

Electronic supplementary information

Table S1. Relative energies calculated at different levels of theory. Shady cells correspond to CO₂H_{bonded} structures (see definition in Figure 3 and in the manuscript). ff99(HF) and ff99(DFT) refer to relative energies calculated with the ff99 force field using HF/6-31G* and B3LYP/cc-pVTZ sets of RESP charges, respectively. Labelling of structures corresponds to Figure S1. WG dipeptide.

CCSDT/CBS ^a		MP2/CBS ^b		SCS-MP2/CBS ^b		MP3/CBS ^c		TPSS-D/LP ₁ ^d		PBE-D/LP ₁ ^d			
WG_01	0.00	WG_02	0.00	WG_01	0.00	WG_01	0.00	WG_01	0.00	WG_01	0.00		
WG_02	0.40	WG_01	0.03	WG_02	0.52	WG_05	0.94	WG_03	0.62	WG_04	0.97		
WG_03	0.90	WG_03	0.42	WG_05	1.06	WG_02	1.17	WG_02	0.74	WG_05	1.30		
WG_05	1.26	WG_07	0.61	WG_03	1.10	WG_04	1.19	WG_04	1.32	WG_02	1.67		
WG_04	1.26	WG_10	0.70	WG_10	1.19	WG_03	1.79	WG_05	1.53	WG_03	2.00		
WG_06	1.32	WG_06	0.94	WG_09	1.19	WG_09	1.82	WG_06	1.59	WG_06	2.45		
WG_10	1.52	WG_09	1.08	WG_04	1.22	WG_07	1.86	WG_08	1.98	WG_08	2.84		
WG_07	1.53	WG_13	1.11	WG_07	1.37	WG_10	1.98	WG_12	2.41	WG_07	3.06		
WG_09	1.60	WG_04	1.22	WG_06	1.45	WG_06	2.09	WG_10	3.13	WG_12	3.48		
WG_11	2.02	WG_11	1.34	WG_13	1.82	WG_11	2.35	WG_07	3.19	WG_09	3.51		
WG_13	2.03	WG_15	1.59	WG_14	1.84	WG_13	2.36	WG_09	3.40	WG_10	3.52		
WG_08	2.06	WG_05	1.60	WG_11	1.86	WG_08	2.41	WG_11	3.43	WG_11	3.60		
WG_14	2.21	WG_14	1.61	WG_08	1.92	WG_14	2.45	WG_15	3.54	WG_14	3.90		
WG_15	2.41	WG_08	1.74	WG_15	2.22	WG_12	3.15	WG_13	3.60	WG_13	4.08		
WG_12	2.45	WG_12	1.95	WG_12	2.65	WG_15	3.24	WG_14	3.82	WG_15	4.57		
MO6-2X/LP ₂ ^e		BH&H/LP ₃ ^f		B3LYP/LP ₁ ^d		TPSS/LP ₁ ^d		SCC-DF-TB-D		ff99(HF)		ff99(DFT)	
WG_01	0.00	WG_01	0.00	WG_01	0.00	WG_01	0.00	WG_03	0.00	WG_03	0.00	WG_02	0.00
WG_02	0.16	WG_04	1.33	WG_05	0.04	WG_05	0.33	WG_01	0.45	WG_02	0.15	WG_09	0.25
WG_03	0.26	WG_03	1.35	WG_04	1.05	WG_04	1.29	WG_06	0.50	WG_12	0.19	WG_12	0.72
WG_09	0.34	WG_02	1.59	WG_02	3.47	WG_02	3.28	WG_02	0.57	WG_01	1.06	WG_13	1.25
WG_10	0.42	WG_05	1.70	WG_08	3.71	WG_08	3.67	WG_10	0.88	WG_08	2.06	WG_03	1.25
WG_07	0.57	WG_06	2.48	WG_03	4.14	WG_03	3.91	WG_08	1.33	WG_05	2.76	WG_10	1.43
WG_13	0.58	WG_11	2.51	WG_06	4.28	WG_06	4.17	WG_12	1.46	WG_04	3.83	WG_08	1.86
WG_14	0.95	WG_07	2.63	WG_09	4.82	WG_12	4.96	WG_14	1.58	WG_06	4.60	WG_01	2.29
WG_06	1.03	WG_12	3.15	WG_11	4.92	WG_11	5.64	WG_05	1.73	WG_09	4.61	WG_06	2.91
WG_11	1.17	WG_08	3.35	WG_07	5.20	WG_07	5.92	WG_04	1.76	WG_15	4.74	WG_05	2.95
WG_05	1.17	WG_10	3.37	WG_12	5.29	WG_09	5.95	WG_09	1.82	WG_13	4.83	WG_15	3.10
WG_15	1.29	WG_15	3.55	WG_14	5.37	WG_14	6.49	WG_07	1.90	WG_10	5.01	WG_14	3.32
WG_04	1.32	WG_13	3.80	WG_10	5.52	WG_10	6.52	WG_13	2.08	WG_11	5.74	WG_11	3.68
WG_08	1.83	WG_09	3.85	WG_13	6.17	WG_13	6.82	WG_15	2.33	WG_07	7.55	WG_04	3.99
WG_12	1.85	WG_14	4.38	WG_15	6.89	WG_15	7.34	WG_11	3.46	WG_14	9.46	WG_07	4.23

^a $E_{\text{CBS}}^{\text{CCSD(T)}} = E_{\text{CBS}}^{\text{MP2}} + (E_{\text{6-31G}^*}^{\text{CCSD(T)}} - E_{\text{6-31G}^*}^{\text{MP2}})$. ^bRelative energies extrapolated to the CBS limit. ^c $E_{\text{CBS}}^{\text{MP3}} = E_{\text{CBS}}^{\text{MP2}} + (E_{\text{6-31G}^*}^{\text{MP3}} - E_{\text{6-31G}^*}^{\text{MP2}})$. ^dLP₁ stands for 6-311++G(3df,3pd) Pople basis set. ^eLP₂ stands for 6-311+G(2df,2pd) Pople basis set. ^fLP₃ stands for 6-311++G(d,p) Pople basis set.

Table S1. (cont.). WGG tripeptide.

CCSDT/CBS ^a		MP2/CBS ^b		SCS-MP2/CBS ^b		MP3/CBS ^c		TPSS-D/LP ₁ ^d		PBE-D/LP ₁ ^d			
WGG_01	0.00	WGG_02	0.00	WGG_01	0.00	WGG_01	0.00	WGG_01	0.00	WGG_01	0.00		
WGG_02	0.26	WGG_01	0.43	WGG_02	0.25	WGG_02	0.39	WGG_02	0.39	WGG_02	0.56		
WGG_03	1.09	WGG_07	1.37	WGG_05	1.92	WGG_05	2.36	WGG_06	2.14	WGG_03	2.32		
WGG_05	1.71	WGG_14	1.37	WGG_03	2.01	WGG_04	2.51	WGG_03	2.17	WGG_06	2.42		
WGG_04	2.09	WGG_05	1.46	WGG_04	2.18	WGG_03	2.61	WGG_12	2.92	WGG_12	3.14		
WGG_07	2.37	WGG_04	2.06	WGG_07	2.39	WGG_09	2.81	WGG_04	2.94	WGG_08	3.17		
WGG_14	2.38	WGG_03	2.24	WGG_14	2.39	WGG_06	3.15	WGG_15	2.97	WGG_15	3.21		
WGG_06	2.52	WGG_06	2.56	WGG_09	2.43	WGG_11	3.29	WGG_08	3.10	WGG_09	3.48		
WGG_09	2.78	WGG_10	2.79	WGG_06	2.58	WGG_07	3.34	WGG_07	3.19	WGG_04	3.49		
WGG_08	2.96	WGG_09	2.81	WGG_08	2.83	WGG_14	3.34	WGG_14	3.20	WGG_07	4.27		
WGG_11	3.34	WGG_11	3.04	WGG_11	2.85	WGG_12	3.38	WGG_09	3.26	WGG_14	4.29		
WGG_12	3.36	WGG_08	3.13	WGG_12	3.03	WGG_08	3.40	WGG_05	4.49	WGG_11	4.58		
WGG_15	3.37	WGG_13	3.55	WGG_15	3.04	WGG_15	3.40	WGG_11	4.72	WGG_05	5.40		
WGG_10	3.83	WGG_12	3.69	WGG_10	3.98	WGG_10	4.76	WGG_10	4.98	WGG_10	5.92		
WGG_13	4.24	WGG_15	3.71	WGG_13	4.15	WGG_13	5.07	WGG_13	5.35	WGG_13	6.00		
MO6-2X/LP ₂ ^e		BH&H/LP ₃ ^f		B3LYP/LP ₁ ^d		TPSS/LP ₁ ^d		SCC-DF-TB-D		ff99(HF)		ff99(DFT)	
WGG_05	0.00	WGG_01	0.00	WGG_01	0.00	WGG_01	0.00	WGG_01	0.00	WGG_01	0.00	WGG_03	0.00
WGG_02	0.04	WGG_02	0.21	WGG_02	2.52	WGG_02	2.16	WGG_06	0.46	WGG_06	0.32	WGG_01	0.08
WGG_01	0.31	WGG_04	2.83	WGG_12	3.25	WGG_12	3.65	WGG_04	1.23	WGG_10	0.91	WGG_06	0.27
WGG_07	1.38	WGG_06	3.27	WGG_15	3.32	WGG_15	3.70	WGG_03	1.34	WGG_15	1.06	WGG_10	0.54
WGG_14	1.38	WGG_05	3.59	WGG_03	3.94	WGG_03	3.90	WGG_08	1.41	WGG_03	1.20	WGG_15	0.64
WGG_04	1.53	WGG_07	3.78	WGG_09	4.59	WGG_06	4.70	WGG_02	1.55	WGG_04	3.93	WGG_14	2.46
WGG_03	2.28	WGG_14	3.80	WGG_08	4.66	WGG_09	4.78	WGG_15	2.43	WGG_14	4.04	WGG_07	2.52
WGG_09	2.56	WGG_03	3.96	WGG_06	4.70	WGG_08	4.80	WGG_10	2.50	WGG_07	4.09	WGG_04	2.60
WGG_06	2.63	WGG_12	4.49	WGG_04	5.56	WGG_04	5.19	WGG_05	3.25	WGG_02	4.38	WGG_12	3.18
WGG_10	2.63	WGG_15	4.57	WGG_11	6.37	WGG_11	6.93	WGG_07	3.46	WGG_12	5.25	WGG_08	3.36
WGG_11	2.81	WGG_08	4.75	WGG_07	8.27	WGG_07	7.62	WGG_14	3.47	WGG_08	5.32	WGG_02	3.90
WGG_08	3.11	WGG_09	4.83	WGG_14	8.28	WGG_14	7.64	WGG_09	3.97	WGG_09	9.35	WGG_13	5.85
WGG_13	3.12	WGG_11	5.03	WGG_05	8.38	WGG_05	8.79	WGG_11	4.85	WGG_13	9.47	WGG_09	6.57
WGG_12	3.33	WGG_10	5.55	WGG_13	9.34	WGG_13	9.00	WGG_12	5.19	WGG_11	10.76	WGG_11	8.97
WGG_15	3.36	WGG_13	6.45	WGG_10	10.09	WGG_10	9.26	WGG_13	5.21	WGG_05	13.42	WGG_05	10.50

^a $E_{\text{CBS}}^{\text{CCSD}(1)} = E_{\text{CBS}}^{\text{MP2}} + (E_{6-31\text{G}^*}^{\text{CCSD}(1)} - E_{6-31\text{G}^*}^{\text{MP2}})$. ^bRelative energies extrapolated to the CBS limit. ^c $E_{\text{CBS}}^{\text{MP3}} = E_{\text{CBS}}^{\text{MP2}} + (E_{6-31\text{G}^*}^{\text{MP3}} - E_{6-31\text{G}^*}^{\text{MP2}})$. ^dLP₁ stands for 6-311++G(3df,3pd) Pople basis set. ^eLP₂ stands for 6-311+G(2df,2pd) Pople basis set. ^fLP₃ stands for 6-311++G(d,p) Pople basis set.

Table S1. (cont.). FGG tripeptide.

CCSDT/CBS ^a		MP2/CBS ^b		SCS-MP2/CBS ^b		MP3/CBS ^c		TPSS-D/LP ₁ ^d		PBE-D/LP ₁ ^d			
FGG_099	0.00	FGG_099	0.00	FGG_099	0.00	FGG_099	0.00	FGG_444	0.00	FGG_444	0.00		
FGG_444	0.69	FGG_357	0.74	FGG_366	0.64	FGG_444	0.27	FGG_357	0.64	FGG_357	1.18		
FGG_357	1.18	FGG_444	1.09	FGG_444	0.68	FGG_366	0.40	FGG_215	0.90	FGG_215	1.24		
FGG_215	1.29	FGG_215	1.55	FGG_357	0.96	FGG_357	0.73	FGG_114	1.39	FGG_224	2.04		
FGG_366	1.51	FGG_114	1.57	FGG_300	1.06	FGG_215	0.97	FGG_099	1.54	FGG_099	2.31		
FGG_114	2.03	FGG_412	2.35	FGG_215	1.28	FGG_691	1.47	FGG_224	1.54	FGG_114	2.39		
FGG_691	2.36	FGG_366	2.46	FGG_691	1.61	FGG_114	1.62	FGG_080	2.09	FGG_380	2.45		
FGG_412	2.36	FGG_080	2.47	FGG_114	1.66	FGG_470	1.66	FGG_055	2.25	FGG_055	2.47		
FGG_224	2.43	FGG_224	2.65	FGG_470	1.81	FGG_300	2.08	FGG_380	2.25	FGG_080	2.74		
FGG_470	2.52	FGG_470	2.81	FGG_252	1.97	FGG_252	2.20	FGG_412	2.80	FGG_366	2.80		
FGG_080	2.71	FGG_380	3.05	FGG_412	2.08	FGG_412	2.20	FGG_300	3.03	FGG_300	2.84		
FGG_252	2.73	FGG_691	3.12	FGG_224	2.23	FGG_080	2.23	FGG_366	3.05	FGG_470	3.25		
FGG_380	2.77	FGG_252	3.23	FGG_080	2.27	FGG_224	2.28	FGG_470	3.44	FGG_412	3.44		
FGG_055	3.04	FGG_055	3.39	FGG_380	2.49	FGG_380	2.40	FGG_691	3.59	FGG_691	3.46		
FGG_300	3.12	FGG_300	4.25	FGG_055	2.82	FGG_055	2.84	FGG_252	3.88	FGG_252	4.45		
MO6-2X/LP ₂ ^e		BH&H/LP ₃ ^f		B3LYP/LP ₁ ^d		TPSS/LP ₁ ^d		SCC-DF-TB-D		ff99(HF)		ff99(DFT)	
FGG_099	0.00	FGG_444	0.00	FGG_366	0.00	FGG_444	0.00	FGG_444	0.00	FGG_380	0.00	FGG_380	0.00
FGG_357	2.20	FGG_099	0.41	FGG_444	0.55	FGG_366	0.94	FGG_215	0.33	FGG_224	0.07	FGG_224	0.22
FGG_412	2.51	FGG_357	0.74	FGG_300	0.63	FGG_300	1.43	FGG_099	0.34	FGG_055	0.91	FGG_055	0.30
FGG_114	2.61	FGG_215	1.05	FGG_691	1.34	FGG_215	1.58	FGG_224	0.42	FGG_215	1.38	FGG_215	1.59
FGG_300	2.72	FGG_114	2.17	FGG_215	2.15	FGG_691	1.86	FGG_055	0.87	FGG_444	2.22	FGG_444	2.60
FGG_444	2.80	FGG_300	2.47	FGG_470	2.94	FGG_357	2.55	FGG_380	1.45	FGG_366	4.89	FGG_366	4.25
FGG_366	2.82	FGG_224	2.81	FGG_380	2.98	FGG_224	2.71	FGG_357	1.53	FGG_080	5.19	FGG_099	4.30
FGG_215	3.09	FGG_366	2.92	FGG_224	3.07	FGG_380	2.80	FGG_470	1.59	FGG_099	5.44	FGG_412	4.57
FGG_080	3.57	FGG_412	3.14	FGG_252	3.20	FGG_055	3.05	FGG_300	1.71	FGG_412	5.63	FGG_080	4.61
FGG_470	3.57	FGG_380	3.24	FGG_357	3.45	FGG_470	3.72	FGG_080	1.80	FGG_252	5.80	FGG_252	4.67
FGG_691	3.93	FGG_080	3.24	FGG_055	3.68	FGG_114	3.77	FGG_412	2.03	FGG_114	6.40	FGG_300	5.68
FGG_252	4.05	FGG_470	3.37	FGG_114	4.53	FGG_252	3.79	FGG_252	2.12	FGG_300	6.59	FGG_470	5.81
FGG_224	4.16	FGG_691	3.67	FGG_099	4.57	FGG_080	3.99	FGG_114	2.21	FGG_470	8.02	FGG_114	5.89
FGG_380	4.37	FGG_055	4.11	FGG_080	4.60	FGG_099	4.78	FGG_691	2.39	FGG_357	8.26	FGG_357	7.82
FGG_055	4.90	FGG_252	4.70	FGG_412	5.50	FGG_412	5.51	FGG_366	2.54	FGG_691	9.03	FGG_691	8.05

^a $E_{\text{CBS}}^{\text{CCSD}(1)} = E_{\text{CBS}}^{\text{MP2}} + (E_{6-31\text{G}^*}^{\text{CCSD}(1)} - E_{6-31\text{G}^*}^{\text{MP2}})$. ^bRelative energies extrapolated to the CBS limit. ^c $E_{\text{CBS}}^{\text{MP3}} = E_{\text{CBS}}^{\text{MP2}} + (E_{6-31\text{G}^*}^{\text{MP3}} - E_{6-31\text{G}^*}^{\text{MP2}})$. ^dLP₁ stands for 6-311++G(3df,3pd) Pople basis set. ^eLP₂ stands for 6-311+G(2df,2pd) Pople basis set. ^fLP₃ stands for 6-311++G(d,p) Pople basis set.

Table S1. (cont.). GGF tripeptide.

CCSDT/CBS ^a		MP2/CBS ^b		SCS-MP2/CBS ^b		MP3/CBS ^c		TPSS-D/LP ₁ ^d		PBE-D/LP ₁ ^d			
GGF_15	0.00	GGF_15	0.00	GGF_15	0.00	GGF_15	0.00	GGF_14	0.00	GGF_15	0.00		
GGF_14	0.39	GGF_14	0.00	GGF_14	0.43	GGF_14	0.67	GGF_13	0.28	GGF_14	0.10		
GGF_13	0.75	GGF_13	0.42	GGF_12	0.67	GGF_13	1.02	GGF_15	0.55	GGF_13	0.62		
GGF_12	1.06	GGF_11	0.92	GGF_13	0.76	GGF_11	1.03	GGF_11	1.47	GGF_11	0.90		
GGF_11	1.23	GGF_12	0.94	GGF_11	1.10	GGF_12	1.39	GGF_06	2.78	GGF_06	2.40		
GGF_10	1.73	GGF_10	1.43	GGF_10	1.19	GGF_10	1.66	GGF_10	3.04	GGF_07	2.56		
GGF_09	2.14	GGF_09	1.63	GGF_03	1.51	GGF_03	2.19	GGF_07	3.11	GGF_10	2.64		
GGF_08	2.33	GGF_05	1.77	GGF_09	1.72	GGF_09	2.20	GGF_01	3.44	GGF_01	2.80		
GGF_07	2.35	GGF_08	1.77	GGF_08	1.73	GGF_07	2.35	GGF_12	3.82	GGF_08	3.69		
GGF_06	2.42	GGF_06	2.06	GGF_07	1.86	GGF_08	2.38	GGF_03	3.98	GGF_04	3.81		
GGF_05	2.44	GGF_07	2.11	GGF_01	2.02	GGF_04	2.44	GGF_08	4.10	GGF_02	3.87		
GGF_04	2.49	GGF_01	2.15	GGF_04	2.05	GGF_06	2.49	GGF_04	4.13	GGF_12	3.90		
GGF_03	2.59	GGF_03	2.19	GGF_02	2.37	GGF_05	2.82	GGF_09	4.14	GGF_03	3.93		
GGF_02	2.77	GGF_04	2.20	GGF_05	2.52	GGF_01	2.90	GGF_02	4.24	GGF_09	3.97		
GGF_01	2.93	GGF_02	2.33	GGF_06	2.55	GGF_02	2.94	GGF_05	4.81	GGF_05	5.48		
MO6-2X/LP ₂ ^e		BH&H/LP ₃ ^f		B3LYP/LP ₁ ^d		TPSS/LP ₁ ^d		SCC-DF-TB-D		ff99(HF)		ff99(DFT)	
GGF_15	0.00	GGF_15	0.00	GGF_15	0.00	GGF_15	0.00	GGF_15	0.00	GGF_14	0.00	GGF_14	0.00
GGF_12	0.25	GGF_11	0.75	GGF_11	1.04	GGF_14	0.90	GGF_14	0.71	GGF_15	1.26	GGF_01	0.24
GGF_13	0.54	GGF_14	0.84	GGF_14	1.13	GGF_11	1.04	GGF_13	1.23	GGF_13	1.60	GGF_15	0.65
GGF_14	0.66	GGF_13	1.20	GGF_13	1.59	GGF_13	1.31	GGF_07	1.47	GGF_01	1.91	GGF_13	1.39
GGF_05	0.77	GGF_01	2.43	GGF_03	2.15	GGF_10	3.09	GGF_10	1.87	GGF_12	4.02	GGF_12	3.06
GGF_11	1.05	GGF_12	2.77	GGF_10	2.38	GGF_07	3.14	GGF_12	1.90	GGF_03	4.51	GGF_03	3.46
GGF_09	1.37	GGF_06	3.27	GGF_07	2.70	GGF_06	3.45	GGF_11	2.26	GGF_11	6.87	GGF_10	6.09
GGF_01	1.55	GGF_07	3.30	GGF_12	3.30	GGF_03	3.50	GGF_01	2.54	GGF_07	7.71	GGF_07	6.26
GGF_04	1.66	GGF_10	3.38	GGF_06	3.86	GGF_01	4.00	GGF_08	2.65	GGF_10	8.03	GGF_11	6.31
GGF_03	1.69	GGF_04	3.70	GGF_08	3.88	GGF_12	4.15	GGF_09	2.69	GGF_02	8.98	GGF_08	6.59
GGF_10	1.77	GGF_02	3.91	GGF_01	3.88	GGF_04	4.37	GGF_02	2.84	GGF_08	9.15	GGF_09	6.98
GGF_08	1.81	GGF_08	4.06	GGF_04	3.92	GGF_08	4.77	GGF_04	3.25	GGF_09	9.72	GGF_02	8.37
GGF_07	2.20	GGF_03	4.16	GGF_09	4.11	GGF_09	4.93	GGF_03	3.53	GGF_06	9.81	GGF_06	8.73
GGF_02	2.32	GGF_09	4.22	GGF_02	4.19	GGF_02	4.95	GGF_06	4.15	GGF_04	12.65	GGF_05	10.59
GGF_06	2.97	GGF_05	4.57	GGF_05	6.85	GGF_05	7.03	GGF_05	4.27	GGF_05	13.37	GGF_04	10.66

^a $E_{\text{CBS}}^{\text{CCSD}(1)} = E_{\text{CBS}}^{\text{MP2}} + (E_{6-31\text{G}^*}^{\text{CCSD}(1)} - E_{6-31\text{G}^*}^{\text{MP2}})$. ^bRelative energies extrapolated to the CBS limit. ^c $E_{\text{CBS}}^{\text{MP3}} = E_{\text{CBS}}^{\text{MP2}} + (E_{6-31\text{G}^*}^{\text{MP3}} - E_{6-31\text{G}^*}^{\text{MP2}})$. ^dLP₁ stands for 6-311++G(3df,3pd) Pople basis set. ^eLP₂ stands for 6-311+G(2df,2pd) Pople basis set. ^fLP₃ stands for 6-311++G(d,p) Pople basis set.

