Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Synthesis, Luminescence and Electrochemical Properties of Luminescent Dinuclear Mixed-Valence Gold Complexes with Alkynyl Bridges

Ling-Ling Hung, Wai Han Lam, Keith Man-Chung Wong, Eddie Chung-Chin Cheng, Nianyong Zhu, Vivian Wing-Wah Yam*

Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong, P. R. China

Fax: (852)2857-1586

Tel: (852)2859-2153

E-mail: wwyam@hku.hk

Supplementary Information

Table S1. Selected singlet excited states (S_n) in **3**–**7** computed by TDDFT/CPCM (CH_2Cl_2)

Complex	S_n	Excitation[a]	Coefficient[b]	Vertical excitation energies (eV)	f[c]
3	S_1	H → L	0.70	3.26	0.000
	S_2	H–1 → L	0.70	3.34	0.113
	S_3	H–2 → L	0.70	3.75	0.172
4	S_1	H → L	0.69	3.05	0.000
	S_2	H–2 → L	0.70	3.36	0.057
	S_3	H–1 → L	0.69	3.40	0.282
5	S_1	H → L	0.69	3.10	0.000
	S_2	H–2 → L	0.70	3.30	0.117
	S_3	H–1 → L	0.69	3.45	0.249
6	S_1	H → L	0.70	3.17	0.563
	S_2	H–1 → L	0.70	3.36	0.055
	S_3	H–2 → L	0.70	3.48	0.002
7	S_1	H → L	0.69	3.23	0.568
	S_2	H–1 → L	0.69	3.30	0.113
	S_3	H–2 → L	0.70	3.49	0.000

[a] The orbitals involved in the excitations (H = HOMO and L = LUMO).
[b] The coefficient in the configuration interaction (CI) expansion.
[c] Oscillator strengths.

Table S2. Selected triplet excited states (T_n) in **3**–**7** computed by TDDFT/CPCM (CH_2Cl_2)

Complex	**T_n**	**Excitation**[a]	**Coefficient**[b]	**Vertical excitation energies (eV)**
3	T_1	H–1 → L+1	0.56	2.71
	T_2	H–1 → L	0.64	2.73
4	T_1	H–2 → L	0.64	2.73
	T_2	H–2 → L+1	0.53	2.74
5	T_1	H–2 → L	0.64	2.70
	T_2	H–2 → L+1	0.55	2.70
6	T_1	H → L+2	0.48	2.48
	T_2	H–1 → L	0.64	2.74
7	T_1	H → L+2	0.47	2.48
	T_2	H–1 → L	0.64	2.70

[a] The orbitals involved in the excitations (H = HOMO and L = LUMO).
[b] The largest coefficients in the configuration interaction (CI) expansion.

Table S3. Relative energy of the optimized triplet excited state with respect to the optimized ground state in CH_2Cl_2.

Complex	$\Delta E(T_1–S_0)$ / eV
3	2.66
4	2.68
5	2.65
6	2.47
7	2.48

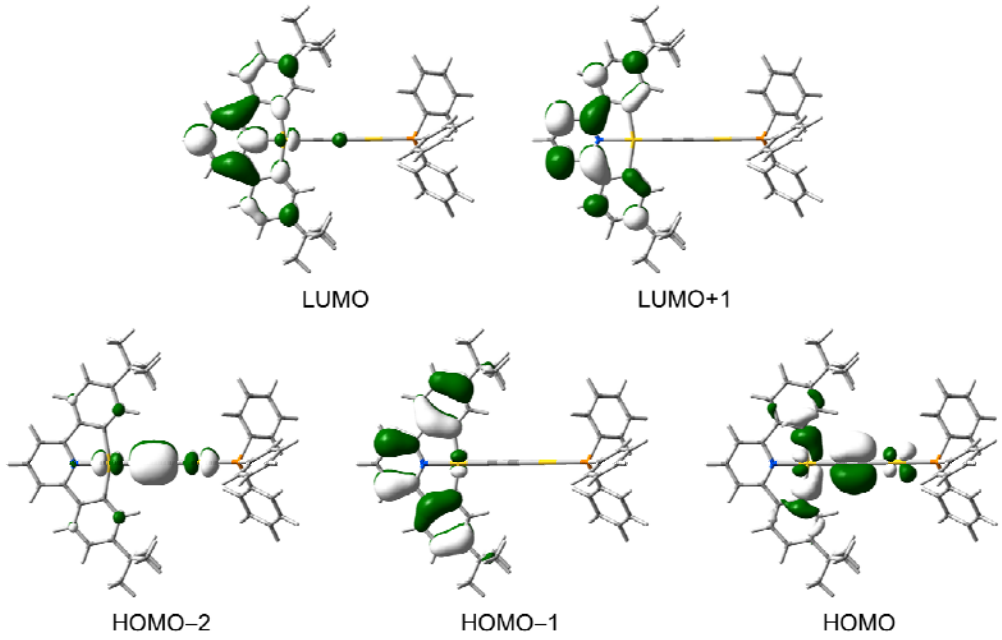

Figure S1. Spatial plots (isovalue = 0.03) of selected molecular orbitals of **3**.

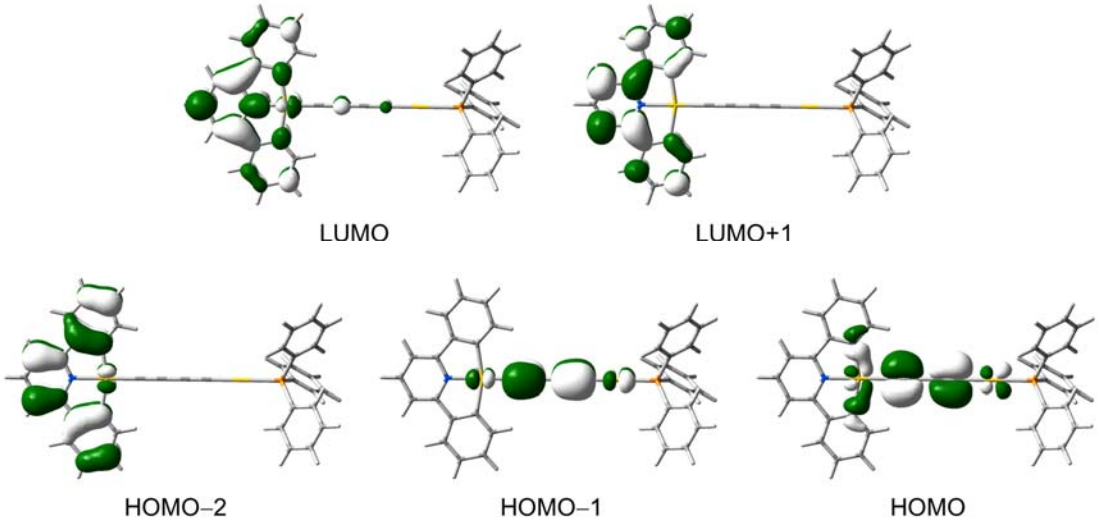

Figure S2. Spatial plots (isovalue = 0.03) of selected molecular orbitals of **4**.

