Supporting Information

Chirality Engineering in Layered Metal Hydroxides for Enhanced Electrocatalytic Oxygen Evolution and Reaction Mechanism Revelation

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Experimental Section

General materials

Cobalt nitrate hexahydrate ($Co(NO_3)_2 \cdot 6H_2O$, ≥99%) was purchased from Aladdin. L-threonine (L-Thr, ≥99%), D-threonine (D-Thr, ≥99%), triethylamine ($C_6H_{15}N$, ≥99%), titanium sulfate ($Ti(SO_4)_2$, ≥96%), anhydrous sodium sulfate (Na_2SO_4, ≥99%) , potassium hydroxide (KOH, ≥95%) were purchased from Macklin. Anhydrous ethanol (≥99.7%) was purchased from Tianjin Fuyu Fine Chemical Co., Ltd. Nafion solution (D520, 5%) was purchased from DuPont Company. All reagents were used as received without further purification.

Synthesis

Chiral $Co(OH)_2$ nanomaterials were synthesized using a liquid phase synthesis method. Co nitrate hexahydrate (1.2 g) and chiral L/D-Thr at varying concentrations (0, 1, 3, 5, and 10 mmol) were dissolved in water (40 mL). The mixture was subjected to magnetic stirring at room temperature until complete dissolution and homogeneity were achieved. Subsequently, triethylamine (5 mL) was added dropwise to the solution. Following an additional 3 min of stirring, the solution was transferred to a hydrothermal reactor and heated at 180 ℃ for 10 h. The resulting products were then centrifuged at 6000 rpm for 3 min and washed with water and anhydrous ethanol for three times. Finally, the products were dried overnight at 60 °C to yield $Co(OH)_2$ nanomaterials, denoted as **0L**, **0D**, **1L**, **1D**, **3L**, **3D**, **5L**, **5D**, **10L**, and **10D**.

Characterization

X-ray diffraction (XRD) patterns of materials were measured using a diffractometer with a Cu-Kα radiation source operating at 40 kV and 40 mA (D8-Advance, Bruker). Morphologies of materials were taken using a scanning electron microscopy (SEM) at 15 kV and 0.2 nA (Apreo HiVac, FEI) and a transmission electron microscopy (TEM, Talos F200x, FEI). The thickness and spin polarization of materials were measured by an atomic force microscopy (AFM, Dimension Icon, Bruker). Specific surface areas of materials were measured by a fully automatic gas adsorption analyzer (ASAP 2460, Micromeritics). Laser confocal Raman spectra

of materials were measured by a Raman spectrometer (Reinshaw inVa). Ultraviolet-visible (UV-vis) spectra of materials were measured with a spectrophotometer (Pulsar TU-1901). Circular dichroism (CD) spectra of materials were measured by a spectroscopy using a 150 W xenon lamp with the spectrum of anhydrous ethanol as a baseline (Chirascan, Applied Photophysics). X-ray photoelectron spectroscopy (XPS) results of materials were obtained with a spectrometer (PHI Versaprobe 4). X-ray absorption fine structure spectroscopy (XAFS) results of materials were measured by a spectrometer (easyXAFS300+).

Electrochemical Studies

In a typical procedure, 4 mg of catalysts (**1L**, **3L**, **5L**, and **10L**), 375 μL water, 125 μL anhydrous ethanol, and 50 μL Nafion (5 wt%) were mixed in a vortex mixer. The samples were then sonicated for 1 h to obtain a suspension. A drop of the obtained suspension (5 μL) was coated on a GC electrode (0.07 cm^2) and dried naturally in air. Electrochemical tests were carried out with an electrochemical analyzer (CHI 660e) using a typical three-electrode system, with a catalyst-loaded GC electrode as the working electrode, a carbon rod as the counter electrode, and a Hg/HgO electrode as the reference electrode. Linear scanning voltammetry (LSV) data were obtained at 0.005 V s^{-1} with 100% *iR* compensation. Tafel plots were obtained by measuring LSV at a low scan rate. Electrochemical impedance spectroscopy (EIS) was performed at 0.696 V (vs Hg/HgO) with an amplitude of 0.005 V in the range of 1 ~ 1×10^5 Hz. Cyclic voltammetry (CV) tests with different scan rates were conducted between 0.02 and 0.10 V s^{-1} without *iR* compensation. Stability tests were performed by loading the catalyst ink on a carbon cloth electrode. The potential *E* (versus reversible hydrogen electrode, vs RHE) was calculated with Equation (S1).

$$E\left(vs\ \mathrm{RHE}\right)=E\left(vs\ \mathrm{Hg/HgO}\right)+V_{\mathrm{Hg/HgO}}\left(0.098\,\mathrm{V}\right)+0.059\times\mathrm{pH} \quad \text{(S1)}$$

The potential *E* (versus normal hydrogen electrode, vs NHE) was calculated with Equation (S2).

$$E\left(vs\ \mathrm{NHE}\right)=E\left(vs\ \mathrm{Hg/HgO}\right)+V_{\mathrm{Hg/HgO}}\left(0.098\,\mathrm{V}\right) \quad \text{(S2)}$$

Titanium sulfate photometric method for detecting hydrogen peroxide

The catalyst material (**1L** and **10L**) was coated on a glassy carbon electrode as the working electrode. A carbon rod was selected as the counter electrode and Ag/AgCl was selected as the reference electrode. The electrolysis was carried out in neutral solution (0.5 M Na_2SO_4) at E = 1.7 V (vs RHE) for 1h. Then, the electrolyte (5 mL) was mixed with acidic $Ti(SO_4)_2$ solution (0.3 mol L^{-1} H_2SO_4 and 3 mmol L^{-1} $Ti(SO_4)_2$) for 5 min. The content of H_2O_2 was detected using a UV-visible spectrophotometer.

Theoretical Calculations

Adsorption energy calculations were carried out with the CASTEP module in the Materials Studio 8.0 software package. Crystal structures of $Co(OH)_2$ with different crystal planes were constructed. Generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) and projector augmented wave (PAW) pseudopotential were selected to describe interactions between core and electrons. An energy cutoff of 300 eV was used for the plane-wave expansion. The Monkhorst Pack of a 2 × 2 × 1 k-point grid was selected. The predicted crystal habit of $Co(OH)_2$ was obtained by the crystal morphology prediction model with the Bravais Friedel Donnay Harker (BFDH) method.

Density of states of $Co(OH)_2$ with different spin states and calculations of intermediate adsorption energy in reaction processes were carried out using the Vienna Ab initio Simulation Package (VASP 6.3.2). The GGA of PBE function was used to describe the exchange-correlation energy. The PAW method and pseudopotentials were used to describe the interactions between valence electrons and ions. A 3 × 2 × 1 k-point grid under Monkhorst-Pack was used in the optimization process. The truncation energy of 500 eV was set. The lattice parameters and ionic positions of all crystal structures were fully relaxed. The convergence criteria for the total energy of all relaxed atoms and the final force were 10^{-5} eV and 0.03 eV $Å^{-1}$, respectively. To correct for the localization effect of d-orbital electrons in transition metal atoms, the Hubbard+U method was used, and the effective U value of Co was 2.5 eV. In the

low spin state formed by the strong crystal field, the initial magnetic moment of Co ion was set to 1 μB. However, in the corresponding high-spin state under the weak crystal field condition, the initial magnetic moment configuration is 3 μB.

Calculation of anisotropy factor (g-factor)

The *g*-factor represents the degree of asymmetry extinction of the circularly polarized light and can be used as an index to evaluate the chiroptical activity of substances among different systems. The *g*-factor was calculated with Equation (S3).

$$g-\text{factor}=\frac{A_{LCP}-A_{RCP}}{A_{LCP}+A_{RCP}}=\frac{\Delta A}{A_{total}}\approx\frac{\text{CD}\left(\text{mdeg}\right)}{32980\cdot\text{Abs}} \qquad \text{(S3)}$$

The CD values and extinction values were obtained from circular dichroism spectra and the corresponding UV-vis spectra at the same concentration, respectively.

Calculation of adsorption energy

The adsorption energies of threonine on different crystalline surfaces were calculated with Equation (S4).

$$\Delta G=E_{\text{total}}-E_{\text{surface}}-E_{\text{adsorbate}} \quad \text{(S4)}$$

Calculation of spin polarization (*P*)

Spin polarization (*P*) can be quantified using the Equation S5.

$$P=\frac{I_{\text{up}}-I_{\text{down}}}{I_{\text{up}}+I_{\text{down}}}\times 100\% \qquad \text{(S5)}$$

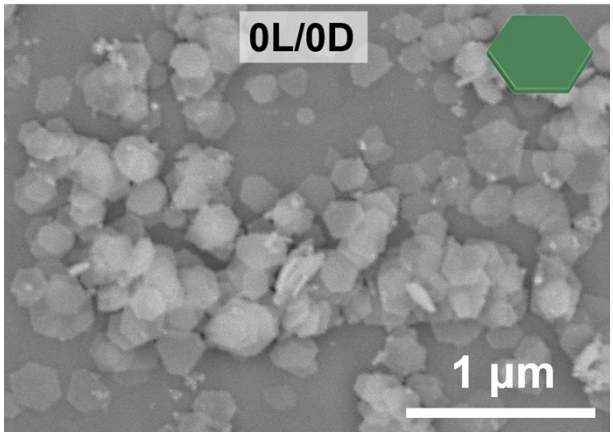

Fig. S1. SEM image of $Co(OH)_2$ obtained without adding amino acids.

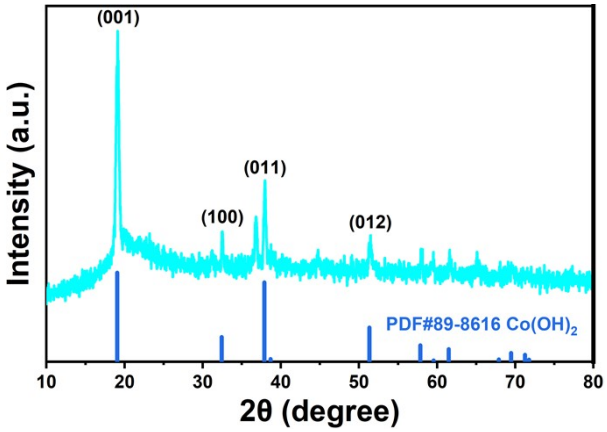

Fig. S2. XRD pattern of $Co(OH)_2$ obtained without adding amino acids.

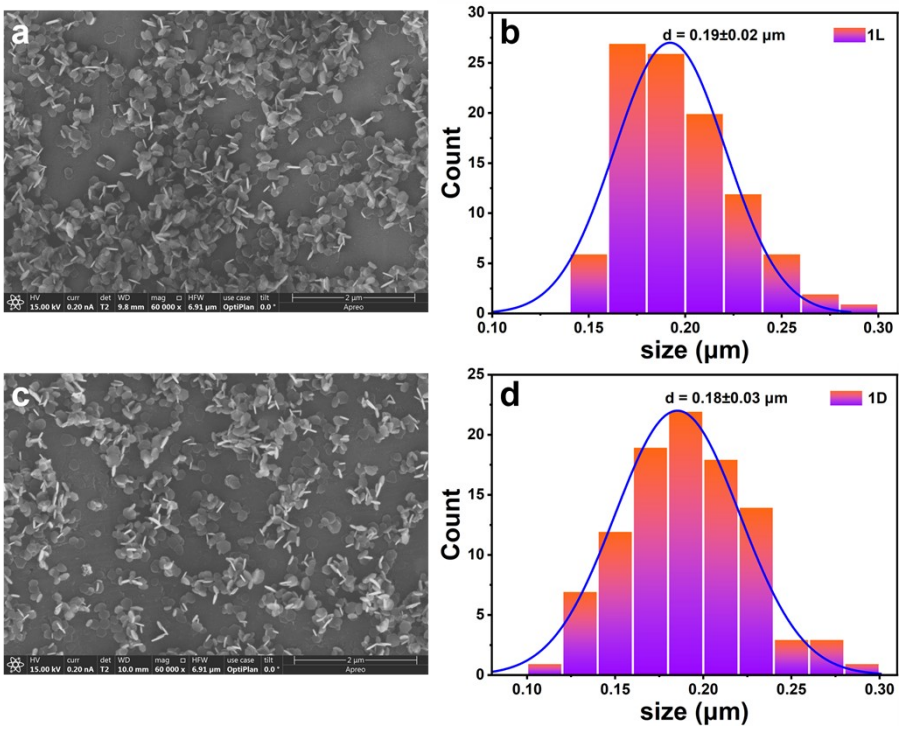

Fig. S3. (a, c) SEM images and (b, d) size distribution diagrams of **1L** (a, b) and **1D** (c, d).

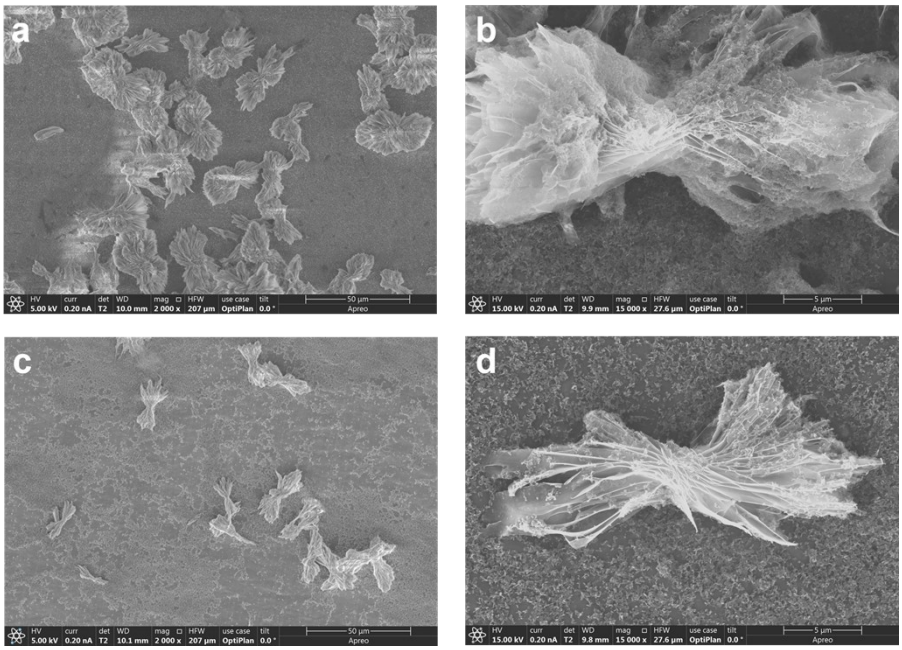

Fig. S4. SEM images of (a, b) **3L** and **3D** (c, d).

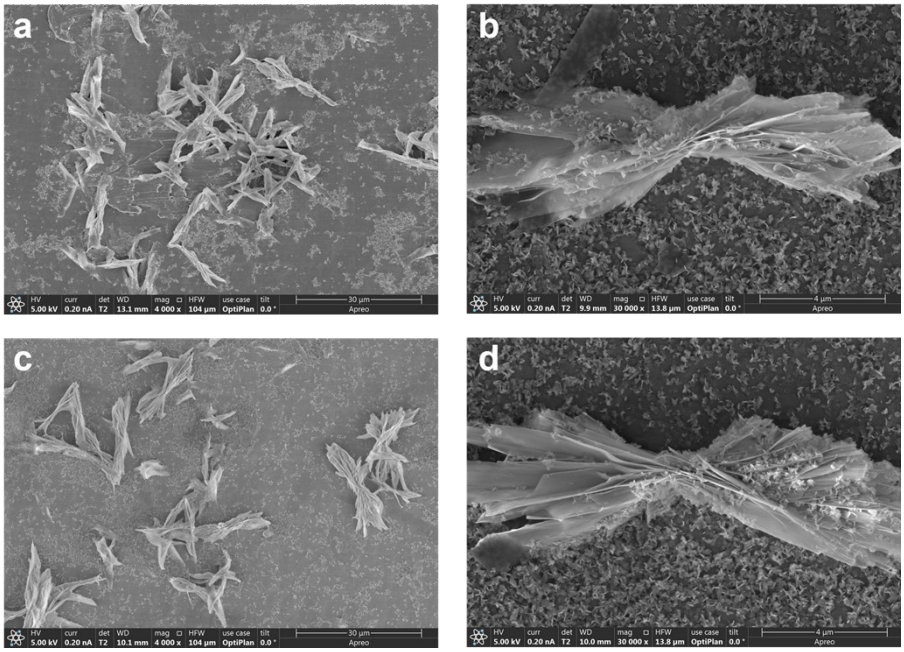

Fig. S5. SEM images of (a, b) **5L** and (c, d) **5D**.

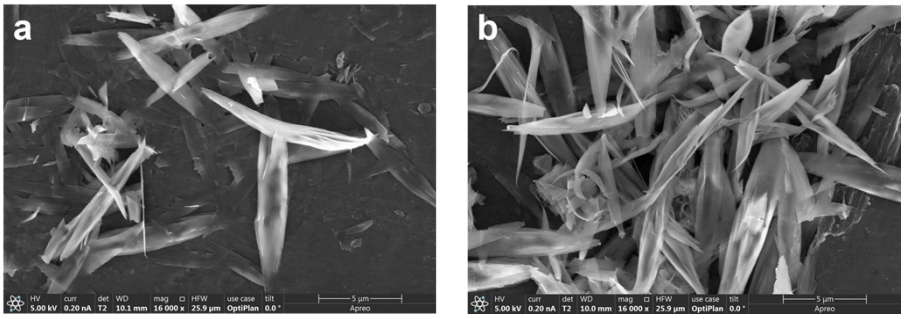

Fig. S6. SEM images of (a) **10L** and (b) **10D**.

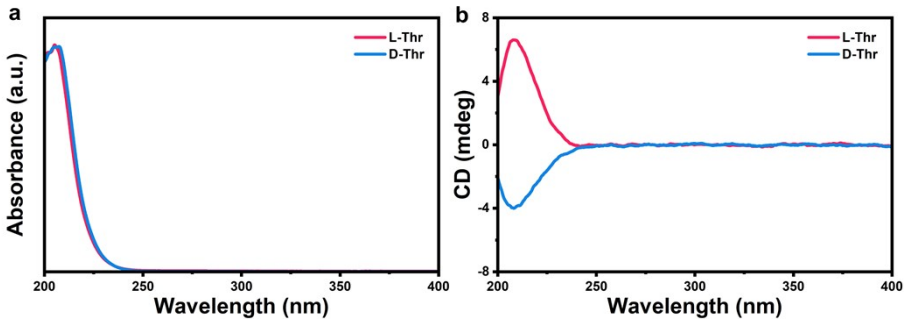

Fig. S7. (a) UV-vis and (b) CD spectra of L/D-Thr. Dissolve a quantity of L/D-Thr in deionised water to make a 0.1 M solution and test for UV-vis and CD in the 200 ~ 400 nm range.

