SUPPORTING INFORMATION

Fullerene-enhanced Raman scattering: ZnO-covered C_{60} as ultrasensitive CO gas sensor

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Table SI. A comparison of structural properties, energetics, and electronic behavior for the $C_{60}ZnO$ fullerene of Fig. 1a obtained by fully relaxing the structure within both PBE/6-31g** (second column) and PBE0/6-311g**+GD3 (third column) methodologies. In the fourth column we present additional data by following the two step procedure discussed in Sec. II (see text).

	PBE/6-31g**	PBE0/6-311g**+GD3	PBE0/6-311G**+GD3 (pre-opt)
Zn—O	1.85 Å	1.89 Å	
Zn—C	2.01 Å	2.05 Å	
O—C	1.44 Å	1.4 Å	
C—C	1.61 Å	1.6 Å	
$ZnO \rightarrow C_{60}$ charge transfer	0.21	0.29	0.34
E_{ads}	2.4 eV	3.2 eV	3.35 eV
HOMO-LUMO $C_{60}ZnO$	1.12 eV	2.39 eV	2.46 eV
HOMO-LUMO C_{60}	1.66 eV	3 eV	2.93 eV

Table SII. Calculated HOMO—LUMO energy gaps obtained within the PBE0/6-311g**+GD3 methodology for the model $C_{60}(ZnO)_n$ structures shown in Fig. 1 (see text).

Atomic configuration	HOMO—LUMO energy gap (eV)
Fig. 1a	2.46
Fig. 1b	2.15
Fig. 1c	1.31
Fig. 1d	0.7
Fig. 1e	0.7
Fig. 1f	1.18

Table SIII. Calculated HOMO—LUMO energy gaps obtained within the PBE0/6-311g**+GD3 methodology for the model $C_{60}(ZnO)_n$ structures shown in Fig. 2 (see text).

Atomic configuration	HOMO—LUMO energy gap (eV)
Fig. 2a	0.97
Fig. 2b	1.1
Fig. 2c	0.63
Fig. 2d	0.75
Fig. 2e	1.38
Fig. 2f	1.45
Fig. 2g	1.33
Fig. 2h	1.14

Table SIV. A comparison of calculated and measured Raman-active vibrations for the C_{60} molecule (see text).

No. of Raman frequency	Frequency (cm^{-1}) PBE/6-31g**	Frequency (cm^{-1}) PBE0/6-311g**+GD3	Exp. (cm^{-1})
1	257	268	273
2	420	439	433
3	488	509	498
4	688	724	711
5	772	805	775
6	1103	1147	1101
7	1257	1306	1251
8	1436	1488	1427
9	1487	1542	1470
10	1571	1646	1578

Table SV. Calculated CO adsorption energies E_{ads} obtained within the PBE0/6-311g**+GD3 methodology for the model $C_{60}(ZnO)_nCO$ structures shown in Fig. 6 (see text).

Atomic configuration	E_{ads}(CO) (eV)
Fig. 6a	2.21
Fig. 6b	0.73
Fig. 6c	0.33
Fig. 6d	0.64
Fig. 6e	0.71
Fig. 6f	0.38

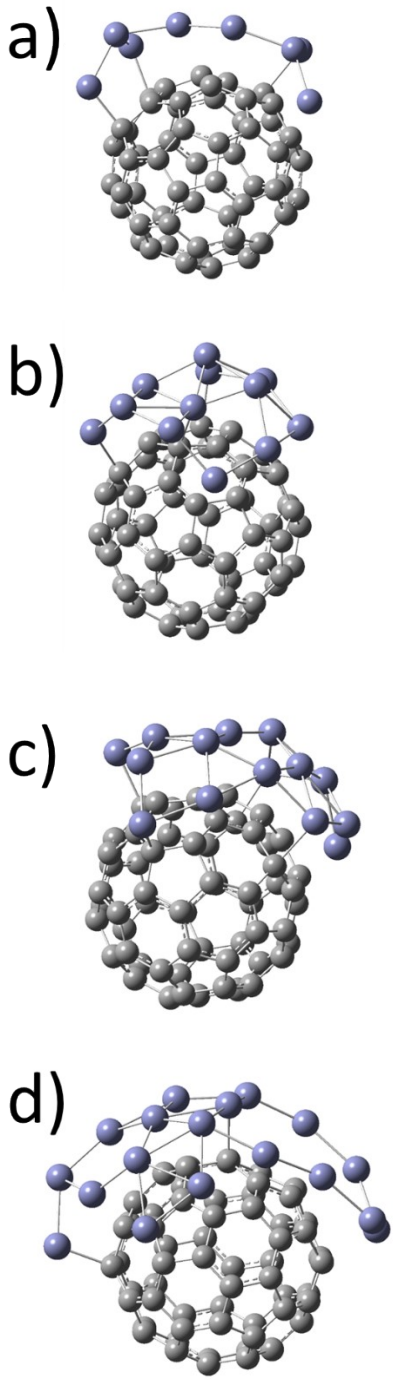

Figure S1. Optimized atomic configurations for the following fullerene compounds: a) $C_{60}(Zn)_8$, b) $C_{60}(Zn)_{12}$, c) $C_{60}(Zn)_{15}$, and d) $C_{60}(Zn)_{18}$ (see text).

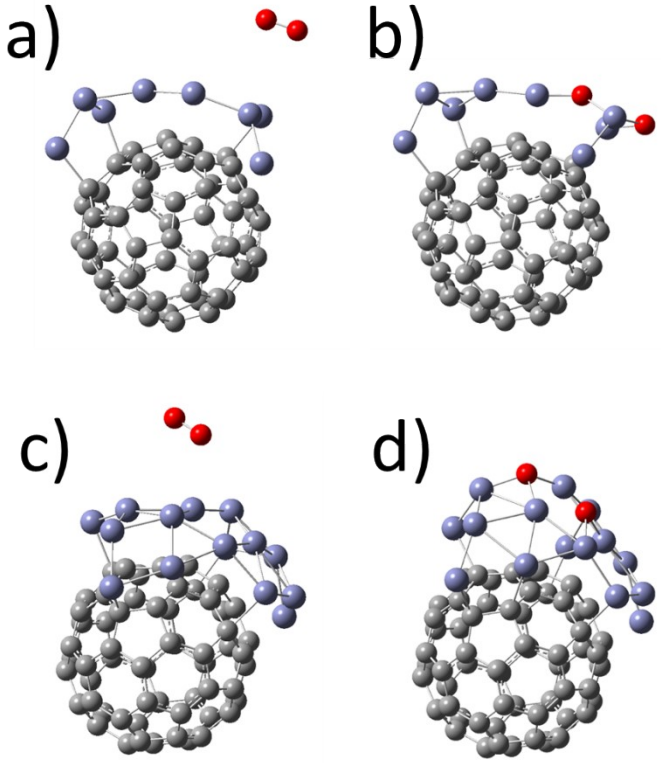

Figure S2. Interaction of a single oxygen molecule with $C_{60}(Zn)_n$ fullerenes. In a) and c) we show the initial atomic configurations for $C_{60}(Zn)_8+O_2$ and $C_{60}(Zn)_{15}+O_2$ systems, respectively. In b) and d) we present the corresponding optimized atomic configurations.

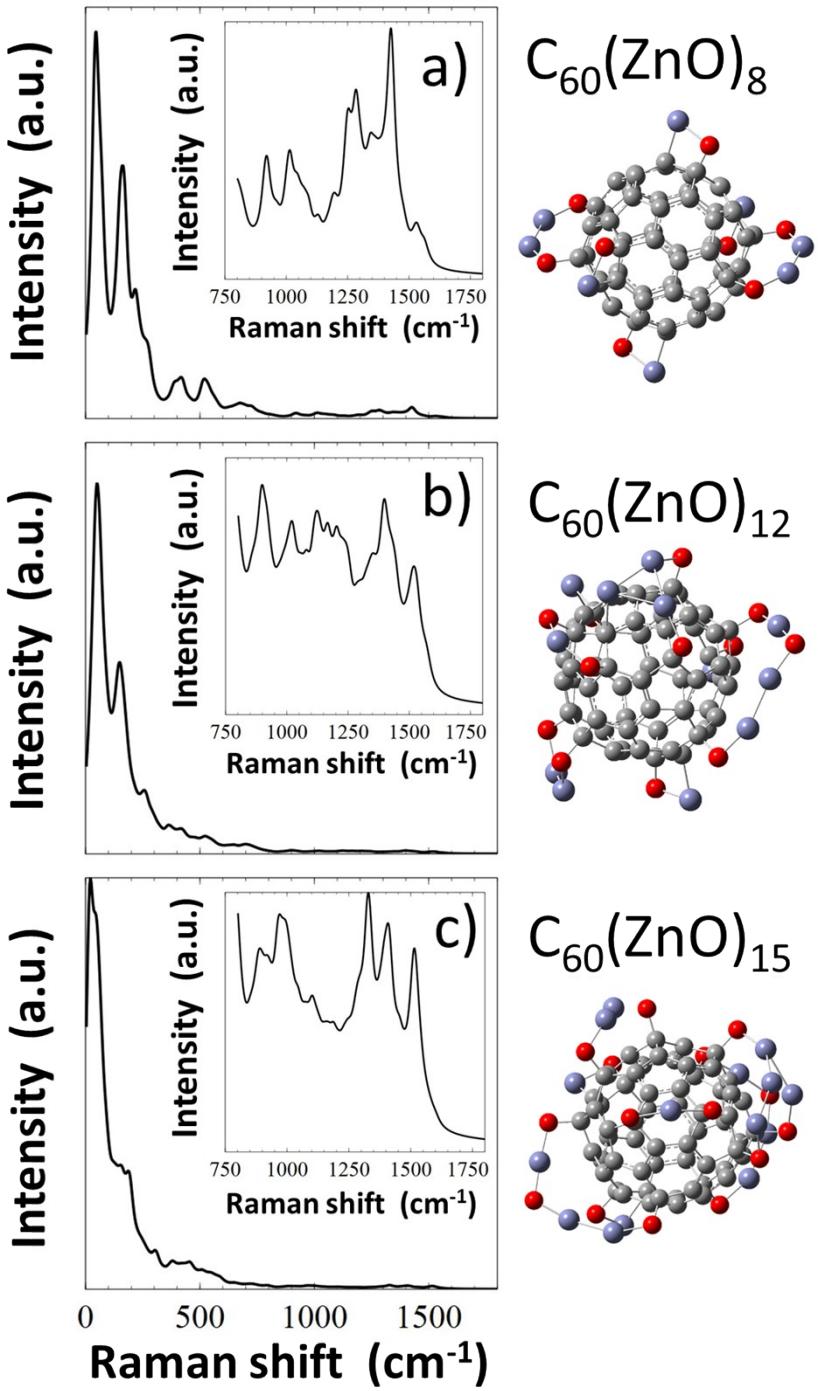

Figure S3. Calculated Raman spectra (assuming a 2000 nm laser wavelength) for the optimized fullerene compounds a) $C_{60}(ZnO)_8$, b) $C_{60}(ZnO)_{12}$, and c) $C_{60}(ZnO)_{15}$ as presented in Figs. 1c, 1e, and 1f, respectively. For clarity, simulated spectra in the 800—1800 cm^{-1} frequency range are plotted as insets.

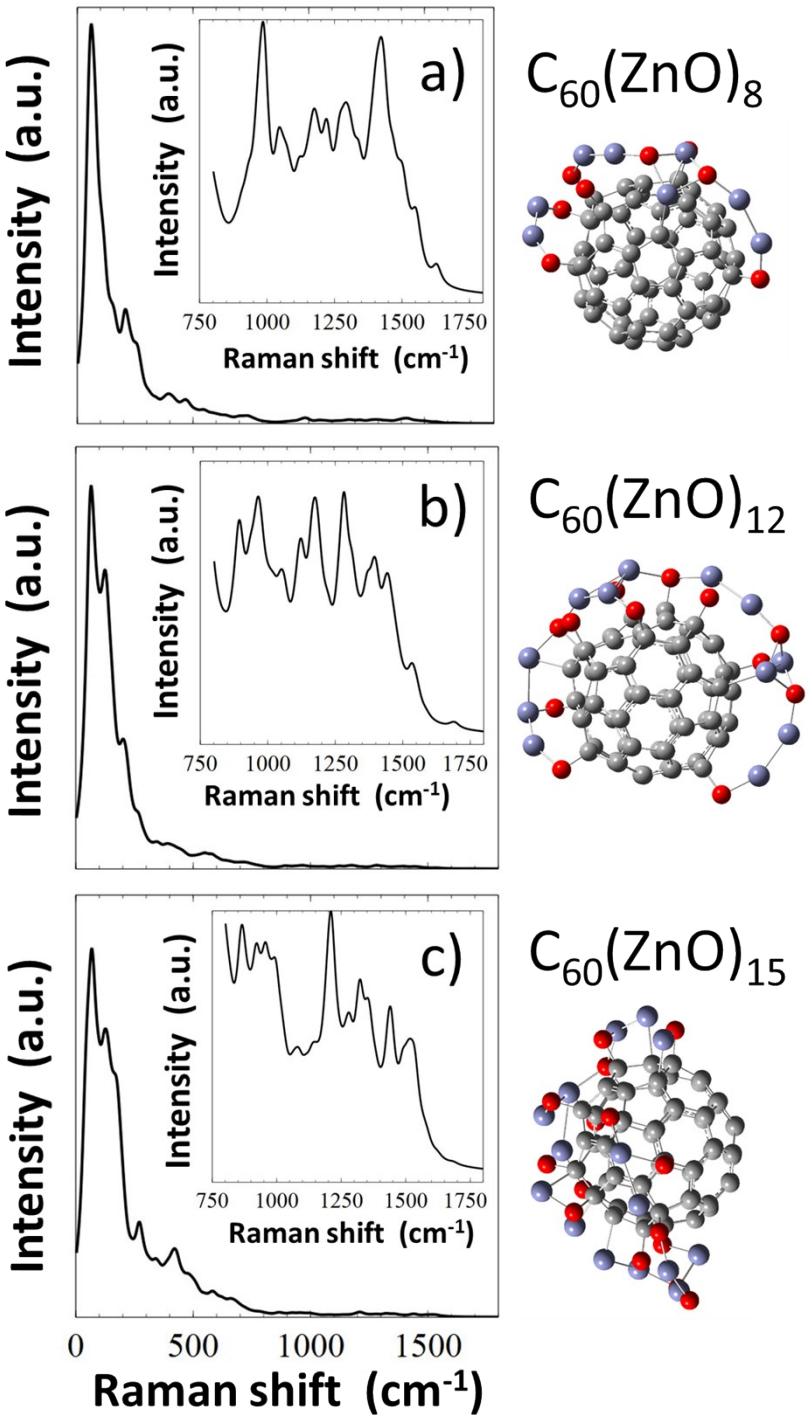

Figure S4. Calculated Raman spectra (assuming a 2000 nm laser wavelength) for the optimized fullerene compounds a) $C_{60}(ZnO)_8$, b) $C_{60}(ZnO)_{12}$, and c) $C_{60}(ZnO)_{15}$ as presented in Figs. 2a, 2c, and 2d, respectively. For clarity, simulated spectra in the 800—1800 cm^{-1} frequency range are plotted as insets.

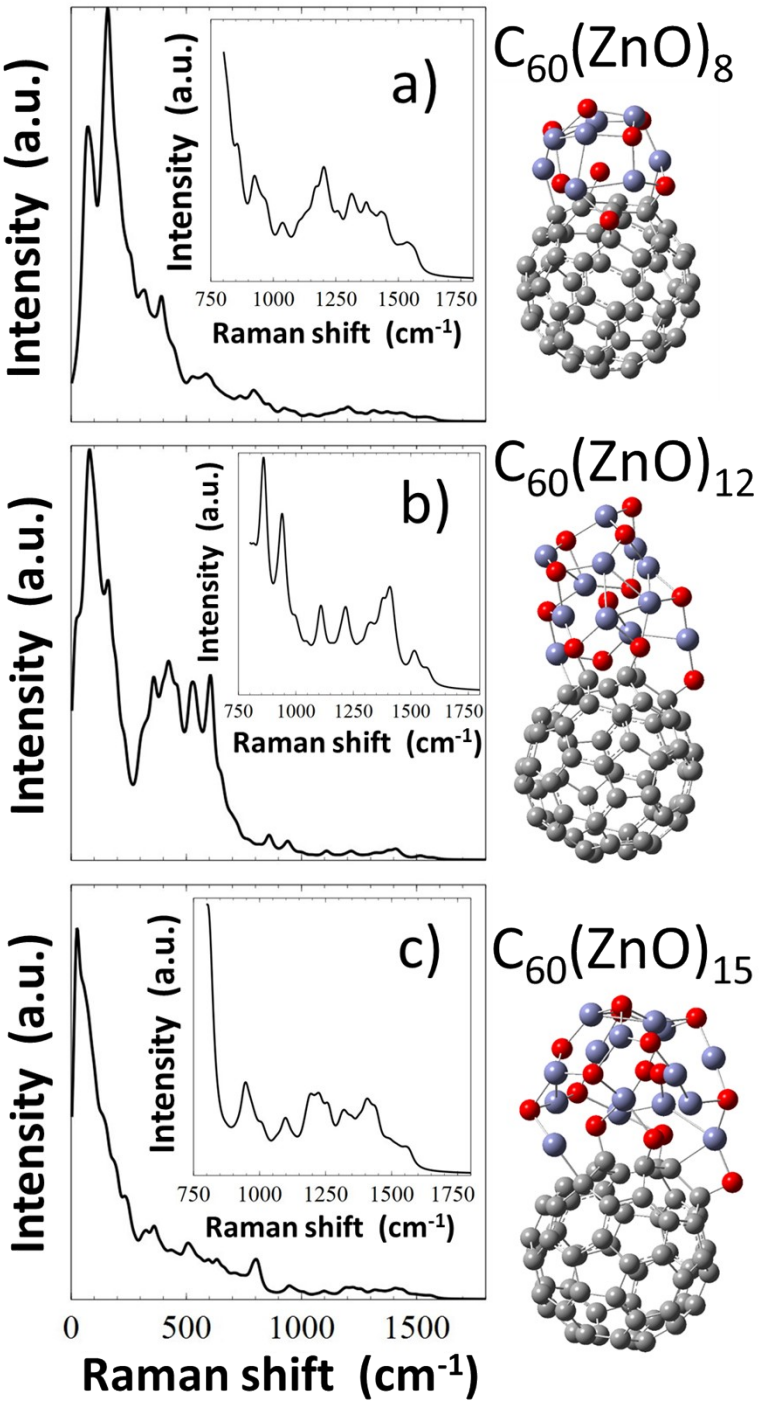

Figure S5. Calculated Raman spectra (assuming a 2000 nm laser wavelength) for the optimized fullerene compounds a) $C_{60}(ZnO)_8$, b) $C_{60}(ZnO)_{12}$, and c) $C_{60}(ZnO)_{15}$ as presented in Figs. 2e, 2g, and 2h, respectively. For clarity, simulated spectra in the 800—1800 cm^{-1} frequency range are plotted as insets.