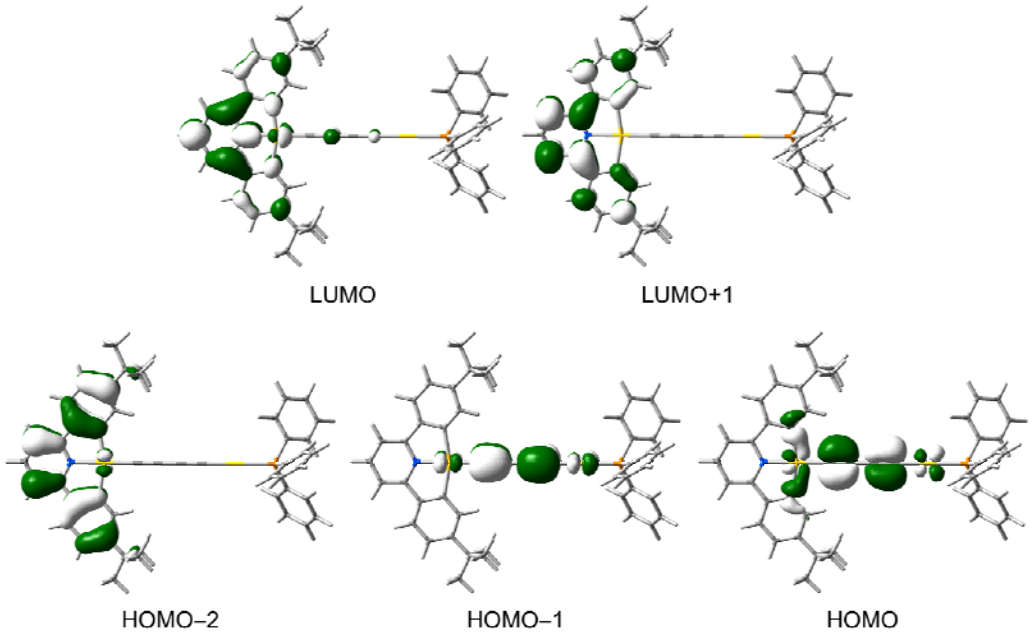

Figure S3. Spatial plots (isovalue = 0.03) of selected molecular orbitals of **5**.

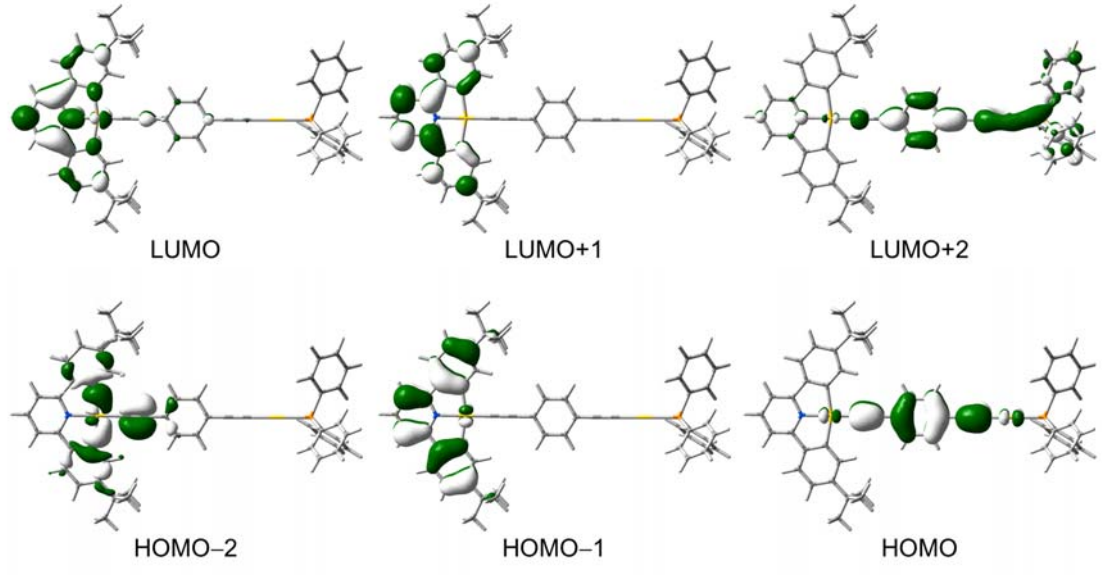

Figure S4. Spatial plots (isovalue = 0.03) of selected molecular orbitals of **7**.