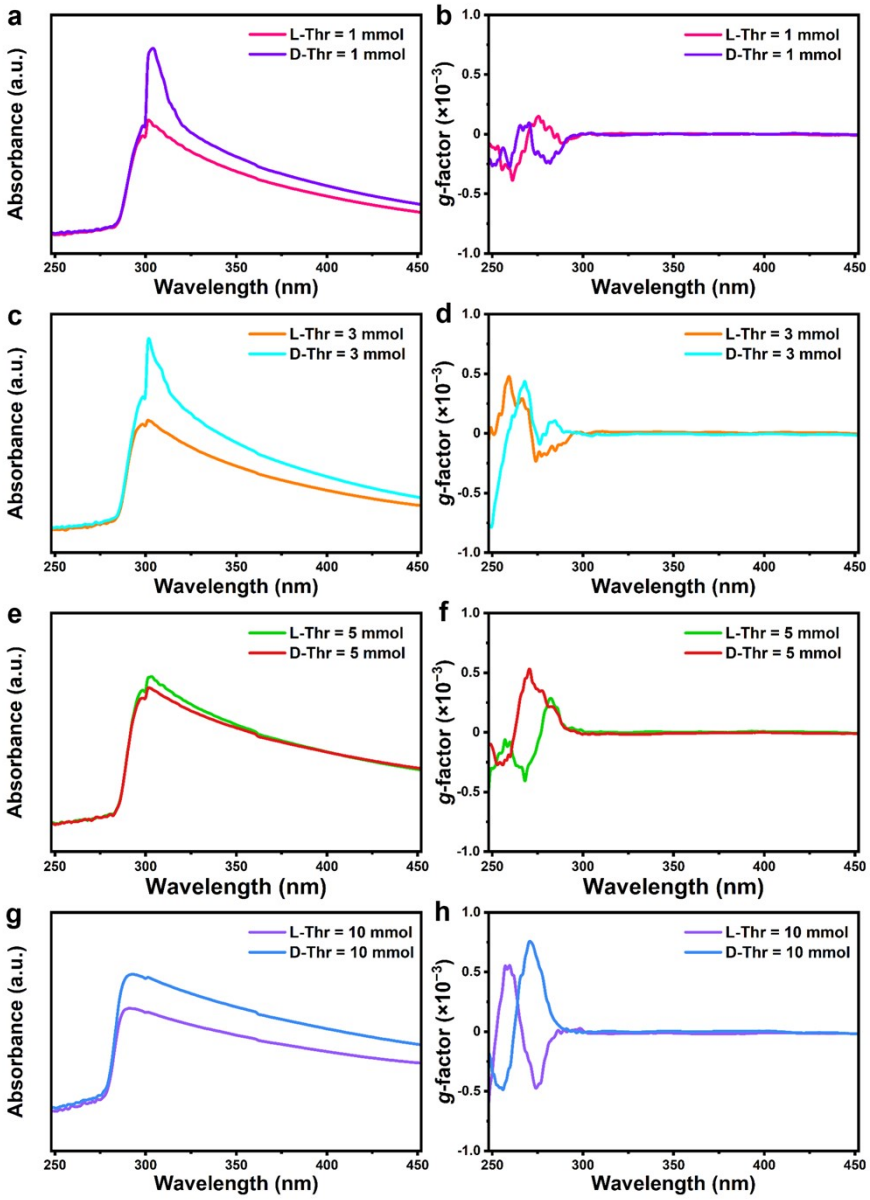

Fig. S8. (a, c, e, and g) UV-vis spectra and (b, d, f, and h) *g*-factor of (a and b) **1L**/**1D**, (c and d) **3L**/**3D**, (e and f) **5L**/**5D**, and (g and h) **10L**/**10D.**

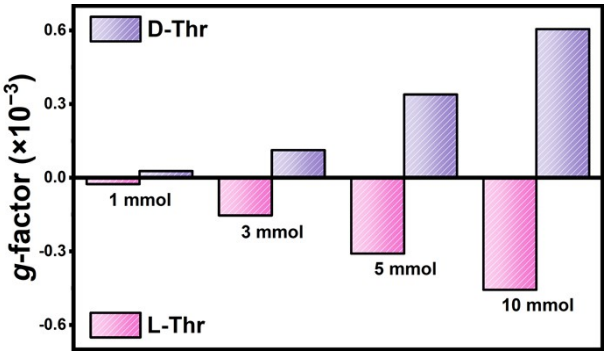

Fig. S9. Peak values of *g*-factors.

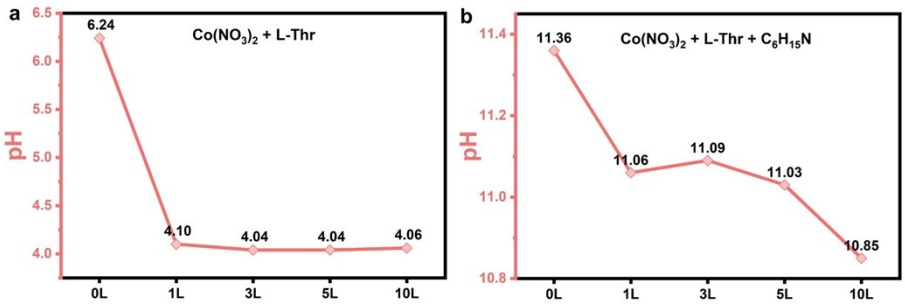

Fig. S10. The pH values of precursor solutions before (a) and after (b) the addition of triethylamine. The 0L stands for the adding amount of L-Thr is 0 mmol.

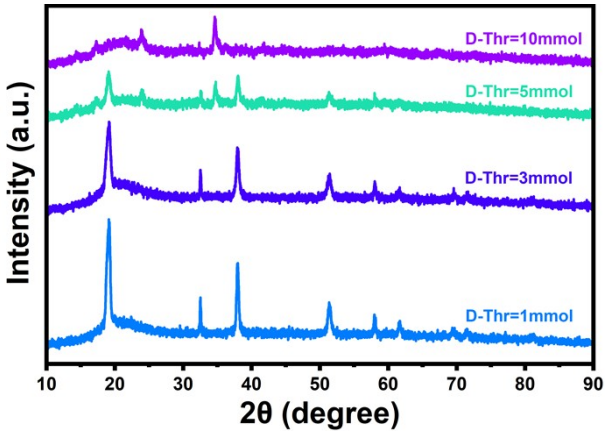

Fig. S11. XRD patterns of Co-based nanomaterials (**1D**, **3D**, **5D**, and **10D**).

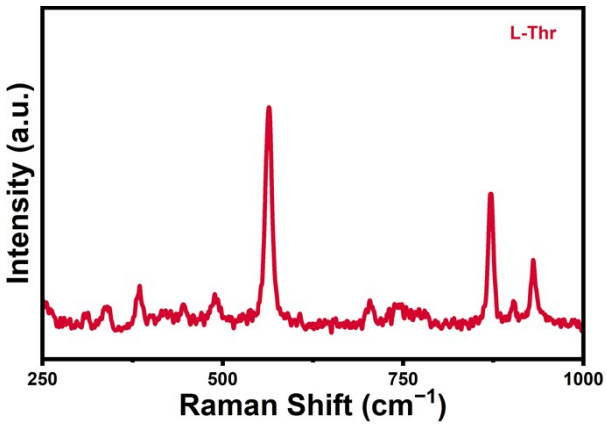

Fig. S12. Raman spectrum of L-Thr.

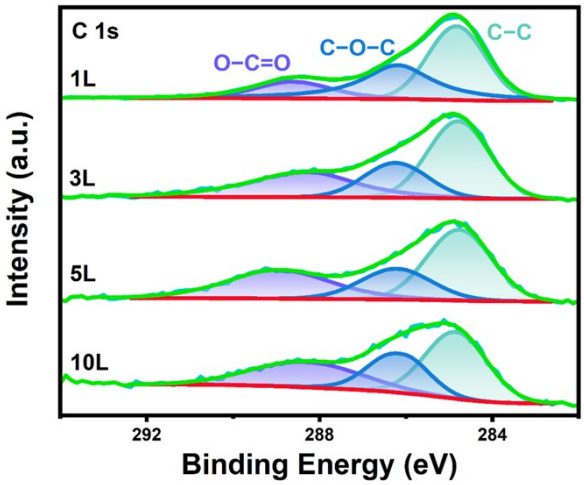

Fig. S13. XPS C 1s spectra of Co-based nanomaterials (**1D**, **3D**, **5D**, and **10D**).

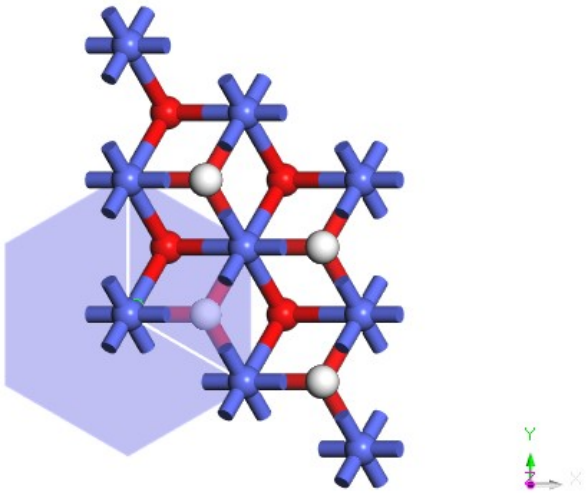

Fig. S14. Calculated crystal habit based on the crsytal structure of $Co(OH)_2$.

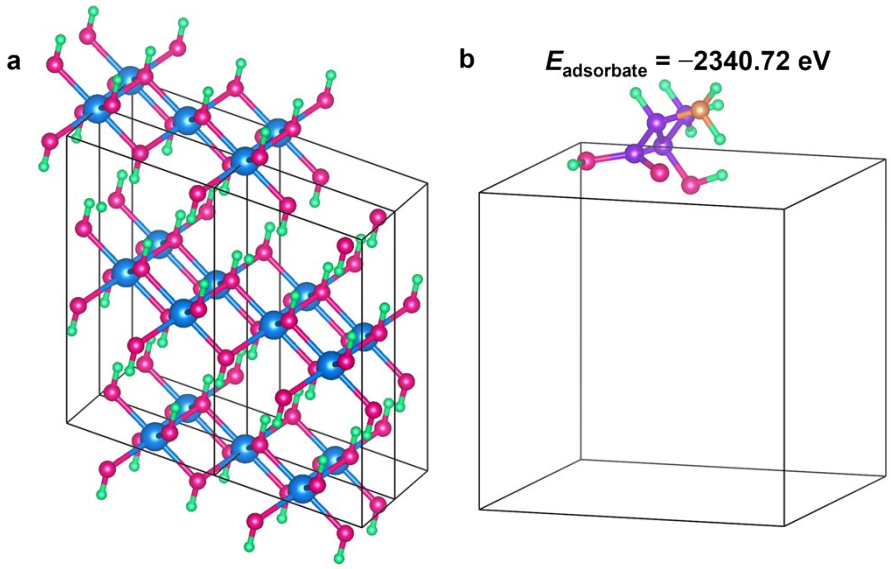

Fig. S15. Computational models of (a) $Co(OH)_2$ supercell and (b) Thr molecule.

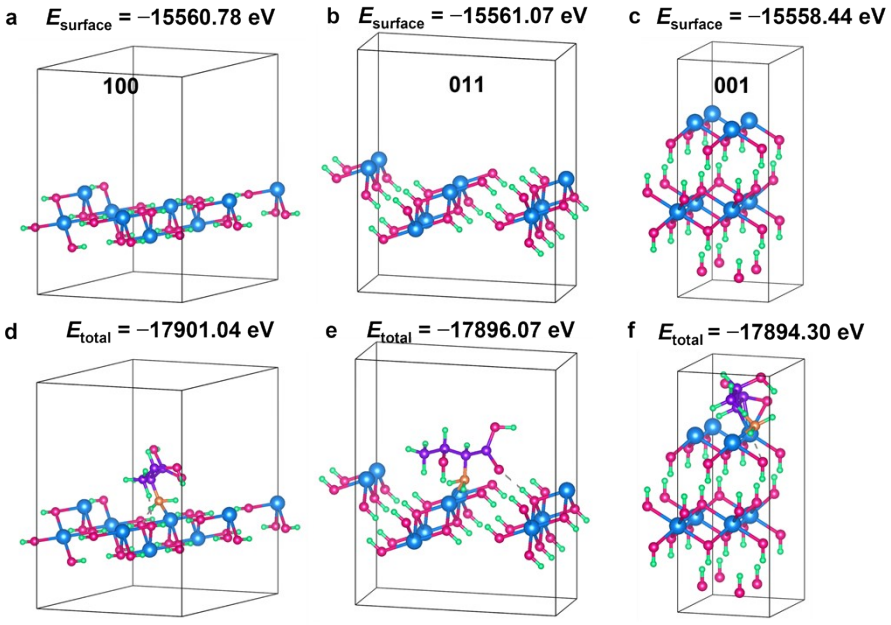

Fig. S16. Computational models of (a) (100), (b) (011), and (c) (001) crystal surface of $Co(OH)_2$ supercell. Computational models for Thr adsorption on the crystal surface (d) (100), (e) (011), and (f) (001) of $Co(OH)_2$ supercells.

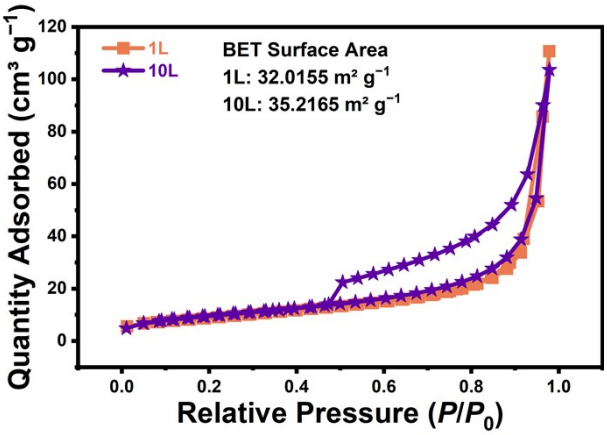

Fig. S17. N_2 isothermal adsorption and desorption data of **1L** and **10L**.

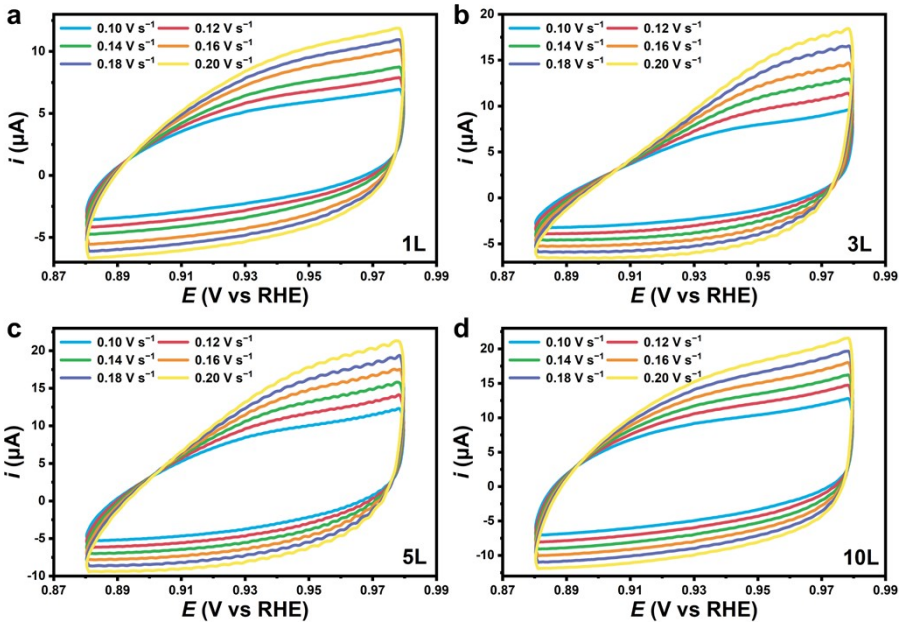

Fig. S18. CV data of (a) **1L**, (b) **3L**, (c) **5L**, and (d) **10L** in the non-Faradaic region with different scan rates (0.10, 0.12, 0.14, 0.18, and 0.20 V s^{-1}).

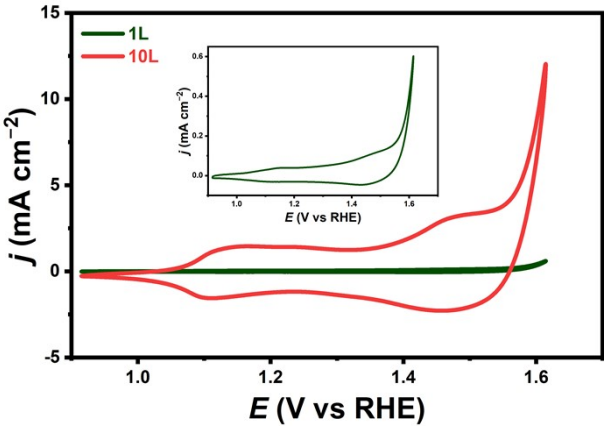

Fig. S19. CV data of **1L** and **10L** at 0.50 V s^{-1}. The insert Fig. is the enlarged CV data of **1L**.

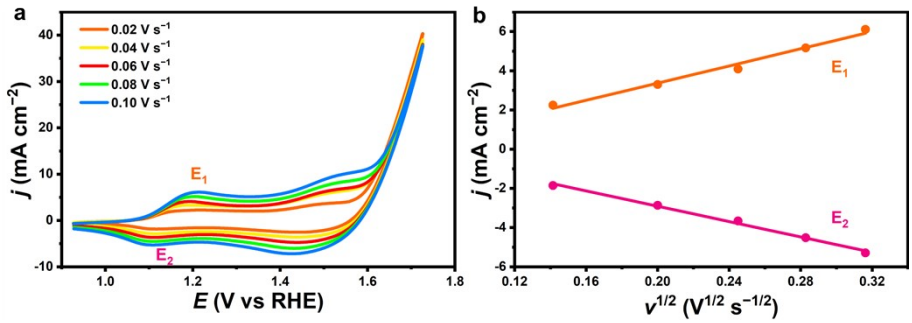

Fig. S20. (a) CV data of **10L** at different scan rates and (b) the relationship between scan rates and redox peak current densities.

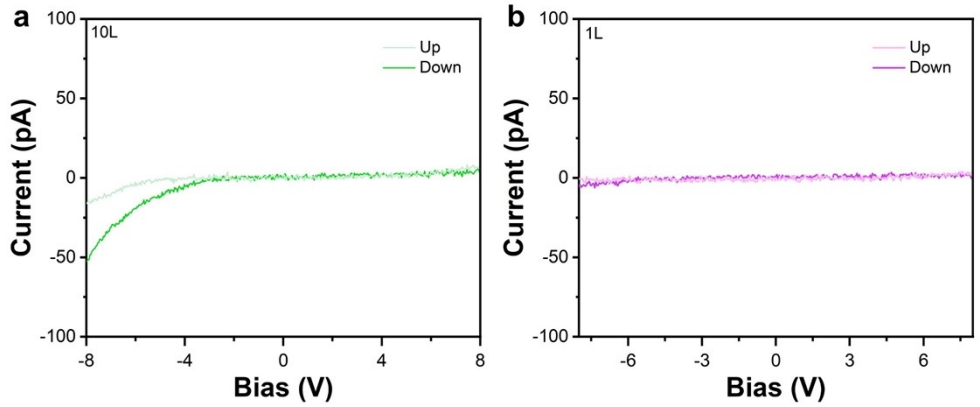

Fig. S21. *I-V* curves of **10L** (a) and **1L** (b) measured with conductive AFM (c-AFM).

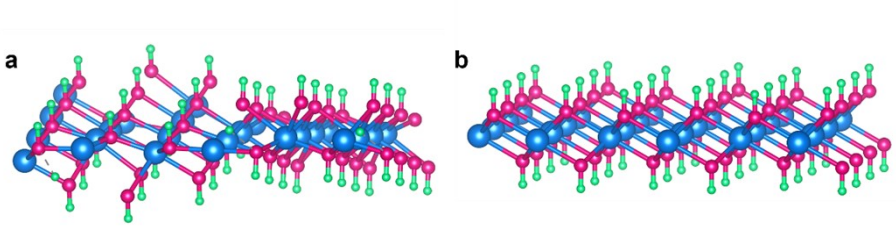

Fig. S22. Computational modellings of $Co(OH)_2$ with (a) high spin state and (b) low spin state.

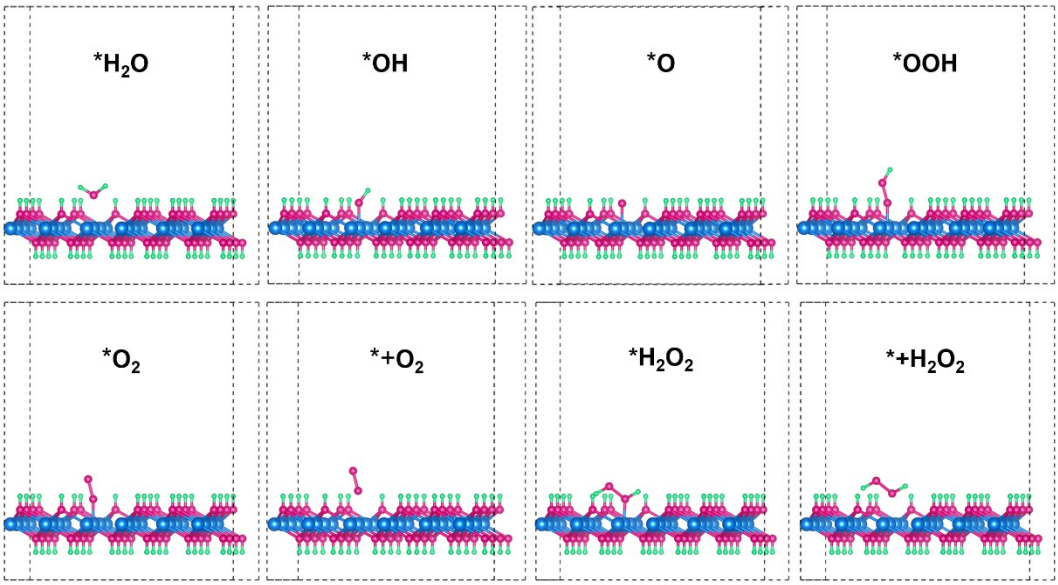

Fig. S23. Computational models of the adsorption of different reaction intermediates on $Co(OH)_2$ with low spin state.

