

Supplementary Information for
“Theoretical Calculation of the OH Vibrational
Overtone Spectra of 1-5 Pentanediol and 1-6
Hexanediol”

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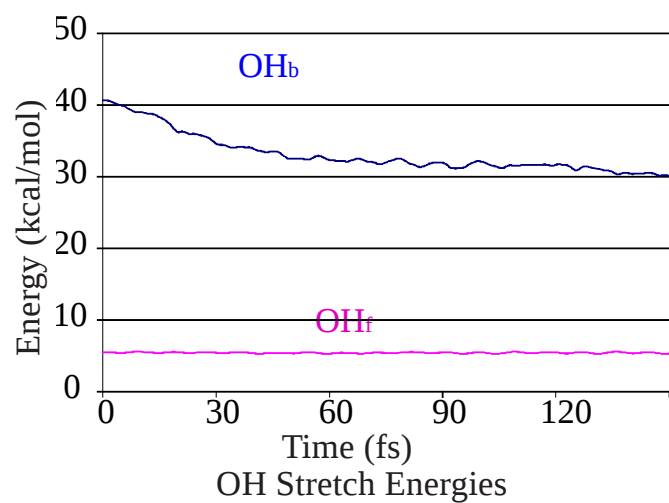
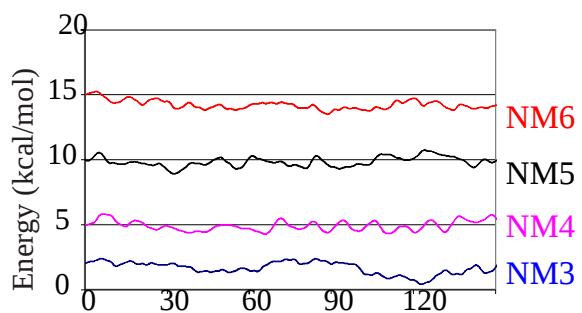
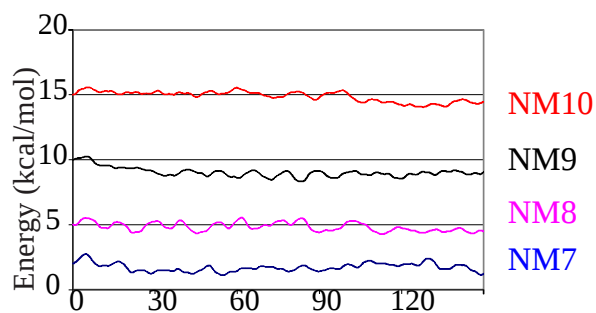


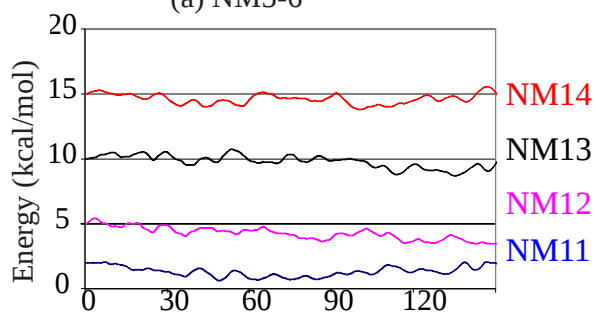
Figure S1: Time dependence of energy in the OH bonds calculated by the local mode model for the $\Delta\nu_{\text{OH}} = 4$ excitation for the OH_b in HD. NM1 is mainly OH_f stretching vibration and NM2 is mainly OH_b stretching vibration.



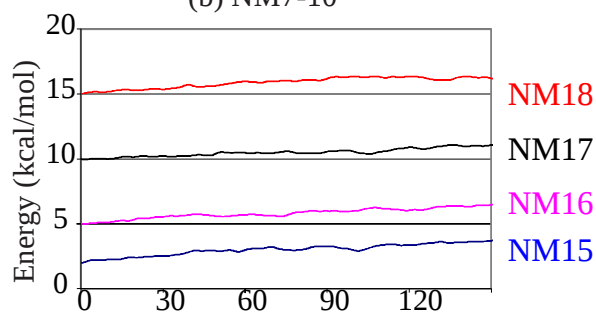
Time (fs)
(a) NM3-6



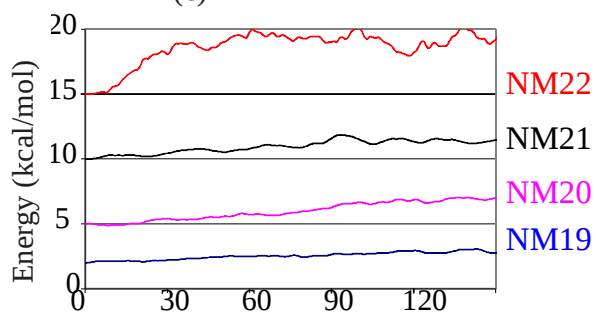
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(b) NM7-10



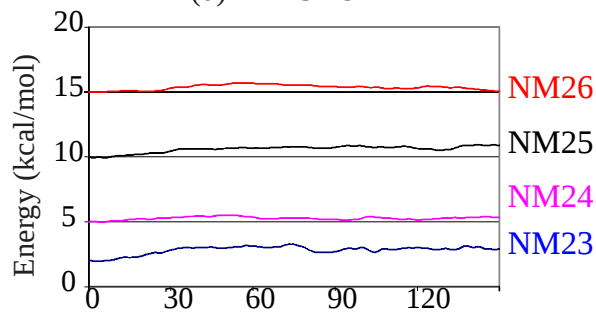
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(c) NM 11-14



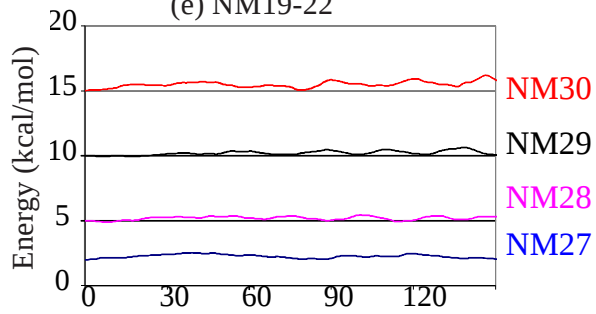
Time (fs)
(d) NM15-18



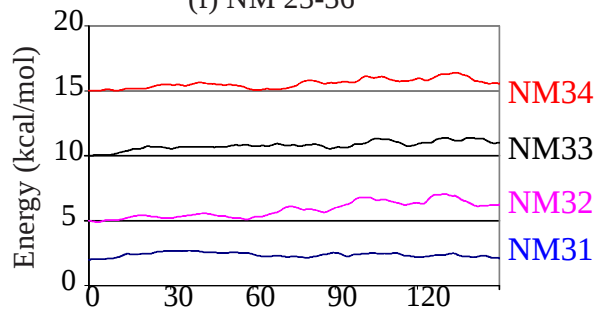
Time (fs)
(e) NM19-22



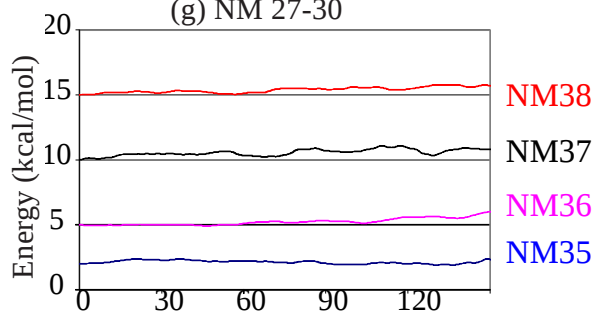
Time (fs)
(f) NM 23-36



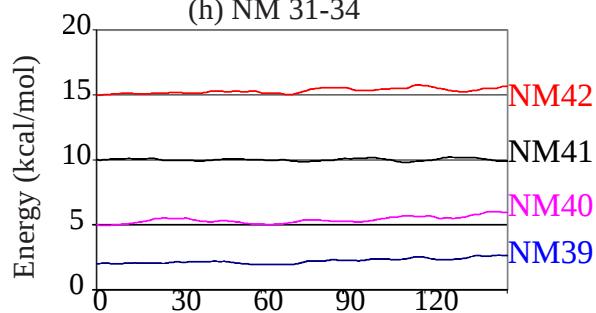
Time (fs)
(g) NM 27-30



Time (fs)
(h) NM 31-34



Time (fs)
(i) NM 35-38



Time (fs)
(j) NM 39-42

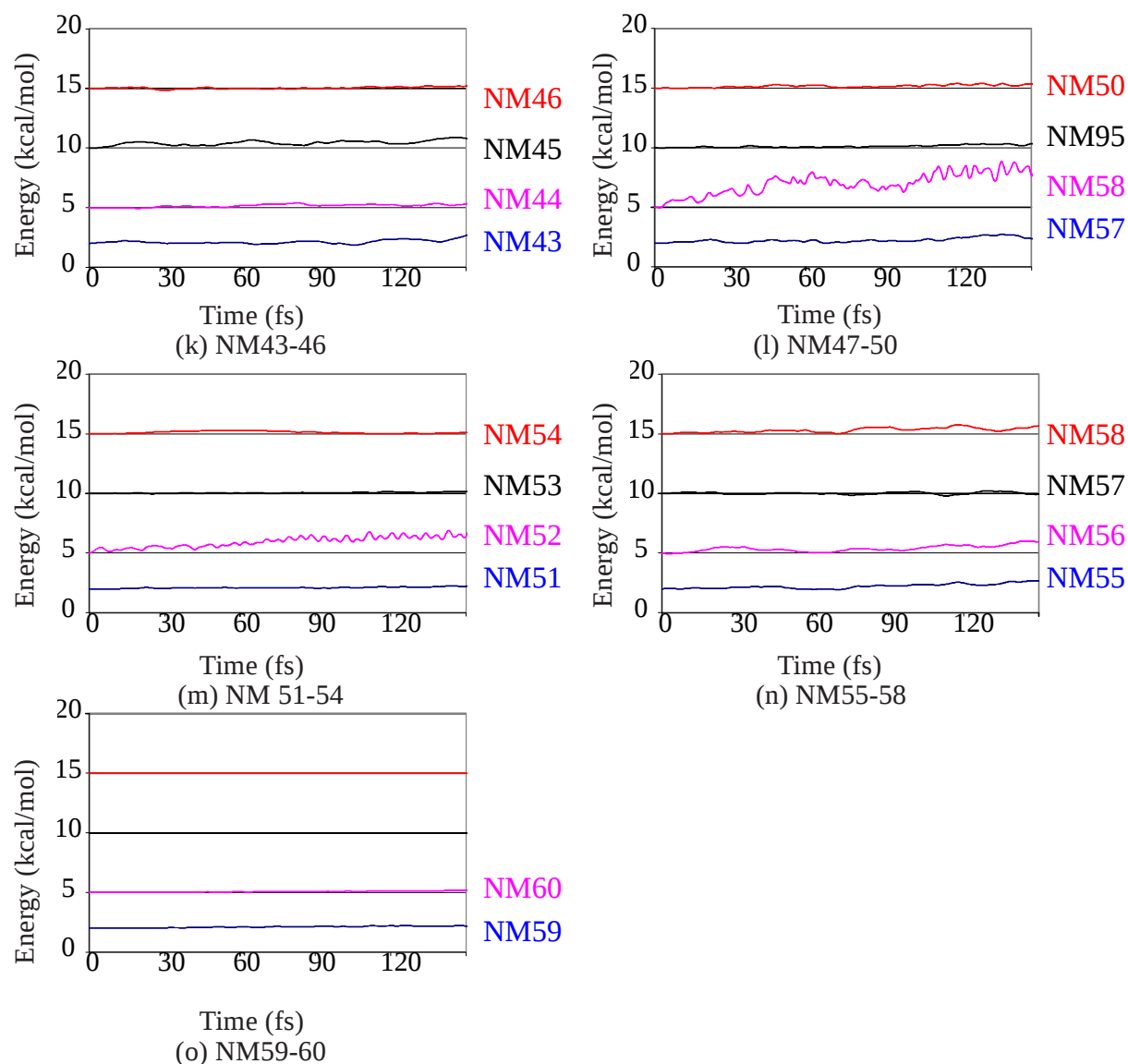


Figure S2: Time dependence of the energy in the 58 normal mode coordinates for the $\Delta\nu_{\text{OH}} = 4$ excitation for the OH_b in HD. Modes are numbered in decending order of frequency. Modes 3-14 mainly correspond to CH stretching vibrations, 15-36 mainly corresponds to CH and OH bend vibrations, 37-49 mainly corresponds to CH wag vibrations. 50-60 mainly corresponds to frame bending modes and OH torsion vibrations.

Table S1: Relative electronic energies in kcal/mol for the 109 low energy distinct conformers of 1-5 pentanediol calculated by MP2/6-311++G(3df,3pd), B3LYP/6-31+G(d,p), MP2/6-31+G(d,p), and B3LYP/6-311++G(3df,3pd). “63” stands for 6-31+G(d,p) and “a63” stands for 6-311++G(3df,3pd).

name	DE MP2/a63	DE B3LYP/63	DE MP2/63	DE B3LYP/a63
tG+G-G+G+g-	0.00	0.00	0.00	0.14
g+G+G-G-G+t	0.43	0.28	0.43	0.51
g+G+G+G-G+g-	0.62	0.58	0.78	0.72
tG-TTG-t	1.35	0.37	1.46	0.00
tG+TTG+g-	1.52	0.53	1.73	0.15
tG+TG-G-t	1.54	1.27	1.84	0.82
tG-TTG+g-	1.55	0.57	1.83	0.16
tG+TG+G+g-	1.57	1.15	1.98	0.77
tG+TG-G-g-	1.65	1.21	1.96	0.77
tTTTG-t	1.68	0.45	1.94	0.04
tG-TTTg-	1.68	0.36	1.83	0.00
tG-TTG-g-	1.69	0.63	1.90	0.22
tTTG-G-t	1.73	1.16	2.11	0.70
tG-G-G-G-g-	1.73	2.18	2.33	1.69
tG-G-TG+g-	1.75	1.39	2.16	0.92
tG+TTTg-	1.78	0.48	1.96	0.10
tG+G+TTg-	1.79	1.19	2.10	0.76
tG+TTG-t	1.80	0.87	2.05	0.42
g-G+TTG-g-	1.80	0.72	2.15	0.28
tG+G+TG+g-	1.81	1.40	2.19	0.94
tG+G+TG-g-	1.85	1.47	2.20	1.00
tG+TTG-g-	1.86	0.79	2.11	0.36
tG-G-TTg-	1.88	1.23	2.23	0.78
g+G+TTG+g-	1.89	0.80	2.21	0.36
tTTTG-g-	1.94	0.61	2.28	0.17
tG+G-G-G-t	1.94	2.22	2.16	1.92
g-G-TG-G-g-	1.96	1.48	2.26	1.05
g-G-TG+G+g+	1.97	1.44	2.35	0.97
tG-G-TG-g-	2.01	1.67	2.28	1.22
g+TTG-G-g-	2.02	1.26	2.37	0.81
tG+G+G+Tg-	2.09	2.05	2.62	1.62
g-TTTG-g-	2.09	0.69	2.37	0.27
g+TTTG-g-	2.09	0.69	2.37	0.27
g-G+TG-G-g-	2.09	1.59	2.57	1.07
g+G+TTG+g+	2.09	0.96	2.44	0.48
t+G-TG+G+g-	2.11	1.71	2.64	1.25
tTTG-G-g-	2.14	1.40	2.59	0.89

tTTTG+g-	2.14	0.89	2.58	0.41
tG-TG-G-t	2.16	1.80	2.55	1.27
tG+G-G-G-g-	2.17	2.31	2.45	1.99
g+G-TG-G-g+	2.18	1.84	2.80	1.35
tTTTTg-	2.19	0.63	2.53	0.21
g+G-TTG-g+	2.20	1.17	2.63	0.67
g+TTTG+g-	2.21	0.87	2.55	0.43
tTG-G-G-t	2.22	2.26	2.85	1.77
tTG-TG-t	2.24	1.40	2.59	0.96
tG+TG+Tg-	2.25	1.33	2.52	0.94
g-G-TTG+g+	2.26	1.12	2.64	0.63
g+TTTG-g+	2.27	0.94	2.64	0.48
tG-TG+Tg-	2.28	1.35	2.58	0.95
g+TTTTg+	2.29	0.64	2.54	0.24
g-TTG-G-g-	2.29	1.49	2.72	0.99
g+G+TG+G+g-	2.32	1.85	2.97	1.33
tG-TG-G-g-	2.33	1.93	2.73	1.38
g+TTTTg-	2.35	0.71	2.61	0.30
g+G-TTG+g-	2.35	1.33	2.84	0.81
tTG+TG-t	2.37	1.55	2.75	1.09
g+G+G+TG+g-	2.37	1.82	2.86	1.28
tTTG+G+g-	2.38	1.75	2.99	1.24
tG+TG-Tg-	2.41	1.45	2.69	1.06
tG-G-G-Tg-	2.42	2.40	2.97	1.94
tG-TG-Tg-	2.47	1.53	2.74	1.13
g-G+G+TG-g-	2.47	1.96	3.06	1.45
g+TG-G-G-g-	2.53	2.31	3.14	1.84
g-TG+TG-g-	2.53	1.50	2.87	1.08
g+TTG+G+g-	2.55	1.82	3.15	1.33
tG-TG+G-t	2.56	1.78	2.64	1.46
tTTG-Tt	2.58	1.53	3.03	1.06
tG+G-TG-g-	2.58	1.71	2.59	1.42
tTG+TG-g-	2.59	1.66	3.01	1.18
tTG+TG+g-	2.59	1.74	3.05	1.26
tG+G-G-Tg-	2.61	2.35	2.88	2.09
g+G-TG+G+g-	2.62	2.18	3.33	1.62
tG-TG+G-g-	2.62	1.79	2.83	1.46
tTG-G-G-g-	2.62	2.51	3.30	1.98
g+TG-TG-g-	2.63	1.59	2.99	1.15

tG+TG+G-t	2.66	1.91	2.72	1.58
tTG-TTg-	2.66	1.53	3.08	1.08
g+TTG-G-g+	2.67	1.96	3.30	1.44
tG-G+TG-g-	2.70	1.80	2.78	1.49
tTG-TG-g-	2.71	1.77	3.18	1.27
tTTG+Tg-	2.71	1.58	3.14	1.13
g+TG-TG-g+	2.76	1.83	3.18	1.37
tTTG-Tg-	2.76	1.57	3.15	1.15
tTG-TG+g-	2.76	1.90	3.31	1.37
g+TG+TG-g-	2.77	1.72	3.12	1.29
g+TTG+Tg-	2.78	1.56	3.16	1.14
tTG+TTg-	2.79	1.69	3.25	1.21
g+TTG-Tg+	2.83	1.62	3.24	1.19
g+TG-TG+g-	2.84	1.88	3.35	1.39
g-G-TG-G+g+	2.85	1.90	3.03	1.57
g-TG-TG-g-	2.86	1.80	3.23	1.36
g+TG+TG+g-	2.89	1.91	3.30	1.46
tTG+G+Tg-	2.90	2.43	3.50	1.98
tG-G+TTg-	2.92	1.80	3.03	1.49
g+TTG-Tg-	2.93	1.70	3.31	1.27
g+G+TG-G+g+	2.95	2.04	3.20	1.67
g+TTG+Tg+	2.95	1.70	3.33	1.27
t+G+TG+G-g-	2.97	2.25	3.22	1.85
tG+G-TG+g-	3.01	2.19	3.22	1.82
g-TTG+G-g-	3.04	1.88	3.31	1.54
tG-G+TG+g-	3.09	2.30	3.30	1.93
tG+G-TTg-	3.11	1.99	3.24	1.66
g+G+G-TG+g-	3.18	2.31	3.56	1.89
tG-TG-G+g-	3.26	2.61	3.71	2.21
tTTG+G-t	3.32	2.33	3.61	1.90
tTTG+G-g-	3.39	2.30	3.79	1.87
g-G+TG+G-g-	3.45	2.67	3.87	2.22
g+TTG+G-g-	3.47	2.35	3.82	1.94

Table S2: Relative electronic energies in kcal/mol and relative population at 313 K for the 381 distinct conformers of 1-6 hexanediol calculated by MP2/6-31+G(d,p), B3LYP/6-31+G(d,p).