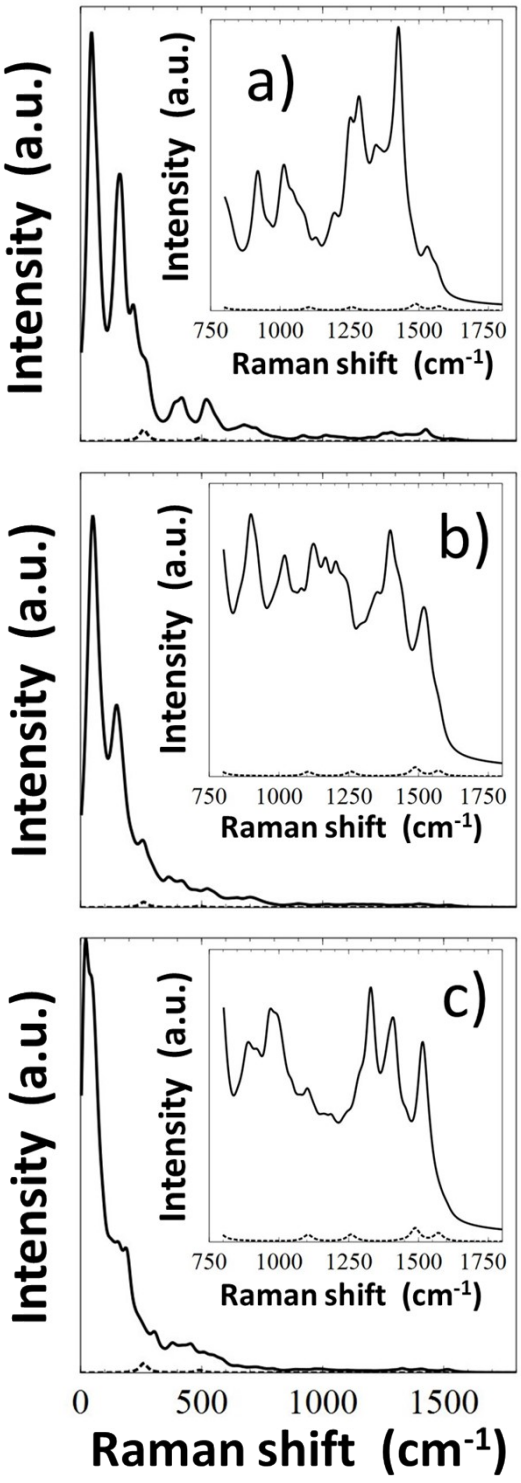

Figure S6. A comparison of the calculated Raman spectra (assuming a 2000 nm laser wavelength) for the optimized a) $C_{60}(ZnO)_8$, b) $C_{60}(ZnO)_{12}$, and c) $C_{60}(ZnO)_{15}$ fullerene compounds presented in Figs. 1c, 1e, and 1f, respectively with the spectrum obtained for the C_{60} molecule (dashed line). For clarity, insets show the simulated spectra in the 800—1800 cm^{-1} frequency range.

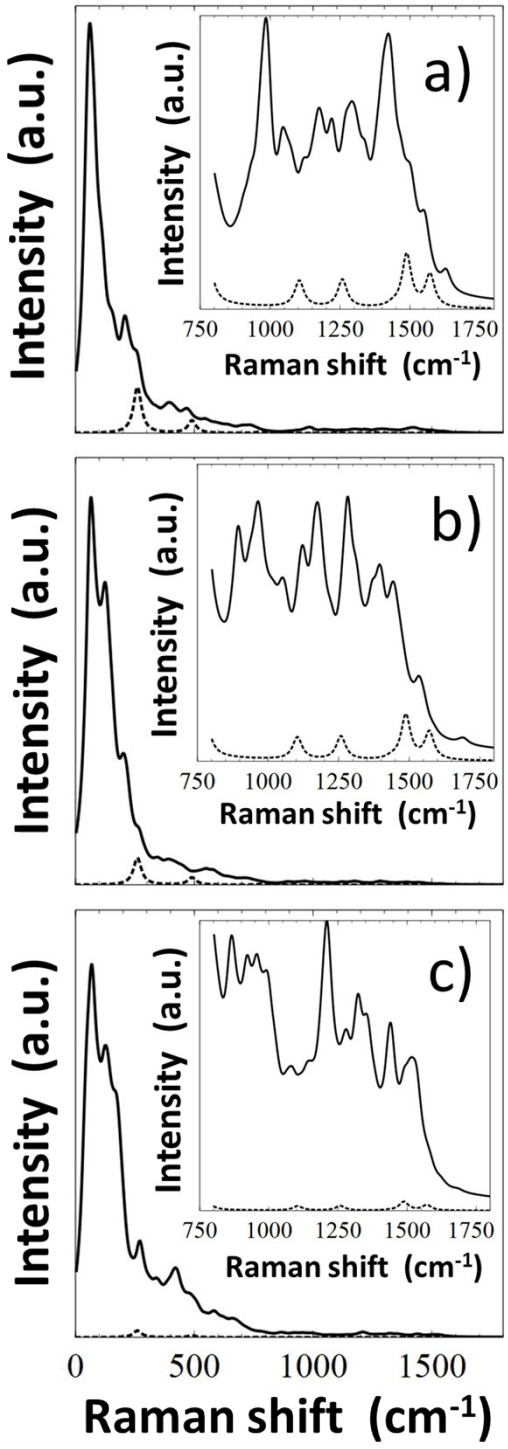

Figure S7. A comparison of the calculated Raman spectra (assuming a 2000 nm laser wavelength) for the optimized a) $C_{60}(ZnO)_8$, b) $C_{60}(ZnO)_{12}$, and c) $C_{60}(ZnO)_{15}$ fullerene compounds presented in Figs. 2a, 2c, and 2d, respectively with the spectrum obtained for the C_{60} molecule (dashed line). For clarity, insets show the simulated spectra in the 800—1800 cm^{-1} frequency range.

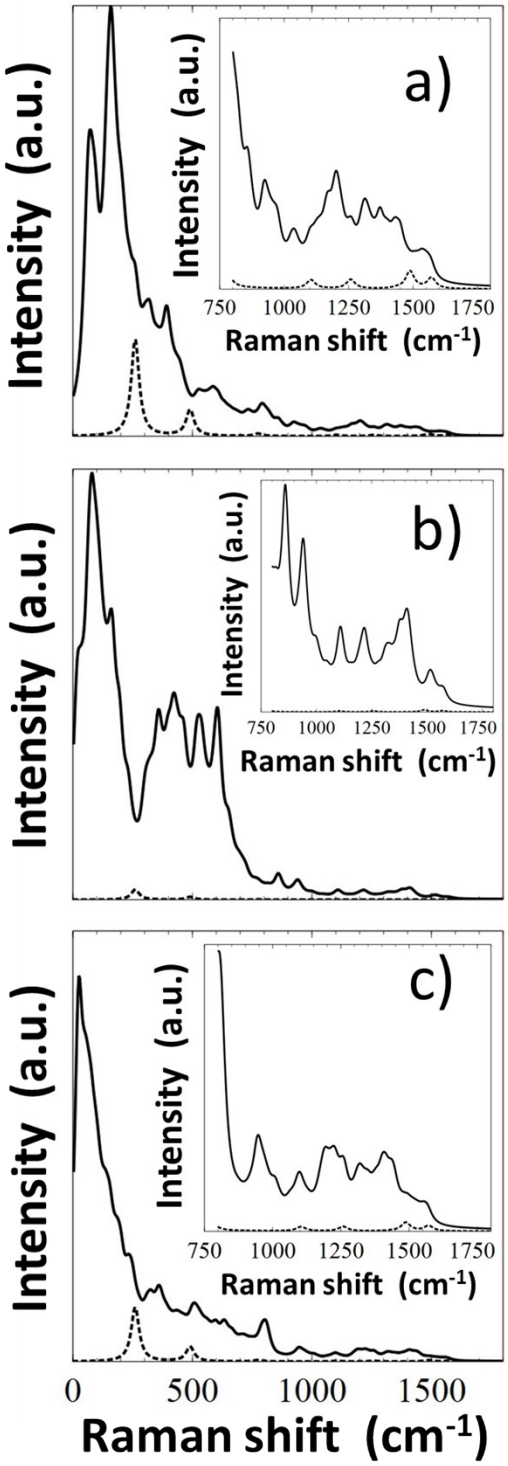

Figure S8. A comparison of the calculated Raman spectra (assuming a 2000 nm laser wavelength) for the optimized a) $C_{60}(ZnO)_8$, b) $C_{60}(ZnO)_{12}$, and c) $C_{60}(ZnO)_{15}$ fullerene compounds presented in Figs. 2e, 2g, and 2h, respectively with the spectrum obtained for the C_{60} molecule (dashed line). For clarity, insets show the simulated spectra in the 800—1800 cm^{-1} frequency range.

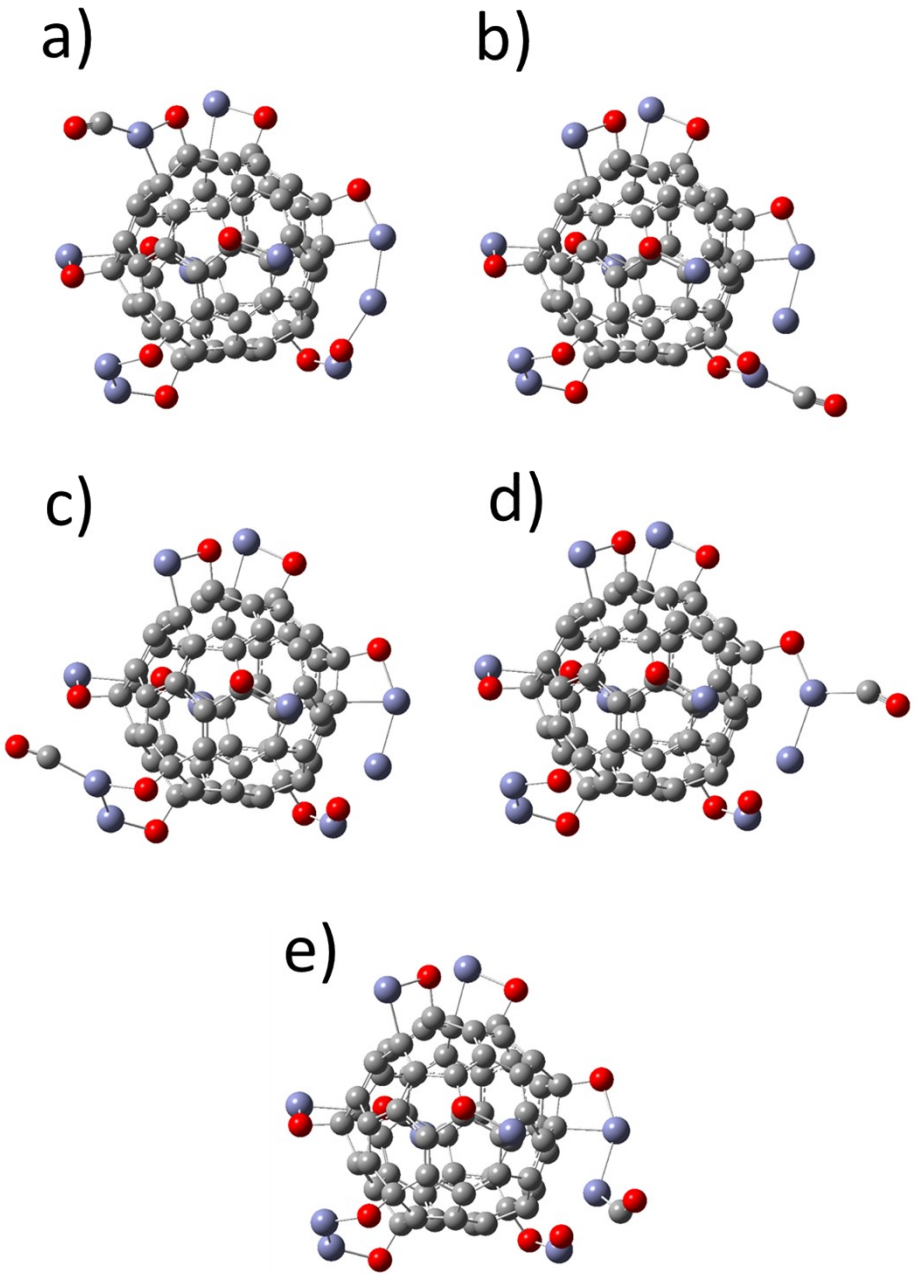

Figure S9. Optimized atomic configurations of a single CO molecule chemisorbed at five different Zn sites in the $C_{60}(ZnO)_{10}$ fullerene compound shown in Fig 1d.

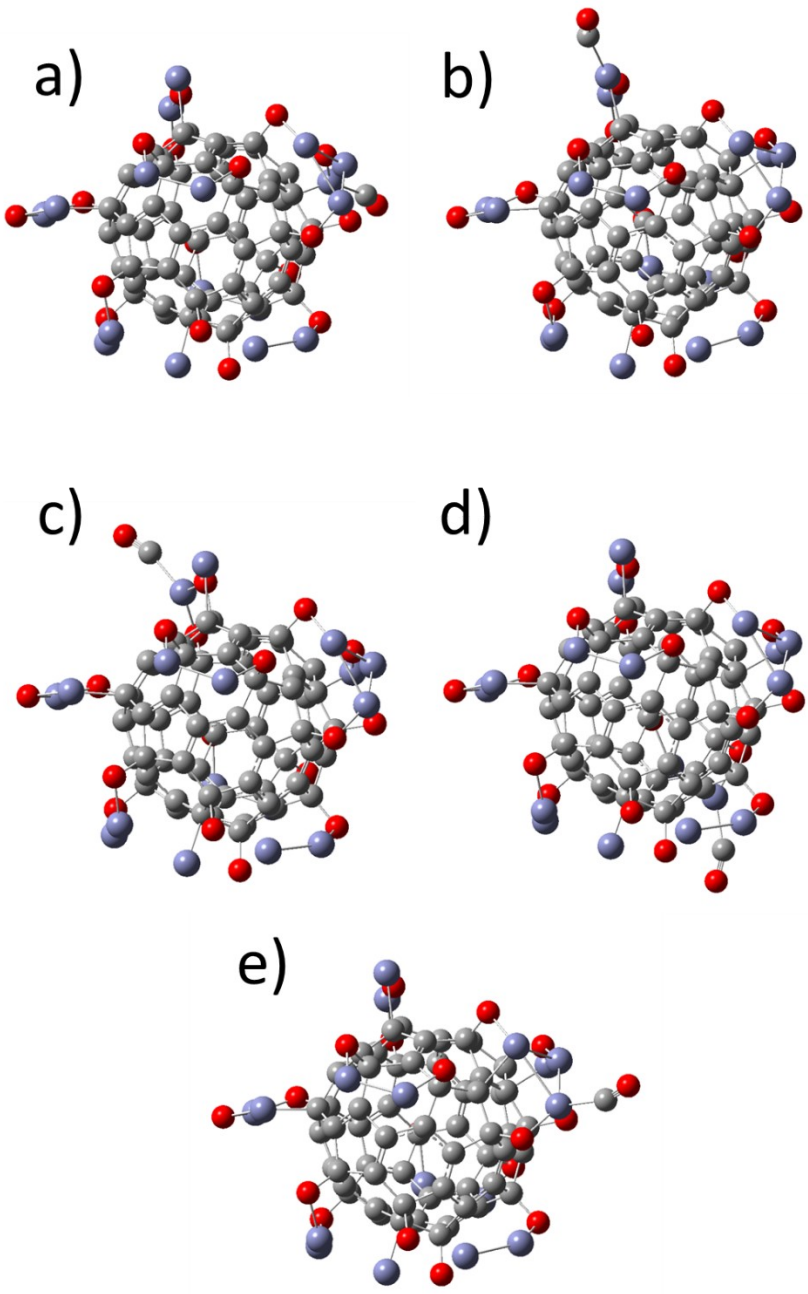

Figure S10. Optimized atomic configurations for a single CO molecule chemisorbed at five different Zn sites in the $C_{60}(ZnO)_{17}$ fullerene compound.

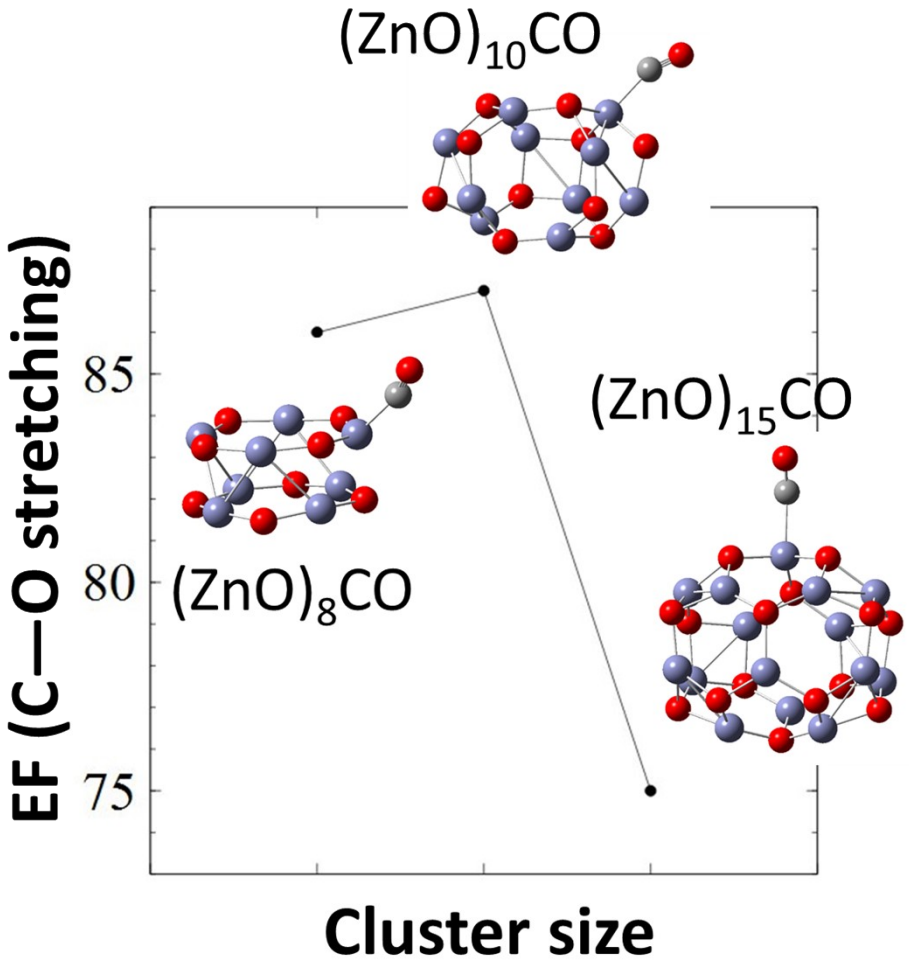

Figure S11. The behavior of the EF value for the C—O stretching mode in the $(ZnO)_8CO$, $(ZnO)_{10}CO$, and $(ZnO)_{15}CO$ clusters shown a insets in the figure (see text).

