

SUPPORTING INFORMATION

Hierarchical structures and magnetism of Co clusters: A perspective from integration of deep learning and hybrid differential evolution algorithm

Wei-Hua Yang ^a, Fang-Qi Yu ^a, Zi-Wen Guo ^b, Rao Huang ^{a,*}, Jun-Ren Chen ^c, Feng-Qiang Gao ^c, Gui-Fang Shao ^d, Tun-Dong Liu ^d, and Yu-Hua Wen ^{a,*}

^a *Department of Physics, Xiamen University, Xiamen 361005, China*

^b *Institute of Artificial Intelligence, Xiamen University, Xiamen 361005, China*

^c *Xiamen University Tan Kah Kee College, Zhangzhou, 363105, China*

^d *Pen-Tung Sah Institute of Micro-Nano Science and Technology, Xiamen University, Xiamen 361102, China*

*Correspondence should be addressed to Y. H. W. (yhwen@xmu.edu.cn), and R. H. (huangrao@xmu.edu.cn).

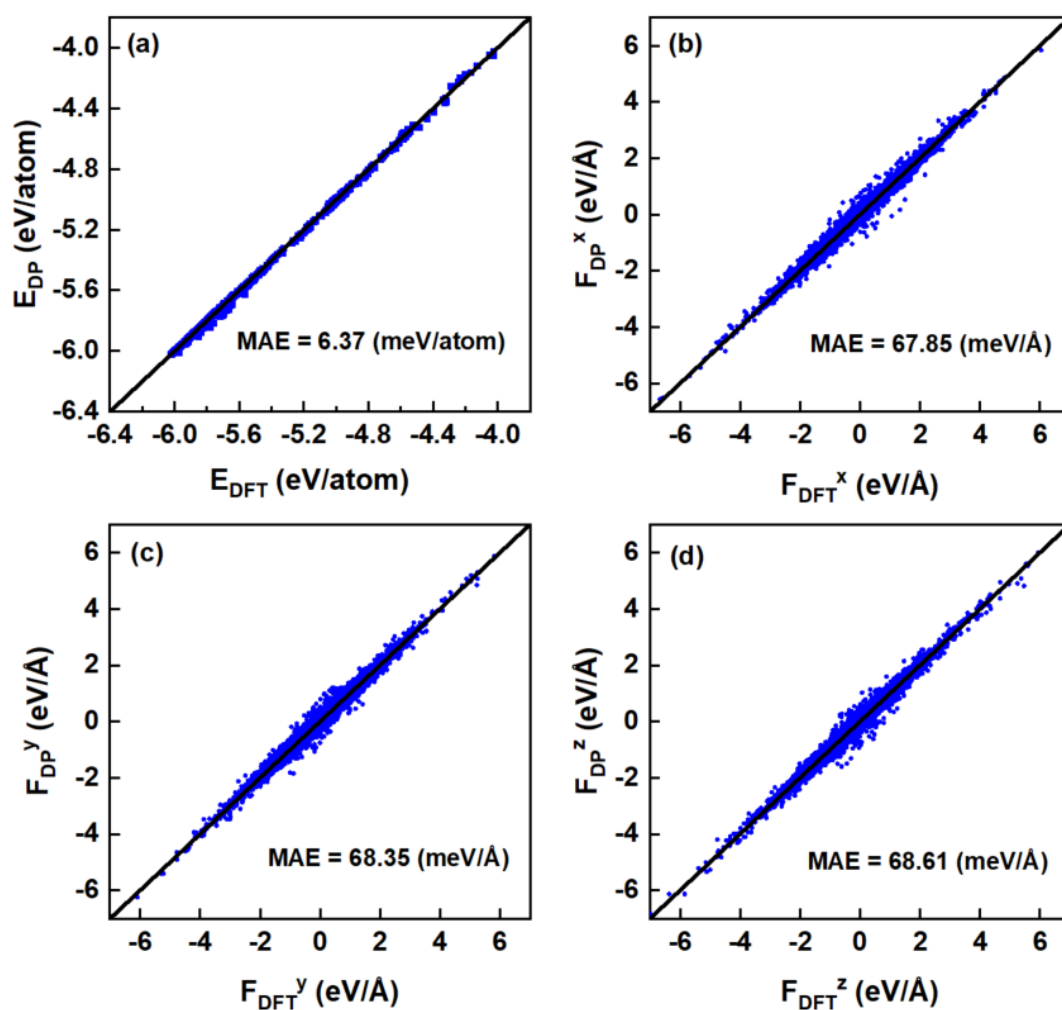


Fig. S1 Comparison of the results from the DP model and DFT calculations: (a) total energy of cluster, and forces on atom along the (b) x , (c) y , and (d) z directions.

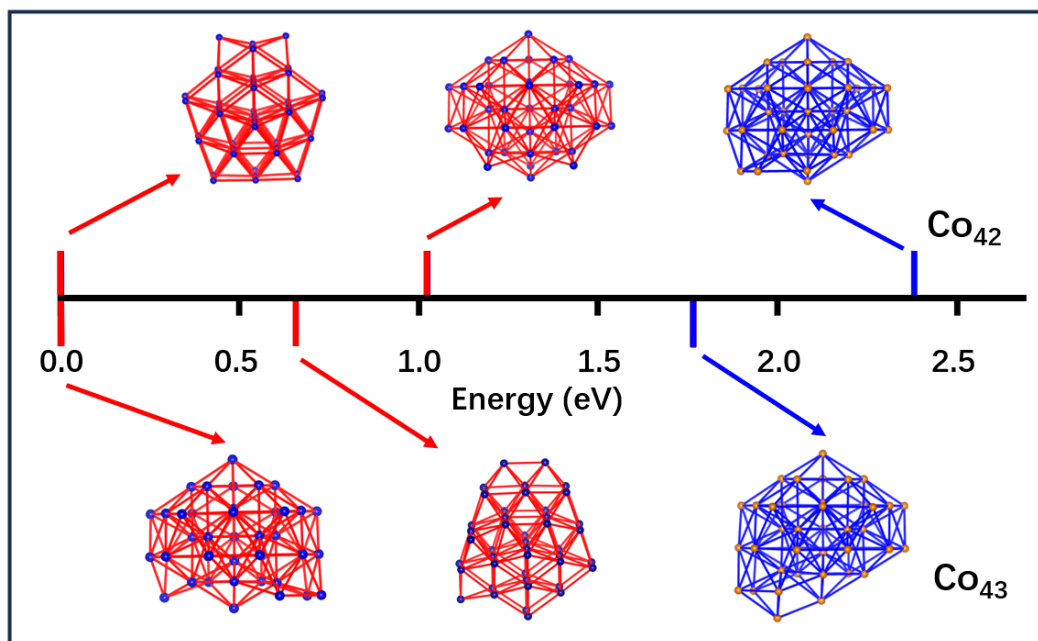


Fig. S2 Structures and relative energy distribution of Co_{42} and Co_{43} obtained by DP model. Colors indicate prediction comparisons: blue bonds represent structures already recorded in the CCD, while red bonds denote those newly identified using our DP model.