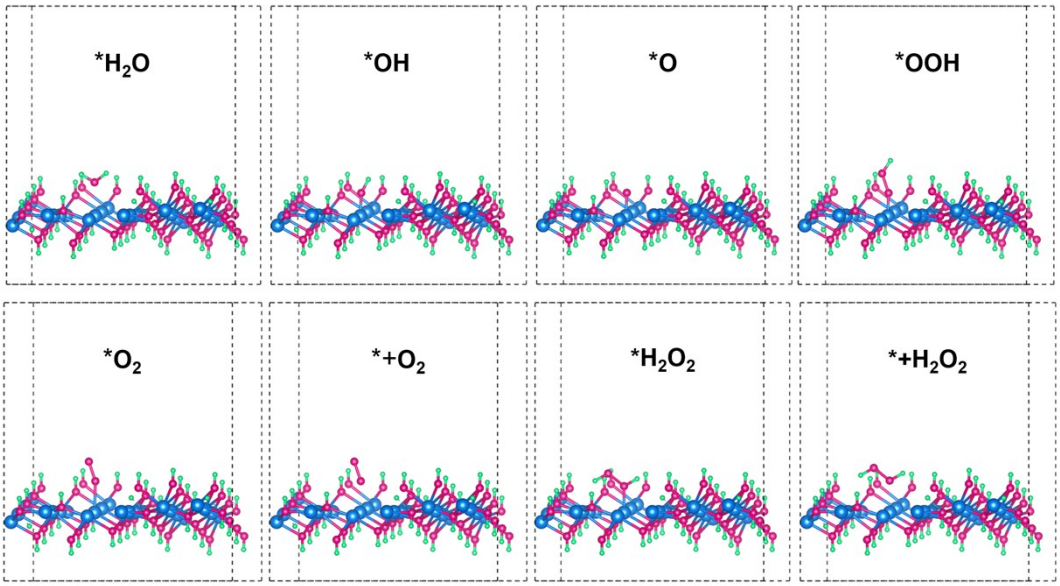

Fig. S24. Computational models of the adsorption of different reaction intermediates on $Co(OH)_2$ with high spin state.

Structure parameters

$Co(OH)_2$

			x	*y*	*z*
1	Co	Co0	0.31106	0.25048	0.50022
2	Co	Co1	0.06033	0.00021	0.99975
3	Co	Co2	0.81032	0.74983	0.49981
4	Co	Co3	0.56055	0.49988	0.00018
5	H	H4	0.42049	0.02525	0.71178
6	H	H5	0.17959	0.77650	0.21212
7	H	H6	0.91430	0.53014	0.71256
8	H	H7	0.67624	0.27364	0.21189
9	H	H8	0.95330	0.22568	0.78797
10	H	H9	0.71839	0.97145	0.28761
11	H	H10	0.45281	0.72308	0.78792
12	H	H11	0.20925	0.47300	0.28811
13	O	O12	0.36762	0.97435	0.60927
14	O	O13	0.11843	0.72374	0.10972
15	O	O14	0.85955	0.47506	0.61011
16	O	O15	0.61953	0.22311	0.10947
17	O	O16	0.00427	0.27671	0.89044
18	O	O17	0.76317	0.02596	0.39010
19	O	O18	0.50207	0.77652	0.89040
20	O	O19	0.25453	0.52540	0.39060

$Co(OH)_2$ (1 0 0)

			x	*y*	*z*

1	Co	Co1	0.00025	0.99642	0.39997
2	Co	Co2	0.37806	0.50919	0.34682
3	Co	Co3	0.25581	0.02246	0.29383
4	Co	Co4	0.13377	0.53602	0.24089
5	H	H5	0.39810	0.25502	0.21121
6	H	H6	0.26481	0.71526	0.37210
7	H	H7	0.14475	0.22972	0.31587
8	H	H8	0.01929	0.74162	0.26541
9	H	H9	0.49206	0.30307	0.32414
10	H	H10	0.36770	0.81512	0.27435
11	H	H11	0.24664	0.32946	0.21806
12	H	H12	0.11271	0.78969	0.37839
13	O	O13	0.37327	0.15530	0.20000
14	O	O14	0.23915	0.61610	0.35914
15	O	O15	0.11785	0.13016	0.30427
16	O	O16	0.49469	0.64219	0.25340
17	O	O17	0.01697	0.40285	0.33494
18	O	O18	0.39443	0.91524	0.28384
19	O	O19	0.27278	0.42933	0.22850
20	O	O20	0.13838	0.88979	0.38798
21	Co	Co21	0.50025	0.99642	0.39997
22	Co	Co22	0.87806	0.50919	0.34682
23	Co	Co23	0.75581	0.02246	0.29383
24	Co	Co24	0.63377	0.53602	0.24089
25	H	H25	0.89810	0.25502	0.21121
26	H	H26	0.76481	0.71526	0.37210

27	H	H27	0.64475	0.22972	0.31587
28	H	H28	0.51929	0.74162	0.26541
29	H	H29	0.99206	0.30307	0.32414
30	H	H30	0.86770	0.81512	0.27435
31	H	H31	0.74664	0.32946	0.21806
32	H	H32	0.61271	0.78969	0.37839
33	O	O33	0.87327	0.15530	0.20000
34	O	O34	0.73915	0.61610	0.35914
35	O	O35	0.61785	0.13016	0.30427
36	O	O36	0.99469	0.64219	0.25340
37	O	O37	0.51697	0.40285	0.33494
38	O	O38	0.89443	0.91524	0.28384
39	O	O39	0.77278	0.42933	0.22850
40	O	O40	0.63838	0.88979	0.38798
41	C	C41	0.70397	-0.46434	-0.43992
42	C	C42	0.57250	-0.47270	-0.40356
43	C	C43	0.47388	-0.56115	-0.46747
44	C	C44	0.34193	-0.56858	-0.43250
45	H	H45	0.71464	-0.41528	-0.50912
46	H	H46	0.77778	-0.39813	-0.39334
47	H	H47	0.71641	-0.57349	-0.44431
48	O	O48	0.55549	-0.32835	-0.39818
49	H	H49	0.56538	-0.28164	-0.46584
50	H	H50	0.56070	-0.52218	-0.33449
51	N	N51	0.49205	-0.49314	-0.55814
52	H	H52	0.58797	-0.48651	-0.58232

53	H	H53	0.48048	-0.38676	-0.55243
54	O	O54	0.26342	-0.48854	-0.47922
55	O	O55	0.28646	-0.66653	-0.35729
56	H	H56	0.18419	-0.70953	-0.36814
57	H	H57	0.48598	-0.67041	-0.47221

$Co(OH)_2$ (0 0 1)

			x	*y*	*z*
1	Co	Co1	0.00084	0.00228	0.69743
2	Co	Co2	0.49340	0.00054	0.35796
3	Co	Co3	0.25057	0.50184	0.69715
4	Co	Co4	0.24341	0.50000	0.35826
5	H	H5	0.24133	0.16859	0.16264
6	H	H6	0.00299	0.67137	0.50201
7	H	H7	0.48805	0.67309	0.16317
8	H	H8	0.25137	0.16862	0.50186
9	H	H9	0.48978	0.33118	0.21432
10	H	H10	0.25460	0.82883	0.55322
11	H	H11	0.23955	0.82860	0.21429
12	H	H12	0.49992	0.33013	0.55356
13	O	O13	0.23905	0.16859	0.09310
14	O	O14	0.49654	0.66946	0.43256
15	O	O15	0.48481	0.66888	0.09368
16	O	O16	0.24715	0.16896	0.43239
17	O	O17	0.49113	0.33132	0.28382
18	O	O18	0.25284	0.83245	0.62274

19	O	O19	0.24003	0.83115	0.28379
20	O	O20	0.49841	0.33164	0.62308
21	Co	Co21	0.50084	0.00228	0.69743
22	Co	Co22	0.99340	0.00054	0.35796
23	Co	Co23	0.75057	0.50184	0.69715
24	Co	Co24	0.74341	0.50000	0.35826
25	H	H25	0.74133	0.16859	0.16264
26	H	H26	0.50299	0.67137	0.50201
27	H	H27	0.98805	0.67309	0.16317
28	H	H28	0.75137	0.16862	0.50186
29	H	H29	0.98978	0.33118	0.21432
30	H	H30	0.75460	0.82883	0.55322
31	H	H31	0.73955	0.82860	0.21429
32	H	H32	0.99992	0.33013	0.55356
33	O	O33	0.73905	0.16859	0.09310
34	O	O34	0.99654	0.66946	0.43256
35	O	O35	0.98481	0.66888	0.09368
36	O	O36	0.74715	0.16896	0.43239
37	O	O37	0.99113	0.33132	0.28382
38	O	O38	0.75284	0.83245	0.62274
39	O	O39	0.74003	0.83115	0.28379
40	O	O40	0.99841	0.33164	0.62308
41	C	C41	-1.19687	0.50606	0.87829
42	C	C42	-1.42647	0.48429	0.90759
43	C	C43	-1.55763	0.43546	0.81787
44	C	C44	-1.78806	0.41688	0.84606

45	H	H45	-1.17966	0.65988	0.82499
46	H	H46	-1.09848	0.54402	0.94423
47	H	H47	-1.14319	0.33048	0.84387
48	O	O48	-1.49836	0.71711	0.95269
49	H	H49	-1.48209	0.86559	0.90019
50	H	H50	-1.44548	0.33021	0.96061
51	N	N51	-1.52897	0.64207	0.74918
52	H	H52	-1.36206	0.65620	0.73025
53	H	H53	-1.58062	0.81146	0.78415
54	O	O54	-1.93675	0.61794	0.82073
55	O	O55	-1.86899	0.18788	0.89027
56	H	H56	-2.02960	0.15500	0.86478
57	H	H57	-1.50442	0.26018	0.78306

$Co(OH)_2$ (0 1 1)

			x	*y*	*z*
1	Co	Co1	0.00020	0.00269	0.47573
2	Co	Co2	0.42435	0.28552	0.26655
3	Co	Co3	0.28288	0.85784	0.33612
4	Co	Co4	0.14148	0.43007	0.40589
5	H	H5	0.05582	0.78717	0.47192
6	H	H6	0.48473	0.06986	0.26339
7	H	H7	0.33532	0.64308	0.33419
8	H	H8	0.20028	0.21415	0.40184
9	H	H9	0.36993	0.50126	0.27037
10	H	H10	0.23629	0.07277	0.33874

11	H	H11	0.08688	0.64550	0.40894
12	H	H12	0.01456	0.92792	0.20000
13	O	O13	0.03950	0.84520	0.42917
14	O	O14	0.46438	0.12728	0.22016
15	O	O15	0.31834	0.69986	0.29029
16	O	O16	0.18201	0.27223	0.35923
17	O	O17	0.38529	0.44329	0.31313
18	O	O18	0.24832	0.01580	0.38249
19	O	O19	0.10123	0.58822	0.45238
20	O	O20	0.02699	0.87033	0.24316
21	Co	Co21	0.50020	0.00269	0.47573
22	Co	Co22	0.92435	0.28552	0.26655
23	Co	Co23	0.78288	0.85784	0.33612
24	Co	Co24	0.64148	0.43007	0.40589
25	H	H25	0.55582	0.78717	0.47192
26	H	H26	0.98473	0.06986	0.26339
27	H	H27	0.83532	0.64308	0.33419
28	H	H28	0.70028	0.21415	0.40184
29	H	H29	0.86993	0.50126	0.27037
30	H	H30	0.73629	0.07277	0.33874
31	H	H31	0.58688	0.64550	0.40894
32	H	H32	0.51456	0.92792	0.20000
33	O	O33	0.53950	0.84520	0.42917
34	O	O34	0.96438	0.12728	0.22016
35	O	O35	0.81834	0.69986	0.29029
36	O	O36	0.68201	0.27223	0.35923

37	O	O37	0.88529	0.44329	0.31313
38	O	O38	0.74832	0.01580	0.38249
39	O	O39	0.60123	0.58822	0.45238
40	O	O40	0.52699	0.87033	0.24316
41	C	C41	-1.48073	0.29316	0.59442
42	C	C42	-1.42042	0.40122	0.62426
43	C	C43	-1.58568	0.48937	0.58962
44	C	C44	-1.52542	0.59798	0.61792
45	H	H45	-1.48845	0.29083	0.51851
46	H	H46	-1.35834	0.22730	0.61922
47	H	H47	-1.64012	0.28171	0.62336
48	O	O48	-1.20993	0.41689	0.58558
49	H	H49	-1.21910	0.41505	0.51171
50	H	H50	-1.41314	0.40452	0.70013
51	N	N51	-1.59168	0.48281	0.48920
52	H	H52	-1.63246	0.40377	0.46938
53	H	H53	-1.43497	0.49338	0.46230
54	O	O54	-1.44365	0.66958	0.54942
55	O	O55	-1.56784	0.63714	0.71196
56	H	H56	-1.61298	0.72423	0.71106
57	H	H57	-1.74551	0.47823	0.61827

$Co(OH)_2$-High Spin

			x	*y*	*z*
1	Co	Co1	0.02156	0.00011	0.29532
2	Co	Co2	0.14012	0.16660	0.24790

3	H	H3	0.05365	0.22372	0.39548
4	H	H4	0.17575	0.05614	0.38006
5	H	H5	-0.00734	0.11032	0.19643
6	H	H6	0.11581	0.27613	0.18386
7	O	O7	0.03736	0.22308	0.34796
8	O	O8	0.16055	0.05625	0.33241
9	O	O9	0.00644	0.11037	0.24427
10	O	O10	0.12917	0.27698	0.23175
11	Co	Co11	0.26777	0.00011	0.26737
12	Co	Co12	0.39012	0.16660	0.24790
13	H	H13	0.29985	0.22372	0.36752
14	H	H14	0.42195	0.05614	0.35211
15	H	H15	0.23886	0.11032	0.16847
16	H	H16	0.36201	0.27613	0.15591
17	O	O17	0.28356	0.22308	0.32000
18	O	O18	0.40676	0.05625	0.30445
19	O	O19	0.25264	0.11037	0.21631
20	O	O20	0.37537	0.27698	0.20380
21	Co	Co21	0.51397	0.00011	0.23941
22	Co	Co22	0.64012	0.16660	0.24790
23	H	H23	0.54605	0.22372	0.33957
24	H	H24	0.66815	0.05614	0.32415
25	H	H25	0.48506	0.11032	0.14052
26	H	H26	0.60822	0.27613	0.12795
27	O	O27	0.52976	0.22308	0.29205
28	O	O28	0.65296	0.05625	0.27650

29	O	O29	0.49884	0.11037	0.18836
30	O	O30	0.62158	0.27698	0.17585
31	Co	Co31	0.76017	0.00011	0.21146
32	Co	Co32	0.89012	0.16660	0.24790
33	H	H33	0.79226	0.22372	0.31161
34	H	H34	0.91435	0.05614	0.29620
35	H	H35	0.73126	0.11032	0.11256
36	H	H36	0.85442	0.27613	0.10000
37	O	O37	0.77597	0.22308	0.26409
38	O	O38	0.89916	0.05625	0.24854
39	O	O39	0.74504	0.11037	0.16040
40	O	O40	0.86778	0.27698	0.14789
41	Co	Co41	0.00997	0.33345	0.27373
42	Co	Co42	0.14012	0.49993	0.24790
43	H	H43	-0.00066	0.55705	0.29852
44	H	H44	0.16953	0.38947	0.38337
45	H	H45	0.00153	0.44366	0.17230
46	H	H46	0.17013	0.60947	0.11343
47	O	O47	0.00927	0.55642	0.25028
48	O	O48	0.15434	0.38958	0.33571
49	O	O49	0.00878	0.44371	0.22073
50	O	O50	0.15725	0.61032	0.16138
51	Co	Co51	0.25902	0.33345	0.25970
52	Co	Co52	0.39012	0.49993	0.24790
53	H	H53	0.24554	0.55705	0.32647
54	H	H54	0.41573	0.38947	0.35541

55	H	H55	0.25058	0.44366	0.15827
56	H	H56	0.41633	0.60947	0.14138
57	O	O57	0.25548	0.55642	0.27823
58	O	O58	0.40054	0.38958	0.30776
59	O	O59	0.25783	0.44371	0.20670
60	O	O60	0.40345	0.61032	0.18933
61	Co	Co61	0.50807	0.33345	0.24567
62	Co	Co62	0.64012	0.49993	0.24790
63	H	H63	0.49174	0.55705	0.35443
64	H	H64	0.66193	0.38947	0.32746
65	H	H65	0.49963	0.44366	0.14423
66	H	H66	0.66254	0.60947	0.16934
67	O	O67	0.50168	0.55642	0.30618
68	O	O68	0.64674	0.38958	0.27980
69	O	O69	0.50688	0.44371	0.19267
70	O	O70	0.64965	0.61032	0.21728
71	Co	Co71	0.75712	0.33345	0.23164
72	Co	Co72	0.89012	0.49993	0.24790
73	H	H73	0.73794	0.55705	0.38238
74	H	H74	0.90813	0.38947	0.29950
75	H	H75	0.74868	0.44366	0.13020
76	H	H76	0.90874	0.60947	0.19729
77	O	O77	0.74788	0.55642	0.33414
78	O	O78	0.89294	0.38958	0.25185
79	O	O79	0.75593	0.44371	0.17863
80	O	O80	0.89585	0.61032	0.24524

81	Co	Co81	0.01674	0.66678	0.22378
82	Co	Co82	0.14135	0.83327	0.22960
83	H	H83	-0.00061	0.89039	0.29783
84	H	H84	0.12161	0.72281	0.31301
85	H	H85	0.04708	0.77699	0.10020
86	H	H86	0.17018	0.94280	0.11274
87	O	O87	0.00932	0.88975	0.24959
88	O	O88	0.13264	0.72292	0.26488
89	O	O89	0.03462	0.77704	0.14819
90	O	O90	0.15730	0.94365	0.16069
91	Co	Co91	0.26579	0.66678	0.23781
92	Co	Co92	0.39040	0.83327	0.24363
93	H	H93	0.24559	0.89039	0.32578
94	H	H94	0.36781	0.72281	0.34096
95	H	H95	0.29328	0.77699	0.12815
96	H	H96	0.41638	0.94280	0.14070
97	O	O97	0.25552	0.88975	0.27754
98	O	O98	0.37885	0.72292	0.29283
99	O	O99	0.28082	0.77704	0.17614
100	O	O100	0.40350	0.94365	0.18864
101	Co	Co101	0.51484	0.66678	0.25184
102	Co	Co102	0.63945	0.83327	0.25766
103	H	H103	0.49179	0.89039	0.35374
104	H	H104	0.61401	0.72281	0.36891
105	H	H105	0.53948	0.77699	0.15611
106	H	H106	0.66259	0.94280	0.16865

107	O	O107	0.50173	0.88975	0.30550
108	O	O108	0.62505	0.72292	0.32079
109	O	O109	0.52702	0.77704	0.20410
110	O	O110	0.64970	0.94365	0.21660
111	Co	Co111	0.76389	0.66678	0.26587
112	Co	Co112	0.88850	0.83327	0.27169
113	H	H113	0.73799	0.89039	0.38169
114	H	H114	0.86021	0.72281	0.39687
115	H	H115	0.78568	0.77699	0.18406
116	H	H116	0.90879	0.94280	0.19660
117	O	O117	0.74793	0.88975	0.33345
118	O	O118	0.87125	0.72292	0.34874
119	O	O119	0.77322	0.77704	0.23205
120	O	O120	0.89590	0.94365	0.24455

$Co(OH)_2$-Low Spin

			x	*y*	*z*
1	Co	Co1	0.01511	0.00011	0.20057
2	Co	Co2	0.14012	0.16660	0.20078
3	H	H3	0.01991	0.22372	0.30141
4	H	H4	0.14410	0.05614	0.30130
5	H	H5	0.01330	0.11032	0.10002
6	H	H6	0.13819	0.27613	0.10000
7	O	O7	0.01668	0.22308	0.25279
8	O	O8	0.14199	0.05625	0.25267
9	O	O9	0.01397	0.11037	0.14868

10	O	O10	0.13843	0.27698	0.14866
11	Co	Co11	0.26511	0.00011	0.20057
12	Co	Co12	0.39012	0.16660	0.20078
13	H	H13	0.26991	0.22372	0.30141
14	H	H14	0.39410	0.05614	0.30130
15	H	H15	0.26330	0.11032	0.10002
16	H	H16	0.38819	0.27613	0.10000
17	O	O17	0.26668	0.22308	0.25279
18	O	O18	0.39199	0.05625	0.25267
19	O	O19	0.26397	0.11037	0.14868
20	O	O20	0.38843	0.27698	0.14866
21	Co	Co21	0.51511	0.00011	0.20057
22	Co	Co22	0.64012	0.16660	0.20078
23	H	H23	0.51991	0.22372	0.30141
24	H	H24	0.64410	0.05614	0.30130
25	H	H25	0.51330	0.11032	0.10002
26	H	H26	0.63819	0.27613	0.10000
27	O	O27	0.51668	0.22308	0.25279
28	O	O28	0.64199	0.05625	0.25267
29	O	O29	0.51397	0.11037	0.14868
30	O	O30	0.63843	0.27698	0.14866
31	Co	Co31	0.76511	0.00011	0.20057
32	Co	Co32	0.89012	0.16660	0.20078
33	H	H33	0.76991	0.22372	0.30141
34	H	H34	0.89410	0.05614	0.30130
35	H	H35	0.76330	0.11032	0.10002