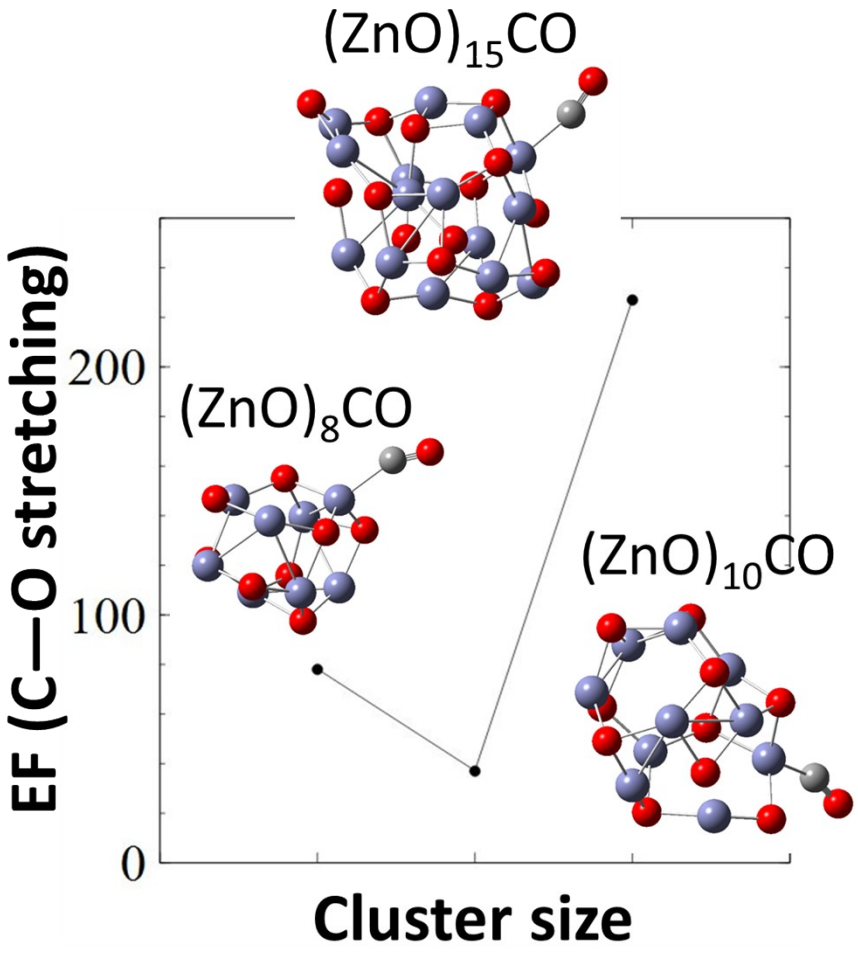

Figure S12. The behavior of the EF value for the C—O stretching mode in the $(ZnO)_8CO$, $(ZnO)_{10}CO$, and $(ZnO)_{15}CO$ clusters shown a insets in the figure (see text).

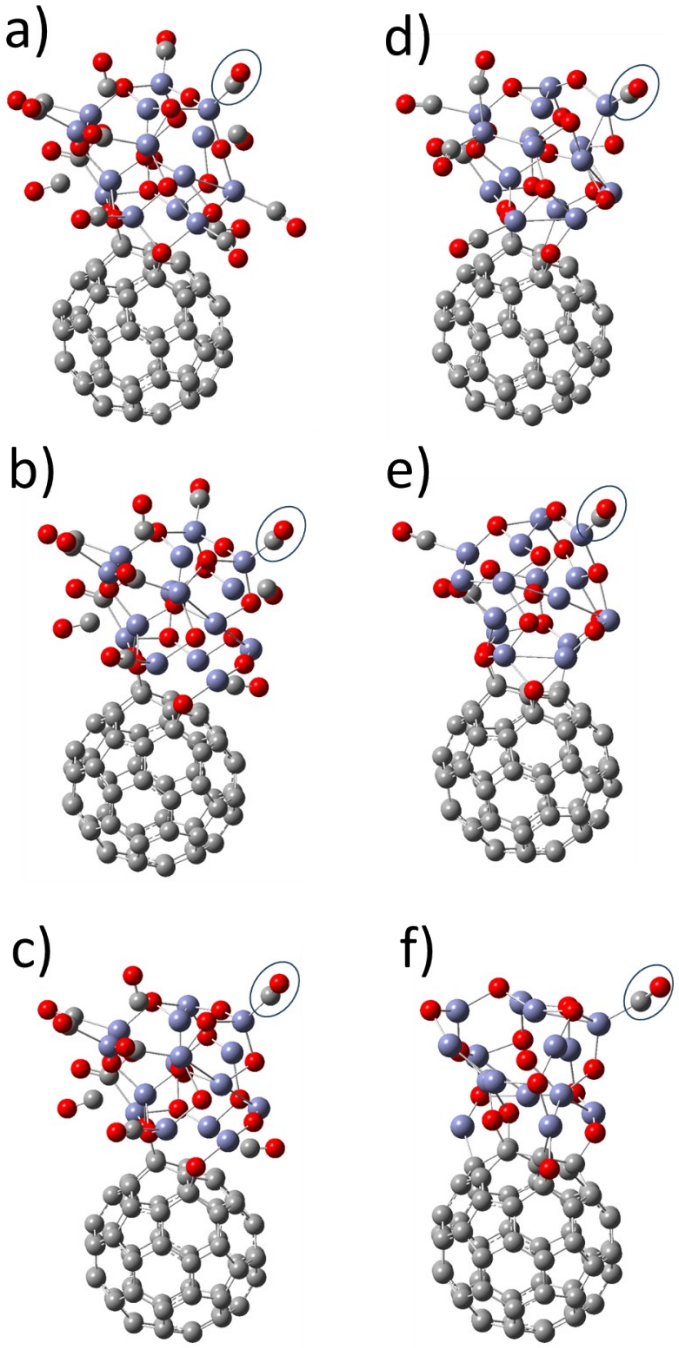

Figure S13. Optimized atomic configurations for the a) $C_{60}(ZnO)_{15}(CO)_{14}$, b) $C_{60}(ZnO)_{15}(CO)_{12}$, c) $C_{60}(ZnO)_{15}(CO)_{10}$, d) $C_{60}(ZnO)_{15}(CO)_{7}$, e) $C_{60}(ZnO)_{15}(CO)_{3}$, and f) $C_{60}(ZnO)_{15}(CO)_{1}$ fullerene compounds. The selected CO probe molecule is specified in all the figures (see text).

Optimized Cartesian atomic coordinates (Å) of the optimized structures at the PBE/6-31g** level of theory.

Figure 1a

C	1.23715	-0.02494	-3.48363
C	1.93017	-1.22743	-3.04009
C	1.19326	-2.34485	-2.60962
C	-0.25993	-2.30073	-2.60519
C	-0.93185	-1.13333	-3.01732
C	-0.16659	0.02132	-3.46704
C	2.00635	1.13036	-3.04028
C	3.16779	0.64263	-2.31415
C	3.12018	-0.81538	-2.31365
C	3.53411	-1.53194	-1.17773
C	1.62389	-3.08953	-1.43225
C	-0.72741	-3.01355	-1.43173
C	-1.84153	-2.526	-0.72538
C	-2.54956	-1.34044	-1.16626
C	-2.09258	-0.65232	-2.29298
C	-2.04557	0.82075	-2.29165
C	-0.85452	1.22273	-3.02189
C	-0.11062	2.34176	-2.60634
C	1.34314	2.29268	-2.60957
C	3.62794	1.33081	-1.17821
C	2.94156	2.53325	-0.72847
C	1.8202	3.00671	-1.43097
C	0.65839	3.49351	-0.70188
C	-0.53274	3.0784	-1.43128
C	-1.67829	2.66121	-0.72872
C	-2.46503	1.54173	-1.18166
C	-3.24385	0.94227	0.
C	-3.17482	-0.66906	-0.00004
C	0.43373	-3.50445	-0.70248
C	-0.93188	-1.13348	3.01726
C	-0.25995	-2.30085	2.60507
C	1.19324	-2.34498	2.60951
C	1.93014	-1.22758	3.04004
C	1.23712	-0.02511	3.48363
C	-0.85455	1.22259	3.02193
C	-2.04559	0.82064	2.29166
C	-2.09261	-0.65243	2.29292
C	-2.54957	-1.3405	1.16617
C	-1.84154	-2.52604	0.72523
C	-0.72743	-3.01362	1.43157
C	1.62388	-3.0896	1.43211
C	2.77186	-2.68896	0.72874
C	3.5341	-1.53199	1.17769
C	3.12016	-0.81549	2.31364
C	3.16777	0.64252	2.31421
C	2.00632	1.13021	3.04035

C	1.34312	2.29256	2.60969
C	-0.11065	2.34164	2.60645
C	-2.46505	1.54168	1.1817
C	-1.67829	2.66117	0.72883
C	-0.53276	3.07833	1.43142
C	0.65838	3.49347	0.70205
C	1.82018	3.00664	1.43113
C	2.94156	2.53322	0.72861
C	3.62793	1.33075	1.17831
C	4.05227	0.58745	0.00003
C	4.00543	-0.81742	0.
C	0.43372	-3.50449	0.70231
C	2.77186	-2.68892	-0.72885
C	-0.16663	0.02115	3.46704
O	-4.60478	1.41347	-0.00001
Zn	-5.16116	-0.35467	0.

Figure 1b

C	-0.92818	3.75983	-0.03139
C	-0.06714	3.34292	-1.23011
C	-0.54695	2.62869	-2.32239
C	-1.86655	1.98074	-2.28047
C	-2.65696	2.0602	-1.12504
C	-2.31812	2.93935	0.01958
C	-0.00053	3.37595	1.1295
C	1.34067	3.21027	0.64961
C	1.30386	3.18712	-0.82273
C	2.19044	2.38875	-1.54184
C	0.34606	1.75938	-3.05983
C	-1.7667	0.72564	-2.98801
C	-2.46587	-0.40709	-2.52114
C	-3.2961	-0.32378	-1.3445
C	-3.36305	0.89279	-0.65345
C	-3.32241	0.91302	0.81235
C	-2.5918	2.0988	1.20636
C	-1.74257	2.05031	2.31807
C	-0.42273	2.6959	2.27033
C	2.26338	2.41118	1.33841
C	1.82666	1.70711	2.51909
C	0.50606	1.84816	2.98775
C	-0.2156	0.68146	3.46535
C	-1.60582	0.81351	3.05246
C	-2.33143	-0.32833	2.65519
C	-3.23067	-0.26991	1.53935
C	-3.40968	-1.67216	0.93967
C	-3.33845	-1.64218	-0.66837
C	-0.40055	0.57949	-3.46645
C	0.00053	-3.37594	-1.1295
C	0.42273	-2.69588	-2.27033
C	1.74256	-2.05029	-2.31807

C	2.59179	-2.09878	-1.20636
C	2.31811	-2.93933	-0.01958
C	0.06713	-3.3429	1.23011
C	-1.30386	-3.18711	0.82273
C	-1.34067	-3.21025	-0.64962
C	-2.26339	-2.41117	-1.33841
C	-1.82667	-1.7071	-2.51909
C	-0.50607	-1.84815	-2.98775
C	1.60582	-0.8135	-3.05246
C	2.33142	0.32835	-2.65518
C	3.23066	0.26993	-1.53934
C	3.3224	-0.91301	-0.81235
C	3.36304	-0.89277	0.65345
C	2.65695	-2.06019	1.12504
C	1.86654	-1.98073	2.28047
C	0.54695	-2.62868	2.32239
C	-2.19045	-2.38873	1.54184
C	-1.68995	-1.6368	2.65696
C	-0.34607	-1.75936	3.05983
C	0.40054	-0.57947	3.46646
C	1.7667	-0.72562	2.98802
C	2.46586	0.40711	2.52114
C	3.29609	0.32379	1.3445
C	3.33844	1.6422	0.66837
C	3.40967	1.67218	-0.93967
C	0.21559	-0.68145	-3.46535
C	1.68994	1.63682	-2.65696
C	0.92817	-3.75981	0.03139
O	-4.63971	-2.26103	1.407
Zn	-5.11838	-2.53413	-0.36227
O	4.6397	2.26105	-1.407
Zn	5.11843	2.53401	0.36227
O	-1.15594	5.18364	-0.04273
Zn	-2.97455	4.84288	0.00896
Zn	2.97454	-4.84287	-0.00896
O	1.15593	-5.18363	0.04273

Figure 1c

C	-2.56095	0.72384	-2.75738
C	-1.89612	-0.65047	-2.96102
C	-2.19925	-1.75067	-2.15285
C	-3.02856	-1.60099	-0.94272
C	-3.48369	-0.30339	-0.57994
C	-3.0665	0.80322	-1.32863
C	-1.32717	1.64616	-2.8974
C	-0.21438	0.92219	-3.42586
C	-0.56501	-0.50904	-3.46842
C	0.40119	-1.48463	-3.22197
C	-1.23313	-2.76764	-1.89477
C	-2.56839	-2.49148	0.03647

C	-2.48786	-2.04471	1.38936
C	-2.9508	-0.78036	1.79709
C	-3.76291	0.12095	0.89283
C	-3.10361	1.52357	0.89553
C	-2.86949	1.93851	-0.45986
C	-1.88343	2.87867	-0.7862
C	-1.08435	2.69621	-1.99967
C	1.10632	1.3027	-3.12444
C	1.32999	2.38845	-2.2132
C	0.25426	3.10257	-1.6674
C	0.29047	3.73059	-0.32362
C	-1.03559	3.39316	0.24932
C	-1.22029	2.92764	1.56042
C	-2.28324	2.00617	1.89315
C	-1.91173	1.22336	3.16942
C	-2.2093	-0.32244	2.95529
C	-1.58647	-3.50116	-0.59395
C	1.32715	-1.64446	2.89724
C	1.08442	-2.69461	1.99967
C	1.88355	-2.87703	0.78624
C	2.86972	-1.93696	0.46
C	3.06703	-0.80157	1.32891
C	1.89631	0.65211	2.9612
C	0.56512	0.51066	3.46846
C	0.2144	-0.92053	3.42582
C	-1.10628	-1.30107	3.12442
C	-1.32992	-2.38685	2.21321
C	-0.2542	-3.10097	1.66741
C	1.0357	-3.39155	-0.24929
C	1.22035	-2.92608	-1.5604
C	2.28324	-2.00455	-1.89304
C	3.10357	-1.52194	-0.8954
C	3.76279	-0.11941	-0.89285
C	3.48322	0.30504	0.57979
C	3.02873	1.60266	0.94279
C	2.19936	1.75228	2.15293
C	-0.40111	1.48622	3.22198
C	-0.06082	2.60851	2.3942
C	1.23321	2.76919	1.89478
C	1.58654	3.50274	0.59396
C	2.56846	2.49309	-0.03647
C	2.48796	2.04634	-1.38939
C	2.9509	0.782	-1.79717
C	2.20926	0.32404	-2.95526
C	1.91178	-1.22174	-3.16934
C	-0.29038	-3.72899	0.32364
C	0.06088	-2.60695	-2.3942
C	2.56105	-0.72229	2.75761
O	-2.55475	1.73476	4.35112
Zn	-3.39809	0.10152	4.56957
O	2.55495	-1.73317	-4.35096
Zn	3.39898	-0.10021	-4.56885

O	-3.66964	1.01487	-3.62373
Zn	-5.17282	0.74528	-2.60487
Zn	5.17235	-0.75222	2.6042
O	3.66903	-1.0142	3.62461
Zn	0.98191	5.61257	-0.14728
O	2.25837	4.74327	0.88168
O	-2.25828	-4.7417	-0.88165
Zn	-0.98173	-5.611	0.1472
Zn	5.86622	-0.338	0.50683
O	5.16896	-0.11386	-1.18425
O	-5.16904	0.11466	1.18446
Zn	-5.86711	0.33116	-0.50738

Figure 1d

C	-1.49804	-3.32015	-0.55186
C	-0.54418	-2.90038	-1.68145
C	0.86405	-2.8994	-1.54821
C	1.46391	-3.04863	-0.2898
C	0.60409	-3.13218	0.87522
C	-0.77831	-3.22376	0.79098
C	-2.54767	-2.18991	-0.64829
C	-2.38395	-1.46781	-1.90164
C	-1.14565	-1.93758	-2.51454
C	-0.37647	-1.01952	-3.31073
C	1.77799	-2.12517	-2.51931
C	2.80539	-2.31673	-0.23555
C	2.9434	-1.4952	0.9917
C	2.12451	-1.64054	2.16559
C	0.98179	-2.43735	2.11675
C	-0.2291	-2.03798	2.78723
C	-1.43263	-2.70723	2.11036
C	-2.47846	-1.65808	1.7654
C	-3.03962	-1.51524	0.45406
C	-2.8401	-0.17486	-2.07565
C	-3.55706	0.54364	-1.02457
C	-3.81126	-0.18976	0.35786
C	-3.17871	0.5654	1.53106
C	-2.52227	-0.38915	2.40134
C	-1.44429	0.03836	3.23139
C	-0.30006	-0.81945	3.42607
C	0.9118	0.05413	3.7805
C	2.20176	-0.41139	2.98272
C	2.75177	-1.50432	-1.51075
C	2.55706	2.56544	0.65165
C	3.40073	2.03278	-0.49462
C	2.51712	2.08645	-1.78367
C	1.3827	2.88496	-1.93118
C	0.92312	3.88252	-0.84902
C	0.55451	3.23234	1.63204
C	1.16288	2.31269	2.53679