Cartesian coordinates for all optimized structures reported in the paper

3 (S_0)					**3** (T_1)				
1	C	4.412798	-0.376859	2.758535	1	C	4.424673	-0.363719	2.759037
2	C	5.087241	0.197032	1.673209	2	C	5.099408	0.207445	1.672468
3	C	6.282967	0.889894	1.891443	3	C	6.296416	0.898609	1.889112
4	C	6.799900	0.999074	3.180267	4	C	6.814302	1.008745	3.177477
5	C	6.129526	0.419412	4.255029	5	C	6.143612	0.431693	4.253454
6	C	4.936283	-0.269079	4.043221	6	C	4.949088	-0.255070	4.043283
7	P	4.376118	-0.008821	0.003821	7	P	4.386495	0.000325	0.003834
8	C	5.101401	-1.551416	-0.651394	8	C	5.111792	-1.542833	-0.650462
9	C	6.277828	-2.101378	-0.131562	9	C	6.288504	-2.092512	-0.130965
10	C	6.804604	-3.267462	-0.682468	10	C	6.814876	-3.259092	-0.681225
11	C	6.163778	-3.888219	-1.752087	11	C	6.173366	-3.880705	-1.749937
12	C	4.989714	-3.345404	-2.271825	12	C	4.999003	-3.338233	-2.269349
13	C	4.456005	-2.184325	-1.721594	13	C	4.465716	-2.176671	-1.719708
14	Au	2.057402	-0.010742	-0.006809	14	Au	2.067967	-0.001939	-0.006469
15	C	0.075872	-0.009034	-0.011760	15	C	0.086999	-0.001877	-0.011487
16	C	-1.159695	-0.004874	-0.010011	16	C	-1.149151	-0.000351	-0.009802
17	Au	-3.113922	0.004589	-0.003358	17	Au	-3.109670	-0.001388	-0.003523
18	C	-3.425426	2.049773	-0.001994	18	C	-3.426576	2.027785	-0.002293
19	C	-4.814874	2.354014	0.003676	19	C	-4.876669	2.324511	0.003175
20	C	-5.233387	3.684641	0.005664	20	C	-5.292049	3.704904	0.004836
21	C	-4.296942	4.714980	0.002224	21	C	-4.361078	4.703378	0.001905
22	C	-2.924074	4.447911	-0.003231	22	C	-2.954710	4.437476	-0.002948
23	C	-2.518208	3.100242	-0.005294	23	C	-2.542492	3.079506	-0.004997
24	C	-5.744859	1.216437	0.007449	24	C	-5.746679	1.236075	0.006624
25	N	-5.127979	0.015478	0.004809	25	N	-5.102961	-0.006893	0.004104
26	C	-5.757787	-1.178733	0.007722	26	C	-5.737375	-1.182864	0.007198
27	C	-7.152412	-1.186871	0.013738	27	C	-7.144475	-1.201530	0.013066
28	C	-7.828615	0.030057	0.016509	28	C	-7.855009	0.029047	0.015701
29	C	-7.139331	1.239636	0.013447	29	C	-7.180834	1.222976	0.012614
30	C	-4.840195	-2.326307	0.004181	30	C	-4.835785	-2.334356	0.004105
31	C	-3.447511	-2.037174	-0.001588	31	C	-3.439014	-2.041812	-0.001482
32	C	-2.551846	-3.097534	-0.004730	32	C	-2.545317	-3.104407	-0.004206
33	C	-2.972393	-4.440712	-0.002376	33	C	-2.968972	-4.445897	-0.001662
34	C	-4.348097	-4.692783	0.003189	34	C	-4.347389	-4.700011	0.003722
35	C	-5.273233	-3.652281	0.006450	35	C	-5.271532	-3.662057	0.006593
36	C	5.096737	1.333011	-1.003435	36	C	5.107798	1.341080	-1.004663
37	C	4.428445	2.563282	-1.044835	37	C	4.440130	2.571675	-1.046565
38	C	4.957717	3.622097	-1.776072	38	C	4.969543	3.629805	-1.778694
39	C	6.150662	3.457815	-2.478077	39	C	6.162056	3.464540	-2.481211
40	C	6.814800	2.233724	-2.446929	40	C	6.825572	2.240130	-2.449643
41	C	6.292085	1.171986	-1.712194	41	C	6.302695	1.179113	-1.713950
42	H	-1.488936	-2.869311	-0.009064	42	H	-1.481978	-2.878674	-0.008374
43	H	-4.717962	-5.712134	0.005146	43	H	-4.714921	-5.720013	0.005818
44	H	-6.333957	-3.889967	0.010829	44	H	-6.332350	-3.898327	0.010849
45	H	-7.698541	-2.122578	0.016277	45	H	-7.677309	-2.144452	0.015613
46	H	-8.914335	0.035913	0.021214	46	H	-8.939523	0.016402	0.020276
47	H	-7.675387	2.181165	0.015753	47	H	-7.722782	2.162423	0.014767
48	H	-1.457875	2.860287	-0.009538	48	H	-1.479756	2.850031	-0.008821
49	H	-4.655704	5.738296	0.003953	49	H	-4.706490	5.731526	0.003370
50	H	-6.291426	3.933939	0.009957	50	H	-6.349069	3.953386	0.008507
51	H	3.490684	2.687626	-0.508450	51	H	3.502637	2.696686	-0.509859
52	H	4.433483	4.572660	-1.804383	52	H	4.445767	4.580619	-1.807329
53	H	6.559346	4.282573	-3.054452	53	H	6.570862	4.288744	-3.058298
54	H	7.741661	2.101638	-2.997162	54	H	7.752083	2.107233	-3.000279
55	H	6.812430	0.218672	-1.695357	55	H	6.822594	0.225558	-1.696784
56	H	6.780654	-1.624033	0.704512	56	H	6.791895	-1.614546	0.704414
57	H	7.716608	-3.691007	-0.272427	57	H	7.727109	-3.682355	-0.271386
58	H	6.575707	-4.798603	-2.177496	58	H	6.584978	-4.791464	-2.174861
59	H	4.483610	-3.830685	-3.101007	59	H	4.492320	-3.824165	-3.097802
60	H	3.532728	-1.769355	-2.118992	60	H	3.542148	-1.761984	-2.116738
61	H	6.808220	1.347999	1.058312	61	H	6.821949	1.354698	1.055044
62	H	7.727051	1.540440	3.343305	62	H	7.742450	1.548799	3.339221
63	H	6.533654	0.509091	5.259065	63	H	6.548493	0.522088	5.257127
64	H	4.407160	-0.715723	4.879698	64	H	4.419691	-0.699654	4.880691
65	H	3.475014	-0.902932	2.596508	65	H	3.485830	-0.888271	2.598189
66	C	-1.867758	5.554390	-0.006868	66	C	-1.910435	5.544990	-0.005809
67	C	-2.488430	6.954043	-0.003663	67	C	-2.534211	6.943698	-0.002949
68	H	-1.692475	7.705635	-0.006471	68	H	-1.738951	7.695752	-0.005175
69	H	-3.109526	7.126328	-0.889053	69	H	-3.154021	7.116055	-0.889157
70	H	-3.102363	7.125401	0.886886	70	H	-3.148066	7.115043	0.887586
71	C	-0.994087	5.416265	-1.265193	71	C	-1.032183	5.409033	-1.263990
72	H	-0.486338	4.447735	-1.303050	72	H	-0.522575	4.441698	-1.302214
73	H	-1.597380	5.517492	-2.173521	73	H	-1.632834	5.512558	-2.173535
74	H	-0.226757	6.198377	-1.277391	74	H	-0.266529	6.192857	-1.269598
75	C	-0.984061	5.414972	1.244300	75	C	-1.023855	5.407606	1.246366
76	H	-1.580139	5.514980	2.157509	76	H	-1.618508	5.509932	2.159977
77	H	-0.475748	4.446557	1.277006	77	H	-0.513841	4.440323	1.280067
78	H	-0.216840	6.197244	1.251358	78	H	-0.258279	6.191517	1.247924
79	C	-1.928177	-5.558648	-0.005922	79	C	-1.926985	-5.565301	-0.004796
80	C	-1.053336	-5.430410	-1.264481	80	C	-1.051853	-5.437542	-1.263494
81	H	-0.534769	-4.467649	-1.302517	81	H	-0.531535	-4.475815	-1.301122
82	H	-0.294715	-6.220952	-1.276701	82	H	-0.294928	-6.229640	-1.275206
83	H	-1.657975	-5.525080	-2.172629	83	H	-1.656445	-5.531213	-2.171725
84	C	-1.042676	-5.428539	1.244968	84	C	-1.041609	-5.435153	1.246469
85	H	-0.284177	-6.219256	1.252095	85	H	-0.284784	-6.227395	1.253665
86	H	-0.523511	-4.465892	1.277077	86	H	-0.520742	-4.473510	1.277946
87	H	-1.639626	-5.521567	2.158354	87	H	-1.638809	-5.526844	2.159776
88	C	-2.564123	-6.951429	-0.002174	88	C	-2.563692	-6.957771	-0.000867
89	H	-3.179774	-7.115762	0.888515	89	H	-3.179258	-7.122024	0.889858
90	H	-3.187177	-7.117203	-0.887432	90	H	-3.186410	-7.123805	-0.886276
91	H	-1.776423	-7.711663	-0.004843	91	H	-1.775984	-7.717923	-0.003278