36	H	H36	0.88819	0.27613	0.10000
37	O	O37	0.76668	0.22308	0.25279
38	O	O38	0.89199	0.05625	0.25267
39	O	O39	0.76397	0.11037	0.14868
40	O	O40	0.88843	0.27698	0.14866
41	Co	Co41	0.01511	0.33345	0.20057
42	Co	Co42	0.14012	0.49993	0.20078
43	H	H43	0.01991	0.55705	0.30141
44	H	H44	0.14410	0.38947	0.30130
45	H	H45	0.01330	0.44366	0.10002
46	H	H46	0.13819	0.60947	0.10000
47	O	O47	0.01668	0.55642	0.25279
48	O	O48	0.14199	0.38958	0.25267
49	O	O49	0.01397	0.44371	0.14868
50	O	O50	0.13843	0.61032	0.14866
51	Co	Co51	0.26511	0.33345	0.20057
52	Co	Co52	0.39012	0.49993	0.20078
53	H	H53	0.26991	0.55705	0.30141
54	H	H54	0.39410	0.38947	0.30130
55	H	H55	0.26330	0.44366	0.10002
56	H	H56	0.38819	0.60947	0.10000
57	O	O57	0.26668	0.55642	0.25279
58	O	O58	0.39199	0.38958	0.25267
59	O	O59	0.26397	0.44371	0.14868
60	O	O60	0.38843	0.61032	0.14866
61	Co	Co61	0.51511	0.33345	0.20057

62 Co Co62 0.64012 0.49993 0.20078

63 H H63 0.51991 0.55705 0.30141

64 H H64 0.64410 0.38947 0.30130

65 H H65 0.51330 0.44366 0.10002

66 H H66 0.63819 0.60947 0.10000

67 O O67 0.51668 0.55642 0.25279

68 O O68 0.64199 0.38958 0.25267

69 O O69 0.51397 0.44371 0.14868

70 O O70 0.63843 0.61032 0.14866

71 Co Co71 0.76511 0.33345 0.20057

72 Co Co72 0.89012 0.49993 0.20078

73 H H73 0.76991 0.55705 0.30141

74 H H74 0.89410 0.38947 0.30130

75 H H75 0.76330 0.44366 0.10002

76 H H76 0.88819 0.60947 0.10000

77 O O77 0.76668 0.55642 0.25279

78 O O78 0.89199 0.38958 0.25267

79 O O79 0.76397 0.44371 0.14868

80 O O80 0.88843 0.61032 0.14866

81 Co Co81 0.01511 0.66678 0.20057

82 Co Co82 0.14012 0.83327 0.20078

83 H H83 0.01991 0.89039 0.30141

84 H H84 0.14410 0.72281 0.30130

85 H H85 0.01330 0.77699 0.10002

86 H H86 0.13819 0.94280 0.10000

87 O O87 0.01668 0.88975 0.25279

88	O	O88	0.14199	0.72292	0.25267
89	O	O89	0.01397	0.77704	0.14868
90	O	O90	0.13843	0.94365	0.14866
91	Co	Co91	0.26511	0.66678	0.20057
92	Co	Co92	0.39012	0.83327	0.20078
93	H	H93	0.26991	0.89039	0.30141
94	H	H94	0.39410	0.72281	0.30130
95	H	H95	0.26330	0.77699	0.10002
96	H	H96	0.38819	0.94280	0.10000
97	O	O97	0.26668	0.88975	0.25279
98	O	O98	0.39199	0.72292	0.25267
99	O	O99	0.26397	0.77704	0.14868
100	O	O100	0.38843	0.94365	0.14866
101	Co	Co101	0.51511	0.66678	0.20057
102	Co	Co102	0.64012	0.83327	0.20078
103	H	H103	0.51991	0.89039	0.30141
104	H	H104	0.64410	0.72281	0.30130
105	H	H105	0.51330	0.77699	0.10002
106	H	H106	0.63819	0.94280	0.10000
107	O	O107	0.51668	0.88975	0.25279
108	O	O108	0.64199	0.72292	0.25267
109	O	O109	0.51397	0.77704	0.14868
110	O	O110	0.63843	0.94365	0.14866
111	Co	Co111	0.76511	0.66678	0.20057
112	Co	Co112	0.89012	0.83327	0.20078
113	H	H113	0.76991	0.89039	0.30141

114	H	H114	0.89410	0.72281	0.30130
115	H	H115	0.76330	0.77699	0.10002
116	H	H116	0.88819	0.94280	0.10000
117	O	O117	0.76668	0.88975	0.25279
118	O	O118	0.89199	0.72292	0.25267
119	O	O119	0.76397	0.77704	0.14868
120	O	O120	0.88843	0.94365	0.14866

$Co(OH)_2$-High Spin-*H_2O

			x	*y*	*z*
1	Co	Co1	0.02156	0.00011	0.29532
2	Co	Co2	0.14012	0.16660	0.24790
3	H	H3	0.05365	0.22372	0.39548
4	H	H4	0.17575	0.05614	0.38006
5	H	H5	-0.00734	0.11032	0.19643
6	H	H6	0.11581	0.27613	0.18386
7	O	O7	0.03736	0.22308	0.34796
8	O	O8	0.16055	0.05625	0.33241
9	O	O9	0.00644	0.11037	0.24427
10	O	O10	0.12917	0.27698	0.23175
11	Co	Co11	0.26777	0.00011	0.26737
12	Co	Co12	0.39012	0.16660	0.24790
13	H	H13	0.29985	0.22372	0.36752
14	H	H14	0.42195	0.05614	0.35211
15	H	H15	0.23886	0.11032	0.16847
16	H	H16	0.36201	0.27613	0.15591

17	O	O17	0.28356	0.22308	0.32000
18	O	O18	0.40676	0.05625	0.30445
19	O	O19	0.25264	0.11037	0.21631
20	O	O20	0.37537	0.27698	0.20380
21	Co	Co21	0.51397	0.00011	0.23941
22	Co	Co22	0.64012	0.16660	0.24790
23	H	H23	0.66815	0.05614	0.32415
24	H	H24	0.48506	0.11032	0.14052
25	H	H25	0.60822	0.27613	0.12795
26	O	O26	0.65296	0.05625	0.27650
27	O	O27	0.49884	0.11037	0.18836
28	O	O28	0.62158	0.27698	0.17585
29	Co	Co29	0.76017	0.00011	0.21146
30	Co	Co30	0.89012	0.16660	0.24790
31	H	H31	0.79226	0.22372	0.31161
32	H	H32	0.91435	0.05614	0.29620
33	H	H33	0.73126	0.11032	0.11256
34	H	H34	0.85442	0.27613	0.10000
35	O	O35	0.77597	0.22308	0.26409
36	O	O36	0.89916	0.05625	0.24854
37	O	O37	0.74504	0.11037	0.16040
38	O	O38	0.86778	0.27698	0.14789
39	Co	Co39	0.00997	0.33345	0.27373
40	Co	Co40	0.14012	0.49993	0.24790
41	H	H41	-0.00066	0.55705	0.29852
42	H	H42	0.16953	0.38947	0.38337

43	H	H43	0.00153	0.44366	0.17230
44	H	H44	0.17013	0.60947	0.11343
45	O	O45	0.00927	0.55642	0.25028
46	O	O46	0.15434	0.38958	0.33571
47	O	O47	0.00878	0.44371	0.22073
48	O	O48	0.15725	0.61032	0.16138
49	Co	Co49	0.25902	0.33345	0.25970
50	Co	Co50	0.39012	0.49993	0.24790
51	H	H51	0.24554	0.55705	0.32647
52	H	H52	0.25058	0.44366	0.15827
53	H	H53	0.41633	0.60947	0.14138
54	O	O54	0.25548	0.55642	0.27823
55	O	O55	0.25783	0.44371	0.20670
56	O	O56	0.40345	0.61032	0.18933
57	Co	Co57	0.50807	0.33345	0.24567
58	Co	Co58	0.64012	0.49993	0.24790
59	H	H59	0.49174	0.55705	0.35443
60	H	H60	0.49963	0.44366	0.14423
61	H	H61	0.66254	0.60947	0.16934
62	O	O62	0.50168	0.55642	0.30618
63	O	O63	0.50688	0.44371	0.19267
64	O	O64	0.64965	0.61032	0.21728
65	Co	Co65	0.75712	0.33345	0.23164
66	Co	Co66	0.89012	0.49993	0.24790
67	H	H67	0.73794	0.55705	0.38238
68	H	H68	0.74868	0.44366	0.13020

69	H	H69	0.90874	0.60947	0.19729
70	O	O70	0.74788	0.55642	0.33414
71	O	O71	0.75593	0.44371	0.17863
72	O	O72	0.89585	0.61032	0.24524
73	Co	Co73	0.01674	0.66678	0.22378
74	Co	Co74	0.14135	0.83327	0.22960
75	H	H75	-0.00061	0.89039	0.29783
76	H	H76	0.12161	0.72281	0.31301
77	H	H77	0.04708	0.77699	0.10020
78	H	H78	0.17018	0.94280	0.11274
79	O	O79	0.00932	0.88975	0.24959
80	O	O80	0.13264	0.72292	0.26488
81	O	O81	0.03462	0.77704	0.14819
82	O	O82	0.15730	0.94365	0.16069
83	Co	Co83	0.26579	0.66678	0.23781
84	Co	Co84	0.39040	0.83327	0.24363
85	H	H85	0.24559	0.89039	0.32578
86	H	H86	0.36781	0.72281	0.34096
87	H	H87	0.29328	0.77699	0.12815
88	H	H88	0.41638	0.94280	0.14070
89	O	O89	0.25552	0.88975	0.27754
90	O	O90	0.37885	0.72292	0.29283
91	O	O91	0.28082	0.77704	0.17614
92	O	O92	0.40350	0.94365	0.18864
93	Co	Co93	0.51484	0.66678	0.25184
94	Co	Co94	0.63945	0.83327	0.25766

95	H	H95	0.49179	0.89039	0.35374
96	H	H96	0.61401	0.72281	0.36891
97	H	H97	0.53948	0.77699	0.15611
98	H	H98	0.66259	0.94280	0.16865
99	O	O99	0.50173	0.88975	0.30550
100	O	O100	0.62505	0.72292	0.32079
101	O	O101	0.52702	0.77704	0.20410
102	O	O102	0.64970	0.94365	0.21660
103	Co	Co103	0.76389	0.66678	0.26587
104	Co	Co104	0.88850	0.83327	0.27169
105	H	H105	0.73799	0.89039	0.38169
106	H	H106	0.86021	0.72281	0.39687
107	H	H107	0.78568	0.77699	0.18406
108	H	H108	0.90879	0.94280	0.19660
109	O	O109	0.74793	0.88975	0.33345
110	O	O110	0.87125	0.72292	0.34874
111	O	O111	0.77322	0.77704	0.23205
112	O	O112	0.89590	0.94365	0.24455
113	O	O113	0.50272	0.32959	0.36676
114	H	H114	0.51585	0.38222	0.39967
115	H	H115	0.51922	0.27361	0.39498

$Co(OH)_2$-High Spin-*OH

			x	*y*	*z*
1	Co	Co1	0.02156	0.00011	0.29532
2	Co	Co2	0.14012	0.16660	0.24790

3	H	H3	0.05365	0.22372	0.39548
4	H	H4	0.17575	0.05614	0.38006
5	H	H5	-0.00734	0.11032	0.19643
6	H	H6	0.11581	0.27613	0.18386
7	O	O7	0.03736	0.22308	0.34796
8	O	O8	0.16055	0.05625	0.33241
9	O	O9	0.00644	0.11037	0.24427
10	O	O10	0.12917	0.27698	0.23175
11	Co	Co11	0.26777	0.00011	0.26737
12	Co	Co12	0.39012	0.16660	0.24790
13	H	H13	0.29985	0.22372	0.36752
14	H	H14	0.42195	0.05614	0.35211
15	H	H15	0.23886	0.11032	0.16847
16	H	H16	0.36201	0.27613	0.15591
17	O	O17	0.28356	0.22308	0.32000
18	O	O18	0.40676	0.05625	0.30445
19	O	O19	0.25264	0.11037	0.21631
20	O	O20	0.37537	0.27698	0.20380
21	Co	Co21	0.51397	0.00011	0.23941
22	Co	Co22	0.64012	0.16660	0.24790
23	H	H23	0.66815	0.05614	0.32415
24	H	H24	0.48506	0.11032	0.14052
25	H	H25	0.60822	0.27613	0.12795
26	O	O26	0.65296	0.05625	0.27650
27	O	O27	0.49884	0.11037	0.18836
28	O	O28	0.62158	0.27698	0.17585

29	Co	Co29	0.76017	0.00011	0.21146
30	Co	Co30	0.89012	0.16660	0.24790
31	H	H31	0.79226	0.22372	0.31161
32	H	H32	0.91435	0.05614	0.29620
33	H	H33	0.73126	0.11032	0.11256
34	H	H34	0.85442	0.27613	0.10000
35	O	O35	0.77597	0.22308	0.26409
36	O	O36	0.89916	0.05625	0.24854
37	O	O37	0.74504	0.11037	0.16040
38	O	O38	0.86778	0.27698	0.14789
39	Co	Co39	0.00997	0.33345	0.27373
40	Co	Co40	0.14012	0.49993	0.24790
41	H	H41	-0.00066	0.55705	0.29852
42	H	H42	0.16953	0.38947	0.38337
43	H	H43	0.00153	0.44366	0.17230
44	H	H44	0.17013	0.60947	0.11343
45	O	O45	0.00927	0.55642	0.25028
46	O	O46	0.15434	0.38958	0.33571
47	O	O47	0.00878	0.44371	0.22073
48	O	O48	0.15725	0.61032	0.16138
49	Co	Co49	0.25902	0.33345	0.25970
50	Co	Co50	0.39012	0.49993	0.24790
51	H	H51	0.24554	0.55705	0.32647
52	H	H52	0.25058	0.44366	0.15827
53	H	H53	0.41633	0.60947	0.14138
54	O	O54	0.25548	0.55642	0.27823

55	O	O55	0.25783	0.44371	0.20670
56	O	O56	0.40345	0.61032	0.18933
57	Co	Co57	0.50807	0.33345	0.24567
58	Co	Co58	0.64012	0.49993	0.24790
59	H	H59	0.49174	0.55705	0.35443
60	H	H60	0.49963	0.44366	0.14423
61	H	H61	0.66254	0.60947	0.16934
62	O	O62	0.50168	0.55642	0.30618
63	O	O63	0.50688	0.44371	0.19267
64	O	O64	0.64965	0.61032	0.21728
65	Co	Co65	0.75712	0.33345	0.23164
66	Co	Co66	0.89012	0.49993	0.24790
67	H	H67	0.73794	0.55705	0.38238
68	H	H68	0.74868	0.44366	0.13020
69	H	H69	0.90874	0.60947	0.19729
70	O	O70	0.74788	0.55642	0.33414
71	O	O71	0.75593	0.44371	0.17863
72	O	O72	0.89585	0.61032	0.24524
73	Co	Co73	0.01674	0.66678	0.22378
74	Co	Co74	0.14135	0.83327	0.22960
75	H	H75	-0.00061	0.89039	0.29783
76	H	H76	0.12161	0.72281	0.31301
77	H	H77	0.04708	0.77699	0.10020
78	H	H78	0.17018	0.94280	0.11274
79	O	O79	0.00932	0.88975	0.24959
80	O	O80	0.13264	0.72292	0.26488

81	O	O81	0.03462	0.77704	0.14819
82	O	O82	0.15730	0.94365	0.16069
83	Co	Co83	0.26579	0.66678	0.23781
84	Co	Co84	0.39040	0.83327	0.24363
85	H	H85	0.24559	0.89039	0.32578
86	H	H86	0.36781	0.72281	0.34096
87	H	H87	0.29328	0.77699	0.12815
88	H	H88	0.41638	0.94280	0.14070
89	O	O89	0.25552	0.88975	0.27754
90	O	O90	0.37885	0.72292	0.29283
91	O	O91	0.28082	0.77704	0.17614
92	O	O92	0.40350	0.94365	0.18864
93	Co	Co93	0.51484	0.66678	0.25184
94	Co	Co94	0.63945	0.83327	0.25766
95	H	H95	0.49179	0.89039	0.35374
96	H	H96	0.61401	0.72281	0.36891
97	H	H97	0.53948	0.77699	0.15611
98	H	H98	0.66259	0.94280	0.16865
99	O	O99	0.50173	0.88975	0.30550
100	O	O100	0.62505	0.72292	0.32079
101	O	O101	0.52702	0.77704	0.20410
102	O	O102	0.64970	0.94365	0.21660
103	Co	Co103	0.76389	0.66678	0.26587
104	Co	Co104	0.88850	0.83327	0.27169
105	H	H105	0.73799	0.89039	0.38169
106	H	H106	0.86021	0.72281	0.39687

107	H	H107	0.78568	0.77699	0.18406
108	H	H108	0.90879	0.94280	0.19660
109	O	O109	0.74793	0.88975	0.33345
110	O	O110	0.87125	0.72292	0.34874
111	O	O111	0.77322	0.77704	0.23205
112	O	O112	0.89590	0.94365	0.24455
113	O	O113	0.50674	0.33682	0.32833
114	H	H114	0.49327	0.36661	0.37723

$Co(OH)_2$-High Spin-*O

			x	*y*	*z*
1	Co	Co1	0.02156	0.00011	0.29532
2	Co	Co2	0.14012	0.16660	0.24790
3	H	H3	0.05365	0.22372	0.39548
4	H	H4	0.17575	0.05614	0.38006
5	H	H5	-0.00734	0.11032	0.19643
6	H	H6	0.11581	0.27613	0.18386
7	O	O7	0.03736	0.22308	0.34796
8	O	O8	0.16055	0.05625	0.33241
9	O	O9	0.00644	0.11037	0.24427
10	O	O10	0.12917	0.27698	0.23175
11	Co	Co11	0.26777	0.00011	0.26737
12	Co	Co12	0.39012	0.16660	0.24790
13	H	H13	0.29985	0.22372	0.36752
14	H	H14	0.42195	0.05614	0.35211
15	H	H15	0.23886	0.11032	0.16847

16	H	H16	0.36201	0.27613	0.15591
17	O	O17	0.28356	0.22308	0.32000
18	O	O18	0.40676	0.05625	0.30445
19	O	O19	0.25264	0.11037	0.21631
20	O	O20	0.37537	0.27698	0.20380
21	Co	Co21	0.51397	0.00011	0.23941
22	Co	Co22	0.64012	0.16660	0.24790
23	H	H23	0.66815	0.05614	0.32415
24	H	H24	0.48506	0.11032	0.14052
25	H	H25	0.60822	0.27613	0.12795
26	O	O26	0.65296	0.05625	0.27650
27	O	O27	0.49884	0.11037	0.18836
28	O	O28	0.62158	0.27698	0.17585
29	Co	Co29	0.76017	0.00011	0.21146
30	Co	Co30	0.89012	0.16660	0.24790
31	H	H31	0.79226	0.22372	0.31161
32	H	H32	0.91435	0.05614	0.29620
33	H	H33	0.73126	0.11032	0.11256
34	H	H34	0.85442	0.27613	0.10000
35	O	O35	0.77597	0.22308	0.26409
36	O	O36	0.89916	0.05625	0.24854
37	O	O37	0.74504	0.11037	0.16040
38	O	O38	0.86778	0.27698	0.14789
39	Co	Co39	0.00997	0.33345	0.27373
40	Co	Co40	0.14012	0.49993	0.24790
41	H	H41	-0.00066	0.55705	0.29852

42	H	H42	0.16953	0.38947	0.38337
43	H	H43	0.00153	0.44366	0.17230
44	H	H44	0.17013	0.60947	0.11343
45	O	O45	0.00927	0.55642	0.25028
46	O	O46	0.15434	0.38958	0.33571
47	O	O47	0.00878	0.44371	0.22073
48	O	O48	0.15725	0.61032	0.16138
49	Co	Co49	0.25902	0.33345	0.25970
50	Co	Co50	0.39012	0.49993	0.24790
51	H	H51	0.24554	0.55705	0.32647
52	H	H52	0.25058	0.44366	0.15827
53	H	H53	0.41633	0.60947	0.14138
54	O	O54	0.25548	0.55642	0.27823
55	O	O55	0.25783	0.44371	0.20670
56	O	O56	0.40345	0.61032	0.18933
57	Co	Co57	0.50807	0.33345	0.24567
58	Co	Co58	0.64012	0.49993	0.24790
59	H	H59	0.49174	0.55705	0.35443
60	H	H60	0.49963	0.44366	0.14423
61	H	H61	0.66254	0.60947	0.16934
62	O	O62	0.50168	0.55642	0.30618
63	O	O63	0.50688	0.44371	0.19267
64	O	O64	0.64965	0.61032	0.21728
65	Co	Co65	0.75712	0.33345	0.23164
66	Co	Co66	0.89012	0.49993	0.24790
67	H	H67	0.73794	0.55705	0.38238