C	2.43137	1.88603	1.91932
C	2.82633	0.56103	2.08119
C	3.32507	-0.13743	0.91121
C	3.51949	0.51443	-0.32417
C	2.50968	0.80346	-2.41915
C	1.45758	0.35971	-3.2462
C	0.31476	1.20582	-3.42908
C	0.2774	2.434	-2.73372
C	-0.95937	2.86169	-2.10057
C	-0.6781	3.7162	-0.94459
C	-1.42776	3.38722	0.23368
C	-0.89999	3.57087	1.6466
C	0.41246	1.42972	3.31237
C	-1.00991	1.40221	3.17437
C	-1.75519	2.42536	2.45896
C	-2.717	1.8622	1.48051
C	-2.53743	2.52222	0.19311
C	-2.87941	1.84709	-1.00348
C	-2.08196	2.03893	-2.16044
C	-2.25135	0.83148	-3.07754
C	-0.86277	0.34569	-3.64286
C	3.07091	-0.16607	-1.50387
C	1.01446	-1.01919	-3.20799
C	1.3888	3.34923	0.48766
O	1.14532	0.09001	5.19786
Zn	2.86222	-0.5656	4.90522
O	-3.19433	1.14283	-4.1295
Zn	-1.92312	0.54015	-5.34828
Zn	-2.30484	4.14097	3.38771
O	-1.11997	4.89647	2.16467
O	4.75664	2.51598	-0.59887
Zn	5.5977	0.82867	-0.56572
Zn	3.74715	-3.4357	-2.19953
O	2.48581	-3.01551	-3.45286
O	-2.02329	-3.67777	2.99174
Zn	-3.67748	-3.90604	2.22012
Zn	-5.60282	0.46573	-1.03597
O	-5.20628	-0.42725	0.56908
O	1.35717	5.21676	-1.05985
Zn	-0.41872	5.78323	-1.2313
O	4.16464	-3.15847	-0.37766
Zn	5.30173	-1.49508	-0.27937
Zn	-3.71011	-4.4218	0.05849
O	-2.11624	-4.58917	-0.83964

Figure 1e

C	-2.86049	-1.20328	-2.45669
C	-1.37608	-1.35205	-2.83061
C	-0.52717	-2.37005	-2.31706
C	-0.95793	-3.13087	-1.23989

C	-2.2421	-2.85784	-0.63542
C	-3.1387	-1.93708	-1.14602
C	-2.9172	0.32066	-2.19776
C	-1.72668	0.95464	-2.73041
C	-0.80198	-0.11448	-3.09779
C	0.6223	0.08653	-2.94043
C	1.01464	-2.35989	-2.46003
C	0.20387	-3.76962	-0.47391
C	0.01533	-3.52835	1.00924
C	-1.27575	-3.27933	1.61403
C	-2.37805	-2.96042	0.82199
C	-3.3595	-1.98296	1.22802
C	-4.07241	-1.41599	-0.01029
C	-4.00601	0.10219	0.00542
C	-3.5564	0.8834	-1.10743
C	-1.28001	2.19287	-2.29172
C	-2.00686	2.95082	-1.2715
C	-3.34052	2.3363	-0.66337
C	-3.24508	2.14094	0.85309
C	-3.79565	0.84273	1.19469
C	-3.37562	0.17419	2.38129
C	-3.17599	-1.26317	2.3811
C	-2.15929	-1.62109	3.46819
C	-1.09142	-2.68554	2.95475
C	1.39445	-2.91712	-1.0446
C	1.95735	-0.4147	2.89035
C	2.89592	-1.07427	1.92092
C	3.00668	-0.12638	0.70845
C	2.8811	1.24707	0.71156
C	2.39405	1.992	1.98257
C	0.4291	1.23204	3.46808
C	-0.15996	-0.02298	3.81241
C	0.80604	-1.07388	3.43394
C	0.3288	-2.29808	2.95235
C	0.98721	-2.92022	1.81802
C	2.17701	-2.31725	1.25856
C	2.75583	-0.86421	-0.48831
C	2.70246	-0.28823	-1.88526
C	2.2325	1.17895	-1.69394
C	2.51393	1.94911	-0.50718
C	1.44129	2.88329	-0.08422
C	1.29502	2.86903	1.33779
C	0.04428	3.08656	1.90844
C	-0.36083	2.49191	3.26487
C	-1.52708	-0.24615	3.71468
C	-2.38242	0.78545	3.20285
C	-1.93949	2.15353	2.99995
C	-2.27173	2.69174	1.65869
C	-1.08886	3.31089	1.07027
C	-0.94032	3.34529	-0.32877
C	0.33818	3.14374	-0.90556
C	0.19968	2.60876	-2.3393

C	1.08319	1.38473	-2.44411
C	2.02619	-2.02334	-0.13875
C	1.49895	-0.92585	-2.62148
C	1.69621	0.98807	2.88904
O	-2.8203	-2.07002	4.66655
Zn	-1.81896	-3.63323	4.59015
O	0.49696	3.5819	-3.34261
Zn	2.26303	3.88926	-2.88677
Zn	-2.02361	3.46458	4.54746
O	-0.17964	3.36336	4.39031
O	4.19207	-1.47835	2.39038
Zn	4.30347	-2.78056	1.054
Zn	0.96807	-4.766	-2.53086
O	1.43676	-3.28926	-3.51052
O	-5.45428	-1.80681	-0.01841
Zn	-6.19597	-0.69241	-1.26999
Zn	-3.36003	4.31175	-1.92962
O	-4.48711	3.12293	-1.01979
O	3.43352	2.69766	2.65099
Zn	4.44864	3.31414	1.30349
O	0.38235	-5.17895	-0.82843
Zn	3.15423	-3.94423	-0.71729
Zn	-5.21701	-0.57994	-3.25391
O	-3.70193	-1.55469	-3.56878
Zn	4.50142	-1.86045	-1.35675
O	3.99432	-0.4758	-2.49663
O	5.22214	3.90917	-0.14829
Zn	3.9853	3.66157	-1.43996

Figure 1f

C	-2.00654	-1.49884	-3.12683
C	-0.47426	-1.44896	-3.35129
C	0.43797	-2.29718	-2.68364
C	-0.02328	-3.09259	-1.62141
C	-1.36252	-3.06498	-1.20439
C	-2.28155	-2.20533	-1.81236
C	-2.29989	-0.00541	-2.94409
C	-1.17142	0.80266	-3.3616
C	-0.05892	-0.12234	-3.56667
C	1.26832	0.28548	-3.19949
C	1.96666	-2.07789	-2.57996
C	1.09193	-3.48883	-0.66474
C	0.66357	-3.29278	0.75216
C	-0.68773	-3.15668	1.12253
C	-1.80779	-3.47618	0.1977
C	-2.92086	-2.39896	0.4643
C	-3.19805	-1.76055	-0.83531
C	-3.68855	-0.42757	-0.94919
C	-3.21651	0.44365	-2.0358
C	-1.00552	2.10213	-2.91832

C	-1.99199	2.72983	-2.03232
C	-3.28575	1.8941	-1.58614
C	-3.35133	1.70316	-0.06899
C	-3.72158	0.36294	0.22439
C	-3.6938	-0.24385	1.61152
C	-3.04134	-1.65885	1.61898
C	-2.0651	-1.76653	2.82193
C	-0.79664	-2.3692	2.30091
C	2.20559	-2.52068	-1.09373
C	1.85685	0.08773	2.89491
C	2.96337	-0.45263	1.99231
C	3.09966	0.46065	0.74971
C	2.76259	1.81504	0.70325
C	1.98664	2.47097	1.86378
C	-0.03967	1.42637	3.05774
C	-0.48402	0.18469	3.51495
C	0.75605	-0.78248	3.54091
C	0.47746	-1.94344	2.65652
C	1.39947	-2.48965	1.69226
C	2.46387	-1.7221	1.27314
C	3.24223	-0.3105	-0.42071
C	3.22176	0.23752	-1.83655
C	2.52166	1.62253	-1.77004
C	2.40162	2.37666	-0.55132
C	1.20611	3.19624	-0.33005
C	0.86263	3.17009	1.06038
C	-0.47288	3.20882	1.43496
C	-0.97407	2.54334	2.71815
C	-1.77366	-0.27487	3.04236
C	-2.68154	0.55329	2.43559
C	-2.41998	1.96924	2.24319
C	-2.61998	2.43491	0.86321
C	-1.49281	3.23236	0.42793
C	-1.14882	3.28479	-0.9429
C	0.21237	3.28042	-1.31191
C	0.39397	2.71441	-2.72506
C	1.44513	1.62009	-2.65204
C	2.77157	-1.66192	-0.13264
C	2.22572	-0.58035	-2.68966
C	1.35451	1.36771	2.70059
O	-2.46365	-2.37633	4.05757
Zn	-1.00443	-1.88854	5.11244
O	0.79883	3.67792	-3.69513
Zn	2.49819	4.06807	-3.06775
Zn	-2.94623	3.20437	3.76777
O	-1.07826	3.36906	3.88379
O	4.25948	-0.73296	2.54527
Zn	4.96832	-1.69165	1.11059
Zn	3.03061	-4.33551	-2.1945
O	2.65085	-2.9517	-3.46063
O	-7.02249	-0.2428	-0.83018
Zn	-5.96602	-0.45184	-2.26629

Zn	-3.47268	3.86519	-2.82525
O	-4.50021	2.4868	-2.08321
O	2.80679	3.34596	2.63223
Zn	3.94478	3.993	1.3912
O	1.42055	-4.94322	-0.94066
Zn	4.46375	-3.37711	-0.62296
Zn	-4.46168	-1.3273	-3.70916
O	-2.81127	-2.04718	-4.1654
Zn	5.3071	-0.89534	-1.10642
O	4.55763	0.22557	-2.37773
O	4.89311	4.66056	0.07491
Zn	4.05372	4.41084	-1.47945
O	-5.03318	-0.19507	2.12123
Zn	-6.09613	-0.19993	0.65505
Zn	-0.29167	0.28754	5.75496
O	0.91135	-1.22641	4.92309
O	-2.05246	-4.91495	0.19216
Zn	-0.3177	-5.36246	-0.28374

Figure 2a

C	-2.69081	-1.11586	1.14893
C	-3.55618	0.19559	1.64085
C	-3.72582	1.27103	0.5819
C	-3.58293	1.04019	-0.7881
C	-2.73197	-0.04587	-1.15429
C	-2.31849	-1.0238	-0.30775
C	-1.42209	-1.0755	1.96759
C	-1.43719	-0.02535	2.92858
C	-2.60654	0.80394	2.72593
C	-2.4467	2.18627	2.89558
C	-3.67848	2.69336	0.80539
C	-3.42956	2.29356	-1.4967
C	-2.56694	2.35989	-2.60584
C	-1.86072	1.17894	-3.07683
C	-2.19973	-0.21684	-2.56491
C	-0.92044	-1.03005	-2.21005
C	-1.19882	-1.83601	-0.93239
C	-0.05833	-1.69444	0.03796
C	-0.20576	-1.5362	1.44536
C	-0.18947	0.5043	3.41219
C	1.06251	0.02668	2.94128
C	1.1935	-1.20941	2.06313
C	1.93454	-0.79603	0.79704
C	1.20877	-1.24316	-0.34241
C	1.58321	-0.91201	-1.70853
C	0.34579	-0.60127	-2.52895
C	0.55813	0.70969	-3.14831
C	-0.55378	1.56719	-3.42865
C	-3.46594	3.33998	-0.48985
C	0.78686	4.59554	-1.76283

C	-0.42996	5.06902	-1.2502
C	-0.56583	5.31044	0.18332
C	0.52749	5.07986	1.03956
C	1.78815	4.59724	0.50747
C	2.62493	3.18208	-1.34211
C	1.92691	2.6711	-2.46637
C	0.79032	3.54985	-2.75915
C	-0.41247	3.01446	-3.22678
C	-1.6722	3.51016	-2.71665
C	-1.68306	4.51992	-1.73471
C	-1.90324	4.91541	0.583
C	-2.11355	4.28754	1.83237
C	-0.98017	4.04294	2.71104
C	0.31072	4.44141	2.33164
C	1.44178	3.56536	2.5941
C	2.35797	3.66212	1.47225
C	3.05507	2.52928	1.03393
C	3.49302	2.32325	-0.44334
C	1.78965	1.26696	-2.68554
C	2.3912	0.34316	-1.73387
C	3.11512	0.8199	-0.64461
C	2.83256	0.24127	0.67501
C	2.8296	1.28322	1.689
C	1.94844	1.15461	2.80659
C	1.25178	2.34565	3.26762
C	-0.08382	1.93797	3.6488
C	-1.18215	2.75396	3.35858
C	-2.60124	4.43612	-0.60158
C	-3.0175	3.16188	1.94538
C	1.92468	4.34491	-0.8732
Zn	5.47801	0.82502	-0.40189
O	4.89278	2.54354	-0.64488
O	-1.5242	-3.22572	-1.09555
Zn	-0.11323	-4.23415	-0.01207
Zn	2.60867	-3.22747	1.11413
O	1.87161	-2.33577	2.61262
Zn	-2.17966	-3.65037	0.90817
O	-3.45421	-2.31666	1.40666
O	-3.25871	-0.89336	-3.22656
Zn	-4.45192	-1.46406	-1.84335
Zn	2.51047	-2.79658	-1.41179
O	1.69986	-4.19695	-0.33362
O	4.02847	-2.83804	-0.18125
Zn	5.0514	-1.35586	-0.08769
Zn	-5.05631	-1.45743	0.40707
O	-4.86909	-0.20769	1.90533

Figure 2b

C	1.45574	-1.88049	1.22992
C	-0.07921	-2.06919	1.74932

C	-1.10171	-1.66524	0.73211
C	-0.83481	-1.5402	-0.57781
C	0.49304	-1.48629	-1.05323
C	1.55567	-1.54396	-0.23016
C	1.95327	-0.71196	2.03736
C	0.94711	-0.26547	2.99372
C	-0.24562	-0.99787	2.8396
C	-1.50855	-0.28881	2.92523
C	-2.57542	-1.5408	1.00075
C	-2.04474	-1.59124	-1.47021
C	-1.68507	-0.60958	-2.59152
C	-0.36146	-0.42075	-3.02753
C	0.80411	-1.25248	-2.5089
C	2.09515	-0.41749	-2.22853
C	2.76643	-0.93917	-0.92582
C	3.14374	0.19106	0.03242
C	2.77836	0.21057	1.44487
C	0.95455	1.11552	3.39454
C	1.89566	2.03737	2.89239
C	3.05079	1.61448	2.01484
C	3.04419	2.43708	0.72265
C	3.1492	1.53365	-0.38199
C	2.94071	1.9443	-1.78773
C	2.15493	0.9097	-2.56816
C	1.04931	1.61028	-3.23338
C	-0.17791	0.95386	-3.4631
C	-3.10132	-1.06801	-0.42412
C	-2.44298	3.46626	-1.9037
C	-3.57112	2.5706	-1.41973
C	-3.51841	2.51761	0.12016
C	-2.96911	3.49502	0.9536
C	-2.05546	4.43156	0.3823
C	-0.39154	4.53183	-1.49045
C	-0.19607	3.679	-2.63367
C	-1.45533	2.99613	-2.85968
C	-1.42058	1.65348	-3.28461
C	-2.35617	0.67622	-2.70891
C	-3.23525	1.10302	-1.74099
C	-3.59034	1.18334	0.55872
C	-3.52893	0.72112	2.00003
C	-2.66345	1.77657	2.75649
C	-2.47306	3.07484	2.27977
C	-1.22286	3.7842	2.49176
C	-0.96406	4.60995	1.32598
C	0.36412	4.76019	0.87163
C	0.6436	4.70858	-0.56507
C	1.03536	2.98722	-2.80329
C	2.12067	3.19496	-1.87542
C	1.91434	4.03517	-0.76707
C	2.39808	3.64715	0.55383
C	1.44866	4.10793	1.5667
C	1.20562	3.29748	2.69721

C	-0.16713	3.15462	3.1761
C	-0.3295	1.79321	3.60726
C	-1.53201	1.11614	3.36266
C	-3.44923	0.28915	-0.55597
C	-2.61787	-0.50391	2.08817
C	-1.77994	4.36047	-1.03376
O	-4.91854	2.81843	-1.8647
Zn	-5.75421	1.3691	-1.03775
Zn	-1.7266	-3.7655	0.19212
O	-3.15892	-2.87798	1.24959
O	3.86503	-1.85016	-1.12094
Zn	5.46012	-1.04289	-0.14727
Zn	5.36448	1.13198	1.14513
O	4.38241	1.64561	2.59805
O	-2.13318	-3.00981	-1.77884
Zn	-4.78279	-2.24243	0.23569
Zn	3.96739	-2.56314	0.80951
O	2.20832	-3.14063	1.38966
Zn	-5.76341	-0.05004	0.79561
O	-4.86402	0.42839	2.39923
O	0.89597	-2.55156	-3.08121
Zn	-0.12907	-3.63358	-1.88245
Zn	4.93253	1.64521	-1.76805
O	6.08144	0.77684	-0.5624
Zn	0.75469	-4.15415	0.40965
O	-0.35737	-3.45975	1.93513

Figure 2c

C	0.01291	2.74683	1.17268
C	1.50402	2.30901	1.6831
C	2.26056	1.5064	0.67328
C	1.94294	1.45878	-0.63148
C	0.69305	1.91179	-1.09885
C	-0.24241	2.41007	-0.27086
C	-0.91458	1.91696	2.03141
C	-0.1556	1.12187	2.98423
C	1.2328	1.29864	2.80523
C	2.09833	0.1428	2.91219
C	3.55017	0.7857	0.94302
C	3.05233	0.98454	-1.52877
C	2.31766	0.20198	-2.61945
C	1.01427	0.53005	-3.02625
C	0.28889	1.77504	-2.54453
C	-1.2263	1.53508	-2.22165
C	-1.59989	2.33121	-0.94066
C	-2.38675	1.49266	0.06041
C	-2.06135	1.38521	1.47317
C	-0.71019	-0.12746	3.44067
C	-1.95026	-0.60861	2.97417
C	-2.87388	0.21147	2.08608