Name	DE MP2	POP MP2	DE B3LYP	POP B3LYP
g-G+G+TG+G+t	0.00	0.47	0.30	0.02
g+G-G-TG-G-g-	0.45	0.75	0.54	0.03
tG+G-TG-G-g+	0.67	0.45	0.55	0.03
g+G+G+TG+G-g+	1.13	0.07	0.71	0.01
tG+G-G-G+G-g+	1.15	0.20	0.74	0.02
g+G+G-TG-G-g+	1.22	0.19	0.79	0.02
tG-G+G+G-G-g+	1.43	0.19	0.79	0.03
tG-TG-G-G+g-	1.48	0.48	1.22	0.04
tG-G+G-G-G+g+	1.57	0.10	1.21	0.01
tG-G+G+TG+C+	1.58	0.22	1.41	0.02
g-G+TG+G+G-g-	1.80	0.17	1.49	0.01
tG+TTTG-t	1.82	2.20	0.02	2.42
g+G+TG+G+G-g+	1.97	0.12	1.54	0.01
tG-TTTG-t	2.01	1.78	0.20	2.00
tG-TTG-G-t	2.09	2.14	0.86	0.94
tG+TTTG-g+	2.17	2.57	0.23	3.57
tG+TTTG+g+	2.18	2.04	0.20	2.99
tG-TTTG+g+	2.19	2.21	0.21	3.24
tG-TTTTg+	2.19	1.81	0.00	3.74
tG+TTG+G+g+	2.25	1.35	0.83	0.80
tG-TTTG-g+	2.28	1.52	0.30	2.22
tG+TTG-G-t	2.28	1.66	0.91	0.92
tG+TTTTg+	2.29	1.78	0.10	3.70
tG-G-TTG+g+	2.32	1.22	0.88	0.74
tG-TTTTt	2.35	1.01	0.13	2.19
tG-TG-G-G-t	2.36	1.11	1.69	0.20
tG+G+TTG+g+	2.39	1.27	0.96	0.77
tG+G+G-G-G+g+	2.41	0.02	2.13	0.00
tG+G+TTTg+	2.49	1.58	0.87	1.34
tG-G-TTG-g+	2.50	0.92	1.09	0.53
tG-TG-TG-t	2.51	0.66	1.05	0.42
tG+TTG-G-g+	2.52	0.88	1.03	0.59
g+G+TTTG-g-	2.54	0.70	0.39	1.36
tG-TG+TG-t	2.55	0.61	1.07	0.40
tG-G-TTTg+	2.59	1.39	0.93	1.23
tG-G-G-TG-g+	2.60	0.58	1.85	0.11
g+G-G-G+G+G-g-	2.61	0.03	1.90	0.01
tG+G+TG-G-T+	2.63	1.10	1.71	0.30

tG+TG-TG-t	2.64	1.11	1.13	0.77
tG-G-TG-G-t	2.66	0.70	1.70	0.20
tG+G+TTG-g+	2.67	0.75	1.20	0.48
g+G+TTTG-g+	2.67	0.51	0.53	0.97
tTTTG-G-t	2.70	1.59	1.03	1.45
g+G-TTTG-g-	2.70	0.39	0.54	0.76
g+G+G-G-G+G-g-	2.70	0.02	2.06	0.00
g+G+TTTTg+	2.71	0.39	0.32	1.11
tG-TG-TG+g+	2.73	0.61	1.08	0.51
g+G-TTG-G-g-	2.73	0.56	1.16	0.42
tG-TG+TTt	2.73	0.42	0.92	0.47
g+G+TTG-G-g-	2.75	0.68	1.07	0.62
tG-TTG+G+g+	2.75	0.78	1.17	0.61
tG+TG-TG-g+	2.76	0.63	1.14	0.51
g+TTTG+G+g+	2.76	0.65	0.92	0.75
tTTTTt	2.77	0.17	0.16	1.40
tTG+TTG-t	2.79	0.73	0.95	0.85
tTTTTG+g+	2.79	0.85	0.38	2.52
tG-TG-TG-g+	2.79	0.54	1.22	0.41
tTTTTTg+	2.80	0.68	0.17	2.80
tG+TG-G-G-t	2.80	0.72	1.97	0.17
tG-TG+TTg+	2.81	0.60	0.95	0.73
g-G+TTTG+g-	2.82	0.41	0.68	0.78
tG+TTG-Tg+	2.83	0.63	0.94	0.79
tG+TG-TTg+	2.84	0.59	0.99	0.69
tG+TG-TG+g+	2.84	0.66	1.21	0.55
g+G-TTTTg-	2.84	0.49	0.48	1.36
tG+G+G+TTg+	2.85	0.59	1.74	0.21
tG-TG+TG-g+	2.85	0.61	1.18	0.55
tTTG-G-G-t	2.86	0.59	1.78	0.20
tG+TG+TG+g+	2.86	0.81	1.21	0.71
tG-TTG-Tg+	2.87	0.64	0.98	0.81
tG+TG+G+G+g+	2.87	0.33	1.94	0.09
tG-TG-G-G-g+	2.88	0.57	2.02	0.14
tTTTG+G+g+	2.88	0.91	1.06	1.05
tG+TTG+Tg+	2.89	0.55	0.99	0.70
g+TTTG-G-g-	2.91	0.75	1.08	0.88
tTG-G-TG-t	2.91	0.62	1.84	0.21
tG-TG+G+G+g+	2.91	0.18	1.94	0.05

tG-G-TG+G+g+	2.92	0.38	1.81	0.14
g+G-TG-G-G-g-	2.94	0.37	2.00	0.10
tG-TG-TTt	2.95	0.35	1.15	0.38
g+G+G+TTG-g+	2.95	0.47	1.35	0.38
tG-TTG+Tg+	2.96	0.62	1.04	0.83
tG-TG-TTg+	2.96	0.60	1.10	0.74
tTG-TTG-t	2.96	0.68	1.13	0.79
tTG-TG-G-t	2.97	0.61	1.77	0.26
tG-G+TTG-g+	2.97	0.35	1.33	0.29
tG-G-G-G-G-t	2.98	0.11	2.71	0.01
tG-TG+TG+g+	2.98	0.55	1.31	0.49
tG+G+G+TG-g+	3.02	0.32	2.02	0.09
C-G-TG-G+G-t	3.02	0.02	2.59	0.00
tG+TG+TG-g+	3.02	0.17	1.31	0.16
tG-TG+G+G-t	3.03	0.40	2.28	0.08
tG-G-G-TG+g+	3.03	0.21	2.05	0.06
tG+G-G-TTg+	3.04	0.31	2.01	0.10
tG-G-TG-Tg+	3.04	0.46	1.80	0.21
tG-G-G-TTg+	3.04	0.37	1.88	0.14
tTTG-TG+g+	3.06	0.42	1.10	0.60
tTTG+G+G+g+	3.07	0.33	1.82	0.15
g+G-G+G-G-G+g-	3.07	0.01	2.34	0.00
g+G+TG-TG-g+	3.08	0.32	1.33	0.32
tG+G+TG+G+g+	3.09	0.76	1.93	0.30
tG+G+G+TG+g+	3.09	0.23	2.12	0.07
tG+TG-G-Tg+	3.09	0.27	1.76	0.14
tG+TG-G-G-g+	3.10	0.39	2.12	0.11
tG+G+TG+Tg+	3.11	0.24	1.83	0.12
g+G+G+TG-G-g-	3.15	0.40	1.83	0.21
g+G+TTG-G-g+	3.15	0.18	1.44	0.18
tG+G-TTG-g+	3.16	0.18	1.49	0.16
tTTG-TTg+	3.20	0.41	1.03	0.83
g+G-TG-TG-g-	3.21	0.22	1.59	0.18
g+G-TG-TG-g-	3.21	0.26	1.43	0.27
tG+G+G+G+G+g+	3.21	0.21	2.85	0.02
tG+G-G-TG+g+	3.22	0.24	2.33	0.06
tG+TG+G+Tg+	3.22	0.41	1.95	0.19
tTG+G+TG-t	3.22	0.13	1.92	0.06
g+G+TG-TG-g-	3.23	0.37	1.41	0.42

g+G-G-TTG-g-	3.23	0.13	1.48	0.14
g-G-G-G-TG+g-	3.24	0.28	2.14	0.10
g+G+TG-TTg+	3.24	0.13	1.22	0.21
g-G+G+TG-G-t	3.25	0.18	2.09	0.07
g+TTG-G-G-g-	3.26	0.24	1.95	0.12
g+G-TG+TG-g-	3.27	0.28	1.43	0.33
tTTG-TTt	3.27	0.24	1.12	0.47
tG-G+G+TG-g+	3.27	0.19	2.34	0.05
g+G+TG-G-G-g-	3.28	0.17	2.15	0.06
g+G+G+TG+Tg-	3.28	0.14	1.86	0.08
tTG-G-G-G-t	3.29	0.15	2.65	0.02
tTG+TG+G+g+	3.30	0.35	1.86	0.22
tTG+TTG+g+	3.31	0.38	1.30	0.58
tTTG+TG-g+	3.31	0.31	1.28	0.49
g+TG-TTG+g+	3.32	0.30	1.24	0.51
g-G+G+G+G+G+t	3.33	0.14	2.91	0.02
tTTG+TTg+	3.33	0.36	1.13	0.75
tTTG-TG-g+	3.33	0.31	1.38	0.44
g+G-TG-TTg-	3.34	0.15	1.36	0.22
g+TG+TTG-g-	3.35	0.33	1.25	0.60
g-G+TG+TG+g-	3.35	0.13	1.64	0.12
g+G+TG+TG+g+	3.35	0.12	1.51	0.14
g+G+G+G+G+G+g+	3.36	0.14	2.83	0.02
tG+TTG+G-t	3.37	0.33	1.78	0.26
tTTTG-Tg+	3.38	0.35	1.08	0.88
g+G-TG-TTg+	3.39	0.12	1.38	0.18
tG-TG+G+Tg+	3.41	0.17	2.05	0.09
tTTTG-G-g+	3.41	0.32	1.40	0.49
tG+G-TTTg+	3.41	0.31	1.48	0.43
tG-G+TTTg+	3.42	0.32	1.49	0.43
g-TG-TG+G+t	3.42	0.10	1.91	0.07
g+G+TG+TG-g+	3.42	0.14	1.55	0.17
g+G-TG+TG+g+	3.42	0.29	1.55	0.36
g+TG-G-TG-g-	3.42	0.23	2.04	0.13
tG+G-G-G-G-t	3.43	0.17	3.28	0.01
tG+G+TG-Tg+	3.43	0.21	1.93	0.14
tTG-TTTg+	3.44	0.30	1.17	0.71
g+TTTG-Tg+	3.45	0.24	1.14	0.60
g+G-TG+TTg-	3.45	0.10	1.38	0.17

tG-G+G+TTg+	3.46	0.18	2.30	0.07
g-G+TTG+G+g-	3.46	0.10	1.68	0.11
tTG-TTG-g+	3.46	0.28	1.41	0.46
tG-G+G+G+G+g+	3.47	0.16	3.16	0.02
g+TTTG-G-g+	3.47	0.25	1.45	0.39
tTG+G+TG+g+	3.47	0.23	2.08	0.13
g+G-TTG+G-g-	3.48	0.14	1.67	0.15
tTTTG-Tt	3.48	0.39	1.20	0.92
tTG+TG-G-t	3.49	0.22	2.00	0.15
g+TG+TG+G+g+	3.49	0.12	2.02	0.08
tTG+TTTg+	3.49	0.29	1.22	0.68
tTTTG+G-t	3.49	0.35	1.55	0.49
g-G+TG-TG+g-	3.49	0.05	1.60	0.13
tTG-G-TG+g+	3.49	0.14	2.04	0.09
g+G-G-G-TG-g-	3.50	0.18	2.40	0.06
g+G+TG-G-G-g+	3.50	0.09	2.34	0.04
tG-TTG+G-g+	3.52	0.08	1.84	0.07
g+TG-G-G-G-g-	3.54	0.05	2.70	0.01
tTTG+G+G-t	3.55	0.23	2.39	0.09
tTTTG+Tg+	3.57	0.27	1.24	0.70
tG+TG+G-G-t	3.57	0.07	3.07	0.01
tTTG-G-G-g+	3.61	0.16	2.24	0.09
g+TTTG-Tg-	3.61	0.21	1.28	0.54
tTG+G+G+G+g+	3.63	0.09	2.81	0.02
g+G+G-TTG-g+	3.63	0.18	1.80	0.20
g+G+G+TG-G-g+	3.65	0.20	2.26	0.11
tTG+G+TTg+	3.68	0.22	2.08	0.18
tG-G+TG+G+g+	3.68	0.15	2.59	0.05
tTTG+G+Tg+	3.69	0.10	2.08	0.08
g+G-G-G-G-G-g-	3.69	0.10	3.13	0.02
g+G+G+TG-Tg+	3.70	0.09	2.02	0.08
tTG-G-TTg+	3.70	0.24	2.08	0.20
tG-G+TTG+g+	3.71	0.16	1.94	0.17
tTTG-G-Tg+	3.71	0.24	2.07	0.21
tTTG-G-Tt	3.72	0.26	2.14	0.20
g-G+TG+G+G+g-	3.73	0.13	2.60	0.05
g+TTTG+G-g-	3.75	0.21	1.63	0.39
g+G+TTG+G-g-	3.77	0.14	1.81	0.19
g+TG-G-TG+g-	3.78	0.04	2.21	0.03

g+TTG-G-G-g+	3.79	0.13	2.35	0.08
g+TG+G+TG-g-	3.80	0.08	2.27	0.05
tTG+G+TG-g+	3.81	0.09	2.27	0.06
g+TG+TG-G-g-	3.81	0.11	2.06	0.11
tTTG-G-G+g+	3.81	0.09	2.46	0.05
tG+G-TG-G-t	3.81	0.14	2.87	0.04
tG+TTG+G-g+	3.82	0.05	2.18	0.04
tG+TG-G-G+g+	3.83	0.11	2.78	0.04
tG+G+TG+G-g+	3.84	0.09	2.68	0.03
tTTTG-G+g+	3.84	0.10	1.72	0.18
g+TTTG-G+g+	3.85	0.09	1.73	0.17
g+TTG+G+Tg+	3.86	0.16	2.17	0.15
tG-G+TG-G-t	3.86	0.11	2.71	0.04
tG+G-TG+G+g+	3.87	0.11	2.56	0.05
tTG-TG+G+g+	3.87	0.16	2.17	0.15
g+G+TG+G-G-g-	3.88	0.05	3.20	0.01
g+TG+G+TG+g+	3.89	0.13	2.43	0.08
g+TG+G+G+G+g+	3.91	0.06	3.01	0.01
tG+G-TTG+g+	3.92	0.19	2.14	0.20
g+TTG+G+G-g-	3.94	0.07	2.52	0.04
g+TG-TG-Tg+	3.95	0.04	1.98	0.06
tG+G-TG-Tg+	3.95	0.10	2.36	0.08
tG+G-G-G-Tg+	3.96	0.08	3.22	0.02
tG+G+TG-G+g+	3.98	0.13	2.62	0.07
tG-G+G+G+Tg+	3.98	0.05	3.28	0.01
g+G-G+G+G-G-g-	3.98	0.00	2.98	0.00
g+TTG-G-Tg-	3.99	0.14	2.31	0.12
tG+TG+G+G-t	4.00	0.08	3.31	0.02
tTG-TG-Tg+	4.01	0.10	2.07	0.14
tTG-TG-Tg+	4.01	0.05	2.07	0.07
tTG-TG-G-g+	4.01	0.10	2.43	0.08
tG-G+G+G+G-t	4.02	0.05	3.75	0.00
tTG-TG-Tt	4.02	0.13	2.13	0.17
g+TG+G+TG-g+	4.03	0.05	2.44	0.04
g+G-TG+G+G-g-	4.03	0.03	2.81	0.01
tTG-G-G-Tt	4.05	0.02	2.93	0.02
g+TG-TG-G-g+	4.06	0.07	2.41	0.06
tG+TTG-G+g+	4.06	0.15	2.22	0.17
g-TG-TG-Tt	4.08	0.05	2.15	0.06

g-G+G+G+G+Tt	4.10	0.05	3.19	0.01
g+G-G+TTG-g-	4.11	0.07	2.24	0.09
tG+TG-G+G+g+	4.12	0.02	3.32	0.01
g+G+G-TG-G-g-	4.13	0.03	2.93	0.01
tG-G+TG+Tg+	4.14	0.08	2.53	0.06
g-TG-G-G-Tt	4.15	0.02	2.96	0.01
tG+G+G-G-G-t	4.16	0.05	3.87	0.00
g+TG-G-G-G-g+	4.17	0.04	3.20	0.01
tTG-G-G-Tg+	4.18	0.02	2.98	0.01
g+G+TG-G-G+g+	4.19	0.03	2.99	0.01
tG-G+TG-G-g+	4.19	0.08	2.76	0.05
tTG+TG+G-t	4.21	0.08	2.62	0.06
g-G+G+TG-Tt	4.21	0.04	2.43	0.04
g+TG+TG+Tg+	4.24	0.07	2.24	0.11
g-G+G+G+G+G+g-	4.25	0.04	3.53	0.01
tTG+G+G+G-t	4.26	0.07	3.53	0.01
tTG+TG-Tt	4.28	0.12	2.24	0.19
tG+G+G-TG-g+	4.29	0.04	3.42	0.01
tTG+TG-Tg+	4.30	0.09	2.21	0.16
tG-G-G-G-G+g+	4.30	0.04	3.76	0.01
tG+G-G-G-G+g+	4.32	0.02	3.91	0.00
tG-G-G+TG+g+	4.34	0.04	3.56	0.01
tG-TG+G-G-t	4.34	0.06	3.54	0.01
g+G+TTG+G-g+	4.34	0.04	2.49	0.05
tG+G+G+G+G+g+	4.35	0.03	3.84	0.00
tG-G+TG+G-t	4.37	0.05	3.12	0.02
g+G+G-G-G-G-g-	4.37	0.04	3.69	0.01
g+TTG-G+G+g+	4.38	0.02	3.27	0.01
tG+G-TG+Tg+	4.39	0.08	2.68	0.07
g+G-G-TG+Tg+	4.39	0.03	2.55	0.03
tTG-TG+G-t	4.42	0.10	2.72	0.09
tG-G-G+TTg+	4.42	0.03	3.24	0.01
g-TG-TG+Tt	4.43	0.04	2.33	0.07
g+TG+TG-Tg+	4.44	0.06	2.29	0.12
g+G+G+G-G-G-g-	4.45	0.01	3.81	0.00
tTG-TG-G+g+	4.46	0.04	2.65	0.05
tG+G+G-TG+g+	4.50	0.02	3.52	0.01
tG+G+G-G-Tg+	4.50	0.02	3.88	0.00
tG+TG+G-G-g+	4.51	0.02	3.49	0.01