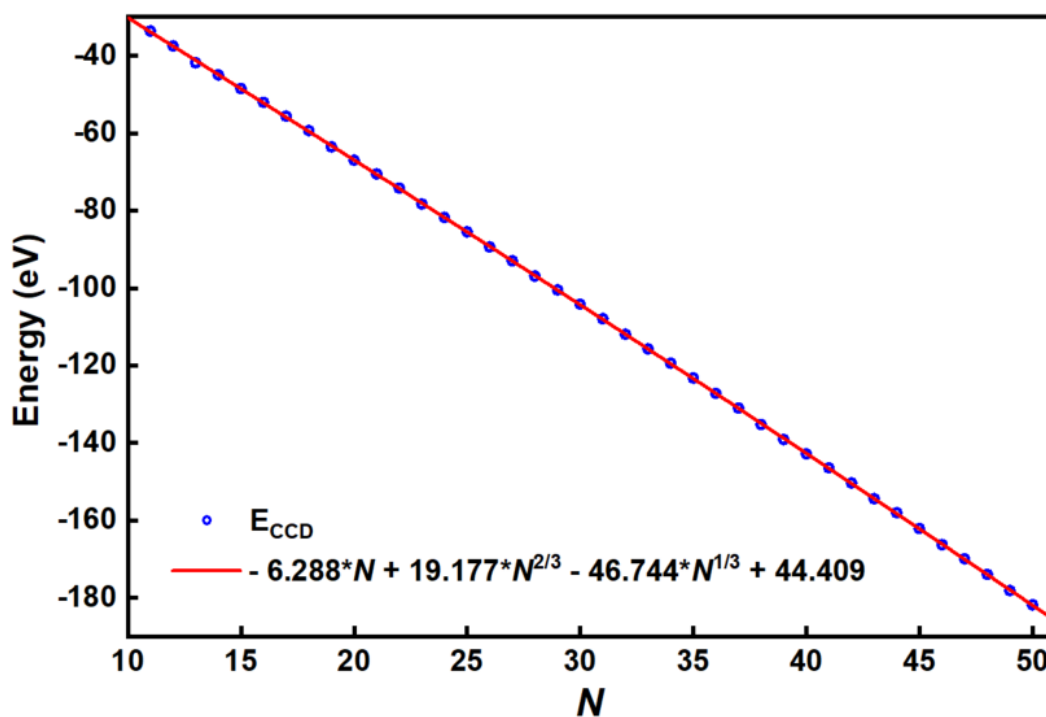


Fig. S3 The fitting curve of Gupta potential energy for Co_N ($N = 11-50$) in CCD.

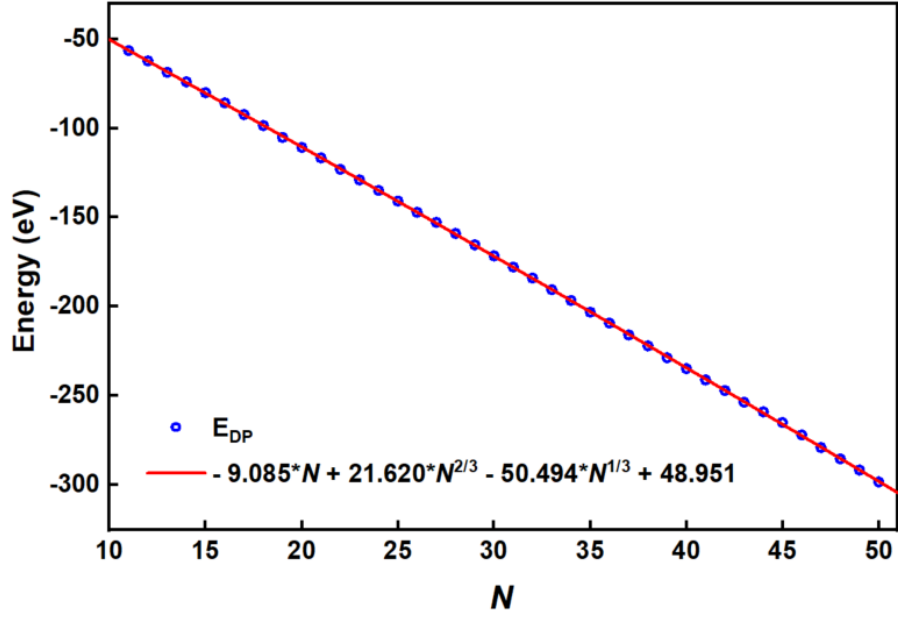


Fig. S4 The fitting curve of DP energy for Co_N ($N = 11\text{--}50$) in our work.

Table S1 Spin gaps (δ_1 , δ_2) of the lowest-energy Co_N ($N = 11\text{--}50$) clusters

	δ_1	δ_2	N	δ_1	δ_2	N	δ_1	δ_2	N	δ_1	δ_2
11	0.300	0.145	21	0.151	0.448	31	0.220	0.101	41	0.339	0.188
12	0.362	0.159	22	0.301	0.438	32	0.207	0.170	42	0.076	0.324
13	0.265	0.615	23	0.413	0.427	33	0.193	0.207	43	0.258	0.333
14	0.131	0.149	24	0.377	0.355	34	0.104	0.074	44	0.080	0.046
15	0.384	0.118	25	0.450	0.111	35	0.126	0.095	45	0.036	0.129
16	0.069	0.687	26	0.388	0.162	36	0.081	0.048	46	0.344	0.037
17	0.251	0.178	27	0.327	0.169	37	0.051	0.326	47	0.218	0.177
18	0.332	0.056	28	0.731	0.068	38	0.037	0.317	48	0.359	0.100
19	0.279	0.816	29	0.282	0.186	39	0.359	0.347	49	0.429	0.066
20	0.262	0.832	30	0.249	0.157	40	0.348	0.304	50	0.160	0.086

Table S2 Coordinates of the the lowest-energy Co_N ($N = 11-50$) clusters

Coordinates for Co_{11}			Coordinates for Co_{12}		
X	Y	Z	X	Y	Z
8.087924	6.467290	5.689802	8.271992	7.174581	7.252826
7.241415	8.803744	5.671938	6.478629	6.410141	8.616311
8.862679	7.339734	9.526357	7.997046	4.878896	7.801463
8.590343	8.005454	7.334650	7.071352	7.993193	10.247223
7.027134	4.890864	6.937045	6.066899	7.144552	6.361414
7.721095	10.134991	7.515176	8.380602	9.481716	6.696376
5.628069	9.389213	7.203298	6.264268	9.426329	5.845909
7.068237	6.063465	8.928614	8.795654	8.745004	8.956176
8.985427	5.770985	7.753699	7.794342	7.930744	5.052466
6.925975	8.459266	8.901014	7.598804	5.591776	5.613916
6.361699	7.174993	7.038410	8.607448	6.481051	9.499656
			6.672964	8.742019	8.056268

Coordinates for Co_{13}			Coordinates for Co_{14}		
X	Y	Z	X	Y	Z
8.396292	7.376436	7.295969	10.861840	10.049307	9.672716
6.008394	5.077733	6.982282	8.517179	7.735269	9.175551
6.602929	6.611996	8.659454	8.822189	9.301350	10.819402
8.121346	5.080751	7.844606	10.510499	7.785419	10.316188
7.195652	8.195048	10.290366	9.716857	10.495850	12.558064
6.191199	7.346407	6.404557	8.742689	10.041379	8.582975
8.504902	9.683571	6.739519	11.046910	12.347520	9.126762
6.388568	9.628184	5.889052	8.985237	12.306757	8.166100
8.919954	8.946859	8.999319	11.341628	11.641817	11.389373
7.918642	8.132599	5.095609	10.579133	10.807234	7.453288
7.723104	5.793631	5.657059	10.335440	8.451779	8.024966
8.731748	6.682906	9.542799	11.532137	9.329493	11.829890
6.797264	8.943874	8.099411	9.251933	11.614129	10.381416
			9.756329	8.092694	12.503308