Table S1. (cont.). GFA tripeptide.

CCSDT/CBS ^a		MP2/CBS ^b		SCS-MP2/CBS ^b		MP3/CBS ^c		TPSS-D/LP ₁ ^d		PBE-D/LP ₁ ^d			
GFA_15	0.00	GFA_15	0.00	GFA_10	0.00	GFA_07	0.00	GFA_15	0.00	GFA_07	0.00		
GFA_10	0.25	GFA_10	0.02	GFA_09	0.09	GFA_10	0.16	GFA_12	0.64	GFA_15	0.21		
GFA_07	0.30	GFA_09	0.12	GFA_07	0.13	GFA_15	0.21	GFA_16	0.79	GFA_12	0.48		
GFA_09	0.34	GFA_07	0.91	GFA_15	0.21	GFA_09	0.25	GFA_07	0.87	GFA_06	0.55		
GFA_12	0.56	GFA_12	0.98	GFA_03	0.29	GFA_04	0.37	GFA_10	1.12	GFA_11	0.76		
GFA_11	0.81	GFA_02	1.03	GFA_04	0.36	GFA_12	0.41	GFA_09	1.25	GFA_08	0.77		
GFA_14	0.85	GFA_03	1.10	GFA_01	0.41	GFA_05	0.44	GFA_06	1.56	GFA_10	0.78		
GFA_06	0.85	GFA_01	1.22	GFA_05	0.45	GFA_06	0.45	GFA_11	1.56	GFA_09	0.88		
GFA_08	0.88	GFA_11	1.29	GFA_02	0.46	GFA_11	0.74	GFA_08	1.64	GFA_16	1.41		
GFA_13	0.96	GFA_16	1.40	GFA_12	0.49	GFA_02	0.76	GFA_02	2.94	GFA_02	1.98		
GFA_02	1.12	GFA_08	1.41	GFA_06	0.61	GFA_08	0.81	GFA_13	3.34	GFA_04	2.42		
GFA_04	1.18	GFA_04	1.45	GFA_13	0.84	GFA_14	0.86	GFA_03	3.43	GFA_05	2.50		
GFA_05	1.25	GFA_05	1.53	GFA_14	0.89	GFA_03	0.87	GFA_01	3.54	GFA_03	2.70		
GFA_03	1.43	GFA_06	1.60	GFA_11	0.91	GFA_13	0.93	GFA_04	3.85	GFA_01	2.77		
GFA_01	1.56	GFA_13	1.68	GFA_08	0.99	GFA_01	0.99	GFA_14	3.87	GFA_13	3.21		
GFA_16	1.56	GFA_14	1.82	GFA_16	1.75	GFA_16	1.81	GFA_05	3.94	GFA_14	3.43		
MO6-2X/LP ₂ ^e		BH&H/LP ₃ ^f		B3LYP/LP ₁ ^d		TPSS/LP ₁ ^d		SCC-DF-TB-D		ff99(HF)		ff99(DFT)	
GFA_10	0.00	GFA_15	0.00	GFA_06	0.00	GFA_07	0.00	GFA_07	0.00	GFA_13	0.00	GFA_07	0.00
GFA_09	0.09	GFA_11	0.22	GFA_07	0.18	GFA_06	0.04	GFA_15	0.17	GFA_07	0.13	GFA_13	0.05
GFA_15	0.54	GFA_08	0.34	GFA_12	0.86	GFA_12	0.57	GFA_11	0.31	GFA_12	0.27	GFA_12	0.58
GFA_14	0.72	GFA_07	0.44	GFA_11	1.15	GFA_11	0.70	GFA_08	0.43	GFA_15	0.44	GFA_06	1.05
GFA_04	0.76	GFA_12	0.86	GFA_08	1.18	GFA_08	0.76	GFA_06	0.70	GFA_16	0.83	GFA_15	1.08
GFA_05	0.81	GFA_10	1.04	GFA_04	2.33	GFA_15	1.55	GFA_12	0.92	GFA_06	1.25	GFA_16	1.85
GFA_07	0.82	GFA_06	1.09	GFA_05	2.40	GFA_10	2.58	GFA_10	1.09	GFA_11	1.70	GFA_11	1.96
GFA_02	1.13	GFA_09	1.10	GFA_15	2.42	GFA_09	2.67	GFA_09	1.12	GFA_08	2.10	GFA_08	2.24
GFA_03	1.14	GFA_14	1.31	GFA_14	2.77	GFA_16	2.79	GFA_02	1.20	GFA_09	4.32	GFA_02	2.40
GFA_13	1.16	GFA_16	1.50	GFA_10	2.86	GFA_04	3.47	GFA_16	1.92	GFA_10	4.39	GFA_09	3.14
GFA_01	1.26	GFA_13	2.35	GFA_09	2.94	GFA_05	3.53	GFA_13	2.04	GFA_14	4.39	GFA_10	3.21
GFA_12	1.33	GFA_04	2.75	GFA_13	3.20	GFA_14	3.55	GFA_14	2.27	GFA_02	4.63	GFA_01	4.17
GFA_11	1.39	GFA_05	2.77	GFA_03	3.32	GFA_13	3.93	GFA_04	2.36	GFA_04	6.15	GFA_14	4.22
GFA_08	1.41	GFA_02	2.79	GFA_01	3.38	GFA_02	4.36	GFA_05	2.40	GFA_05	6.45	GFA_03	4.24
GFA_06	1.50	GFA_03	4.08	GFA_02	3.49	GFA_03	4.44	GFA_03	2.76	GFA_01	7.44	GFA_04	4.57
GFA_16	2.09	GFA_01	4.14	GFA_16	3.91	GFA_01	4.50	GFA_01	2.80	GFA_03	7.48	GFA_05	4.86

^a $E_{\text{CBS}}^{\text{CCSD(T)}} = E_{\text{CBS}}^{\text{MP2}} + (E^{\text{CCSD(T)}} - E^{\text{MP2}})_{|6-31\text{G}^*}$. ^bRelative energies extrapolated to the CBS limit. ^c $E_{\text{CBS}}^{\text{MP3}} = E_{\text{CBS}}^{\text{MP2}} + (E^{\text{MP3}} - E^{\text{MP2}})_{|6-31\text{G}^*}$. ^dLP₁ stands for 6-311++G(3df,3pd) Pople basis set. ^eLP₂ stands for 6-311+G(2df,2pd) Pople basis set. ^fLP₃ stands for 6-311++G(d,p) Pople basis set.

Figure S1. RI-MP2/cc-pVTZ geometries of the different peptides here studied. For the sake of simplicity, the nomenclature used is equivalent to that of previous publications (see Refs. 2, 3, 27 and 36).

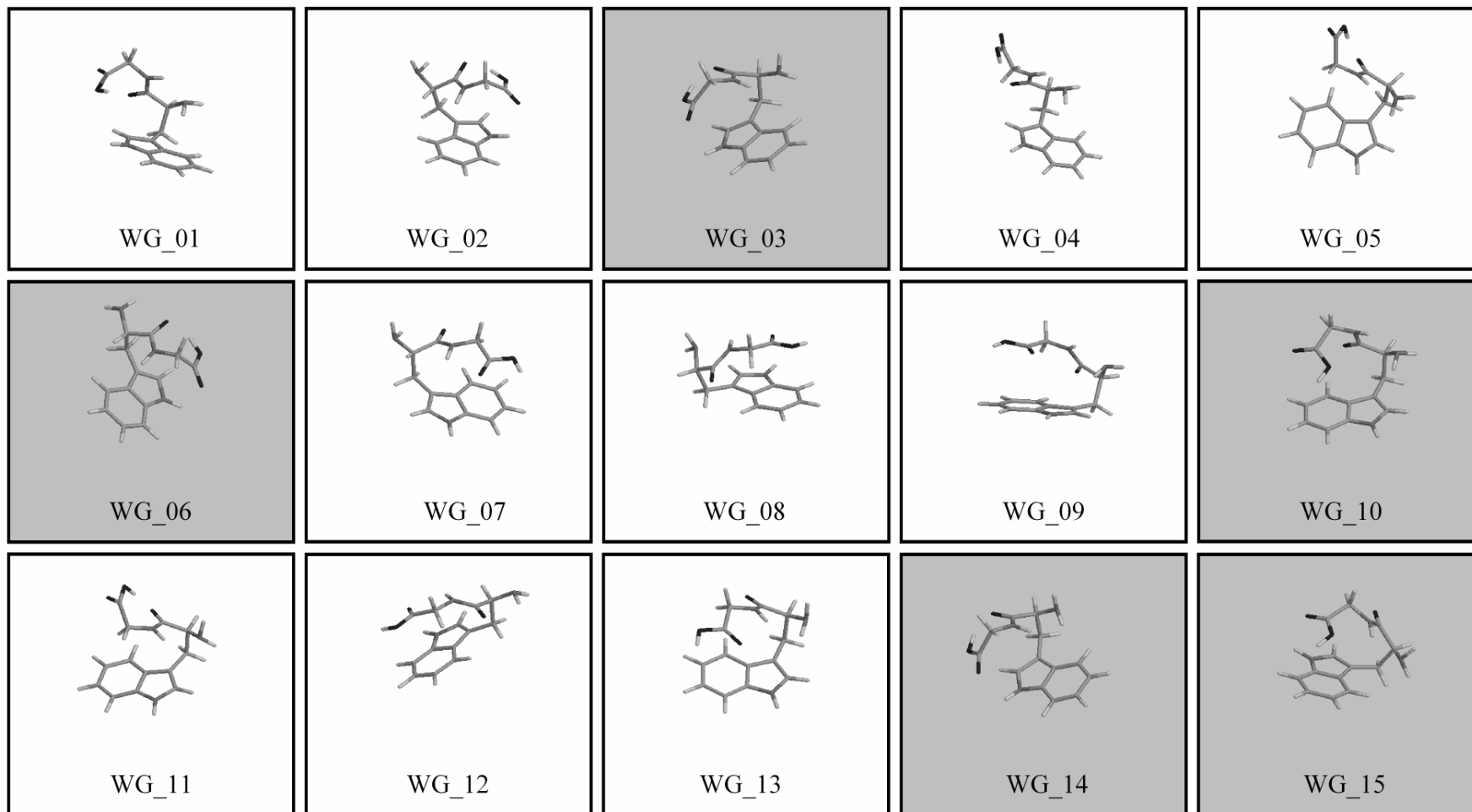


Figure S1. (cont.).

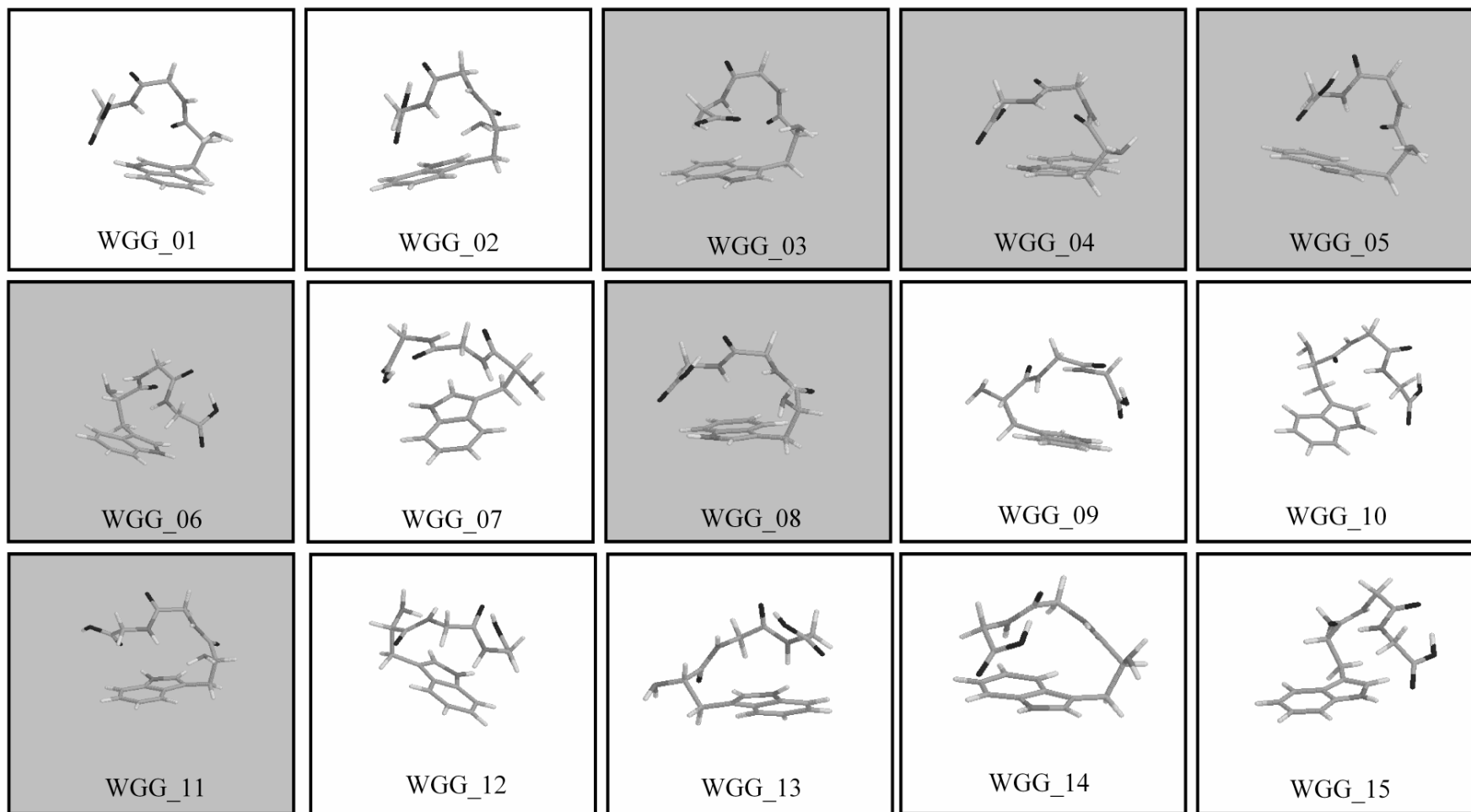


Figure S1. (cont.).

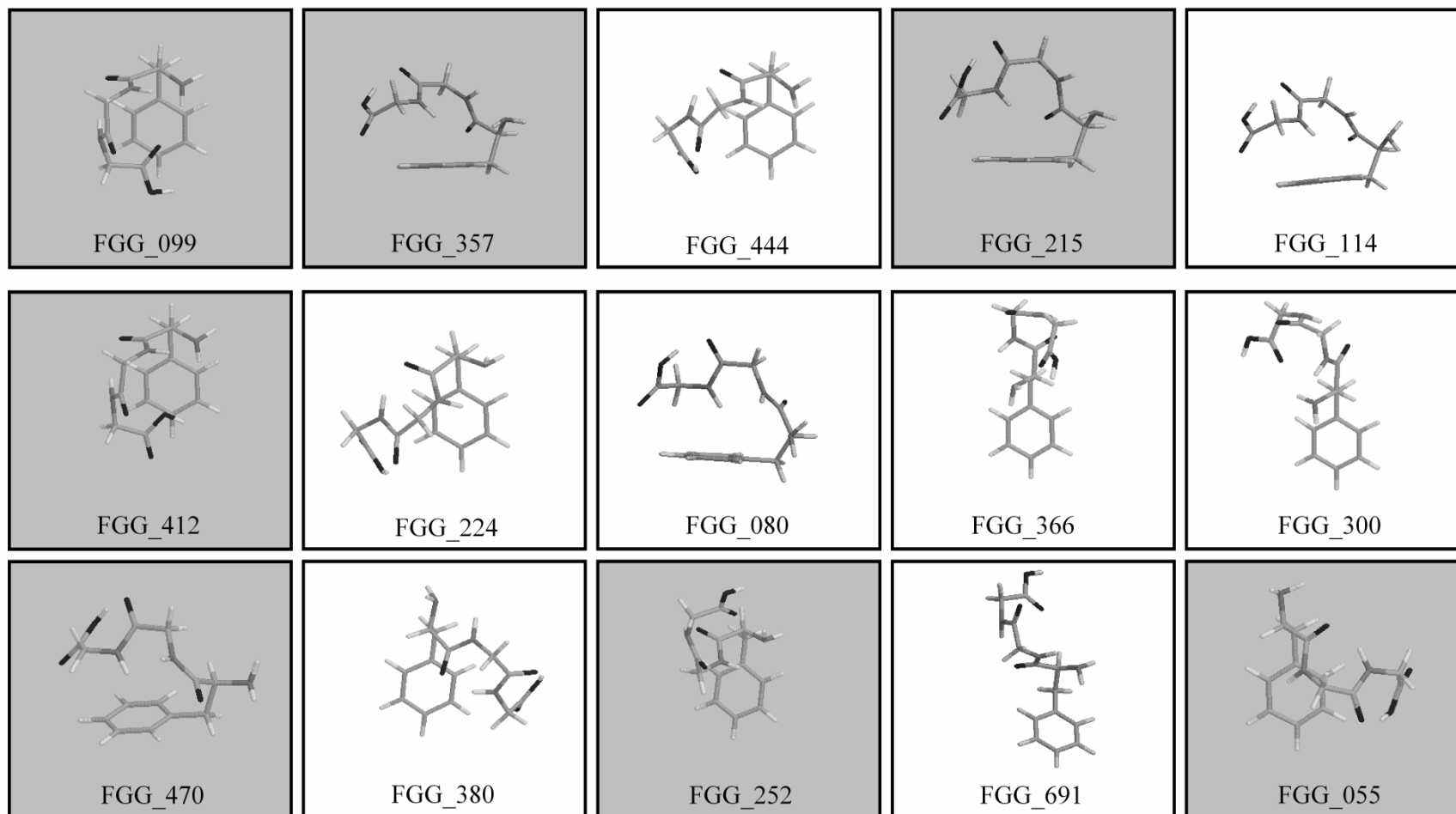
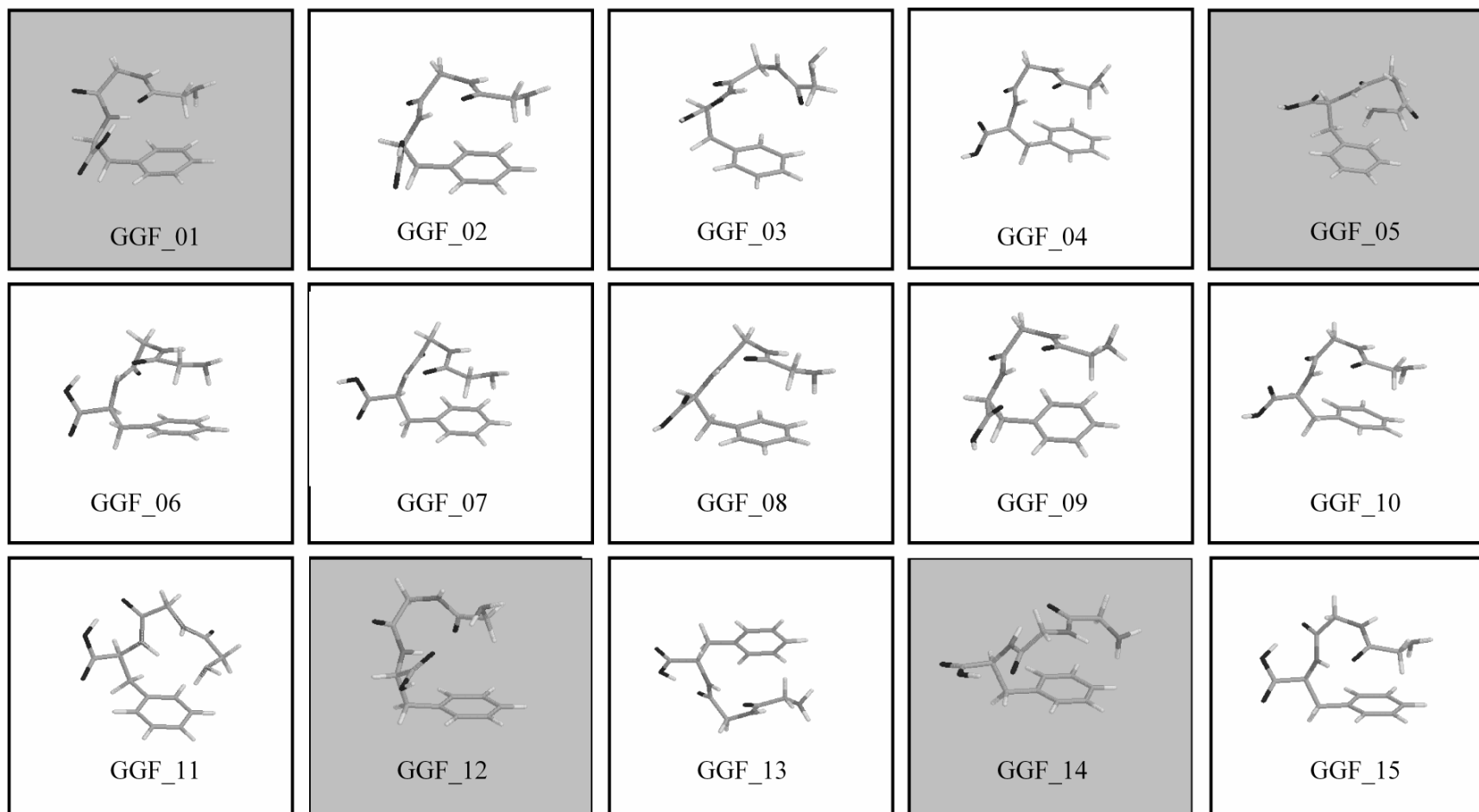


Figure S1. (cont.).