g+TG+G+G-G-g-	4.53	0.02	3.73	0.00
tG-G-G+G+G+g+	4.55	0.02	3.99	0.00
g+TG+TG-Tg-	4.55	0.05	2.39	0.11
tTG-G-G+G+g+	4.55	0.01	3.92	0.00
tTTTG+G-g+	4.57	0.03	2.40	0.05
tG-TG+G-Tg+	4.59	0.01	3.08	0.01
tG+G-TG+G-t	4.61	0.04	3.20	0.02
g+G-G+G+TG-g-	4.61	0.02	3.23	0.01
tTG+G-TG-t	4.63	0.03	3.30	0.01
tTG-G-G-G+g+	4.64	0.04	3.63	0.01
tG-G-G+G+Tg+	4.64	0.02	3.91	0.00
g+G-G-TG+G-g-	4.64	0.05	3.02	0.04
g-G+G+TG+G+g-	4.66	0.04	3.08	0.03
tTG-G+TG-t	4.67	0.03	3.21	0.02
g+TTTG+G-g+	4.70	0.04	2.52	0.07
g+G+G+G+G+G-g+	4.70	0.02	4.00	0.00
tG-TG+G-G-g+	4.70	0.02	3.57	0.01
tG+G+G-G-G-g+	4.71	0.02	4.27	0.00
tG-TG-G+Tg+	4.73	0.03	3.26	0.02
g+G+G-G-G-G-g+	4.75	0.02	3.95	0.00
tTTG+G-G-t	4.75	0.01	3.24	0.01
tG+TG+G-Tg+	4.77	0.02	3.29	0.01
g-G-G+TG-G+t	4.84	0.02	3.26	0.02
tTG+TG-G+g+	4.85	0.03	2.93	0.04
C+G+TG+G-Tg+	4.85	0.02	3.39	0.02
g+G+TG-G+G+g+	4.88	0.02	3.40	0.01
g+TTG+G-G-g-	4.91	0.01	3.24	0.01
g+TG-G+TG-g-	4.95	0.02	3.29	0.01
g+G+TG+G-G-g+	4.97	0.01	3.82	0.00
g+G-G+TG-G-g-	4.98	0.01	3.36	0.01
tTTG+G-Tt	5.01	0.02	3.22	0.02
g+TTG-G+G-g-	5.01	0.01	3.63	0.00
tG+TG-G+G-t	5.02	0.01	3.92	0.00
tTTG-G+G+g+	5.02	0.02	3.41	0.01
tG+G-G+TTg+	5.03	0.01	3.85	0.00
tG+G+G-TTg+	5.03	0.02	3.46	0.02
tTTG-G+G-t	5.04	0.01	3.87	0.00
g+G+G+G-G-G-g+	5.04	0.01	4.46	0.00
tG-G+G-TTg+	5.05	0.03	3.76	0.02

tTG+G-TTg+	5.06	0.01	3.27	0.01
tTG+G-TG+g+	5.07	0.02	3.45	0.01
tG-G-G+TG-g+	5.09	0.01	3.65	0.00
tG+G-G+TG-g+	5.10	0.02	4.04	0.01
tG+G+G+G-Tg+	5.11	0.01	4.14	0.00
tTG-G+TG+g+	5.12	0.02	3.56	0.01
g+G+G-TG+G-G-	5.12	0.02	3.33	0.02
tTTG+G-G-g+	5.13	0.01	3.61	0.00
tG+TG-G+Tg+	5.14	0.02	3.45	0.02
tTG+TG+G-g+	5.14	0.01	3.34	0.01
tTTG-G+Tg+	5.15	0.01	3.30	0.02
g+G-G-G+TG-g-	5.18	0.01	3.85	0.00
g+TG-TG-G+g-	5.18	0.01	3.33	0.01
tTG-G+TG-g+	5.19	0.01	3.53	0.01
g+TG+G-TG+g+	5.20	0.01	3.49	0.01
tTTG+G-Tg+	5.21	0.01	3.34	0.01
g+G-G-TG-G+g-	5.23	0.01	3.77	0.01
g-G+G-TG-G+t	5.24	0.01	3.73	0.01
g+TTG+G+G-g+	5.24	0.01	3.56	0.01
g+TG-G+TG-g+	5.25	0.00	3.53	0.00
g+TTG+G-Tg-	5.26	0.01	3.34	0.01
tG-G-G-G+Tg+	5.28	0.01	4.26	0.00
tG-G+G+G+G-g+	5.28	0.00	4.61	0.00
g+G-TG+G-G-g-	5.29	0.01	3.73	0.01
g+TTG+G-Tg+	5.30	0.01	3.37	0.01
tG-G+G-TG+g+	5.31	0.00	4.04	0.00
g+G+G-G-G-G+g+	5.32	0.01	4.52	0.00
g+G+TG-G+G-g-	5.33	0.01	3.95	0.00
g-G+G-TG+G-t	5.35	0.01	3.82	0.00
g+TTG+G-G-g+	5.38	0.01	3.79	0.00
g+TG-G+G+G+g+	5.39	0.00	4.25	0.00
tTG-G+TTg+	5.40	0.02	3.42	0.03
g-G+G+TG-G+g-	5.47	0.01	3.77	0.01
g+TG+G-TG+g-	5.47	0.01	3.71	0.01
g-G-G+G-TG+g-	5.47	0.01	4.20	0.00
tTG+G-G-Tg+	5.49	0.01	4.18	0.00
tG+G+G+G-G-g+	5.52	0.01	4.62	0.00
tTG-G+G+G+g+	5.53	0.01	4.42	0.00
g+TG-TG+G-g+	5.54	0.01	3.55	0.01

tG+TG+G-G+g+	5.54	0.01	4.13	0.00
g+G+G-TG-G+g-	5.62	0.01	3.91	0.01
g+G-G+TG+G-g-	5.62	0.00	3.91	0.00
g+TG+G-G-G-g-	5.65	0.00	4.46	0.00
tTG+G-G-Tt	5.66	0.01	4.35	0.00
g+TG+TG-G+g-	5.69	0.01	3.68	0.01
tTG-G-G+Tg+	5.69	0.00	4.32	0.00
tTTG+G-G+g+	5.78	0.00	4.42	0.00
tTG+G+G-Tg+	5.81	0.00	4.43	0.00
tTG-G+G+G-t	5.83	0.00	4.65	0.00
g+TG+G-G-Tg+	5.86	0.00	4.42	0.00
g+G+G+G+G-G-g+	5.88	0.00	4.80	0.00
tG+G+G+G-G+g+	5.94	0.00	4.82	0.00
tG+G-G+G+G+g+	5.95	0.00	4.85	0.00
g+G-G+TG-G+g+	5.96	0.00	4.14	0.00
tTG+G-G-G-g+	5.97	0.00	4.75	0.00
tG+G-G-G+Tg+	5.97	0.00	4.73	0.00
g+TG-G+G+G+g-	5.98	0.00	4.73	0.00
tG-G+G-G-G-t	6.00	0.00	5.00	0.00
tTG-G+G+Tg+	6.01	0.00	4.61	0.00
tG-G+G-G-Tg+	6.03	0.00	4.82	0.00
g+TG+G-G-G-g+	6.13	0.00	4.84	0.00
tTG+G+G-G-g+	6.13	0.00	4.98	0.00
tG-TG-G+G-t	6.22	0.00	4.82	0.00
g+G-TG-G+G-g-	6.24	0.00	4.65	0.00
tTG-G-G+G-t	6.27	0.00	5.14	0.00
tG+G-G+G+Tg+	6.41	0.00	5.15	0.00
g+TG+G+G-G-g+	6.45	0.00	5.18	0.00
g+TG+G-G-G+g+	6.53	0.00	5.18	0.00
tTG+G-G-G+g+	6.92	0.00	5.39	0.00
g+G-G+TG-G+g-	7.05	0.00	5.15	0.00

Optimized geometries for all the molecules calculated in the paper are given in the following in Angstrom xyz format.

Optimized Cartesian Geometries calculated by MP2/6-311++G(3df,3pd)

1-5 Pentanediol

tTTTG-t	C	2.3179756	-0.5099852	0.2335409
	C	1.1978800	0.4206282	-0.1724046
	C	-0.1630542	-0.0953886	0.2742623

C	-1.2946405	0.8371617	-0.1368896	
C	-2.6551029	0.3369967	0.2966653	
O	3.5446921	0.0562005	-0.2151925	
O	-2.8963863	-0.8985080	-0.3698847	
H	2.1606047	-1.4952843	-0.2153380	
H	2.3246079	-0.6293172	1.3214528	
H	1.3899982	1.4053465	0.2585852	
H	1.2168384	0.5351309	-1.2578325	
H	-0.1734332	-0.2107727	1.3623888	
H	-0.3452615	-1.0832885	-0.1512140	
H	-1.2985933	0.9567507	-1.2223536	
H	-1.1357924	1.8267651	0.2982192	
H	-3.4243424	1.0685780	0.0358916	
H	-2.6701093	0.1950870	1.3821326	
H	4.2582992	-0.5375450	0.0271803	
H	-3.7594750	-1.2224101	-0.1043116	
tG-TTTg-	C	-2.6563071	0.3376182	0.2890708
	C	-1.2946697	0.8404806	-0.1380726
	C	-0.1632418	-0.0869584	0.2850505
	C	1.2001615	0.4185895	-0.1676158
	C	2.3223898	-0.5088247	0.2602209
	O	-2.8905211	-0.8979056	-0.3796362
	O	3.6103245	-0.0292078	-0.1039021
	H	-3.4258250	1.0675239	0.0245502
	H	-2.6763008	0.1954234	1.3743222
	H	-1.2933933	0.9538867	-1.2243818
	H	-1.1413872	1.8329206	0.2923995
	H	-0.3462383	-1.0812676	-0.1248799
	H	-0.1705742	-0.1860667	1.3747006
	H	1.3924945	1.4127175	0.2410840
	H	1.2085240	0.5115639	-1.2579635
	H	2.1529806	-1.5104715	-0.1471799
	H	2.3424077	-0.5936007	1.3458235
	H	-3.7498082	-1.2297949	-0.1115209
	H	3.6395481	0.0350427	-1.0611534
tG+TTTg-	C	2.6541708	0.3494793	0.2910806
	C	1.2931336	0.8381328	-0.1543242
	C	0.1635214	-0.0890305	0.2742362
	C	-1.2000075	0.4060560	-0.1895827
	C	-2.3207652	-0.5188881	0.2473080
	O	2.8976523	-0.8977816	-0.3513240
	O	-3.5979422	-0.1070822	-0.2221662
	H	2.6678285	0.2288992	1.3791446
	H	3.4221802	1.0775501	0.0171424
	H	1.1320132	1.8362138	0.2604384
	H	1.2986162	0.9353321	-1.2420268
	H	0.1698205	-0.1804872	1.3646536
	H	0.3495416	-1.0857354	-0.1282530
	H	-1.2189726	0.4889709	-1.2778772
	H	-1.3841951	1.4073158	0.2129932
	H	-2.3224819	-0.6129899	1.3380806

H	-2.1660368	-1.5130586	-0.1690290	
H	3.7589931	-1.2181335	-0.0758795	
H	-3.7750072	0.7657030	0.1358461	
tTTTG-g-	C	2.3228977	-0.4938618	0.2522267
	C	1.1964602	0.4140664	-0.1866883
	C	-0.1590604	-0.0828847	0.2963673
	C	-1.2987840	0.8297266	-0.1347602
	C	-2.6610093	0.3226989	0.3057369
	O	3.5417658	0.0478962	-0.2445926
	O	-2.9804967	-0.9473383	-0.2502884
	H	2.1599427	-1.5019452	-0.1407478
	H	2.3451699	-0.5547578	1.3446205
	H	1.3900512	1.4184885	0.1951285
	H	1.2063054	0.4774018	-1.2766144
	H	-0.1576422	-0.1545706	1.3879770
	H	-0.3450243	-1.0889673	-0.0834123
	H	-1.2931751	0.9376372	-1.2240368
	H	-1.1498462	1.8311210	0.2783318
	H	-3.4357088	1.0543652	0.0608145
	H	-2.6730678	0.1743398	1.3849715
	H	4.2611812	-0.5253171	0.0282385
	H	-3.0619893	-0.8387556	-1.2007265
tG+TTG+g-	C	-2.4748222	0.0174792	-0.5219891
	C	-1.2387925	0.8483032	-0.2556698
	C	0.0039427	-0.0001883	-0.0210062
	C	1.2430820	0.8457137	0.2388798
	C	2.4808749	0.0139841	0.5268506
	O	-2.7269892	-0.7686006	0.6383810
	O	2.8841376	-0.7816267	-0.5808549
	H	-2.3090051	-0.6263616	-1.3918545
	H	-3.3260883	0.6691044	-0.7354806
	H	-1.0775156	1.5115063	-1.1088907
	H	-1.4248340	1.4791632	0.6162178
	H	0.1619791	-0.6300393	-0.9018271
	H	-0.1726666	-0.6661308	0.8260436
	H	1.0615038	1.4970159	1.0984048
	H	1.4436538	1.4885665	-0.6211405
	H	2.3089467	-0.6139675	1.4070573
	H	3.3293657	0.6610734	0.7400526
	H	-3.5184094	-1.2891096	0.4862168
	H	2.2125407	-1.4516219	-0.7233088
tTTTTg-	C	-2.5179623	0.4617316	0.0159267
	C	-1.2638485	-0.3824911	-0.0149020
	C	-0.0002082	0.4669726	0.0126403
	C	1.2678266	-0.3766011	-0.0249848
	C	2.5224815	0.4761956	0.0150619
	O	-3.6364741	-0.4169873	-0.0061130
	O	3.7168037	-0.2869491	-0.0853093
	H	-2.5353832	1.1308580	-0.8498576
	H	-2.5283785	1.0770715	0.9209493
	H	-1.2789912	-1.0597997	0.8409725

H	-1.2807634	-0.9999544	-0.9146774	
H	0.0025601	1.0878859	0.9130976	
H	-0.0014790	1.1514589	-0.8403620	
H	1.2863896	-0.9863520	-0.9299690	
H	1.2722970	-1.0634512	0.8266634	
H	2.5290370	1.0872117	0.9235249	
H	2.5401477	1.1535693	-0.8376061	
H	-4.4375713	0.1109265	0.0066022	
H	3.7461976	-0.8881036	0.6624375	
tG-TTG-g-	C	-2.4666307	0.0194003	0.5582220
	C	-1.2234692	0.8312709	0.2663981
	C	-0.0043082	-0.0370812	-0.0117570
	C	1.2298322	0.7873831	-0.3484226
	C	2.4703837	-0.0642459	-0.5549520
	O	-2.7904501	-0.7139687	-0.6191382
	O	2.8436128	-0.7830557	0.6153844
	H	-3.2920796	0.6809123	0.8345237
	H	-2.2768161	-0.6617183	1.3937522
	H	-1.4273574	1.4769703	-0.5910310
	H	-1.0279855	1.4820050	1.1225242
	H	-0.2252585	-0.7108203	-0.8411329
	H	0.2059401	-0.6615781	0.8588129
	H	1.4258754	1.5116251	0.4495575
	H	1.0513762	1.3674689	-1.2581609
	H	3.3019683	0.5533078	-0.9054550
	H	2.2785325	-0.8252905	-1.3102697
	H	-3.5588259	-1.2581781	-0.4353807
	H	3.0945321	-0.1414698	1.2840048
tG-TTG+g-	C	2.5275370	-0.2290668	0.2593493
	C	1.2622835	-0.8709963	-0.2668271
	C	-0.0002828	-0.2056121	0.2643369
	C	-1.2699545	-0.8586759	-0.2651557
	C	-2.5364365	-0.2118323	0.2689375
	O	2.5456378	1.1227306	-0.1877088
	O	-2.7083139	1.1252197	-0.1798472
	H	3.4035039	-0.7672748	-0.1119000
	H	2.5375876	-0.2702995	1.3533943
	H	1.2732020	-0.8200672	-1.3576046
	H	1.2699605	-1.9280507	0.0100140
	H	0.0298880	0.8489700	-0.0148825
	H	0.0012742	-0.2500704	1.3584519
	H	-1.2795774	-1.9160069	0.0145951
	H	-1.2850414	-0.8095429	-1.3560397
	H	-2.5403417	-0.2529350	1.3636448
	H	-3.4136910	-0.7486063	-0.0866115
	H	3.3544272	1.5347131	0.1230653
	H	-1.9721654	1.6457768	0.1487160
g+TTTG-g-	C	2.3245902	-0.5075834	0.2578440
	C	1.1995305	0.4027804	-0.1988438
	C	-0.1597821	-0.0769483	0.2925256
	C	-1.2969747	0.8306273	-0.1556870

C	-2.6600188	0.3375858	0.2987195	
O	3.5961436	-0.1127081	-0.2397801	
O	-2.9821645	-0.9450474	-0.2246708	
H	2.1650852	-1.5153684	-0.1225256	
H	2.3377330	-0.5646964	1.3509652	
H	1.3868321	1.4165991	0.1688858	
H	1.2103964	0.4504800	-1.2895561	
H	-0.1584229	-0.1305522	1.3851652	
H	-0.3468549	-1.0892125	-0.0697482	
H	-1.2933333	0.9150152	-1.2470038	
H	-1.1445507	1.8402808	0.2359165	
H	-3.4332446	1.0648102	0.0365169	
H	-2.6709064	0.2165844	1.3813913	
H	3.7859720	0.7645114	0.1003881	
H	-3.0734140	-0.8596099	-1.1765868	
g-TTTG-g-	C	2.3270650	-0.4977308	0.2688039
	C	1.2001408	0.4131106	-0.1824133
	C	-0.1590470	-0.0780475	0.2978995
	C	-1.2981127	0.8323833	-0.1396548
	C	-2.6606243	0.3254065	0.3006788
	O	3.6113664	-0.0268965	-0.1177203
	O	-2.9780113	-0.9458440	-0.2534388
	H	2.1579751	-1.5126703	-0.1044844
	H	2.3528529	-0.5470237	1.3564101
	H	1.3941667	1.4205912	0.1910581
	H	1.2015088	0.4698368	-1.2754590
	H	-0.1571046	-0.1427784	1.3898641
	H	-0.3446940	-1.0868020	-0.0749673
	H	-1.2914859	0.9353686	-1.2295094
	H	-1.1506646	1.8355647	0.2696154
	H	-3.4356595	1.0560299	0.0540379
	H	-2.6729893	0.1792661	1.3801851
	H	3.6392248	-0.0014924	-1.0767873
	H	-3.0793382	-0.8356449	-1.2017145
tTTTG+g-	C	-2.3196256	-0.5202244	0.2092017
	C	-1.2009692	0.4283557	-0.1584227
	C	0.1649338	-0.1117524	0.2438091
	C	1.2977732	0.8340678	-0.1336285
	C	2.6641971	0.3336411	0.3013466
	O	-3.5466319	0.0736243	-0.1958167
	O	3.0540819	-0.8628671	-0.3602724
	H	-2.3147414	-0.6982186	1.2892113
	H	-2.1706780	-1.4808368	-0.2938377
	H	-1.2306728	0.6032273	-1.2353403
	H	-1.3824840	1.3879192	0.3291681
	H	0.3171409	-1.0804342	-0.2411139
	H	0.1868087	-0.2865775	1.3242445
	H	1.1244876	1.8079871	0.3320311
	H	1.3065314	0.9862287	-1.2147297
	H	2.6814165	0.1944267	1.3874386
	H	3.4297574	1.0642880	0.0484487