Coordinates for Co_{15}			Coordinates for Co_{16}		
X	Y	Z	X	Y	Z
10.997013	10.201316	9.445552	13.056553	10.946611	10.090562
8.722201	7.730611	9.368689	9.088220	7.416613	9.456260
9.097287	9.511468	10.867211	7.873736	8.923789	10.799664
10.806657	7.955735	10.317043	12.304122	8.860240	9.520575
9.657746	11.268573	12.335602	8.755180	11.028239	11.385989
8.845664	9.959814	8.487333	8.280026	9.359769	8.518923
11.078272	12.400342	8.647347	10.524530	11.248873	12.900340
8.990725	12.156529	7.746648	11.342901	10.719329	8.514403

11.415863	11.951027	10.997238	10.947654	11.667523	10.674592
10.615630	10.650763	7.180161	9.578548	10.538222	6.991483
10.472859	8.384854	8.006669	10.443272	8.617049	7.948257
11.273459	9.721044	11.797420	11.857089	9.795594	11.695499
9.327035	11.780223	10.013916	9.141284	11.453376	9.069824
9.126340	7.318812	11.685942	10.111991	9.407018	10.164710
9.573248	9.008889	13.103229	9.657084	9.176231	12.457985
			7.037809	10.841524	9.810932

Coordinates for Co ₁₇			Coordinates for Co ₁₈		
X	Y	Z	X	Y	Z
12.962361	11.215213	9.940094	13.134234	10.502769	9.623523
9.282601	7.480296	9.555830	9.630100	7.642248	9.796604
7.891033	8.962373	10.790534	7.860916	8.921562	10.754309
12.232333	9.063724	9.462010	11.428783	11.766101	10.616652
8.651433	11.156140	11.330120	8.154686	11.269725	11.162544
8.216003	9.395247	8.481163	7.669335	8.086444	8.598971
10.425785	11.427079	12.835148	10.100739	10.860218	12.370394
11.217449	10.941815	8.401464	11.201192	10.909075	8.372885
10.825181	11.879478	10.585459	9.629911	9.146876	7.918665
9.447079	10.607146	6.904590	9.224119	11.325572	7.196644
10.423558	8.750845	7.900103	9.895611	9.989477	10.164622
11.820620	10.018766	11.593809	11.923960	9.542138	11.379187
8.960054	11.556852	8.974891	9.414274	12.190013	9.366313
10.020560	9.671034	10.042089	11.703886	8.710450	9.205913
9.699808	9.275252	12.352442	9.881156	8.496444	12.008205
6.910504	10.819012	9.799644	7.899745	10.388952	8.881491
11.013639	7.779728	11.050610	11.583365	7.262816	11.028279
			9.663987	12.989120	11.554798

Coordinates for Co ₁₉			Coordinates for Co ₂₀		
X	Y	Z	X	Y	Z
10.000000	10.000000	10.000000	10.129069	10.055949	10.133132
10.804826	9.546436	7.780302	9.001562	6.993103	9.712190
9.195174	10.453564	12.219698	7.922622	9.037625	9.824837
9.361872	11.428707	8.174592	11.918634	9.612829	8.585863
9.181003	8.089837	8.791262	9.111995	12.236183	10.204381
12.976761	9.586823	8.635996	7.661576	8.986339	7.587967
11.414356	10.467324	12.945087	10.496685	11.493260	12.011863
7.738049	9.972108	9.185553	10.904569	11.789328	8.654304
10.638128	8.571293	11.825408	11.232087	13.137449	10.520375
12.261951	10.027892	10.814447	10.486094	10.324814	6.872804
8.376177	8.543401	11.010961	9.785734	8.573186	8.213763
8.585644	9.532676	7.054913	12.281615	11.048311	10.468395

8.557046	11.882271	10.394291	8.727611	10.844249	8.285177
11.442954	8.117729	9.605709	11.144122	7.874605	10.067231
7.023239	10.413177	11.364004	9.358586	8.319705	11.611223
10.818997	11.910163	11.208738	7.050209	11.181315	9.843889
9.824440	6.759133	10.598569	8.340524	10.504784	11.679933
11.623823	11.456599	8.989039	11.510405	9.317499	11.943446
10.175560	13.240867	9.401431	9.730674	9.767854	13.392047
			13.205628	8.901613	10.387179

Coordinates for Co ₂₁			Coordinates for Co ₂₂		
X	Y	Z	X	Y	Z
10.308590	10.158392	9.404421	10.174830	10.163111	9.469897
11.021023	9.469387	7.268536	10.865566	9.365063	7.377679
9.539910	10.864201	11.657172	9.436523	10.918708	11.707322
9.618292	11.380334	7.500138	9.541737	11.358614	7.555435
9.451062	8.141465	8.445641	9.211016	8.163079	8.578772
12.566807	10.239195	10.149740	12.435078	10.154799	10.254682
11.831692	10.918569	12.282118	11.725480	10.935600	12.347177
8.021259	10.051418	8.685508	7.890912	10.151353	8.755999
11.002465	8.892244	11.396339	10.760073	8.922612	11.529914
9.392275	7.643360	12.524924	9.112498	7.770073	12.695604
8.653067	8.785653	10.644886	8.480160	8.920890	10.777683
8.792508	9.381268	6.606586	8.609465	9.373185	6.686758
8.882882	12.070855	9.669006	8.843538	12.139209	9.684061
11.720656	8.256021	9.183903	13.089662	9.376546	8.164793
7.313053	10.743254	10.827843	7.215707	10.932466	10.860074
11.164510	12.157375	10.401454	11.114283	12.140884	10.433235
10.141230	6.956533	10.352543	9.834642	6.986896	10.507439
11.877971	11.477867	8.246698	11.820684	11.360377	8.307523
10.467974	13.308155	8.519044	10.487648	13.295836	8.513094
8.006995	9.507557	12.757175	7.830541	9.702132	12.868601
10.225780	9.596897	13.476328	10.037830	9.703938	13.596578
			11.482125	8.164633	9.327682

Coordinates for Co ₂₃			Coordinates for Co ₂₄		
X	Y	Z	X	Y	Z
11.220225	10.362333	8.041617	9.641844	8.574284	7.513188
9.529786	9.797041	6.525712	13.047872	10.542763	8.593996
9.551039	10.276703	9.803391	10.140731	10.845915	7.045573
12.852995	8.234671	11.203114	11.321326	12.151216	8.621781
9.853817	8.359805	8.343531	11.892137	9.274261	7.057818
11.958690	10.235115	10.378074	10.854705	9.872129	9.060339
12.555851	10.069831	12.611964	9.037758	11.542782	9.046250
7.875049	9.711055	8.218852	7.927558	10.201409	7.487485

11.253814	8.161642	12.899654	6.874680	10.842834	9.587303
7.927634	10.170500	11.552007	11.472857	7.635825	8.694096
8.206358	8.306203	10.126558	12.063119	11.199273	10.668138
6.331640	9.647695	9.958742	8.492479	9.123691	9.511791
9.223255	11.686906	7.920960	8.825160	11.142698	13.174477
12.152314	8.368071	8.916769	8.077548	12.102829	11.160304
7.588343	11.595561	9.668273	12.656876	8.932875	10.274542
9.282444	12.156030	11.252656	10.289490	12.779823	10.679635
10.569901	8.199787	10.684933	9.805226	10.511483	11.153379
10.899152	12.252602	9.531573	9.286837	6.925888	9.169609
8.944116	13.476386	9.381504	7.596452	9.820361	11.592438
8.907421	8.202068	12.362007	8.233958	7.567313	11.269428
10.274559	10.137352	12.153627	9.409674	8.892739	12.808826
11.566106	12.098480	11.774559	10.443373	8.155604	10.785715
11.475493	8.494161	6.689923	10.983301	11.800523	12.711494
			11.625040	9.561481	12.332395