4 (S_0)				
1	C	-5.434948	0.381788	2.757155
2	C	-6.109774	-0.201238	1.676976
3	C	-7.300325	-0.900793	1.901959
4	C	-7.811887	-1.007684	3.193046
5	C	-7.141161	-0.419441	4.262904
6	C	-5.953116	0.275786	4.044070
7	P	-5.408818	0.000882	0.003664
8	C	-6.136254	1.540025	-0.654951
9	C	-7.310419	2.090433	-0.130501
10	C	-7.841408	3.253644	-0.683235
11	C	-7.206852	3.870915	-1.758601
12	C	-6.035105	3.327399	-2.282756
13	C	-5.497217	2.168935	-1.731245
14	Au	-3.089820	0.009700	-0.014477
15	C	-1.110516	0.013954	-0.024354
16	C	0.122815	0.013157	-0.023658
17	C	1.489291	0.011295	-0.020755
18	C	2.717463	0.008759	-0.016822
19	Au	4.666273	0.002224	-0.005356
20	C	4.977885	-2.042141	-0.003238
21	C	6.366283	-2.347471	0.005854
22	C	6.803577	-3.675453	0.008767
23	C	5.874216	-4.710834	0.002699
24	C	4.511049	-4.422293	-0.006176
25	C	4.069103	-3.096545	-0.009105
26	C	7.293143	-1.205114	0.011958
27	N	6.673922	-0.005172	0.007704
28	C	7.301965	1.190165	0.011985
29	C	8.695786	1.200235	0.021420
30	C	9.374457	-0.015123	0.026019
31	C	8.686860	-1.225455	0.021384
32	C	6.383556	2.339323	0.005920
33	C	4.992937	2.044254	-0.003164
34	C	4.091987	3.105369	-0.008968
35	C	4.543743	4.427815	-0.005982
36	C	5.909008	4.706256	0.002877
37	C	6.830679	3.664026	0.008876
38	C	-6.123693	-1.347512	-0.997359
39	C	-5.450468	-2.575125	-1.036814
40	C	-5.977511	-3.637726	-1.764076
41	C	-7.172895	-3.479796	-2.463334
42	C	-7.841905	-2.258313	-2.433698
43	C	-7.321454	-1.192525	-1.703390
44	H	3.024501	2.901615	-0.015865
45	H	6.257331	5.734671	0.005175
46	H	7.893456	3.890107	0.015820
47	H	9.240642	2.136499	0.025145
48	H	10.460033	-0.019119	0.033390
49	H	9.224805	-2.165713	0.025075
50	H	3.003158	-2.884868	-0.016012
51	H	6.214918	-5.741800	0.004958
52	H	7.864645	-3.909408	0.015726
53	H	-4.511180	-2.695172	-0.502216
54	H	-5.449568	-4.586216	-1.791457
55	H	-7.579796	-4.307650	-3.036491
56	H	-8.770689	-2.131368	-2.981832
57	H	-7.845222	-0.241088	-1.688074
58	H	-7.807924	1.616025	0.710376
59	H	-8.751637	3.677798	-0.269976
60	H	-7.621952	4.779279	-2.185193
61	H	-5.533911	3.810164	-3.116326
62	H	-4.576190	1.753322	-2.132998
63	H	-7.825488	-1.365921	1.072713
64	H	-8.735001	-1.554148	3.361682
65	H	-7.541028	-0.507576	5.268761
66	H	-5.423794	0.729077	4.876794
67	H	-4.501528	0.913911	2.590075
68	H	3.787180	-5.232987	-0.010846
69	H	3.825892	5.243843	-0.010599

4 (T_1)				
1	C	-5.441297	0.375419	2.759433
2	C	-6.117692	-0.202430	1.677472
3	C	-7.310178	-0.899366	1.900399
4	C	-7.822070	-1.008730	3.191146
5	C	-7.149747	-0.425559	4.262786
6	C	-5.959776	0.267006	4.046036
7	P	-5.415972	0.002799	0.004757
8	C	-6.142166	1.544142	-0.650383
9	C	-7.315037	2.095373	-0.123927
10	C	-7.844839	3.260350	-0.674114
11	C	-7.210394	3.878595	-1.748976
12	C	-6.039913	3.334284	-2.275139
13	C	-5.503214	2.174077	-1.726141
14	Au	-3.097216	0.009601	-0.013748
15	C	-1.118163	0.012775	-0.024166
16	C	0.115438	0.011755	-0.023785
17	C	1.481954	0.010094	-0.021333
18	C	2.710740	0.008169	-0.017459
19	Au	4.665193	-0.001404	-0.006308
20	C	4.980682	-2.041735	-0.004277
21	C	6.374926	-2.346147	0.004628
22	C	6.819674	-3.674750	0.007479
23	C	5.894898	-4.710293	0.001569
24	C	4.527946	-4.423822	-0.007102
25	C	4.077562	-3.102405	-0.009982
26	C	7.280343	-1.197048	0.010501
27	N	6.651674	-0.016960	0.006251
28	C	7.303186	1.222846	0.010787
29	C	8.737837	1.200340	0.020399
30	C	9.405352	0.003500	0.024793
31	C	8.686681	-1.222050	0.019915
32	C	6.442442	2.317786	0.005391
33	C	4.987769	2.022651	-0.004010
34	C	4.103359	3.084822	-0.009512
35	C	4.556406	4.411934	-0.006404
36	C	5.955278	4.696402	0.002636
37	C	6.878290	3.692364	0.008450
38	C	-6.132835	-1.342406	-0.999271
39	C	-5.460723	-2.570504	-1.042174
40	C	-5.989078	-3.630863	-1.771763
41	C	-7.184712	-3.470185	-2.469966
42	C	-7.852634	-2.248190	-2.436937
43	C	-7.330848	-1.184671	-1.704271
44	H	3.034855	2.886093	-0.016330
45	H	6.284035	5.731536	0.004931
46	H	7.938601	3.924951	0.015344
47	H	9.284873	2.136612	0.024194
48	H	10.489529	-0.015966	0.032084
49	H	9.214514	-2.167664	0.023460
50	H	3.010422	-2.897449	-0.016718
51	H	6.236147	-5.740910	0.003747
52	H	7.881585	-3.903770	0.014257
53	H	-4.521209	-2.692596	-0.508430
54	H	-5.461961	-4.579733	-1.801793
55	H	-7.592649	-4.296261	-3.044950
56	H	-8.781604	-2.119075	-2.984256
57	H	-7.853757	-0.232801	-1.686364
58	H	-7.812488	1.620211	0.716553
59	H	-8.754072	3.685092	-0.259264
60	H	-7.624569	4.788304	-2.173604
61	H	-5.538772	3.817775	-3.108324
62	H	-4.583122	1.757850	-2.129406
63	H	-7.836608	-1.360588	1.069771
64	H	-8.746687	-1.553159	3.358132
65	H	-7.549872	-0.515616	5.268373
66	H	-5.429187	0.716301	4.880121
67	H	-4.506344	0.905332	2.593912
68	H	3.808381	-5.238433	-0.011646
69	H	3.844957	5.231896	-0.010836