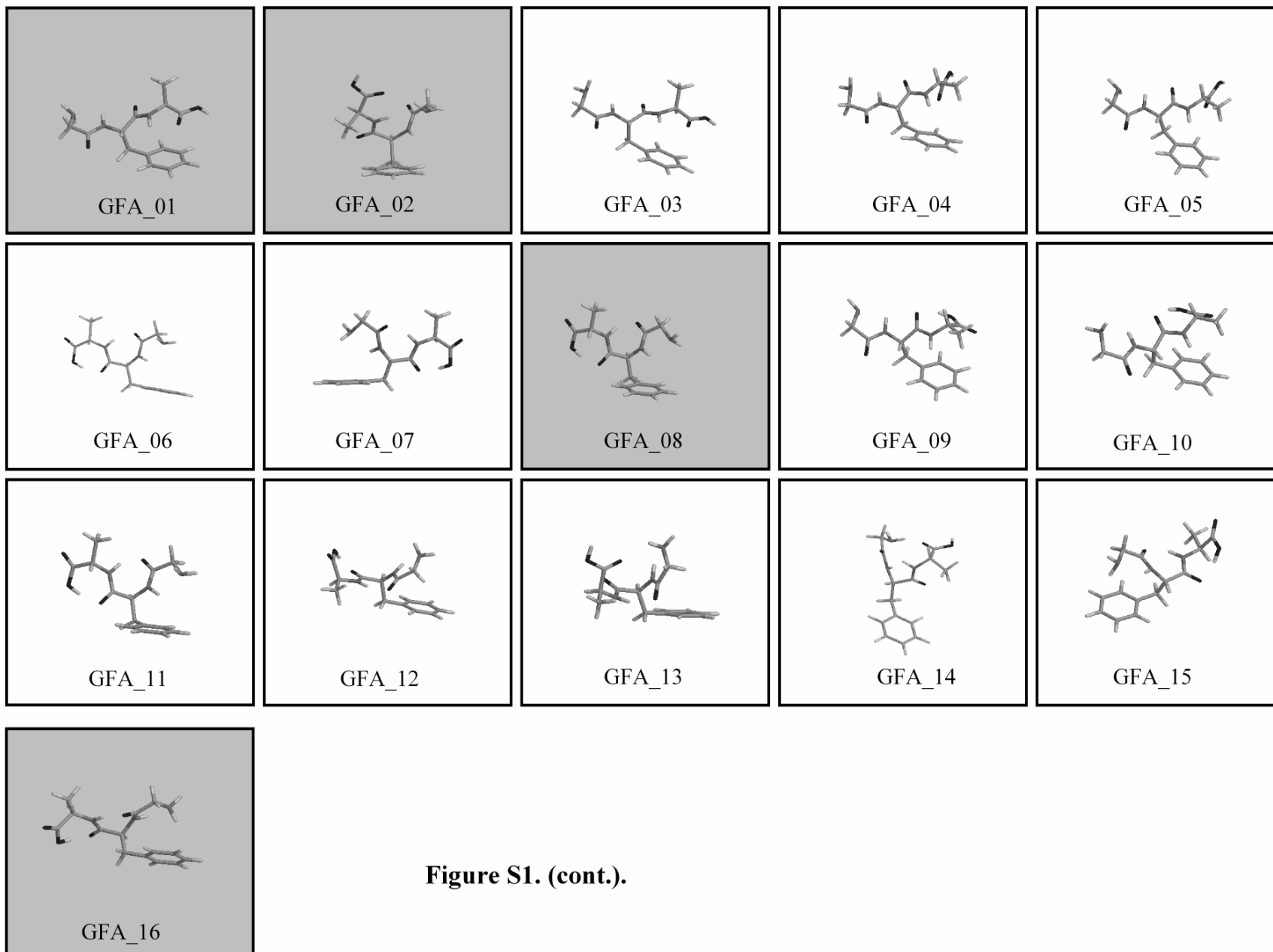


Figure S1. (cont.).

WG_01.xyz

o	-2.94633	-0.91974	1.27713
c	-3.05690	0.40279	1.46300
o	-3.06064	0.90573	2.56045
h	-2.92094	-1.09730	0.30175
c	-3.19688	1.21568	0.17725
h	-3.31758	2.25675	0.45414
h	-4.08614	0.87620	-0.35823
n	-2.04164	1.09342	-0.69124
h	-1.43228	1.87639	-0.89206
c	-1.78708	-0.01064	-1.39973
o	-2.46335	-1.04878	-1.30858
c	-0.57570	0.06734	-2.31929
h	-0.96543	-0.03415	-3.33428
n	0.08130	1.36756	-2.19209
h	0.49463	1.64309	-3.07240
h	0.83831	1.30020	-1.51788
c	0.33378	-1.13578	-2.00146
h	1.13981	-1.16748	-2.73648
h	-0.25309	-2.04727	-2.10628
c	0.88961	-1.01564	-0.62052
c	0.26881	-1.41492	0.54777
h	-0.65968	-1.94098	0.68964
n	1.02447	-1.03326	1.62709
h	0.76527	-1.18388	2.58697
c	2.14551	-0.37490	1.19591
c	3.19880	0.19464	1.91508
h	3.22285	0.16948	2.99663
c	4.21625	0.79584	1.19000
h	5.04656	1.24721	1.71531
c	4.19197	0.82489	-0.21890
h	5.00873	1.29469	-0.74975
c	3.14690	0.26014	-0.93197
h	3.14882	0.28002	-2.01495
c	2.09310	-0.35011	-0.22641

WG_02.xyz

o	-1.81194	2.32920	-0.57670
c	-0.86763	2.44672	0.36389
o	0.07899	3.18970	0.23470
h	-2.41971	1.59349	-0.31813
c	-1.07877	1.57557	1.59963
h	-2.07107	1.76509	2.00987
h	-0.32560	1.84248	2.33296
n	-0.96261	0.15457	1.31220
h	-0.05242	-0.27489	1.40634
c	-1.88528	-0.50499	0.58373
o	-2.92583	0.03883	0.18356
c	-1.57751	-1.95739	0.24695
h	-0.86201	-2.34488	0.97349
n	-2.75262	-2.81132	0.24966
h	-3.12019	-2.88549	1.19140
h	-3.47612	-2.34268	-0.28719
c	-0.92714	-1.99063	-1.15268
h	-1.70307	-1.75887	-1.88575

h	-0.59514	-3.01322	-1.33514
c	0.17613	-0.99387	-1.24653
c	0.11364	0.22658	-1.88519
h	-0.65005	0.61869	-2.53608
n	1.20709	0.98828	-1.55366
h	1.28672	1.97419	-1.74390
c	1.97665	0.30306	-0.65108
c	3.13733	0.68586	0.02495
h	3.58260	1.65968	-0.12880
c	3.69010	-0.22621	0.91213
h	4.58631	0.03968	1.45558
c	3.10915	-1.49383	1.11750
h	3.57572	-2.18126	1.80994
c	1.95716	-1.87468	0.44539
h	1.53096	-2.85838	0.60031
c	1.36654	-0.96836	-0.45470

WG_03.xyz

o	0.73424	-2.98815	-0.60355
c	1.51429	-2.06656	-0.52464
o	2.30484	-1.89287	0.53984
h	2.75228	-1.01132	0.45701
c	1.69112	-1.03133	-1.63555
h	1.08899	-1.34522	-2.48093
h	2.74251	-1.00692	-1.92742
n	1.28065	0.30633	-1.24919
h	0.38857	0.68092	-1.54694
c	1.93957	1.03258	-0.33614
o	2.96595	0.63995	0.24042
c	1.30218	2.36459	0.01184
h	2.12361	3.04948	0.24098
n	0.43637	2.81242	-1.07520
h	-0.12040	3.59866	-0.76286
h	0.99343	3.14514	-1.85423
c	0.46734	2.15631	1.29960
h	-0.15218	3.04593	1.44421
h	1.16181	2.10725	2.13856
c	-0.34292	0.90408	1.26454
c	0.05942	-0.27880	1.85148
h	0.91362	-0.46986	2.47930
n	-0.78959	-1.29342	1.49615
h	-0.59963	-2.27091	1.64532
c	-1.74693	-0.80320	0.64694
c	-2.79487	-1.46338	0.00181
h	-2.94337	-2.52848	0.11897
c	-3.63326	-0.70185	-0.79695
h	-4.45449	-1.17969	-1.31330
c	-3.43421	0.68527	-0.94664
h	-4.11425	1.25027	-1.56976
c	-2.38649	1.33630	-0.31563
h	-2.24561	2.39909	-0.45229
c	-1.50885	0.59246	0.49372

WG_04.xyz

o	0.75486	-0.31786	-3.95151
c	-0.41911	-0.87974	-3.64399
o	-1.15083	-1.35649	-4.47817

h	1.19072	-0.01023	-3.11971
c	-0.75335	-0.90357	-2.15434
h	-0.02722	-1.53755	-1.64043
h	-1.74092	-1.33680	-2.04241
n	-0.74379	0.40398	-1.52716
h	-1.59502	0.87803	-1.25559
c	0.38327	1.05791	-1.23654
o	1.50940	0.67335	-1.59403
c	0.21670	2.32187	-0.40855
h	0.66512	3.11946	-1.00221
n	-1.19408	2.62114	-0.17883
h	-1.44718	2.33743	0.76343
h	-1.36804	3.61342	-0.25683
c	1.03789	2.16852	0.89274
h	1.11429	3.15206	1.35981
h	2.04403	1.84494	0.62592
c	0.39668	1.21060	1.83948
c	-0.43316	1.55154	2.89161
h	-0.69002	2.52876	3.26900
n	-0.90897	0.41641	3.49985
h	-1.50581	0.39812	4.30790
c	-0.40090	-0.68786	2.86176
c	-0.59398	-2.04631	3.12257
h	-1.23284	-2.38261	3.92874
c	0.07190	-2.95095	2.31044
h	-0.05229	-4.01108	2.48359
c	0.91653	-2.51267	1.27121
h	1.43411	-3.24779	0.66962
c	1.10593	-1.16487	1.01025
h	1.76270	-0.84219	0.21407
c	0.42984	-0.22238	1.80655

WG_05.xyz

o	-4.53484	-0.61725	0.05155
c	-4.30941	0.51296	0.73050
o	-5.19622	1.25928	1.06803
h	-3.67335	-1.07561	-0.09970
c	-2.84415	0.77503	1.07292
h	-2.49951	-0.01690	1.74160
h	-2.78920	1.72774	1.58738
n	-1.97150	0.81419	-0.08396
h	-1.56903	1.67564	-0.42945
c	-1.58935	-0.29215	-0.72916
o	-2.03683	-1.41947	-0.46252
c	-0.56602	-0.08340	-1.83757
h	-1.11122	-0.22996	-2.77292
n	-0.06059	1.28773	-1.81146
h	0.24338	1.56701	-2.73470
h	0.75536	1.33403	-1.20779
c	0.51002	-1.17432	-1.70776
h	1.17854	-1.10805	-2.56775
h	0.01942	-2.14600	-1.73820
c	1.28143	-1.01382	-0.43973
c	0.94051	-1.52653	0.79699
h	0.11163	-2.16171	1.06312
n	1.85119	-1.11001	1.73723
h	1.83514	-1.36667	2.70872

c	2.80019	-0.32051	1.14147
c	3.91590	0.32333	1.68131
h	4.15607	0.25200	2.73409
c	4.70906	1.05990	0.81486
h	5.58091	1.57116	1.19895
c	4.40384	1.15033	-0.55807
h	5.05091	1.72802	-1.20384
c	3.29694	0.51128	-1.09245
h	3.08230	0.58056	-2.15164
c	2.46702	-0.23888	-0.23913

WG_06.xyz

o	-1.87571	2.28771	-0.57870
c	-0.94129	2.42361	0.36930
o	-0.01044	3.18770	0.24946
h	-2.46669	1.53558	-0.32830
c	-1.14244	1.54267	1.60044
h	-2.14407	1.70219	2.00059
h	-0.40486	1.82705	2.34284
n	-0.98186	0.12779	1.30756
h	-0.06966	-0.28662	1.43491
c	-1.88066	-0.55483	0.57496
o	-2.92843	-0.03859	0.15895
c	-1.52627	-1.98748	0.23258
h	-0.78609	-2.34628	0.94950
n	-2.73189	-2.78926	0.35992
h	-2.59904	-3.68046	-0.10260
h	-3.48061	-2.30720	-0.12647
c	-0.88249	-1.98273	-1.17882
h	-1.66598	-1.74385	-1.90098
h	-0.53052	-2.99589	-1.38995
c	0.21115	-0.97393	-1.25713
c	0.12920	0.25399	-1.87952
h	-0.64029	0.64206	-2.52595
n	1.20681	1.03055	-1.53247
h	1.26862	2.02040	-1.70840
c	1.98567	0.34655	-0.63708
c	3.13832	0.74074	0.04625
h	3.56608	1.72452	-0.09332
c	3.70655	-0.17333	0.92127
h	4.59693	0.10109	1.47001
c	3.14825	-1.45399	1.10777
h	3.62558	-2.14242	1.79180
c	2.00440	-1.84591	0.42846
h	1.59510	-2.83842	0.57208
c	1.39767	-0.93806	-0.45932

WG_07.xyz

o	2.32132	0.53962	2.52641
c	1.18070	0.90914	1.90787
o	1.13529	1.71874	1.01123
h	3.03134	1.00480	2.05850
c	-0.01389	0.22031	2.52352
h	-0.10495	0.56471	3.55642
h	0.14948	-0.85551	2.55037
n	-1.18862	0.48105	1.74736
h	-1.34735	1.40231	1.36582

c	-1.90651	-0.52023	1.19370
o	-1.80833	-1.70226	1.51414
c	-2.83011	-0.08675	0.06084
h	-3.82113	-0.46649	0.30952
n	-2.88931	1.36642	-0.07160
h	-2.22616	1.66210	-0.78290
h	-3.80760	1.65680	-0.37830
c	-2.33828	-0.80038	-1.22280
h	-3.08313	-0.64055	-2.00515
h	-2.28399	-1.87000	-1.02127
c	-1.01384	-0.27158	-1.66443
c	-0.81527	0.76252	-2.56152
h	-1.53612	1.28863	-3.16738
n	0.52398	1.04924	-2.65877
h	0.92423	1.76008	-3.24487
c	1.22783	0.21582	-1.82842
c	2.60016	0.13974	-1.58543
h	3.29914	0.80145	-2.08040
c	3.03500	-0.82041	-0.68431
h	4.09272	-0.91557	-0.47714
c	2.12332	-1.68497	-0.04599
h	2.49883	-2.42701	0.64590
c	0.75993	-1.60584	-0.28442
h	0.07000	-2.26975	0.21808
c	0.28759	-0.63450	-1.18565

WG_08.xyz

o	0.72964	-0.57108	3.57367
c	1.16814	0.56959	3.02977
o	1.78641	1.39430	3.65953
h	0.26660	-1.09903	2.87884
c	0.85614	0.73570	1.54609
h	1.38878	-0.03408	0.98051
h	1.21515	1.71175	1.23895
n	-0.56223	0.64639	1.23826
h	-1.04207	1.42069	0.79951
c	-1.20114	-0.52924	1.16301
o	-0.72674	-1.59434	1.58374
c	-2.54358	-0.49440	0.45897
h	-3.17769	-1.23154	0.95791
n	-3.08830	0.86147	0.46116
h	-3.88073	0.90929	-0.16836
h	-3.44048	1.09338	1.38333
c	-2.31568	-0.95873	-0.99546
h	-3.26960	-0.88237	-1.52376
h	-2.04640	-2.01498	-0.97090
c	-1.25348	-0.17584	-1.68995
c	-1.39664	1.03180	-2.34064
h	-2.28894	1.60005	-2.54556
n	-0.16454	1.49834	-2.73194
h	-0.00573	2.33558	-3.26434
c	0.80490	0.60387	-2.35109
c	2.19118	0.64445	-2.51666
h	2.67784	1.46991	-3.01973
c	2.92406	-0.41885	-2.01052
h	3.99987	-0.42085	-2.11949
c	2.29240	-1.49769	-1.36022

h	2.89709	-2.31027	-0.98106
c	0.91678	-1.53570	-1.19321
h	0.44787	-2.36064	-0.67373
c	0.14761	-0.46912	-1.69083

WG_09.xyz

o	0.39506	2.35394	2.54175
c	0.90194	1.31466	1.85598
o	1.77166	1.41854	1.01958
h	0.83025	3.14297	2.18468
c	0.27676	0.01616	2.29032
h	-0.80838	0.09250	2.24066
h	0.54407	-0.15866	3.33477
n	0.73368	-1.03923	1.42296
h	1.49115	-0.78509	0.80348
c	-0.13144	-2.00064	1.00648
o	-1.22558	-2.19000	1.53068
c	0.32995	-2.83062	-0.18441
h	1.41763	-2.78591	-0.26782
n	-0.07760	-4.22566	-0.08962
h	-1.05373	-4.22759	0.19380
h	0.41582	-4.66211	0.68157
c	-0.27982	-2.22419	-1.46046
h	-1.36588	-2.32171	-1.38534
h	0.04307	-2.84588	-2.29560
c	0.09344	-0.79585	-1.67879
c	1.19083	-0.33319	-2.37763
h	1.93956	-0.88781	-2.92022
n	1.22826	1.03941	-2.33494
h	1.94693	1.61193	-2.74087
c	0.16747	1.50114	-1.60176
c	-0.20200	2.80501	-1.26762
h	0.37187	3.65891	-1.60414
c	-1.33324	2.96531	-0.48046
h	-1.65208	3.96125	-0.20350
c	-2.08156	1.85352	-0.04305
h	-2.95907	2.01769	0.56783
c	-1.71708	0.55881	-0.38052
h	-2.29519	-0.28684	-0.03008
c	-0.57113	0.36509	-1.17197

WG_10.xyz

o	2.21545	-2.41704	0.62579
c	1.06224	-1.83210	0.99982
o	0.96777	-1.06612	1.93215
h	2.89697	-2.05388	1.21133
c	-0.07957	-2.28755	0.13041
h	-0.24693	-3.34970	0.32563
h	0.19349	-2.18988	-0.91937
n	-1.24132	-1.48630	0.40120
h	-1.25520	-0.94340	1.25628
c	-1.99387	-1.01310	-0.62032
o	-1.92224	-1.42060	-1.77578
c	-2.90976	0.13990	-0.24541
h	-3.81352	0.02261	-0.84982
n	-3.15361	0.18151	1.19393
h	-3.66310	1.02608	1.42607

h	-3.74435	-0.59488	1.46903
c	-2.21228	1.44197	-0.68621
h	-2.86363	2.27850	-0.41838
h	-2.14228	1.42686	-1.77436
c	-0.85696	1.62311	-0.08727
c	-0.55877	2.21105	1.12431
h	-1.21792	2.66628	1.84497
n	0.79470	2.16049	1.34871
h	1.25064	2.45536	2.19378
c	1.40549	1.51835	0.30480
c	2.75056	1.20744	0.09809
h	3.51116	1.48619	0.81639
c	3.07589	0.52290	-1.06422
h	4.10810	0.26441	-1.25876
c	2.08479	0.16378	-1.99979
h	2.37541	-0.37095	-2.89401
c	0.74959	0.47819	-1.79687
h	-0.00333	0.17938	-2.51450
c	0.38861	1.16695	-0.62495

WG_11.xyz

o	1.48588	-0.45255	-1.36612
c	2.48674	0.11691	-0.66551
o	3.39322	-0.49754	-0.15595
h	1.56085	-1.41224	-1.22189
c	2.36094	1.63012	-0.62970
h	2.90468	2.03149	-1.48435
h	2.84852	1.96552	0.28120
n	1.00514	2.10619	-0.64944
h	0.49200	2.23847	-1.50752
c	0.27409	2.14685	0.48581
o	0.74137	1.95764	1.60599
c	-1.20821	2.45593	0.28637
h	-1.37330	3.42563	0.75896
n	-1.54519	2.56756	-1.13128
h	-2.32540	3.19886	-1.25704
h	-1.84511	1.65550	-1.46606
c	-2.03856	1.39815	1.04951
h	-3.07723	1.73445	1.06991
h	-1.67780	1.35631	2.07656
c	-1.94946	0.05660	0.40160
c	-2.77898	-0.41391	-0.60071
h	-3.67761	0.02370	-1.00608
n	-2.33734	-1.63825	-1.04012
h	-2.78629	-2.19898	-1.74245
c	-1.21427	-1.99328	-0.33698
c	-0.40209	-3.12442	-0.44865
h	-0.61501	-3.90666	-1.16609
c	0.68743	-3.21275	0.40874
h	1.33743	-4.07576	0.35466
c	0.95226	-2.20395	1.35763
h	1.81266	-2.30455	2.00414
c	0.15226	-1.07727	1.45833
h	0.38576	-0.29395	2.16545
c	-0.94690	-0.94940	0.59090

WG_12.xyz

o	1.56405	-2.83351	-0.49169
c	2.14792	-1.77473	-0.43434
o	2.85947	-1.40897	0.63701
h	3.09777	-0.45267	0.53418
c	2.13038	-0.75424	-1.57100
h	1.68712	-1.22611	-2.44109
h	3.15156	-0.44956	-1.80146
n	1.35744	0.43157	-1.24241
h	0.39453	0.47622	-1.53516
c	1.77176	1.32194	-0.31989
o	2.85881	1.20638	0.26522
c	0.82034	2.46557	0.00830
h	1.45952	3.32729	0.20561
n	-0.15046	2.83062	-1.00762
h	-0.87246	2.12794	-1.10945
h	0.28589	2.97459	-1.90906
c	0.08889	2.09201	1.31948
h	-0.64338	2.87619	1.51605
h	0.81823	2.09531	2.12927
c	-0.53941	0.74078	1.22064
c	0.06452	-0.42821	1.63989
h	0.97670	-0.56343	2.19620
n	-0.66001	-1.51229	1.21572
h	-0.32594	-2.46213	1.25388
c	-1.73691	-1.07956	0.48880
c	-2.74137	-1.80565	-0.15594
h	-2.74087	-2.88764	-0.15523
c	-3.74162	-1.08795	-0.79353
h	-4.53359	-1.61911	-1.30328
c	-3.75277	0.32125	-0.77747
h	-4.56243	0.84740	-1.26462
c	-2.75579	1.04314	-0.14035
h	-2.79265	2.12544	-0.11856
c	-1.70813	0.34587	0.49381