68	H	H68	0.74868	0.44366	0.13020
69	H	H69	0.90874	0.60947	0.19729
70	O	O70	0.74788	0.55642	0.33414
71	O	O71	0.75593	0.44371	0.17863
72	O	O72	0.89585	0.61032	0.24524
73	Co	Co73	0.01674	0.66678	0.22378
74	Co	Co74	0.14135	0.83327	0.22960
75	H	H75	-0.00061	0.89039	0.29783
76	H	H76	0.12161	0.72281	0.31301
77	H	H77	0.04708	0.77699	0.10020
78	H	H78	0.17018	0.94280	0.11274
79	O	O79	0.00932	0.88975	0.24959
80	O	O80	0.13264	0.72292	0.26488
81	O	O81	0.03462	0.77704	0.14819
82	O	O82	0.15730	0.94365	0.16069
83	Co	Co83	0.26579	0.66678	0.23781
84	Co	Co84	0.39040	0.83327	0.24363
85	H	H85	0.24559	0.89039	0.32578
86	H	H86	0.36781	0.72281	0.34096
87	H	H87	0.29328	0.77699	0.12815
88	H	H88	0.41638	0.94280	0.14070
89	O	O89	0.25552	0.88975	0.27754
90	O	O90	0.37885	0.72292	0.29283
91	O	O91	0.28082	0.77704	0.17614
92	O	O92	0.40350	0.94365	0.18864
93	Co	Co93	0.51484	0.66678	0.25184

94	Co	Co94	0.63945	0.83327	0.25766
95	H	H95	0.49179	0.89039	0.35374
96	H	H96	0.61401	0.72281	0.36891
97	H	H97	0.53948	0.77699	0.15611
98	H	H98	0.66259	0.94280	0.16865
99	O	O99	0.50173	0.88975	0.30550
100	O	O100	0.62505	0.72292	0.32079
101	O	O101	0.52702	0.77704	0.20410
102	O	O102	0.64970	0.94365	0.21660
103	Co	Co103	0.76389	0.66678	0.26587
104	Co	Co104	0.88850	0.83327	0.27169
105	H	H105	0.73799	0.89039	0.38169
106	H	H106	0.86021	0.72281	0.39687
107	H	H107	0.78568	0.77699	0.18406
108	H	H108	0.90879	0.94280	0.19660
109	O	O109	0.74793	0.88975	0.33345
110	O	O110	0.87125	0.72292	0.34874
111	O	O111	0.77322	0.77704	0.23205
112	O	O112	0.89590	0.94365	0.24455
113	O	O113	0.50674	0.33682	0.32833

$Co(OH)_2$-High Spin-*OOH

			x	*y*	*z*
1	Co	Co1	0.02156	0.00011	0.29532
2	Co	Co2	0.14012	0.16660	0.24790
3	H	H3	0.05365	0.22372	0.39548

4	H	H4	0.17575	0.05614	0.38006
5	H	H5	-0.00734	0.11032	0.19643
6	H	H6	0.11581	0.27613	0.18386
7	O	O7	0.03736	0.22308	0.34796
8	O	O8	0.16055	0.05625	0.33241
9	O	O9	0.00644	0.11037	0.24427
10	O	O10	0.12917	0.27698	0.23175
11	Co	Co11	0.26777	0.00011	0.26737
12	Co	Co12	0.39012	0.16660	0.24790
13	H	H13	0.29985	0.22372	0.36752
14	H	H14	0.42195	0.05614	0.35211
15	H	H15	0.23886	0.11032	0.16847
16	H	H16	0.36201	0.27613	0.15591
17	O	O17	0.28356	0.22308	0.32000
18	O	O18	0.40676	0.05625	0.30445
19	O	O19	0.25264	0.11037	0.21631
20	O	O20	0.37537	0.27698	0.20380
21	Co	Co21	0.51397	0.00011	0.23941
22	Co	Co22	0.64012	0.16660	0.24790
23	H	H23	0.66815	0.05614	0.32415
24	H	H24	0.48506	0.11032	0.14052
25	H	H25	0.60822	0.27613	0.12795
26	O	O26	0.65296	0.05625	0.27650
27	O	O27	0.49884	0.11037	0.18836
28	O	O28	0.62158	0.27698	0.17585
29	Co	Co29	0.76017	0.00011	0.21146

30 Co Co30 0.89012 0.16660 0.24790

31 H H31 0.79226 0.22372 0.31161

32 H H32 0.91435 0.05614 0.29620

33 H H33 0.73126 0.11032 0.11256

34 H H34 0.85442 0.27613 0.10000

35 O O35 0.77597 0.22308 0.26409

36 O O36 0.89916 0.05625 0.24854

37 O O37 0.74504 0.11037 0.16040

38 O O38 0.86778 0.27698 0.14789

39 Co Co39 0.00997 0.33345 0.27373

40 Co Co40 0.14012 0.49993 0.24790

41 H H41 -0.00066 0.55705 0.29852

42 H H42 0.16953 0.38947 0.38337

43 H H43 0.00153 0.44366 0.17230

44 H H44 0.17013 0.60947 0.11343

45 O O45 0.00927 0.55642 0.25028

46 O O46 0.15434 0.38958 0.33571

47 O O47 0.00878 0.44371 0.22073

48 O O48 0.15725 0.61032 0.16138

49 Co Co49 0.25902 0.33345 0.25970

50 Co Co50 0.39012 0.49993 0.24790

51 H H51 0.24554 0.55705 0.32647

52 H H52 0.25058 0.44366 0.15827

53 H H53 0.41633 0.60947 0.14138

54 O O54 0.25548 0.55642 0.27823

55 O O55 0.25783 0.44371 0.20670

56	O	O56	0.40345	0.61032	0.18933
57	Co	Co57	0.50807	0.33345	0.24567
58	Co	Co58	0.64012	0.49993	0.24790
59	H	H59	0.49174	0.55705	0.35443
60	H	H60	0.49963	0.44366	0.14423
61	H	H61	0.66254	0.60947	0.16934
62	O	O62	0.50168	0.55642	0.30618
63	O	O63	0.50688	0.44371	0.19267
64	O	O64	0.64965	0.61032	0.21728
65	Co	Co65	0.75712	0.33345	0.23164
66	Co	Co66	0.89012	0.49993	0.24790
67	H	H67	0.73794	0.55705	0.38238
68	H	H68	0.74868	0.44366	0.13020
69	H	H69	0.90874	0.60947	0.19729
70	O	O70	0.74788	0.55642	0.33414
71	O	O71	0.75593	0.44371	0.17863
72	O	O72	0.89585	0.61032	0.24524
73	Co	Co73	0.01674	0.66678	0.22378
74	Co	Co74	0.14135	0.83327	0.22960
75	H	H75	-0.00061	0.89039	0.29783
76	H	H76	0.12161	0.72281	0.31301
77	H	H77	0.04708	0.77699	0.10020
78	H	H78	0.17018	0.94280	0.11274
79	O	O79	0.00932	0.88975	0.24959
80	O	O80	0.13264	0.72292	0.26488
81	O	O81	0.03462	0.77704	0.14819

82	O	O82	0.15730	0.94365	0.16069
83	Co	Co83	0.26579	0.66678	0.23781
84	Co	Co84	0.39040	0.83327	0.24363
85	H	H85	0.24559	0.89039	0.32578
86	H	H86	0.36781	0.72281	0.34096
87	H	H87	0.29328	0.77699	0.12815
88	H	H88	0.41638	0.94280	0.14070
89	O	O89	0.25552	0.88975	0.27754
90	O	O90	0.37885	0.72292	0.29283
91	O	O91	0.28082	0.77704	0.17614
92	O	O92	0.40350	0.94365	0.18864
93	Co	Co93	0.51484	0.66678	0.25184
94	Co	Co94	0.63945	0.83327	0.25766
95	H	H95	0.49179	0.89039	0.35374
96	H	H96	0.61401	0.72281	0.36891
97	H	H97	0.53948	0.77699	0.15611
98	H	H98	0.66259	0.94280	0.16865
99	O	O99	0.50173	0.88975	0.30550
100	O	O100	0.62505	0.72292	0.32079
101	O	O101	0.52702	0.77704	0.20410
102	O	O102	0.64970	0.94365	0.21660
103	Co	Co103	0.76389	0.66678	0.26587
104	Co	Co104	0.88850	0.83327	0.27169
105	H	H105	0.73799	0.89039	0.38169
106	H	H106	0.86021	0.72281	0.39687
107	H	H107	0.78568	0.77699	0.18406

108	H	H108	0.90879	0.94280	0.19660
109	O	O109	0.74793	0.88975	0.33345
110	O	O110	0.87125	0.72292	0.34874
111	O	O111	0.77322	0.77704	0.23205
112	O	O112	0.89590	0.94365	0.24455
113	O	O113	0.50674	0.33682	0.32833
114	O	O114	0.51230	0.30906	0.39854
115	H	H115	0.50360	0.34498	0.44495

$Co(OH)_2$-High Spin-*O_2

			x	*y*	*z*
1	Co	Co1	0.02156	0.00011	0.29532
2	Co	Co2	0.14012	0.16660	0.24790
3	H	H3	0.05365	0.22372	0.39548
4	H	H4	0.17575	0.05614	0.38006
5	H	H5	-0.00734	0.11032	0.19643
6	H	H6	0.11581	0.27613	0.18386
7	O	O7	0.03736	0.22308	0.34796
8	O	O8	0.16055	0.05625	0.33241
9	O	O9	0.00644	0.11037	0.24427
10	O	O10	0.12917	0.27698	0.23175
11	Co	Co11	0.26777	0.00011	0.26737
12	Co	Co12	0.39012	0.16660	0.24790
13	H	H13	0.29985	0.22372	0.36752
14	H	H14	0.42195	0.05614	0.35211
15	H	H15	0.23886	0.11032	0.16847

16	H	H16	0.36201	0.27613	0.15591
17	O	O17	0.28356	0.22308	0.32000
18	O	O18	0.40676	0.05625	0.30445
19	O	O19	0.25264	0.11037	0.21631
20	O	O20	0.37537	0.27698	0.20380
21	Co	Co21	0.51397	0.00011	0.23941
22	Co	Co22	0.64012	0.16660	0.24790
23	H	H23	0.66815	0.05614	0.32415
24	H	H24	0.48506	0.11032	0.14052
25	H	H25	0.60822	0.27613	0.12795
26	O	O26	0.65296	0.05625	0.27650
27	O	O27	0.49884	0.11037	0.18836
28	O	O28	0.62158	0.27698	0.17585
29	Co	Co29	0.76017	0.00011	0.21146
30	Co	Co30	0.89012	0.16660	0.24790
31	H	H31	0.79226	0.22372	0.31161
32	H	H32	0.91435	0.05614	0.29620
33	H	H33	0.73126	0.11032	0.11256
34	H	H34	0.85442	0.27613	0.10000
35	O	O35	0.77597	0.22308	0.26409
36	O	O36	0.89916	0.05625	0.24854
37	O	O37	0.74504	0.11037	0.16040
38	O	O38	0.86778	0.27698	0.14789
39	Co	Co39	0.00997	0.33345	0.27373
40	Co	Co40	0.14012	0.49993	0.24790
41	H	H41	-0.00066	0.55705	0.29852

42	H	H42	0.16953	0.38947	0.38337
43	H	H43	0.00153	0.44366	0.17230
44	H	H44	0.17013	0.60947	0.11343
45	O	O45	0.00927	0.55642	0.25028
46	O	O46	0.15434	0.38958	0.33571
47	O	O47	0.00878	0.44371	0.22073
48	O	O48	0.15725	0.61032	0.16138
49	Co	Co49	0.25902	0.33345	0.25970
50	Co	Co50	0.39012	0.49993	0.24790
51	H	H51	0.24554	0.55705	0.32647
52	H	H52	0.25058	0.44366	0.15827
53	H	H53	0.41633	0.60947	0.14138
54	O	O54	0.25548	0.55642	0.27823
55	O	O55	0.25783	0.44371	0.20670
56	O	O56	0.40345	0.61032	0.18933
57	Co	Co57	0.50807	0.33345	0.24567
58	Co	Co58	0.64012	0.49993	0.24790
59	H	H59	0.49174	0.55705	0.35443
60	H	H60	0.49963	0.44366	0.14423
61	H	H61	0.66254	0.60947	0.16934
62	O	O62	0.50168	0.55642	0.30618
63	O	O63	0.50688	0.44371	0.19267
64	O	O64	0.64965	0.61032	0.21728
65	Co	Co65	0.75712	0.33345	0.23164
66	Co	Co66	0.89012	0.49993	0.24790
67	H	H67	0.73794	0.55705	0.38238

68	H	H68	0.74868	0.44366	0.13020
69	H	H69	0.90874	0.60947	0.19729
70	O	O70	0.74788	0.55642	0.33414
71	O	O71	0.75593	0.44371	0.17863
72	O	O72	0.89585	0.61032	0.24524
73	Co	Co73	0.01674	0.66678	0.22378
74	Co	Co74	0.14135	0.83327	0.22960
75	H	H75	-0.00061	0.89039	0.29783
76	H	H76	0.12161	0.72281	0.31301
77	H	H77	0.04708	0.77699	0.10020
78	H	H78	0.17018	0.94280	0.11274
79	O	O79	0.00932	0.88975	0.24959
80	O	O80	0.13264	0.72292	0.26488
81	O	O81	0.03462	0.77704	0.14819
82	O	O82	0.15730	0.94365	0.16069
83	Co	Co83	0.26579	0.66678	0.23781
84	Co	Co84	0.39040	0.83327	0.24363
85	H	H85	0.24559	0.89039	0.32578
86	H	H86	0.36781	0.72281	0.34096
87	H	H87	0.29328	0.77699	0.12815
88	H	H88	0.41638	0.94280	0.14070
89	O	O89	0.25552	0.88975	0.27754
90	O	O90	0.37885	0.72292	0.29283
91	O	O91	0.28082	0.77704	0.17614
92	O	O92	0.40350	0.94365	0.18864
93	Co	Co93	0.51484	0.66678	0.25184

94	Co	Co94	0.63945	0.83327	0.25766
95	H	H95	0.49179	0.89039	0.35374
96	H	H96	0.61401	0.72281	0.36891
97	H	H97	0.53948	0.77699	0.15611
98	H	H98	0.66259	0.94280	0.16865
99	O	O99	0.50173	0.88975	0.30550
100	O	O100	0.62505	0.72292	0.32079
101	O	O101	0.52702	0.77704	0.20410
102	O	O102	0.64970	0.94365	0.21660
103	Co	Co103	0.76389	0.66678	0.26587
104	Co	Co104	0.88850	0.83327	0.27169
105	H	H105	0.73799	0.89039	0.38169
106	H	H106	0.86021	0.72281	0.39687
107	H	H107	0.78568	0.77699	0.18406
108	H	H108	0.90879	0.94280	0.19660
109	O	O109	0.74793	0.88975	0.33345
110	O	O110	0.87125	0.72292	0.34874
111	O	O111	0.77322	0.77704	0.23205
112	O	O112	0.89590	0.94365	0.24455
113	O	O113	0.50674	0.33682	0.32833
114	O	O114	0.51230	0.30906	0.39854

$Co(OH)_2$-High Spin-*+O_2

			x	*y*	*z*
1	Co	Co1	0.02156	0.00011	0.29532
2	Co	Co2	0.14012	0.16660	0.24790

3	H	H3	0.05365	0.22372	0.39548
4	H	H4	0.17575	0.05614	0.38006
5	H	H5	-0.00734	0.11032	0.19643
6	H	H6	0.11581	0.27613	0.18386
7	O	O7	0.03736	0.22308	0.34796
8	O	O8	0.16055	0.05625	0.33241
9	O	O9	0.00644	0.11037	0.24427
10	O	O10	0.12917	0.27698	0.23175
11	Co	Co11	0.26777	0.00011	0.26737
12	Co	Co12	0.39012	0.16660	0.24790
13	H	H13	0.29985	0.22372	0.36752
14	H	H14	0.42195	0.05614	0.35211
15	H	H15	0.23886	0.11032	0.16847
16	H	H16	0.36201	0.27613	0.15591
17	O	O17	0.28356	0.22308	0.32000
18	O	O18	0.40676	0.05625	0.30445
19	O	O19	0.25264	0.11037	0.21631
20	O	O20	0.37537	0.27698	0.20380
21	Co	Co21	0.51397	0.00011	0.23941
22	Co	Co22	0.64012	0.16660	0.24790
23	H	H23	0.66815	0.05614	0.32415
24	H	H24	0.48506	0.11032	0.14052
25	H	H25	0.60822	0.27613	0.12795
26	O	O26	0.65296	0.05625	0.27650
27	O	O27	0.49884	0.11037	0.18836
28	O	O28	0.62158	0.27698	0.17585

29	Co	Co29	0.76017	0.00011	0.21146
30	Co	Co30	0.89012	0.16660	0.24790
31	H	H31	0.79226	0.22372	0.31161
32	H	H32	0.91435	0.05614	0.29620
33	H	H33	0.73126	0.11032	0.11256
34	H	H34	0.85442	0.27613	0.10000
35	O	O35	0.77597	0.22308	0.26409
36	O	O36	0.89916	0.05625	0.24854
37	O	O37	0.74504	0.11037	0.16040
38	O	O38	0.86778	0.27698	0.14789
39	Co	Co39	0.00997	0.33345	0.27373
40	Co	Co40	0.14012	0.49993	0.24790
41	H	H41	-0.00066	0.55705	0.29852
42	H	H42	0.16953	0.38947	0.38337
43	H	H43	0.00153	0.44366	0.17230
44	H	H44	0.17013	0.60947	0.11343
45	O	O45	0.00927	0.55642	0.25028
46	O	O46	0.15434	0.38958	0.33571
47	O	O47	0.00878	0.44371	0.22073
48	O	O48	0.15725	0.61032	0.16138
49	Co	Co49	0.25902	0.33345	0.25970
50	Co	Co50	0.39012	0.49993	0.24790
51	H	H51	0.24554	0.55705	0.32647
52	H	H52	0.25058	0.44366	0.15827
53	H	H53	0.41633	0.60947	0.14138
54	O	O54	0.25548	0.55642	0.27823

55	O	O55	0.25783	0.44371	0.20670
56	O	O56	0.40345	0.61032	0.18933
57	Co	Co57	0.50807	0.33345	0.24567
58	Co	Co58	0.64012	0.49993	0.24790
59	H	H59	0.49174	0.55705	0.35443
60	H	H60	0.49963	0.44366	0.14423
61	H	H61	0.66254	0.60947	0.16934
62	O	O62	0.50168	0.55642	0.30618
63	O	O63	0.50688	0.44371	0.19267
64	O	O64	0.64965	0.61032	0.21728
65	Co	Co65	0.75712	0.33345	0.23164
66	Co	Co66	0.89012	0.49993	0.24790
67	H	H67	0.73794	0.55705	0.38238
68	H	H68	0.74868	0.44366	0.13020
69	H	H69	0.90874	0.60947	0.19729
70	O	O70	0.74788	0.55642	0.33414
71	O	O71	0.75593	0.44371	0.17863
72	O	O72	0.89585	0.61032	0.24524
73	Co	Co73	0.01674	0.66678	0.22378
74	Co	Co74	0.14135	0.83327	0.22960
75	H	H75	-0.00061	0.89039	0.29783
76	H	H76	0.12161	0.72281	0.31301
77	H	H77	0.04708	0.77699	0.10020
78	H	H78	0.17018	0.94280	0.11274
79	O	O79	0.00932	0.88975	0.24959
80	O	O80	0.13264	0.72292	0.26488

81	O	O81	0.03462	0.77704	0.14819
82	O	O82	0.15730	0.94365	0.16069
83	Co	Co83	0.26579	0.66678	0.23781
84	Co	Co84	0.39040	0.83327	0.24363
85	H	H85	0.24559	0.89039	0.32578
86	H	H86	0.36781	0.72281	0.34096
87	H	H87	0.29328	0.77699	0.12815
88	H	H88	0.41638	0.94280	0.14070
89	O	O89	0.25552	0.88975	0.27754
90	O	O90	0.37885	0.72292	0.29283
91	O	O91	0.28082	0.77704	0.17614
92	O	O92	0.40350	0.94365	0.18864
93	Co	Co93	0.51484	0.66678	0.25184
94	Co	Co94	0.63945	0.83327	0.25766
95	H	H95	0.49179	0.89039	0.35374
96	H	H96	0.61401	0.72281	0.36891
97	H	H97	0.53948	0.77699	0.15611
98	H	H98	0.66259	0.94280	0.16865
99	O	O99	0.50173	0.88975	0.30550
100	O	O100	0.62505	0.72292	0.32079
101	O	O101	0.52702	0.77704	0.20410
102	O	O102	0.64970	0.94365	0.21660
103	Co	Co103	0.76389	0.66678	0.26587
104	Co	Co104	0.88850	0.83327	0.27169
105	H	H105	0.73799	0.89039	0.38169
106	H	H106	0.86021	0.72281	0.39687