C	-3.1322	-0.58927	0.82086
C	-2.91849	0.25372	-0.31616
C	-2.94303	-0.26885	-1.67848
C	-1.83685	0.3345	-2.51476
C	-1.09905	-0.77771	-3.12445
C	0.29552	-0.67791	-3.40904
C	3.80189	0.09945	-0.46651
C	1.36011	-3.82089	-1.7872
C	2.74216	-3.44031	-1.32782
C	2.76295	-3.33178	0.20957
C	1.8698	-3.95576	1.06615
C	0.62353	-4.44728	0.52102
C	-0.96029	-4.00483	-1.3148
C	-0.78892	-3.14403	-2.42668
C	0.65748	-3.03265	-2.71339
C	1.15641	-1.79386	-3.22594
C	2.40399	-1.25559	-2.69316
C	3.04356	-1.97416	-1.70015
C	3.40832	-2.13421	0.60464
C	3.52549	-1.62742	2.03293
C	2.31972	-2.21866	2.81844
C	1.61239	-3.34141	2.38324
C	0.18589	-3.47161	2.6205
C	-0.42096	-4.15691	1.49512
C	-1.70378	-3.79748	1.06146
C	-2.17279	-3.9506	-0.41277
C	-1.63479	-2.0231	-2.65618
C	-2.69326	-1.73886	-1.70619
C	-2.90546	-2.58238	-0.61465
C	-3.08024	-1.95721	0.69351
C	-2.38543	-2.73341	1.71891
C	-1.82672	-2.04653	2.82856
C	-0.51183	-2.45321	3.29617
C	0.19365	-1.25827	3.67527
C	1.5609	-1.13815	3.39978
C	3.54061	-1.28469	-0.54102
C	3.18554	-0.14132	2.06879
C	0.35868	-4.36272	-0.87169
Zn	-4.66141	-4.14904	-0.34934
O	-3.08264	-5.04615	-0.57268
O	3.85263	-4.25666	-1.77061
Zn	5.24486	-3.32261	-0.97977
Zn	3.67651	3.14469	0.07327
O	4.67034	1.75023	1.13269
O	-2.23773	3.59491	-1.17854
Zn	-3.95693	3.3182	-0.09871
Zn	-5.27095	0.78328	1.10948
O	-4.13428	0.6305	2.61214
O	3.72515	2.22849	-1.86451
Zn	5.77728	0.42283	0.13711
Zn	-2.01784	4.39732	0.73476
O	-0.13928	4.20286	1.25953

Zn	5.81535	-2.00895	0.849
O	4.87064	-1.86968	2.46612
O	0.73187	2.97357	-3.16708
Zn	2.11641	3.59638	-1.99938
Zn	-4.91911	0.49078	-1.39376
O	-5.31069	2.0946	-0.36234
O	-6.07228	-0.48494	-0.16228
Zn	-5.85426	-2.27242	-0.05263
Zn	1.57208	4.50935	0.27655
O	2.33795	3.46457	1.82968

Figure 2d

C	3.52551	-1.87389	0.98064
C	2.28673	-2.94825	1.05196
C	1.15203	-2.60126	0.14124
C	1.2806	-1.7471	-0.89297
C	2.39387	-0.89716	-1.02929
C	3.38316	-0.85833	-0.12031
C	3.4284	-1.15641	2.29001
C	2.38528	-1.69527	3.11665
C	1.67536	-2.7371	2.44843
C	0.24705	-2.77681	2.58957
C	-0.21517	-3.2425	0.15597
C	0.2077	-1.88419	-1.93009
C	-0.03614	-0.52511	-2.61993
C	1.04391	0.47437	-2.40336
C	2.4855	0.10595	-2.14388
C	3.23355	1.17933	-1.27221
C	4.13961	0.44587	-0.25115
C	4.08431	1.01073	1.17811
C	3.64955	0.22993	2.28731
C	1.77127	-0.85078	4.10977
C	2.11734	0.5382	4.19012
C	3.06359	1.09202	3.2932
C	2.96375	2.4015	2.75968
C	3.76176	2.46319	1.43522
C	2.93869	3.15245	0.27537
C	2.70118	2.40695	-1.0014
C	1.36141	2.90869	-1.63309
C	0.5609	1.70863	-2.05571
C	-0.90484	-2.37124	-0.96544
C	-2.76211	2.17322	-0.24362
C	-3.12823	0.61181	-0.31357
C	-2.90267	-0.10867	1.00989
C	-2.89059	0.47178	2.25572
C	-2.52999	1.88008	2.35269
C	-1.23298	3.51266	1.10926
C	-0.76732	3.67791	-0.32208
C	-1.49527	2.49134	-0.99567
C	-0.84334	1.61717	-1.81046

C	-1.41061	0.31499	-2.35333
C	-2.27004	-0.27432	-1.27583
C	-2.41053	-1.4273	0.76927
C	-2.01837	-2.35865	1.89204
C	-1.65897	-1.53801	3.11962
C	-2.28995	-0.27703	3.39758
C	-1.46395	0.7169	4.11372
C	-1.63667	2.0162	3.48188
C	-0.5495	2.91855	3.39677
C	-0.34607	3.6728	2.18641
C	0.71194	3.51653	-0.41254
C	1.59188	3.66412	0.63438
C	1.09119	3.7902	1.96766
C	1.77612	3.12444	3.03264
C	0.753	2.56515	3.92533
C	0.92187	1.30114	4.5053
C	-0.19118	0.36506	4.60037
C	0.36032	-0.95921	4.33905
C	-0.38658	-1.88966	3.58838
C	-1.76251	-1.35447	-0.49849
C	-0.70452	-3.0566	1.56863
C	-2.34694	2.63807	1.18198
O	1.36452	3.88605	-2.68956
Zn	-0.40342	4.53137	-2.78918
O	-4.52713	0.40745	-0.64819
Zn	-3.97873	-1.47611	-1.51677
Zn	1.54125	-4.22617	-1.32927
O	-0.1947	-4.62953	-0.40611
O	5.50232	0.33755	-0.68408
Zn	6.17246	1.35345	1.14478
O	-6.7056	1.63411	0.76717
Zn	-5.94728	0.04141	1.11009
O	0.75426	-2.90552	-2.8103
Zn	-1.90634	-4.04621	-1.41033
Zn	6.07669	-1.00311	0.69202
O	4.80523	-2.54628	0.67364
Zn	-4.3346	-2.57762	0.61465
O	-3.22866	-3.14308	2.22932
O	-5.5207	-1.57559	1.86173
Zn	-4.11423	-1.56676	3.13582
O	-1.16833	4.91402	-0.95921
Zn	-2.69776	4.15271	-2.14104
O	3.09857	-0.5724	-3.2312
Zn	2.84984	-2.42136	-2.79157
Zn	4.50765	4.41682	0.24505
O	5.12554	3.10508	1.52511
Zn	3.96833	-3.50423	-0.87182
O	2.70282	-4.2244	0.53042
Zn	-0.86251	-0.59061	-4.41365
O	-2.12111	0.55182	-3.58085
Zn	-5.40651	2.22948	-0.31708
O	-3.80012	3.02522	-0.82487

Figure 2e

C	-0.61369	1.49507	-0.06096
C	-0.93513	0.24638	-0.90471
C	-0.94597	-1.06941	-0.14526
C	-0.63971	-1.19345	1.37005
C	-0.36148	0.10884	2.16937
C	-0.26627	1.38498	1.38804
C	0.10668	2.56133	-0.93716
C	0.57431	1.72302	-2.09866
C	0.06466	0.42565	-2.01193
C	0.63558	-0.67166	-2.66958
C	-0.27389	-2.28049	-0.87894
C	0.45052	-2.23273	1.44852
C	1.43486	-2.21154	2.44231
C	1.65695	-0.99527	3.23475
C	0.86496	0.12806	2.99767
C	1.49873	1.43008	2.94924
C	0.83886	2.21113	1.93893
C	1.55284	3.10486	1.1385
C	1.27488	3.21507	-0.28603
C	1.79308	1.93187	-2.7918
C	2.79452	2.76865	-2.20784
C	2.52328	3.38224	-0.9415
C	3.59422	3.41764	0.06698
C	2.98479	3.26381	1.36659
C	3.635	2.50627	2.36215
C	2.88129	1.58595	3.19092
C	3.69474	0.41408	3.44133
C	3.08346	-0.85546	3.44567
C	0.64515	-2.88705	0.20505
C	5.2169	-2.45236	0.8702
C	4.22373	-3.26047	0.28372
C	3.96828	-3.18369	-1.15077
C	4.72021	-2.2916	-1.93822
C	5.74215	-1.45282	-1.32977
C	6.21218	-0.31753	0.82061
C	5.59049	-0.48664	2.12571
C	4.97225	-1.80629	2.15287
C	3.73987	-1.98549	2.79925
C	2.71168	-2.81456	2.1901
C	2.9463	-3.43792	0.94417
C	2.53736	-3.33891	-1.36242
C	1.88968	-2.56925	-2.34407
C	2.68019	-1.65464	-3.17263
C	4.06132	-1.51407	-2.97935
C	4.67285	-0.19155	-3.01213
C	5.71036	-0.15687	-1.98945
C	5.9192	1.0184	-1.24426
C	6.18354	0.93762	0.18597
C	4.96454	0.60192	2.75957

C	4.92854	1.90235	2.09745
C	5.51938	2.05916	0.82981
C	4.83978	2.8338	-0.19855
C	5.09591	2.1921	-1.48696
C	4.09663	2.16771	-2.47039
C	3.88586	0.94927	-3.24601
C	2.45593	0.80123	-3.43491
C	1.87788	-0.47182	-3.39646
C	1.89787	-3.47943	-0.05508
C	0.61141	-1.95534	-2.07028
C	5.9934	-1.53555	0.05238
Zn	-3.84656	1.1622	-1.53268
Zn	-4.75429	-0.62838	1.38006
Zn	-3.90168	1.87983	0.85058
Zn	-2.62564	-2.34866	0.31997
Zn	-2.26837	0.01212	2.77495
O	-1.84609	-1.80058	2.04843
O	-3.52112	2.91199	-0.72999
O	-3.9528	0.75471	2.3923
O	-1.43469	-3.10423	-1.3189
O	-4.55514	-2.21078	0.42397
O	-2.16439	0.29814	-1.76527
Zn	-4.72573	-1.19328	-1.2306
O	-5.11853	0.54824	-0.22123
Zn	-1.74486	3.33428	-1.03829
O	-1.57187	2.02572	0.94106
Zn	-2.57155	-1.66722	-2.08645

Figure 2f

C	-0.01888	1.73391	-0.83978
C	-0.07419	0.36122	-1.7283
C	-0.29439	-1.0293	-0.98087
C	-0.29366	-1.13372	0.58081
C	-0.19227	0.18971	1.38305
C	-0.06911	1.56236	0.71041
C	1.2467	2.41747	-1.31847
C	1.81113	1.75889	-2.45106
C	1.18987	0.47328	-2.56276
C	1.94403	-0.60182	-3.0282
C	0.63855	-2.25333	-1.48857
C	0.77374	-2.13211	0.93058
C	1.44877	-2.13754	2.16029
C	1.44883	-0.94263	2.97482
C	0.74716	0.19638	2.4998
C	1.36768	1.49364	2.61814
C	0.96596	2.27457	1.47065
C	1.89631	3.19166	0.92043
C	2.03277	3.24854	-0.53414
C	3.15452	1.97847	-2.83504
C	3.98615	2.81878	-2.00839

C	3.43219	3.43602	-0.86675
C	4.17329	3.46786	0.37673
C	3.21759	3.30267	1.47379
C	3.59862	2.55546	2.61611
C	2.64571	1.63831	3.20291
C	3.36495	0.46794	3.6718
C	2.77026	-0.80213	3.5467
C	1.26738	-2.79218	-0.19551
C	5.48903	-2.41264	1.60421
C	4.6823	-3.21949	0.78997
C	4.79194	-3.13932	-0.66356
C	5.71447	-2.24652	-1.24335
C	6.56185	-1.41807	-0.40479
C	6.47412	-0.27957	1.79391
C	5.5331	-0.44153	2.89656
C	4.92981	-1.76228	2.78399
C	3.57511	-1.93754	3.10151
C	2.73964	-2.77061	2.25302
C	3.27505	-3.39948	1.11542
C	3.45811	-3.26528	-1.21174
C	3.07305	-2.49683	-2.3455
C	4.05338	-1.58859	-2.95408
C	5.3445	-1.46823	-2.42047
C	5.96484	-0.15552	-2.3016
C	6.71352	-0.1228	-1.05453
C	6.73732	1.05059	-0.28034
C	6.61788	0.9741	1.16979
C	4.76722	0.65018	3.3399
C	4.91016	1.94984	2.68607
C	5.82044	2.10035	1.61867
C	5.44707	2.88052	0.44932
C	6.0181	2.23439	-0.72815
C	5.30489	2.20886	-1.93746
C	5.27821	0.98946	-2.74167
C	3.94283	0.85177	-3.29525
C	3.34354	-0.41362	-3.40068
C	2.51947	-3.43447	-0.12069
C	1.79211	-1.88293	-2.40242
C	6.44394	-1.48994	0.99655
Zn	-1.93147	2.57026	0.59291
Zn	-3.04638	-2.37412	0.30598
Zn	-4.53522	1.30837	1.33472
Zn	-1.75957	-2.49841	-2.1401
Zn	-2.12479	-0.06183	2.02721
O	-1.48586	-1.87763	1.21552
O	-3.75153	2.88303	0.60989
O	-3.86413	0.27555	2.92707
O	-0.12174	-3.27824	-2.18422
O	-3.5146	-2.04562	-1.60125
O	-1.19287	0.47203	-2.68383
Zn	-4.99026	-0.93422	-0.50222
O	-3.19107	0.01314	0.3322

Zn	-2.45954	1.98305	-2.42597
O	-1.09655	2.63258	-1.19185
Zn	-2.35259	-0.33195	-1.30883
Zn	-4.63493	-1.21345	2.26553
O	-4.89272	-2.37359	0.91418
O	-5.68275	0.79423	-0.24488
Zn	-4.38625	1.96274	-1.11901

Figure 2g

C	-0.63962	-1.43479	-1.08275
C	-0.43372	0.17582	-1.34475
C	-0.24732	1.12785	-0.08397
C	-0.4868	0.52076	1.3773
C	-0.85585	-0.95373	1.47243
C	-1.05428	-1.78119	0.31209
C	-1.82055	-1.80341	-2.01512
C	-2.24865	-0.66429	-2.77167
C	-1.61732	0.50025	-2.22793
C	-2.24618	1.73407	-2.28131
C	-1.07588	2.51598	-0.09608
C	-1.51702	1.40066	2.03123
C	-2.36583	0.93797	3.05359
C	-2.53246	-0.48679	3.28609
C	-1.81833	-1.4066	2.48996
C	-2.49606	-2.56783	1.96239
C	-2.00143	-2.79436	0.6157
C	-2.85416	-3.34723	-0.37798
C	-2.76608	-2.79386	-1.72803
C	-3.53289	-0.5785	-3.36132
C	-4.50052	-1.61164	-3.06707
C	-4.12617	-2.69558	-2.25403
C	-5.03257	-3.16959	-1.22699
C	-4.23324	-3.56755	-0.06476
C	-4.73338	-3.31665	1.24397
C	-3.84156	-2.8269	2.28082
C	-4.57307	-1.88831	3.11524
C	-3.92325	-0.7351	3.60471
C	-1.8455	2.51038	1.23825
C	-6.29161	1.76696	2.23284
C	-5.35358	2.76246	1.92827
C	-5.2725	3.31407	0.57682
C	-6.1512	2.8292	-0.42234
C	-7.11721	1.79907	-0.10864
C	-7.36645	-0.15507	1.39608
C	-6.57696	-0.5498	2.55843
C	-5.9166	0.63891	3.07859
C	-4.61347	0.54859	3.58807
C	-3.63889	1.58174	3.26248
C	-3.99826	2.66981	2.45056
C	-3.88247	3.55752	0.28482

C	-3.37178	3.28487	-1.01805
C	-4.29565	2.78925	-2.05346
C	-5.65075	2.57404	-1.76565
C	-6.31913	1.38491	-2.2839
C	-7.22734	0.90489	-1.2574
C	-7.39544	-0.47675	-1.06038
C	-7.46945	-1.02041	0.28918
C	-5.92044	-1.79017	2.57997
C	-6.0174	-2.68358	1.42487
C	-6.77807	-2.29542	0.30105
C	-6.28064	-2.55205	-1.04296
C	-6.66742	-1.42747	-1.88716
C	-5.79537	-0.96818	-2.88631
C	-5.6169	0.46686	-3.0875
C	-4.21472	0.69927	-3.37501
C	-3.57623	1.84283	-2.8654
C	-3.08805	3.15259	1.43231
C	-2.1155	2.65508	-1.18908
C	-7.18818	1.26837	1.1961
Zn	2.08028	-2.16062	-0.18872
Zn	1.71978	1.17231	0.58716
Zn	4.67393	-2.59712	0.56237
Zn	1.34615	3.09062	-0.89801
Zn	0.95779	-1.35388	2.31887
O	0.78572	0.62097	2.19689
O	3.77389	-2.82524	-1.00796
O	2.59584	-2.03533	1.72968
O	-0.19506	3.67443	-0.18694
O	2.97194	2.54017	-1.57283
O	0.62649	0.33992	-2.33926
Zn	4.26791	1.47946	-0.5704
O	2.81001	-0.19918	-0.31366
Zn	1.65377	-1.31074	-2.73047
O	0.56818	-2.21777	-1.42002
Zn	2.51571	0.80575	-2.25216
Zn	3.76697	-0.4367	1.53279
O	3.71356	1.56862	1.42308
O	5.45727	0.14979	-1.25524
Zn	4.08517	-1.08678	-1.88305
Zn	6.46431	0.02506	0.39062
O	5.53756	-1.29253	1.49856
Zn	5.45922	1.95457	1.84765
O	7.07887	1.56476	1.27733

Figure 2h

C	0.56695	-0.86527	0.47816
C	0.53993	0.72261	0.85591
C	0.81219	1.72222	-0.3455
C	1.19771	1.14445	-1.74195
C	1.5249	-0.31387	-1.80326

