-0.28493
O	14.36031	19.20732	-4.79369
O	14.41173	21.18784	1.84985
O	13.67206	18.31496	-1.93047
O	13.70020	18.72068	0.25231

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