WG_13.xyz

o	-2.44506	-0.58138	-2.41105
c	-1.83022	-0.94021	-1.27007
o	-0.94466	-1.76418	-1.21200
h	-1.99060	-1.06533	-3.11741
c	-2.41827	-0.22610	-0.08082
h	-3.45870	-0.54200	0.02394
h	-2.41998	0.84920	-0.25069
n	-1.63067	-0.52850	1.08430
h	-1.02631	-1.33169	0.99536
c	-1.23227	0.46596	1.92218
o	-1.72568	1.58917	1.91194
c	-0.09134	0.11406	2.87322
h	-0.35303	0.57376	3.82677
n	0.20211	-1.29148	3.09521
h	-0.63536	-1.81719	3.30969
h	0.62831	-1.69636	2.26865
c	1.18057	0.80947	2.34895
h	1.96264	0.66563	3.09514
h	0.97787	1.87718	2.26783
c	1.61679	0.25998	1.03056
c	2.49804	-0.78557	0.82703

h	3.07345	-1.34251	1.54929
n	2.61025	-1.04729	-0.51716
h	3.18740	-1.76325	-0.92153
c	1.80592	-0.18649	-1.21764
c	1.58201	-0.07469	-2.59088
h	2.07831	-0.72473	-3.29979
c	0.69482	0.90423	-3.01386
h	0.50211	1.02601	-4.07150
c	0.05109	1.75382	-2.09144
h	-0.63120	2.50850	-2.45924
c	0.27513	1.64286	-0.72755
h	-0.22913	2.29741	-0.02830
c	1.16388	0.65459	-0.26880

WG_14.xyz

o	0.39444	2.33042	2.57271
c	0.89858	1.30331	1.86669
o	1.76525	1.42204	1.02919
h	0.83017	3.12527	2.22950
c	0.27500	-0.00250	2.28092
h	-0.81031	0.07490	2.23766
h	0.54605	-0.19570	3.32129
n	0.72858	-1.04054	1.39384
h	1.49527	-0.78992	0.78575
c	-0.11904	-2.01868	0.99342
o	-1.20588	-2.22554	1.52619
c	0.33807	-2.82725	-0.20710
h	1.42323	-2.74725	-0.30821
n	-0.02905	-4.21288	0.03167
h	-0.95481	-4.21321	0.44816
h	-0.09305	-4.71100	-0.84763
c	-0.30850	-2.20894	-1.46921
h	-1.39188	-2.29987	-1.36178
h	-0.01297	-2.82278	-2.32369
c	0.07375	-0.78540	-1.69886
c	1.17100	-0.32615	-2.40034
h	1.91321	-0.88114	-2.95148
n	1.21755	1.04611	-2.34874
h	1.93624	1.61658	-2.75760
c	0.16452	1.51020	-1.60554
c	-0.19307	2.81400	-1.25811
h	0.38342	3.66682	-1.59277
c	-1.31519	2.97515	-0.45817
h	-1.62476	3.97098	-0.17047
c	-2.06606	1.86503	-0.02076
h	-2.93481	2.03054	0.60218
c	-1.71370	0.57061	-0.37193
h	-2.29265	-0.27435	-0.02077
c	-0.57823	0.37646	-1.17784

WG_15.xyz

o	-2.71118	0.86135	0.39915
c	-2.18688	0.29275	-0.53102
o	-1.49440	0.91617	-1.50557
h	-1.33704	1.83351	-1.21734
c	-2.20083	-1.20082	-0.77450
h	-2.85275	-1.41046	-1.62424

h	-2.58635	-1.70399	0.10653
n	-0.85859	-1.67883	-1.02123
h	-0.25172	-1.12858	-1.61557
c	-0.21844	-2.45605	-0.11089
o	-0.76240	-3.04102	0.81811
c	1.29187	-2.50435	-0.29318
h	1.59501	-3.54148	-0.12440
n	1.69731	-1.98103	-1.59699
h	2.70480	-1.87639	-1.61709
h	1.46724	-2.64743	-2.32599
c	1.89523	-1.64226	0.83737
h	2.94895	-1.46205	0.60602
h	1.86421	-2.23818	1.74909
c	1.16913	-0.36099	1.08930
c	0.27935	-0.17584	2.12902
h	-0.02163	-0.87477	2.89225
n	-0.23875	1.09302	2.08683
h	-1.03338	1.40334	2.61959
c	0.26030	1.74557	0.99251
c	-0.03683	3.01708	0.49578
h	-0.74214	3.66637	0.99798
c	0.60297	3.41168	-0.67278
h	0.39987	4.39059	-1.08592
c	1.52225	2.56088	-1.32127
h	2.00458	2.90253	-2.22694
c	1.81254	1.29957	-0.82602
h	2.49627	0.64961	-1.35305
c	1.16870	0.86012	0.34346

WGG_01.xyz

o	-3.01979	-1.26222	-1.35597
c	-2.41969	-0.40759	-1.97690
o	-2.51449	0.88202	-1.66692
h	-1.91615	1.39941	-2.26496
c	-1.50225	-0.73649	-3.14763
h	-1.87212	-0.22734	-4.03943
h	-1.53049	-1.80856	-3.30774
n	-0.12815	-0.33253	-2.91476
h	0.57882	-0.99938	-2.60385
c	0.23853	0.95833	-2.95059
o	-0.56080	1.88612	-3.14056
c	1.72183	1.20180	-2.72474
h	1.92079	2.24477	-2.94748
h	2.30421	0.56343	-3.39038
n	2.10359	0.92796	-1.35617
h	2.32404	1.66229	-0.69486
c	2.31169	-0.32084	-0.90694
o	2.11223	-1.33268	-1.59101
c	2.83777	-0.40123	0.52293
h	3.88271	-0.70744	0.42715
n	2.80326	0.91995	1.14988
h	3.51777	0.98767	1.86239
h	1.91067	1.04123	1.62104
c	2.06376	-1.49295	1.28100
h	2.54493	-1.64714	2.24889
h	2.14124	-2.42222	0.71777
c	0.63361	-1.10805	1.46539

c	-0.40986	-1.39323	0.60295
h	-0.41023	-1.99461	-0.29089
n	-1.56815	-0.82505	1.06177
h	-2.44401	-0.86644	0.55672
c	-1.31189	-0.14600	2.21997
c	-2.16517	0.59273	3.04387
h	-3.21237	0.71529	2.80109
c	-1.61988	1.16169	4.18421
h	-2.25279	1.73952	4.84366
c	-0.25716	0.99542	4.50537
h	0.12880	1.44322	5.41113
c	0.59108	0.26746	3.68680
h	1.63258	0.13832	3.95530
c	0.07290	-0.31275	2.51336

WGG_02.xyz

o	1.98266	-1.14174	-2.86388
c	2.49334	-0.36484	-2.07979
o	3.72050	-0.54472	-1.60714
h	3.90076	0.15177	-0.92519
c	1.77500	0.87707	-1.56219
h	0.83196	0.98836	-2.08599
h	2.40237	1.74967	-1.75115
n	1.50999	0.80150	-0.13755
h	0.59295	0.52999	0.18916
c	2.49501	0.97468	0.75823
o	3.67306	1.16295	0.42656
c	2.10611	0.92117	2.22353
h	2.53911	1.79648	2.70359
h	2.57707	0.03341	2.64517
n	0.69323	0.83950	2.46113
h	0.09544	1.65308	2.51477
c	0.07840	-0.34817	2.69566
o	0.66784	-1.42076	2.75295
c	-1.43925	-0.24520	2.83490
h	-1.66853	-0.48596	3.87490
n	-1.89517	1.12127	2.57180
h	-2.76663	1.29641	3.05454
h	-2.08629	1.23132	1.58062
c	-2.06178	-1.31832	1.92298
h	-3.14767	-1.27747	2.03034
h	-1.72732	-2.29531	2.26886
c	-1.66564	-1.12760	0.49406
c	-0.60979	-1.75924	-0.14203
h	0.08293	-2.48278	0.25606
n	-0.52481	-1.33755	-1.44439
h	0.22736	-1.55820	-2.08929
c	-1.49655	-0.40352	-1.68017
c	-1.78252	0.32096	-2.84154
h	-1.19674	0.18854	-3.74212
c	-2.85764	1.19582	-2.79913
h	-3.10980	1.77090	-3.67939
c	-3.63982	1.33586	-1.63488
h	-4.48509	2.01036	-1.64695
c	-3.35391	0.61991	-0.48312
h	-3.98222	0.72431	0.39300
c	-2.25089	-0.25574	-0.47970

WGG_03.xyz

o	-2.03423	3.20190	0.50767
c	-0.84682	3.05474	0.70923
o	0.05880	3.30341	-0.23634
h	0.95167	3.01596	0.09396
c	-0.28851	2.55362	2.03459
h	-1.11501	2.45091	2.72855
h	0.42412	3.28584	2.42021
n	0.37237	1.26634	1.90706
h	-0.01592	0.43053	2.34046
c	1.57677	1.15261	1.32818
o	2.15324	2.09860	0.77094
c	2.21977	-0.22149	1.42676
h	2.39319	-0.45048	2.47881
h	3.17150	-0.16774	0.90767
n	1.43250	-1.29619	0.85736
h	1.55056	-1.51336	-0.12260
c	0.38084	-1.84279	1.50668
o	0.00149	-1.43905	2.61269
c	-0.30639	-3.01296	0.81535
h	0.35274	-3.40026	0.03862
n	-0.61521	-4.10038	1.73216
h	0.24462	-4.51287	2.07630
h	-1.06759	-3.69513	2.54622
c	-1.61009	-2.51984	0.16904
h	-2.32844	-2.33581	0.97132
h	-2.00229	-3.33849	-0.43671
c	-1.41662	-1.26835	-0.61792
c	-2.03508	-0.05589	-0.38614
h	-2.80361	0.19700	0.32663
n	-1.53755	0.89688	-1.23660
h	-1.79398	1.87259	-1.20509
c	-0.55420	0.34360	-2.00806
c	0.28859	0.93330	-2.95304
h	0.21954	1.98814	-3.18235
c	1.22410	0.11799	-3.57272
h	1.89645	0.54290	-4.30522
c	1.30957	-1.25625	-3.27225
h	2.03473	-1.86609	-3.79422
c	0.47314	-1.84186	-2.33198
h	0.53109	-2.90683	-2.14225
c	-0.47005	-1.03680	-1.66392

WGG_04.xyz

o	-1.41580	2.24029	-1.97265
c	-0.81092	2.51546	-0.95936
o	-1.39054	3.17448	0.04662
h	-0.71161	3.34088	0.74631
c	0.66060	2.16324	-0.74605
h	1.22615	3.09627	-0.68920
h	1.00084	1.58285	-1.59666
n	0.90660	1.39020	0.46158
h	1.18209	0.41804	0.37633
c	0.86303	1.95819	1.67812
o	0.54329	3.14370	1.84985
c	1.17691	1.04708	2.85330

h	1.08058	1.63832	3.75826
h	2.19145	0.65999	2.76827
n	0.27277	-0.07845	2.89272
h	-0.66800	0.00555	3.25254
c	0.53403	-1.19953	2.18758
o	1.59679	-1.38572	1.59430
c	-0.59567	-2.22351	2.17794
h	-0.35808	-2.95651	2.95294
n	-1.84982	-1.57322	2.55592
h	-2.21343	-1.07884	1.74574
h	-2.53925	-2.27012	2.80869
c	-0.62060	-2.93661	0.81589
h	-1.41849	-3.68165	0.84840
h	0.31906	-3.47176	0.68423
c	-0.81945	-1.99979	-0.33302
c	-2.00674	-1.41891	-0.74985
h	-3.00561	-1.53606	-0.36005
n	-1.79260	-0.66632	-1.87731
h	-2.43402	0.01355	-2.25290
c	-0.46526	-0.71965	-2.21040
c	0.21337	-0.12963	-3.27967
h	-0.30166	0.50860	-3.98386
c	1.57371	-0.37765	-3.38138
h	2.13478	0.06296	-4.19454
c	2.23973	-1.19178	-2.44107
h	3.30244	-1.36079	-2.55132
c	1.56279	-1.78450	-1.38656
h	2.08625	-2.39583	-0.66557
c	0.18092	-1.55183	-1.25673

WGG_05.xyz

o	-0.74911	-1.68409	0.31482
c	-1.68066	-1.21278	-0.29642
o	-2.38751	-1.91138	-1.21349
h	-1.99331	-2.79630	-1.21851
c	-2.21765	0.19581	-0.15874
h	-3.29601	0.12795	-0.02810
h	-2.01567	0.73306	-1.08462
n	-1.61772	0.88363	0.94746
h	-0.74947	1.37991	0.79129
c	-1.85023	0.39466	2.19932
o	-2.76480	-0.37758	2.45448
c	-0.81865	0.81994	3.23330
h	-1.17062	0.51819	4.21443
h	-0.64999	1.89474	3.20721
n	0.43812	0.16096	2.93382
h	0.54298	-0.83273	3.09343
c	1.28327	0.67626	2.01858
o	1.16903	1.81349	1.55430
c	2.42732	-0.25146	1.61947
h	3.24604	-0.02683	2.30923
n	2.03049	-1.63654	1.84646
h	2.83385	-2.24778	1.77485
h	1.36395	-1.91306	1.12962
c	2.91691	0.07958	0.19699
h	3.85396	-0.46048	0.04398
h	3.14289	1.14443	0.14979

c	1.95351	-0.28736	-0.88394
c	1.84606	-1.53220	-1.47320
h	2.41827	-2.42700	-1.28855
n	0.86561	-1.51752	-2.43470
h	0.64354	-2.28206	-3.04745
c	0.32457	-0.26031	-2.51052
c	-0.65942	0.24461	-3.36389
h	-1.15139	-0.38438	-4.09433
c	-0.98459	1.58717	-3.23704
h	-1.74177	2.01403	-3.88067
c	-0.34214	2.40387	-2.28298
h	-0.61854	3.44737	-2.21388
c	0.63444	1.90139	-1.43622
h	1.11542	2.53345	-0.70342
c	0.98477	0.54192	-1.53670

WGG_06.xyz

o	-1.78047	-3.44014	0.00012
c	-0.63353	-3.17132	0.29468
o	0.34282	-3.17739	-0.60940
h	1.17306	-2.83066	-0.18519
c	-0.21642	-2.78650	1.70723
h	0.55191	-3.48351	2.04977
h	-1.08899	-2.86792	2.34553
n	0.29651	-1.43089	1.79603
h	-0.20748	-0.70908	2.31218
c	1.51738	-1.11533	1.34197
o	2.22751	-1.90328	0.69940
c	2.01993	0.26938	1.72569
h	2.99851	0.38775	1.27183
h	2.12162	0.30075	2.81228
n	1.17828	1.36977	1.30989
h	1.41473	1.91634	0.49259
c	0.02593	1.68801	1.92380
o	-0.46216	1.03019	2.85071
c	-0.67767	2.91458	1.37296
h	-1.14910	3.39687	2.23402
n	0.26535	3.77848	0.66504
h	0.86628	4.25744	1.32646
h	-0.24760	4.49863	0.17013
c	-1.79768	2.45146	0.41564
h	-2.10408	3.32127	-0.17432
h	-2.65541	2.16765	1.02618
c	-1.45158	1.29081	-0.45893
c	-2.07117	0.05862	-0.36456
h	-2.87156	-0.25185	0.28827
n	-1.53300	-0.81199	-1.27202
h	-1.77651	-1.78961	-1.34040
c	-0.52908	-0.18348	-1.95672
c	0.32999	-0.68711	-2.93640
h	0.26805	-1.71913	-3.25361
c	1.26704	0.18265	-3.47082
h	1.95156	-0.17257	-4.22893
c	1.34230	1.52253	-3.04136
h	2.07821	2.17781	-3.48811
c	0.49603	2.01877	-2.06144
h	0.58006	3.04447	-1.73359

c	-0.45922	1.15953	-1.48475
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WGG_07.xyz

o	1.30576	0.11577	3.54184
c	0.71633	0.92843	2.86112
o	1.36345	1.82927	2.12422
h	0.69539	2.39970	1.66258
c	-0.80871	0.99897	2.78857
h	-1.12975	1.96535	3.18095
h	-1.21527	0.20408	3.40305
n	-1.33309	0.85460	1.43989
h	-1.66099	-0.05810	1.14478
c	-1.21500	1.84189	0.54187
o	-0.63128	2.90807	0.80003
c	-1.75718	1.59177	-0.84359
h	-2.37931	2.44282	-1.12447
h	-2.34835	0.68013	-0.91346
n	-0.60664	1.45586	-1.70958
h	0.28993	1.83659	-1.43441
c	-0.58588	0.57129	-2.72873
o	-1.57178	-0.02891	-3.14731
c	0.80602	0.30363	-3.28081
h	0.69879	0.20341	-4.36418
n	1.74871	1.34354	-2.87352
h	1.63132	2.16890	-3.44995
h	2.69838	1.02384	-3.02054
c	1.25744	-1.06033	-2.72781
h	2.26890	-1.25282	-3.09573
h	0.60976	-1.81943	-3.16776
c	1.22054	-1.17985	-1.23820
c	2.24772	-0.91695	-0.35258
h	3.24141	-0.54769	-0.54728
n	1.85652	-1.21334	0.92880
h	2.36224	-0.97891	1.76979
c	0.56049	-1.65328	0.91316
c	-0.25698	-2.08399	1.96235
h	0.10897	-2.10972	2.97918
c	-1.55929	-2.44883	1.64560
h	-2.22374	-2.78292	2.43158
c	-2.02757	-2.40440	0.31416
h	-3.04768	-2.69769	0.10452
c	-1.20073	-2.01724	-0.73212
h	-1.57252	-1.98840	-1.74743
c	0.12127	-1.63331	-0.44208

WGG_08.xyz

o	0.46590	3.20973	2.01925
c	0.68983	3.05568	0.83656
o	-0.23969	3.29415	-0.08784
h	0.10882	3.00255	-0.97271
c	2.02789	2.55769	0.30589
h	2.70682	2.46273	1.14573
h	2.42349	3.28814	-0.40307
n	1.91999	1.26663	-0.35102
h	2.34751	0.43436	0.05112
c	1.36445	1.14378	-1.56563
o	0.81312	2.08405	-2.15675

c	1.48257	-0.23264	-2.19936
h	2.53873	-0.46139	-2.34589
h	0.98704	-0.18524	-3.16373
n	0.89438	-1.30235	-1.42033
h	-0.07198	-1.54597	-1.58212
c	1.52071	-1.84603	-0.35673
o	2.61226	-1.43637	0.05465
c	0.81169	-3.00033	0.32348
h	0.02745	-3.36799	-0.33808
n	1.79551	-4.06106	0.49888
h	2.61301	-3.65385	0.94132
h	1.42958	-4.75876	1.13598
c	0.16944	-2.48994	1.62948
h	0.97562	-2.28439	2.33703
h	-0.43336	-3.30372	2.04335
c	-0.63660	-1.25212	1.42172
c	-0.41880	-0.03242	2.03167
h	0.28621	0.23274	2.80318
n	-1.27206	0.90922	1.51870
h	-1.24667	1.88790	1.76469
c	-2.03159	0.34139	0.53456
c	-2.97599	0.91733	-0.31833
h	-3.21314	1.97106	-0.25876
c	-3.58421	0.09039	-1.25085
h	-4.31578	0.50456	-1.93088
c	-3.27227	-1.28195	-1.32421
h	-3.78402	-1.90132	-2.04854
c	-2.33227	-1.85362	-0.47822
h	-2.13236	-2.91688	-0.53061
c	-1.67596	-1.03711	0.46365

WGG_09.xyz

o	-1.44525	-0.79696	-3.67117
c	-0.18864	-0.68052	-3.25296
o	0.62627	-1.57042	-3.39743
h	-1.94283	0.01205	-3.39631
c	0.14242	0.64302	-2.57447
h	-0.13066	1.46038	-3.24371
h	1.20476	0.68568	-2.36627
n	-0.58314	0.81223	-1.33001
h	-0.13331	0.59066	-0.45067
c	-1.87528	1.17598	-1.34834
o	-2.51255	1.31380	-2.40033
c	-2.53957	1.44006	-0.01276
h	-3.40806	0.78718	0.04968
h	-2.89043	2.47113	-0.02727
n	-1.71641	1.18697	1.14085
h	-1.05777	1.87842	1.45669
c	-1.85315	0.03189	1.85952
o	-2.66365	-0.83625	1.56386
c	-0.92568	-0.12134	3.05471
h	-0.34337	0.79149	3.19678
n	-1.64405	-0.40411	4.29127
h	-2.23780	0.38139	4.53311
h	-2.27469	-1.17905	4.10821
c	0.02165	-1.28779	2.75823

h	-0.58322	-2.19612	2.72463
h	0.70874	-1.37879	3.60103
c	0.75802	-1.13331	1.47125
c	0.62375	-1.91736	0.34173
h	-0.03749	-2.75085	0.16742
n	1.50145	-1.50242	-0.63014
h	1.48609	-1.81146	-1.59622
c	2.19969	-0.41787	-0.16818
c	3.18565	0.35516	-0.79074
h	3.53223	0.12550	-1.79042
c	3.71934	1.41279	-0.06915
h	4.48382	2.03028	-0.52041
c	3.29777	1.68706	1.24798
h	3.75026	2.51032	1.78387
c	2.33181	0.91274	1.87125
h	2.04176	1.11757	2.89436
c	1.75401	-0.15498	1.15946