C	1.28478	-1.20238	-0.78192
C	1.27676	-1.60181	1.71904
C	1.85186	-0.48174	2.53026
C	1.54555	0.77464	1.98441
C	2.36187	1.89861	2.22013
C	1.81881	2.96421	-0.0698
C	2.44225	1.92173	-2.19246
C	3.43241	1.36335	-3.03192
C	3.45544	-0.07985	-3.32356
C	2.49977	-0.89936	-2.73317
C	2.84999	-2.20543	-2.22739
C	2.07685	-2.40418	-1.01605
C	2.62148	-3.09107	0.06906
C	2.33732	-2.60926	1.40583
C	3.03932	-0.63188	3.31054
C	3.88449	-1.77064	3.13635
C	3.52544	-2.75112	2.15911
C	4.57052	-3.34076	1.30781
C	3.99989	-3.57021	0.00082
C	4.76753	-3.33616	-1.157
C	4.18117	-2.65934	-2.30387
C	5.1903	-1.79317	-2.88859
C	4.83136	-0.52988	-3.40466
C	2.80749	2.88914	-1.23433
C	7.21188	1.50042	-1.40543
C	6.38858	2.62381	-1.20899
C	6.12261	3.10692	0.14235
C	6.70231	2.44662	1.24428
C	7.54896	1.28455	1.0357
C	7.80533	-0.60756	-0.54441
C	7.21997	-0.81622	-1.86254
C	6.84601	0.4907	-2.39261
C	5.67138	0.63115	-3.14465
C	4.80033	1.78172	-2.92693
C	5.16027	2.76058	-1.97006
C	4.74466	3.55748	0.19464
C	3.97025	3.30671	1.33757
C	4.57474	2.63594	2.48211
C	5.91019	2.21431	2.44593
C	6.26986	0.90692	2.98076
C	7.28193	0.33535	2.10497
C	7.27587	-1.04812	1.83446
C	7.55198	-1.5274	0.48791
C	6.41145	-1.93748	-2.10783
C	6.14623	-2.89083	-1.03678
C	6.70139	-2.68156	0.23908
C	5.89778	-2.91384	1.43074
C	6.2592	-1.90152	2.42277
C	5.27415	-1.35127	3.25905
C	5.28389	0.07745	3.54028
C	3.8983	0.51715	3.56704
C	3.56022	1.76158	3.04017

C	4.14333	3.31955	-1.12009
C	2.60109	2.85865	1.21468
C	7.81037	0.82114	-0.27081
Zn	-2.18028	-0.27811	1.27922
Zn	-1.53579	1.21433	-1.28487
Zn	-2.98276	-3.03698	1.13327
Zn	-0.53074	3.36717	-0.35201
Zn	-0.64975	-0.56472	-2.96225
O	0.00665	1.22256	-2.62043
O	-3.2959	-1.53771	2.1875
O	-1.39146	-2.25674	-2.61478
O	1.09979	4.19994	-0.05985
O	-2.28287	3.77378	0.22002
O	-0.72925	1.02843	1.47442
Zn	-5.00792	0.64325	-0.36681
O	-3.03713	1.03803	-0.00794
Zn	-0.24644	-2.85346	1.85315
O	-0.79337	-1.32689	0.28731
Zn	-2.32284	2.35905	1.63527
Zn	-3.18165	-1.58033	-2.32196
O	-2.45199	0.35091	-2.87129
O	-5.81447	-0.66016	0.74519
Zn	-4.96937	-0.54699	2.46983
Zn	-5.08034	-1.87823	-0.46205
O	-3.54805	-2.92756	-0.73044
Zn	-4.22194	0.95197	-2.71865
O	-4.92401	-0.76419	-2.09824
Zn	-3.79918	1.73508	3.26264
O	-5.12882	0.6807	3.801
O	-5.04943	2.23409	-1.56547
Zn	-3.69676	3.06649	-0.66651
O	-1.33012	-3.96141	0.82289
Zn	-1.34989	-2.9955	-0.87732

Figure 6a

C	1.68427	1.17878	-3.32965
C	0.15382	0.97135	-3.46426
C	-0.79689	1.82524	-2.85882
C	-0.34977	2.7498	-1.88374
C	0.99131	2.88085	-1.5457
C	1.96016	2.04746	-2.11638
C	2.12903	-0.25527	-3.01196
C	1.07719	-1.20718	-3.29612
C	-0.13099	-0.41329	-3.5422
C	-1.36752	-0.89041	-3.04845
C	-2.24045	1.45421	-2.59188
C	-1.45778	3.18586	-0.94205
C	-0.96354	3.21396	0.48349
C	0.413	3.17765	0.78612
C	1.45939	3.48551	-0.22734

C	2.67945	2.54128	0.09007
C	2.96044	1.79388	-1.1542
C	3.56222	0.50337	-1.15278
C	3.12807	-0.5194	-2.1162
C	1.04847	-2.45712	-2.71131
C	2.1152	-2.88954	-1.80585
C	3.34593	-1.90168	-1.52162
C	3.45804	-1.54149	-0.03843
C	3.71615	-0.15108	0.09407
C	3.69815	0.59787	1.41015
C	2.92273	1.94414	1.30522
C	1.99157	2.09663	2.53724
C	0.64809	2.52938	2.02644
C	-2.53631	2.10775	-1.1986
C	-1.7322	-0.06486	3.0055
C	-2.92386	0.28829	2.12691
C	-3.06163	-0.76356	0.99422
C	-2.60097	-2.09062	1.06628
C	-1.70474	-2.54269	2.24296
C	0.27727	-1.21073	3.21428
C	0.62681	0.10634	3.50897
C	-0.6907	0.96039	3.50407
C	-0.56429	2.04068	2.49083
C	-1.57982	2.41921	1.53957
C	-2.56089	1.5086	1.24929
C	-3.22408	-0.13311	-0.24403
C	-3.25934	-0.80861	-1.57247
C	-2.46687	-2.13497	-1.42437
C	-2.24293	-2.7526	-0.14069
C	-0.9603	-3.42918	0.09622
C	-0.55817	-3.22524	1.45649
C	0.79078	-3.11202	1.76461
C	1.2898	-2.27385	2.94374
C	1.84971	0.62009	2.9313
C	2.8011	-0.19028	2.36709
C	2.65808	-1.63549	2.33706
C	2.83476	-2.22663	1.00236
C	1.76672	-3.15878	0.71457
C	1.36942	-3.38716	-0.6226
C	-0.00144	-3.53901	-0.92028
C	-0.28506	-3.15859	-2.37715
C	-1.42818	-2.15508	-2.36344
C	-2.95586	1.27485	-0.13074
C	-2.40079	-0.04419	-2.60702
C	-1.13219	-1.30798	2.91961
O	2.37316	2.88184	3.67447
Zn	1.08013	2.32482	4.90106
O	-0.62559	-4.26852	-3.20835
Zn	-2.19157	-4.80019	-2.39274
Zn	3.35895	-2.66948	3.94149
O	1.51547	-2.94887	4.18638
O	-4.17179	0.57976	2.76198

Zn	-4.94569	1.63871	1.44924
Zn	-3.53386	3.69257	-2.34508
O	-3.2272	2.08	-3.57987
O	6.89931	0.61248	-1.20036
Zn	5.74902	0.57893	-2.58121
Zn	3.66548	-3.99517	-2.51395
O	4.58481	-2.43603	-2.02115
O	-2.39223	-3.38286	3.1645
Zn	-3.48227	-4.32794	2.08587
O	-1.90734	4.53021	-1.36478
Zn	-4.76372	2.76424	-0.56842
Zn	4.11426	1.18566	-4.02183
O	2.38039	1.6792	-4.46809
Zn	-4.32645	0.49881	-3.33433
O	-4.64843	-0.82884	-2.05443
O	-4.37246	-5.29374	0.92362
Zn	-3.6211	-5.0806	-0.68095
O	5.05978	0.71359	1.84578
Zn	6.04903	0.64414	0.32966
Zn	0.51948	0.20427	5.75828
O	-0.82438	1.53921	4.83187
O	1.52828	4.91535	-0.36004
Zn	-0.31737	5.3235	-0.42734
C	-0.9892	7.07828	0.32171
O	-1.43083	7.93615	0.9418

Figure 6b

C	-2.04512	-0.75864	-3.31224
C	-0.52885	-0.58865	-3.56472
C	0.43301	-1.54924	-3.18619
C	0.04136	-2.62199	-2.36544
C	-1.2773	-2.75291	-1.90524
C	-2.24672	-1.79838	-2.2255
C	-2.38584	0.61836	-2.72572
C	-1.29103	1.55104	-2.95168
C	-0.16233	0.76388	-3.43485
C	1.168	1.11032	-3.01494
C	1.95667	-1.30617	-3.07688
C	1.20707	-3.21504	-1.58982
C	0.83777	-3.4243	-0.1586
C	-0.49789	-3.44814	0.28266
C	-1.64866	-3.54581	-0.65478
C	-2.77757	-2.62317	-0.06779
C	-3.13525	-1.66956	-1.13396
C	-3.67565	-0.37581	-0.86658
C	-3.27187	0.77469	-1.69523
C	-1.1337	2.67586	-2.16677
C	-2.09544	2.99387	-1.10061
C	-3.33067	2.04818	-0.86151
C	-3.35988	1.45158	0.5481

C	-3.67714	0.06682	0.47944
C	-3.55588	-0.89174	1.64883
C	-2.86431	-2.22746	1.24752
C	-1.83523	-2.61936	2.34178
C	-0.57522	-3.01194	1.6338
C	2.26803	-2.1216	-1.77671
C	2.03243	-0.70442	2.77586
C	3.11336	-0.93736	1.72361
C	3.16991	0.28323	0.77099
C	2.79624	1.58739	1.10524
C	2.05145	1.87088	2.42781
C	0.10888	0.46524	3.36445
C	-0.27871	-0.87016	3.48314
C	0.98629	-1.75931	3.20134
C	0.70051	-2.64651	2.04461
C	1.5932	-2.87456	0.93634
C	2.61848	-1.98509	0.70536
C	3.27155	-0.13925	-0.56886
C	3.17692	0.76858	-1.78087
C	2.44407	2.05737	-1.31772
C	2.36635	2.45418	0.06363
C	1.15709	3.13461	0.54195
C	0.87597	2.72045	1.88457
C	-0.44293	2.60164	2.30149
C	-0.86946	1.59554	3.37179
C	-1.57425	-1.23335	2.94839
C	-2.5294	-0.30719	2.61815
C	-2.31779	1.11586	2.80715
C	-2.59414	1.92724	1.61292
C	-1.50776	2.85733	1.37694
C	-1.22373	3.28721	0.06183
C	0.11806	3.44089	-0.34595
C	0.24588	3.28234	-1.86789
C	1.33628	2.25809	-2.1346
C	2.85982	-1.53631	-0.642
C	2.16754	0.17512	-2.78879
C	1.48615	0.55915	2.95202
O	-2.16556	-3.55303	3.37901
Zn	-0.68154	-3.30524	4.48336
O	0.54519	4.5003	-2.55308
Zn	2.22113	4.83208	-1.8446
Zn	-2.81364	1.88166	4.62381
O	-0.94651	2.06948	4.72123
O	4.43977	-1.30576	2.13619
Zn	5.11809	-1.79746	0.47128
Zn	3.09845	-3.54582	-3.34941
O	2.63543	-1.88383	-4.17997
O	-7.02742	-0.7181	-0.5737
Zn	-6.03671	-0.55527	-2.05566
Zn	-3.532	4.30103	-1.65377
O	-4.51518	2.82945	-1.16684
O	2.87771	2.52191	3.38857

Zn	3.90315	3.58528	2.35881
O	1.56852	-4.53166	-2.25639
Zn	4.58606	-2.97882	-1.64215
Zn	-4.52418	-0.77632	-3.71322
O	-2.852	-1.06637	-4.44566
Zn	5.33269	-0.43529	-1.45868
O	4.48908	0.95333	-2.34809
O	4.73359	4.67516	1.26439
Zn	3.81156	4.79724	-0.25716
O	-4.86177	-1.04732	2.22207
Zn	-6.00795	-0.87975	0.83954
Zn	0.03233	-1.37675	5.66891
O	1.21604	-2.55476	4.40192
O	-1.85443	-4.93739	-1.04339
Zn	-0.13347	-5.17157	-1.69103
C	-3.46071	6.0814	-2.35993
O	-2.99828	7.11617	-2.58593

Figure 6c

C	-2.09144	3.06017	1.7726
C	-0.56358	3.17556	1.99631
C	0.34744	3.52545	0.97493
C	-0.10729	3.57335	-0.35478
C	-1.43674	3.28499	-0.69437
C	-2.35444	2.89682	0.28634
C	-2.36453	1.71757	2.46149
C	-1.23135	1.30647	3.26648
C	-0.13458	2.2089	2.92394
C	1.20374	1.69432	2.85982
C	1.88057	3.31609	1.02116
C	1.0177	3.38629	-1.36086
C	0.61968	2.42055	-2.42905
C	-0.72043	2.06899	-2.67286
C	-1.86145	2.82597	-2.08851
C	-2.95481	1.76337	-1.70955
C	-3.24859	1.9615	-0.27716
C	-3.72445	0.91471	0.56568
C	-3.25796	0.81569	1.95695
C	-1.03827	-0.01357	3.62998
C	-1.99801	-1.05197	3.24317
C	-3.29662	-0.63906	2.40002
C	-3.33976	-1.33509	1.03762
C	-3.72647	-0.39943	0.04013
C	-3.68347	-0.67643	-1.44802
C	-3.04624	0.5019	-2.25105
C	-2.04562	-0.07137	-3.29759
C	-0.79464	0.75627	-3.22218
C	2.13273	2.8481	-0.45257
C	1.88731	-1.54017	-2.2597
C	2.97654	-0.57272	-1.82943

C	3.10785	-0.62839	-0.29143
C	2.7949	-1.73478	0.50332
C	2.05021	-2.95119	-0.09254
C	0.03091	-2.82984	-1.70006
C	-0.43069	-2.01389	-2.74387
C	0.80442	-1.21828	-3.30621
C	0.49383	0.23682	-3.27872
C	1.38605	1.24523	-2.75698
C	2.44577	0.86753	-1.96146
C	3.21446	0.67017	0.24151
C	3.17835	1.01235	1.71863
C	2.50064	-0.18764	2.43647
C	2.41726	-1.50043	1.85353
C	1.23594	-2.32797	2.12182
C	0.91767	-3.09623	0.95486
C	-0.41071	-3.36571	0.65383
C	-0.9041	-3.56205	-0.78377
C	-1.72721	-1.39725	-2.60407
C	-2.64228	-1.77257	-1.66204
C	-2.36734	-2.83928	-0.71633
C	-2.58151	-2.45013	0.68435
C	-1.44745	-2.83872	1.49442
C	-1.12732	-2.10445	2.65962
C	0.22615	-1.86437	2.97287
C	0.3722	-0.59842	3.82554
C	1.41046	0.28711	3.15934
C	2.73107	1.61468	-0.76174
C	2.15715	2.14575	1.95731
C	1.41751	-2.52604	-1.40786
O	-2.43552	-0.34942	-4.64063
Zn	-1.15054	-1.62916	-5.14121
O	0.76354	-0.84451	5.17464
Zn	2.46074	-1.52599	4.89666
Zn	-2.88281	-4.72941	-1.24238
O	-1.00589	-4.90999	-1.26178
O	4.2768	-0.63256	-2.4422
Zn	4.95594	0.97163	-1.77638
Zn	2.92274	4.98449	-0.57053
O	2.54696	4.54463	1.25598
O	-7.06215	0.64442	0.52494
Zn	-6.02956	1.66988	1.57611
Zn	-3.47213	-1.58259	4.52888
O	-4.50898	-0.87621	3.1399
O	2.89636	-4.08992	-0.22652
Zn	4.032	-3.8888	1.16038
O	1.322	4.75213	-1.94683
Zn	4.40583	3.3398	-1.29759
Zn	-4.55885	3.23493	2.27998
O	-2.91326	4.08828	2.31503
Zn	5.2652	1.58909	0.49805
O	4.50339	1.35698	2.16981
O	4.96728	-3.66636	2.62848

Zn	4.05375	-2.6454	3.77112
O	-5.01223	-1.03182	-1.85194
Zn	-6.10326	-0.22024	-0.65801
Zn	0.094	-3.45544	-4.33843
O	1.02843	-1.72382	-4.64786
O	-2.12777	4.01351	-2.89525
Zn	-0.40894	4.6892	-2.74035
C	0.61298	-5.21552	-3.63944
O	0.63651	-6.36761	-3.55931

Figure 6d

C	-1.79456	-1.47884	-3.31252
C	-0.28639	-1.15064	-3.47499
C	0.75883	-1.90768	-2.86014
C	0.40931	-2.84079	-1.88284
C	-0.9432	-3.074	-1.50979
C	-1.97025	-2.33151	-2.07165
C	-2.35157	-0.07855	-3.01977
C	-1.37264	0.94237	-3.32789
C	-0.11529	0.23421	-3.56602
C	1.11045	0.83391	-3.09845
C	2.20931	-1.41309	-2.65582
C	1.54926	-3.17696	-0.92041
C	1.01864	-3.07029	0.4852
C	-0.31023	-3.25606	0.83001
C	-1.35362	-3.66578	-0.15394
C	-2.62474	-2.80858	0.16312
C	-2.98453	-2.12568	-1.09232
C	-3.68143	-0.89892	-1.11364
C	-3.35106	0.12932	-2.1124
C	-1.44005	2.2059	-2.77127
C	-2.5322	2.57603	-1.86761
C	-3.67422	1.50229	-1.54338
C	-3.73672	1.16811	-0.04877
C	-3.892	-0.22533	0.12481
C	-3.79028	-0.93783	1.45842
C	-2.9047	-2.21388	1.37158
C	-1.95479	-2.26622	2.59882
C	-0.58455	-2.60092	2.08671
C	2.53668	-2.02331	-1.22812
C	1.57938	0.19885	2.97955
C	2.79565	-0.07292	2.09185
C	2.83058	0.95409	0.93865
C	2.25142	2.20685	0.97781
C	1.34498	2.6384	2.15255
C	-0.51528	1.18616	3.19303
C	-0.75598	-0.14738	3.53119
C	0.63022	-0.89253	3.51979
C	0.57289	-2.00048	2.53184
C	1.59036	-2.25993	1.53568

C	2.53493	-1.32424	1.23793
C	3.05249	0.29234	-0.31749
C	3.00293	0.98286	-1.65787
C	2.08476	2.22031	-1.51664
C	1.81068	2.81745	-0.25709
C	0.50754	3.41639	-0.01075
C	0.1414	3.20399	1.36058
C	-1.19022	2.99188	1.68801
C	-1.61326	2.15578	2.89579
C	-1.93327	-0.77338	2.96331
C	-2.9515	-0.05872	2.38646
C	-2.92645	1.39196	2.31762
C	-3.16326	1.9342	0.97451
C	-2.17461	2.9295	0.64778
C	-1.81366	3.16367	-0.70459
C	-0.47093	3.42188	-1.02254
C	-0.17141	3.02532	-2.47396
C	1.05108	2.12668	-2.45768
C	2.83264	-1.09582	-0.17576
C	2.17265	0.09737	-2.60323
C	0.87878	1.38805	2.88126
O	-2.25478	-3.0631	3.75049
Zn	-0.93545	-2.43285	4.9175
O	0.07301	4.12898	-3.34578
Zn	1.64324	4.78283	-2.63042
Zn	-3.70363	2.39562	3.91242
O	-1.89422	2.86476	4.10644
O	4.06754	-0.2205	2.71706
Zn	5.01879	-1.23233	1.49428
Zn	4.30633	-2.5619	-2.26528
O	3.16179	-1.90484	-3.60321
O	-6.99853	-1.27896	-1.1091
Zn	-5.9006	-1.22221	-2.52445
Zn	-4.16874	3.53298	-2.58726
O	-4.95818	1.92641	-2.03391
O	1.98916	3.57659	3.00941
Zn	3.0287	4.49512	1.86077
O	1.99978	-4.54666	-1.1919
Zn	5.8069	-2.16591	-0.44867
Zn	-4.23202	-1.71511	-3.96453
O	-2.46833	-2.06981	-4.41746
Zn	5.22291	-0.27738	-1.74236
O	4.3297	1.28032	-2.11874
O	3.87505	5.39665	0.61928
Zn	3.10801	5.17864	-0.97587
O	-5.12959	-1.16853	1.91898
Zn	-6.13003	-1.19973	0.41017
Zn	-0.64407	-0.24286	5.77808
O	0.83714	-1.42344	4.86092
O	-1.40561	-5.116	-0.25818
Zn	0.36278	-5.28295	-0.74709
C	6.8635	-3.77482	-0.59017