107	H	H107	0.78568	0.77699	0.18406
108	H	H108	0.90879	0.94280	0.19660
109	O	O109	0.74793	0.88975	0.33345
110	O	O110	0.87125	0.72292	0.34874
111	O	O111	0.77322	0.77704	0.23205
112	O	O112	0.89590	0.94365	0.24455
113	O	O113	0.50675	0.33672	0.35833
114	O	O114	0.51231	0.30896	0.42854

$Co(OH)_2$-High Spin-*H_2O_2

			x	*y*	*z*
1	Co	Co1	0.02156	0.00011	0.29532
2	Co	Co2	0.14012	0.16660	0.24790
3	H	H3	0.05365	0.22372	0.39548
4	H	H4	0.17575	0.05614	0.38006
5	H	H5	-0.00734	0.11032	0.19643
6	H	H6	0.11581	0.27613	0.18386
7	O	O7	0.03736	0.22308	0.34796
8	O	O8	0.16055	0.05625	0.33241
9	O	O9	0.00644	0.11037	0.24427
10	O	O10	0.12917	0.27698	0.23175
11	Co	Co11	0.26777	0.00011	0.26737
12	Co	Co12	0.39012	0.16660	0.24790
13	H	H13	0.29985	0.22372	0.36752
14	H	H14	0.42195	0.05614	0.35211
15	H	H15	0.23886	0.11032	0.16847

16	H	H16	0.36201	0.27613	0.15591
17	O	O17	0.28356	0.22308	0.32000
18	O	O18	0.40676	0.05625	0.30445
19	O	O19	0.25264	0.11037	0.21631
20	O	O20	0.37537	0.27698	0.20380
21	Co	Co21	0.51397	0.00011	0.23941
22	Co	Co22	0.64012	0.16660	0.24790
23	H	H23	0.66815	0.05614	0.32415
24	H	H24	0.48506	0.11032	0.14052
25	H	H25	0.60822	0.27613	0.12795
26	O	O26	0.65296	0.05625	0.27650
27	O	O27	0.49884	0.11037	0.18836
28	O	O28	0.62158	0.27698	0.17585
29	Co	Co29	0.76017	0.00011	0.21146
30	Co	Co30	0.89012	0.16660	0.24790
31	H	H31	0.79226	0.22372	0.31161
32	H	H32	0.91435	0.05614	0.29620
33	H	H33	0.73126	0.11032	0.11256
34	H	H34	0.85442	0.27613	0.10000
35	O	O35	0.77597	0.22308	0.26409
36	O	O36	0.89916	0.05625	0.24854
37	O	O37	0.74504	0.11037	0.16040
38	O	O38	0.86778	0.27698	0.14789
39	Co	Co39	0.00997	0.33345	0.27373
40	Co	Co40	0.14012	0.49993	0.24790
41	H	H41	-0.00066	0.55705	0.29852

42	H	H42	0.16953	0.38947	0.38337
43	H	H43	0.00153	0.44366	0.17230
44	H	H44	0.17013	0.60947	0.11343
45	O	O45	0.00927	0.55642	0.25028
46	O	O46	0.15434	0.38958	0.33571
47	O	O47	0.00878	0.44371	0.22073
48	O	O48	0.15725	0.61032	0.16138
49	Co	Co49	0.25902	0.33345	0.25970
50	Co	Co50	0.39012	0.49993	0.24790
51	H	H51	0.24554	0.55705	0.32647
52	H	H52	0.25058	0.44366	0.15827
53	H	H53	0.41633	0.60947	0.14138
54	O	O54	0.25548	0.55642	0.27823
55	O	O55	0.25783	0.44371	0.20670
56	O	O56	0.40345	0.61032	0.18933
57	Co	Co57	0.50807	0.33345	0.24567
58	Co	Co58	0.64012	0.49993	0.24790
59	H	H59	0.49174	0.55705	0.35443
60	H	H60	0.49963	0.44366	0.14423
61	H	H61	0.66254	0.60947	0.16934
62	O	O62	0.50168	0.55642	0.30618
63	O	O63	0.50688	0.44371	0.19267
64	O	O64	0.64965	0.61032	0.21728
65	Co	Co65	0.75712	0.33345	0.23164
66	Co	Co66	0.89012	0.49993	0.24790
67	H	H67	0.73794	0.55705	0.38238

68	H	H68	0.74868	0.44366	0.13020
69	H	H69	0.90874	0.60947	0.19729
70	O	O70	0.74788	0.55642	0.33414
71	O	O71	0.75593	0.44371	0.17863
72	O	O72	0.89585	0.61032	0.24524
73	Co	Co73	0.01674	0.66678	0.22378
74	Co	Co74	0.14135	0.83327	0.22960
75	H	H75	-0.00061	0.89039	0.29783
76	H	H76	0.12161	0.72281	0.31301
77	H	H77	0.04708	0.77699	0.10020
78	H	H78	0.17018	0.94280	0.11274
79	O	O79	0.00932	0.88975	0.24959
80	O	O80	0.13264	0.72292	0.26488
81	O	O81	0.03462	0.77704	0.14819
82	O	O82	0.15730	0.94365	0.16069
83	Co	Co83	0.26579	0.66678	0.23781
84	Co	Co84	0.39040	0.83327	0.24363
85	H	H85	0.24559	0.89039	0.32578
86	H	H86	0.36781	0.72281	0.34096
87	H	H87	0.29328	0.77699	0.12815
88	H	H88	0.41638	0.94280	0.14070
89	O	O89	0.25552	0.88975	0.27754
90	O	O90	0.37885	0.72292	0.29283
91	O	O91	0.28082	0.77704	0.17614
92	O	O92	0.40350	0.94365	0.18864
93	Co	Co93	0.51484	0.66678	0.25184

94	Co	Co94	0.63945	0.83327	0.25766
95	H	H95	0.49179	0.89039	0.35374
96	H	H96	0.61401	0.72281	0.36891
97	H	H97	0.53948	0.77699	0.15611
98	H	H98	0.66259	0.94280	0.16865
99	O	O99	0.50173	0.88975	0.30550
100	O	O100	0.62505	0.72292	0.32079
101	O	O101	0.52702	0.77704	0.20410
102	O	O102	0.64970	0.94365	0.21660
103	Co	Co103	0.76389	0.66678	0.26587
104	Co	Co104	0.88850	0.83327	0.27169
105	H	H105	0.73799	0.89039	0.38169
106	H	H106	0.86021	0.72281	0.39687
107	H	H107	0.78568	0.77699	0.18406
108	H	H108	0.90879	0.94280	0.19660
109	O	O109	0.74793	0.88975	0.33345
110	O	O110	0.87125	0.72292	0.34874
111	O	O111	0.77322	0.77704	0.23205
112	O	O112	0.89590	0.94365	0.24455
113	O	O113	0.49304	0.26202	0.38599
114	O	O114	0.49620	0.33190	0.34038
115	H	H115	0.46631	0.38586	0.36679
116	H	H116	0.52293	0.20807	0.35958

$Co(OH)_2$-High Spin-*+H_2O_2

	x	*y*	*z*

1	Co	Co1	0.02156	0.00011	0.29532
2	Co	Co2	0.14012	0.16660	0.24790
3	H	H3	0.05365	0.22372	0.39548
4	H	H4	0.17575	0.05614	0.38006
5	H	H5	-0.00734	0.11032	0.19643
6	H	H6	0.11581	0.27613	0.18386
7	O	O7	0.03736	0.22308	0.34796
8	O	O8	0.16055	0.05625	0.33241
9	O	O9	0.00644	0.11037	0.24427
10	O	O10	0.12917	0.27698	0.23175
11	Co	Co11	0.26777	0.00011	0.26737
12	Co	Co12	0.39012	0.16660	0.24790
13	H	H13	0.29985	0.22372	0.36752
14	H	H14	0.42195	0.05614	0.35211
15	H	H15	0.23886	0.11032	0.16847
16	H	H16	0.36201	0.27613	0.15591
17	O	O17	0.28356	0.22308	0.32000
18	O	O18	0.40676	0.05625	0.30445
19	O	O19	0.25264	0.11037	0.21631
20	O	O20	0.37537	0.27698	0.20380
21	Co	Co21	0.51397	0.00011	0.23941
22	Co	Co22	0.64012	0.16660	0.24790
23	H	H23	0.66815	0.05614	0.32415
24	H	H24	0.48506	0.11032	0.14052
25	H	H25	0.60822	0.27613	0.12795
26	O	O26	0.65296	0.05625	0.27650

27	O	O27	0.49884	0.11037	0.18836
28	O	O28	0.62158	0.27698	0.17585
29	Co	Co29	0.76017	0.00011	0.21146
30	Co	Co30	0.89012	0.16660	0.24790
31	H	H31	0.79226	0.22372	0.31161
32	H	H32	0.91435	0.05614	0.29620
33	H	H33	0.73126	0.11032	0.11256
34	H	H34	0.85442	0.27613	0.10000
35	O	O35	0.77597	0.22308	0.26409
36	O	O36	0.89916	0.05625	0.24854
37	O	O37	0.74504	0.11037	0.16040
38	O	O38	0.86778	0.27698	0.14789
39	Co	Co39	0.00997	0.33345	0.27373
40	Co	Co40	0.14012	0.49993	0.24790
41	H	H41	-0.00066	0.55705	0.29852
42	H	H42	0.16953	0.38947	0.38337
43	H	H43	0.00153	0.44366	0.17230
44	H	H44	0.17013	0.60947	0.11343
45	O	O45	0.00927	0.55642	0.25028
46	O	O46	0.15434	0.38958	0.33571
47	O	O47	0.00878	0.44371	0.22073
48	O	O48	0.15725	0.61032	0.16138
49	Co	Co49	0.25902	0.33345	0.25970
50	Co	Co50	0.39012	0.49993	0.24790
51	H	H51	0.24554	0.55705	0.32647
52	H	H52	0.25058	0.44366	0.15827

53	H	H53	0.41633	0.60947	0.14138
54	O	O54	0.25548	0.55642	0.27823
55	O	O55	0.25783	0.44371	0.206701
56	O	O56	0.40345	0.61032	0.18933
57	Co	Co57	0.50807	0.33345	0.24567
58	Co	Co58	0.64012	0.49993	0.24790
59	H	H59	0.49174	0.55705	0.35443
60	H	H60	0.49963	0.44366	0.14423
61	H	H61	0.66254	0.60947	0.16934
62	O	O62	0.50168	0.55642	0.30618
63	O	O63	0.50688	0.44371	0.19267
64	O	O64	0.64965	0.61032	0.21728
65	Co	Co65	0.75712	0.33345	0.23164
66	Co	Co66	0.89012	0.49993	0.24790
67	H	H67	0.73794	0.55705	0.38238
68	H	H68	0.74868	0.44366	0.13020
69	H	H69	0.90874	0.60947	0.19729
70	O	O70	0.74788	0.55642	0.33414
71	O	O71	0.75593	0.44371	0.17863
72	O	O72	0.89585	0.61032	0.24524
73	Co	Co73	0.01674	0.66678	0.22378
74	Co	Co74	0.14135	0.83327	0.22960
75	H	H75	-0.00061	0.89039	0.29783
76	H	H76	0.12161	0.72281	0.31301
77	H	H77	0.04708	0.77699	0.10020
78	H	H78	0.17018	0.94280	0.11274

79	O	O79	0.00932	0.88975	0.24959
80	O	O80	0.13264	0.72292	0.26488
81	O	O81	0.03462	0.77704	0.14819
82	O	O82	0.15730	0.94365	0.16069
83	Co	Co83	0.26579	0.66678	0.23781
84	Co	Co84	0.39040	0.83327	0.24363
85	H	H85	0.24559	0.89039	0.32578
86	H	H86	0.36781	0.72281	0.34096
87	H	H87	0.29328	0.77699	0.12815
88	H	H88	0.41638	0.94280	0.14070
89	O	O89	0.25552	0.88975	0.27754
90	O	O90	0.37885	0.72292	0.29283
91	O	O91	0.28082	0.77704	0.17614
92	O	O92	0.40350	0.94365	0.18864
93	Co	Co93	0.51484	0.66678	0.25184
94	Co	Co94	0.63945	0.83327	0.25766
95	H	H95	0.49179	0.89039	0.35374
96	H	H96	0.61401	0.72281	0.36891
97	H	H97	0.53948	0.77699	0.15611
98	H	H98	0.66259	0.94280	0.16865
99	O	O99	0.50173	0.88975	0.30550
100	O	O100	0.62505	0.72292	0.32079
101	O	O101	0.52702	0.77704	0.20410
102	O	O102	0.64970	0.94365	0.21660
103	Co	Co103	0.76389	0.66678	0.26587
104	Co	Co104	0.88850	0.83327	0.27169

105	H	H105	0.73799	0.89039	0.38169
106	H	H106	0.86021	0.72281	0.39687
107	H	H107	0.78568	0.77699	0.18406
108	H	H108	0.90879	0.94280	0.19660
109	O	O109	0.74793	0.88975	0.33345
110	O	O110	0.87125	0.72292	0.34874
111	O	O111	0.77322	0.77704	0.23205
112	O	O112	0.89590	0.94365	0.24455
113	O	O113	0.49282	0.26204	0.40599
114	O	O114	0.49599	0.33193	0.36038
115	H	H115	0.46609	0.38588	0.38679
116	H	H116	0.52271	0.20809	0.37958

$Co(OH)_2$-Low Spin-*H_2O

			x	*y*	*z*
1	Co	Co1	0.01511	0.00011	0.20057
2	Co	Co2	0.14012	0.16660	0.20078
3	H	H3	0.01991	0.22372	0.30141
4	H	H4	0.14410	0.05614	0.30130
5	H	H5	0.01330	0.11032	0.10002
6	H	H6	0.13819	0.27613	0.10000
7	O	O7	0.01668	0.22308	0.25279
8	O	O8	0.14199	0.05625	0.25267
9	O	O9	0.01397	0.11037	0.14868
10	O	O10	0.13843	0.27698	0.14866
11	Co	Co11	0.26511	0.00011	0.20057

12 Co Co12 0.39012 0.16660 0.20078

13 H H13 0.26991 0.22372 0.30141

14 H H14 0.39410 0.05614 0.30130

15 H H15 0.26330 0.11032 0.10002

16 H H16 0.38819 0.27613 0.10000

17 O O17 0.26668 0.22308 0.25279

18 O O18 0.39199 0.05625 0.25267

19 O O19 0.26397 0.11037 0.14868

20 O O20 0.38843 0.27698 0.14866

21 Co Co21 0.51511 0.00011 0.20057

22 Co Co22 0.64012 0.16660 0.20078

23 H H23 0.64410 0.05614 0.30130

24 H H24 0.51330 0.11032 0.10002

25 H H25 0.63819 0.27613 0.10000

26 O O26 0.64199 0.05625 0.25267

27 O O27 0.51397 0.11037 0.14868

28 O O28 0.63843 0.27698 0.14866

29 Co Co29 0.76511 0.00011 0.20057

30 Co Co30 0.89012 0.16660 0.20078

31 H H31 0.76991 0.22372 0.30141

32 H H32 0.89410 0.05614 0.30130

33 H H33 0.76330 0.11032 0.10002

34 H H34 0.88819 0.27613 0.10000

35 O O35 0.76668 0.22308 0.25279

36 O O36 0.89199 0.05625 0.25267

37 O O37 0.76397 0.11037 0.14868

38 O O38 0.88843 0.27698 0.14866

39 Co Co39 0.01511 0.33345 0.20057

40 Co Co40 0.14012 0.49993 0.20078

41 H H41 0.01991 0.55705 0.30141

42 H H42 0.14410 0.38947 0.30130

43 H H43 0.01330 0.44366 0.10002

44 H H44 0.13819 0.60947 0.10000

45 O O45 0.01668 0.55642 0.25279

46 O O46 0.14199 0.38958 0.25267

47 O O47 0.01397 0.44371 0.14868

48 O O48 0.13843 0.61032 0.14866

49 Co Co49 0.26511 0.33345 0.20057

50 Co Co50 0.39012 0.49993 0.20078

51 H H51 0.26991 0.55705 0.30141

52 H H52 0.26330 0.44366 0.10002

53 H H53 0.38819 0.60947 0.10000

54 O O54 0.26668 0.55642 0.25279

55 O O55 0.26397 0.44371 0.14868

56 O O56 0.38843 0.61032 0.14866

57 Co Co57 0.51511 0.33345 0.20057

58 Co Co58 0.64012 0.49993 0.20078

59 H H59 0.51991 0.55705 0.30141

60 H H60 0.51330 0.44366 0.10002

61 H H61 0.63819 0.60947 0.10000

62 O O62 0.51668 0.55642 0.25279

63 O O63 0.51397 0.44371 0.14868

64 O O64 0.63843 0.61032 0.14866

65 Co Co65 0.76511 0.33345 0.20057

66 Co Co66 0.89012 0.49993 0.20078

67 H H67 0.76991 0.55705 0.30141

68 H H68 0.76330 0.44366 0.10002

69 H H69 0.88819 0.60947 0.10000

70 O O70 0.76668 0.55642 0.25279

71 O O71 0.76397 0.44371 0.14868

72 O O72 0.88843 0.61032 0.14866

73 Co Co73 0.01511 0.66678 0.20057

74 Co Co74 0.14012 0.83327 0.20078

75 H H75 0.01991 0.89039 0.30141

76 H H76 0.14410 0.72281 0.30130

77 H H77 0.01330 0.77699 0.10002

78 H H78 0.13819 0.94280 0.10000

79 O O79 0.01668 0.88975 0.25279

80 O O80 0.14199 0.72292 0.25267

81 O O81 0.01397 0.77704 0.14868

82 O O82 0.13843 0.94365 0.14866

83 Co Co83 0.26511 0.66678 0.20057

84 Co Co84 0.39012 0.83327 0.20078

85 H H85 0.26991 0.89039 0.30141

86 H H86 0.39410 0.72281 0.30130

87 H H87 0.26330 0.77699 0.10002

88 H H88 0.38819 0.94280 0.10000

89 O O89 0.26668 0.88975 0.25279

90	O	O90	0.39199	0.72292	0.25267
91	O	O91	0.26397	0.77704	0.14868
92	O	O92	0.38843	0.94365	0.14866
93	Co	Co93	0.51511	0.66678	0.20057
94	Co	Co94	0.64012	0.83327	0.20078
95	H	H95	0.51991	0.89039	0.30141
96	H	H96	0.64410	0.72281	0.30130
97	H	H97	0.51330	0.77699	0.10002
98	H	H98	0.63819	0.94280	0.10000
99	O	O99	0.51668	0.88975	0.25279
100	O	O100	0.64199	0.72292	0.25267
101	O	O101	0.51397	0.77704	0.14868
102	O	O102	0.63843	0.94365	0.14866
103	Co	Co103	0.76511	0.66678	0.20057
104	Co	Co104	0.89012	0.83327	0.20078
105	H	H105	0.76991	0.89039	0.30141
106	H	H106	0.89410	0.72281	0.30130
107	H	H107	0.76330	0.77699	0.10002
108	H	H108	0.88819	0.94280	0.10000
109	O	O109	0.76668	0.88975	0.25279
110	O	O110	0.89199	0.72292	0.25267
111	O	O111	0.76397	0.77704	0.14868
112	O	O112	0.88843	0.94365	0.14866
113	O	O113	0.53029	0.33740	0.32052
114	H	H114	0.54342	0.39003	0.35342
115	H	H115	0.54679	0.28142	0.34873

$Co(OH)_2$-Low Spin-*OH

		x	*y*	*z*
1	Co Co1	0.01511	0.00011	0.20057
2	Co Co2	0.14012	0.16660	0.20078
3	H H3	0.01991	0.22372	0.30141
4	H H4	0.14410	0.05614	0.30130
5	H H5	0.01330	0.11032	0.10002
6	H H6	0.13819	0.27613	0.10000
7	O O7	0.01668	0.22308	0.25279
8	O O8	0.14199	0.05625	0.25267
9	O O9	0.01397	0.11037	0.14868
10	O O10	0.13843	0.27698	0.14866
11	Co Co11	0.26511	0.00011	0.20057
12	Co Co12	0.39012	0.16660	0.20078
13	H H13	0.26991	0.22372	0.30141
14	H H14	0.39410	0.05614	0.30130
15	H H15	0.26330	0.11032	0.10002
16	H H16	0.38819	0.27613	0.10000
17	O O17	0.26668	0.22308	0.25279
18	O O18	0.39199	0.05625	0.25267
19	O O19	0.26397	0.11037	0.14868
20	O O20	0.38843	0.27698	0.14866
21	Co Co21	0.51511	0.00011	0.20057
22	Co Co22	0.64012	0.16660	0.20078
23	H H23	0.64410	0.05614	0.30130