Coordinates for CO ₂₅			Coordinates for CO ₂₆		
X	Y	Z	X	Y	Z
9.515742	8.644710	7.559650	9.161679	8.973104	7.569630
12.899554	10.710956	8.674455	13.080740	10.042231	8.101947
9.968570	10.943496	7.105994	10.085669	11.126202	7.145701
11.117331	12.273311	8.707682	11.811755	11.991938	8.526087
11.768338	9.401596	7.109516	11.405526	9.202011	6.762245
10.719925	9.962404	9.119677	10.921073	9.844836	8.945570
8.862199	11.580267	9.125524	9.572823	11.890167	9.348702
7.776572	10.236750	7.552156	7.857761	10.917830	8.002228
6.715538	10.829997	9.658613	6.484577	9.425306	10.637866
11.373581	7.718517	8.749173	10.893355	7.552358	8.377145
11.890270	11.322452	10.758605	12.648498	10.721953	10.358108
8.374891	9.153560	9.569267	6.951497	8.785435	8.474613
8.655325	11.149802	13.251986	8.189823	10.304943	12.072262
7.885048	12.104215	11.243551	7.376662	11.577133	10.231174
12.546519	9.056865	10.367268	12.619442	8.418094	9.757531
10.074009	12.845849	10.772039	11.326139	12.657430	10.775959
9.654342	10.557477	11.224685	10.426563	10.522516	11.236646
9.194522	6.964503	9.214477	8.665448	7.343987	9.233672
7.461596	9.810301	11.656346	8.652364	9.632648	9.817784
8.138396	7.574517	11.313923	8.184349	8.003290	11.462618
9.287654	8.915192	12.867053	9.926640	8.877154	12.855964
10.327311	8.216656	10.848515	10.427177	8.109833	10.651298
10.794205	11.871376	12.793605	12.109897	11.372683	12.599889
11.486646	9.647042	12.419257	12.133826	9.083587	12.007403
13.511917	8.508187	8.336984	9.967764	11.172334	13.423440

9.118953 12.450997 11.624519

Coordinates for Co ₂₇			Coordinates for Co ₂₈		
X	Y	Z	X	Y	Z
9.022976	8.962953	7.527392	9.106465	9.459352	7.345530
12.961200	10.095768	8.113092	13.064917	10.001983	8.264477
9.900477	11.121992	7.092538	10.383970	11.430579	6.934474
11.603759	12.041616	8.451880	12.044213	12.148681	8.455065
11.302920	9.232400	6.737206	10.809366	10.192181	8.855717
10.755776	9.877124	8.891019	11.427729	9.297950	6.791909
9.390509	11.877795	9.305676	9.723285	12.361581	9.064931
7.690089	10.884043	7.958534	8.119184	11.590955	7.481927
6.319036	9.394484	10.601881	6.602303	9.129926	10.328516
10.762467	7.576296	8.346175	10.554882	7.828022	8.417893
12.495863	10.857357	10.294791	12.542984	10.894574	10.402242
6.797218	8.747967	8.433789	6.835614	9.565716	7.938310
8.027860	10.308321	12.039449	8.238914	9.953299	11.850510
7.198271	11.549025	10.188655	8.355088	10.402455	9.471409
12.496384	8.460425	9.721429	12.214565	8.543990	9.921292
11.102384	12.719475	10.725307	11.406997	13.014638	10.583210
10.246930	10.565063	11.198252	9.952250	10.654419	13.313197
8.541842	7.345585	9.200986	9.895591	8.709649	10.570512
8.487939	9.625462	9.778189	8.208859	8.003054	9.029981
8.049780	8.010768	11.431844	8.019458	7.594332	11.371732
9.775672	8.910242	12.820096	9.687595	8.325242	12.877508
10.276730	8.154513	10.611284	9.663932	6.436320	10.101860
11.987445	11.412316	12.528576	10.240024	11.061811	11.045896
11.996792	9.135704	11.986375	11.637322	9.425204	12.101813
9.837646	11.213436	13.381361	11.296647	7.133095	11.582823
8.911361	12.459288	11.577598	8.196905	12.207497	10.947672
14.060673	9.460581	11.056624	9.838289	12.871105	12.396052
			11.932649	11.762391	12.553546

Coordinates for Co ₂₉			Coordinates for Co ₃₀		
X	Y	Z	X	Y	Z
9.411341	9.829375	6.130424	10.569555	9.680683	6.097359
12.573999	10.702613	8.682542	9.751521	11.074064	10.567431
10.608420	11.415822	7.469690	10.319318	11.921605	6.585918
11.778126	12.979423	8.849322	12.047658	11.766076	8.191812
11.371166	9.171333	7.286907	12.271901	9.446563	7.702841
10.147789	7.375946	8.262140	9.979889	8.686936	10.038039
9.372291	12.935131	8.869219	9.935938	12.691598	8.798500
8.230082	11.395404	7.470807	8.222425	11.527695	7.598084
6.954271	9.386525	10.796782	8.343662	9.413912	11.736345

8.226070	8.089911	7.075281	10.367381	8.007544	7.781031
12.562525	11.867267	10.822309	10.585387	11.901073	12.588754
8.136221	11.196562	9.864840	8.465843	9.239649	7.063428
8.144829	9.675712	12.841533	7.922929	9.882379	9.325845
7.019219	9.618383	8.436065	6.533200	10.671115	10.980499
13.385532	9.666173	10.631763	12.918953	8.638428	11.512882
10.570790	13.235972	10.907641	11.659520	12.452612	10.466346
10.139290	10.383240	13.836179	8.244412	7.625615	8.822050
8.125955	7.772639	9.448624	8.622644	7.152343	11.147699
9.369432	9.587916	8.450347	12.097708	7.818782	9.457765
8.047596	7.504621	11.823172	10.158750	10.349257	8.282033
10.109597	8.267431	12.777698	9.444374	7.957580	13.204091
10.116841	7.096569	10.641303	10.178351	6.370101	9.500730
11.383000	12.208467	12.844736	10.860053	9.558004	12.202824
11.416724	10.052563	11.873970	9.223006	10.314506	13.721063
10.583003	11.175762	9.836007	10.995595	7.261613	11.565429
9.362292	11.475200	11.915847	7.816060	12.230760	9.836600
12.123006	7.813330	11.638206	9.537788	13.419741	11.041078
9.295541	9.286325	10.862327	12.706020	11.021919	12.031336
11.435051	8.834385	9.654317	8.204540	11.766784	12.175578
			12.015620	10.151064	9.976609

Coordinates for Co ₃₁			Coordinates for Co ₃₂		
X	Y	Z	X	Y	Z
10.792974	9.961397	6.448988	10.539320	10.494611	6.863168
10.148731	11.856446	12.465032	8.384863	11.383798	12.582338
9.187631	11.579605	7.221038	8.652953	11.937177	6.915043
11.502523	11.722197	7.921212	12.607082	11.307467	7.824513
12.350376	9.492788	8.202423	11.974393	9.018190	8.125941
7.787836	9.239659	9.363369	11.325055	6.765000	8.489595
9.931350	13.350407	8.603753	10.647660	12.702589	7.904291
7.021262	10.843423	7.820701	6.741848	11.350781	8.317914
7.237640	9.364055	11.686022	9.139206	9.111069	12.728077
10.560241	7.956398	7.751730	9.957624	8.180020	7.153024
7.825808	11.714651	11.791812	10.207234	12.066793	11.273644
8.599463	9.229009	7.115247	8.586928	9.923625	8.102430
6.328449	10.912126	10.146034	6.815380	9.368666	9.594005
11.666812	9.559993	10.509613	6.911653	9.567730	11.988016
13.205447	9.099586	12.185156	13.190917	9.229653	12.081996
10.873748	11.932432	10.203231	12.099856	12.532683	9.857799
8.394073	7.206729	8.327252	8.074474	7.615657	8.520888
7.695839	7.275970	10.670782	8.175097	7.845683	10.891928
12.164854	7.484279	9.478932	12.284436	7.970515	10.285259
10.062985	10.040617	8.747331	12.931785	10.275579	9.966207