WGG_10.xyz

o	1.51913	-0.81284	3.29989
c	2.23207	-0.38545	2.41387
o	3.23757	-1.09651	1.91575
h	3.69212	-0.55887	1.21426
c	2.04998	1.00752	1.81734
h	2.93174	1.59970	2.07518
h	1.17517	1.45515	2.27588
n	1.86785	1.02310	0.37776
h	0.97525	1.30334	-0.02879
c	2.87376	0.76801	-0.46877
o	4.00007	0.40350	-0.09622
c	2.55352	0.96253	-1.94329
h	3.44479	0.69501	-2.50093
h	2.31878	2.01505	-2.11458
n	1.44306	0.15140	-2.39935
h	1.58000	-0.59340	-3.06751
c	0.16294	0.52225	-2.18536
o	-0.14772	1.49463	-1.49326
c	-0.87352	-0.40048	-2.79610
h	-1.78294	0.19743	-2.88866
n	-0.38028	-0.96104	-4.05486
h	-0.94320	-1.76342	-4.31177
h	-0.47694	-0.28911	-4.80728
c	-1.13167	-1.56782	-1.82302
h	-0.27631	-2.24420	-1.89155
h	-2.00790	-2.11206	-2.18877
c	-1.31774	-1.14050	-0.41079
c	-0.42368	-1.35343	0.61925
h	0.50645	-1.90008	0.61860
n	-0.88371	-0.76029	1.76724
h	-0.37221	-0.76708	2.64010
c	-2.08247	-0.14822	1.50849
c	-2.92716	0.57868	2.35149
h	-2.68372	0.73546	3.39420
c	-4.09428	1.08676	1.80179
h	-4.77150	1.65371	2.42585
c	-4.41702	0.87672	0.44595
h	-5.33757	1.28816	0.05474

c	-3.57853	0.15698	-0.38945
h	-3.84155	0.00286	-1.42849
c	-2.38829	-0.37114	0.13717

WGG_11.xyz

o	-4.55726	-0.11785	0.01359
c	-3.27579	0.24449	0.19290
o	-2.92110	1.40147	0.26135
h	-5.06527	0.70668	-0.03053

c	-2.37888	-0.97513	0.22945
h	-2.16607	-1.25505	-0.80228
h	-2.93713	-1.78016	0.70264
n	-1.14471	-0.75988	0.92613
h	-0.29614	-0.54697	0.42502
c	-1.17966	-0.64726	2.28095
o	-2.22556	-0.71506	2.91333
c	0.15942	-0.46132	2.97546
h	0.13138	-1.06984	3.87867
h	0.25494	0.58091	3.28022
n	1.28882	-0.76649	2.14082
h	1.42928	-1.68311	1.73802
c	2.26315	0.13379	1.86963
o	2.33522	1.25052	2.37102
c	3.24053	-0.32072	0.78619
h	4.23294	-0.34378	1.23855
n	2.91661	-1.66650	0.30685
h	2.28521	-1.60458	-0.48589
h	3.75265	-2.12891	-0.02496
c	3.20416	0.76471	-0.30980
h	3.88189	0.47434	-1.11487
h	3.56844	1.69673	0.11954
c	1.81181	0.95119	-0.82120
c	0.87408	1.81904	-0.28951
h	0.98364	2.50898	0.53093
n	-0.31845	1.69291	-0.95435
h	-1.20463	2.02451	-0.59519
c	-0.20211	0.71270	-1.90264
c	-1.14710	0.21282	-2.80444
h	-2.15584	0.60532	-2.83519
c	-0.73728	-0.78748	-3.67410
h	-1.44251	-1.19562	-4.38516
c	0.58854	-1.26735	-3.66171
h	0.87683	-2.03388	-4.36808
c	1.52857	-0.76547	-2.77556
h	2.54874	-1.12936	-2.79798
c	1.13982	0.23018	-1.85848

WGG_12.xyz

o	-1.38319	-3.45732	-0.02886
c	-0.82919	-2.78755	-0.87324
o	-1.51079	-2.00621	-1.71271
h	-0.86899	-1.58972	-2.34372
c	0.68788	-2.77687	-1.06325
h	0.91595	-3.18424	-2.04980
h	1.13031	-3.40637	-0.30000
n	1.27497	-1.44928	-0.96739

h	1.67755	-1.16284	-0.08147
c	1.11763	-0.55132	-1.94729
o	0.44792	-0.79035	-2.96791
c	1.69881	0.82674	-1.74415
h	2.28260	1.09067	-2.62679
h	2.32699	0.90677	-0.85932
n	0.55556	1.69696	-1.56562
h	-0.31438	1.41635	-1.98561
c	0.54161	2.69168	-0.64566
o	1.55412	3.10289	-0.08775
c	-0.84371	3.21683	-0.27451
h	-0.77435	4.30494	-0.27470
n	-1.96981	2.82241	-1.10209
h	-1.83676	3.05655	-2.07700
h	-2.14742	1.82748	-1.02185
c	-1.10866	2.75741	1.17201
h	-2.07628	3.16319	1.46810
h	-0.34420	3.19410	1.81349
c	-1.10025	1.26891	1.31998
c	-2.17733	0.41053	1.18534
h	-3.20796	0.63940	0.96502
n	-1.78694	-0.88191	1.43449
h	-2.33910	-1.70821	1.26136
c	-0.44740	-0.90195	1.71426
c	0.38483	-1.97241	2.05558
h	-0.00280	-2.97900	2.12669
c	1.72589	-1.68964	2.28039
h	2.40076	-2.49224	2.54744
c	2.22038	-0.37008	2.18681
h	3.26959	-0.18611	2.37647
c	1.38451	0.69695	1.88511
h	1.77414	1.70365	1.82156
c	0.02279	0.44073	1.64122

WGG_13.xyz

o	-1.50023	2.30969	1.66163
c	-0.70619	3.00699	0.84908
o	0.22587	3.65805	1.26973
h	-2.20374	1.87240	1.11660
c	-1.06164	2.92482	-0.63552
h	-0.33642	3.50772	-1.19142
h	-2.05755	3.34743	-0.77860
n	-1.05970	1.56616	-1.15504
h	-0.23122	1.23572	-1.63710
c	-2.03445	0.70378	-0.84160
o	-2.96837	1.00073	-0.07691
c	-1.92716	-0.70007	-1.38395
h	-1.12406	-0.82190	-2.10772
h	-2.87625	-0.96479	-1.85203
n	-1.63308	-1.53814	-0.23991
h	-1.94691	-1.22822	0.66483
c	-0.82342	-2.61756	-0.32846
o	-0.44253	-3.08768	-1.39677
c	-0.32926	-3.16119	0.99618
h	-0.93336	-2.75721	1.81211
n	-0.46836	-4.60798	0.96497

h	0.12032	-5.02721	1.67480
h	-0.12398	-4.92795	0.06538
c	1.12627	-2.66751	1.17058
h	1.72101	-3.15628	0.39552
h	1.48542	-3.03422	2.13508
c	1.30683	-1.18674	1.08311
c	1.27239	-0.27558	2.12195
h	1.10105	-0.44293	3.17322
n	1.53064	0.98841	1.65255
h	1.43240	1.84499	2.17642
c	1.72002	0.93585	0.29803
c	2.03356	1.95306	-0.60882
h	2.16769	2.97319	-0.27754
c	2.14409	1.59991	-1.94774
h	2.38405	2.35998	-2.67955
c	1.96606	0.26381	-2.36898
h	2.06338	0.02543	-3.41980
c	1.69764	-0.75176	-1.46075
h	1.57104	-1.77216	-1.79636
c	1.57193	-0.42435	-0.09850

WGG_14.xyz

o	-1.30567	-3.54375	-0.11450
c	-0.71848	-2.86079	-0.92684
o	-1.36823	-2.11773	-1.82101
h	-0.70214	-1.65886	-2.39565
c	0.80638	-2.78891	-1.00373
h	1.12275	-3.17991	-1.97236
h	1.21602	-3.40549	-0.21214
n	1.33202	-1.44079	-0.85981
h	1.66047	-1.14603	0.05281
c	1.21083	-0.54150	-1.84566
o	0.62434	-0.79800	-2.91074
c	1.75411	0.84364	-1.59565
h	2.37434	1.12500	-2.44789
h	2.34701	0.91294	-0.68525
n	0.60369	1.70917	-1.45699
h	-0.29393	1.43359	-1.83481
c	0.58498	2.72797	-0.57192
o	1.57264	3.14668	0.02524
c	-0.80635	3.28032	-0.30180
h	-0.69907	4.36380	-0.20330
n	-1.75183	2.87110	-1.33822
h	-2.70053	3.01688	-1.01523
h	-1.63802	3.44725	-2.16423
c	-1.25262	2.72873	1.06422
h	-2.26285	3.09752	1.26135
h	-0.60073	3.16784	1.82013
c	-1.21732	1.23868	1.18289
c	-2.24648	0.35409	0.92470
h	-3.24119	0.54963	0.55871
n	-1.85505	-0.92776	1.21869
h	-2.36257	-1.76804	0.98542
c	-0.55765	-0.91344	1.65415
c	0.26081	-1.96323	2.08137
h	-0.10581	-2.97975	2.10880
c	1.56408	-1.64728	2.44350

h	2.22846	-2.43370	2.77662
c	2.03253	-0.31587	2.39956
h	3.05331	-0.10675	2.69088
c	1.20541	0.73084	2.01432
h	1.57760	1.74598	1.98549
c	-0.11779	0.44159	1.63393

WGG_15.xyz

o	-1.53804	-3.29311	0.81195
c	-2.24667	-2.40375	0.38460
o	-3.24906	-1.90039	1.09665
h	-3.70042	-1.19709	0.55916
c	-2.06437	-1.80844	-1.00895
h	-2.95063	-2.05705	-1.59825
h	-1.19471	-2.27287	-1.46058
n	-1.87056	-0.37012	-1.02080
h	-0.97565	0.02963	-1.30262
c	-2.87193	0.48295	-0.76823

o	-4.00116	0.11745	-0.40601
c	-2.53783	1.95448	-0.95992
h	-3.42474	2.52043	-0.69516
h	-2.29490	2.12514	-2.01064
n	-1.42642	2.39433	-0.14121
h	-1.55912	3.06897	0.59855
c	-0.14798	2.18355	-0.52220
o	0.15612	1.49438	-1.49843
c	0.89317	2.79057	0.39737
h	1.80313	2.87450	-0.20098
n	0.40826	4.05488	0.95286
h	0.50688	4.80308	0.27643
h	0.97566	4.31312	1.75174
c	1.14377	1.82014	1.56851
h	0.28851	1.89713	2.24410
h	2.02221	2.18122	2.11232
c	1.32013	0.40570	1.14457
c	0.41974	-0.61916	1.35641
h	-0.51069	-0.61332	1.90255
n	0.87270	-1.76905	0.76153
h	0.35666	-2.63928	0.76782
c	2.07236	-1.51671	0.14866
c	2.91113	-2.36388	-0.58012
h	2.66126	-3.40493	-0.73797
c	4.08094	-1.82056	-1.08905
h	4.75387	-2.44798	-1.65742
c	4.41225	-0.46706	-0.87705
h	5.33474	-0.08086	-1.28894
c	3.57952	0.37246	-0.15539
h	3.84949	1.40952	0.00011
c	2.38653	-0.14740	0.37317

FGG_055.xyz

O	-3.065000	0.117000	-2.327000
C	-3.029000	-0.032000	-1.129000
O	-3.155000	0.992000	-0.274000
H	-2.990000	0.658000	0.642000
C	-2.846000	-1.396000	-0.469000

H	-2.855000	-2.147000	-1.251000
H	-3.677000	-1.574000	0.217000
N	-1.595000	-1.507000	0.261000
H	-0.848000	-2.111000	-0.072000
C	-1.402000	-0.890000	1.437000
O	-2.229000	-0.122000	1.947000
C	-0.085000	-1.219000	2.128000
H	-0.040000	-2.292000	2.315000
H	-0.075000	-0.686000	3.073000
N	1.090000	-0.845000	1.364000
H	1.478000	0.078000	1.493000
C	1.524000	-1.574000	0.311000
O	0.952000	-2.605000	-0.059000
C	2.756000	-1.048000	-0.420000
N	3.482000	-2.091000	-1.123000
H	2.807000	-2.631000	-1.655000
H	3.863000	-2.746000	-0.450000
H	3.429000	-0.586000	0.305000
C	2.321000	0.033000	-1.427000
H	3.220000	0.330000	-1.968000
H	1.634000	-0.418000	-2.147000
C	1.675000	1.208000	-0.752000
C	2.433000	2.027000	0.094000
H	3.500000	1.859000	0.183000
C	1.834000	3.059000	0.815000
H	2.435000	3.683000	1.463000
C	0.465000	3.291000	0.690000
H	-0.003000	4.091000	1.247000
C	-0.297000	2.499000	-0.168000
H	-1.357000	2.673000	-0.283000
C	0.307000	1.462000	-0.879000
H	-0.292000	0.849000	-1.543000

FGG_080.xyz

O	3.751000	-1.438000	-0.404000
C	3.370000	-0.309000	-0.200000
O	3.725000	0.719000	-0.980000
H	3.322000	1.542000	-0.615000
C	2.465000	0.063000	0.969000
H	2.993000	0.774000	1.607000
H	2.246000	-0.836000	1.531000
N	1.212000	0.667000	0.548000
H	0.363000	0.120000	0.570000
C	1.171000	1.960000	0.191000
O	2.190000	2.654000	0.084000
C	-0.195000	2.572000	-0.040000
H	-0.063000	3.376000	-0.761000
H	-0.525000	3.004000	0.906000
N	-1.217000	1.655000	-0.469000
H	-1.263000	1.323000	-1.422000
C	-2.254000	1.299000	0.332000
O	-2.344000	1.596000	1.516000
C	-3.315000	0.450000	-0.357000
N	-3.172000	0.496000	-1.814000
H	-3.746000	-0.227000	-2.232000
H	-3.531000	1.376000	-2.167000
H	-4.274000	0.843000	-0.005000

C	-3.196000	-0.991000	0.160000
H	-3.552000	-0.997000	1.189000
H	-3.880000	-1.617000	-0.421000
C	-1.806000	-1.566000	0.126000
C	-1.142000	-1.844000	-1.076000
H	-1.626000	-1.624000	-2.017000
C	0.139000	-2.394000	-1.071000
H	0.644000	-2.593000	-2.006000
C	0.771000	-2.700000	0.134000
H	1.766000	-3.122000	0.130000
C	0.118000	-2.429000	1.336000
H	0.594000	-2.666000	2.278000
C	-1.152000	-1.851000	1.330000
H	-1.651000	-1.633000	2.266000

FGG_099.xyz

O	1.014000	-0.006000	-1.163000
C	2.026000	0.038000	-0.502000
O	3.147000	-0.642000	-0.810000
H	2.931000	-1.160000	-1.600000
C	2.219000	0.850000	0.763000
H	3.104000	1.470000	0.630000
H	2.406000	0.164000	1.586000
N	1.078000	1.673000	1.045000
H	0.270000	1.245000	1.480000
C	0.822000	2.705000	0.186000
O	1.658000	3.166000	-0.577000
C	-0.624000	3.178000	0.212000
H	-0.695000	4.101000	-0.354000
H	-0.970000	3.333000	1.232000
N	-1.460000	2.162000	-0.399000
H	-1.455000	2.031000	-1.402000
C	-1.889000	1.098000	0.308000
O	-1.763000	1.001000	1.532000
C	-2.585000	0.029000	-0.532000
N	-2.036000	0.055000	-1.884000
H	-1.088000	-0.311000	-1.875000
H	-2.588000	-0.528000	-2.500000
H	-3.631000	0.343000	-0.602000
C	-2.566000	-1.329000	0.191000
H	-2.982000	-1.187000	1.188000
H	-3.230000	-2.000000	-0.357000
C	-1.202000	-1.952000	0.286000
C	-0.709000	-2.746000	-0.754000
H	-1.331000	-2.931000	-1.621000
C	0.556000	-3.327000	-0.679000
H	0.913000	-3.947000	-1.491000
C	1.349000	-3.127000	0.449000
H	2.327000	-3.583000	0.517000
C	0.864000	-2.347000	1.499000
H	1.462000	-2.212000	2.391000
C	-0.399000	-1.764000	1.417000
H	-0.780000	-1.166000	2.235000

FGG_114.xyz

O	3.784000	1.428000	-0.288000
C	3.373000	0.316000	-0.054000

O	3.709000	-0.743000	-0.797000
H	3.297000	-1.549000	-0.404000
C	2.449000	0.007000	1.121000
H	2.226000	0.936000	1.633000
H	2.973000	-0.667000	1.802000
N	1.200000	-0.623000	0.734000
H	0.377000	-0.051000	0.603000
C	1.159000	-1.921000	0.393000
O	2.172000	-2.629000	0.337000
C	-0.195000	-2.514000	0.069000
H	-0.232000	-3.486000	0.561000
H	-0.243000	-2.687000	-1.006000
N	-1.315000	-1.684000	0.416000
H	-1.487000	-1.375000	1.363000
C	-2.248000	-1.318000	-0.499000
O	-2.210000	-1.617000	-1.686000
C	-3.354000	-0.430000	0.057000
N	-3.332000	-0.401000	1.521000
H	-3.816000	-1.212000	1.889000
H	-3.846000	0.405000	1.856000
H	-4.289000	-0.822000	-0.352000
C	-3.153000	0.978000	-0.526000
H	-3.358000	0.914000	-1.594000
H	-3.904000	1.640000	-0.087000
C	-1.775000	1.542000	-0.320000
C	-0.814000	1.426000	-1.332000
H	-1.075000	0.914000	-2.250000
C	0.462000	1.965000	-1.171000
H	1.195000	1.872000	-1.961000
C	0.798000	2.630000	0.008000
H	1.789000	3.045000	0.125000
C	-0.147000	2.737000	1.029000
H	0.103000	3.253000	1.947000
C	-1.421000	2.195000	0.866000
H	-2.152000	2.300000	1.658000

FGG_215.xyz

O	3.045000	-2.140000	0.347000
C	2.938000	-0.975000	0.040000
O	3.107000	-0.546000	-1.212000
H	3.057000	0.441000	-1.218000
C	2.648000	0.113000	1.073000
H	3.556000	0.710000	1.190000
H	2.428000	-0.379000	2.015000
N	1.542000	0.998000	0.747000
H	0.699000	0.998000	1.313000
C	1.653000	1.952000	-0.189000
O	2.638000	2.061000	-0.932000
C	0.477000	2.912000	-0.283000
H	0.690000	3.604000	-1.091000
H	0.391000	3.461000	0.656000
N	-0.779000	2.244000	-0.545000
H	-1.200000	2.235000	-1.464000
C	-1.510000	1.683000	0.434000
O	-1.132000	1.622000	1.609000
C	-2.861000	1.137000	-0.017000
N	-2.916000	1.083000	-1.477000

H	-3.878000	1.061000	-1.789000
H	-2.486000	0.219000	-1.794000
H	-3.597000	1.875000	0.314000
C	-3.157000	-0.194000	0.702000
H	-3.157000	-0.010000	1.776000
H	-4.159000	-0.513000	0.411000
C	-2.146000	-1.248000	0.357000
C	-2.260000	-2.008000	-0.814000
H	-3.146000	-1.908000	-1.431000
C	-1.265000	-2.915000	-1.179000
H	-1.368000	-3.487000	-2.091000
C	-0.147000	-3.088000	-0.367000
H	0.639000	-3.774000	-0.650000
C	-0.046000	-2.374000	0.826000
H	0.810000	-2.532000	1.466000
C	-1.032000	-1.459000	1.180000
H	-0.955000	-0.901000	2.104000

FGG_224.xyz

O	3.265000	-1.219000	1.576000
C	3.119000	-0.448000	0.655000
O	3.192000	-0.839000	-0.620000
H	2.963000	-0.071000	-1.200000
C	2.850000	1.038000	0.863000
H	3.638000	1.611000	0.370000
H	2.875000	1.233000	1.929000
N	1.561000	1.466000	0.349000
H	0.813000	1.756000	0.979000
C	1.335000	1.600000	-0.964000
O	2.155000	1.278000	-1.836000
C	0.002000	2.238000	-1.332000
H	-0.044000	2.273000	-2.415000
H	-0.008000	3.256000	-0.939000
N	-1.167000	1.542000	-0.837000
H	-1.755000	0.999000	-1.455000
C	-1.581000	1.622000	0.439000
O	-0.938000	2.182000	1.335000
C	-2.910000	0.948000	0.730000
N	-3.684000	0.789000	-0.499000
H	-4.068000	1.684000	-0.783000
H	-4.477000	0.182000	-0.325000
H	-3.395000	1.579000	1.480000
C	-2.643000	-0.421000	1.381000
H	-2.182000	-0.236000	2.352000
H	-3.612000	-0.892000	1.567000
C	-1.763000	-1.327000	0.568000
C	-0.420000	-1.504000	0.921000
H	-0.030000	-1.007000	1.801000
C	0.416000	-2.331000	0.172000
H	1.443000	-2.473000	0.474000
C	-0.081000	-2.979000	-0.957000
H	0.568000	-3.616000	-1.542000
C	-1.417000	-2.816000	-1.318000
H	-1.813000	-3.330000	-2.184000
C	-2.252000	-2.002000	-0.556000
H	-3.292000	-1.897000	-0.835000

FGG_252.xyz

O	-2.658000	-1.237000	-0.512000
C	-3.698000	-0.698000	-0.210000
O	-4.911000	-1.193000	-0.523000
H	-4.749000	-2.012000	-1.015000
C	-3.832000	0.593000	0.575000
H	-4.345000	0.374000	1.510000
H	-4.458000	1.271000	-0.001000
N	-2.558000	1.201000	0.828000
H	-1.949000	0.761000	1.512000
C	-1.915000	1.776000	-0.234000
O	-2.478000	2.101000	-1.269000
C	-0.410000	1.883000	-0.035000
H	-0.164000	2.236000	0.965000
H	0.001000	2.552000	-0.783000
N	0.150000	0.558000	-0.208000
H	0.381000	0.205000	-1.127000
C	0.104000	-0.359000	0.772000
O	-0.261000	-0.116000	1.928000
C	0.583000	-1.742000	0.369000
N	0.454000	-1.914000	-1.075000
H	-0.532000	-1.990000	-1.306000
H	0.893000	-2.782000	-1.358000
H	-0.026000	-2.440000	0.951000
C	2.048000	-1.910000	0.814000
H	2.059000	-1.926000	1.904000
H	2.398000	-2.885000	0.466000
C	2.943000	-0.815000	0.311000
C	3.523000	-0.872000	-0.958000
H	3.369000	-1.747000	-1.576000
C	4.292000	0.186000	-1.439000
H	4.735000	0.126000	-2.424000
C	4.492000	1.319000	-0.651000
H	5.090000	2.139000	-1.023000
C	3.925000	1.383000	0.620000
H	4.083000	2.255000	1.241000
C	3.158000	0.323000	1.096000
H	2.708000	0.378000	2.080000