24	H	H24	0.51330	0.11032	0.10002
25	H	H25	0.63819	0.27613	0.10000
26	O	O26	0.64199	0.05625	0.25267
27	O	O27	0.51397	0.11037	0.14868
28	O	O28	0.63843	0.27698	0.14866
29	Co	Co29	0.76511	0.00011	0.20057
30	Co	Co30	0.89012	0.16660	0.20078
31	H	H31	0.76991	0.22372	0.30141
32	H	H32	0.89410	0.05614	0.30130
33	H	H33	0.76330	0.11032	0.10002
34	H	H34	0.88819	0.27613	0.10000
35	O	O35	0.76668	0.22308	0.25279
36	O	O36	0.89199	0.05625	0.25267
37	O	O37	0.76397	0.11037	0.14868
38	O	O38	0.88843	0.27698	0.14866
39	Co	Co39	0.01511	0.33345	0.20057
40	Co	Co40	0.14012	0.49993	0.20078
41	H	H41	0.01991	0.55705	0.30141
42	H	H42	0.14410	0.38947	0.30130
43	H	H43	0.01330	0.44366	0.10002
44	H	H44	0.13819	0.60947	0.10000
45	O	O45	0.01668	0.55642	0.25279
46	O	O46	0.14199	0.38958	0.25267
47	O	O47	0.01397	0.44371	0.14868
48	O	O48	0.13843	0.61032	0.14866
49	Co	Co49	0.26511	0.33345	0.20057

50 Co Co50 0.39012 0.49993 0.20078

51 H H51 0.26991 0.55705 0.30141

52 H H52 0.26330 0.44366 0.10002

53 H H53 0.38819 0.60947 0.10000

54 O O54 0.26668 0.55642 0.25279

55 O O55 0.26397 0.44371 0.14868

56 O O56 0.38843 0.61032 0.14866

57 Co Co57 0.51511 0.33345 0.20057

58 Co Co58 0.64012 0.49993 0.20078

59 H H59 0.51991 0.55705 0.30141

60 H H60 0.51330 0.44366 0.10002

61 H H61 0.63819 0.60947 0.10000

62 O O62 0.51668 0.55642 0.25279

63 O O63 0.51397 0.44371 0.14868

64 O O64 0.63843 0.61032 0.14866

65 Co Co65 0.76511 0.33345 0.20057

66 Co Co66 0.89012 0.49993 0.20078

67 H H67 0.76991 0.55705 0.30141

68 H H68 0.76330 0.44366 0.10002

69 H H69 0.88819 0.60947 0.10000

70 O O70 0.76668 0.55642 0.25279

71 O O71 0.76397 0.44371 0.14868

72 O O72 0.88843 0.61032 0.14866

73 Co Co73 0.01511 0.66678 0.20057

74 Co Co74 0.14012 0.83327 0.20078

75 H H75 0.01991 0.89039 0.30141

76	H	H76	0.14410	0.72281	0.30130
77	H	H77	0.01330	0.77699	0.10002
78	H	H78	0.13819	0.94280	0.10000
79	O	O79	0.01668	0.88975	0.25279
80	O	O80	0.14199	0.72292	0.25267
81	O	O81	0.01397	0.77704	0.14868
82	O	O82	0.13843	0.94365	0.14866
83	Co	Co83	0.26511	0.66678	0.20057
84	Co	Co84	0.39012	0.83327	0.20078
85	H	H85	0.26991	0.89039	0.30141
86	H	H86	0.39410	0.72281	0.30130
87	H	H87	0.26330	0.77699	0.10002
88	H	H88	0.38819	0.94280	0.10000
89	O	O89	0.26668	0.88975	0.25279
90	O	O90	0.39199	0.72292	0.25267
91	O	O91	0.26397	0.77704	0.14868
92	O	O92	0.38843	0.94365	0.14866
93	Co	Co93	0.51511	0.66678	0.20057
94	Co	Co94	0.64012	0.83327	0.20078
95	H	H95	0.51991	0.89039	0.30141
96	H	H96	0.64410	0.72281	0.30130
97	H	H97	0.51330	0.77699	0.10002
98	H	H98	0.63819	0.94280	0.10000
99	O	O99	0.51668	0.88975	0.25279
100	O	O100	0.64199	0.72292	0.25267
101	O	O101	0.51397	0.77704	0.14868

102	O	O102	0.63843	0.94365	0.14866
103	Co	Co103	0.76511	0.66678	0.20057
104	Co	Co104	0.89012	0.83327	0.20078
105	H	H105	0.76991	0.89039	0.30141
106	H	H106	0.89410	0.72281	0.30130
107	H	H107	0.76330	0.77699	0.10002
108	H	H108	0.88819	0.94280	0.10000
109	O	O109	0.76668	0.88975	0.25279
110	O	O110	0.89199	0.72292	0.25267
111	O	O111	0.76397	0.77704	0.14868
112	O	O112	0.88843	0.94365	0.14866
113	O	O113	0.51208	0.33321	0.29089
114	H	H114	0.50265	0.37175	0.33577

$Co(OH)_2$-Low Spin-*O

			x	*y*	*z*
1	Co	Co1	0.01511	0.00011	0.20057
2	Co	Co2	0.14012	0.16660	0.20078
3	H	H3	0.01991	0.22372	0.30141
4	H	H4	0.14410	0.05614	0.30130
5	H	H5	0.01330	0.11032	0.10002
6	H	H6	0.13819	0.27613	0.10000
7	O	O7	0.01668	0.22308	0.25279
8	O	O8	0.14199	0.05625	0.25267
9	O	O9	0.01397	0.11037	0.14868
10	O	O10	0.13843	0.27698	0.14866

11	Co	Co11	0.26511	0.00011	0.20057
12	Co	Co12	0.39012	0.16660	0.20078
13	H	H13	0.26991	0.22372	0.30141
14	H	H14	0.39410	0.05614	0.30130
15	H	H15	0.26330	0.11032	0.10002
16	H	H16	0.38819	0.27613	0.10000
17	O	O17	0.26668	0.22308	0.25279
18	O	O18	0.39199	0.05625	0.25267
19	O	O19	0.26397	0.11037	0.14868
20	O	O20	0.38843	0.27698	0.14866
21	Co	Co21	0.51511	0.00011	0.20057
22	Co	Co22	0.64012	0.16660	0.20078
23	H	H23	0.64410	0.05614	0.30130
24	H	H24	0.51330	0.11032	0.10002
25	H	H25	0.63819	0.27613	0.10000
26	O	O26	0.64199	0.05625	0.25267
27	O	O27	0.51397	0.11037	0.14868
28	O	O28	0.63843	0.27698	0.14866
29	Co	Co29	0.76511	0.00011	0.20057
30	Co	Co30	0.89012	0.16660	0.20078
31	H	H31	0.76991	0.22372	0.30141
32	H	H32	0.89410	0.05614	0.30130
33	H	H33	0.76330	0.11032	0.10002
34	H	H34	0.88819	0.27613	0.10000
35	O	O35	0.76668	0.22308	0.25279
36	O	O36	0.89199	0.05625	0.25267

37 O O37 0.76397 0.11037 0.14868

38 O O38 0.88843 0.27698 0.14866

39 Co Co39 0.01511 0.33345 0.20057

40 Co Co40 0.14012 0.49993 0.20078

41 H H41 0.01991 0.55705 0.30141

42 H H42 0.14410 0.38947 0.30130

43 H H43 0.01330 0.44366 0.10002

44 H H44 0.13819 0.60947 0.10000

45 O O45 0.01668 0.55642 0.25279

46 O O46 0.14199 0.38958 0.25267

47 O O47 0.01397 0.44371 0.14868

48 O O48 0.13843 0.61032 0.14866

49 Co Co49 0.26511 0.33345 0.20057

50 Co Co50 0.39012 0.49993 0.20078

51 H H51 0.26991 0.55705 0.30141

52 H H52 0.26330 0.44366 0.10002

53 H H53 0.38819 0.60947 0.10000

54 O O54 0.26668 0.55642 0.25279

55 O O55 0.26397 0.44371 0.14868

56 O O56 0.38843 0.61032 0.14866

57 Co Co57 0.51511 0.33345 0.20057

58 Co Co58 0.64012 0.49993 0.20078

59 H H59 0.51991 0.55705 0.30141

60 H H60 0.51330 0.44366 0.10002

61 H H61 0.63819 0.60947 0.10000

62 O O62 0.51668 0.55642 0.25279

63 O O63 0.51397 0.44371 0.14868

64 O O64 0.63843 0.61032 0.14866

65 Co Co65 0.76511 0.33345 0.20057

66 Co Co66 0.89012 0.49993 0.20078

67 H H67 0.76991 0.55705 0.30141

68 H H68 0.76330 0.44366 0.10002

69 H H69 0.88819 0.60947 0.10000

70 O O70 0.76668 0.55642 0.25279

71 O O71 0.76397 0.44371 0.14868

72 O O72 0.88843 0.61032 0.14866

73 Co Co73 0.01511 0.66678 0.20057

74 Co Co74 0.14012 0.83327 0.20078

75 H H75 0.01991 0.89039 0.30141

76 H H76 0.14410 0.72281 0.30130

77 H H77 0.01330 0.77699 0.10002

78 H H78 0.13819 0.94280 0.10000

79 O O79 0.01668 0.88975 0.25279

80 O O80 0.14199 0.72292 0.25267

81 O O81 0.01397 0.77704 0.14868

82 O O82 0.13843 0.94365 0.14866

83 Co Co83 0.26511 0.66678 0.20057

84 Co Co84 0.39012 0.83327 0.20078

85 H H85 0.26991 0.89039 0.30141

86 H H86 0.39410 0.72281 0.30130

87 H H87 0.26330 0.77699 0.10002

88 H H88 0.38819 0.94280 0.10000

89	O	O89	0.26668	0.88975	0.25279
90	O	O90	0.39199	0.72292	0.25267
91	O	O91	0.26397	0.77704	0.14868
92	O	O92	0.38843	0.94365	0.14866
93	Co	Co93	0.51511	0.66678	0.20057
94	Co	Co94	0.64012	0.83327	0.20078
95	H	H95	0.51991	0.89039	0.30141
96	H	H96	0.64410	0.72281	0.30130
97	H	H97	0.51330	0.77699	0.10002
98	H	H98	0.63819	0.94280	0.10000
99	O	O99	0.51668	0.88975	0.25279
100	O	O100	0.64199	0.72292	0.25267
101	O	O101	0.51397	0.77704	0.14868
102	O	O102	0.63843	0.94365	0.14866
103	Co	Co103	0.76511	0.66678	0.20057
104	Co	Co104	0.89012	0.83327	0.20078
105	H	H105	0.76991	0.89039	0.30141
106	H	H106	0.89410	0.72281	0.30130
107	H	H107	0.76330	0.77699	0.10002
108	H	H108	0.88819	0.94280	0.10000
109	O	O109	0.76668	0.88975	0.25279
110	O	O110	0.89199	0.72292	0.25267
111	O	O111	0.76397	0.77704	0.14868
112	O	O112	0.88843	0.94365	0.14866
113	O	O113	0.51208	0.33321	0.29089

$Co(OH)_2$-Low Spin-*OOH

		x	*y*	*z*
1	Co Co1	0.01511	0.00011	0.20057
2	Co Co2	0.14012	0.16660	0.20078
3	H H3	0.01991	0.22372	0.30141
4	H H4	0.14410	0.05614	0.30130
5	H H5	0.01330	0.11032	0.10002
6	H H6	0.13819	0.27613	0.10000
7	O O7	0.01668	0.22308	0.25279
8	O O8	0.14199	0.05625	0.25267
9	O O9	0.01397	0.11037	0.14868
10	O O10	0.13843	0.27698	0.14866
11	Co Co11	0.26511	0.00011	0.20057
12	Co Co12	0.39012	0.16660	0.20078
13	H H13	0.26991	0.22372	0.30141
14	H H14	0.39410	0.05614	0.30130
15	H H15	0.26330	0.11032	0.10002
16	H H16	0.38819	0.27613	0.10000
17	O O17	0.26668	0.22308	0.25279
18	O O18	0.39199	0.05625	0.25267
19	O O19	0.26397	0.11037	0.14868
20	O O20	0.38843	0.27698	0.14866
21	Co Co21	0.51511	0.00011	0.20057
22	Co Co22	0.64012	0.16660	0.20078
23	H H23	0.64410	0.05614	0.30130
24	H H24	0.51330	0.11032	0.10002

25 H H25 0.63819 0.27613 0.10000

26 O O26 0.64199 0.05625 0.25267

27 O O27 0.51397 0.11037 0.14868

28 O O28 0.63843 0.27698 0.14866

29 Co Co29 0.76511 0.00011 0.20057

30 Co Co30 0.89012 0.16660 0.20078

31 H H31 0.76991 0.22372 0.30141

32 H H32 0.89410 0.05614 0.30130

33 H H33 0.76330 0.11032 0.10002

34 H H34 0.88819 0.27613 0.10000

35 O O35 0.76668 0.22308 0.25279

36 O O36 0.89199 0.05625 0.25267

37 O O37 0.76397 0.11037 0.14868

38 O O38 0.88843 0.27698 0.14866

39 Co Co39 0.01511 0.33345 0.20057

40 Co Co40 0.14012 0.49993 0.20078

41 H H41 0.01991 0.55705 0.30141

42 H H42 0.14410 0.38947 0.30130

43 H H43 0.01330 0.44366 0.10002

44 H H44 0.13819 0.60947 0.10000

45 O O45 0.01668 0.55642 0.25279

46 O O46 0.14199 0.38958 0.25267

47 O O47 0.01397 0.44371 0.14868

48 O O48 0.13843 0.61032 0.14866

49 Co Co49 0.26511 0.33345 0.20057

50 Co Co50 0.39012 0.49993 0.20078

51	H	H51	0.26991	0.55705	0.30141
52	H	H52	0.26330	0.44366	0.10002
53	H	H53	0.38819	0.60947	0.10000
54	O	O54	0.26668	0.55642	0.25279
55	O	O55	0.26397	0.44371	0.14868
56	O	O56	0.38843	0.61032	0.14866
57	Co	Co57	0.51511	0.33345	0.20057
58	Co	Co58	0.64012	0.49993	0.20078
59	H	H59	0.51991	0.55705	0.30141
60	H	H60	0.51330	0.44366	0.10002
61	H	H61	0.63819	0.60947	0.10000
62	O	O62	0.51668	0.55642	0.25279
63	O	O63	0.51397	0.44371	0.14868
64	O	O64	0.63843	0.61032	0.14866
65	Co	Co65	0.76511	0.33345	0.20057
66	Co	Co66	0.89012	0.49993	0.20078
67	H	H67	0.76991	0.55705	0.30141
68	H	H68	0.76330	0.44366	0.10002
69	H	H69	0.88819	0.60947	0.10000
70	O	O70	0.76668	0.55642	0.25279
71	O	O71	0.76397	0.44371	0.14868
72	O	O72	0.88843	0.61032	0.14866
73	Co	Co73	0.01511	0.66678	0.20057
74	Co	Co74	0.14012	0.83327	0.20078
75	H	H75	0.01991	0.89039	0.30141
76	H	H76	0.14410	0.72281	0.30130

77	H	H77	0.01330	0.77699	0.10002
78	H	H78	0.13819	0.94280	0.10000
79	O	O79	0.01668	0.88975	0.25279
80	O	O80	0.14199	0.72292	0.25267
81	O	O81	0.01397	0.77704	0.14868
82	O	O82	0.13843	0.94365	0.14866
83	Co	Co83	0.26511	0.66678	0.20057
84	Co	Co84	0.39012	0.83327	0.20078
85	H	H85	0.26991	0.89039	0.30141
86	H	H86	0.39410	0.72281	0.30130
87	H	H87	0.26330	0.77699	0.10002
88	H	H88	0.38819	0.94280	0.10000
89	O	O89	0.26668	0.88975	0.25279
90	O	O90	0.39199	0.72292	0.25267
91	O	O91	0.26397	0.77704	0.14868
92	O	O92	0.38843	0.94365	0.14866
93	Co	Co93	0.51511	0.66678	0.20057
94	Co	Co94	0.64012	0.83327	0.20078
95	H	H95	0.51991	0.89039	0.30141
96	H	H96	0.64410	0.72281	0.30130
97	H	H97	0.51330	0.77699	0.10002
98	H	H98	0.63819	0.94280	0.10000
99	O	O99	0.51668	0.88975	0.25279
100	O	O100	0.64199	0.72292	0.25267
101	O	O101	0.51397	0.77704	0.14868
102	O	O102	0.63843	0.94365	0.14866

103	Co	Co103	0.76511	0.66678	0.20057
104	Co	Co104	0.89012	0.83327	0.20078
105	H	H105	0.76991	0.89039	0.30141
106	H	H106	0.89410	0.72281	0.30130
107	H	H107	0.76330	0.77699	0.10002
108	H	H108	0.88819	0.94280	0.10000
109	O	O109	0.76668	0.88975	0.25279
110	O	O110	0.89199	0.72292	0.25267
111	O	O111	0.76397	0.77704	0.14868
112	O	O112	0.88843	0.94365	0.14866
113	O	O113	0.51208	0.33321	0.29089
114	O	O114	0.51522	0.31156	0.36263
115	H	H115	0.51005	0.34471	0.41067

$Co(OH)_2$-Low Spin-*O_2

			x	*y*	*z*
1	Co	Co1	0.01511	0.00011	0.20057
2	Co	Co2	0.14012	0.16660	0.20078
3	H	H3	0.01991	0.22372	0.30141
4	H	H4	0.14410	0.05614	0.30130
5	H	H5	0.01330	0.11032	0.10002
6	H	H6	0.13819	0.27613	0.10000
7	O	O7	0.01668	0.22308	0.25279
8	O	O8	0.14199	0.05625	0.25267
9	O	O9	0.01397	0.11037	0.14868
10	O	O10	0.13843	0.27698	0.14866

11	Co	Co11	0.26511	0.00011	0.20057
12	Co	Co12	0.39012	0.16660	0.20078
13	H	H13	0.26991	0.22372	0.30141
14	H	H14	0.39410	0.05614	0.30130
15	H	H15	0.26330	0.11032	0.10002
16	H	H16	0.38819	0.27613	0.10000
17	O	O17	0.26668	0.22308	0.25279
18	O	O18	0.39199	0.05625	0.25267
19	O	O19	0.26397	0.11037	0.14868
20	O	O20	0.38843	0.27698	0.14866
21	Co	Co21	0.51511	0.00011	0.20057
22	Co	Co22	0.64012	0.16660	0.20078
23	H	H23	0.64410	0.05614	0.30130
24	H	H24	0.51330	0.11032	0.10002
25	H	H25	0.63819	0.27613	0.10000
26	O	O26	0.64199	0.05625	0.25267
27	O	O27	0.51397	0.11037	0.14868
28	O	O28	0.63843	0.27698	0.14866
29	Co	Co29	0.76511	0.00011	0.20057
30	Co	Co30	0.89012	0.16660	0.20078
31	H	H31	0.76991	0.22372	0.30141
32	H	H32	0.89410	0.05614	0.30130
33	H	H33	0.76330	0.11032	0.10002
34	H	H34	0.88819	0.27613	0.10000
35	O	O35	0.76668	0.22308	0.25279
36	O	O36	0.89199	0.05625	0.25267

37	O	O37	0.76397	0.11037	0.14868
38	O	O38	0.88843	0.27698	0.14866
39	Co	Co39	0.01511	0.33345	0.20057
40	Co	Co40	0.14012	0.49993	0.20078
41	H	H41	0.01991	0.55705	0.30141
42	H	H42	0.14410	0.38947	0.30130
43	H	H43	0.01330	0.44366	0.10002
44	H	H44	0.13819	0.60947	0.10000
45	O	O45	0.01668	0.55642	0.25279
46	O	O46	0.14199	0.38958	0.25267
47	O	O47	0.01397	0.44371	0.14868
48	O	O48	0.13843	0.61032	0.14866
49	Co	Co49	0.26511	0.33345	0.20057
50	Co	Co50	0.39012	0.49993	0.20078
51	H	H51	0.26991	0.55705	0.30141
52	H	H52	0.26330	0.44366	0.10002
53	H	H53	0.38819	0.60947	0.10000
54	O	O54	0.26668	0.55642	0.25279
55	O	O55	0.26397	0.44371	0.14868
56	O	O56	0.38843	0.61032	0.14866
57	Co	Co57	0.51511	0.33345	0.20057
58	Co	Co58	0.64012	0.49993	0.20078
59	H	H59	0.51991	0.55705	0.30141
60	H	H60	0.51330	0.44366	0.10002
61	H	H61	0.63819	0.60947	0.10000
62	O	O62	0.51668	0.55642	0.25279