O	7.245	-4.87001	-0.60986

Figure 6e

C	1.6759	2.30033	-2.73814
C	0.15471	2.07938	-2.92863
C	-0.82356	2.62116	-2.06465
C	-0.41476	3.22528	-0.86652
C	0.93714	3.30501	-0.50061
C	1.92797	2.7388	-1.30741
C	2.17847	0.86154	-2.90068
C	1.14547	0.01048	-3.45997
C	-0.09122	0.78837	-3.42783
C	-1.3317	0.12652	-3.12873
C	-2.30249	2.17696	-1.97881
C	-1.52335	3.25351	0.17516
C	-0.99857	2.82843	1.51021
C	0.38329	2.80008	1.80302
C	1.4	3.46567	0.94576
C	2.66017	2.52622	0.93977
C	2.94789	2.2284	-0.47535
C	3.60877	1.03759	-0.89524
C	3.19399	0.36255	-2.13534
C	1.1785	-1.36321	-3.30946
C	2.28504	-2.01947	-2.60698
C	3.48053	-1.12648	-2.02102
C	3.60491	-1.25975	-0.50112
C	3.80863	0.02376	0.07327
C	3.7736	0.3057	1.56147
C	2.94063	1.57927	1.89871
C	2.02378	1.28517	3.11759
C	0.66112	1.80012	2.76938
C	-2.54019	2.27233	-0.432
C	-1.60711	-1.08117	2.87215
C	-2.81989	-0.52137	2.13395
C	-2.90441	-1.16261	0.72683
C	-2.3922	-2.40837	0.37113
C	-1.47305	-3.17992	1.34107
C	0.45752	-2.13685	2.68443
C	0.75633	-0.97414	3.39668
C	-0.59779	-0.22064	3.66361
C	-0.52642	1.13171	3.05234
C	-1.56426	1.74316	2.26331
C	-2.52759	0.92988	1.69985
C	-3.19443	-0.18085	-0.24379
C	-3.1923	-0.40295	-1.74383
C	-2.30962	-1.65401	-2.00226
C	-2.03758	-2.64018	-0.98965
C	-0.72532	-3.29528	-0.97813
C	-0.3119	-3.52162	0.37521
C	1.03502	-3.44823	0.70052

C	1.51246	-3.01016	2.08628
C	1.94628	-0.24468	3.008
C	2.92186	-0.78527	2.2117
C	2.84069	-2.14823	1.71599
C	3.02514	-2.27021	0.26292
C	1.99295	-3.10709	-0.30992
C	1.58355	-2.90977	-1.64849
C	0.21658	-3.02407	-1.97805
C	-0.11262	-2.19826	-3.22772
C	-1.2981	-1.30879	-2.89189
C	-2.88749	1.12099	0.32571
C	-2.368	0.71708	-2.41911
C	-0.9491	-2.20286	2.38479
O	2.40129	1.66207	4.45009
Zn	1.06926	0.76386	5.39833
O	-0.42074	-2.98189	-4.37916
Zn	-1.98333	-3.78558	-3.80207
Zn	3.61014	-3.60229	2.90791
O	1.7891	-4.04166	3.04114
O	-4.11362	-0.53213	2.7634
Zn	-4.96656	0.66143	1.60387
Zn	-3.56575	4.31416	-1.22014
O	-3.12858	3.12748	-2.63398
O	6.94249	1.33566	-0.87853
Zn	5.78344	1.71538	-2.19586
Zn	3.85305	-2.74072	-3.6695
O	4.73075	-1.4219	-2.67083
O	-2.12397	-4.30462	1.9239
Zn	-3.22885	-4.83985	0.60409
O	-2.04745	4.67237	0.21051
Zn	-4.66791	2.64347	0.14014
Zn	4.09413	2.64498	-3.3771
O	2.33535	3.17441	-3.64888
Zn	-5.35653	0.27259	-0.73696
O	-4.5494	-0.47742	-2.22646
O	-4.14681	-5.33112	-0.80742
Zn	-3.39389	-4.63601	-2.27042
O	5.13253	0.33727	2.01824
Zn	6.10666	0.8191	0.57059
Zn	0.70607	-1.59418	5.5464
O	-0.73038	-0.10565	5.11517
O	1.45121	4.89303	1.2493
Zn	-0.35007	5.1765	0.92041
C	-4.53634	6.01718	-1.30223
O	-5.35688	6.80389	-1.09326

Figure 6f

C	2.50178	1.84545	-2.71095
C	0.99496	2.02079	-3.02594
C	0.13074	2.83803	-2.26337

C	0.59126	3.36924	-1.04672
C	1.88333	3.10581	-0.56786
C	2.74948	2.26639	-1.27412
C	2.61884	0.31954	-2.79522
C	1.44472	-0.25824	-3.41853
C	0.4569	0.81375	-3.50935
C	-0.93012	0.50624	-3.30048
C	-1.41632	2.78564	-2.28669
C	-0.54612	3.71374	-0.09625
C	-0.25354	3.21469	1.28027
C	1.04352	2.85373	1.69195
C	2.25901	3.20137	0.90937
C	3.22773	1.96871	1.0307
C	3.53522	1.54641	-0.34796
C	3.88516	0.2055	-0.68249
C	3.40931	-0.39272	-1.93806
C	1.1059	-1.58613	-3.23421
C	1.94787	-2.47688	-2.43014
C	3.28644	-1.89872	-1.76526
C	3.25676	-1.99412	-0.23832
C	3.74425	-0.78161	0.32166
C	3.67383	-0.43485	1.79387
C	3.17803	1.02298	2.03014
C	2.12908	1.02688	3.17502
C	0.97666	1.8585	2.70355
C	-1.71852	2.97592	-0.75981
C	-1.95874	-0.32803	2.68025
C	-2.93155	0.48985	1.83496
C	-3.0652	-0.16087	0.43666
C	-2.87285	-1.51505	0.15415
C	-2.26806	-2.45412	1.21396
C	-0.23526	-1.89057	2.69314
C	0.30196	-0.81653	3.40792
C	-0.82612	0.27312	3.53843
C	-0.35945	1.53082	2.9015
C	-1.14155	2.34813	2.00855
C	-2.25222	1.80569	1.39794
C	-3.03399	0.822	-0.57303
C	-2.96319	0.54157	-2.06292
C	-2.42279	-0.90558	-2.21893
C	-2.49446	-1.88546	-1.16444
C	-1.40552	-2.86357	-1.03162
C	-1.17003	-3.13263	0.35556
C	0.12323	-3.39131	0.79087
C	0.5946	-3.0331	2.2019
C	1.66519	-0.43428	3.0978
C	2.52168	-1.24078	2.39545
C	2.12592	-2.5577	1.92581
C	2.38031	-2.78793	0.49679
C	1.21018	-3.35404	-0.14251
C	0.96916	-3.11637	-1.51472
C	-0.35212	-2.88459	-1.95317

C	-0.3587	-2.05647	-3.24404
C	-1.29273	-0.87716	-3.02644
C	-2.45002	2.03483	-0.01023
C	-1.82314	1.37439	-2.69077
C	-1.57926	-1.59983	2.27197
O	2.49114	1.35748	4.52411
Zn	0.89518	0.90279	5.37629
O	-0.76547	-2.78672	-4.39996
Zn	-2.5085	-3.17555	-3.91549
Zn	2.39829	-4.09585	3.22253
O	0.52079	-4.06375	3.19436
O	-4.2339	0.80047	2.35863
Zn	-4.72796	2.08793	1.10175
Zn	-2.28709	5.028	-1.5285
O	-1.93833	3.88102	-3.02034
O	7.16528	-0.40169	-0.413
Zn	6.25568	0.20689	-1.83541
Zn	3.35176	-3.61179	-3.35324
O	4.4631	-2.53686	-2.29524
O	-3.2284	-3.32243	1.78575
Zn	-4.54755	-3.59952	0.56183
O	-0.69689	5.22258	-0.11131
Zn	-3.92588	3.98726	-0.24121
Zn	4.96677	1.50587	-3.16452
O	3.43743	2.47143	-3.58279
Zn	-4.98146	1.73827	-1.23751
O	-4.2437	0.81408	-2.66574
O	-5.26804	-3.78587	-1.05824
Zn	-4.1709	-3.43957	-2.41856
O	4.95739	-0.73381	2.35958
Zn	6.1229	-0.60507	0.97932
Zn	-0.05065	-1.28714	5.56157
O	-1.03815	0.4856	4.96983
O	2.65242	4.57834	1.18828
Zn	1.01839	5.30954	0.70717
C	-6.44306	-3.9296	1.55915
O	-7.5771	-3.78073	1.62496

Figure 7a

C	2.07873	-2.79117	2.08754
C	0.58578	-3.09372	1.82234
C	0.10527	-3.42183	0.5317
C	0.95765	-3.35284	-0.6488
C	2.2176	-2.78141	-0.5023
C	2.70897	-2.38189	0.76893
C	1.94491	-1.54988	2.99182
C	0.57173	-1.41387	3.46781
C	-0.24722	-2.37748	2.71816
C	-1.58118	-2.05099	2.36243
C	-1.2226	-3.06094	0.16226

C	0.08071	-3.12136	-1.88908
C	0.61135	-1.94639	-2.66773
C	1.88399	-1.39501	-2.47608
C	2.95282	-1.99685	-1.60845
C	3.60557	-0.86485	-0.79658
C	3.55642	-1.2597	0.62259
C	3.55162	-0.26855	1.65848
C	2.7528	-0.45305	2.86289
C	0.06098	-0.19392	3.85343
C	0.892	1.02208	3.85814
C	2.40083	0.91948	3.43364
C	2.75442	1.82229	2.24281
C	3.548	1.08175	1.29773
C	3.87507	1.56223	-0.10566
C	3.6789	0.44774	-1.17346
C	2.92928	1.00631	-2.41612
C	1.87559	0.00423	-2.81249
C	-1.31587	-2.85697	-1.28478
C	-1.30784	1.78973	-2.48109
C	-2.30071	0.63771	-2.50665
C	-2.90604	0.46171	-1.09659
C	-2.97051	1.43338	-0.11801
C	-2.31129	2.81555	-0.32354
C	0.06752	3.21647	-1.24667
C	0.93826	2.61308	-2.17251
C	0.07849	1.75304	-3.15678
C	0.59314	0.35589	-3.19325
C	-0.23235	-0.82946	-3.07777
C	-1.51694	-0.68856	-2.60378
C	-2.8448	-0.92154	-0.7338
C	-3.17668	-1.40932	0.64316
C	-2.90216	-0.30122	1.64547
C	-2.99862	1.0629	1.28421
C	-2.06214	1.98942	1.96488
C	-1.56925	2.95123	1.0297
C	-0.27223	3.44207	1.1768
C	0.58501	3.88683	-0.00868
C	2.22489	2.16015	-1.72038
C	2.75952	2.51678	-0.51458
C	2.03932	3.38079	0.41376
C	1.93632	2.84041	1.78096
C	0.55416	2.9536	2.23956
C	0.05038	2.01899	3.16359
C	-1.27884	1.54811	3.03519
C	-1.43044	0.17009	3.70266
C	-2.08387	-0.76287	2.69565
C	-1.99922	-1.61417	-1.62672
C	-2.18007	-2.54359	1.10557
C	-1.26691	2.67771	-1.42223
O	3.5989	1.49624	-3.57618
Zn	2.33321	2.50855	-4.52884
O	-2.12991	0.22324	4.94371

Zn	-3.76879	1.01778	4.67173
Zn	2.50585	5.31712	0.09698
O	0.69537	5.31719	-0.25723
O	-3.34518	0.63088	-3.47562
Zn	-4.64478	-0.57988	-2.91008
Zn	-2.7996	-3.95411	-2.10163
O	-4.29335	-4.06425	-1.01608
O	6.82891	-0.88825	0.85856
Zn	5.71985	-2.33079	0.90609
Zn	1.69082	1.42588	5.66312
O	3.18189	1.22358	4.62118
O	-3.24953	3.84061	-0.61778
Zn	-4.77589	3.42584	0.2944
O	-0.15391	-4.37183	-2.72158
Zn	-5.09081	-2.24845	-1.26395
Zn	4.6118	-3.75148	2.38474
O	2.79065	-3.86525	2.6751
Zn	-3.90914	-3.75874	0.83816
O	-4.56252	-1.88174	0.67333
O	-5.7427	2.77547	1.62845
Zn	-4.73881	1.71424	2.69977
O	5.19217	2.11578	-0.10095
Zn	6.29468	0.71687	0.3204
Zn	0.78124	4.17346	-3.62263
O	0.2333	2.41448	-4.45885
O	3.85759	-2.83669	-2.36651
Zn	2.54902	-3.94223	-3.00309
C	0.93442	-4.93163	-3.38427
O	0.73629	-5.9089	-4.08144
C	-6.43815	-0.10896	-3.87648
C	-4.16745	-5.01573	2.33077
C	8.32195	1.07002	-0.39285
C	4.16283	6.27673	0.04529
C	-6.21943	3.70526	-1.2898
C	-4.80972	1.45858	6.3623
C	0.83427	1.6895	7.35297
C	2.84589	3.26544	-6.29853
O	-6.78398	3.08275	-2.07495
O	-7.58872	-0.15973	-3.76637
O	3.09924	4.06176	-7.09886
O	-0.06895	1.92188	8.04064
O	-5.66397	2.03636	6.88464
O	-3.80823	-5.68488	3.20101
O	5.27348	6.49814	0.28822
O	9.25827	0.65847	-0.91452
C	5.71049	-5.21597	3.25724
O	6.73628	-5.74064	3.37167
C	-7.13349	-2.16326	-1.08639
C	-0.1511	5.80598	-3.05955
C	5.80199	-3.45749	-0.85701
C	-2.69027	-4.57636	-3.98338
O	-8.14163	-1.75639	-1.48009

O	-0.25891	6.94886	-2.89987
O	6.25073	-4.40473	-1.34607
O	-2.56083	-4.66559	-5.12263

Figure 7b

C	1.56052	-3.04514	2.07762
C	0.11553	-3.25213	1.57167
C	-0.17423	-3.42915	0.1909
C	0.85294	-3.28705	-0.83922
C	2.09247	-2.80355	-0.45565
C	2.39221	-2.54812	0.9113
C	1.34113	-1.89106	3.07391
C	-0.08024	-1.73048	3.34698
C	-0.81315	-2.58209	2.39817
C	-2.06478	-2.14616	1.87657
C	-1.40543	-2.96861	-0.32824
C	0.19457	-2.89132	-2.16474
C	0.88397	-1.67806	-2.73966
C	2.13348	-1.21178	-2.31447
C	3.01909	-1.96016	-1.35222
C	3.57997	-0.96207	-0.33088
C	3.29622	-1.47234	1.01537
C	3.17968	-0.57463	2.12545
C	2.1979	-0.82767	3.17575
C	-0.59209	-0.51885	3.75533
C	0.26201	0.64635	4.00541
C	1.82464	0.50153	3.82883
C	2.38348	1.49312	2.78845
C	3.28908	0.80169	1.90648
C	3.82306	1.38618	0.60806
C	3.72163	0.374	-0.55181
C	3.29384	1.07033	-1.85251
C	2.25483	0.21127	-2.54366
C	-1.27262	-2.62831	-1.76483
C	-0.91653	2.0968	-2.46234
C	-1.93692	1.01549	-2.76068
C	-2.76618	0.74413	-1.4862
C	-2.93521	1.61506	-0.43889
C	-2.19894	2.97481	-0.4014
C	0.3243	3.29308	-0.92054
C	1.27842	2.75398	-1.77467
C	0.55436	2.08233	-2.97661
C	1.05318	0.6666	-3.06727
C	0.1611	-0.48152	-3.16026
C	-1.17359	-0.32127	-2.85518
C	-2.80475	-0.68277	-1.25846
C	-3.35526	-1.27647	0.01084
C	-3.19243	-0.27631	1.14436
C	-3.19882	1.11447	0.90908
C	-2.33384	1.92517	1.80439

C	-1.66427	2.9372	1.04782
C	-0.3817	3.33498	1.42442
C	0.64896	3.86164	0.42631
C	2.52374	2.26778	-1.22918
C	2.8306	2.44348	0.11928
C	2.0165	3.23619	1.00693
C	1.68818	2.58424	2.29649
C	0.25612	2.72021	2.5436
C	-0.41959	1.73422	3.28622
C	-1.73394	1.34973	2.92669
C	-2.02329	-0.07159	3.42885
C	-2.56905	-0.87631	2.26229
C	-1.81991	-1.30378	-2.04142
C	-2.48459	-2.4956	0.50297
C	-1.00537	2.88293	-1.34042
O	4.3599	1.49405	-2.69122
Zn	4.10578	3.33966	-2.69599
O	-2.87356	-0.09983	4.58793
Zn	-4.4562	0.76525	4.17588
Zn	2.54883	5.18928	0.78501
O	0.74892	5.29144	0.28814
O	-2.80329	1.15278	-3.88067
Zn	-4.29217	0.0766	-3.59217
Zn	-2.61982	-3.74428	-2.68131
O	-4.35437	-3.7153	-2.05365
O	6.70996	-1.25231	1.44975
Zn	5.64577	-2.70337	1.2251
Zn	0.79953	0.87623	5.91633
O	2.46671	0.60731	5.12269
O	-3.03113	4.07871	-0.71543
Zn	-4.63142	3.83427	0.10165
O	0.0391	-4.04256	-3.14058
Zn	-4.79315	-1.77243	-2.25365
Zn	4.01275	-3.908	2.27802
O	2.20105	-4.19382	2.61917
Zn	-4.22626	-3.58521	-0.1249
O	-4.74895	-1.67738	-0.20864
O	-5.80557	3.05322	1.18325
Zn	-5.03795	1.73834	2.16728
O	5.15274	1.8781	0.79547
Zn	6.19479	0.39645	1.05728
Zn	1.98716	4.09597	-3.51765
O	0.74456	2.87158	-4.15725
O	3.99307	-2.76656	-2.05912
Zn	2.75831	-3.67225	-3.06255
C	1.17698	-4.56649	-3.73041
O	1.0302	-5.47254	-4.53516
C	-6.01773	0.79059	-4.49504
C	-4.74891	-4.96593	1.17906
C	8.25663	0.81637	0.45159
C	-6.18402	5.02122	-0.81629
C	-5.70381	1.08129	5.75253