H	-4.2626805	-0.5243087	0.0285938	
H	2.4736769	-1.5682001	-0.0676028	
tG+TTG-t	C	0.3504288	0.0033887	2.5303352
	C	0.3579762	-0.8231341	1.2627726
	C	0.3384250	0.0269933	0.0000000
	C	0.3579764	-0.8231340	-1.2627727
	C	0.3504288	0.0033888	-2.5303353
	O	-0.8772853	0.7223136	2.5743610
	O	-0.8772853	0.7223136	-2.5743609
	H	1.1995689	0.6947180	2.5265223
	H	0.4434299	-0.6480143	3.4036953
	H	1.2485580	-1.4572079	1.2724442
	H	-0.5109811	-1.4848739	1.2768479
	H	1.2088954	0.6911109	0.0000001
	H	-0.5471511	0.6598839	0.0000000
	H	-0.5109808	-1.4848741	-1.2768479
	H	1.2485583	-1.4572077	-1.2724441
	H	0.4434298	-0.6480144	-3.4036953
	H	1.1995689	0.6947180	-2.5265224
	H	-0.8850748	1.2608598	3.3682025
	H	-0.8850749	1.2608597	-3.3682025
tG+TTG-g-	C	-2.5287637	-0.2272164	0.2638118
	C	-1.2630530	-0.8612924	-0.2709589
	C	0.0006286	-0.2208377	0.2868444
	C	1.2647424	-0.8438499	-0.2876885
	C	2.5380900	-0.2222847	0.2595922
	O	-2.5661590	1.1191473	-0.1980239
	O	2.6420788	1.1667838	-0.0246251
	H	-2.5254254	-0.2575045	1.3580997
	H	-3.4041354	-0.7773931	-0.0917682
	H	-1.2809676	-1.9268087	-0.0279553
	H	-1.2721079	-0.7780216	-1.3602931
	H	0.0106785	-0.3309811	1.3756678
	H	-0.0094854	0.8475913	0.0775855
	H	1.2604469	-0.7458060	-1.3782979
	H	1.2861038	-1.9164342	-0.0730043
	H	3.4129895	-0.7580342	-0.1198601
	H	2.5503415	-0.2934499	1.3466916
	H	-3.3447772	1.5440153	0.1674629
	H	2.6521536	1.2711787	-0.9790818
g+TTTTg-	C	-0.0058166	0.4725571	2.5228091
	C	-0.0074985	-0.3805870	1.2674880
	C	-0.0084270	0.4646420	0.0000000
	C	-0.0074989	-0.3805866	-1.2674883
	C	-0.0058153	0.4725578	-2.5228092
	O	-0.0693866	-0.2954172	3.7162891
	O	-0.0693871	-0.2954160	-3.7162894
	H	-0.8893102	1.1090915	2.5413873
	H	0.8728691	1.1256241	2.5287903
	H	0.8743190	-1.0284604	1.2721915
	H	-0.8841228	-1.0304470	1.2863128

	H	0.8648958	1.1231943	0.0000000
	H	-0.8892214	1.1128102	0.0000002
	H	-0.8841241	-1.0304455	-1.2863138
	H	0.8743178	-1.0284612	-1.2721915
	H	0.8728719	1.1256229	-2.5287903
	H	-0.8893074	1.1090942	-2.5413871
	H	0.7119549	-0.8518021	3.7516419
	H	0.7119514	-0.8518053	-3.7516406
tG-TTG-t	C	0.0073275	2.5282792	0.0052631
	C	0.0171215	1.2630026	-0.8241734
	C	0.0000013	0.0000001	0.0256293
	C	-0.0171206	-1.2630024	-0.8241733
	C	-0.0073285	-2.5282790	0.0052633
	O	-1.2258490	2.5710376	0.7179509
	O	1.2258481	-2.5710393	0.7179509
	H	0.1032216	3.4038672	-0.6423892
	H	0.8516539	2.5209964	0.7016949
	H	-0.8499782	1.2796214	-1.4887859
	H	0.9093889	1.2718611	-1.4550976
	H	-0.8781752	0.0153400	0.6735074
	H	0.8781791	-0.0153396	0.6735056
	H	0.8499790	-1.2796224	-1.4887858
	H	-0.9093881	-1.2718597	-1.4550975
	H	-0.1032243	-3.4038669	-0.6423889
	H	-0.8516547	-2.5209946	0.7016953
	H	-1.2307512	3.3581325	1.2663609
	H	1.2307490	-3.3581342	1.2663609
g+TTTG+g-	C	-2.3222270	-0.5275814	0.2214381
	C	-1.2041836	0.4303755	-0.1470066
	C	0.1653544	-0.1066036	0.2490957
	C	1.2971745	0.8393373	-0.1305432
	C	2.6654240	0.3349409	0.2946368
	O	-3.6130048	-0.0174097	-0.0795753
	O	3.0475621	-0.8602090	-0.3737820
	H	-2.3240859	-0.7019141	1.2966243
	H	-2.1626738	-1.4928953	-0.2701047
	H	-1.2241886	0.6092354	-1.2261875
	H	-1.3877460	1.3890125	0.3416460
	H	0.3170674	-1.0754504	-0.2354120
	H	0.1874955	-0.2813476	1.3294544
	H	1.1281062	1.8121178	0.3390606
	H	1.3013816	0.9947632	-1.2113712
	H	2.6896643	0.1925722	1.3800124
	H	3.4304235	1.0652051	0.0388399
	H	-3.6621969	0.1219901	-1.0280271
	H	2.4870560	-1.5717279	-0.0583089
g-G+TTG-g-	C	-2.5414697	-0.2227104	0.2373650
	C	-1.2670273	-0.8540226	-0.2967728
	C	-0.0057957	-0.2247332	0.2788872
	C	1.2676440	-0.8704841	-0.2490779
	C	2.5270010	-0.2090931	0.2841510

O	-2.6937903	1.1341207	-0.1566174	
O	2.6189318	1.1638950	-0.0758673	
H	-2.5713127	-0.3116419	1.3285110	
H	-3.4131581	-0.7375035	-0.1616402	
H	-1.2850407	-1.9211841	-0.0579424	
H	-1.2627987	-0.7636200	-1.3852462	
H	-0.0228334	-0.3082811	1.3703310	
H	0.0285528	0.8400407	0.0411346	
H	1.2756568	-0.8254987	-1.3426825	
H	1.2888361	-1.9300324	0.0205131	
H	3.4134817	-0.7545006	-0.0505477	
H	2.5216561	-0.2200678	1.3735815	
H	-1.9945088	1.6446419	0.2569438	
H	2.7207222	1.2120001	-1.0293967	
g+G+TTG+g-	C	-2.4767893	-0.0270921	-0.5334827
	C	-1.2402997	0.8229676	-0.2982396
	C	0.0076347	-0.0085639	-0.0348939
	C	1.2372190	0.8489448	0.2321450
	C	2.4785537	0.0290470	0.5392215
	O	-2.8010587	-0.8445589	0.5848189
	O	2.9025722	-0.7661821	-0.5605429
	H	-2.3016305	-0.7209080	-1.3550082
	H	-3.3260866	0.6049661	-0.8063719
	H	-1.0836689	1.4598927	-1.1731042
	H	-1.4226592	1.4930918	0.5479261
	H	0.1820902	-0.6471827	-0.9057630
	H	-0.1743213	-0.6694509	0.8154818
	H	1.0424226	1.5064270	1.0842695
	H	1.4424388	1.4863798	-0.6306885
	H	2.3016097	-0.5973228	1.4195736
	H	3.3179428	0.6850807	0.7609560
	H	-3.0633801	-0.2664876	1.3050671
	H	2.2489826	-1.4546796	-0.6985406
g+TTTG-g+	C	2.3223400	-0.5278622	0.2237685
	C	1.2032961	0.4156719	-0.1774693
	C	-0.1649565	-0.1048507	0.2443600
	C	-1.2965387	0.8349226	-0.1512693
	C	-2.6633405	0.3460476	0.2963240
	O	3.6013935	-0.0903501	-0.2116854
	O	-3.0568286	-0.8614965	-0.3418709
	H	2.1748546	-1.5002080	-0.2443639
	H	2.3126845	-0.6777886	1.3083767
	H	1.3763865	1.3945989	0.2797676
	H	1.2329849	0.5560573	-1.2594099
	H	-0.1821631	-0.2542083	1.3286983
	H	-0.3210054	-1.0844644	-0.2164066
	H	-1.3072705	0.9637245	-1.2353913
	H	-1.1215249	1.8185533	0.2932266
	H	-3.4273609	1.0738685	0.0308321
	H	-2.6788241	0.2279944	1.3849118
	H	3.7817680	0.7560513	0.2035582

H	-2.4874989	-1.5661665	-0.0267004	
g-G-TTG+g+	C	-0.3471300	0.0118825	2.5361254
C	-0.3538015	-0.8204726	1.2653176	
C	-0.3650133	0.0253580	0.0000000	
C	-0.3538015	-0.8204726	-1.2653176	
C	-0.3471299	0.0118825	-2.5361254	
O	0.8048539	0.8378587	2.6476935	
O	0.8048538	0.8378588	-2.6476935	
H	-0.4421168	-0.6348301	3.4129292	
H	-1.1930627	0.6983568	2.5360688	
H	0.5238619	-1.4754867	1.2653278	
H	-1.2296567	-1.4756064	1.2861467	
H	0.4918791	0.6976730	0.0000001	
H	-1.2586237	0.6567004	0.0000001	
H	-1.2296569	-1.4756062	-1.2861467	
H	0.5238617	-1.4754868	-1.2653277	
H	-1.1930628	0.6983567	-2.5360690	
H	-0.4421166	-0.6348302	-3.4129292	
H	1.5715780	0.2643705	2.7179015	
H	1.5715780	0.2643707	-2.7179016	
tTTG-G-t	C	-2.1926577	0.0447735	0.4348715
C	-0.8666858	0.1047105	-0.2891351	
C	0.1817912	0.8547498	0.5222299	
C	1.4994439	1.0496976	-0.2231019	
C	2.1581203	-0.2513349	-0.6320821	
O	-3.1052580	-0.6854610	-0.3783685	
O	2.3508139	-1.0291464	0.5456549	
H	-2.5638507	1.0584229	0.6145733	
H	-2.0609935	-0.4463911	1.4036641	
H	-0.5412379	-0.9177699	-0.4827541	
H	-1.0185095	0.5891852	-1.2565703	
H	0.3772351	0.3166362	1.4505313	
H	-0.2089741	1.8376147	0.7971928	
H	2.1951492	1.6057472	0.4074693	
H	1.3322781	1.6431064	-1.1253561	
H	3.1159049	-0.0417140	-1.1152759	
H	1.5294247	-0.7888072	-1.3465926	
H	-3.9467103	-0.7331265	0.0800998	
H	2.7737002	-1.8536428	0.2968298	
g+TTTTg+	C	-0.0469142	2.5225673	0.4724591
C	-0.0199227	1.2671683	-0.3801051	
C	-0.0000006	0.0000000	0.4653320	
C	0.0199221	-1.2671683	-0.3801052	
C	0.0469147	-2.5225673	0.4724591	
O	-0.0000025	3.7164945	-0.2960793	
O	0.0000036	-3.7164946	-0.2960793	
H	0.8331513	2.5566308	1.1131646	
H	-0.9285768	2.5138406	1.1213525	
H	-0.8988315	1.2555811	-1.0315190	
H	0.8589937	1.3019390	-1.0264590	
H	-0.8769260	-0.0165065	1.1186968	

H	0.8769244	0.0165064	1.1186975	
H	0.8988308	-1.2555806	-1.0315194	
H	-0.8589944	-1.3019396	-1.0264588	
H	-0.8331506	-2.5566314	1.1131648	
H	0.9285775	-2.5138400	1.1213522	
H	-0.7816259	3.7403698	-0.8527119	
H	0.7816272	-3.7403696	-0.8527117	
tG-G-TTg-	C	-2.1569524	-0.2275564	0.6493770
	C	-1.4954585	1.0578158	0.1972592
	C	-0.1819789	0.8349380	-0.5475725
	C	0.8727118	0.1094449	0.2787746
	C	2.1966360	0.0222494	-0.4583969
	O	-2.3557978	-1.0402199	-0.5028269
	O	3.1850587	-0.7083917	0.2563315
	H	-3.1120816	0.0004095	1.1294935
	H	-1.5275484	-0.7448977	1.3782613
	H	-2.1919312	1.5957223	-0.4479736
	H	-1.3232773	1.6796470	1.0793586
	H	0.2098509	1.8063315	-0.8592302
	H	-0.3822118	0.2648076	-1.4554616
	H	0.5468332	-0.9042041	0.5136460
	H	1.0241037	0.6337393	1.2284607
	H	2.5577662	1.0275808	-0.6976557
	H	2.0629680	-0.5128329	-1.3972786
	H	-2.7823108	-1.8548448	-0.2288285
	H	3.3479151	-0.2494204	1.0833890
tG+TG-G-g-	C	2.1634034	-0.7588731	0.0474376
	C	0.8129235	-0.3083265	0.5601477
	C	0.0546868	0.5275772	-0.4624905
	C	-1.2560173	1.0933844	0.0749578
	C	-2.2328571	0.0331209	0.5566159
	O	2.9585835	0.4024930	-0.1738692
	O	-2.5084826	-0.9533373	-0.4307010
	H	2.0358070	-1.3193729	-0.8839997
	H	2.6424775	-1.4142634	0.7794878
	H	0.2387299	-1.1994143	0.8198223
	H	0.9644076	0.2667202	1.4774267
	H	-0.1502030	-0.0898650	-1.3393424
	H	0.6913412	1.3498786	-0.7883863
	H	-1.7394337	1.6920279	-0.7027466
	H	-1.0545233	1.7726070	0.9081245
	H	-3.1580083	0.5069276	0.8966124
	H	-1.8195270	-0.5155595	1.4004367
	H	3.8116132	0.1244492	-0.5134808
	H	-2.9000912	-0.5101321	-1.1873739
tG+TG-G-t	C	2.1534851	-0.7676206	0.0604726
	C	0.8004531	-0.3058365	0.5566509
	C	0.0557316	0.5251979	-0.4797146
	C	-1.2556001	1.1082951	0.0382403
	C	-2.2337062	0.0626874	0.5319812
	O	2.9620974	0.3868914	-0.1462560

O	-2.4607416	-0.8605253	-0.5293391	
H	2.0324826	-1.3236470	-0.8745505	
H	2.6177352	-1.4297575	0.7963460	
H	0.2191789	-1.1923233	0.8176212	
H	0.9471765	0.2739179	1.4718846	
H	-0.1505626	-0.0965115	-1.3524634	
H	0.7006382	1.3406984	-0.8068319	
H	-1.7353142	1.6830198	-0.7557755	
H	-1.0558631	1.7984732	0.8618448	
H	-3.1689904	0.5447985	0.8284655	
H	-1.8300931	-0.4547094	1.4068562	
H	3.8110668	0.1035957	-0.4914586	
H	-3.1154471	-1.4987872	-0.2386969	
tG+G+TTg-	C	-2.1560034	-0.2602903	-0.6257678
	C	-1.5084267	1.0520143	-0.2352792
	C	-0.1822103	0.8791137	0.5003280
	C	0.8603989	0.1033163	-0.2949611
	C	2.2002082	0.0793488	0.4177095
	O	-2.3027832	-1.0426261	0.5558890
	O	3.2044111	-0.6182516	-0.3077860
	H	-1.5378823	-0.7870811	-1.3577024
	H	-3.1296325	-0.0674581	-1.0831294
	H	-1.3560242	1.6373952	-1.1452875
	H	-2.2035130	1.6076559	0.3961834
	H	-0.3661675	0.3711939	1.4477062
	H	0.2133269	1.8693287	0.7395940
	H	0.9966271	0.5458884	-1.2844941
	H	0.5233165	-0.9262513	-0.4399291
	H	2.0794945	-0.3465821	1.4187432
	H	2.5795901	1.0935303	0.5338797
	H	-2.7587321	-1.8547180	0.3251624
	H	2.9181929	-1.5296339	-0.4009508
g+G-TTG+g-	C	-0.3459849	0.0052766	2.5415790
	C	-0.3637172	-0.8206540	1.2665145
	C	-0.3045151	0.0239343	0.0000001
	C	-0.3637166	-0.8206545	-1.2665140
	C	-0.3459841	0.0052757	-2.5415788
	O	0.8718674	0.7145087	2.7277810
	O	0.8718669	0.7145109	-2.7277785
	H	-0.4353354	-0.6444728	3.4096742
	H	-1.1970762	0.6941177	2.5512879
	H	0.4791715	-1.5142161	1.2849355
	H	-1.2794727	-1.4181077	1.2578869
	H	0.6240015	0.6021130	-0.0000003
	H	-1.1361387	0.7370770	-0.0000002
	H	-1.2794719	-1.4181086	-1.2578865
	H	0.4791725	-1.5142163	-1.2849343
	H	-1.1970771	0.6941145	-2.5512898
	H	-0.4353311	-0.6444744	-3.4096738
	H	0.9254245	1.3987410	2.0579197
	H	0.9254167	1.3987491	-2.0579227

tG+TG+G+g-	C	-0.0465250	-0.2533935	-2.0605869
	C	-1.1276367	-0.4341028	-1.0175354
	C	-1.1665488	0.7138441	0.0059909
	C	-1.0312101	0.2588835	1.4572742
	C	0.2994805	-0.4230372	1.7517430
	O	1.2162428	-0.2830872	-1.3872952
	O	1.4094315	0.3899676	1.4161660
	H	-0.1747572	0.7046532	-2.5721335
	H	-0.0892764	-1.0542950	-2.8018331
	H	-2.0830627	-0.5204114	-1.5367214
	H	-0.9574554	-1.3903357	-0.5197666
	H	-2.0957364	1.2735517	-0.1034363
	H	-0.3599710	1.4175505	-0.2051391
	H	-1.8416904	-0.4312058	1.7107215
	H	-1.1260693	1.1270953	2.1115907
	H	0.3632770	-1.3817497	1.2284610
	H	0.3726457	-0.6308876	2.8187302
	H	1.9135300	-0.1484155	-2.0331879
	H	1.5115584	0.3160924	0.4591219
tTTG-G-g-	C	-2.1984763	0.0281941	0.4554382
	C	-0.8850363	0.1098080	-0.2893152
	C	0.1808390	0.8260062	0.5301155
	C	1.4861447	1.0356470	-0.2319367
	C	2.1563932	-0.2592698	-0.6615707
	O	-3.1312068	-0.6550373	-0.3747112
	O	2.4016704	-1.1383264	0.4295918
	H	-2.5568536	1.0356722	0.6884676
	H	-2.0545913	-0.5087928	1.3978419
	H	-0.5680196	-0.9054860	-0.5283473
	H	-1.0515594	0.6326632	-1.2340112
	H	0.3843525	0.2545638	1.4372677
	H	-0.2001674	1.8006369	0.8449015
	H	2.1843727	1.6036663	0.3897204
	H	1.3026102	1.6384529	-1.1256991
	H	3.0849842	-0.0373907	-1.1942917
	H	1.5153511	-0.8170082	-1.3405678
	H	-3.9635437	-0.7226683	0.0975716
	H	3.0168653	-0.7035262	1.0249996
tTTG-Tt	C	-2.4212439	0.2559282	0.1943324
	C	-1.0003319	-0.1017671	-0.1799905
	C	-0.0264237	1.0176795	0.1710351
	C	1.3974305	0.7651251	-0.3154305
	C	2.0259265	-0.4646805	0.3037825
	O	-3.2536572	-0.8493429	-0.1377808
	O	3.3841295	-0.5097425	-0.1208684
	H	-2.7331072	1.1520210	-0.3507289
	H	-2.4777920	0.4730470	1.2655512
	H	-0.7364932	-1.0246704	0.3373933
	H	-0.9612531	-0.3090663	-1.2514877
	H	-0.0187511	1.1677930	1.2543168
	H	-0.3836149	1.9517133	-0.2689279