9.206449	8.090648	12.295549	8.715802	12.206062	9.255325
9.858322	7.874315	10.020593	10.050847	8.438610	9.475995
10.976203	9.629058	12.814648	11.034353	9.722920	11.364499
8.721239	10.166842	13.402487	10.601593	10.881537	13.347906
11.486530	7.551545	11.755635	10.434955	7.394507	11.615716
9.368343	10.109502	11.078802	8.763307	10.167915	10.606315
9.233116	13.419648	10.947282	10.216978	13.886363	9.859894
12.425464	11.303964	11.924516	12.444893	11.487488	11.975085
8.418901	11.761691	9.476875	6.920013	11.559316	10.655489
13.863604	9.034319	9.976141	10.698250	10.770019	9.186559
13.103788	11.236698	9.647812	9.495771	6.202908	9.797808
			11.375474	8.635068	13.393332

Coordinates for Co ₃₃			Coordinates for Co ₃₄		
X	Y	Z	X	Y	Z
9.564819	11.406635	7.107066	9.620168	11.688117	6.998526
9.272766	9.079227	6.531698	9.338263	9.367826	6.410185
11.495905	9.922628	6.904775	11.560097	10.156751	6.910601
10.046740	9.768047	8.712236	9.971997	10.044641	8.604640
11.767146	12.220691	7.391660	11.479794	8.670816	9.941399
7.990678	12.457087	8.595350	7.989051	12.726141	8.419193
10.307885	12.219211	9.216711	10.277156	12.428064	9.137193
12.261120	9.082019	12.140495	12.879503	7.317581	11.205283
10.833053	7.752135	7.811349	10.821497	8.000575	7.712896
11.461191	11.117194	13.165851	11.219346	11.363306	13.158654
10.044322	6.539376	9.735790	9.969523	6.807850	9.642369
11.664944	8.308754	9.970320	12.264764	6.668659	9.065199
10.992886	12.736520	11.436213	10.852210	12.997551	11.408855
10.764102	7.209670	11.917784	10.587003	7.456737	11.828789
9.287211	8.543684	10.682500	9.104003	8.832824	10.559613
12.503680	12.906588	9.624446	12.078391	9.322892	12.199999
9.981176	9.248383	12.887667	10.621559	10.735013	10.912218
8.490368	7.424874	12.559965	8.273906	7.675744	12.397354
10.783480	10.454135	10.945644	12.793995	11.464720	11.320846
13.032339	8.574952	8.094254	13.023888	8.751676	8.190996
7.708503	9.620891	12.159219	7.495991	9.896760	11.968885
6.267780	11.172311	9.600113	6.189347	11.464550	9.340559
8.483473	10.859711	10.236163	8.364232	11.130218	10.082607
12.342592	10.626920	9.034658	12.246685	10.873332	9.047926
8.710458	13.127381	10.777344	8.626937	13.388578	10.619703
8.527784	7.894914	8.481746	8.470476	8.159343	8.311654
13.768874	9.260849	10.327040	13.643035	9.428906	10.392355
7.793482	6.775900	10.447374	7.666036	7.029288	10.244792
9.200760	11.497203	12.454283	8.985614	11.764308	12.340175

12.935572	11.263316	11.269088	12.425396	13.089400	9.705369
7.002877	8.963778	10.020131	6.886088	9.241892	9.782122
7.747368	10.143734	8.048361	7.740650	10.432574	7.852531
6.964666	11.821285	11.712705	6.797333	12.118803	11.480950
			9.736064	9.504563	12.805566

Coordinates for Co ₃₅			Coordinates for Co ₃₆		
X	Y	Z	X	Y	Z
9.428917	11.525986	7.049347	9.440539	11.436919	7.050542
9.159309	9.185817	6.522231	9.157988	9.120900	6.508652
11.387454	10.020952	6.928249	11.393764	9.958483	6.944200
9.878770	9.947122	8.696517	9.867842	9.821856	8.696546
11.630178	12.335379	7.340493	11.650112	12.269412	7.397390
7.831848	12.593769	8.503430	7.858767	12.528795	8.553315
10.146347	12.386899	9.155717	10.140963	12.204649	9.171516
12.118068	9.341254	12.211262	12.104409	9.169078	12.208146
10.717691	7.872540	7.816271	10.707652	7.778791	7.782662
11.269706	11.399199	13.145572	11.266036	11.203997	13.188313
9.958452	6.729870	9.806021	9.927913	6.607191	9.746524
11.455538	8.619050	9.997706	11.442369	8.483823	9.981184
10.806529	12.970824	11.372892	10.813103	12.835949	11.466452
10.641319	7.446061	11.949156	10.623121	7.279211	11.903269
9.095321	8.766354	10.700517	9.070279	8.622243	10.684285
12.344363	13.084416	9.581916	12.296709	13.017590	9.632727
9.799948	9.506532	12.897468	9.782290	9.315393	12.895038
8.348161	7.641511	12.596396	8.324466	7.458469	12.552461
10.593025	10.696232	10.938159	10.580569	10.536614	10.964312
12.935911	8.671562	8.187841	12.925351	8.564745	8.178157
7.526077	9.839963	12.141775	7.506711	9.677721	12.143396
6.093961	11.325524	9.524007	6.105746	11.266182	9.543313
8.298275	11.045243	10.192923	8.283682	10.903068	10.224489
12.198184	10.810169	9.028850	12.196856	10.694392	9.058015
8.525536	13.321308	10.680522	8.544927	13.190241	10.735719
8.398093	8.036267	8.497836	8.373479	7.946939	8.463577
13.629598	9.399100	10.364933	13.616965	9.268537	10.369306
7.674809	6.935299	10.483124	7.637162	6.810383	10.424577
8.997576	11.739190	12.404205	8.987955	11.558440	12.456945
12.765066	11.465790	11.251794	12.748898	11.325770	11.284975
6.843209	9.123772	9.998639	6.821543	9.019733	9.973921
7.597199	10.270476	8.009214	7.598741	10.209006	8.014018
6.765056	12.029367	11.630192	6.760146	11.896500	11.684230
12.234706	6.606680	9.144319	12.208976	6.479522	9.096733
12.905800	7.310523	11.250504	12.891771	7.152622	11.208529
			10.342202	14.386839	9.812567