63 O O63 0.51397 0.44371 0.14868

64 O O64 0.63843 0.61032 0.14866

65 Co Co65 0.76511 0.33345 0.20057

66 Co Co66 0.89012 0.49993 0.20078

67 H H67 0.76991 0.55705 0.30141

68 H H68 0.76330 0.44366 0.10002

69 H H69 0.88819 0.60947 0.10000

70 O O70 0.76668 0.55642 0.25279

71 O O71 0.76397 0.44371 0.14868

72 O O72 0.88843 0.61032 0.14866

73 Co Co73 0.01511 0.66678 0.20057

74 Co Co74 0.14012 0.83327 0.20078

75 H H75 0.01991 0.89039 0.30141

76 H H76 0.14410 0.72281 0.30130

77 H H77 0.01330 0.77699 0.10002

78 H H78 0.13819 0.94280 0.10000

79 O O79 0.01668 0.88975 0.25279

80 O O80 0.14199 0.72292 0.25267

81 O O81 0.01397 0.77704 0.14868

82 O O82 0.13843 0.94365 0.14866

83 Co Co83 0.26511 0.66678 0.20057

84 Co Co84 0.39012 0.83327 0.20078

85 H H85 0.26991 0.89039 0.30141

86 H H86 0.39410 0.72281 0.30130

87 H H87 0.26330 0.77699 0.10002

88 H H88 0.38819 0.94280 0.10000

89	O	O89	0.26668	0.88975	0.25279
90	O	O90	0.39199	0.72292	0.25267
91	O	O91	0.26397	0.77704	0.14868
92	O	O92	0.38843	0.94365	0.14866
93	Co	Co93	0.51511	0.66678	0.20057
94	Co	Co94	0.64012	0.83327	0.20078
95	H	H95	0.51991	0.89039	0.30141
96	H	H96	0.64410	0.72281	0.30130
97	H	H97	0.51330	0.77699	0.10002
98	H	H98	0.63819	0.94280	0.10000
99	O	O99	0.51668	0.88975	0.25279
100	O	O100	0.64199	0.72292	0.25267
101	O	O101	0.51397	0.77704	0.14868
102	O	O102	0.63843	0.94365	0.14866
103	Co	Co103	0.76511	0.66678	0.20057
104	Co	Co104	0.89012	0.83327	0.20078
105	H	H105	0.76991	0.89039	0.30141
106	H	H106	0.89410	0.72281	0.30130
107	H	H107	0.76330	0.77699	0.10002
108	H	H108	0.88819	0.94280	0.10000
109	O	O109	0.76668	0.88975	0.25279
110	O	O110	0.89199	0.72292	0.25267
111	O	O111	0.76397	0.77704	0.14868
112	O	O112	0.88843	0.94365	0.14866
113	O	O113	0.51208	0.33321	0.29089
114	O	O114	0.51522	0.31156	0.36263

$Co(OH)_2$-Low Spin-*+O_2

		x	*y*	*z*
1	Co	Co1	0.01511	0.00011	0.20057
2	Co	Co2	0.14012	0.16660	0.20078
3	H	H3	0.01991	0.22372	0.30141
4	H	H4	0.14410	0.05614	0.30130
5	H	H5	0.01330	0.11032	0.10002
6	H	H6	0.13819	0.27613	0.10000
7	O	O7	0.01668	0.22308	0.25279
8	O	O8	0.14199	0.05625	0.25267
9	O	O9	0.01397	0.11037	0.14868
10	O	O10	0.13843	0.27698	0.14866
11	Co	Co11	0.26511	0.00011	0.20057
12	Co	Co12	0.39012	0.16660	0.20078
13	H	H13	0.26991	0.22372	0.30141
14	H	H14	0.39410	0.05614	0.30130
15	H	H15	0.26330	0.11032	0.10002
16	H	H16	0.38819	0.27613	0.10000
17	O	O17	0.26668	0.22308	0.25279
18	O	O18	0.39199	0.05625	0.25267
19	O	O19	0.26397	0.11037	0.14868
20	O	O20	0.38843	0.27698	0.14866
21	Co	Co21	0.51511	0.00011	0.20057
22	Co	Co22	0.64012	0.16660	0.20078
23	H	H23	0.64410	0.05614	0.30130

24	H	H24	0.51330	0.11032	0.10002
25	H	H25	0.63819	0.27613	0.10000
26	O	O26	0.64199	0.05625	0.25267
27	O	O27	0.51397	0.11037	0.14868
28	O	O28	0.63843	0.27698	0.14866
29	Co	Co29	0.76511	0.00011	0.20057
30	Co	Co30	0.89012	0.16660	0.20078
31	H	H31	0.76991	0.22372	0.30141
32	H	H32	0.89410	0.05614	0.30130
33	H	H33	0.76330	0.11032	0.10002
34	H	H34	0.88819	0.27613	0.10000
35	O	O35	0.76668	0.22308	0.25279
36	O	O36	0.89199	0.05625	0.25267
37	O	O37	0.76397	0.11037	0.14868
38	O	O38	0.88843	0.27698	0.14866
39	Co	Co39	0.01511	0.33345	0.20057
40	Co	Co40	0.14012	0.49993	0.20078
41	H	H41	0.01991	0.55705	0.30141
42	H	H42	0.14410	0.38947	0.30130
43	H	H43	0.01330	0.44366	0.10002
44	H	H44	0.13819	0.60947	0.10000
45	O	O45	0.01668	0.55642	0.25279
46	O	O46	0.14199	0.38958	0.25267
47	O	O47	0.01397	0.44371	0.14868
48	O	O48	0.13843	0.61032	0.14866
49	Co	Co49	0.26511	0.33345	0.20057

50 Co Co50 0.39012 0.49993 0.20078

51 H H51 0.26991 0.55705 0.30141

52 H H52 0.26330 0.44366 0.10002

53 H H53 0.38819 0.60947 0.10000

54 O O54 0.26668 0.55642 0.25279

55 O O55 0.26397 0.44371 0.14868

56 O O56 0.38843 0.61032 0.14866

57 Co Co57 0.51511 0.33345 0.20057

58 Co Co58 0.64012 0.49993 0.20078

59 H H59 0.51991 0.55705 0.30141

60 H H60 0.51330 0.44366 0.10002

61 H H61 0.63819 0.60947 0.10000

62 O O62 0.51668 0.55642 0.25279

63 O O63 0.51397 0.44371 0.14868

64 O O64 0.63843 0.61032 0.14866

65 Co Co65 0.76511 0.33345 0.20057

66 Co Co66 0.89012 0.49993 0.20078

67 H H67 0.76991 0.55705 0.30141

68 H H68 0.76330 0.44366 0.10002

69 H H69 0.88819 0.60947 0.10000

70 O O70 0.76668 0.55642 0.25279

71 O O71 0.76397 0.44371 0.14868

72 O O72 0.88843 0.61032 0.14866

73 Co Co73 0.01511 0.66678 0.20057

74 Co Co74 0.14012 0.83327 0.20078

75 H H75 0.01991 0.89039 0.30141

76	H	H76	0.14410	0.72281	0.30130
77	H	H77	0.01330	0.77699	0.10002
78	H	H78	0.13819	0.94280	0.10000
79	O	O79	0.01668	0.88975	0.25279
80	O	O80	0.14199	0.72292	0.25267
81	O	O81	0.01397	0.77704	0.14868
82	O	O82	0.13843	0.94365	0.14866
83	Co	Co83	0.26511	0.66678	0.20057
84	Co	Co84	0.39012	0.83327	0.20078
85	H	H85	0.26991	0.89039	0.30141
86	H	H86	0.39410	0.72281	0.30130
87	H	H87	0.26330	0.77699	0.10002
88	H	H88	0.38819	0.94280	0.10000
89	O	O89	0.26668	0.88975	0.25279
90	O	O90	0.39199	0.72292	0.25267
91	O	O91	0.26397	0.77704	0.14868
92	O	O92	0.38843	0.94365	0.14866
93	Co	Co93	0.51511	0.66678	0.20057
94	Co	Co94	0.64012	0.83327	0.20078
95	H	H95	0.51991	0.89039	0.30141
96	H	H96	0.64410	0.72281	0.30130
97	H	H97	0.51330	0.77699	0.10002
98	H	H98	0.63819	0.94280	0.10000
99	O	O99	0.51668	0.88975	0.25279
100	O	O100	0.64199	0.72292	0.25267
101	O	O101	0.51397	0.77704	0.14868

102	O	O102	0.63843	0.94365	0.14866
103	Co	Co103	0.76511	0.66678	0.20057
104	Co	Co104	0.89012	0.83327	0.20078
105	H	H105	0.76991	0.89039	0.30141
106	H	H106	0.89410	0.72281	0.30130
107	H	H107	0.76330	0.77699	0.10002
108	H	H108	0.88819	0.94280	0.10000
109	O	O109	0.76668	0.88975	0.25279
110	O	O110	0.89199	0.72292	0.25267
111	O	O111	0.76397	0.77704	0.14868
112	O	O112	0.88843	0.94365	0.14866
113	O	O113	0.51168	0.33381	0.32089
114	O	O114	0.51482	0.31217	0.39263

$Co(OH)_2$-Low Spin-*H_2O_2

			x	*y*	*z*
1	Co	Co1	0.01511	0.00011	0.20057
2	Co	Co2	0.14012	0.16660	0.20078
3	H	H3	0.01991	0.22372	0.30141
4	H	H4	0.14410	0.05614	0.30130
5	H	H5	0.01330	0.11032	0.10002
6	H	H6	0.13819	0.27613	0.10000
7	O	O7	0.01668	0.22308	0.25279
8	O	O8	0.14199	0.05625	0.25267
9	O	O9	0.01397	0.11037	0.14868
10	O	O10	0.13843	0.27698	0.14866

11	Co	Co11	0.26511	0.00011	0.20057
12	Co	Co12	0.39012	0.16660	0.20078
13	H	H13	0.26991	0.22372	0.30141
14	H	H14	0.39410	0.05614	0.30130
15	H	H15	0.26330	0.11032	0.10002
16	H	H16	0.38819	0.27613	0.10000
17	O	O17	0.26668	0.22308	0.25279
18	O	O18	0.39199	0.05625	0.25267
19	O	O19	0.26397	0.11037	0.14868
20	O	O20	0.38843	0.27698	0.14866
21	Co	Co21	0.51511	0.00011	0.20057
22	Co	Co22	0.64012	0.16660	0.20078
23	H	H23	0.64410	0.05614	0.30130
24	H	H24	0.51330	0.11032	0.10002
25	H	H25	0.63819	0.27613	0.10000
26	O	O26	0.64199	0.05625	0.25267
27	O	O27	0.51397	0.11037	0.14868
28	O	O28	0.63843	0.27698	0.14866
29	Co	Co29	0.76511	0.00011	0.20057
30	Co	Co30	0.89012	0.16660	0.20078
31	H	H31	0.76991	0.22372	0.30141
32	H	H32	0.89410	0.05614	0.30130
33	H	H33	0.76330	0.11032	0.10002
34	H	H34	0.88819	0.27613	0.10000
35	O	O35	0.76668	0.22308	0.25279
36	O	O36	0.89199	0.05625	0.25267

37	O	O37	0.76397	0.11037	0.14868
38	O	O38	0.88843	0.27698	0.14866
39	Co	Co39	0.01511	0.33345	0.20057
40	Co	Co40	0.14012	0.49993	0.20078
41	H	H41	0.01991	0.55705	0.30141
42	H	H42	0.14410	0.38947	0.30130
43	H	H43	0.01330	0.44366	0.10002
44	H	H44	0.13819	0.60947	0.10000
45	O	O45	0.01668	0.55642	0.25279
46	O	O46	0.14199	0.38958	0.25267
47	O	O47	0.01397	0.44371	0.14868
48	O	O48	0.13843	0.61032	0.14866
49	Co	Co49	0.26511	0.33345	0.20057
50	Co	Co50	0.39012	0.49993	0.20078
51	H	H51	0.26991	0.55705	0.30141
52	H	H52	0.26330	0.44366	0.10002
53	H	H53	0.38819	0.60947	0.10000
54	O	O54	0.26668	0.55642	0.25279
55	O	O55	0.26397	0.44371	0.14868
56	O	O56	0.38843	0.61032	0.14866
57	Co	Co57	0.51511	0.33345	0.20057
58	Co	Co58	0.64012	0.49993	0.20078
59	H	H59	0.51991	0.55705	0.30141
60	H	H60	0.51330	0.44366	0.10002
61	H	H61	0.63819	0.60947	0.10000
62	O	O62	0.51668	0.55642	0.25279

63 O O63 0.51397 0.44371 0.14868

64 O O64 0.63843 0.61032 0.14866

65 Co Co65 0.76511 0.33345 0.20057

66 Co Co66 0.89012 0.49993 0.20078

67 H H67 0.76991 0.55705 0.30141

68 H H68 0.76330 0.44366 0.10002

69 H H69 0.88819 0.60947 0.10000

70 O O70 0.76668 0.55642 0.25279

71 O O71 0.76397 0.44371 0.14868

72 O O72 0.88843 0.61032 0.14866

73 Co Co73 0.01511 0.66678 0.20057

74 Co Co74 0.14012 0.83327 0.20078

75 H H75 0.01991 0.89039 0.30141

76 H H76 0.14410 0.72281 0.30130

77 H H77 0.01330 0.77699 0.10002

78 H H78 0.13819 0.94280 0.10000

79 O O79 0.01668 0.88975 0.25279

80 O O80 0.14199 0.72292 0.25267

81 O O81 0.01397 0.77704 0.14868

82 O O82 0.13843 0.94365 0.14866

83 Co Co83 0.26511 0.66678 0.20057

84 Co Co84 0.39012 0.83327 0.20078

85 H H85 0.26991 0.89039 0.30141

86 H H86 0.39410 0.72281 0.30130

87 H H87 0.26330 0.77699 0.10002

88 H H88 0.38819 0.94280 0.10000

89	O	O89	0.26668	0.88975	0.25279
90	O	O90	0.39199	0.72292	0.25267
91	O	O91	0.26397	0.77704	0.14868
92	O	O92	0.38843	0.94365	0.14866
93	Co	Co93	0.51511	0.66678	0.20057
94	Co	Co94	0.64012	0.83327	0.20078
95	H	H95	0.51991	0.89039	0.30141
96	H	H96	0.64410	0.72281	0.30130
97	H	H97	0.51330	0.77699	0.10002
98	H	H98	0.63819	0.94280	0.10000
99	O	O99	0.51668	0.88975	0.25279
100	O	O100	0.64199	0.72292	0.25267
101	O	O101	0.51397	0.77704	0.14868
102	O	O102	0.63843	0.94365	0.14866
103	Co	Co103	0.76511	0.66678	0.20057
104	Co	Co104	0.89012	0.83327	0.20078
105	H	H105	0.76991	0.89039	0.30141
106	H	H106	0.89410	0.72281	0.30130
107	H	H107	0.76330	0.77699	0.10002
108	H	H108	0.88819	0.94280	0.10000
109	O	O109	0.76668	0.88975	0.25279
110	O	O110	0.89199	0.72292	0.25267
111	O	O111	0.76397	0.77704	0.14868
112	O	O112	0.88843	0.94365	0.14866
113	O	O113	0.50718	0.26796	0.33697
114	O	O114	0.51035	0.33784	0.29137

115	H	H115	0.48045	0.39179	0.31778
116	H	H116	0.53707	0.21400	0.31056

$Co(OH)_2$-Low Spin-*+H_2O_2

			x	*y*	*z*
1	Co	Co1	0.01511	0.00011	0.20057
2	Co	Co2	0.14012	0.16660	0.20078
3	H	H3	0.01991	0.22372	0.30141
4	H	H4	0.14410	0.05614	0.30130
5	H	H5	0.01330	0.11032	0.10002
6	H	H6	0.13819	0.27613	0.10000
7	O	O7	0.01668	0.22308	0.25279
8	O	O8	0.14199	0.05625	0.25267
9	O	O9	0.01397	0.11037	0.14868
10	O	O10	0.13843	0.27698	0.14866
11	Co	Co11	0.26511	0.00011	0.20057
12	Co	Co12	0.39012	0.16660	0.20078
13	H	H13	0.26991	0.22372	0.30141
14	H	H14	0.39410	0.05614	0.30130
15	H	H15	0.26330	0.11032	0.10002
16	H	H16	0.38819	0.27613	0.10000
17	O	O17	0.26668	0.22308	0.25279
18	O	O18	0.39199	0.05625	0.25267
19	O	O19	0.26397	0.11037	0.14868
20	O	O20	0.38843	0.27698	0.14866
21	Co	Co21	0.51511	0.00011	0.20057

22	Co	Co22	0.64012	0.16660	0.20078
23	H	H23	0.64410	0.05614	0.30130
24	H	H24	0.51330	0.11032	0.10002
25	H	H25	0.63819	0.27613	0.10000
26	O	O26	0.64199	0.05625	0.25267
27	O	O27	0.51397	0.11037	0.14868
28	O	O28	0.63843	0.27698	0.14866
29	Co	Co29	0.76511	0.00011	0.20057
30	Co	Co30	0.89012	0.16660	0.20078
31	H	H31	0.76991	0.22372	0.30141
32	H	H32	0.89410	0.05614	0.30130
33	H	H33	0.76330	0.11032	0.10002
34	H	H34	0.88819	0.27613	0.10000
35	O	O35	0.76668	0.22308	0.25279
36	O	O36	0.89199	0.05625	0.25267
37	O	O37	0.76397	0.11037	0.14868
38	O	O38	0.88843	0.27698	0.14866
39	Co	Co39	0.01511	0.33345	0.20057
40	Co	Co40	0.14012	0.49993	0.20078
41	H	H41	0.01991	0.55705	0.30141
42	H	H42	0.14410	0.38947	0.30130
43	H	H43	0.01330	0.44366	0.10002
44	H	H44	0.13819	0.60947	0.10000
45	O	O45	0.01668	0.55642	0.25279
46	O	O46	0.14199	0.38958	0.25267
47	O	O47	0.01397	0.44371	0.14868

48 O O48 0.13843 0.61032 0.14866

49 Co Co49 0.26511 0.33345 0.20057

50 Co Co50 0.39012 0.49993 0.20078

51 H H51 0.26991 0.55705 0.30141

52 H H52 0.26330 0.44366 0.10002

53 H H53 0.38819 0.60947 0.10000

54 O O54 0.26668 0.55642 0.25279

55 O O55 0.26397 0.44371 0.14868

56 O O56 0.38843 0.61032 0.14866

57 Co Co57 0.51511 0.33345 0.20057

58 Co Co58 0.64012 0.49993 0.20078

59 H H59 0.51991 0.55705 0.30141

60 H H60 0.51330 0.44366 0.10002

61 H H61 0.63819 0.60947 0.10000

62 O O62 0.51668 0.55642 0.25279

63 O O63 0.51397 0.44371 0.14868

64 O O64 0.63843 0.61032 0.14866

65 Co Co65 0.76511 0.33345 0.20057

66 Co Co66 0.89012 0.49993 0.20078

67 H H67 0.76991 0.55705 0.30141

68 H H68 0.76330 0.44366 0.10002

69 H H69 0.88819 0.60947 0.10000

70 O O70 0.76668 0.55642 0.25279

71 O O71 0.76397 0.44371 0.14868

72 O O72 0.88843 0.61032 0.14866

73 Co Co73 0.01511 0.66678 0.20057

74 Co Co74 0.14012 0.83327 0.20078

75 H H75 0.01991 0.89039 0.30141

76 H H76 0.14410 0.72281 0.30130

77 H H77 0.01330 0.77699 0.10002

78 H H78 0.13819 0.94280 0.10000

79 O O79 0.01668 0.88975 0.25279

80 O O80 0.14199 0.72292 0.25267

81 O O81 0.01397 0.77704 0.14868

82 O O82 0.13843 0.94365 0.14866

83 Co Co83 0.26511 0.66678 0.20057

84 Co Co84 0.39012 0.83327 0.20078

85 H H85 0.26991 0.89039 0.30141

86 H H86 0.39410 0.72281 0.30130

87 H H87 0.26330 0.77699 0.10002

88 H H88 0.38819 0.94280 0.10000

89 O O89 0.26668 0.88975 0.25279

90 O O90 0.39199 0.72292 0.25267

91 O O91 0.26397 0.77704 0.14868

92 O O92 0.38843 0.94365 0.14866

93 Co Co93 0.51511 0.66678 0.20057

94 Co Co94 0.64012 0.83327 0.20078

95 H H95 0.51991 0.89039 0.30141

96 H H96 0.64410 0.72281 0.30130

97 H H97 0.51330 0.77699 0.10002

98 H H98 0.63819 0.94280 0.10000

99 O O99 0.51668 0.88975 0.25279

100 O O100 0.64199 0.72292 0.25267

101 O O101 0.51397 0.77704 0.14868

102 O O102 0.63843 0.94365 0.14866

103 Co Co103 0.76511 0.66678 0.20057

104 Co Co104 0.89012 0.83327 0.20078

105 H H105 0.76991 0.89039 0.30141

106 H H106 0.89410 0.72281 0.30130

107 H H107 0.76330 0.77699 0.10002

108 H H108 0.88819 0.94280 0.10000

109 O O109 0.76668 0.88975 0.25279

110 O O110 0.89199 0.72292 0.25267

111 O O111 0.76397 0.77704 0.14868

112 O O112 0.88843 0.94365 0.14866

113 O O113 0.53569 0.27966 0.35709

114 O O114 0.53886 0.34954 0.31149

115 H H115 0.50896 0.40350 0.33789

116 H H116 0.56558 0.22571 0.33068