5 (S_0)				
1	C	5.826254	-0.388083	2.758524
2	C	6.500998	0.194916	1.678277
3	C	7.691677	0.894287	1.903133
4	C	8.203449	1.001015	3.194155
5	C	7.532811	0.412786	4.264073
6	C	6.344634	-0.282257	4.045368
7	P	5.799625	-0.007013	0.005102
8	C	6.526599	-1.546380	-0.653558
9	C	7.700697	-2.097074	-0.129254
10	C	8.231338	-3.260416	-0.682047
11	C	7.596512	-3.877540	-1.757336
12	C	6.424822	-3.333750	-2.281338
13	C	5.887280	-2.175154	-1.729763
14	Au	3.480659	-0.014927	-0.012659
15	C	1.501502	-0.017847	-0.022183
16	C	0.268151	-0.015557	-0.021404
17	C	-1.098356	-0.011770	-0.018522
18	C	-2.326649	-0.007146	-0.014373
19	Au	-4.275710	0.003947	-0.003320
20	C	-4.582716	2.050296	-0.001161
21	C	-5.971348	2.355363	0.007325
22	C	-6.388192	3.686274	0.010093
23	C	-5.450142	4.715055	0.004675
24	C	-4.077635	4.446787	-0.003546
25	C	-3.673026	3.098415	-0.006361
26	C	-6.900585	1.218472	0.012943
27	N	-6.284071	0.016437	0.008976
28	C	-6.915472	-1.177821	0.012933
29	C	-8.309699	-1.184076	0.021710
30	C	-8.984999	0.033217	0.026014
31	C	-8.294644	1.242051	0.021726
32	C	-6.000491	-2.326199	0.007329
33	C	-4.608161	-2.038463	-0.001146
34	C	-3.711667	-3.097907	-0.006280
35	C	-4.133127	-4.441121	-0.003421
36	C	-5.508880	-4.692215	0.004770
37	C	-6.433991	-3.651783	0.010125
38	C	6.514835	1.341072	-0.996120
39	C	5.841705	2.568717	-1.036082
40	C	6.368968	3.631086	-1.763529
41	C	7.564497	3.472896	-2.462476
42	C	8.233430	2.251377	-2.432342
43	C	7.712751	1.185832	-1.701849
44	H	-2.648116	-2.873068	-0.012647
45	H	-5.878961	-5.711393	0.007173
46	H	-7.494692	-3.889123	0.016522
47	H	-8.856165	-2.119505	0.025165
48	H	-10.070643	0.039965	0.032881
49	H	-8.829512	2.184175	0.025198
50	H	-2.612380	2.860236	-0.012748
51	H	-5.807498	5.738768	0.007060
52	H	-7.445814	3.936907	0.016513
53	H	4.902305	2.688944	-0.501717
54	H	5.841084	4.579597	-1.791302
55	H	7.971577	4.300557	-3.035783
56	H	9.162328	2.124224	-2.980235
57	H	8.236455	0.234362	-1.686172
58	H	8.198422	-1.622778	0.711557
59	H	9.141522	-3.684781	-0.268905
60	H	8.011357	-4.785994	-2.183988
61	H	5.923412	-3.816391	-3.114852
62	H	4.966297	-1.759321	-2.131395
63	H	8.216789	1.359389	1.073839
64	H	9.126665	1.547342	3.362678
65	H	7.932852	0.500796	5.269873
66	H	5.815373	-0.735535	4.878137
67	H	4.892722	-0.920041	2.591538
68	C	-3.020703	5.552553	-0.009347
69	C	-3.641207	6.952259	-0.005235
70	H	-2.844851	7.703345	-0.009657
71	H	-4.263704	7.124782	-0.889588
72	H	-4.253265	7.124179	0.886491
73	C	-2.149564	5.413907	-1.269389
74	H	-1.640161	4.446435	-1.307740
75	H	-2.754876	5.514242	-2.176434
76	H	-1.383018	6.196632	-1.283388
77	C	-2.134953	5.413019	1.240373
78	H	-2.729678	5.512658	2.154470
79	H	-1.625120	4.445535	1.272086
80	H	-1.368325	6.195767	1.246051
81	C	-3.090065	-5.560003	-0.009122
82	C	-2.217118	-5.432229	-1.269060
83	H	-1.695699	-4.471183	-1.307385
84	H	-1.460370	-6.224427	-1.282941
85	H	-2.823546	-5.525060	-2.176161
86	C	-2.202819	-5.431545	1.240722
87	H	-1.445976	-6.223751	1.246457
88	H	-1.680993	-4.470484	1.272553
89	H	-2.798882	-5.523828	2.154722
90	C	-3.728012	-6.951844	-0.005110
91	H	-4.342229	-7.116126	0.886570
92	H	-4.352554	-7.116520	-0.889519
93	H	-2.941106	-7.712822	-0.009515