Coordinates for Co ₃₇			Coordinates for Co ₃₈		
X	Y	Z	X	Y	Z
9.675391	11.683908	7.236193	9.539913	11.585254	6.862183
9.391092	9.430505	6.418174	9.157338	9.229882	6.449804
11.604388	10.182887	7.093297	11.426758	10.037694	6.681531
8.455475	8.053828	8.181254	10.001276	10.024666	8.530167
11.829611	12.459937	7.869248	11.768166	12.350919	6.999942
8.032879	12.617680	8.754240	8.071261	12.753180	8.372661
10.247006	12.110905	9.562275	10.403320	12.459935	8.917214
11.936749	8.762273	12.301431	12.492969	9.525119	11.942192
10.830940	7.924533	7.637476	10.774050	7.934299	7.687806
11.058967	10.694055	13.452745	11.748631	11.628064	12.863346
9.898092	6.549536	9.401964	10.121362	6.830110	9.750452
11.404225	8.346096	9.964137	13.196191	7.440847	11.000389
9.937843	13.906975	8.099685	11.233453	13.152586	11.053755
10.439155	6.959434	11.683995	10.980747	7.625450	11.877460
8.991042	8.454319	10.516856	9.418105	5.898654	11.768700
12.376394	12.874170	10.175408	12.640436	13.158184	9.158840
9.559634	8.890318	12.838250	10.229012	9.764677	12.788138
8.092010	7.111428	12.191927	8.683390	7.897025	12.677180
12.690659	11.005825	11.674844	10.906724	10.862638	10.771185
13.010896	8.616835	8.279468	13.017484	8.701758	7.896469
7.357869	9.399235	11.980183	7.888290	10.155377	12.206742
6.150412	11.295086	9.459398	6.325507	11.601021	9.547185
8.273531	10.788615	10.267689	8.567751	11.253668	10.109901
10.533349	10.289350	11.174894	12.349028	10.865402	8.727316
8.573941	13.027579	11.036271	8.925264	13.543540	10.486348
9.943777	9.842701	8.688262	8.497190	8.161917	8.501818
13.557679	9.031068	10.585628	13.866943	9.487913	9.998910
7.560213	6.708548	9.948974	7.840713	7.117148	10.591526
8.849592	11.200313	12.591677	9.454506	12.023595	12.247901
12.252028	10.623279	9.354098	13.118421	11.603288	10.868455
6.815124	8.988062	9.691056	7.012891	9.345215	10.040099
7.745433	10.363823	7.934681	7.727955	10.425712	7.974626
6.682210	11.697965	11.702352	7.155723	12.369366	11.601998
12.233111	6.439723	8.896753	12.368422	6.674767	8.951632
12.761675	6.840153	11.126069	11.655023	8.728713	9.806679
10.466407	14.307405	10.329001	5.660827	10.539321	11.551511
10.781200	12.521648	11.900148	9.339948	8.936717	10.664272
			6.435012	8.306378	12.073666

Coordinates for Co ₃₉			Coordinates for Co ₄₀		
X	Y	Z	X	Y	Z
8.809662	11.401265	7.388218	8.937524	11.447831	7.297272
8.119915	9.115211	6.968091	8.228621	9.168221	6.873802
12.790558	10.267000	6.781550	12.914490	10.281046	6.727966
10.471970	9.692772	6.856004	10.586374	9.726036	6.785255
11.157028	11.978230	7.263401	11.288145	12.001525	7.197135
7.758748	12.652444	9.173919	7.888443	12.710784	9.067111
10.051121	12.008024	9.382307	10.167869	12.048091	9.308328
12.248937	8.769772	11.905432	12.322842	8.804417	11.862706
9.767179	7.601828	7.903236	9.856243	7.643680	7.827035
11.880085	10.884789	13.031909	11.962323	10.925234	12.982614
9.309785	6.497912	10.008172	9.379271	6.546182	9.926162
12.587433	6.694151	10.770376	12.656593	6.719765	10.730671
9.504934	13.643910	7.833494	9.654005	13.691775	7.740400
10.526476	7.070501	11.970264	10.593546	7.117598	11.912872
11.732510	10.279920	8.843984	11.833233	10.307326	8.791136
12.373719	12.550819	9.225492	12.496764	12.570280	9.174591
10.151044	9.185991	13.084871	10.227152	9.240377	13.033576
7.250931	6.956834	11.182660	7.298249	6.999061	11.090013
10.694859	14.203903	9.752421	10.836915	14.248432	9.675793
12.115622	8.174520	7.778998	12.205670	8.202320	7.728979
7.669285	8.018047	9.082675	7.747646	8.073566	8.976788
6.081256	11.598116	10.553529	6.182622	11.686931	10.428174
8.299085	10.961107	10.774260	8.396118	11.032714	10.683263
13.980483	10.826991	8.700477	14.097921	10.837948	8.664209
8.975439	13.225033	11.136010	9.100355	13.281089	11.049955
8.897655	8.585973	11.096212	8.967320	8.634141	11.024021
13.332313	8.747109	9.741090	13.414366	8.771111	9.706559
10.647029	10.304499	11.043429	10.748303	10.353043	11.015193
11.291420	12.569209	11.390414	11.401719	12.607437	11.329010
12.953729	10.860715	10.858200	13.050118	10.885429	10.816254
6.617089	9.265422	10.870281	6.667060	9.343475	10.757929
7.077507	10.366229	8.764376	7.180290	10.437707	8.651903
7.271181	12.158108	12.472456	7.374401	12.247760	12.378076
11.397508	6.134159	8.851449	11.472278	6.162448	8.792980
11.019629	8.164976	9.903236	11.095427	8.203462	9.847195
8.440856	7.516827	13.101587	8.493900	7.561712	13.046250
9.352971	9.695501	8.956571	9.427017	9.731270	8.853402
7.833780	9.838011	12.832372	7.899281	9.923336	12.773999
9.559266	11.534172	12.766572	9.652812	11.601231	12.697265
			6.296776	8.224209	12.774160

Coordinates for Co ₄₁			Coordinates for Co ₄₂		
X	Y	Z	X	Y	Z
8.938875	11.364044	7.433487	9.067664	11.344172	7.370436
8.158785	9.135606	6.915073	8.264480	9.122502	6.860586
12.913132	9.969354	7.107845	13.025293	9.906500	7.059907
10.540244	9.543766	6.987762	10.649223	9.507728	6.939965
11.335820	11.795880	7.465121	11.469280	11.751782	7.403530
7.841977	12.644987	9.176245	7.984791	12.656135	9.096852
10.825780	14.021082	10.028679	10.980392	13.994120	9.951740
11.862450	8.435112	12.163717	11.954625	8.413199	12.115243
10.071524	11.868013	9.548904	10.200154	11.844822	9.485925
9.297409	11.350795	12.877671	9.426682	11.362448	12.823466
8.939163	6.400689	9.984119	9.019773	6.392097	9.942025
12.151655	6.352844	11.012432	12.229027	6.321880	10.972497
9.745483	13.570023	7.989528	9.898959	13.543912	7.915061
10.034150	6.857882	12.050999	10.117784	6.849206	12.009925
11.697386	10.019895	9.096362	11.802267	9.982240	9.046960
12.475344	12.271669	9.616069	12.609664	12.226532	9.551231
9.713056	8.968352	13.182188	9.816235	8.967135	13.134873
6.829155	6.964244	11.005610	6.917525	6.976102	10.951608
12.069999	13.957237	8.028021	12.227276	13.907421	7.953628
12.007556	7.909970	8.016798	12.102481	7.864017	7.975863
7.480160	8.036045	8.967410	7.574713	8.033974	8.913383
6.001981	11.676584	10.401620	6.117594	11.723685	10.321815
8.166844	10.899672	10.772158	8.277707	10.910099	10.713324
13.993429	10.420414	9.146996	14.106078	10.356437	9.095364
9.264230	9.603813	8.974550	9.364740	9.590259	8.926077
8.588193	8.493217	11.081244	8.686626	8.487622	11.031685
13.108840	8.369793	10.095564	13.203637	8.322435	10.049686
8.943260	13.104810	11.255011	9.090830	13.116586	11.179871
11.191674	12.304662	11.685835	11.323950	12.283480	11.619732
12.793044	10.484384	11.240110	12.902831	10.445920	11.184216
6.377573	9.312450	10.697112	6.448865	9.319349	10.635118
7.062699	10.417730	8.659466	7.176197	10.425556	8.585095
7.074277	12.124303	12.425669	7.201765	12.175033	12.363651
11.079360	5.905125	8.988384	11.157324	5.875722	8.954143
10.758663	7.953551	10.050751	10.846118	7.933764	10.007471
7.901579	7.412016	13.029899	7.997638	7.425761	12.985801
9.627739	7.502046	7.945513	9.718400	7.482243	7.903729
7.472559	9.769643	12.763992	7.566774	9.784742	12.740492
10.461879	10.103871	11.235213	10.563156	10.089168	11.183072
11.546864	10.550241	13.310358	11.659827	10.536008	13.255092