O	-7.27422	5.11006	-1.16294
O	-7.17311	0.81529	-4.43692
O	-6.60651	1.63439	6.21576
O	-4.51873	-5.72167	2.02335
O	9.21151	0.44824	-0.06929
C	1.86489	6.07088	-3.13743
C	5.87907	-3.60259	-0.65133
O	2.25003	6.96101	-2.50157
O	6.26967	-4.53025	-1.22001
C	4.60764	4.63596	-1.28011
O	4.17869	5.4712	-0.54441
O	-7.39437	-1.72196	-1.88952
C	-8.39218	-1.19352	-2.11757
C	-2.15035	-0.00815	7.00096
O	-0.99561	0.13731	7.09609
O	-2.39078	-5.1719	-4.42242
C	-1.81179	-5.88592	-5.12914
C	3.04831	-6.24971	4.65849
O	4.01433	-5.9442	4.11014
O	6.29358	3.22359	-3.8993
C	6.89271	2.27477	-4.16711

Figure 9a

C	-0.56238	1.32602	-0.34369
C	-0.78463	-0.0572	-0.97786
C	-0.73805	-1.22631	-0.01572
C	-0.47195	-1.07876	1.50778
C	-0.2908	0.35133	2.08798
C	-0.25103	1.48666	1.10744
C	0.10357	2.28493	-1.37172
C	0.65242	1.30549	-2.37725
C	0.22811	0.00625	-2.08518
C	0.88099	-1.1438	-2.54427
C	0.02702	-2.4944	-0.52457
C	0.6787	-2.01922	1.77582
C	1.63529	-1.77098	2.76731
C	1.76199	-0.43051	3.35383
C	0.9074	0.58485	2.923
C	1.46389	1.8996	2.66902
C	0.78792	2.45903	1.53139
C	1.46121	3.25849	0.60722
C	1.21175	3.11331	-0.8208
C	1.87501	1.4768	-3.07424
C	2.80762	2.4601	-2.61778
C	2.46506	3.2528	-1.47495
C	3.50528	3.52338	-0.46958
C	2.87375	3.54539	0.82806
C	3.54322	3.00393	1.94519
C	2.82699	2.18396	2.9032
C	3.70441	1.12457	3.35603

C	3.17162	-0.16442	3.55999
C	0.95182	-2.85092	0.65893
C	5.46808	-2.01684	1.31593
C	4.54268	-2.97354	0.8552
C	4.32011	-3.14836	-0.5763
C	5.03618	-2.3507	-1.48832
C	5.98695	-1.35836	-1.01048
C	6.32893	0.14074	0.93077
C	5.6852	0.14695	2.2361
C	5.14887	-1.18789	2.4706
C	3.91292	-1.33915	3.11727
C	2.95421	-2.32147	2.6366
C	3.26122	-3.12262	1.51484
C	2.90818	-3.43018	-0.78245
C	2.24036	-2.87507	-1.88842
C	2.99489	-2.05879	-2.84458
C	4.35902	-1.79876	-2.65509
C	4.88714	-0.46164	-2.89556
C	5.89309	-0.19274	-1.87581
C	6.00886	1.09933	-1.33084
C	6.23933	1.27053	0.09708
C	4.97662	1.281	2.67144
C	4.87778	2.45102	1.80351
C	5.49028	2.43619	0.53654
C	4.79195	2.98734	-0.61585
C	5.12125	2.16185	-1.77647
C	4.15124	1.91145	-2.75744
C	4.03665	0.5717	-3.32561
C	2.62406	0.30171	-3.51199
C	2.12698	-0.98414	-3.27383
C	2.24459	-3.3957	0.51937
C	0.91992	-2.31175	-1.74079
C	6.2069	-1.19753	0.37035
Zn	-3.69466	0.54783	-1.62925
Zn	-4.54088	-0.83241	1.39426
Zn	-4.31295	1.75109	0.49249
Zn	-2.33739	-2.55358	0.64571
Zn	-2.21821	0.27874	2.61366
O	-1.6658	-1.62906	2.2453
O	-3.58235	2.44551	-1.2402
O	-3.96	0.78461	2.14822
O	-1.0683	-3.45731	-0.83144
O	-4.27996	-2.5351	0.72434
O	-1.98811	-0.21457	-1.86594
Zn	-4.49868	-1.83882	-1.08478
O	-5.06309	0.05973	-0.37071
Zn	-1.81519	2.89249	-1.56352
O	-1.56866	1.9412	0.55323
Zn	-2.28912	-2.23448	-1.82042
C	-5.28535	3.56689	0.67697
O	-5.58618	4.65545	0.49116

Figure 9b

C	-0.08753	-0.76634	1.83535
C	-0.17905	0.73729	1.2279
C	-0.31308	0.87108	-0.28272
C	-0.25606	-0.26692	-1.29736
C	-0.02784	-1.66931	-0.7123
C	0.22521	-1.79604	0.73436
C	1.15377	-0.64997	2.76016
C	1.60061	0.70681	2.88077
C	0.95083	1.47232	1.86675
C	1.57101	2.55982	1.26114
C	0.35703	2.10378	-0.98931
C	0.75842	0.13509	-2.32883
C	1.54962	-0.7714	-3.0334
C	1.69572	-2.13023	-2.52612
C	0.9907	-2.52129	-1.37105
C	1.68194	-3.2734	-0.35959
C	1.20932	-2.80015	0.9359
C	2.11222	-2.79466	2.04206
C	2.07797	-1.6687	2.97022
C	2.9051	1.0455	3.31223
C	3.85958	-0.01979	3.52561
C	3.45313	-1.35552	3.35052
C	4.32007	-2.28418	2.6566
C	3.47903	-3.17359	1.85035
C	3.94124	-3.60771	0.57956
C	3.02045	-3.67692	-0.53826
C	3.73741	-3.28772	-1.73808
C	3.07957	-2.51718	-2.71563
C	1.09127	1.49565	-2.18967
C	5.49363	0.2986	-2.80369
C	4.5646	1.33094	-3.00082
C	4.5197	2.47343	-2.08741
C	5.42859	2.52679	-1.00532
C	6.38643	1.45927	-0.79949
C	6.58862	-0.98397	-1.1602
C	5.76541	-1.8864	-1.96101
C	5.09286	-1.09311	-2.97978
C	3.77619	-1.40302	-3.3509
C	2.81827	-0.32724	-3.55405
C	3.20031	1.01577	-3.38524
C	3.139	2.85514	-1.91843
C	2.65536	3.25758	-0.63935
C	3.61429	3.31551	0.47726
C	4.96339	2.96637	0.29853
C	5.64774	2.17626	1.31644
C	6.52757	1.24081	0.63524
C	6.68876	-0.06311	1.13723
C	6.72018	-1.19715	0.22528
C	5.10393	-2.96506	-1.35493

C	5.2301	-3.17847	0.0848
C	6.02197	-2.30288	0.85594
C	5.56668	-1.86086	2.16684
C	5.98416	-0.47547	2.34305
C	5.14554	0.42922	3.01204
C	4.97162	1.78175	2.48488
C	3.58069	2.15002	2.6659
C	2.92345	2.90108	1.66878
C	2.31966	1.94763	-2.70413
C	1.37787	2.85066	-0.14782
C	6.42085	0.35784	-1.67887
Zn	-2.75364	-2.07548	2.03036
Zn	-2.18426	1.76203	-2.13175
Zn	-4.63339	-1.95676	-0.1682
Zn	-1.70136	3.02627	0.35251
Zn	-1.94357	-2.17026	-1.24037
O	-1.56096	-0.21202	-2.11474
O	-4.58351	-2.39835	1.76643
O	-3.76691	-2.43277	-1.91232
O	-0.77357	2.99945	-1.42761
O	-3.32417	2.26298	-0.36145
O	-1.39031	1.50565	1.78222
Zn	-4.80755	1.14537	-0.9423
O	-2.74162	-1.23803	0.26836
Zn	-2.67881	0.44623	2.78336
O	-1.23893	-1.07831	2.67583
Zn	-2.36236	0.56577	0.06863
Zn	-3.67654	-0.76537	-2.67833
O	-3.95549	1.03808	-2.70429
O	-5.52969	-0.1765	0.12508
Zn	-4.72193	-0.38629	1.88651
C	-1.25212	4.62923	1.44996
O	-0.85431	5.51911	2.05251

Figure 9c

C	-0.68835	1.02066	0.22961
C	-0.65059	-0.34596	1.12526
C	-0.8598	-1.69879	0.32441
C	-1.18436	-1.64068	-1.19719
C	-1.53102	-0.30013	-1.76319
C	-1.35337	0.88885	-1.09558
C	-1.46553	2.11146	1.11889
C	-2.05933	1.31502	2.24058
C	-1.70737	-0.04261	2.16568
C	-2.51866	-1.04426	2.73585
C	-1.8548	-2.80238	0.96551
C	-2.39354	-2.56341	-1.40717
C	-3.35171	-2.35263	-2.42429
C	-3.3834	-1.09406	-3.18917
C	-2.46998	-0.09379	-2.87353

C	-2.86338	1.29526	-2.85517
C	-2.15049	1.91613	-1.75439
C	-2.75528	2.91328	-0.98844
C	-2.52613	2.92041	0.44169
C	-3.28555	1.68342	2.87586
C	-4.13963	2.67042	2.29311
C	-3.75069	3.27212	1.05576
C	-4.7643	3.50722	0.01557
C	-4.13673	3.29873	-1.26894
C	-4.84554	2.66289	-2.30741
C	-4.19611	1.65548	-3.13234
C	-5.16314	0.61252	-3.42735
C	-4.76092	-0.7395	-3.47011
C	-2.78908	-3.15906	-0.19194
C	-7.20095	-2.0449	-0.99444
C	-6.3702	-3.01003	-0.39676
C	-6.16032	-2.99951	1.04745
C	-6.80048	-2.02242	1.83614
C	-7.65484	-1.02601	1.21367
C	-7.86645	0.21058	-0.92348
C	-7.2233	-0.02119	-2.21047
C	-6.80489	-1.41853	-2.25082
C	-5.59389	-1.76913	-2.86454
C	-4.7169	-2.75218	-2.23663
C	-5.10604	-3.35924	-1.01866
C	-4.77944	-3.36366	1.30285
C	-4.06341	-2.71658	2.32186
C	-4.73042	-1.71632	3.14552
C	-6.069	-1.37304	2.91742
C	-6.47324	0.02646	2.96274
C	-7.45303	0.23661	1.90724
C	-7.45556	1.44644	1.1836
C	-7.67566	1.43244	-0.25559
C	-6.42105	0.97508	-2.78914
C	-6.22133	2.24268	-2.09691
C	-6.83195	2.45977	-0.84778
C	-6.08861	3.10552	0.2243
C	-6.4808	2.4791	1.4863
C	-5.52695	2.27492	2.49687
C	-5.52753	1.02604	3.24583
C	-4.13774	0.66364	3.47308
C	-3.75603	-0.67459	3.41284
C	-4.12123	-3.56718	0.00916
C	-2.69738	-2.29483	2.10737
C	-7.8632	-1.04074	-0.18171
Zn	2.02807	0.81501	1.27297
Zn	1.55734	-1.47162	-0.68858
Zn	2.79727	3.36161	0.22319
Zn	0.51212	-3.19294	0.90736
Zn	0.66107	-0.37867	-2.87286
O	0.04787	-1.97341	-1.95334
O	3.13451	2.31028	1.71356

O	1.33439	1.36536	-3.10315
O	-1.11233	-3.9359	1.42149
O	2.2534	-3.36047	1.61743
O	0.59426	-0.3885	1.85611
Zn	4.876	-0.54705	-0.01462
O	2.94854	-0.8326	0.53569
Zn	0.03302	3.38048	0.87456
O	0.66831	1.43927	-0.05674
Zn	2.22753	-1.54898	2.48629
Zn	3.12083	0.87212	-2.51908
O	2.49104	-1.12551	-2.42202
O	5.6978	1.03928	0.66472
Zn	4.82517	1.48822	2.31381
Zn	4.99322	1.81272	-0.87325
O	3.43388	2.65807	-1.48262
Zn	4.32759	-1.65829	-2.30496
O	4.8886	0.20474	-2.05942
Zn	3.6477	-0.38103	3.83985
O	4.96269	0.81043	3.99504
O	4.9693	-2.4372	-0.60012
Zn	3.64745	-2.95205	0.53126
O	1.15153	4.10352	-0.42851
Zn	1.22297	2.6332	-1.71057
C	5.27937	-3.02731	-3.40835
O	5.8895	-3.93645	-3.73864

Figure 10c

C	-1.24388	1.00355	1.27764
C	-1.40614	-0.59501	1.57089
C	-1.7	-1.46839	0.37702
C	-1.69068	-1.04455	-1.04994
C	-1.77351	0.44225	-1.24805
C	-1.54932	1.3983	-0.1845
C	-2.31555	1.62074	2.19998
C	-2.88641	0.63816	3.07194
C	-2.50122	-0.66144	2.60554
C	-3.38674	-1.73932	2.72859
C	-2.59708	-2.73178	0.50398
C	-2.89856	-1.74928	-1.67574
C	-3.69934	-1.18915	-2.68372
C	-3.59758	0.23532	-2.95029
C	-2.66558	1.01877	-2.22429
C	-3.05685	2.33415	-1.75249
C	-2.41078	2.54832	-0.47738
C	-3.09835	3.26339	0.52499
C	-3.04694	2.76918	1.9046
C	-4.12799	0.8513	3.71821
C	-4.88471	2.04259	3.40496
C	-4.35514	2.98731	2.50824
C	-5.20995	3.58599	1.50167

C	-4.42715	3.75995	0.27941
C	-5.05188	3.56196	-0.97763
C	-4.34414	2.84341	-2.01637
C	-5.29771	2.03096	-2.74934
C	-4.92465	0.74784	-3.20585
C	-3.41478	-2.71738	-0.7846
C	-7.66276	-1.14585	-1.57605
C	-6.92275	-2.29601	-1.26321
C	-6.86077	-2.78517	0.11504
C	-7.5644	-2.09139	1.12678
C	-8.32	-0.89862	0.80098
C	-8.27253	0.99282	-0.80092
C	-7.49302	1.16174	-2.02151
C	-7.11942	-0.16161	-2.50375
C	-5.85976	-0.36554	-3.08752
C	-5.09738	-1.56216	-2.76559
C	-5.61986	-2.50769	-1.86825
C	-5.53465	-3.30108	0.34874
C	-4.892	-3.07456	1.60375
C	-5.63077	-2.35073	2.65131
C	-6.92976	-1.87475	2.41902
C	-7.31241	-0.55188	2.89849
C	-8.17202	0.05373	1.89721
C	-8.07378	1.43091	1.62689
C	-8.12747	1.91292	0.25441
C	-6.60504	2.24226	-2.15129
C	-6.45226	3.19798	-1.05612
C	-7.19461	3.02019	0.12769
C	-6.56708	3.23027	1.42445
C	-7.11525	2.24973	2.35481
C	-6.28998	1.66934	3.33053
C	-6.38967	0.23894	3.60887
C	-5.04867	-0.26006	3.84132
C	-4.68125	-1.53168	3.36339
C	-4.76087	-3.11347	-0.86629
C	-3.51842	-2.73357	1.69362
C	-8.37473	-0.42877	-0.52666
Zn	1.40627	0.00392	1.94028
Zn	1.44307	-1.70477	-0.96139
Zn	2.98102	3.49253	-0.43192
Zn	-0.51597	-3.62172	-1.07745
Zn	0.69858	-0.78463	-3.24994
O	-0.46373	-1.67243	-1.79205
O	3.53188	3.25057	1.48833
O	1.22378	0.92932	-2.61794
O	-1.65785	-3.90422	0.50227
O	1.116	-3.4996	0.03885
O	-0.1823	-1.13029	2.27256
Zn	4.27666	-0.82804	0.14292
O	2.32481	-0.8588	0.46333
Zn	0.87285	3.14129	1.43174
O	0.05521	1.43291	1.70298

Zn	-0.14298	-2.79699	1.3286
Zn	3.10358	1.10398	-2.47242
O	2.08363	-1.99543	-2.78493
O	5.28848	0.68997	0.80473
Zn	4.26596	1.5128	2.16795
Zn	5.35604	1.35828	-0.96952
O	4.06306	2.61536	-1.67312
Zn	3.9301	-1.99754	-2.30587
O	4.46539	-0.14515	-1.92237
Zn	3.66199	-1.34372	3.35557
O	2.96927	0.35587	3.03119
O	4.29937	-2.69457	-0.52816
Zn	2.94095	-3.13089	0.72571
O	1.06278	3.34838	-0.4626
Zn	0.17057	1.93001	-1.3727
C	4.2663	-1.93635	5.28594
C	4.95639	2.18711	4.022
C	7.00361	2.38776	-1.50145
C	2.70263	5.57624	-0.67004
C	3.06168	2.1624	-4.36117
C	-0.66977	3.2744	-2.86856
C	-0.52075	-0.89717	-4.81545
C	5.30412	-1.79263	2.00664
C	3.07848	-3.25101	2.7435
C	-0.54576	-4.58444	-2.81355
C	5.19565	-3.31335	-3.16751
C	2.5226	3.63703	2.38734
O	7.63704	3.32202	-1.70042
O	2.12547	6.5386	-0.90159
O	-0.65275	4.13557	-3.62963
O	6.40073	-2.15184	2.16854
O	2.90223	-4.18973	3.47016
O	-0.61789	-4.95524	-3.89824
O	5.85597	-4.25211	-3.20998
O	2.81926	3.92358	3.5352
O	2.69408	3.1145	-4.88848
O	-1.44076	-1.08132	-5.47955
O	4.05897	-2.93851	5.83829
O	5.10842	2.35562	5.14526