5 (T_1)				
1	C	5.836490	-0.381655	2.759629
2	C	6.512266	0.197085	1.677756
3	C	7.704707	0.894115	1.900637
4	C	8.217162	1.002689	3.191227
5	C	7.545453	0.418623	4.262767
6	C	6.355528	-0.274039	4.046075
7	P	5.809733	-0.007141	0.005248
8	C	6.536236	-1.547748	-0.651339
9	C	7.709470	-2.099046	-0.125773
10	C	8.239430	-3.263418	-0.677094
11	C	7.604791	-3.880986	-1.752230
12	C	6.433946	-3.336607	-2.277519
13	C	5.897086	-2.177020	-1.727369
14	Au	3.491055	-0.014230	-0.012401
15	C	1.512186	-0.016799	-0.022106
16	C	0.278516	-0.014547	-0.021391
17	C	-1.087990	-0.011219	-0.018632
18	C	-2.317027	-0.007370	-0.014519
19	Au	-4.271559	0.004355	-0.003583
20	C	-4.586681	2.047144	-0.001237
21	C	-5.981279	2.347809	0.007204
22	C	-6.408426	3.678373	0.010156
23	C	-5.477500	4.709792	0.004956
24	C	-4.100549	4.447213	-0.003218
25	C	-3.685104	3.102979	-0.006189
26	C	-6.887668	1.201963	0.012533
27	N	-6.258401	0.020652	0.008458
28	C	-6.911062	-1.218235	0.012500
29	C	-8.343500	-1.196149	0.021597
30	C	-9.011648	0.001500	0.025833
31	C	-8.293077	1.227044	0.021309
32	C	-6.048397	-2.312770	0.007142
33	C	-4.598309	-2.023531	-0.001442
34	C	-3.718105	-3.079081	-0.006062
35	C	-4.137617	-4.434450	-0.003146
36	C	-5.545525	-4.693128	0.004654
37	C	-6.471212	-3.690001	0.009599
38	C	6.525872	1.338976	-0.998134
39	C	5.853565	2.567017	-1.039685
40	C	6.381308	3.628008	-1.768798
41	C	7.576518	3.468039	-2.467893
42	C	8.244630	2.246114	-2.436217
43	C	7.723459	1.181966	-1.704021
44	H	-2.653672	-2.858167	-0.012174
45	H	-5.895896	-5.719460	0.006764
46	H	-7.529497	-3.932737	0.015421
47	H	-8.890254	-2.132758	0.025199
48	H	-10.095914	0.020577	0.032759
49	H	-8.820050	2.173292	0.024638
50	H	-2.622653	2.873476	-0.012530
51	H	-5.838275	5.732111	0.007437
52	H	-7.467606	3.921476	0.016558
53	H	4.914362	2.688565	-0.505268
54	H	5.854035	4.576827	-1.797767
55	H	7.983967	4.294612	-3.042509
56	H	9.173272	2.117549	-2.984223
57	H	8.246536	0.230169	-1.687143
58	H	8.207110	-1.624393	0.714884
59	H	9.148956	-3.688205	-0.262929
60	H	8.019109	-4.790208	-2.177762
61	H	5.932668	-3.819557	-3.110939
62	H	4.976715	-1.760725	-2.129936
63	H	8.230654	1.356035	1.070089
64	H	9.141737	1.547203	3.358177
65	H	7.946019	0.508066	5.268234
66	H	5.825409	-0.724017	4.880091
67	H	4.901555	-0.911613	2.594136
68	C	-3.052251	5.560521	-0.008832
69	C	-3.681499	6.956362	-0.004711
70	H	-2.889429	7.711894	-0.009037
71	H	-4.304677	7.125458	-0.889206
72	H	-4.294383	7.124840	0.887064
73	C	-2.180094	5.427163	-1.269053
74	H	-1.663443	4.463626	-1.306901
75	H	-2.785976	5.522939	-2.176158
76	H	-1.419724	6.215823	-1.282659
77	C	-2.165739	5.426223	1.241236
78	H	-2.761222	5.521238	2.155279
79	H	-1.648647	4.462687	1.272411
80	H	-1.405302	6.214915	1.246793
81	C	-3.099941	-5.548004	-0.008220
82	C	-2.223632	-5.417042	-1.268341
83	H	-1.706097	-4.454128	-1.307166
84	H	-1.463904	-6.206451	-1.275715
85	H	-2.827117	-5.515846	-2.176483
86	C	-2.210282	-5.415894	1.242396
87	H	-1.450540	-6.205324	1.242462
88	H	-1.692346	-4.452959	1.274798
89	H	-2.804088	-5.513805	2.156991
90	C	-3.732392	-6.942781	-0.004215
91	H	-4.345223	-7.110777	0.887646
92	H	-4.354805	-7.111551	-0.889270
93	H	-2.941441	-7.699270	-0.008152

6 (S_0)				
1	C	-7.551081	2.411290	-1.384411
2	C	-8.236195	1.635294	-0.440809
3	C	-9.423036	2.118112	0.120868
4	C	-9.920817	3.360481	-0.265123
5	C	-9.240075	4.124872	-1.210026
6	C	-8.055511	3.649297	-1.769875
7	P	-7.549239	0.002217	-0.001897
8	C	-8.279642	-1.175657	-1.189904
9	C	-9.460313	-0.892794	-1.884952
10	C	-9.993828	-1.833480	-2.762900
11	C	-9.354982	-3.056883	-2.951283
12	C	-8.176814	-3.341929	-2.263121
13	C	-7.636748	-2.404183	-1.388652
14	Au	-5.230084	-0.025426	0.005129
15	C	-3.248402	-0.039121	0.009679
16	C	-2.019454	-0.040013	0.010699
17	C	-0.594760	-0.037220	0.010894
18	C	0.123063	1.172283	-0.037090
19	C	1.508255	1.176013	-0.037653
20	C	2.232712	-0.028915	0.009248
21	C	1.515436	-1.238026	0.057355
22	C	0.130104	-1.242444	0.058430
23	C	3.658183	-0.023694	0.007574
24	C	4.881658	-0.016445	0.005541
25	Au	6.833121	-0.001463	0.001035
26	C	7.168384	-2.041695	-0.005066
27	C	8.560565	-2.330662	-0.009147
28	C	9.013808	-3.653289	-0.013543
29	C	8.097040	-4.699883	-0.013971
30	C	6.730462	-4.427811	-0.010042
31	C	6.272846	-3.107382	-0.005638
32	C	9.474322	-1.177398	-0.008480
33	N	8.841163	0.015050	-0.003908
34	C	9.454680	1.217749	-0.002455
35	C	10.848387	1.244517	-0.005886
36	C	11.541386	0.037214	-0.010627
37	C	10.868258	-1.181285	-0.011975
38	C	8.522095	2.355841	0.002742
39	C	7.134860	2.043988	0.005488
40	C	6.221888	3.094743	0.010452
41	C	6.657648	4.422534	0.012639
42	C	8.019555	4.717111	0.009893
43	C	8.953449	3.685777	0.004924
44	C	-8.274978	-0.419856	1.618775
45	C	-7.603380	-0.004479	2.775613
46	C	-8.137492	-0.279821	4.030499
47	C	-9.338465	-0.978841	4.139389
48	C	-10.005939	-1.401219	2.991970
49	C	-9.478357	-1.124122	1.732982
50	H	2.048081	2.117378	-0.075007
51	H	-0.422185	2.110345	-0.073958
52	H	-0.409500	-2.183740	0.095910
53	H	2.060789	-2.176224	0.094013
54	H	5.156826	2.877853	0.012597
55	H	5.930259	5.230122	0.016503
56	H	8.355747	5.749570	0.011589
57	H	10.013475	3.924534	0.002791
58	H	11.382264	2.187118	-0.004871
59	H	12.626962	0.046113	-0.013325
60	H	11.417512	-2.114987	-0.015684
61	H	5.204351	-2.908113	-0.002578
62	H	6.016494	-5.247296	-0.010397
63	H	8.450201	-5.726655	-0.017375
64	H	10.077641	-3.874499	-0.016640
65	H	-6.659684	0.529250	2.691664
66	H	-7.610733	0.044022	4.923099
67	H	-9.751015	-1.199583	5.119437
68	H	-10.939051	-1.950479	3.074477
69	H	-10.000897	-1.460538	0.842161
70	H	-9.960638	0.061193	-1.745893
71	H	-10.909118	-1.607155	-3.301623
72	H	-9.771855	-3.786640	-3.639086
73	H	-7.672313	-4.291673	-2.413347
74	H	-6.710862	-2.622964	-0.862089
75	H	-9.955822	1.528830	0.861624
76	H	-10.841158	3.731285	0.176108
77	H	-9.629381	5.094480	-1.506237
78	H	-7.518369	4.245965	-2.501013
79	H	-6.620142	2.046748	-1.812079