13.656212 12.154188 7.586515 13.792852 12.085190 7.525144
5.458805 10.663015 12.264719

Coordinates for Co ₄₃			Coordinates for Co ₄₄		
X	Y	Z	X	Y	Z
8.107428	11.203161	7.502797	10.251249	6.625630	8.769104
7.750479	8.816545	7.109636	12.235515	6.808535	10.303136
12.171022	10.743741	6.433813	13.452827	8.269280	11.891378
9.966754	9.782338	6.756633	12.465713	12.245703	7.314502
10.319498	12.161943	7.156735	8.079408	13.954524	8.728154
7.072307	12.263242	9.432750	10.019003	14.153985	10.229525
9.434868	11.967687	9.357456	13.452378	12.257613	11.421393
13.580906	8.130472	11.717772	6.822069	9.881568	8.234497
9.729649	7.584761	7.840963	11.024744	12.287827	11.420219
11.302549	8.650008	12.189856	12.450032	7.319546	7.898276
9.648825	12.361944	11.815425	8.043301	6.024302	9.695142
11.912519	6.654782	10.992270	10.023173	10.185278	10.894576
8.491121	13.573726	7.945491	9.062052	12.030211	9.795921
9.935681	6.714229	12.376633	8.206455	7.802591	8.008993
11.277081	10.547989	8.608408	10.006068	6.119188	11.171518
12.536357	12.436728	8.139339	9.051940	8.122681	10.307781
9.403262	10.085980	12.938432	12.352924	10.188449	10.965590
7.730395	6.523059	11.424435	10.896773	10.401918	13.075256
10.703408	13.829794	8.865668	9.591317	7.088873	13.335993
11.930013	8.546982	7.477241	11.218262	8.757818	9.382717
7.723833	7.647864	9.257053	8.219565	11.821562	7.510017
5.710106	10.942677	10.972442	6.383546	11.579478	11.837118
8.048213	10.646264	10.882974	6.651648	12.064221	9.420022
13.562205	10.149347	8.343375	6.329985	9.085100	12.128144
8.618331	13.902952	10.313306	10.431907	8.459776	7.084179
9.052541	8.424147	11.105911	7.671723	7.027172	11.899793
13.329912	7.996379	9.405694	6.632397	8.046023	9.898847
11.605250	11.109255	12.599106	8.397451	9.640383	6.365692
11.696261	12.299065	10.389337	14.761180	10.200535	11.132590
13.981628	11.844509	9.885190	10.277892	13.141926	7.985995
6.689379	8.714130	11.183955	5.320448	10.127747	10.160807
6.714078	9.883637	9.045653	12.482318	9.777518	7.562729
7.251513	12.613369	11.828763	9.221061	9.903392	8.614440
11.041123	8.361051	9.687488	13.651039	8.743785	9.490338
11.700349	6.381379	8.586292	7.705557	10.145001	10.498577
7.999512	8.167517	13.143287	12.243056	13.299761	9.542151
9.046579	9.568464	8.916938	10.438399	10.952481	6.792879
7.008325	10.359415	12.940910	7.749704	13.507412	11.109967
12.751307	10.048772	10.700460	11.037804	8.254947	11.857719
8.416313	12.024491	13.756674	11.226951	11.202531	9.094014

9.700669	6.426422	9.986759	8.705581	9.180435	12.595957
14.934634	9.543382	10.153621	13.661002	11.232869	9.194069
10.413818	10.366399	10.833057	8.774198	11.648795	12.288526
			13.320436	10.431532	13.091786

Coordinates for Co ₄₅			Coordinates for Co ₄₆		
X	Y	Z	X	Y	Z
11.047884	12.664264	8.403883	12.791647	8.989090	10.821239
9.548602	8.658385	6.483524	11.463143	5.987546	9.621630
12.410375	6.508647	9.490808	7.549345	10.882465	7.803689
8.008666	10.487668	7.021466	7.434608	12.275716	11.599704
10.413178	10.950298	6.761763	8.961773	6.906542	12.781484
8.081035	7.818129	10.896351	10.546544	8.451311	6.590971
8.484930	8.748977	8.623029	13.481168	7.415381	9.105875
10.891171	9.228021	8.340904	14.326478	9.743034	9.097710
6.284241	9.662293	8.560105	8.860270	9.126300	11.955476
8.852449	6.679989	7.664218	9.073139	10.322938	5.961253
10.130679	7.142920	9.611072	11.194790	13.055230	12.760659
13.763501	10.201569	9.938345	12.099428	10.528091	8.904617
8.866182	12.772594	7.295711	6.575690	9.910408	11.607719
7.152933	11.944221	8.831100	10.578006	9.791901	10.518028
11.222237	13.168202	10.796804	8.333103	10.605723	10.089268
11.216903	7.109450	7.480109	9.442071	13.704700	11.150294
11.949341	9.108210	6.254912	6.102209	11.414501	9.714768
12.048929	8.589907	10.413934	9.667051	6.616116	8.051192
6.728950	7.325342	9.007201	10.308979	11.989960	9.665827
10.056253	10.482739	14.327560	13.712790	11.278140	7.291754
12.883482	11.609839	11.789254	9.799242	10.066920	8.236919
11.168698	9.905259	12.379896	7.933883	10.762210	13.508685
9.048307	13.273245	9.693767	6.672873	9.044948	9.267630
14.250624	7.851429	10.389255	11.235142	9.561128	12.787726
10.390785	7.635249	11.984171	8.832478	13.071535	13.457671
9.222503	13.753603	12.077362	8.059332	12.863136	9.254621
7.321841	12.458033	11.220814	9.561153	12.311249	7.357201
13.433548	9.300502	12.183223	7.197268	7.523551	11.171268
6.556005	10.539937	12.474968	11.911629	12.797215	8.030042
9.525859	11.556012	11.304883	11.268926	8.241289	8.912482
8.702295	9.533161	12.597087	7.344741	6.701014	8.857748
8.425302	11.810596	13.312105	12.021547	6.620960	7.307835
13.217814	12.540162	9.530216	8.174694	8.493086	7.370085
9.817818	9.332101	10.504107	9.409235	8.911608	14.250194
5.900496	8.735243	10.762472	11.865484	13.610013	10.426488
7.619996	10.220887	10.452283	12.898069	8.938101	7.237045
9.345792	11.086359	8.866347	13.696110	12.136259	9.600381
10.918799	12.244821	13.054858	9.690747	11.413128	11.947735

5.464152	11.095870	10.373289	12.174338	11.360491	11.325134
12.651395	6.983069	11.908678	7.141185	8.414256	13.473502
11.526939	10.965302	10.002148	11.405462	10.816520	6.582931
7.159278	8.210554	6.789413	8.959376	8.273575	9.678437
12.586661	10.839275	7.880832	10.797467	7.569446	11.338218
12.566656	10.790212	13.972160	10.077957	14.227172	8.832254
13.136518	8.477453	8.293612	9.115214	6.036862	10.452232
			10.254270	11.239312	14.242478