FGG_300.xyz

O	-1.243000	-1.485000	0.285000
C	-2.219000	-2.010000	-0.204000
O	-2.452000	-3.335000	-0.158000
H	-1.710000	-3.723000	0.330000
C	-3.321000	-1.296000	-0.962000
H	-4.273000	-1.610000	-0.541000
H	-3.287000	-1.624000	-1.999000
N	-3.194000	0.130000	-0.882000
H	-2.474000	0.582000	-1.437000
C	-3.456000	0.717000	0.325000
O	-4.071000	0.162000	1.224000
C	-2.830000	2.095000	0.475000
H	-3.290000	2.600000	1.317000
H	-2.951000	2.687000	-0.431000
N	-1.412000	1.922000	0.726000
H	-1.081000	1.666000	1.648000
C	-0.556000	1.637000	-0.277000

O	-0.863000	1.697000	-1.470000
C	0.842000	1.240000	0.188000
N	0.763000	0.680000	1.535000
H	1.697000	0.574000	1.913000
H	0.364000	-0.253000	1.475000
H	1.426000	2.163000	0.253000
C	1.492000	0.329000	-0.863000
H	0.879000	-0.568000	-0.962000
H	1.481000	0.844000	-1.822000
C	2.890000	-0.033000	-0.460000
C	3.159000	-1.233000	0.205000
H	2.350000	-1.933000	0.375000
C	4.450000	-1.541000	0.633000
H	4.640000	-2.477000	1.141000
C	5.492000	-0.646000	0.404000
H	6.495000	-0.884000	0.733000
C	5.238000	0.553000	-0.259000
H	6.045000	1.249000	-0.448000
C	3.947000	0.855000	-0.685000
H	3.756000	1.785000	-1.207000

FGG_357.xyz

O	-3.542000	1.728000	0.307000
C	-3.284000	0.574000	0.058000
O	-3.757000	-0.441000	0.787000
H	-3.443000	-1.290000	0.394000
C	-2.406000	0.162000	-1.121000
H	-2.065000	1.061000	-1.621000
H	-3.009000	-0.433000	-1.809000
N	-1.246000	-0.624000	-0.738000
H	-0.355000	-0.166000	-0.618000
C	-1.357000	-1.918000	-0.396000
O	-2.445000	-2.503000	-0.332000
C	-0.070000	-2.652000	-0.073000
H	-0.129000	-3.626000	-0.558000
H	-0.040000	-2.816000	1.004000
N	1.123000	-1.939000	-0.436000
H	1.436000	-1.861000	-1.394000
C	2.011000	-1.501000	0.493000
O	1.881000	-1.658000	1.700000
C	3.187000	-0.720000	-0.093000
N	3.099000	-0.642000	-1.551000
H	2.594000	0.196000	-1.819000
H	4.024000	-0.566000	-1.954000
H	4.083000	-1.284000	0.167000
C	3.244000	0.648000	0.620000
H	3.385000	0.469000	1.685000
H	4.110000	1.194000	0.243000
C	1.984000	1.435000	0.391000
C	0.901000	1.312000	1.273000
H	1.002000	0.679000	2.145000
C	-0.293000	1.990000	1.035000
H	-1.120000	1.893000	1.726000
C	-0.431000	2.798000	-0.094000
H	-1.366000	3.311000	-0.272000
C	0.642000	2.939000	-0.972000
H	0.555000	3.582000	-1.838000

C	1.841000	2.266000	-0.727000
H	2.684000	2.416000	-1.392000

FGG_366.xyz

O	-1.902000	1.592000	0.373000
C	-3.032000	1.852000	0.027000
O	-3.612000	3.052000	0.225000
H	-2.953000	3.598000	0.679000
C	-3.976000	0.909000	-0.692000
H	-4.189000	1.321000	-1.676000
H	-4.908000	0.877000	-0.132000
N	-3.429000	-0.412000	-0.806000
H	-2.672000	-0.557000	-1.468000
C	-3.345000	-1.157000	0.338000
O	-3.988000	-0.914000	1.350000
C	-2.306000	-2.265000	0.261000
H	-2.341000	-2.777000	-0.699000
H	-2.478000	-2.968000	1.069000
N	-0.996000	-1.660000	0.412000
H	-0.662000	-1.385000	1.328000
C	-0.403000	-1.014000	-0.613000
O	-0.805000	-1.058000	-1.779000
C	0.852000	-0.250000	-0.232000
N	0.800000	0.139000	1.173000
H	1.710000	0.482000	1.460000
H	0.140000	0.903000	1.281000
H	0.904000	0.594000	-0.925000
C	2.066000	-1.156000	-0.481000
H	1.985000	-2.026000	0.172000
H	2.022000	-1.499000	-1.516000
C	3.351000	-0.426000	-0.220000
C	4.034000	-0.580000	0.989000
H	3.653000	-1.277000	1.726000
C	5.197000	0.143000	1.250000
H	5.716000	0.008000	2.190000
C	5.693000	1.032000	0.300000
H	6.597000	1.591000	0.498000
C	5.021000	1.193000	-0.912000
H	5.405000	1.876000	-1.657000
C	3.859000	0.470000	-1.167000
H	3.342000	0.593000	-2.111000

FGG_380.xyz

O	-2.543000	-2.593000	0.779000
C	-2.741000	-1.438000	0.481000
O	-3.262000	-0.560000	1.343000
H	-3.401000	0.299000	0.875000
C	-2.440000	-0.887000	-0.911000
H	-3.392000	-0.653000	-1.393000
H	-1.937000	-1.666000	-1.473000
N	-1.600000	0.298000	-0.920000
H	-0.655000	0.254000	-1.293000
C	-2.067000	1.500000	-0.550000
O	-3.201000	1.674000	-0.081000
C	-1.101000	2.660000	-0.736000
H	-1.602000	3.555000	-0.383000
H	-0.870000	2.764000	-1.798000

N	0.138000	2.483000	-0.009000
H	0.339000	3.003000	0.833000
C	1.144000	1.732000	-0.500000
O	1.054000	1.083000	-1.545000
C	2.383000	1.683000	0.375000
N	2.486000	2.897000	1.185000
H	2.852000	3.664000	0.632000
H	3.139000	2.749000	1.944000
H	3.224000	1.519000	-0.304000
C	2.273000	0.478000	1.325000
H	3.200000	0.437000	1.906000
H	1.458000	0.672000	2.025000
C	2.050000	-0.825000	0.616000
C	3.060000	-1.384000	-0.172000
H	4.019000	-0.885000	-0.246000
C	2.849000	-2.574000	-0.861000
H	3.640000	-2.993000	-1.467000
C	1.620000	-3.225000	-0.765000
H	1.456000	-4.154000	-1.295000
C	0.607000	-2.686000	0.026000
H	-0.346000	-3.187000	0.127000
C	0.825000	-1.489000	0.709000
H	0.040000	-1.078000	1.333000

FGG_412.xyz

O	3.437000	0.225000	0.523000
C	2.386000	-0.336000	0.324000
O	1.276000	-0.123000	1.062000
H	1.526000	0.582000	1.682000
C	2.185000	-1.346000	-0.790000
H	2.886000	-2.157000	-0.599000
H	2.482000	-0.860000	-1.717000
N	0.860000	-1.881000	-0.914000
H	0.146000	-1.358000	-1.408000
C	0.434000	-2.811000	-0.014000
O	1.178000	-3.394000	0.761000
C	-1.073000	-3.026000	-0.034000
H	-1.304000	-3.863000	0.616000
H	-1.416000	-3.236000	-1.047000
N	-1.761000	-1.842000	0.438000
H	-1.890000	-1.668000	1.426000
C	-2.030000	-0.804000	-0.373000
O	-1.785000	-0.802000	-1.583000
C	-2.715000	0.373000	0.320000
N	-2.394000	0.357000	1.745000
H	-1.462000	0.736000	1.879000
H	-3.031000	0.957000	2.254000
H	-3.788000	0.178000	0.230000
C	-2.419000	1.686000	-0.423000
H	-2.711000	1.558000	-1.465000
H	-3.055000	2.461000	0.011000
C	-0.981000	2.112000	-0.342000
C	-0.511000	2.836000	0.761000
H	-1.204000	3.129000	1.540000
C	0.827000	3.226000	0.848000
H	1.167000	3.795000	1.704000
C	1.715000	2.906000	-0.176000

H	2.752000	3.202000	-0.112000
C	1.254000	2.202000	-1.288000
H	1.934000	1.969000	-2.097000
C	-0.078000	1.801000	-1.366000
H	-0.436000	1.255000	-2.228000

FGG_444.xyz

O	2.261000	-2.612000	1.127000
C	2.571000	-1.683000	0.417000
O	2.497000	-1.750000	-0.916000
H	2.776000	-0.881000	-1.295000
C	3.072000	-0.354000	0.971000
H	4.083000	-0.176000	0.599000
H	3.094000	-0.430000	2.053000
N	2.233000	0.771000	0.601000
H	1.562000	1.171000	1.256000
C	2.247000	1.283000	-0.639000
O	2.917000	0.807000	-1.565000
C	1.371000	2.512000	-0.830000
H	1.573000	2.902000	-1.822000
H	1.630000	3.261000	-0.080000
N	-0.042000	2.209000	-0.725000
H	-0.663000	2.260000	-1.521000
C	-0.655000	2.051000	0.459000
O	-0.059000	2.025000	1.542000
C	-2.175000	1.935000	0.384000
N	-2.628000	1.919000	-1.006000
H	-3.533000	2.362000	-1.087000
H	-2.744000	0.956000	-1.311000
H	-2.540000	2.851000	0.853000
C	-2.649000	0.739000	1.233000
H	-2.153000	0.796000	2.201000
H	-3.724000	0.842000	1.393000
C	-2.362000	-0.568000	0.551000
C	-3.338000	-1.169000	-0.253000
H	-4.322000	-0.720000	-0.315000
C	-3.069000	-2.348000	-0.946000
H	-3.838000	-2.801000	-1.557000
C	-1.815000	-2.943000	-0.841000
H	-1.603000	-3.861000	-1.372000
C	-0.835000	-2.364000	-0.035000
H	0.133000	-2.834000	0.070000
C	-1.108000	-1.182000	0.650000
H	-0.350000	-0.745000	1.289000

FGG_470.xyz

O	-2.447000	0.883000	1.775000
C	-2.938000	0.993000	0.676000
O	-3.762000	2.004000	0.328000
H	-3.856000	2.552000	1.122000
C	-2.717000	0.061000	-0.480000
H	-2.303000	0.635000	-1.314000
H	-3.681000	-0.319000	-0.820000
N	-1.847000	-1.008000	-0.082000
H	-1.362000	-0.963000	0.808000
C	-1.536000	-1.979000	-0.971000
O	-2.023000	-2.045000	-2.095000

C	-0.512000	-2.983000	-0.459000
H	-0.462000	-3.796000	-1.176000
H	-0.819000	-3.365000	0.515000
N	0.801000	-2.387000	-0.322000
H	1.518000	-2.495000	-1.025000
C	1.152000	-1.689000	0.771000
O	0.390000	-1.472000	1.717000
C	2.598000	-1.195000	0.775000
N	3.202000	-1.359000	-0.546000
H	2.985000	-0.548000	-1.117000
H	4.209000	-1.398000	-0.467000
H	3.124000	-1.859000	1.465000
C	2.656000	0.233000	1.350000
H	2.164000	0.226000	2.322000
H	3.706000	0.496000	1.498000
C	2.002000	1.231000	0.439000
C	0.641000	1.534000	0.565000
H	0.068000	1.082000	1.364000
C	0.033000	2.430000	-0.311000
H	-1.013000	2.681000	-0.189000
C	0.767000	3.026000	-1.337000
H	0.290000	3.720000	-2.015000
C	2.123000	2.739000	-1.467000
H	2.707000	3.211000	-2.246000
C	2.734000	1.853000	-0.580000
H	3.798000	1.661000	-0.663000

FGG_691.xyz

O	2.772000	-1.458000	0.254000
C	3.803000	-1.029000	-0.208000
O	4.964000	-1.718000	-0.212000
H	4.772000	-2.562000	0.223000
C	3.980000	0.322000	-0.871000
H	4.274000	0.161000	-1.907000
H	4.791000	0.842000	-0.367000
N	2.784000	1.111000	-0.800000
H	1.983000	0.812000	-1.350000
C	2.471000	1.681000	0.401000
O	3.272000	1.831000	1.313000
C	1.003000	2.064000	0.519000
H	0.642000	2.520000	-0.401000
H	0.887000	2.754000	1.349000
N	0.220000	0.870000	0.774000
H	0.120000	0.494000	1.708000
C	-0.085000	0.009000	-0.211000
O	0.135000	0.226000	-1.408000
C	-0.708000	-1.302000	0.258000
N	-1.025000	-1.250000	1.683000
H	-1.005000	-2.180000	2.079000
H	-1.967000	-0.894000	1.810000
H	0.091000	-2.034000	0.120000
C	-1.886000	-1.673000	-0.661000
H	-1.538000	-1.619000	-1.692000
H	-2.177000	-2.703000	-0.449000
C	-3.056000	-0.758000	-0.445000
C	-4.094000	-1.118000	0.421000
H	-4.080000	-2.098000	0.884000

C	-5.152000	-0.247000	0.677000
H	-5.948000	-0.547000	1.346000
C	-5.185000	1.004000	0.067000
H	-6.005000	1.682000	0.260000
C	-4.160000	1.373000	-0.804000
H	-4.185000	2.339000	-1.289000
C	-3.104000	0.502000	-1.057000
H	-2.309000	0.788000	-1.734000

GFA_01.xyz

o	-1.54480	-0.50820	-3.05665
c	-0.57715	-1.23521	-3.04406
o	0.05816	-1.64892	-4.15788
h	-0.42775	-1.25613	-4.89914
c	0.04795	-1.82219	-1.80300
c	-0.24677	-3.31849	-1.71079
h	0.20216	-3.70280	-0.79882
h	-1.32210	-3.48555	-1.67678
h	0.17229	-3.84394	-2.56617
h	1.12828	-1.67387	-1.84993
n	-0.47724	-1.08967	-0.67438
h	-1.19240	-0.40717	-0.88414
c	0.25768	-0.96421	0.45349
o	1.25468	-1.64335	0.68873
c	-0.18518	0.14073	1.38971
h	-1.23498	0.39487	1.23612
n	-0.01030	-0.30594	2.74426
h	0.65808	-1.03629	2.95121
c	-0.64458	0.30524	3.76675
o	-1.43201	1.23681	3.62394
c	-0.33924	-0.27905	5.13737
h	-1.19300	-0.90329	5.40030
h	-0.32889	0.55863	5.83684
n	0.86534	-1.10526	5.13767
h	1.68773	-0.52893	5.26008
h	0.84942	-1.75496	5.91128
c	0.67535	1.39173	1.09240
h	0.32601	2.18580	1.75236
h	1.70604	1.14525	1.35106
c	0.57413	1.78856	-0.34951
c	1.53677	1.36669	-1.27259
h	2.40038	0.81539	-0.91939
c	1.39083	1.64217	-2.63093
h	2.14818	1.31511	-3.33129
c	0.27352	2.34226	-3.08415
h	0.15643	2.55695	-4.13756
c	-0.69070	2.76958	-2.17316
h	-1.55816	3.31489	-2.51898
c	-0.53922	2.49511	-0.81550
h	-1.28777	2.83094	-0.10721

GFA_02.xyz

o	2.66007	0.56601	1.48191
c	2.75523	1.43545	0.64042
o	3.72022	2.36941	0.65215
h	4.26489	2.18426	1.43246
c	1.80330	1.62918	-0.51522

c	1.01622	2.92996	-0.34824
h	0.33962	3.03004	-1.19267
h	0.43181	2.89608	0.57025
h	1.68849	3.78465	-0.32202
h	2.38021	1.67944	-1.44026
n	0.95144	0.47210	-0.54554
h	0.96266	-0.12782	0.26266
c	0.24912	0.10719	-1.63822
o	0.20874	0.76618	-2.67268
c	-0.54157	-1.19594	-1.48546
h	-0.23259	-1.83700	-2.31022
n	-0.24959	-1.88914	-0.25577
h	-0.64935	-1.56781	0.61786
c	0.83929	-2.69944	-0.14062
o	1.51493	-3.07915	-1.08674
c	1.14207	-3.11415	1.29352
h	2.21006	-3.33285	1.32903
h	0.60977	-4.04749	1.47885
n	0.68080	-2.10807	2.25026
h	0.57559	-2.51523	3.16930
h	1.37104	-1.36979	2.33668
c	-2.04124	-0.88478	-1.59841
h	-2.20046	-0.38976	-2.55547
h	-2.58795	-1.82798	-1.59902
c	-2.50018	-0.00805	-0.46843
c	-2.40325	1.38478	-0.56779
h	-2.05218	1.82255	-1.49396
c	-2.75395	2.20009	0.50529
h	-2.68057	3.27527	0.40939
c	-3.20504	1.63470	1.69752
h	-3.47857	2.26794	2.53036
c	-3.31447	0.25014	1.80591
h	-3.67473	-0.19620	2.72286
c	-2.96686	-0.56284	0.72810
h	-3.06768	-1.63869	0.81011

GFA_03.xyz

o	-3.02386	0.54922	-1.56780
c	-3.01380	1.26674	-0.59307
o	-4.12987	1.69169	0.03070
h	-4.87017	1.31407	-0.46854
c	-1.77285	1.83116	0.05261
c	-1.65513	3.32769	-0.23167
h	-2.50879	3.86276	0.17857
h	-0.74428	3.69612	0.23260
h	-1.60360	3.50064	-1.30540
h	-1.83655	1.67724	1.13131
n	-0.64802	1.08517	-0.46185
h	-0.85871	0.40942	-1.18316
c	0.46742	0.93739	0.28812
o	0.69934	1.60727	1.29218
c	1.39258	-0.17957	-0.14756
h	1.25324	-0.42329	-1.20157
n	2.75161	0.24568	0.04751
h	2.96484	0.91755	0.77311
c	3.77190	-0.38546	-0.57258
o	3.62115	-1.29179	-1.38722

c	5.15466	0.10811	-0.17795
h	5.74559	0.14213	-1.09551
h	5.58774	-0.67128	0.44861
n	5.11170	1.35263	0.58429
h	5.97072	1.48005	1.10076
h	5.02823	2.14456	-0.03977
c	1.06372	-1.43204	0.69905
h	1.71339	-2.23498	0.35056
h	1.31500	-1.19970	1.73480
c	-0.38372	-1.80257	0.57789
c	-0.84854	-2.49363	-0.54561
h	-0.13721	-2.83732	-1.28770
c	-2.20896	-2.74245	-0.71560
h	-2.55377	-3.27591	-1.59081
c	-3.12399	-2.30458	0.24003
h	-4.17963	-2.49906	0.10840
c	-2.67201	-1.62054	1.36776
h	-3.37564	-1.28598	2.11879
c	-1.31081	-1.37083	1.53231
h	-0.95839	-0.83193	2.40402

GFA_04.xyz

o	1.71530	1.45965	-2.02042
c	2.31205	0.43112	-2.23375
o	3.53989	0.38307	-2.79172
h	3.79421	1.30515	-2.94848
c	1.78247	-0.97128	-1.98404
c	1.21310	-1.53306	-3.28113
h	0.37533	-0.92173	-3.61780
h	1.97416	-1.54368	-4.05707
h	0.85987	-2.54903	-3.11847
h	2.61886	-1.57702	-1.64023
n	0.75733	-0.95913	-0.97139
h	-0.20216	-0.87200	-1.27624
c	1.06640	-0.48314	0.26511
o	2.22196	-0.27138	0.61584
c	-0.12469	-0.21772	1.16794
h	-0.78054	-1.09063	1.18928
n	0.37240	0.01705	2.49284
h	1.35282	0.22466	2.63028
c	-0.44324	-0.09891	3.55913
o	-1.63758	-0.38118	3.47434
c	0.21772	0.17264	4.90054
h	-0.22036	-0.53261	5.60964
h	-0.10297	1.16902	5.20427
n	1.67489	0.15425	4.81877
h	2.01884	-0.79617	4.86134
h	2.08011	0.64523	5.60318
c	-0.95374	0.98330	0.64997
h	-1.57255	1.30135	1.48914
h	-0.27797	1.79746	0.38442
c	-1.83398	0.61537	-0.50969
c	-1.60060	1.11019	-1.79711
h	-0.77503	1.79062	-1.95881
c	-2.40696	0.71505	-2.86475
h	-2.21839	1.10970	-3.85443
c	-3.45369	-0.18185	-2.65846

h	-4.07811	-0.48861	-3.48639
c	-3.69794	-0.67504	-1.37665
h	-4.51512	-1.36307	-1.20727
c	-2.89470	-0.27795	-0.31058
h	-3.08785	-0.65122	0.68881

GFA_05.xyz

o	-2.00681	1.45437	-1.71698
c	-2.25313	0.42373	-2.29729
o	-2.83146	0.37393	-3.51554
h	-2.97136	1.29620	-3.77870
c	-2.02796	-0.97779	-1.75415
c	-3.33003	-1.50480	-1.16322
h	-3.18526	-2.52025	-0.80096
h	-3.64318	-0.87741	-0.32825
h	-4.11509	-1.50672	-1.91492
h	-1.70744	-1.60046	-2.58740
n	-1.00285	-0.97607	-0.74153
h	-1.29368	-0.86992	0.22028
c	0.24031	-0.53325	-1.07168
o	0.58169	-0.34430	-2.23381
c	1.16372	-0.27490	0.10554
h	1.17057	-1.13968	0.77275
n	2.48676	-0.07172	-0.41185
h	2.61974	0.03596	-1.40924
c	3.55982	-0.19079	0.39539
o	3.48172	-0.42062	1.60118
c	4.90268	-0.03676	-0.29938
h	5.32663	-1.03854	-0.36562
h	5.54060	0.53319	0.37925
n	4.77746	0.51012	-1.64666
h	4.70563	1.51861	-1.61275
h	5.59911	0.29525	-2.19394
c	0.68214	0.94937	0.92270
h	1.53682	1.26128	1.52287
h	0.42118	1.75653	0.23680
c	-0.47016	0.61873	1.82706
c	-1.75206	1.13238	1.60402
h	-1.91442	1.79974	0.76799
c	-2.81365	0.77260	2.43467
h	-3.79906	1.18127	2.25371
c	-2.60657	-0.10697	3.49576
h	-3.42982	-0.38655	4.13882
c	-1.33017	-0.61896	3.72948
h	-1.16026	-1.29403	4.55729
c	-0.27017	-0.25738	2.90190
h	0.72534	-0.64490	3.08653