6 (T_1)				
1	C	-7.523596	2.410415	-1.387116
2	C	-8.211801	1.636991	-0.443658
3	C	-9.398183	2.122988	0.116271
4	C	-9.892373	3.366286	-0.271267
5	C	-9.208442	4.128366	-1.215725
6	C	-8.024361	3.649501	-1.773801
7	P	-7.531346	0.002160	-0.002260
8	C	-8.260547	-1.176237	-1.190238
9	C	-9.436796	-0.889682	-1.891171
10	C	-9.970219	-1.830022	-2.769592
11	C	-9.335837	-3.056563	-2.952266
12	C	-8.162170	-3.345290	-2.257855
13	C	-7.622036	-2.408007	-1.383049
14	Au	-5.211923	-0.028227	0.006480
15	C	-3.238331	-0.042660	0.012514
16	C	-1.987509	-0.043224	0.014289
17	C	-0.613798	-0.040126	0.015494
18	C	0.139985	1.207973	0.015142
19	C	1.491073	1.213075	0.014374
20	C	2.254304	-0.030405	0.013844
21	C	1.499477	-1.279017	0.015492
22	C	0.148293	-1.283070	0.016281
23	C	3.627369	-0.024770	0.011308
24	C	4.873020	-0.017047	0.008636
25	Au	6.814519	-0.001488	0.001789
26	C	7.149341	-2.041137	-0.000646
27	C	8.542023	-2.330666	-0.005757
28	C	8.993426	-3.654878	-0.008009
29	C	8.076440	-4.700282	-0.005246
30	C	6.709024	-4.427246	-0.000271
31	C	6.252741	-3.107223	0.002007
32	C	9.452637	-1.178340	-0.008462
33	N	8.814452	0.015590	-0.005399
34	C	9.432207	1.220238	-0.007052
35	C	10.824984	1.245393	-0.012234
36	C	11.520287	0.038648	-0.015501
37	C	10.845618	-1.179756	-0.013667
38	C	8.502062	2.356859	-0.002978
39	C	7.114534	2.043570	0.001837
40	C	6.199841	3.094142	0.005800
41	C	6.633435	4.421774	0.005067
42	C	7.995978	4.718177	0.000352
43	C	8.930715	3.688613	-0.003694
44	C	-8.260950	-0.417013	1.617636
45	C	-7.592954	0.000389	2.775765
46	C	-8.131041	-0.272848	4.029368
47	C	-9.332299	-0.971841	4.135601
48	C	-9.996179	-1.396124	2.986820
49	C	-9.464720	-1.121042	1.729010
50	H	2.040499	2.149629	0.013927
51	H	-0.416057	2.140606	0.015325
52	H	-0.401317	-2.219506	0.017332
53	H	2.055195	-2.211848	0.015891
54	H	5.134838	2.876552	0.009498
55	H	5.904996	5.228446	0.008199
56	H	8.330666	5.751178	-0.000195
57	H	9.990544	3.928571	-0.007369
58	H	11.357899	2.188707	-0.013700
59	H	12.605751	0.047889	-0.019555
60	H	11.394515	-2.113842	-0.016256
61	H	5.184168	-2.907914	0.005910
62	H	5.994506	-5.246276	0.001862
63	H	8.428752	-5.727403	-0.006987
64	H	10.057220	-3.876639	-0.011888
65	H	-6.648874	0.533822	2.693789
66	H	-7.607176	0.052557	4.923099
67	H	-9.747873	-1.191060	5.114705
68	H	-10.929507	-1.945301	3.067296
69	H	-9.984570	-1.458758	0.837124
70	H	-9.933760	0.066647	-1.756317
71	H	-10.882002	-1.600917	-3.313045
72	H	-9.752641	-3.786031	-3.640402
73	H	-7.661262	-4.297641	-2.403477
74	H	-6.699634	-2.629930	-0.851709
75	H	-9.933371	1.535545	0.856732
76	H	-10.812391	3.739623	0.168467
77	H	-9.594965	5.098724	-1.513093
78	H	-7.484873	4.244321	-2.504703
79	H	-6.593398	2.042909	-1.813905

7 (S_0)				
1	C	-8.259811	-1.742865	-2.160056
2	C	-8.896771	-0.664436	-1.532708
3	C	-10.071929	-0.140952	-2.081949
4	C	-10.605911	-0.696713	-3.242341
5	C	-9.973354	-1.774182	-3.858019
6	C	-8.800642	-2.297415	-3.315709
7	P	-8.165102	-0.001879	0.002781
8	C	-8.880088	-0.996793	1.355695
9	C	-10.079795	-1.700557	1.205356
10	C	-10.599960	-2.426122	2.274514
11	C	-9.928749	-2.453298	3.494858
12	C	-8.731443	-1.756330	3.648230
13	C	-8.204717	-1.033820	2.582215
14	Au	-5.845987	-0.023719	-0.010027
15	C	-3.864314	-0.036041	-0.017233
16	C	-2.635357	-0.036610	-0.018049
17	C	-1.210647	-0.033442	-0.017718
18	C	-0.485483	-1.239444	-0.018444
19	C	0.899861	-1.234664	-0.016606
20	C	1.616894	-0.024391	-0.013986
21	C	0.892078	1.181311	-0.013813
22	C	-0.493121	1.177203	-0.015634
23	C	3.042269	-0.018696	-0.010863
24	C	4.265821	-0.010729	-0.007433
25	Au	6.217448	0.006757	-0.000434
26	C	6.516173	2.053411	0.000819
27	C	7.903753	2.364217	0.005967
28	C	8.314998	3.696914	0.007524
29	C	7.372644	4.721943	0.004089
30	C	6.001201	4.448029	-0.000924
31	C	5.602587	3.097999	-0.002484
32	C	8.837859	1.230732	0.009417
33	N	8.226040	0.026421	0.007058
34	C	8.861268	-1.165674	0.009382
35	C	10.255580	-1.167044	0.014646
36	C	10.926442	0.052795	0.017244
37	C	10.231915	1.259330	0.014678
38	C	7.949576	-2.317239	0.005907
39	C	6.556152	-2.033726	0.000781
40	C	5.663333	-3.096155	-0.002498
41	C	6.088512	-4.438078	-0.000945
42	C	7.465080	-4.684952	0.004022
43	C	8.387057	-3.641560	0.007437
44	C	-8.863168	1.673286	0.199806
45	C	-8.189076	2.749376	-0.391629
46	C	-8.704518	4.037725	-0.289949
47	C	-9.889099	4.262188	0.409414
48	C	-10.559049	3.196499	1.006022
49	C	-10.050228	1.903959	0.903384
50	H	1.445589	-2.173564	-0.016898
51	H	-1.024928	-2.181584	-0.020156
52	H	-1.038669	2.115824	-0.015131
53	H	1.431799	2.123694	-0.011927
54	H	4.599137	-2.873973	-0.006375
55	H	7.838334	-5.702993	0.005325
56	H	9.448485	-3.875792	0.011295
57	H	10.805579	-2.100424	0.016688
58	H	12.012078	0.063389	0.021351
59	H	10.763686	2.203240	0.016742
60	H	4.542996	2.854800	-0.006390
61	H	7.725856	5.747117	0.005427
62	H	9.371560	3.952085	0.011413
63	H	-7.258350	2.577831	-0.927073
64	H	-8.175838	4.867221	-0.749869
65	H	-10.286848	5.269175	0.494180
66	H	-11.479459	3.369527	1.555668
67	H	-10.574838	1.077983	1.374908
68	H	-10.605358	-1.687096	0.254880
69	H	-11.530285	-2.972459	2.151142
70	H	-10.335467	-3.022722	4.325371
71	H	-8.201824	-1.781764	4.595843
72	H	-7.264014	-0.500924	2.698779
73	H	-10.567887	0.701549	-1.608784
74	H	-11.516905	-0.284197	-3.665574
75	H	-10.390766	-2.203116	-4.764217
76	H	-8.301017	-3.132614	-3.797292
77	H	-7.338042	-2.143846	-1.745324
78	C	4.939197	5.548945	-0.004656
79	C	5.553244	6.951501	-0.002311
80	H	4.753579	7.699064	-0.005145
81	H	6.166574	7.126334	0.887960
82	H	6.173009	7.126492	-0.888084
83	C	4.056584	5.405724	1.246861
84	H	3.550580	4.436095	1.279267
85	H	4.652632	5.507133	2.159888
86	H	3.286845	6.185380	1.254429
87	C	4.065605	5.405961	-1.262513
88	H	4.668201	5.507562	-2.171210
89	H	3.559851	4.436338	-1.298747
90	H	3.295931	6.185611	-1.275458
91	C	5.048348	-5.559701	-0.004611
92	C	4.163329	-5.433949	1.247077
93	H	3.638419	-4.474441	1.279705
94	H	3.409032	-6.228552	1.254690
95	H	4.761446	-5.523773	2.159965
96	C	4.171965	-5.433866	-1.262348
97	H	3.417725	-6.228457	-1.275181
98	H	3.647292	-4.474355	-1.298553
99	H	4.776340	-5.523663	-2.171106
100	C	5.689911	-6.949886	-0.002458
101	H	6.312938	-7.112508	-0.888298
102	H	6.306621	-7.112675	0.887760
103	H	4.905140	-7.713068	-0.005315