H	2.0299833	1.6199309	-0.0718647	
H	1.4089550	0.6555364	-1.4013454	
H	1.4985251	-1.3671525	-0.0131871	
H	1.9645008	-0.3989386	1.3954180	
H	-4.1584075	-0.6266504	0.0911702	
H	3.7774310	-1.3194873	0.2109415	
tG+G+TG+g-	C	-2.1485501	-0.0779967	0.5366855
	C	-1.4113532	-0.9968986	-0.4156378
	C	0.0242081	-0.5569848	-0.6907917
	C	0.9118021	-0.5615247	0.5481551
	C	2.3626294	-0.2425663	0.2291333
	O	-2.1305936	1.2289912	-0.0270417
	O	2.5498786	1.0904494	-0.2247685
	H	-1.6682223	-0.0787179	1.5186061
	H	-3.1760649	-0.4290583	0.6630275
	H	-1.4169301	-2.0045500	0.0073412
	H	-1.9673517	-1.0350607	-1.3538469
	H	-0.0073933	0.4430446	-1.1268572
	H	0.4585533	-1.2257292	-1.4390186
	H	0.8721199	-1.5483444	1.0193934
	H	0.5548833	0.1673692	1.2771772
	H	2.7451038	-0.9569908	-0.5081782
	H	2.9748018	-0.3288017	1.1246700
	H	-2.5783362	1.8263714	0.5755989
	H	2.0186501	1.2120233	-1.0147657
tTG-TG-t	C	-1.9452659	-0.5342682	0.0551513
	C	-1.2802715	0.7709473	-0.3258079
	C	0.2194165	0.6280990	-0.5658071
	C	1.0048031	0.2478545	0.6844968
	C	2.4969297	0.2001778	0.4370347
	O	-3.3474603	-0.2960723	0.1283459
	O	2.7447796	-0.8356612	-0.5085829
	H	-1.5716607	-0.8916051	1.0177007
	H	-1.7201648	-1.2936402	-0.7006820
	H	-1.7672419	1.1373594	-1.2307207
	H	-1.4710315	1.5047697	0.4602047
	H	0.6081807	1.5767745	-0.9443095
	H	0.4016946	-0.1155052	-1.3431576
	H	0.6938183	-0.7304670	1.0540205
	H	0.8075884	0.9737798	1.4777708
	H	3.0274655	-0.0008172	1.3715397
	H	2.8393657	1.1643458	0.0475534
	H	-3.7779057	-1.1102141	0.3973938
	H	3.6881745	-0.8709232	-0.6791156
tG-TG+Tg-	C	2.4089130	-0.6571103	0.1833859
	C	0.9614456	-0.5803220	-0.2532127
	C	0.2209240	0.5865460	0.3913198
	C	-1.2039777	0.7587731	-0.1274297
	C	-2.1083425	-0.4137769	0.2088156
	O	3.0606161	0.5310907	-0.2547409
	O	-3.4417084	-0.2277566	-0.2482888

H	2.8853361	-1.5376893	-0.2549511	
H	2.4632839	-0.7438138	1.2733713	
H	0.9310668	-0.4794420	-1.3406651	
H	0.4842574	-1.5288950	-0.0006876	
H	0.7850265	1.4996625	0.2042600	
H	0.2009250	0.4439965	1.4762050	
H	-1.1950852	0.8983763	-1.2101805	
H	-1.6374989	1.6637640	0.3079243	
H	-2.0909762	-0.5945626	1.2892960	
H	-1.7658632	-1.3209578	-0.2838330	
H	3.9819854	0.4854137	0.0084869	
H	-3.7725507	0.5862395	0.1385425	
tG-G-TG+g-	C	-2.2436981	0.0343125	0.5217151
	C	-1.2701246	1.1035743	0.0710538
	C	0.0560668	0.5441510	-0.4380682
	C	0.8141019	-0.2718078	0.6006206
	C	2.1581632	-0.7662881	0.0923295
	O	-2.4378779	-0.8629371	-0.5672651
	O	3.0749435	0.2865593	-0.1787263
	H	-3.1895567	0.4991164	0.8112399
	H	-1.8505424	-0.4992457	1.3909948
	H	-1.7429631	1.6904928	-0.7179996
	H	-1.0901768	1.7760099	0.9133296
	H	0.6705840	1.3885135	-0.7597921
	H	-0.1327478	-0.0763836	-1.3159698
	H	0.2251142	-1.1472686	0.8829530
	H	0.9765108	0.3241766	1.5020936
	H	2.0108910	-1.3858689	-0.7980401
	H	2.6427106	-1.3803545	0.8487610
	H	-3.0800824	-1.5248837	-0.3027107
	H	2.7496179	0.7743298	-0.9377842
g+TTG-G-g-	C	-2.2030355	0.0864307	0.4294865
	C	-0.8674422	0.1028597	-0.2912403
	C	0.1839280	0.8754542	0.4956951
	C	1.5027083	1.0414386	-0.2541554
	C	2.1455832	-0.2771784	-0.6526794
	O	-3.2132162	-0.6090386	-0.2889115
	O	2.3137692	-1.1629095	0.4477620
	H	-2.5780831	1.1023249	0.5451634
	H	-2.0784248	-0.3377827	1.4308391
	H	-0.5356941	-0.9279838	-0.4369658
	H	-1.0070390	0.5456708	-1.2801759
	H	0.3701661	0.3641175	1.4414073
	H	-0.2062519	1.8662759	0.7409536
	H	2.2049206	1.6066118	0.3653081
	H	1.3438809	1.6296245	-1.1621656
	H	3.1020807	-0.0901051	-1.1478657
	H	1.5134593	-0.8133209	-1.3572354
	H	-2.9290822	-1.5208855	-0.3851242
	H	2.9213976	-0.7518641	1.0674331
tTTG-Tg-	C	-2.4242444	0.2583992	0.2002281

C	-1.0103704	-0.1033021	-0.1958163	
C	-0.0264742	1.0101517	0.1462024	
C	1.3964872	0.7404844	-0.3364228	
C	2.0496217	-0.4400174	0.3616914	
O	-3.2673476	-0.8333488	-0.1466502	
O	3.4170305	-0.5949511	0.0039573	
H	-2.7343273	1.1681281	-0.3232489	
H	-2.4683575	0.4541314	1.2761600	
H	-0.7435633	-1.0314988	0.3099423	
H	-0.9890367	-0.3027514	-1.2694826	
H	-0.0142479	1.1692520	1.2283771	
H	-0.3775341	1.9438269	-0.2994815	
H	2.0211158	1.6179851	-0.1635316	
H	1.3860861	0.5601924	-1.4156907	
H	1.4979594	-1.3622377	0.1647571	
H	2.0482631	-0.2772560	1.4392600	
H	-4.1670328	-0.6144579	0.1049858	
H	3.4552835	-0.7902601	-0.9350598	
tTG+TG-t	C	2.1052337	0.4035564	0.1902943
	C	1.2002780	-0.7749266	-0.0964953
	C	-0.2233614	-0.5783763	0.4148052
	C	-0.9569427	0.5811364	-0.2509028
	C	-2.4083687	0.6661365	0.1711988
	O	3.4210326	0.0467290	-0.2224094
	O	-3.0605445	-0.5223746	-0.2653570
	H	2.0852668	0.6297029	1.2617891
	H	1.7668961	1.2902340	-0.3512445
	H	1.1895471	-0.9550529	-1.1731507
	H	1.6437198	-1.6553992	0.3705691
	H	-0.2053214	-0.4170298	1.4970230
	H	-0.7927179	-1.4911128	0.2426009
	H	-0.9170620	0.4672643	-1.3368799
	H	-0.4806926	1.5322786	-0.0056427
	H	-2.8778637	1.5454325	-0.2773758
	H	-2.4726719	0.7601615	1.2600660
	H	3.9952944	0.8033200	-0.0874868
	H	-3.9820357	-0.4755988	-0.0028685
tG+TG-Tg-	C	2.4140619	0.6613909	0.1586259
	C	0.9639802	0.5756765	-0.2672790
	C	0.2224159	-0.5666261	0.4189691
	C	-1.2038043	-0.7636870	-0.0867748
	C	-2.1190097	0.4070165	0.2255876
	O	3.0618601	-0.5349800	-0.2602981
	O	-3.4714021	0.1566150	-0.1352396
	H	2.4749251	0.7702037	1.2463529
	H	2.8878579	1.5333192	-0.2998944
	H	0.4916222	1.5343423	-0.0463945
	H	0.9301471	0.4381464	-1.3510182
	H	0.2023483	-0.3852560	1.4981235
	H	0.7877897	-1.4854334	0.2660535
	H	-1.6378168	-1.6574917	0.3637364

H	-1.1849323	-0.9269930	-1.1690012	
H	-1.7610529	1.3197221	-0.2578185	
H	-2.1343800	0.5864446	1.3004882	
H	3.9800187	-0.4959559	0.0151618	
H	-3.4975719	-0.0044860	-1.0811854	
tG+TG+Tg-	C	-2.4957337	0.1976033	0.4398238
C	-1.0037274	0.2362526	0.6896397	
C	-0.2171102	0.6313908	-0.5552056	
C	1.2821629	0.7693984	-0.3054388	
C	1.9457777	-0.5454713	0.0663878	
O	-2.7444888	-0.8141704	-0.5310020	
O	3.3493686	-0.4159358	0.2517844	
H	-2.8361408	1.1716123	0.0736381	
H	-3.0267969	-0.0248335	1.3690157	
H	-0.8047984	0.9500870	1.4932911	
H	-0.6956308	-0.7481488	1.0446851	
H	-0.6058562	1.5834855	-0.9251879	
H	-0.3961064	-0.1049013	-1.3402870	
H	1.4713697	1.4959941	0.4876364	
H	1.7630289	1.1517738	-1.2104419	
H	1.7214716	-1.2995828	-0.6954588	
H	1.5686064	-0.9148493	1.0171732	
H	-3.6893324	-0.8537843	-0.6923914	
H	3.7248903	-0.0932204	-0.5705941	
g+G+TTG+g+	C	-0.0082848	2.5337503	0.0321738
C	-0.0387136	1.2654871	-0.8033937	
C	-0.0000006	0.0000003	0.0412016	
C	0.0387120	-1.2654864	-0.8033935	
C	0.0082862	-2.5337496	0.0321746	
O	1.1858026	2.6590190	0.7952927	
O	-1.1858027	-2.6590218	0.7952909	
H	-0.8157545	2.5177554	0.7631696	
H	-0.1500562	3.4117603	-0.6040363	
H	-0.9441925	1.2760761	-1.4169531	
H	0.8079734	1.2778784	-1.4979336	
H	-0.8754898	-0.0277411	0.6925630	
H	0.8754896	0.0277420	0.6925622	
H	0.9441893	-1.2760744	-1.4169548	
H	-0.8079770	-1.2778796	-1.4979320	
H	0.8157541	-2.5177512	0.7631723	
H	0.1500621	-3.4117597	-0.6040347	
H	1.9164572	2.7609930	0.1809662	
H	-1.9164549	-2.7609982	0.1809631	
tTG-TTg-	C	2.0338418	-0.4538033	0.3164824
C	1.3950597	0.7559768	-0.3310789	
C	-0.0270117	1.0148486	0.1572209	
C	-1.0056888	-0.1081574	-0.1706603	
C	-2.4281967	0.2585720	0.2123740	
O	3.3845581	-0.5121721	-0.1288409	
O	-3.3548593	-0.7943141	-0.0155944	
H	1.5019667	-1.3662080	0.0370894	

	H	1.9896064	-0.3533896	1.4061599
	H	2.0248591	1.6200175	-0.1146953
	H	1.4009999	0.6178045	-1.4139424
	H	-0.3873003	1.9422915	-0.2939411
	H	-0.0167547	1.1800291	1.2382276
	H	-0.7379703	-1.0264959	0.3526974
	H	-0.9646005	-0.3228287	-1.2433246
	H	-2.7343973	1.1659210	-0.3178920
	H	-2.4836555	0.4663643	1.2800344
	H	3.7889757	-1.3024578	0.2350376
	H	-3.3562344	-0.9866435	-0.9559598
tTTG+Tg-	C	2.4201608	0.2655790	0.2006984
	C	1.0046004	-0.1008438	-0.1855599
	C	0.0227764	1.0156322	0.1521993
	C	-1.3974116	0.7430984	-0.3367831
	C	-2.0297156	-0.4714890	0.3205272
	O	3.2608444	-0.8348117	-0.1249883
	O	-3.3676694	-0.6883979	-0.1070297
	H	2.4665176	0.4828335	1.2723737
	H	2.7313784	1.1635863	-0.3417040
	H	0.9765264	-0.3116977	-1.2565992
	H	0.7402222	-1.0231785	0.3321843
	H	0.3752528	1.9481702	-0.2947409
	H	0.0092898	1.1751921	1.2341858
	H	-1.4020603	0.6002178	-1.4189209
	H	-2.0235101	1.6146537	-0.1254957
	H	-1.9819008	-0.3686469	1.4102054
	H	-1.4953624	-1.3790530	0.0501959
	H	4.1622253	-0.6090501	0.1141130
	H	-3.8759161	0.0972603	0.1074357
g-G+TG-G-g-	C	2.1728855	-0.7543505	0.0821245
	C	0.8289532	-0.2732696	0.6030206
	C	0.0529335	0.5368131	-0.4271668
	C	-1.2683608	1.0876271	0.1024459
	C	-2.2411237	0.0103219	0.5546256
	O	3.0763680	0.3077640	-0.1990671
	O	-2.4954560	-0.9595155	-0.4544248
	H	2.0243236	-1.3774166	-0.8054668
	H	2.6702961	-1.3619607	0.8352465
	H	0.2511326	-1.1539671	0.8910206
	H	0.9941615	0.3251214	1.5022850
	H	-0.1417538	-0.0894302	-1.3004006
	H	0.6591946	1.3825278	-0.7604033
	H	-1.7471313	1.6935380	-0.6720832
	H	-1.0798408	1.7544517	0.9483528
	H	-3.1735861	0.4706431	0.8918175
	H	-1.8325972	-0.5491610	1.3931851
	H	2.7465102	0.7836769	-0.9635447
	H	-2.9333220	-0.5169299	-1.1854777
g-TTG-G-g-	C	2.2049957	0.0300786	-0.4685274
	C	0.8847600	0.1058190	0.2768926

C	-0.1816349	0.8192413	-0.5453236	
C	-1.4852301	1.0448904	0.2149263	
C	-2.1536463	-0.2411674	0.6735122	
O	3.2048655	-0.6884266	0.2411233	
O	-2.3924587	-1.1471165	-0.3962565	
H	2.5540552	1.0387003	-0.7124204	
H	2.0708711	-0.5087421	-1.4052844	
H	0.5697949	-0.9097242	0.5175561	
H	1.0363782	0.6360985	1.2231334	
H	-0.3872054	0.2361372	-1.4444240	
H	0.2041498	1.7873621	-0.8741871	
H	-2.1844573	1.5996455	-0.4173537	
H	-1.3006714	1.6667946	1.0954647	
H	-3.0841906	-0.0090375	1.1984586	
H	-1.5128647	-0.7805544	1.3677198	
H	3.3641075	-0.2302675	1.0693584	
H	-3.0110226	-0.7318561	-1.0021333	
tG-TG-Tg-	C	2.4970392	0.2419113	0.4325497
	C	1.0045461	0.3020548	0.6751848
	C	0.2191048	0.5783746	-0.6023138
	C	-1.2828633	0.7307723	-0.3771882
	C	-1.9537989	-0.5583253	0.0647998
	O	2.7487355	-0.8641342	-0.4280325
	O	-3.3689670	-0.4366118	0.1447312
	H	3.0274363	0.1180834	1.3803974
	H	2.8354866	1.1738524	-0.0318721
	H	0.6976364	-0.6447175	1.1216280
	H	0.8047147	1.0885428	1.4079312
	H	0.4040609	-0.2243883	-1.3177865
	H	0.6054543	1.4947631	-1.0555973
	H	-1.7658309	1.0579414	-1.2990805
	H	-1.4653571	1.5068299	0.3734241
	H	-1.5484956	-0.9009030	1.0200086
	H	-1.7698948	-1.3400919	-0.6712280
	H	3.6925270	-0.9118037	-0.5937498
	H	-3.5691430	0.2320957	0.8035729
g-G-TG+G+g+	C	-2.1738141	-0.7585161	0.0323411
	C	-0.8110431	-0.3157791	0.5372034
	C	-0.0495145	0.5032432	-0.4959389
	C	1.2487563	1.0994918	0.0383648
	C	2.2265871	0.0634647	0.5689969
	O	-3.0346977	0.3349878	-0.2648288
	O	2.5181875	-0.9562751	-0.3784467
	H	-2.6454628	-1.4312408	0.7536842
	H	-2.0632508	-1.3010852	-0.9057513
	H	-0.9433041	0.2668611	1.4557991
	H	-0.2425385	-1.2086661	0.8064182
	H	-0.6927930	1.3069874	-0.8550334
	H	0.1714933	-0.1360881	-1.3525696
	H	1.0317702	1.8050248	0.8456219
	H	1.7373533	1.6752637	-0.7530746

H	1.8061132	-0.4567700	1.4273164	
H	3.1449724	0.5548617	0.9022415	
H	-3.2285410	0.7868437	0.5596457	
H	2.9237262	-0.5407094	-1.1434009	
tG+G+TG-g-	C	2.2290215	0.0864052	0.5433921
	C	1.2495916	1.1102132	0.0078273
	C	-0.0510014	0.5009271	-0.5067629
	C	-0.8024201	-0.3083579	0.5412187
	C	-2.1656546	-0.7666617	0.0515126
	O	2.4743250	-0.8641362	-0.4885920
	O	-3.0381468	0.3166332	-0.2482631
	H	1.8180091	-0.4088268	1.4277315
	H	3.1571548	0.5836088	0.8373091
	H	1.0365874	1.8236277	0.8082363
	H	1.7342078	1.6641607	-0.7978117
	H	0.1697129	-0.1442467	-1.3583327
	H	-0.6995231	1.2993607	-0.8684792
	H	-0.9330660	0.2840813	1.4539844
	H	-0.2275113	-1.1949000	0.8188420
	H	-2.6263952	-1.4365224	0.7828939
	H	-2.0581370	-1.3164276	-0.8827415
	H	3.1297991	-1.4899159	-0.1734977
	H	-3.2140038	0.7852505	0.5709140
g+G-TTG-g+	C	0.0066704	2.5402322	-0.0177221
	C	-0.0164599	1.2668514	-0.8451471
	C	-0.0000006	0.0000000	0.0007495
	C	0.0164593	-1.2668512	-0.8451472
	C	-0.0066694	-2.5402320	-0.0177223
	O	-1.1631037	2.7093264	0.7724174
	O	1.1631055	-2.7093250	0.7724166
	H	0.0414147	3.4106103	-0.6697256
	H	0.9021215	2.5595621	0.6123100
	H	-0.9058794	1.2757229	-1.4785290
	H	0.8551907	1.2692046	-1.5051351
	H	-0.8821212	-0.0252758	0.6485932
	H	0.8821195	0.0252757	0.6485940
	H	0.9058785	-1.2757219	-1.4785295
	H	-0.8551916	-1.2692050	-1.5051349
	H	-0.0414132	-3.4106102	-0.6697257
	H	-0.9021201	-2.5595628	0.6123105
	H	-1.1618468	2.0377488	1.4571496
	H	1.1618457	-2.0377504	1.4571518
tTG+TTg-	C	-2.0299084	-0.4689794	0.2977272
	C	-1.3962759	0.7665895	-0.3044616
	C	0.0277684	1.0089051	0.1866185
	C	1.0070698	-0.0987000	-0.1891429
	C	2.4303617	0.2570876	0.2007961
	O	-3.3875237	-0.5033758	-0.1290418
	O	3.3745975	-0.7388909	-0.1685813
	H	-1.9693596	-0.4180869	1.3901748
	H	-1.5060846	-1.3694906	-0.0312999