GFA_06.xyz

o	0.75900	5.30664	0.88023
c	0.85823	4.33774	0.16665
o	2.03513	3.92632	-0.32062
h	1.89147	3.11637	-0.86448
c	-0.34673	3.49357	-0.26893
c	-1.63976	4.05321	0.28288
h	-2.48358	3.45697	-0.05908
h	-1.61600	4.05114	1.37047

h	-1.76931	5.08128	-0.04169
h	-0.35754	3.49429	-1.36295
n	-0.19608	2.10798	0.16403
h	-0.84725	1.72284	0.84844
c	0.58681	1.23442	-0.48500
o	1.37611	1.56009	-1.38285
c	0.42870	-0.21412	-0.02269
h	0.51652	-0.22649	1.06778
n	-0.89460	-0.71132	-0.35227
h	-1.02100	-1.43840	-1.04723
c	-1.96190	-0.49210	0.43572
o	-1.97013	0.29276	1.38855
c	-3.18620	-1.31881	0.08200
h	-4.05288	-0.66210	0.16813
h	-3.27526	-2.06443	0.87165
n	-3.05117	-1.99331	-1.20663
h	-3.55117	-2.87060	-1.20492
h	-3.44686	-1.43097	-1.94794
c	1.49093	-1.11348	-0.64359
h	1.42756	-1.03636	-1.72933
h	2.46920	-0.72716	-0.35895
c	1.31502	-2.53530	-0.19346
c	1.65904	-2.91408	1.10796
h	2.10359	-2.18531	1.77546
c	1.44515	-4.21607	1.55127
h	1.72192	-4.49397	2.55912
c	0.87984	-5.16140	0.69590
h	0.71584	-6.17372	1.03847
c	0.53689	-4.79795	-0.60396
h	0.10647	-5.52751	-1.27644
c	0.75395	-3.49254	-1.04219
h	0.49766	-3.21701	-2.05846

GFA_07.xyz

o	-0.54482	0.90121	5.35887
c	-0.74005	0.20465	4.39221
o	-1.97006	-0.16556	4.01486
h	-1.90342	-0.71687	3.20016
c	0.39230	-0.34112	3.51269
c	1.74836	0.08073	4.03500
h	2.53730	-0.34094	3.41518
h	1.83066	1.16550	4.03336
h	1.87478	-0.25745	5.05906
h	0.29830	-1.43110	3.51131
n	0.24452	0.10979	2.13263
h	0.93972	0.74049	1.73297
c	-0.62421	-0.45348	1.28113
o	-1.48848	-1.27171	1.62519
c	-0.46294	0.00422	-0.16761
h	-0.46530	1.09835	-0.16812
n	0.81864	-0.41404	-0.70319
h	0.87293	-1.12632	-1.42183
c	1.93930	0.31057	-0.53291
o	2.03700	1.25190	0.25957
c	3.10755	-0.12750	-1.39804
h	3.79377	-0.67512	-0.75233
h	3.61891	0.78633	-1.70659

n	2.67709	-1.00332	-2.48450
h	3.45966	-1.52979	-2.84748
h	2.30411	-0.45912	-3.25338
c	-1.58783	-0.52221	-1.05283
h	-1.63765	-1.60675	-0.95423
h	-2.53149	-0.12831	-0.67650
c	-1.35552	-0.12295	-2.48233
c	-0.91188	-1.05606	-3.42277
h	-0.80487	-2.09419	-3.13116
c	-0.61758	-0.67075	-4.73023
h	-0.28252	-1.40863	-5.44676
c	-0.76363	0.66083	-5.11267
h	-0.53972	0.96325	-6.12637
c	-1.21361	1.60030	-4.18492
h	-1.33953	2.63371	-4.47784
c	-1.50596	1.20906	-2.88131
h	-1.85739	1.94372	-2.16651

GFA_08.xyz

o	-0.11029	5.17822	-0.54130
c	-0.12813	4.02691	-0.90372
o	0.53079	3.60962	-1.99245
h	0.38676	2.64079	-2.10102
c	-0.91429	2.93074	-0.17168
c	-1.66357	3.49006	1.01824
h	-2.24861	2.70598	1.49492
h	-0.96522	3.90766	1.74055
h	-2.32509	4.29009	0.69955
h	-1.60645	2.49646	-0.89821
n	-0.03251	1.85796	0.27388
h	0.22881	1.79192	1.25880
c	0.42922	0.91084	-0.55268
o	0.26921	0.94924	-1.78231
c	1.22107	-0.20218	0.14370
h	2.08191	0.29427	0.60176
n	0.47028	-0.82348	1.21725
h	0.01716	-1.71949	1.06894
c	0.33449	-0.28473	2.44006
o	0.75879	0.83132	2.75850
c	-0.42860	-1.14447	3.43215
h	-1.39336	-0.65769	3.57309
h	0.10255	-1.06869	4.38269
n	-0.64343	-2.50275	2.94529
h	0.12095	-3.10655	3.21645
h	-1.48399	-2.89776	3.34198
c	1.71466	-1.26783	-0.84207
h	2.03296	-0.75708	-1.74912
h	2.58571	-1.75275	-0.40097
c	0.68022	-2.31633	-1.15517
c	-0.33659	-2.09314	-2.09119
h	-0.36399	-1.15224	-2.62216
c	-1.30075	-3.06908	-2.33103
h	-2.07671	-2.88469	-3.06168
c	-1.26931	-4.27953	-1.63965
h	-2.01962	-5.03452	-1.83010
c	-0.26008	-4.51434	-0.70969
h	-0.21999	-5.45366	-0.17500

c	0.70590	-3.53801	-0.47287
h	1.49962	-3.72842	0.24012

GFA_09.xyz

o	1.59159	3.75212	0.44006
c	1.84810	2.58276	0.28301
o	2.28682	1.81033	1.28698
h	2.40991	0.89066	0.95504
c	1.70702	1.86729	-1.06903
c	1.28039	2.83191	-2.15378
h	1.21699	2.31682	-3.11014
h	0.31119	3.26323	-1.90622
h	1.99241	3.64815	-2.23050
h	2.67158	1.41196	-1.30376
n	0.73394	0.78211	-0.98860
h	-0.21853	0.99186	-1.25556
c	0.96336	-0.36726	-0.33215
o	2.04742	-0.62549	0.21237
c	-0.21109	-1.31741	-0.23679
h	-0.80614	-1.28683	-1.15107
n	0.29327	-2.64830	-0.05745
h	1.23588	-2.79827	0.27750
c	-0.48328	-3.71874	-0.33118
o	-1.63673	-3.63371	-0.74420
c	0.19543	-5.06217	-0.11795
h	0.44750	-5.43587	-1.11010
h	-0.56212	-5.73296	0.29095
n	1.41961	-4.95088	0.67037
h	2.03534	-5.72905	0.48124
h	1.20767	-4.98267	1.65892
c	-1.12728	-0.89103	0.93912
h	-1.91762	-1.63997	0.99386
h	-0.54227	-0.92858	1.85932
c	-1.68382	0.48146	0.71014
c	-1.16005	1.59267	1.37741
h	-0.40888	1.44935	2.14442
c	-1.56232	2.88324	1.03858
h	-1.12581	3.73114	1.54723
c	-2.50140	3.07580	0.02604
h	-2.80981	4.07656	-0.24352
c	-3.04744	1.97395	-0.63322
h	-3.78761	2.11743	-1.40894
c	-2.64054	0.68482	-0.29197
h	-3.06198	-0.17230	-0.80498

GFA_10.xyz

o	-0.41823	1.60875	-3.74723
c	-0.28988	1.85548	-2.57226
o	-1.31646	2.26935	-1.81637
h	-1.00550	2.38812	-0.88884
c	1.05013	1.73025	-1.83099
c	2.16083	1.33165	-2.77782
h	2.24139	2.05283	-3.58560
h	3.10779	1.27938	-2.24443
h	1.93843	0.36271	-3.22320
h	1.25888	2.69437	-1.36224
n	0.96537	0.74565	-0.75649

h	1.25218	-0.20025	-0.96993
c	0.28198	0.95259	0.38138
o	-0.28683	2.02451	0.63831
c	0.18980	-0.23120	1.32038
h	1.11533	-0.80865	1.30448
n	-0.01843	0.25826	2.65233
h	-0.44339	1.16357	2.80403
c	0.25472	-0.52287	3.72004
o	0.72289	-1.65474	3.63228
c	-0.07948	0.10402	5.06352
h	0.72845	-0.17020	5.74450
h	-0.97720	-0.40129	5.41889
n	-0.35246	1.53489	4.96206
h	-0.91298	1.84522	5.74315
h	0.50951	2.06330	4.99508
c	-0.96053	-1.16613	0.86598
h	-1.01034	-1.96664	1.60451
h	-1.89362	-0.60151	0.89625
c	-0.69917	-1.70105	-0.50936
c	0.32583	-2.63412	-0.70857
h	0.83398	-3.05592	0.15131
c	0.69630	-3.01681	-1.99705
h	1.48967	-3.73867	-2.13730
c	0.04371	-2.46991	-3.10244
h	0.33589	-2.75924	-4.10256
c	-0.99160	-1.55506	-2.91439
h	-1.49559	-1.11822	-3.76488
c	-1.35964	-1.17704	-1.62447
h	-2.14453	-0.44403	-1.48411

GFA_11.xyz

o	-5.15272	0.53849	-0.15388
c	-4.00327	0.90713	-0.15095
o	-3.60085	1.98907	0.52866
h	-2.63025	2.10241	0.40206
c	-2.89239	0.19199	-0.93105
c	-3.43550	-0.98731	-1.70858
h	-4.22499	-0.66042	-2.37870
h	-2.64022	-1.45287	-2.28738
h	-3.86280	-1.72164	-1.02888
h	-2.44823	0.93061	-1.60386
n	-1.83249	-0.26443	-0.03931
h	-1.77589	-1.25088	0.21979
c	-0.89602	0.55823	0.44976
o	-0.93535	1.78982	0.30475
c	0.20337	-0.14169	1.25702
h	-0.30367	-0.57921	2.12281
n	0.82143	-1.23046	0.52398
h	1.75690	-1.11791	0.14630
c	0.27960	-2.45281	0.39823
o	-0.85671	-2.75279	0.77975
c	1.18380	-3.48057	-0.26120
h	0.55557	-4.06316	-0.93707
h	1.50180	-4.15522	0.53319
n	2.35972	-2.87354	-0.87582
h	3.12764	-3.52859	-0.90677
h	2.16730	-2.60283	-1.83114

c	1.27919	0.83814	1.74077
h	0.77647	1.74789	2.06377
h	1.76960	0.39357	2.60702
c	2.31813	1.14520	0.69484
c	3.52746	0.44044	0.69322
h	3.71764	-0.28798	1.47280
c	4.49161	0.66978	-0.28688
h	5.42058	0.11627	-0.26829
c	4.25823	1.61593	-1.28125
h	5.00468	1.80149	-2.04134
c	3.06079	2.33069	-1.28435
h	2.87778	3.07435	-2.04822
c	2.09625	2.09736	-0.30728
h	1.16529	2.64606	-0.31322

GFA_12.xyz

o	5.07601	-0.77361	-0.02599
c	4.24489	0.07480	-0.24448
o	4.08694	0.62403	-1.45548
h	3.34035	1.26746	-1.41949
c	3.29819	0.61758	0.83394
c	3.59816	0.01157	2.18742
h	2.93853	0.43484	2.94240
h	3.46221	-1.06734	2.15433
h	4.63060	0.20564	2.46253
h	3.42318	1.70359	0.85639
n	1.90744	0.34912	0.48430
h	1.38412	-0.36795	0.99122
c	1.25103	1.05644	-0.44388
o	1.78151	1.94060	-1.13361
c	-0.23569	0.75536	-0.59043
h	-0.53681	1.25989	-1.50598
n	-0.52915	-0.65443	-0.79206
h	-0.99837	-0.95012	-1.64076
c	-0.49619	-1.61083	0.14890
o	-0.01115	-1.48182	1.27936
c	-1.14707	-2.91792	-0.27120
h	-2.09225	-2.95701	0.27111
h	-0.52162	-3.72418	0.11391
n	-1.41304	-2.97494	-1.70537
h	-0.64165	-3.40743	-2.19584
h	-2.23383	-3.53096	-1.89693
c	-1.02768	1.36045	0.58523
h	-0.65085	0.95507	1.52228
h	-0.84196	2.43609	0.57904
c	-2.49129	1.06415	0.44197
c	-3.27122	1.76057	-0.48610
h	-2.82505	2.56262	-1.06277
c	-4.61466	1.44235	-0.66802
h	-5.20706	1.99430	-1.38505
c	-5.19639	0.41849	0.07855
h	-6.24037	0.17279	-0.05906
c	-4.42951	-0.27823	1.01025
h	-4.87842	-1.06479	1.60205
c	-3.08459	0.04233	1.18855
h	-2.48700	-0.49539	1.91460

GFA_13.xyz

o	1.03615	-0.51563	-2.94171
c	0.04518	-0.23286	-3.57889
o	-0.13562	-0.59516	-4.86369
h	0.65506	-1.09657	-5.11422
c	-1.11572	0.61230	-3.07847
c	-0.94865	2.04086	-3.58236
h	-0.90904	2.06178	-4.66855
h	-1.78774	2.64527	-3.24604
h	-0.02904	2.47198	-3.18696
h	-2.03064	0.17239	-3.46924
n	-1.15355	0.60106	-1.63782
h	-0.52141	1.24270	-1.16173
c	-1.32677	-0.60659	-1.02445
o	-1.78618	-1.58784	-1.59538
c	-0.82730	-0.66468	0.41751
h	-1.09694	-1.65380	0.78350
n	0.62998	-0.62793	0.38416
h	1.13486	-1.50390	0.30559
c	1.38051	0.43531	0.04502
o	0.96509	1.59391	-0.07462
c	2.84522	0.10276	-0.17814
h	3.37043	0.29982	0.75743
h	3.20406	0.81964	-0.91839
n	3.01756	-1.30142	-0.53728
h	2.75903	-1.42783	-1.50919
h	3.98445	-1.57811	-0.43882
c	-1.44440	0.38542	1.34898
h	-1.26083	1.38455	0.96297
h	-2.52285	0.21555	1.35363
c	-0.88605	0.25525	2.73640
c	-1.37842	-0.71630	3.61226
h	-2.20253	-1.34695	3.29907
c	-0.82990	-0.87402	4.88261
h	-1.22589	-1.62587	5.55185
c	0.22380	-0.05845	5.29218
h	0.64957	-0.17695	6.27914
c	0.72080	0.91399	4.42659
h	1.53455	1.55359	4.74124
c	0.17008	1.06847	3.15588
h	0.55459	1.82136	2.47914

GFA_14.xyz

o	0.41782	-3.00991	-0.66409
c	0.08581	-2.59359	-1.75242
o	0.58935	-3.07351	-2.90427
h	1.23024	-3.75313	-2.64502
c	-0.99646	-1.54344	-1.98550
c	-0.84785	-0.77191	-3.28977
h	-0.88452	-1.44694	-4.14040
h	-1.66453	-0.05791	-3.36674
h	0.09458	-0.23369	-3.30141
h	-1.93002	-2.10996	-2.01580
n	-1.07936	-0.67558	-0.82908
h	-1.73584	-0.92756	-0.09654
c	0.06343	-0.08439	-0.38355
o	1.09714	-0.03034	-1.04135

c	-0.01963	0.37828	1.06973
h	-1.03663	0.69132	1.30562
n	0.26734	-0.80415	1.86745
h	1.22270	-1.13694	1.94162
c	-0.66575	-1.76879	2.03740
o	-1.86088	-1.62502	1.77429
c	-0.12113	-3.06805	2.60208
h	-0.75504	-3.85909	2.19830
h	-0.27027	-3.04390	3.68206
n	1.30393	-3.20815	2.31776
h	1.41950	-3.49478	1.35256
h	1.71249	-3.92492	2.90104
c	0.96424	1.49873	1.36436
h	0.99762	1.64497	2.44478
h	1.95422	1.19233	1.02495
c	0.54269	2.76797	0.67743
c	-0.40949	3.60088	1.27333
h	-0.80603	3.34229	2.24832
c	-0.84412	4.75943	0.63467
h	-1.57749	5.39549	1.11162
c	-0.32947	5.09969	-0.61510
h	-0.66296	5.99994	-1.11284
c	0.61946	4.27619	-1.21758
h	1.02394	4.53570	-2.18665
c	1.05122	3.11663	-0.57684
h	1.77707	2.46785	-1.04825

GFA_15.xyz

o	-0.92773	-0.33774	5.14434
c	-0.03045	-0.31061	4.33670
o	0.85051	-1.31129	4.21414
h	1.47894	-1.09700	3.48484
c	0.20541	0.87054	3.38618
c	-0.78057	1.98941	3.64188
h	-1.79700	1.63959	3.47436
h	-0.71107	2.31898	4.67423
h	-0.57554	2.82906	2.98055
h	1.23208	1.21106	3.54751
n	0.10043	0.44704	1.99374
h	-0.69268	0.75514	1.42561
c	1.07639	-0.22822	1.37641
o	2.09987	-0.63341	1.94908
c	0.90989	-0.44298	-0.12204
h	1.61773	-1.23048	-0.37088
n	-0.39605	-0.93672	-0.53100
h	-0.41775	-1.73466	-1.15769
c	-1.50791	-0.18459	-0.64149
o	-1.69671	0.88909	-0.06002
c	-2.56379	-0.77739	-1.55993
h	-3.06801	0.07297	-2.02360
h	-3.29544	-1.28406	-0.92996
n	-1.98012	-1.74036	-2.48822
h	-2.69177	-2.34949	-2.86743
h	-1.55024	-1.25421	-3.26822
c	1.30381	0.83421	-0.89873
h	0.74305	1.68327	-0.51099
h	2.36493	1.01557	-0.72071

c	1.00976	0.64908	-2.35936
c	1.75328	-0.25286	-3.12755
h	2.60542	-0.75576	-2.68528
c	1.41140	-0.51233	-4.45246
h	1.99739	-1.21173	-5.03306
c	0.31801	0.13254	-5.03126
h	0.05449	-0.06439	-6.06147
c	-0.42040	1.04641	-4.28047
h	-1.25866	1.56457	-4.72723
c	-0.07730	1.29858	-2.95199
h	-0.65764	1.99959	-2.36532

GFA_16.xyz

o	-5.02826	0.25885	-1.62397
c	-4.25024	0.42846	-0.71420
o	-4.09678	1.61216	-0.11553
h	-3.42062	1.53234	0.60411
c	-3.43338	-0.73661	-0.14616
c	-4.03361	-1.20852	1.17638
h	-3.50862	-2.09748	1.52077
h	-3.95569	-0.43786	1.93872
h	-5.08372	-1.45439	1.02986
h	-3.52645	-1.52728	-0.88527
n	-2.00120	-0.46724	-0.03288
h	-1.35119	-1.00106	-0.61504
c	-1.44614	0.40437	0.81518
o	-2.07987	1.20903	1.51822
c	0.07526	0.44238	0.84393
h	0.32007	0.94326	1.77799
n	0.73781	-0.85231	0.89851
h	1.47959	-0.96302	1.58260
c	0.91636	-1.66602	-0.16085
o	0.21638	-1.66157	-1.17878
c	2.07437	-2.63791	-0.00598
h	2.47901	-2.78261	-1.00977
h	1.65904	-3.59298	0.31702
n	3.03051	-2.16823	0.99168
h	3.64226	-1.46949	0.58205
h	3.61519	-2.92798	1.31189
c	0.60248	1.30722	-0.32605
h	0.18135	0.94933	-1.26414
h	0.25088	2.32725	-0.16390
c	2.10105	1.23497	-0.37521
c	2.74306	0.51127	-1.38462
h	2.15071	0.06954	-2.17601
c	4.12923	0.35334	-1.37725
h	4.61181	-0.20035	-2.17176
c	4.89057	0.91236	-0.35157
h	5.96536	0.79262	-0.34425
c	4.26040	1.64526	0.65474
h	4.84599	2.09446	1.44527
c	2.87710	1.80535	0.63934
h	2.39506	2.37972	1.42190

GGF_01.xyz

o	2.08399	-2.95332	0.95935
c	1.10783	-2.27294	0.73806

o	0.32981	-1.82811	1.72273
h	-0.39735	-1.24972	1.41606
c	0.77488	-1.88423	-0.71105
h	0.67256	-2.82946	-1.24281
n	-0.43715	-1.12759	-0.87176
h	-0.37614	-0.12148	-0.85405
c	-1.66783	-1.69433	-0.79556
o	-1.86711	-2.89757	-0.75373
c	-2.82628	-0.70085	-0.77486
h	-3.54201	-1.09733	-0.05577
h	-3.29302	-0.69611	-1.75739
n	-2.44276	0.65061	-0.43235
h	-2.66418	1.45198	-1.00754
c	-1.93581	0.93526	0.78456
o	-1.66608	0.07223	1.62119
c	-1.70525	2.40858	1.05874
h	-0.73732	2.48224	1.55834
h	-2.46454	2.70625	1.78169
n	-1.82982	3.22022	-0.14908
h	-0.92170	3.31135	-0.58843
h	-2.13965	4.15381	0.08169
c	1.94944	-1.08305	-1.29561
h	2.86620	-1.60816	-1.03235
h	1.85695	-1.07038	-2.38154
c	1.95727	0.32832	-0.77365
c	2.32241	0.60785	0.55025
h	2.66190	-0.19400	1.19322
c	2.26468	1.90940	1.04257
h	2.55381	2.10666	2.06589
c	1.85030	2.95716	0.21915
h	1.82584	3.96993	0.59883
c	1.49258	2.69365	-1.10223
h	1.20283	3.50253	-1.76135
c	1.53601	1.38584	-1.58767
h	1.26419	1.18397	-2.61698

GGF_02.xyz

o	1.86491	-2.65909	0.78072
c	0.84807	-2.90817	-0.06805
o	0.95713	-3.62188	-1.03845
h	2.62555	-3.14497	0.42632
c	-0.44301	-2.23455	0.35648
h	-0.99680	-2.99293	0.92042
n	-0.17014	-1.11798	1.22671
h	0.75873	-0.70173	1.25943
c	-1.17312	-0.45130	1.83770
o	-2.35210	-0.79496	1.80472
c	-0.69698	0.78789	2.59089
h	0.08575	0.50408	3.29610
h	-1.54752	1.18930	3.13214
n	-0.17388	1.80934	1.70647
h	-0.70295	2.63750	1.47136
c	1.06777	1.75618	1.19687
o	1.85168	0.82030	1.38082
c	1.47066	2.96454	0.37171
h	1.94747	2.57622	-0.53007
h	2.24037	3.47879	0.94658

n	0.35427	3.87286	0.12175
h	-0.09664	3.62079	-0.74835
h	0.68370	4.82283	0.02413
c	-1.29749	-1.86107	-0.86806
h	-1.23449	-2.68650	-1.57665
h	-2.32713	-1.76619	-0.53240
c	-0.86185	-0.57088	-1.50138
c	-1.65761	0.57086	-1.37249
h	-2.57916	0.50641	-0.80734
c	-1.28939	1.77133	-1.97836
h	-1.94137	2.63238	-1.90055
c	-0.09715	1.85407	-2.69705
h	0.18591	2.77890	-3.18345
c	0.71786	0.72734	-2.81015
h	1.63932	0.78043	-3.37443
c	0.33365	-0.47673	-2.22444
h	0.95118	-1.35650	-2.35194