Coordinates for Co ₄₇			Coordinates for Co ₄₈		
X	Y	Z	X	Y	Z
11.003752	12.757042	8.245066	10.963986	12.764995	8.104493
9.502241	8.764559	6.313616	9.431591	8.615141	6.549783
12.374044	6.584562	9.298854	12.375841	6.661113	9.629652
7.960178	10.594228	6.864678	7.891781	10.470405	6.981586
10.363507	11.047379	6.597155	10.299030	10.912587	6.614955
8.056935	7.875888	10.715369	10.148607	7.338892	9.847541
8.449293	8.862564	8.449714	8.446629	8.899111	8.706273
10.845940	9.327080	8.169946	10.816999	9.331520	8.322063
6.251057	9.761000	8.403245	6.244849	9.765565	8.612996
8.787225	6.791913	7.481669	8.780331	6.707831	7.934986
10.094934	7.232420	9.415206	10.424387	5.281824	8.851498
13.712128	10.265513	9.759973	13.721806	10.399365	9.756529
8.815483	12.867368	7.153758	8.745799	12.768147	7.078526
7.118003	12.032755	8.702128	7.082869	12.057152	8.710284
11.191884	13.231972	10.653586	11.205960	13.448922	10.457785
11.166446	7.202992	7.291459	11.144752	7.133323	7.594420
11.890778	9.203703	6.076514	11.821003	9.056873	6.220595
11.998206	8.657607	10.236210	12.017167	8.845722	10.404743
6.692953	7.422543	8.820955	6.749115	7.398389	9.212920
10.167969	10.347153	14.144613	10.302404	10.925812	14.211252
12.869400	11.702340	11.599560	12.926589	12.011715	11.491652
11.161528	10.092957	12.066351	11.225543	10.436244	12.148810
9.011010	13.357264	9.553695	9.000751	13.477614	9.404999
14.213435	7.919559	10.183233	14.218914	8.066933	10.375954
10.339651	7.708449	11.850334	11.941845	8.981766	13.784746
9.198312	13.800409	11.959883	9.247369	14.116245	11.737848
7.307580	12.517620	11.102481	7.338909	12.750672	11.046593
13.426760	9.361999	12.006308	13.473299	9.688742	12.078254
6.546141	10.605042	12.314343	6.640714	10.955623	12.441643
9.492752	11.635984	11.120462	9.531573	11.880659	11.097330
8.666651	9.556274	12.442284	8.799975	9.971922	12.607170
8.465742	11.815116	13.186660	8.561054	12.266153	13.179405
13.180859	12.616676	9.352360	13.173213	12.705630	9.169193
9.769637	9.400899	10.313923	10.366260	8.109922	12.195014

5.868505	8.818128	10.585205	5.910015	8.986289	10.839663
7.603431	10.301294	10.280447	7.630234	10.472117	10.411822
9.308876	11.177691	8.705132	9.288594	11.218278	8.737596
10.883191	12.308043	12.905349	8.331045	5.927571	10.087636
5.440190	11.172968	10.240397	5.446430	11.275489	10.415426
12.636790	7.088919	11.797613	12.684689	7.429460	12.081521
11.495395	11.052244	9.804908	11.503566	11.198692	9.804522
7.112032	8.324885	6.613854	7.056889	8.208189	6.932148
12.546086	10.921290	7.694982	12.504136	10.885283	7.674601
12.563185	10.780293	13.817803	12.654637	11.252063	13.812323
13.072634	8.557634	8.114872	13.048338	8.555347	8.285288
9.563543	8.099571	13.998895	8.112320	8.075371	11.084305
11.813726	8.476211	13.594953	9.797765	9.602194	10.492876
			10.970430	12.711131	12.778784

Coordinates for Co ₄₉			Coordinates for Co ₅₀		
X	Y	Z	X	Y	Z
11.185789	12.764611	8.083188	8.933362	10.818933	6.164613
9.685375	8.725286	6.256803	8.641863	13.202832	6.717308
12.456109	6.612199	9.420440	6.644300	11.367379	12.477963
8.151682	10.586628	6.696807	7.257044	9.163431	6.959851
10.576399	10.997194	6.482132	9.388707	9.251702	7.866080
8.066499	7.988134	10.651288	10.870590	7.500863	7.236774
8.566555	8.918265	8.353297	8.476653	7.093733	7.601753
10.982599	9.329504	8.133965	7.777525	13.478538	8.957572
6.382356	9.850299	8.207276	10.120335	13.781605	8.605733
8.899396	6.790479	7.488504	9.073767	11.650867	8.392578
10.188796	7.235533	9.467600	7.325819	10.008378	9.171888
13.808855	10.287452	9.786968	10.569408	12.198630	10.292950
9.032106	12.861177	6.925386	11.150029	9.780136	6.357457
7.269797	12.107711	8.459328	12.780275	12.270055	11.163264
11.305945	13.331291	10.474955	7.735371	5.808925	9.569795
11.303009	7.173022	7.354819	7.735640	9.515847	11.595382
12.090079	9.104650	6.083953	10.113357	6.187210	9.198398
12.059649	8.727539	10.269491	11.337542	10.608479	8.560523
6.760534	7.503500	8.704445	12.027657	10.957545	13.126414
10.115070	10.597057	14.052475	10.402844	9.297743	13.924008
12.931247	11.811737	11.538987	9.177966	13.945271	10.901550
11.188214	10.246941	12.002768	13.531926	10.680125	9.433536
9.154847	13.438904	9.311912	8.619244	7.943498	9.822839
14.251047	7.942383	10.329684	8.494959	12.692222	12.895502
11.723439	8.688036	13.629502	12.502412	6.589229	8.825838
9.277855	13.976882	11.694310	11.787946	10.141423	10.934773
7.393417	12.660004	10.844810	13.955948	10.212428	11.807795
13.428383	9.478326	12.061480	10.848546	12.183863	6.884957

6.606852	10.750429	12.145842	10.115309	8.494721	11.721876
9.574174	11.770039	10.943321	8.441294	7.936523	13.219658
7.770991	10.228147	14.321159	11.057805	8.326776	9.440778
8.476794	12.039741	12.983890	12.324761	8.554599	12.596645
13.328479	12.634544	9.262212	9.207207	6.333567	11.479102
9.438952	8.363473	14.044695	12.330634	12.735228	8.792598
5.906302	8.990294	10.419532	8.025794	11.882522	10.682345
7.688742	10.423216	10.100463	8.201980	10.302506	13.817427
9.451775	11.223880	8.547284	13.060917	11.144741	7.068373
10.319745	7.853004	11.881139	10.859320	13.021043	12.487600
5.534648	11.303992	10.002990	9.517466	10.089743	10.079278
12.606591	7.213852	11.922382	11.563384	14.301994	10.519134
11.608684	11.111388	9.721378	7.000235	11.535025	7.384614
7.278040	8.334077	6.482036	12.802087	8.860598	7.937040
12.719271	10.880888	7.652599	10.122276	11.693247	14.427909
12.531053	10.975633	13.788634	9.216405	8.431026	5.684057
13.198679	8.533203	8.189672	7.017354	7.278122	11.349623
8.695024	9.693806	12.291055	10.658865	6.924174	13.365414
10.917443	12.498083	12.746023	6.541750	7.795341	8.827342
9.847989	9.491629	10.226278	9.806700	10.892339	12.251597
8.264723	5.951941	9.560844	13.251372	8.391757	10.316363
			11.596051	6.743520	11.104132