H	-1.4074050	0.6721263	-1.3917361	
H	-2.0262314	1.6199336	-0.0497687	
H	0.0214483	1.1370156	1.2727152	
H	0.3857115	1.9515009	-0.2337216	
H	0.9716748	-0.2814682	-1.2651644	
H	0.7312037	-1.0332147	0.3061763	
H	2.4825027	0.4601860	1.2752648	
H	2.7436743	1.1601867	-0.3207263	
H	-3.7882800	-1.3101785	0.2010118	
H	3.1477209	-1.5470233	0.2969160	
tTG+TG-g-	C	2.1079063	0.4058183	0.1747508
	C	1.1961277	-0.7773327	-0.0678340
	C	-0.2204652	-0.5603778	0.4540993
	C	-0.9595800	0.5846106	-0.2292330
	C	-2.4229627	0.6551786	0.1753431
	O	3.4143302	0.0369856	-0.2550325
	O	-3.1500732	-0.5141180	-0.1808890
	H	2.1081392	0.6562792	1.2408971
	H	1.7598352	1.2805263	-0.3801461
	H	1.1730391	-0.9869206	-1.1391951
	H	1.6421294	-1.6462560	0.4179350
	H	-0.1902988	-0.3711358	1.5311687
	H	-0.7967695	-1.4751287	0.3156915
	H	-0.8948176	0.4679852	-1.3163589
	H	-0.4960162	1.5444164	0.0101072
	H	-2.8925505	1.5440762	-0.2544522
	H	-2.5065026	0.7257603	1.2592871
	H	3.9949658	0.7919809	-0.1399208
	H	-3.1636746	-0.5703051	-1.1392052
tG-TG-G-t	C	-2.3619441	-0.2444997	0.2305942
	C	-0.9101561	-0.5366325	0.5436028
	C	-0.0318964	-0.5352266	-0.7012978
	C	1.3994867	-0.9904343	-0.4313140
	C	2.1482758	-0.1015175	0.5400807
	O	-2.4363568	1.0730149	-0.3026649
	O	2.1701497	1.2132993	-0.0042396
	H	-2.9654247	-0.3237114	1.1391496
	H	-2.7373091	-0.9735568	-0.4950703
	H	-0.5609728	0.2116384	1.2570249
	H	-0.8572762	-1.5115608	1.0372218
	H	-0.0212620	0.4634463	-1.1338119
	H	-0.4754852	-1.2029724	-1.4447584
	H	1.9571301	-1.0151444	-1.3692039
	H	1.3987716	-2.0068155	-0.0281437
	H	3.1656402	-0.4796311	0.6735591
	H	1.6574671	-0.1039882	1.5172566
	H	-3.3522773	1.2611770	-0.5172632
	H	2.6197383	1.7909725	0.6158619
g+TTG-Tg+	C	-2.4282990	0.2658729	0.2091383
	C	-1.0111504	-0.0946053	-0.1989669
	C	-0.0238107	1.0089514	0.1670150

C	1.3969222	0.7465116	-0.3261102	
C	2.0322285	-0.4754747	0.3143371	
O	-3.3807117	-0.7231632	-0.1556405	
O	3.3688496	-0.6870987	-0.1188309	
H	-2.7432270	1.1735933	-0.3034326	
H	-2.4670473	0.4627572	1.2853601	
H	-0.7327305	-1.0310486	0.2907576	
H	-0.9893808	-0.2747273	-1.2756813	
H	-0.0126132	1.1437723	1.2523897	
H	-0.3761640	1.9513929	-0.2584208	
H	2.0208783	1.6163665	-0.1023284	
H	1.4019792	0.6191757	-1.4101263	
H	1.4983190	-1.3803278	0.0336203	
H	1.9867740	-0.3861767	1.4053365	
H	-3.1512623	-1.5363034	0.2998963	
H	3.8775442	0.0964219	0.1024860	
g-TG+TG-g-	C	-2.1098155	-0.4189876	0.1839016
	C	-1.1996254	0.7637371	-0.0966969
	C	0.2168804	0.5695601	0.4364530
	C	0.9627105	-0.5853646	-0.2221895
	C	2.4235922	-0.6426415	0.1932224
	O	-3.4347232	-0.2163355	-0.2893116
	O	3.1475349	0.5236141	-0.1796040
	H	-2.1101385	-0.6373838	1.2574514
	H	-1.7585124	-1.3085933	-0.3340680
	H	-1.1753435	0.9407629	-1.1739266
	H	-1.6383010	1.6538289	0.3632329
	H	0.1821239	0.4003508	1.5167710
	H	0.7896395	1.4841947	0.2829661
	H	0.9045449	-0.4878362	-1.3114020
	H	0.5003344	-1.5419153	0.0313418
	H	2.8995374	-1.5370306	-0.2173276
	H	2.5002521	-0.6934591	1.2787699
	H	-3.7781379	0.5756606	0.1307868
	H	3.1826681	0.5529143	-1.1385486
g+TTG+Tg-	C	2.4274731	0.2720171	0.2081174
	C	1.0075598	-0.1078037	-0.1720170
	C	0.0232111	1.0148106	0.1396555
	C	-1.3958007	0.7366013	-0.3493934
	C	-2.0341754	-0.4633230	0.3287437
	O	3.3591456	-0.7798443	-0.0005962
	O	-3.3669466	-0.6912990	-0.1082413
	H	2.4795833	0.4973701	1.2724082
	H	2.7304862	1.1721720	-0.3362090
	H	0.9691440	-0.3368222	-1.2417044
	H	0.7435209	-1.0202461	0.3630815
	H	0.3798790	1.9389139	-0.3212473
	H	0.0082026	1.1922387	1.2187310
	H	-1.3968521	0.5723608	-1.4286666
	H	-2.0203559	1.6138251	-0.1584795
	H	-1.9974544	-0.3361018	1.4161509

H	-1.4963624	-1.3763934	0.0847672	
H	3.3609063	-0.9909946	-0.9369550	
H	-3.8814273	0.0937215	0.0933433	
g+TTG-Tg-	C	-2.4328719	0.2624581	0.1996309
	C	-1.0136329	-0.1001345	-0.1986514
	C	-0.0271231	1.0043780	0.1668799
	C	1.3971623	0.7478275	-0.3187846
	C	2.0480953	-0.4523961	0.3467698
	O	-3.3842871	-0.7230397	-0.1752817
	O	3.4167029	-0.5963989	-0.0078129
	H	-2.7414272	1.1726562	-0.3128459
	H	-2.4793637	0.4571808	1.2760668
	H	-0.7388728	-1.0355317	0.2949793
	H	-0.9879491	-0.2840694	-1.2749891
	H	-0.0178000	1.1427336	1.2519162
	H	-0.3802848	1.9455980	-0.2608534
	H	2.0209341	1.6200344	-0.1181761
	H	1.3904086	0.5992346	-1.4029104
	H	1.4979984	-1.3688184	0.1188362
	H	2.0408646	-0.3223739	1.4288668
	H	-3.1726007	-1.5330916	0.2940680
	H	3.4619550	-0.7479340	-0.9546192
t+G-TG+G+g-	C	-2.1719573	-0.7523148	0.0904788
	C	-0.8185038	-0.2844828	0.5823552
	C	-0.0520460	0.4965669	-0.4789429
	C	1.2619482	1.0875696	0.0258640
	C	2.2523884	0.0524054	0.5338726
	O	-2.9534047	0.4026176	-0.1939161
	O	2.6398580	-0.8807296	-0.4673229
	H	-2.6574448	-1.3640505	0.8552317
	H	-2.0485052	-1.3629928	-0.8100449
	H	-0.9677305	0.3408232	1.4657687
	H	-0.2555390	-1.1640098	0.9034383
	H	-0.6878977	1.3023724	-0.8442776
	H	0.1370708	-0.1505978	-1.3412598
	H	1.0527453	1.7867947	0.8401570
	H	1.7361885	1.6554572	-0.7760478
	H	1.8501080	-0.4690396	1.4069758
	H	3.1736105	0.5418509	0.8427381
	H	-3.8151388	0.1173796	-0.5045686
	H	1.8559178	-1.3603058	-0.7435057
g+TTG+Tg+	C	2.4305463	0.2623256	0.2104880
	C	1.0134104	-0.1111055	-0.1856984
	C	0.0265808	1.0068300	0.1352270
	C	-1.3955705	0.7341643	-0.3479224
	C	-2.0528424	-0.4367540	0.3624762
	O	3.3644067	-0.7840124	-0.0143325
	O	-3.4199607	-0.5919859	0.0049161
	H	2.4759224	0.4659019	1.2795080
	H	2.7356785	1.1741540	-0.3130066
	H	0.9841907	-0.3227231	-1.2595271

H	0.7460530	-1.0326550	0.3317503	
H	0.3816241	1.9344998	-0.3197979	
H	0.0128400	1.1784175	1.2153766	
H	-1.3837006	0.5416702	-1.4252364	
H	-2.0186068	1.6149894	-0.1867400	
H	-2.0521543	-0.2619020	1.4380847	
H	-1.5032399	-1.3627198	0.1769240	
H	3.3844374	-0.9650450	-0.9567486	
H	-3.4586684	-0.7949940	-0.9324300	
tTG+TG+g-	C	1.9603397	-0.5325752	0.0086510
	C	1.2761188	0.7936037	-0.2450755
	C	-0.2233013	0.6525831	-0.4901232
	C	-0.9934111	0.0997897	0.7045585
	C	-2.4977513	0.1241675	0.4947808
	O	3.3595294	-0.2826352	0.0807254
	O	-2.9221273	-0.7323784	-0.5578970
	H	1.7319950	-1.2257101	-0.8079778
	H	1.6049562	-0.9773718	0.9409645
	H	1.4564047	1.4514939	0.6072340
	H	1.7535468	1.2526515	-1.1119482
	H	-0.3777935	0.0071304	-1.3595273
	H	-0.6308335	1.6342436	-0.7472644
	H	-0.7586635	0.6963197	1.5910721
	H	-0.6939193	-0.9282474	0.9127950
	H	-2.8308130	1.1511493	0.3118777
	H	-3.0089432	-0.2380552	1.3843811
	H	3.8039360	-1.1075604	0.2871445
	H	-2.5982377	-0.3698639	-1.3849032
tTTG+G+g-	C	2.1940718	0.0575963	0.4322457
	C	0.8656548	0.1136827	-0.2882220
	C	-0.1857560	0.8616221	0.5227499
	C	-1.5107011	1.0451297	-0.2129334
	C	-2.1714100	-0.2612899	-0.6235066
	O	3.0997638	-0.6798542	-0.3789458
	O	-2.4614195	-1.1032514	0.4854423
	H	2.0667705	-0.4251330	1.4064116
	H	2.5652143	1.0726016	0.6033292
	H	1.0112197	0.5997778	-1.2551978
	H	0.5505500	-0.9111146	-0.4934953
	H	0.2030197	1.8464906	0.7917912
	H	-0.3639777	0.3417765	1.4680191
	H	-1.3472692	1.6419170	-1.1144815
	H	-2.2036669	1.5978767	0.4232445
	H	-1.5566100	-0.7902704	-1.3562648
	H	-3.1322449	-0.0558874	-1.0911110
	H	3.9488561	-0.7139337	0.0666135
	H	-1.6310122	-1.4399914	0.8284360
tTG-TG+g-	C	2.1026991	-0.3990813	0.2158852
	C	1.2089521	0.7684470	-0.1441111
	C	-0.2250031	0.6018627	0.3508326
	C	-0.9644636	-0.5709518	-0.2834792

C	-2.4095034	-0.6769481	0.1761804	
O	3.4261797	-0.0608048	-0.1838666	
O	-3.2060559	0.4301018	-0.2242796	
H	1.7736966	-1.3084150	-0.2922664	
H	2.0584517	-0.5762069	1.2958560	
H	1.6493385	1.6677091	0.2888118	
H	1.2173562	0.8966674	-1.2279821	
H	-0.7634248	1.5266696	0.1318062	
H	-0.2255537	0.4841689	1.4391419	
H	-0.4670311	-1.5103396	-0.0320992	
H	-0.9464527	-0.4715047	-1.3711149	
H	-2.4449156	-0.8021701	1.2634035	
H	-2.8819229	-1.5477318	-0.2736661	
H	3.9960785	-0.8131903	-0.0116565	
H	-2.9095956	1.2024137	0.2610473	
g+TG-TG-g-	C	-1.9354537	-0.5581822	0.0385766
	C	-1.2878682	0.7798634	-0.2744296
	C	0.2124907	0.6712275	-0.5332033
	C	1.0162298	0.2599604	0.6947744
	C	2.5082631	0.1938845	0.4151405
	O	-3.3376601	-0.4535022	0.2446828
	O	2.8368361	-0.7709619	-0.5772772
	H	-1.5451656	-0.9708428	0.9661314
	H	-1.7124642	-1.2706259	-0.7630637
	H	-1.7750829	1.1961242	-1.1607853
	H	-1.4840256	1.4678932	0.5504898
	H	0.5856163	1.6376522	-0.8803762
	H	0.3993174	-0.0395596	-1.3401992
	H	0.6882589	-0.7155280	1.0635601
	H	0.8441887	0.9749703	1.5045664
	H	3.0596449	-0.0023037	1.3385588
	H	2.8552555	1.1461476	0.0156051
	H	-3.7238623	-0.0787945	-0.5503639
	H	2.6317130	-1.6389437	-0.2219896
g+TG+TG-g-	C	2.1223651	0.4118852	0.2075267
	C	1.2019739	-0.7646054	-0.0661844
	C	-0.2184681	-0.5500043	0.4484012
	C	-0.9670606	0.5762738	-0.2554115
	C	-2.4257018	0.6530861	0.1647201
	O	3.4710380	0.1489104	-0.1581574
	O	-3.1522936	-0.5278085	-0.1514855
	H	2.1471641	0.6189590	1.2771608
	H	1.7617822	1.3125732	-0.2961075
	H	1.1734693	-0.9554054	-1.1438816
	H	1.6381972	-1.6476528	0.4028615
	H	-0.1875121	-0.3409028	1.5219142
	H	-0.7889991	-1.4710797	0.3288868
	H	-0.9161559	0.4309482	-1.3399592
	H	-0.5034169	1.5430463	-0.0475967
	H	-2.9031962	1.5289467	-0.2826151
	H	-2.4960885	0.7528700	1.2473719

H	3.4904704	-0.0299644	-1.1010486	
H	-3.2044566	-0.5937884	-1.1078057	
tTG-TG-g-	C	-1.9416125	-0.5407734	0.0347870
	C	-1.2847151	0.7828595	-0.2928332
	C	0.2155823	0.6615509	-0.5407435
	C	1.0129746	0.2453848	0.6897912
	C	2.5077464	0.1922020	0.4239612
	O	-3.3444997	-0.3140131	0.1191206
	O	2.8540666	-0.7682266	-0.5668927
	H	-1.5651931	-0.9354281	0.9818152
	H	-1.7135137	-1.2669995	-0.7525499
	H	-1.7753237	1.1827860	-1.1813537
	H	-1.4795299	1.4825947	0.5225752
	H	0.5953830	1.6264238	-0.8849782
	H	0.4026755	-0.0483685	-1.3483981
	H	0.6890774	-0.7359285	1.0475031
	H	0.8285304	0.9516964	1.5047089
	H	3.0527379	-0.0008300	1.3520270
	H	2.8502934	1.1480344	0.0290310
	H	-3.7712953	-1.1408272	0.3532383
	H	2.6482726	-1.6380116	-0.2165053
g+G+G+TG+g-	C	2.1473470	-0.1187669	-0.5810093
	C	1.3990596	-0.9871425	0.4178894
	C	-0.0225943	-0.5077024	0.6972846
	C	-0.9318797	-0.5646694	-0.5251037
	C	-2.3805000	-0.2496784	-0.1915388
	O	2.2125636	1.2437596	-0.1789693
	O	-2.5751052	1.0935682	0.2272950
	H	1.6374451	-0.1105572	-1.5419266
	H	3.1503735	-0.5217459	-0.7447227
	H	1.3764729	-2.0113813	0.0350174
	H	1.9669621	-1.0148926	1.3522542
	H	0.0291474	0.5155281	1.0749541
	H	-0.4545717	-1.1265456	1.4887143
	H	-0.8913505	-1.5680895	-0.9595122
	H	-0.5938911	0.1397188	-1.2860967
	H	-2.7439166	-0.9467527	0.5716498
	H	-3.0052789	-0.3677358	-1.0745601
	H	2.7438301	1.2906305	0.6195007
	H	-2.0425641	1.2407590	1.0118220
tG-TG+G-t	C	-2.1351139	0.7112241	0.2517817
	C	-0.7413009	0.4901098	-0.2922431
	C	-0.0993793	-0.7756648	0.2652435
	C	1.2904616	-1.0781443	-0.2913381
	C	2.4084642	-0.2281982	0.2752182
	O	-2.9522677	-0.3824032	-0.1596913
	O	2.2473686	1.1191064	-0.1628187
	H	-2.5397706	1.6523950	-0.1296707
	H	-2.1020820	0.7708501	1.3447766
	H	-0.8007111	0.4189699	-1.3807699
	H	-0.1284076	1.3592591	-0.0592787

H	-0.7587633	-1.6160051	0.0467765	
H	-0.0396913	-0.7012914	1.3562573	
H	1.2893737	-0.9768475	-1.3791580	
H	1.5436230	-2.1177244	-0.0703373	
H	3.3715310	-0.6200771	-0.0634211	
H	2.3865281	-0.2770156	1.3691026	
H	-3.8379184	-0.2424463	0.1811919	
H	2.9952300	1.6282305	0.1572997	
g-G-TG-G-g-	C	-2.3246995	-0.2273042	0.2805512
C	-0.8708586	-0.5540640	0.5772434	
C	-0.0251608	-0.6464476	-0.6848689	
C	1.4320241	-1.0116119	-0.4176316	
C	2.1402776	-0.0488424	0.5233538	
O	-2.4794660	1.0160476	-0.3905461	
O	2.0025954	1.3116076	0.1319688	
H	-2.9095061	-0.2398798	1.2048469	
H	-2.7485692	-0.9716979	-0.3927347	
H	-0.4716969	0.2188476	1.2395766	
H	-0.8313579	-1.4975415	1.1302445	
H	-0.0729614	0.3062648	-1.2101571	
H	-0.4622238	-1.3946682	-1.3508460	
H	1.9755689	-1.0458796	-1.3662058	
H	1.4986659	-2.0140237	0.0148749	
H	3.1958673	-0.3216385	0.6079962	
H	1.7104407	-0.1023240	1.5214511	
H	-2.0771311	1.6956620	0.1563189	
H	2.3868634	1.4081617	-0.7428771	
* tG+G-G+G+g-	C	2.0623882	0.0131065	0.0303420
C	1.0599497	-1.0511468	0.4194539	
C	-0.0737619	-1.2084674	-0.6087007	
C	-1.4739098	-1.0288930	-0.0263910	
C	-1.7136011	0.3628338	0.5462712	
O	1.3777338	1.2702213	0.0104492	
O	-1.4750294	1.3861148	-0.4033773	
H	2.4743663	-0.2032673	-0.9591594	
H	2.8826745	0.0505947	0.7504566	
H	1.6008270	-1.9902041	0.5428184	
H	0.6591463	-0.7926907	1.4009632	
H	-0.0105714	-2.1901564	-1.0786328	
H	0.0561509	-0.4783097	-1.4090116	
H	-1.6496829	-1.7667952	0.7621956	
H	-2.2099101	-1.2095978	-0.8117622	
H	-1.0964813	0.5230490	1.4351667	
H	-2.7546835	0.4548168	0.8533156	
H	1.9962315	1.9535714	-0.2583691	
H	-0.5168339	1.4984832	-0.4347614	
tG-G+TG-g-	C	-2.4095237	0.2221773	0.2563236
C	-1.2856186	1.0820084	-0.2831454	
C	0.0956846	0.7797527	0.2931802	
C	0.7367633	-0.5040826	-0.2206421	
C	2.1515651	-0.6868409	0.2989435	