GGF_03.xyz

o	-1.47542	-2.18469	0.62294
c	-2.09514	-1.27965	1.13268
o	-3.42758	-1.31655	1.34248
h	-3.72271	-2.17555	1.00321
c	-1.50516	0.03522	1.57787
h	-1.79787	0.23505	2.60907
n	-0.07601	-0.08724	1.50953
h	0.30801	-0.72593	0.83150
c	0.73940	0.76125	2.17551
o	0.33867	1.61602	2.95619
c	2.22943	0.57157	1.91083
h	2.69080	0.25547	2.84490
h	2.62934	1.54885	1.64859
n	2.54895	-0.35113	0.85357
h	2.62689	-1.34844	0.99721
c	2.74809	0.07074	-0.42015
o	2.72997	1.24546	-0.76834
c	2.94148	-1.05617	-1.42213
h	3.69392	-0.72292	-2.13797
h	1.99599	-1.12674	-1.96245
n	3.22552	-2.33917	-0.78117
h	4.22306	-2.48269	-0.69822
h	2.86579	-3.10249	-1.33615
c	-2.03414	1.18548	0.68702
h	-3.11492	1.25048	0.81066
h	-1.58768	2.10228	1.07099
c	-1.66415	0.96377	-0.74892
c	-0.41463	1.37073	-1.22716
h	0.26089	1.91756	-0.58301
c	-0.02465	1.08532	-2.53462
h	0.94922	1.41000	-2.87458
c	-0.88723	0.39417	-3.38420
h	-0.59099	0.17824	-4.40189
c	-2.14069	-0.00568	-2.92223
h	-2.81896	-0.53198	-3.58022
c	-2.52332	0.27572	-1.61284
h	-3.49902	-0.03268	-1.25708

GGF_04.xyz

o	-0.40368	1.13468	3.86889
c	0.38512	0.34067	3.41966
o	1.41815	-0.17219	4.12986
h	1.35988	0.23550	5.00727
c	0.40461	-0.18555	1.99856
h	0.56005	-1.26308	2.04399
n	-0.85075	0.04610	1.34586
h	-1.05035	0.96402	0.95800
c	-1.64376	-0.97651	0.94289
o	-1.45529	-2.15535	1.22705
c	-2.75716	-0.52145	0.00821
h	-3.26279	0.35606	0.40975
h	-3.46398	-1.33632	-0.10826
n	-2.19879	-0.17714	-1.28417
h	-2.06530	-0.86788	-2.01150
c	-1.56846	0.99170	-1.49767
o	-1.50797	1.90977	-0.67442
c	-0.87988	1.10042	-2.84462
h	0.18382	1.16771	-2.61604
h	-1.17131	2.05788	-3.27786
n	-1.13230	-0.04719	-3.71376
h	-0.27120	-0.35964	-4.13908
h	-1.77117	0.19154	-4.45915
c	1.54841	0.49944	1.24221
h	1.37616	1.57929	1.26015
h	2.47686	0.31756	1.78728
c	1.71209	0.05621	-0.19077
c	2.43955	0.87243	-1.06449
h	2.81677	1.82348	-0.70835
c	2.69373	0.47796	-2.37583
h	3.27041	1.11948	-3.02873
c	2.20461	-0.74256	-2.84203
h	2.41096	-1.06106	-3.85556
c	1.45755	-1.55213	-1.98865
h	1.06778	-2.49812	-2.34014
c	1.21522	-1.15912	-0.67167
h	0.64193	-1.81445	-0.02903

GGF_05.xyz

o	-1.89914	0.71092	1.97891
c	-2.30783	1.09761	0.90929
o	-3.62315	1.22764	0.62164
h	-4.09329	0.96752	1.42854
c	-1.45721	1.46944	-0.27960
h	-1.73600	2.47036	-0.61106
n	-0.07803	1.48545	0.12600
h	0.21232	0.82220	0.83792
c	0.82124	2.20910	-0.58936
o	0.50465	2.93805	-1.52259
c	2.27574	2.09465	-0.14265
h	2.58535	3.06952	0.23019
h	2.87059	1.86918	-1.02375
n	2.51647	1.06861	0.84275
h	2.02789	1.15813	1.72091
c	2.71031	-0.22587	0.43932
o	3.12183	-0.53508	-0.66959

c	2.33461	-1.24130	1.50913
h	2.99769	-1.10918	2.36500
h	2.50041	-2.23445	1.09262
n	0.95664	-0.97344	1.93275
h	0.30919	-1.44469	1.30774
h	0.78001	-1.34330	2.85713
c	-1.70147	0.49325	-1.45500
h	-2.76525	0.48869	-1.69126
h	-1.16051	0.89687	-2.31008
c	-1.20809	-0.88365	-1.12471
c	0.08738	-1.27116	-1.48113
h	0.71602	-0.58969	-2.03960
c	0.58224	-2.52600	-1.12831
h	1.58906	-2.79643	-1.41443
c	-0.21631	-3.40988	-0.40358
h	0.16165	-4.38606	-0.13101
c	-1.50953	-3.03365	-0.03703
h	-2.13621	-3.71759	0.51948
c	-2.00010	-1.77980	-0.39690
h	-3.00969	-1.49830	-0.12341

GGF_06.xyz

o	-0.55497	1.55657	4.06146
c	-0.38450	0.52584	3.46008
o	-0.60418	-0.67765	4.01663
h	-0.41462	-1.32861	3.31891
c	0.12423	0.48986	2.01802
h	1.19047	0.71453	2.08052
n	0.00848	-0.82698	1.42260
h	-0.85392	-1.04372	0.91398
c	1.11980	-1.46964	0.93505
o	2.26871	-1.16981	1.22036
c	0.76880	-2.59742	-0.02658
h	-0.00907	-3.22970	0.40344
h	1.66478	-3.18386	-0.20107
n	0.29173	-2.06837	-1.28809
h	0.88512	-2.00254	-2.10511
c	-0.96412	-1.62225	-1.45800
o	-1.81089	-1.58132	-0.55837
c	-1.29025	-1.18932	-2.87456
h	-1.90673	-0.29275	-2.79179
h	-1.91600	-1.97624	-3.29612
n	-0.08794	-1.03172	-3.68641
h	0.26635	-0.08721	-3.58507
h	-0.29923	-1.16822	-4.66499
c	-0.60596	1.54017	1.18666
h	-1.67130	1.29640	1.16954
h	-0.51508	2.49307	1.71010
c	-0.10858	1.67354	-0.22926
c	-0.99988	2.08060	-1.22817
h	-2.04334	2.22553	-0.97621
c	-0.56362	2.32193	-2.52919
h	-1.26716	2.65851	-3.27933
c	0.78030	2.14110	-2.85828
h	1.12869	2.34521	-3.86244
c	1.67128	1.69907	-1.88102
h	2.71373	1.54557	-2.12579

c	1.23159	1.47129	-0.57747
h	1.94584	1.13658	0.16260

GGF_07.xyz

o	4.09057	1.44017	0.64458
c	3.44083	0.44648	0.41037
o	3.91523	-0.80338	0.57454
h	4.82714	-0.68585	0.88365
c	2.01918	0.48234	-0.12035
h	2.11357	0.73196	-1.17963
n	1.34054	-0.78052	-0.06265
h	0.93571	-1.09533	0.81708
c	0.89002	-1.39090	-1.18679
o	1.17134	-1.04346	-2.32873
c	-0.05484	-2.54741	-0.88554
h	0.39776	-3.21855	-0.15494
h	-0.23970	-3.08240	-1.81110
n	-1.31411	-2.06537	-0.35434
h	-2.13098	-1.94255	-0.93785
c	-1.46941	-1.70060	0.92913
o	-0.56873	-1.73054	1.77407
c	-2.87512	-1.25499	1.28889
h	-2.76600	-0.39657	1.95431
h	-3.31377	-2.06437	1.87277
n	-3.69312	-1.01004	0.10512
h	-3.56201	-0.05307	-0.20336
h	-4.67361	-1.12138	0.32216
c	1.23276	1.57023	0.61698
h	1.22713	1.33686	1.68442
h	1.77267	2.51151	0.50639
c	-0.18793	1.71753	0.14005
c	-1.18963	2.04745	1.05866
h	-0.93623	2.12984	2.10851
c	-2.49790	2.28831	0.64271
h	-3.25209	2.56299	1.36854
c	-2.82875	2.18515	-0.70865
h	-3.83860	2.38916	-1.04031
c	-1.84642	1.82127	-1.62938
h	-2.09432	1.72485	-2.67784
c	-0.53736	1.59182	-1.20926
h	0.20509	1.30644	-1.94251

GGF_08.xyz

o	-3.98415	-0.77643	-0.59951
c	-2.81268	-0.95550	0.05414
o	-2.31790	-2.04153	0.24095
h	-4.28782	-1.66636	-0.83472
c	-2.22875	0.36558	0.49219
h	-2.98747	0.87601	1.09027
n	-1.07115	0.08601	1.29764
h	-0.65960	-0.84629	1.27033
c	-0.39406	1.08257	1.90822
o	-0.76369	2.25494	1.92055
c	0.88949	0.62322	2.59151
h	0.66339	-0.19294	3.27947
h	1.28510	1.46927	3.14405

n	1.88401	0.16509	1.64419
h	2.68234	0.72805	1.38809
c	1.85561	-1.07701	1.12843
o	0.96274	-1.89523	1.35669
c	3.03291	-1.42514	0.23565
h	2.61554	-1.90558	-0.65113
h	3.60541	-2.18163	0.77146
n	3.88632	-0.27264	-0.04540
h	3.56750	0.18429	-0.89005
h	4.83878	-0.56800	-0.20777
c	-1.91794	1.27696	-0.71940
h	-2.77173	1.24761	-1.39640
h	-1.81928	2.29050	-0.33834
c	-0.65157	0.88672	-1.42446
c	0.47346	1.71133	-1.33715
h	0.41376	2.61879	-0.74928
c	1.65014	1.38845	-2.01106
h	2.49718	2.06102	-1.96192
c	1.72707	0.21348	-2.75840
h	2.63315	-0.03502	-3.29603
c	0.61978	-0.63211	-2.82845
h	0.66965	-1.54412	-3.40787
c	-0.56100	-0.29258	-2.17278
h	-1.42172	-0.94295	-2.26130

GGF_09.xyz

o	-0.26252	-2.06691	-2.12720
c	-0.18692	-1.00268	-2.69327
o	0.37707	-0.84909	-3.91389
h	0.65579	-1.73751	-4.18328
c	-0.68068	0.31719	-2.15278
h	-1.35338	0.75287	-2.89542
n	-1.39220	0.04655	-0.93227
h	-1.32637	-0.88165	-0.51921
c	-2.02378	1.03109	-0.25609
o	-2.13066	2.18432	-0.66804
c	-2.58576	0.59299	1.09261
h	-3.27622	-0.23828	0.94810
h	-3.11585	1.43989	1.51657
n	-1.55100	0.16145	2.00790
h	-1.08440	0.80457	2.63114
c	-1.02370	-1.07672	1.94096
o	-1.40281	-1.93943	1.14800
c	0.11871	-1.33686	2.90220
h	1.01807	-1.34665	2.28600
h	-0.01771	-2.34672	3.29250
n	0.25309	-0.29315	3.91703
h	1.21115	-0.23910	4.23456
h	-0.30977	-0.51493	4.72833
c	0.49237	1.30859	-1.96121
h	1.06205	1.33890	-2.88969
h	0.05145	2.28888	-1.79602
c	1.36789	0.94322	-0.79946
c	2.33009	-0.06726	-0.90133
h	2.46467	-0.58432	-1.84337
c	3.13667	-0.39592	0.18587
h	3.88223	-1.17339	0.08759

c	2.99467	0.28867	1.39280
h	3.63768	0.04883	2.22972
c	2.03391	1.29212	1.50960
h	1.91695	1.82851	2.44136
c	1.22291	1.60906	0.42151
h	0.48031	2.39339	0.50471

GGF_10.xyz

o	-1.22591	4.22910	0.16959
c	-0.17734	3.42580	0.46890
o	0.74879	3.76919	1.16136
h	-1.04973	5.06816	0.62185
c	-0.37136	2.05192	-0.13553
h	-0.67942	2.17643	-1.17260
n	0.85680	1.31440	-0.14007
h	1.22572	0.95010	0.73531
c	1.36998	0.79876	-1.28381
o	0.95253	1.04473	-2.41081
c	2.51345	-0.17421	-1.02401
h	3.23377	0.26754	-0.33498
h	2.99551	-0.39091	-1.97148
n	2.01940	-1.40907	-0.44825
h	1.82578	-2.22423	-1.01439
c	1.70485	-1.52823	0.85328
o	1.81112	-0.61847	1.68073
c	1.22917	-2.91276	1.25624
h	0.42235	-2.76504	1.97658
h	2.05846	-3.37851	1.78897
n	0.87532	-3.72991	0.09950
h	0.94954	-4.71243	0.32326
h	-0.08939	-3.55295	-0.15658
c	-1.45372	1.31516	0.66843
h	-1.15353	1.30018	1.71932
h	-2.38151	1.88759	0.60679
c	-1.68951	-0.10033	0.20916
c	-1.99204	-1.08589	1.15400
h	-1.98609	-0.82887	2.20618
c	-2.31356	-2.38389	0.76090
h	-2.56553	-3.12591	1.50729
c	-2.31914	-2.71974	-0.59315
h	-2.58443	-3.72135	-0.90587
c	-1.98183	-1.75412	-1.54125
h	-1.96794	-2.00751	-2.59269
c	-1.67454	-0.45390	-1.14435
h	-1.41102	0.27642	-1.89741

GGF_11.xyz

o	-0.56432	3.55591	-0.95794
c	0.46913	2.99076	-0.33098
o	1.61544	3.26017	-0.60745
h	-1.41089	3.22499	-0.56711
c	0.07278	2.01678	0.78702
h	-0.51072	2.60455	1.50213
n	-0.79167	0.95926	0.29364
h	-0.39679	0.03651	0.17757
c	-2.09070	1.12797	0.01672
o	-2.65484	2.22906	0.04556

c	-2.85750	-0.13622	-0.32669
h	-3.53196	0.10437	-1.14481
h	-3.45265	-0.39591	0.54950
n	-2.03014	-1.26388	-0.66302
h	-1.72039	-1.44357	-1.60863
c	-1.72725	-2.23272	0.24133
o	-2.03394	-2.18134	1.42539
c	-0.98387	-3.41520	-0.36082
h	-1.73013	-4.19381	-0.52215
h	-0.30009	-3.77894	0.40672
n	-0.36331	-3.07762	-1.63852
h	0.54681	-2.65929	-1.47880
h	-0.20949	-3.91126	-2.18779
c	1.28188	1.40081	1.49623
h	2.04101	2.17664	1.57982
h	0.97279	1.11470	2.50143
c	1.84250	0.18780	0.80054
c	2.63077	0.29879	-0.35241
h	2.84537	1.28157	-0.74861
c	3.13683	-0.84076	-0.97333
h	3.75066	-0.73789	-1.85799
c	2.87572	-2.10738	-0.44862
h	3.29569	-2.98793	-0.91652
c	2.08928	-2.22906	0.69595
h	1.89921	-3.20324	1.12626
c	1.56490	-1.08889	1.30573
h	0.95454	-1.19012	2.19536

GGF_12.xyz

o	1.48858	-3.01289	-0.09219
c	0.93528	-1.83563	0.26748
o	1.58081	-0.83197	0.46489
h	2.44508	-2.85767	-0.12421
c	-0.57938	-1.94589	0.33747
h	-0.81079	-2.86598	0.87225
n	-1.12803	-0.83116	1.06247
h	-1.31632	0.02742	0.55455
c	-0.75982	-0.69197	2.37324
o	-0.26621	-1.60287	3.02410
c	-0.93638	0.71594	2.92184
h	-0.78039	0.68989	3.99535
h	-1.92517	1.10879	2.69352
n	0.04714	1.57872	2.29674
h	1.02409	1.51358	2.55386
c	-0.17491	2.09142	1.06842
o	-1.27589	2.07651	0.51261
c	1.04966	2.68401	0.39716
h	0.99977	3.76605	0.52227
h	0.93439	2.46992	-0.66826
n	2.28078	2.18345	1.00185
h	3.06429	2.76529	0.74063
h	2.46569	1.24771	0.65851
c	-1.15923	-2.02373	-1.08584
h	-0.81717	-2.95491	-1.53654
h	-2.24432	-2.07244	-0.99121
c	-0.75295	-0.85377	-1.93729
c	0.44341	-0.89157	-2.66327

h	1.04191	-1.79447	-2.65361
c	0.86330	0.21108	-3.40166
h	1.78666	0.16339	-3.96307
c	0.09015	1.37189	-3.42251
h	0.41447	2.22969	-3.99597
c	-1.10548	1.41851	-2.70990
h	-1.70845	2.31550	-2.71132
c	-1.52488	0.30982	-1.97805
h	-2.45791	0.35587	-1.43073

GGF_13.xyz

o	-4.22880	-1.30904	0.65471
c	-3.46651	-0.48877	0.20024
o	-3.88553	0.59168	-0.46460
h	-3.10664	1.14406	-0.72269
c	-1.95601	-0.59970	0.42034
h	-1.78344	-1.61655	0.76366
n	-1.16459	-0.44641	-0.79278
h	-0.54806	-1.21110	-1.06848
c	-0.96829	0.71424	-1.43481
o	-1.61795	1.74879	-1.21982
c	0.13173	0.67170	-2.48639
h	0.16143	1.64222	-2.97069
h	-0.11329	-0.09378	-3.22431
n	1.43057	0.37253	-1.92536
h	2.09835	1.09556	-1.69302
c	1.79184	-0.87248	-1.57312
o	1.06463	-1.86304	-1.69932
c	3.17210	-0.98399	-0.95763
h	3.65144	-1.85511	-1.40592
h	2.99993	-1.21791	0.09264
n	3.93958	0.25513	-1.06208
h	4.58641	0.21380	-1.83819
h	4.48805	0.40073	-0.22651
c	-1.53329	0.38025	1.53178
h	-1.83855	1.39035	1.26512
h	-2.08078	0.09352	2.43148
c	-0.05343	0.34596	1.78128
c	0.76241	1.40002	1.36056
h	0.31176	2.24312	0.85101
c	2.13356	1.38640	1.61406
h	2.74755	2.21914	1.29830
c	2.70712	0.30878	2.28662
h	3.76642	0.30601	2.50964
c	1.90620	-0.76007	2.69132
h	2.34399	-1.59773	3.21760
c	0.53694	-0.73973	2.43699
h	-0.08350	-1.56236	2.77257

GGF_14.xyz

o	-4.26934	-0.60313	-1.30318
c	-3.49169	-0.17338	-0.48379
o	-3.89032	0.46214	0.62136
h	-3.10115	0.69690	1.17024
c	-1.98513	-0.39392	-0.62941
h	-1.83554	-0.69674	-1.66228
n	-1.17916	0.80487	-0.44413

h	-0.53980	1.07694	-1.19276
c	-0.96245	1.39946	0.73770
o	-1.60328	1.15575	1.77118
c	0.14459	2.44425	0.71639
h	0.17193	2.91193	1.69490
h	-0.09434	3.19572	-0.03857
n	1.44467	1.87951	0.42337
h	2.15884	1.78420	1.13291
c	1.83024	1.55613	-0.82230
o	1.09422	1.62218	-1.81223
c	3.27907	1.12451	-0.94379
h	3.78741	1.92665	-1.47845
h	3.28925	0.24736	-1.59325
n	3.90977	0.92673	0.35791
h	4.90462	1.09312	0.30076
h	3.78092	-0.03274	0.65394
c	-1.55121	-1.54220	0.30030
h	-1.86974	-1.33066	1.31932
h	-2.07849	-2.43868	-0.03207
c	-0.06556	-1.76171	0.27364
c	0.58279	-2.14822	-0.90460
h	0.00882	-2.28529	-1.81316
c	1.95452	-2.38618	-0.91853
h	2.43669	-2.70305	-1.83362
c	2.69986	-2.24548	0.25311
h	3.75904	-2.46935	0.25127
c	2.06826	-1.83844	1.42790
h	2.63649	-1.73146	2.34294
c	0.69630	-1.58812	1.43170
h	0.20412	-1.27420	2.34384

GGF_15.xyz

o	3.83330	-1.49153	-1.00528
c	3.34616	-0.68752	-0.24719
o	4.06392	0.27954	0.33529
h	3.46761	0.82235	0.90393
c	1.86498	-0.69314	0.14503
h	1.82912	-0.75851	1.23656
n	1.21678	0.55577	-0.22151
h	0.56296	0.58913	-1.00232
c	1.31199	1.64638	0.55536
o	2.11501	1.74035	1.49343
c	0.34782	2.76745	0.20584
h	0.60003	3.15166	-0.78377
h	0.48092	3.55480	0.94053
n	-1.03414	2.34199	0.19635
h	-1.63809	2.46298	0.99795
c	-1.58320	1.70018	-0.85161
o	-0.95162	1.37875	-1.86218
c	-3.06677	1.42373	-0.70647
h	-3.27068	0.50920	-1.26364
h	-3.58640	2.24042	-1.20921
n	-3.46619	1.39403	0.69776
h	-4.46211	1.54458	0.78432
h	-3.27443	0.47278	1.07741
c	1.11867	-1.85875	-0.48109
h	1.20849	-1.79511	-1.56598

h	1.62563	-2.77807	-0.18695
c	-0.33090	-1.89762	-0.07552
c	-0.70015	-1.93578	1.27440
h	0.06395	-1.92366	2.04184
c	-2.03966	-2.00942	1.64838
h	-2.30368	-2.05045	2.69680
c	-3.03699	-2.05685	0.67254
h	-4.07660	-2.14306	0.95971
c	-2.68177	-2.01503	-0.67466
h	-3.44561	-2.06122	-1.43964
c	-1.33934	-1.92499	-1.04178
h	-1.07020	-1.88348	-2.08937