7 (T_1)				
1	C	-8.250928	-1.758024	-2.146642
2	C	-8.883238	-0.674589	-1.523348
3	C	-10.059722	-0.152043	-2.070634
4	C	-10.599520	-0.713703	-3.225499
5	C	-9.971601	-1.796098	-3.837240
6	C	-8.797717	-2.318509	-3.296557
7	P	-8.144874	-0.002987	0.005049
8	C	-8.857942	-0.987146	1.366991
9	C	-10.060599	-1.687516	1.224297
10	C	-10.580268	-2.404540	2.299417
11	C	-9.905653	-2.426543	3.517991
12	C	-8.705507	-1.732833	3.663705
13	C	-8.179276	-1.018770	2.591786
14	Au	-5.825756	-0.026635	-0.014156
15	C	-3.852368	-0.038843	-0.025605
16	C	-2.601164	-0.039042	-0.027591
17	C	-1.228037	-0.035629	-0.028688
18	C	-0.464705	-1.279068	-0.027654
19	C	0.886111	-1.274484	-0.025404
20	C	1.641207	-0.025352	-0.023886
21	C	0.877200	1.218370	-0.027047
22	C	-0.473519	1.213267	-0.029307
23	C	3.014450	-0.019343	-0.018656
24	C	4.260014	-0.011046	-0.013315
25	Au	6.202196	0.006801	-0.000633
26	C	6.499452	2.053213	0.001753
27	C	7.887105	2.365144	0.010849
28	C	8.296154	3.699269	0.013548
29	C	7.353086	4.722830	0.007435
30	C	5.981166	4.447301	-0.001423
31	C	5.584363	3.097602	-0.004134
32	C	8.819185	1.232699	0.016942
33	N	8.203807	0.026852	0.012557
34	C	8.843190	-1.166404	0.016700
35	C	10.236676	-1.165789	0.026177
36	C	10.908840	0.053914	0.030953
37	C	10.212441	1.259955	0.026417
38	C	7.934033	-2.317316	0.010385
39	C	6.540389	-2.033305	0.001371
40	C	5.646532	-3.095965	-0.004659
41	C	6.070499	-4.437400	-0.002185
42	C	7.447691	-4.685262	0.006584
43	C	8.369944	-3.642912	0.012839
44	C	-8.835249	1.676218	0.192183
45	C	-8.164717	2.744133	-0.417954
46	C	-8.675134	4.034938	-0.323373
47	C	-9.851072	4.270060	0.387105
48	C	-10.517416	3.212524	1.001867
49	C	-10.013651	1.917402	0.906593
50	H	1.442213	-2.207371	-0.024324
51	H	-1.014143	-2.215642	-0.028378
52	H	-1.029757	2.145818	-0.031284
53	H	1.426643	2.155215	-0.027200
54	H	4.582301	-2.873745	-0.011496
55	H	7.820151	-5.703618	0.008705
56	H	9.431292	-3.877684	0.019614
57	H	10.786311	-2.099514	0.029789
58	H	11.994368	0.064765	0.038355
59	H	10.743389	2.204457	0.030213
60	H	4.524849	2.853899	-0.011052
61	H	7.705040	5.748460	0.009740
62	H	9.352512	3.955448	0.020389
63	H	-7.240962	2.564347	-0.962729
64	H	-8.149367	4.858120	-0.797732
65	H	-10.244869	5.279056	0.466121
66	H	-11.431106	3.393849	1.559966
67	H	-10.535457	1.097787	1.392064
68	H	-10.588897	-1.678044	0.275315
69	H	-11.512854	-2.948324	2.182066
70	H	-10.311999	-2.989396	4.353149
71	H	-8.173351	-1.754194	4.609993
72	H	-7.236405	-0.488333	2.702224
73	H	-10.552189	0.694115	-1.600345
74	H	-11.511432	-0.301932	-3.647468
75	H	-10.393534	-2.229595	-4.739155
76	H	-8.301828	-3.157664	-3.775108
77	H	-7.328042	-2.158116	-1.733505
78	C	4.917942	5.547284	-0.008052
79	C	5.530699	6.950434	-0.004012
80	H	4.730446	7.697395	-0.009080
81	H	6.141479	7.125748	0.887920
82	H	6.152862	7.125896	-0.888013
83	C	4.031879	5.403643	1.240952
84	H	3.526514	4.433601	1.271925
85	H	4.625366	5.505319	2.155630
86	H	3.261482	6.182721	1.246610
87	C	4.047713	5.403956	-1.268172
88	H	4.652691	5.505876	-2.175263
89	H	3.542761	4.433933	-1.305778
90	H	3.277445	6.183037	-1.283344
91	C	5.029611	-5.558591	-0.008965
92	C	4.141044	-5.433137	1.240208
93	H	3.616306	-4.473458	1.271570
94	H	3.386453	-6.227534	1.245745
95	H	4.736622	-5.523161	2.154747
96	C	4.156565	-5.432505	-1.268970
97	H	3.402068	-6.226864	-1.284200
98	H	3.632276	-4.472797	-1.306388
99	H	4.763400	-5.522146	-2.176117
100	C	5.670535	-6.949103	-0.005360
101	H	6.296001	-7.111728	-0.889482
102	H	6.284821	-7.112276	0.886465
103	H	4.885512	-7.712052	-0.010535