O	-2.2450543	-1.1147925	-0.2107230	
O	3.0328590	0.3565761	-0.1050473	
H	-3.3690571	0.6223859	-0.0822907	
H	-2.3971698	0.2474485	1.3511063	
H	-1.2679517	0.9897012	-1.3717949	
H	-1.5445483	2.1190917	-0.0572714	
H	0.0259786	0.7332192	1.3847838	
H	0.7640780	1.6107839	0.0637423	
H	0.7578142	-0.4890284	-1.3154732	
H	0.1375265	-1.3688921	0.0620654	
H	2.5450309	-1.6588283	-0.0111520	
H	2.1574191	-0.6590157	1.3883201	
H	-2.9951909	-1.6312946	0.0918702	
H	3.0975022	0.3266493	-1.0624905	
g+TG-TG+g-	C	2.1071044	-0.4035021	0.2414531
	C	1.2128666	0.7518109	-0.1750586
	C	-0.2223305	0.6096083	0.3266991
	C	-0.9687621	-0.5701639	-0.2859788
	C	-2.4096869	-0.6676687	0.1880610
	O	3.4464036	-0.2452578	-0.2052306
	O	-3.2060399	0.4390118	-0.2143854
	H	1.7690237	-1.3356497	-0.2049785
	H	2.0718627	-0.5232407	1.3299033
	H	1.6420947	1.6776933	0.2181964
	H	1.2228021	0.8315535	-1.2636304
	H	-0.7563583	1.5330291	0.0919459
	H	-0.2204470	0.5111179	1.4170723
	H	-0.4706287	-1.5072863	-0.0283355
	H	-0.9606177	-0.4833476	-1.3746934
	H	-2.4358831	-0.7841581	1.2763978
	H	-2.8882982	-1.5407277	-0.2505554
	H	3.7848732	0.5743796	0.1625446
	H	-2.9156857	1.2105124	0.2757360
g+TTG+G+g-	C	-2.1995233	0.0352300	-0.4527024
	C	-0.8730409	0.1166815	0.2817262
	C	0.1845355	0.8402239	-0.5441215
	C	1.5052577	1.0511101	0.1915267
	C	2.1724761	-0.2397578	0.6394491
	O	-3.1810267	-0.7093250	0.2529097
	O	2.4807717	-1.1048966	-0.4461535
	H	-2.0676784	-0.4848132	-1.4006841
	H	-2.5626765	1.0430820	-0.6773816
	H	-1.0171576	0.6410701	1.2316375
	H	-0.5579580	-0.8995406	0.5255912
	H	-0.2051953	1.8139742	-0.8499396
	H	0.3671333	0.2878834	-1.4699079
	H	1.3353512	1.6717112	1.0757875
	H	2.1979545	1.5901061	-0.4566046
	H	1.5552824	-0.7569257	1.3787986
	H	3.1268554	-0.0148714	1.1112171
	H	-3.3650369	-0.2518278	1.0763264

	H	1.6575847	-1.4587354	-0.7894899
tG-G-TG-g-	C	2.1497835	-0.0458968	0.4921997
	C	1.4246564	-1.0148481	-0.4195101
	C	-0.0326004	-0.6390762	-0.6743337
	C	-0.8637633	-0.5237860	0.5958004
	C	-2.3265749	-0.2258504	0.3142731
	O	2.0068681	1.2619492	-0.0534882
	O	-2.5137146	0.9915439	-0.3952145
	H	3.2049604	-0.3232569	0.5568608
	H	1.7303106	-0.0848511	1.5013752
	H	1.9566609	-1.0605237	-1.3710810
	H	1.4839736	-2.0082419	0.0329899
	H	-0.4821054	-1.3959129	-1.3219707
	H	-0.0724585	0.3035594	-1.2167965
	H	-0.4653917	0.2692968	1.2349936
	H	-0.8056080	-1.4523739	1.1723700
	H	-2.8947933	-0.2156555	1.2491320
	H	-2.7509408	-0.9989141	-0.3256591
	H	2.5373357	1.8666705	0.4695033
	H	-2.0823542	1.6902486	0.1031097
g+TG-TG-g+	C	-1.9631147	-0.5451000	-0.0081532
	C	-1.2793962	0.7976826	-0.2015834
	C	0.2194097	0.6705903	-0.4628802
	C	0.9940783	0.0737433	0.7073786
	C	2.4977113	0.1105505	0.4939834
	O	-3.3640687	-0.4191208	0.1907462
	O	2.9209550	-0.7015540	-0.5936240
	H	-1.5935664	-1.0415433	0.8859639
	H	-1.7474015	-1.1960661	-0.8624500
	H	-1.7512929	1.3065495	-1.0468547
	H	-1.4560865	1.4138523	0.6821218
	H	0.6253040	1.6614109	-0.6855162
	H	0.3699306	0.0572765	-1.3559611
	H	0.6976467	-0.9622009	0.8761823
	H	0.7607411	0.6346817	1.6170997
	H	3.0117628	-0.2861432	1.3670212
	H	2.8280308	1.1448791	0.3521595
	H	-3.7357434	0.0036257	-0.5868447
	H	2.6044361	-0.3008722	-1.4056441
tG+G-TG-g-	C	-2.2545176	-0.1225658	-0.4574481
	C	-1.4561511	1.0695481	0.0268619
	C	0.0440478	0.9786092	-0.2548415
	C	0.8249839	0.1809185	0.7836109
	C	2.2921099	0.0412358	0.4208621
	O	-1.8377663	-1.2893414	0.2493382
	O	2.4879909	-0.6851140	-0.7881799
	H	-2.0921336	-0.2545294	-1.5318757
	H	-3.3201390	0.0576171	-0.2917852
	H	-1.8693684	1.9459499	-0.4773750
	H	-1.6330918	1.2057446	1.0963501
	H	0.4633516	1.9872802	-0.2937606

H	0.2027709	0.5401249	-1.2422740	
H	0.3837352	-0.8096123	0.9018725	
H	0.7518055	0.6768470	1.7557724	
H	2.8412130	-0.4297310	1.2411035	
H	2.7359734	1.0202961	0.2415462	
H	-2.3884045	-2.0218205	-0.0359010	
H	2.0817691	-1.5476949	-0.6728576	
g+G+TG+G+g-	C	2.3282059	-0.1881682	0.1510925
C	0.9455160	-0.6966701	0.5226314	
C	0.0057341	-0.7187622	-0.6769957	
C	-1.4483586	-1.0226070	-0.3261719	
C	-2.0987701	0.0371811	0.5499328	
O	2.3010882	1.1759919	-0.2588217	
O	-2.1135392	1.3218277	-0.0554685	
H	2.7150657	-0.7415286	-0.7040841	
H	3.0256216	-0.3246900	0.9810197	
H	1.0326946	-1.7011565	0.9459168	
H	0.5507072	-0.0571111	1.3167163	
H	0.3655814	-1.4682470	-1.3854290	
H	0.0720576	0.2363269	-1.2022865	
H	-1.5105658	-1.9829480	0.1935691	
H	-2.0302176	-1.1119578	-1.2448582	
H	-1.6118676	0.0808933	1.5284750	
H	-3.1434658	-0.2153068	0.7195677	
H	2.1963631	1.7166629	0.5272329	
H	-1.2055459	1.5751794	-0.2386805	
tG+G-TTg-	C	-2.4126386	0.1199427	0.2826514
C	-1.5863543	-0.9566752	-0.3901066	
C	-0.1694714	-1.1210530	0.1562860	
C	0.8008759	-0.0081205	-0.2250525	
C	2.2016306	-0.3047350	0.2766570	
O	-1.8988625	1.3979633	-0.0795590	
O	3.1286409	0.7338972	-0.0104782	
H	-2.3763801	-0.0139444	1.3690610	
H	-3.4546227	0.0292000	-0.0361602	
H	-2.1252844	-1.8982924	-0.2623270	
H	-1.5547593	-0.7509874	-1.4625629	
H	0.2304296	-2.0721752	-0.2060514	
H	-0.2170795	-1.2038889	1.2465682	
H	0.4667793	0.9470929	0.1733307	
H	0.8225485	0.0900434	-1.3151797	
H	2.5530248	-1.2578091	-0.1335695	
H	2.1984539	-0.3959110	1.3623562	
H	-2.4530784	2.0700440	0.3232285	
H	3.1193319	0.8791708	-0.9592971	
g+TTG-G-g+	C	-2.2063821	0.0517409	0.4384464
C	-0.8773351	0.1119762	-0.2933709	
C	0.1828378	0.8435106	0.5230499	
C	1.5043178	1.0405127	-0.2164814	
C	2.1736914	-0.2577253	-0.6377839	
O	-3.2303851	-0.5776939	-0.3183953	

O	2.4903814	-1.0989537	0.4642190	
H	-2.5684229	1.0602136	0.6325351	
H	-2.0777518	-0.4449396	1.4057332	
H	-0.5536268	-0.9089947	-0.5163440	
H	-1.0263963	0.6135010	-1.2518293	
H	0.3621161	0.3106193	1.4611575	
H	-0.2058589	1.8233523	0.8093053	
H	2.1957719	1.5955753	0.4191501	
H	1.3308372	1.6409924	-1.1135390	
H	3.1254579	-0.0417037	-1.1182847	
H	1.5544922	-0.7923874	-1.3630969	
H	-2.9663110	-1.4868059	-0.4768862	
H	1.6677734	-1.3865740	0.8657670	
g-TG-TG-g-	C	-1.9484428	-0.5632983	0.0400267
	C	-1.2867806	0.7500019	-0.3402310
	C	0.2150832	0.6179708	-0.5789380
	C	1.0149537	0.3008581	0.6794353
	C	2.5093279	0.2296477	0.4146953
	O	-3.3629968	-0.4554855	0.1356224
	O	2.8540196	-0.7993054	-0.5045163
	H	-1.5346421	-0.9519041	0.9741237
	H	-1.7657340	-1.3051738	-0.7368074
	H	-1.7753458	1.1191730	-1.2430298
	H	-1.4706349	1.4870723	0.4482055
	H	0.5926819	1.5532787	-0.9989854
	H	0.4019786	-0.1527474	-1.3289089
	H	0.6932142	-0.6490418	1.1145536
	H	0.8324985	1.0697372	1.4362627
	H	3.0559222	0.1053752	1.3534845
	H	2.8499765	1.1548614	-0.0490410
	H	-3.5634384	0.1840916	0.8227903
	H	2.6565232	-1.6425075	-0.0900632
tG-G+TTg-	C	2.4288256	0.1226174	0.2560988
	C	1.5846070	-0.9575195	-0.3874088
	C	0.1780976	-1.1046851	0.1920128
	C	-0.8184860	-0.0537757	-0.2856673
	C	-2.1911990	-0.2760085	0.3199653
	O	1.8744163	1.3999591	-0.0471039
	O	-3.1635134	0.6451682	-0.1565008
	H	3.4522410	0.0566328	-0.1229198
	H	2.4563939	-0.0321771	1.3398984
	H	1.5301835	-0.7693847	-1.4619655
	H	2.1254400	-1.8974730	-0.2556596
	H	0.2403909	-1.0850485	1.2846524
	H	-0.2074518	-2.0919179	-0.0758474
	H	-0.9033165	-0.0935732	-1.3735950
	H	-0.4580323	0.9417849	-0.0260082
	H	-2.1258905	-0.2347598	1.4126140
	H	-2.5700956	-1.2613509	0.0502855
	H	2.4584025	2.0718311	0.3116153
	H	-2.8326362	1.5301285	0.0137547

tG+TG+G-t	C	2.2652526	-0.1226652	-0.4961030
	C	0.7658927	-0.1264365	-0.6956518
	C	0.0809119	0.9829275	0.0941826
	C	-1.4274418	1.0821329	-0.1204004
	C	-2.2380589	-0.0367029	0.5014480
	O	2.5236982	-0.3956305	0.8792484
	O	-2.0447204	-1.2296478	-0.2545641
	H	2.6784366	0.8530515	-0.7735534
	H	2.7296316	-0.8838033	-1.1287593
	H	0.5587963	0.0000031	-1.7613359
	H	0.3692795	-1.0980112	-0.4076310
	H	0.5351947	1.9372624	-0.1884787
	H	0.2865031	0.8459781	1.1575348
	H	-1.6597226	1.1241408	-1.1874582
	H	-1.7833484	2.0169062	0.3190625
	H	-3.2967974	0.2371300	0.5020046
	H	-1.9228992	-0.1856760	1.5393979
	H	3.4737250	-0.4021019	1.0121483
	H	-2.5689124	-1.9261613	0.1468019
tG-TG+G-g-	C	2.1397095	-0.6789065	0.3118769
	C	0.7154087	-0.5167063	-0.1718331
	C	0.1074249	0.8110546	0.2665428
	C	-1.2925215	1.0814703	-0.2775073
	C	-2.3898996	0.1897953	0.2817983
	O	2.9306984	0.3433812	-0.2897102
	O	-2.3092510	-1.1670351	-0.1428971
	H	2.5184665	-1.6657805	0.0337848
	H	2.1729955	-0.5941589	1.4029587
	H	0.7135577	-0.5783668	-1.2631914
	H	0.1188608	-1.3487837	0.1993139
	H	0.7720446	1.6145233	-0.0523608
	H	0.0746250	0.8463219	1.3602928
	H	-1.2890537	1.0014925	-1.3696633
	H	-1.5680997	2.1144251	-0.0485129
	H	-3.3689488	0.6050871	0.0258421
	H	-2.3205988	0.1539236	1.3688878
	H	3.8339502	0.2470086	0.0185650
	H	-2.4032138	-1.1789127	-1.0982102
tG-TG-G-g-	C	-2.3403463	-0.2604526	0.2825812
	C	-0.8743437	-0.5105792	0.5637523
	C	-0.0333371	-0.5219065	-0.7064830
	C	1.4037283	-0.9776584	-0.4715473
	C	2.1669189	-0.1215982	0.5265479
	O	-2.4556671	1.0237404	-0.3208250
	O	2.1656649	1.2585081	0.1874950
	H	-2.9126098	-0.2990490	1.2133539
	H	-2.7252653	-1.0344995	-0.3895920
	H	-0.5184669	0.2647051	1.2436335
	H	-0.7855918	-1.4706939	1.0805332
	H	-0.0391844	0.4757493	-1.1423489
	H	-0.4989171	-1.1906188	-1.4353333

H	1.9456151	-0.9785203	-1.4219987	
H	1.4144149	-2.0094274	-0.1077323	
H	3.1905217	-0.4940507	0.6257656	
H	1.7040814	-0.1742711	1.5098654	
H	-3.3851834	1.2007836	-0.4789896	
H	2.5635118	1.3492910	-0.6817319	
g-TTG+G-g-	C	-2.2006751	-0.3190697	0.2480235
	C	-0.7908442	-0.0199199	-0.2258686
	C	0.1737026	-1.1393541	0.1508427
	C	1.5988256	-0.9587983	-0.3665660
	C	2.3916206	0.1536438	0.3017482
	O	-3.1340594	0.6865465	-0.1236178
	O	1.9231518	1.4637080	0.0020431
	H	-2.2047058	-0.4664979	1.3331578
	H	-2.5671067	-1.2369803	-0.2101144
	H	-0.8065709	0.1079159	-1.3107899
	H	-0.4515257	0.9227231	0.2043629
	H	-0.2191412	-2.0829053	-0.2376023
	H	0.2055257	-1.2437180	1.2395919
	H	1.5835003	-0.7890607	-1.4479583
	H	2.1539677	-1.8875053	-0.2096702
	H	3.4483908	0.0617491	0.0353867
	H	2.3155820	0.0629841	1.3851475
	H	-2.8324596	1.5166912	0.2525495
	H	2.0330344	1.6055647	-0.9410902
g-G+G+TG-g-	C	2.2478075	0.0729576	0.5446464
	C	1.2569753	1.0879426	-0.0017430
	C	-0.0490418	0.4753656	-0.5004900
	C	-0.8232793	-0.2826787	0.5707789
	C	-2.1823679	-0.7544243	0.0800411
	O	2.6558315	-0.8802711	-0.4279645
	O	-3.0301349	0.3189797	-0.3070465
	H	1.8374623	-0.4300798	1.4251489
	H	3.1609933	0.5772977	0.8540256
	H	1.0388075	1.8105545	0.7897227
	H	1.7358427	1.6339106	-0.8160574
	H	0.1506559	-0.1936956	-1.3432776
	H	-0.6867723	1.2653470	-0.8971760
	H	-0.9621135	0.3571258	1.4486379
	H	-0.2653868	-1.1583435	0.9133863
	H	-2.6668909	-1.3714389	0.8415198
	H	-2.0636595	-1.3641045	-0.8152902
	H	1.8810923	-1.3758043	-0.7022177
	H	-3.2524185	0.8183675	0.4821213
g+G-TG+G+g-	C	-2.1650266	-0.7601088	0.1050742
	C	-0.8322308	-0.2411634	0.6196375
	C	-0.0563874	0.5419854	-0.4323413
	C	1.2795545	1.0910320	0.0633206
	C	2.2605448	0.0194085	0.5111912
	O	-3.0745925	0.2783042	-0.2300801
	O	2.5996701	-0.8873687	-0.5301730

H	-2.6636075	-1.3415467	0.8779395	
H	-2.0005353	-1.4192087	-0.7540102	
H	-1.0133092	0.3915584	1.4914992	
H	-0.2508111	-1.1015762	0.9616089	
H	-0.6610028	1.3861953	-0.7710369	
H	0.1086517	-0.0873587	-1.3128605	
H	1.1035956	1.7671941	0.9043415	
H	1.7475007	1.6743370	-0.7311673	
H	1.8744700	-0.5205993	1.3798089	
H	3.1990965	0.4832498	0.8076928	
H	-2.7491998	0.7200541	-1.0167762	
H	1.8220779	-1.4102164	-0.7366959	
g+TG+TG+g-	C	1.9678441	-0.5456189	0.0862470
C	1.2790480	0.7263718	-0.3783217	
C	-0.2215660	0.5488842	-0.5973440	
C	-0.9984455	0.2319165	0.6763216	
C	-2.5019804	0.2237845	0.4582647	
O	3.3820601	-0.4087350	0.1385168	
O	-2.9266392	-0.8115702	-0.4183288	
H	1.7794771	-1.3481996	-0.6262787	
H	1.5803576	-0.8661094	1.0561455	
H	1.4474501	1.5177172	0.3585502	
H	1.7564524	1.0443925	-1.3062346	
H	-0.3741181	-0.2478370	-1.3309469	
H	-0.6253838	1.4657289	-1.0360307	
H	-0.7653347	0.9833724	1.4367158	
H	-0.7051792	-0.7398919	1.0750192	
H	-2.8288098	1.2004353	0.0862078	
H	-3.0179457	0.0359218	1.3976287	
H	3.5899523	0.2541519	0.8007776	
H	-2.6102242	-0.6045309	-1.2999056	
g+G-TG-G-g+	C	-2.3228393	-0.2226194	0.2888793
C	-0.8742297	-0.5807225	0.5742095	
C	-0.0205394	-0.6232128	-0.6872134	
C	1.4378504	-0.9963759	-0.4349672	
C	2.1587843	-0.0312423	0.4948280	
O	-2.4656581	1.0986877	-0.2194322	
O	2.1372080	1.3081131	0.0198813	
H	-2.9043632	-0.2442830	1.2083215	
H	-2.7610111	-0.9498027	-0.4017930	
H	-0.4828978	0.1502520	1.2845229	
H	-0.8447700	-1.5562556	1.0681448	
H	-0.0475827	0.3474243	-1.1887643	
H	-0.4562730	-1.3426946	-1.3854649	
H	1.9717698	-1.0250058	-1.3859706	
H	1.4927421	-1.9976844	0.0012722	
H	3.2107129	-0.3020370	0.5597270	
H	1.7446106	-0.0867530	1.5046563	
H	-2.1640625	1.1026993	-1.1299181	
H	1.2481707	1.6521596	0.1333799	
* g+G+G-G-G+t	C	-1.9716124	-0.2226112	0.0121525

C	-1.0489889	0.6814539	0.8157060
C	-0.0725508	1.5181797	-0.0114921
C	1.0083569	0.7642693	-0.7893883
C	1.9482032	-0.0652808	0.0627345
O	-1.3034204	-1.2431535	-0.7117607
O	1.2692782	-1.2467179	0.5071960
H	-2.5190002	0.3703387	-0.7235789
H	-2.7086730	-0.6656211	0.6899786
H	-1.6869221	1.3643334	1.3832541
H	-0.5070525	0.0806477	1.5473951
H	0.4244856	2.2262565	0.6580233
H	-0.6472032	2.1190153	-0.7215835
H	1.6229440	1.5008992	-1.3125197
H	0.5616040	0.1211175	-1.5462138
H	2.2876847	0.5146154	0.9266773
H	2.8223474	-0.3500457	-0.5264139
H	-0.5095682	-1.4852075	-0.2193777
H	1.9030447	-1.8225351	0.9405563
tG-TG-G+g-	C	-2.2411083	-0.2541421
			-0.4778554
	C	-0.7280487	-0.3003855
			-0.5067715
	C	-0.0980845	0.9917618
			0.0039321
	C	1.4126853	1.0940121
			-0.1947508
	C	2.2280021	0.0013686
			0.4841790
	O	-2.6396335	-0.1091466
			0.8801239
	O	2.3096578	-1.2044092
			-0.2683636
	H	-2.6541203	-1.1723687
			-0.9036779
	H	-2.5941203	0.5921419
			-1.0757495
	H	-0.4228989	-1.1477023
			0.1137574
	H	-0.4065046	-0.4974434
			-1.5327187
	H	-0.3348282	1.1030327
			1.0629748
	H	-0.5753226	1.8309001
			-0.5097853
	H	1.7437349	2.0576301
			0.1999416
	H	1.6600355	1.0840264
			-1.2589232
	H	1.8320770	-0.1947149
			1.4866124
	H	3.2603193	0.3266203
			0.5955038
	H	-3.5980960	-0.0891550
			0.9159537
	H	1.4274148	-1.5724913
			-0.3376347
tTTG+G-t	C	-2.1883646	-0.2762237
			0.3000609
	C	-0.8079953	-0.0240232
			-0.2628321
	C	0.1727007	-1.1050015
			0.1780871
	C	1.5837175	-0.9565571
			-0.3893958
	C	2.4288191	0.1140858
			0.2690837
	O	-3.0536901	0.7502737
			-0.1727060
	O	1.8998834	1.3955487
			-0.0556726
	H	-2.1481790	-0.2709540
			1.3941891
	H	-2.5486519	-1.2594962
			-0.0200224
	H	-0.8730252	-0.0079430
			-1.3526523
	H	-0.4630849	0.9578119
			0.0527940
	H	-0.2210496	-2.0781085
			-0.1279159
	H	0.2316127	-1.1271292
			1.2709606
	H	1.5376319	-0.7559533
			-1.4621268

H	2.1182918	-1.9010550	-0.2642842	
H	3.4599527	0.0305749	-0.0854593	
H	2.4291487	-0.0357343	1.3541018	
H	-3.9300024	0.5952635	0.1857327	
H	2.4689904	2.0632104	0.3333546	
tG+G-TG+g-	C	2.4040442	0.2258434	0.2874618
C	1.3002510	1.0730601	-0.3107899	
C	-0.0999683	0.7828979	0.2291547	
C	-0.7505743	-0.4760182	-0.3340227	
C	-2.1355051	-0.7225140	0.2371112	
O	2.2417438	-1.1259836	-0.1314637	
O	-3.0781910	0.2865140	-0.1084462	
H	2.3659532	0.2934834	1.3799230	
H	3.3733719	0.6090087	-0.0428840	
H	1.5556554	2.1144672	-0.1019126	
H	1.3135988	0.9537119	-1.3964308	
H	-0.7320042	1.6436168	-0.0055632	
H	-0.0548020	0.7137572	1.3215531	
H	-0.1230418	-1.3403500	-0.1202709	
H	-0.8279480	-0.3898019	-1.4201340	
H	-2.0753601	-0.8307610	1.3255170	
H	-2.5466158	-1.6463380	-0.1647375	
H	2.9803463	-1.6358091	0.2086285	
H	-2.8089032	1.1028462	0.3168814	
g+G+TG-G+g+	C	-2.1537462	-0.6544734	0.3411734
C	-0.7165628	-0.5159512	-0.1295815	
C	-0.1035212	0.8166152	0.2842567	
C	1.2909294	1.0852129	-0.2739450	
C	2.3879061	0.1808464	0.2658161	
O	-3.0174476	0.3330412	-0.2134373	
O	2.2998395	-1.1676818	-0.1837028	
H	-2.2094273	-0.5095185	1.4196321	
H	-2.5294315	-1.6571028	0.1202360	
H	-0.1298169	-1.3457038	0.2640925	
H	-0.6904427	-0.6096535	-1.2209078	
H	-0.0615548	0.8629048	1.3769733	
H	-0.7736042	1.6169432	-0.0329560	
H	1.5737810	2.1148134	-0.0388806	
H	1.2762822	1.0138750	-1.3666776	
H	2.3218544	0.1258339	1.3522774	
H	3.3675876	0.5968300	0.0143077	
H	-3.0582860	0.1841007	-1.1609134	
H	2.4274780	-1.1664875	-1.1350673	
tG-G+TG+g-	C	-2.2656635	-0.0099985	0.4694562
C	-1.4203342	1.0802809	-0.1566389	
C	0.0823415	0.9556651	0.0887151	
C	0.7634157	-0.1932142	-0.6473681	
C	2.2738114	-0.1599426	-0.4955892	
O	-2.0616912	-1.2254056	-0.2443343	
O	2.7039228	-0.3566675	0.8471809	
H	-3.3193543	0.2787052	0.4255476	

H	-1.9896182	-0.1318143	1.5222793	
H	-1.6249870	1.1036500	-1.2293736	
H	-1.7663009	2.0310287	0.2554653	
H	0.2453191	0.8550813	1.1663029	
H	0.5588592	1.8931359	-0.2155925	
H	0.5234887	-0.1281590	-1.7122721	
H	0.3835179	-1.1489281	-0.2926342	
H	2.6696674	0.7836346	-0.8869568	
H	2.7267371	-0.9705925	-1.0627276	
H	-2.6245713	-1.8991564	0.1433281	
H	2.4176438	0.4000680	1.3622709	
tTTG+G-g-	C	-2.1902361	-0.2899544	0.2866094
	C	-0.8003395	-0.0125036	-0.2402089
	C	0.1763929	-1.1122703	0.1612004
	C	1.5869270	-0.9460837	-0.4008328
	C	2.4294532	0.1227782	0.2768001
	O	-3.0473097	0.7520956	-0.1653680
	O	1.9460900	1.4479182	0.0999120
	H	-2.1702493	-0.3255116	1.3804509
	H	-2.5408877	-1.2612270	-0.0775969
	H	-0.8517624	0.0552304	-1.3295900
	H	-0.4630638	0.9524378	0.1318829
	H	-0.2207106	-2.0727120	-0.1783684
	H	0.2364511	-1.1711800	1.2522906
	H	1.5365020	-0.7403502	-1.4750078
	H	2.1285380	-1.8899587	-0.2952479
	H	3.4640340	0.0468124	-0.0710291
	H	2.4313728	-0.0389675	1.3545991
	H	-3.9262905	0.5950446	0.1856930
	H	1.9618345	1.6448458	-0.8397307
g-G-TG-G+g+	C	2.2787511	-0.0361281	0.4724610
	C	0.7827415	-0.0058726	0.7304424
	C	0.0651942	1.0036907	-0.1579598
	C	-1.4459161	1.0767891	0.0458177
	C	-2.2251335	-0.1092702	-0.5006867
	O	2.5948110	-0.4477785	-0.8526089
	O	-2.0026541	-1.3271046	0.2034153
	H	2.7755669	-0.6820473	1.2019179
	H	2.7018612	0.9635079	0.5701041
	H	0.3683774	-1.0033640	0.5771947
	H	0.6162730	0.2457551	1.7824928
	H	0.2751434	0.7737425	-1.2046221
	H	0.4948800	1.9912682	0.0314834
	H	-1.8290086	1.9687398	-0.4572757
	H	-1.6790801	1.2010460	1.1087059
	H	-1.9175858	-0.3108711	-1.5265183
	H	-3.2931582	0.1261170	-0.5149791
	H	2.2535917	-1.3380602	-0.9682396
	H	-2.3417749	-1.2148466	1.0945330
g+TTG+G-g-	C	2.2011315	-0.3277681	-0.2593225
	C	0.7873832	0.0010577	0.1844901

C	-0.1686646	-1.1448301	-0.1293651	
C	-1.5938782	-0.9573755	0.3843435	
C	-2.3821044	0.1532480	-0.2932918	
O	3.1166079	0.7370512	-0.0412839	
O	-1.9350879	1.4635402	0.0341772	
H	2.2213374	-0.5101374	-1.3331379	
H	2.5468945	-1.2407063	0.2375184	
H	0.7854098	0.1870255	1.2639067	
H	0.4607319	0.9196425	-0.2983712	
H	0.2345375	-2.0668497	0.2986532	
H	-0.2035156	-1.2979084	-1.2121521	
H	-1.5809776	-0.7778245	1.4642175	
H	-2.1483140	-1.8875863	0.2341800	
H	-3.4445115	0.0471758	-0.0559951	
H	-2.2767422	0.0755497	-1.3753730	
H	3.1042650	0.9469986	0.8952762	
H	-2.0897119	1.6007082	0.9715538	
tTG-G-G-t	C	1.8367149	0.0157560	0.3748614
	C	0.8659786	0.2423223	-0.7625928
	C	-0.2667513	1.1998783	-0.4037469
	C	-1.1339579	0.7485417	0.7720563
	C	-1.7232958	-0.6337419	0.5850078
	O	2.8907978	-0.8072944	-0.1139528
	O	-2.4695620	-0.6261036	-0.6268456
	H	1.3377096	-0.4705868	1.2175637
	H	2.2268267	0.9780816	0.7232071
	H	1.4280480	0.6446142	-1.6064332
	H	0.4655023	-0.7195182	-1.0847889
	H	-0.9061382	1.3253907	-1.2765948
	H	0.1507328	2.1828283	-0.1725050
	H	-1.9524788	1.4580122	0.9039574
	H	-0.5607852	0.7507662	1.7013422
	H	-2.3685211	-0.8768104	1.4334641
	H	-0.9287019	-1.3839947	0.5396682
	H	3.5062883	-0.9687959	0.6040706
	H	-2.8490277	-1.4979967	-0.7549557
tG+G+G+Tg-	C	1.7296861	-0.6290862	0.5736290
	C	1.1393073	0.7517683	0.7686418
	C	0.2617208	1.2044508	-0.3988346
	C	-0.8657292	0.2369213	-0.7505455
	C	-1.8308910	0.0022649	0.3969215
	O	2.4596494	-0.6190752	-0.6488931
	O	-2.8869194	-0.8857726	0.0539794
	H	0.9371624	-1.3822642	0.5390894
	H	2.3868066	-0.8701678	1.4132574
	H	0.5739446	0.7511600	1.7026078
	H	1.9572418	1.4630141	0.8942801
	H	0.8934651	1.3402602	-1.2757681
	H	-0.1628060	2.1821294	-0.1581088
	H	-0.4597338	-0.7211121	-1.0775411
	H	-1.4264307	0.6438218	-1.5969694

H	-2.2285367	0.9608299	0.7485724	
H	-1.3271472	-0.4711978	1.2374888	
H	2.8448114	-1.4883060	-0.7783647	
H	-3.3407336	-0.5197076	-0.7087664	
g+G+G-TG+g-	C	2.3916923	0.2036714	0.3037523
C	1.3013172	1.0736028	-0.3029024	
C	-0.1072259	0.8100868	0.2262311	
C	-0.7279356	-0.5030920	-0.2373164	
C	-2.1411416	-0.6981968	0.2841530	
O	2.3142822	-1.1692116	-0.0625171	
O	-3.0632558	0.2665737	-0.2110716	
H	2.3115359	0.2148349	1.3904952	
H	3.3726523	0.6090390	0.0399535	
H	1.5708468	2.1134020	-0.0996112	
H	1.3144614	0.9600096	-1.3915670	
H	-0.7447391	1.6381438	-0.0947020	
H	-0.0842698	0.8337716	1.3208245	
H	-0.1130503	-1.3384966	0.0964840	
H	-0.7524130	-0.5285417	-1.3296077	
H	-2.1375193	-0.6962602	1.3790578	
H	-2.5298982	-1.6600604	-0.0435231	
H	2.4367672	-1.2262000	-1.0129921	
H	-2.8447355	1.1146396	0.1796112	
t+G+TG+G-g-	C	2.2511545	-0.2012449	-0.4929188
C	0.7447755	-0.2257349	-0.6334686	
C	0.0919378	0.9940145	0.0061330	
C	-1.4210298	1.0769128	-0.1741946	
C	-2.2113526	-0.0226041	0.5199139	
O	2.5599248	-0.2401034	0.8977852	
O	-2.1081676	-1.2942582	-0.1125792	
H	2.6548582	0.7102043	-0.9466609	
H	2.6890148	-1.0622228	-1.0048254	
H	0.5003723	-0.2594440	-1.6988303	
H	0.3587906	-1.1411286	-0.1883757	
H	0.5451060	1.8943522	-0.4191984	
H	0.3256185	1.0040262	1.0720832	
H	-1.6761530	1.0764978	-1.2393581	
H	-1.7704617	2.0331365	0.2242779	
H	-3.2618853	0.2710320	0.5995080	
H	-1.8315528	-0.1721090	1.5302900	
H	3.5142462	-0.2472413	0.9950646	
H	-2.4941675	-1.2156920	-0.9878369	
tG+G-G-G-t	C	2.1246935	0.1147656	-0.2020925
C	0.9262724	0.9654143	-0.5698140	
C	-0.0838692	1.1872862	0.5539463	
C	-0.8003178	-0.0626675	1.0630755	
C	-1.5253037	-0.8230447	-0.0259725	
O	1.7194840	-1.2525028	-0.1184813	
O	-2.4249517	0.0803678	-0.6695327	
H	2.5376061	0.4484559	0.7558454	
H	2.9005142	0.2244780	-0.9642767	

H	1.3056118	1.9406991	-0.8832597	
H	0.4415562	0.5268748	-1.4436675	
H	-0.8353745	1.8941965	0.2018849	
H	0.4279444	1.6637664	1.3945229	
H	-1.5263064	0.2374208	1.8214289	
H	-0.0925707	-0.7462117	1.5307884	
H	-2.0752050	-1.6585542	0.4155303	
H	-0.8066204	-1.2280952	-0.7402707	
H	2.4996570	-1.7837223	0.0562075	
H	-2.8848440	-0.3994190	-1.3612805	
tG+G-G-G-g-	C	2.1304851	0.1229404	-0.1901770
	C	0.9345453	0.9789841	-0.5533610
	C	-0.0855957	1.1779924	0.5657804
	C	-0.7971467	-0.0859186	1.0463139
	C	-1.5095442	-0.8383859	-0.0642736
	O	1.7230112	-1.2440100	-0.1231456
	O	-2.4123518	-0.0158902	-0.7991560
	H	2.5409851	0.4455319	0.7728039
	H	2.9085500	0.2412991	-0.9486249
	H	1.3156403	1.9605143	-0.8442395
	H	0.4571486	0.5573568	-1.4392187
	H	-0.8354302	1.8879476	0.2144253
	H	0.4145739	1.6465759	1.4176289
	H	-1.5268798	0.1941728	1.8125997
	H	-0.0887487	-0.7707260	1.5126261
	H	-2.0318344	-1.7047302	0.3511949
	H	-0.7894848	-1.2063351	-0.7899639
	H	2.5042608	-1.7812832	0.0258910
	H	-3.0884879	0.2929731	-0.1912831
tG-G-G-G-g-	C	1.7756222	0.3109079	-0.7195134
	C	0.8194885	1.0100488	0.2236877
	C	-0.0034680	0.0505769	1.0803055
	C	-0.8042395	-0.9733046	0.2801917
	C	-1.7538799	-0.3553544	-0.7325301
	O	2.6109199	-0.5425632	0.0576774
	O	-2.6437638	0.5900880	-0.1511127
	H	2.3744043	1.0530490	-1.2538830
	H	1.2243738	-0.2731925	-1.4625538
	H	1.3980478	1.6626388	0.8793962
	H	0.1619272	1.6533929	-0.3641493
	H	-0.6864428	0.6388195	1.6936697
	H	0.6649049	-0.4805995	1.7573608
	H	-1.3815942	-1.5938643	0.9717965
	H	-0.1308467	-1.6539853	-0.2462139
	H	-2.3113508	-1.1419134	-1.2492524
	H	-1.2033341	0.2025384	-1.4879959
	H	3.2532767	-0.9502378	-0.5269614
	H	-3.1636775	0.1328047	0.5143634
tG-G-G-Tg-	C	-1.7306649	-0.6046300	0.6059352
	C	-1.1434691	0.7850194	0.7360833
	C	-0.2618205	1.1841599	-0.4478449

C	0.8750676	0.2121233	-0.7548115	
C	1.8401416	0.0285486	0.4018613	
O	-2.4424705	-0.6630946	-0.6255344	
O	2.9724061	-0.7586965	0.0505303	
H	-2.3987121	-0.8022652	1.4481804	
H	-0.9368302	-1.3575744	0.6235393	
H	-1.9632380	1.4996327	0.8238536	
H	-0.5825597	0.8296955	1.6714839	
H	0.1578868	2.1737337	-0.2521066	
H	-0.8905959	1.2768221	-1.3325680	
H	1.4426478	0.5783945	-1.6114580	
H	0.4634535	-0.7590638	-1.0433710	
H	1.3323321	-0.4067402	1.2672611	
H	2.2422381	0.9940200	0.7085019	
H	-2.8632544	-1.5227854	-0.6921669	
H	2.6521538	-1.6095156	-0.2580078	
tTG+G+Tg-	C	-1.7606686	-0.3112303	0.4306882
	C	-1.1501577	0.6461669	-0.5692870
	C	0.0067233	1.4581202	0.0109112
	C	1.1493258	0.6180024	0.5815487
	C	1.7569955	-0.3275207	-0.4389592
	O	-2.8939024	-0.9088220	-0.1891730
	O	2.8329132	-1.0878502	0.0946484
	H	-2.0554822	0.2355538	1.3328103
	H	-1.0377331	-1.0780186	0.7209827
	H	-0.8293038	0.0793335	-1.4440946
	H	-1.9356938	1.3234211	-0.9069513
	H	-0.3753455	2.1128933	0.7971628
	H	0.4008401	2.1124545	-0.7697833
	H	0.8148320	0.0363058	1.4416446
	H	1.9332989	1.2887112	0.9442451
	H	2.0781685	0.2355204	-1.3220291
	H	1.0259529	-1.0634205	-0.7674940
	H	-3.2580903	-1.5622543	0.4117847
	H	3.5025811	-0.4733707	0.4038860
tG+G-G-Tg-	C	-2.0967175	0.3675771	0.0438712
	C	-1.4023064	-0.8224747	-0.5887971
	C	-0.3271820	-1.4736134	0.2825692
	C	0.8251459	-0.5650393	0.7065188
	C	1.6204759	-0.0256516	-0.4680331
	O	-1.2375651	1.5054488	-0.0443869
	O	2.7313868	0.7603256	-0.0487713
	H	-2.3341065	0.1488996	1.0905217
	H	-3.0324739	0.5697941	-0.4826932
	H	-2.1653627	-1.5726110	-0.8073037
	H	-0.9943896	-0.5045673	-1.5493406
	H	0.0789042	-2.3350294	-0.2543375
	H	-0.8079537	-1.8723576	1.1793809
	H	1.5060629	-1.1232438	1.3513421
	H	0.4407259	0.2765565	1.2842645
	H	0.9752852	0.5550733	-1.1286379

H	2.0459175	-0.8490061	-1.0421017	
H	-1.7205173	2.2682595	0.2816220	
H	2.3784804	1.5419126	0.3826776	
* g+G+G+G-G+g-	C	-1.5848293	-0.3561343	-0.5909455
	C	-1.3558656	1.0786687	-0.1524248
	C	-0.0217472	1.3139899	0.5531589
	C	1.2239571	1.0272435	-0.3034548
	C	1.9855619	-0.2272058	0.1045207
	O	-1.4401563	-1.2843400	0.4870839
	O	1.2990569	-1.4338252	-0.1652852
	H	-0.8394724	-0.6620767	-1.3212086
	H	-2.5722270	-0.4603093	-1.0457009
	H	-1.4228768	1.7174376	-1.0371979
	H	-2.1721508	1.3811735	0.5108002
	H	0.0144010	0.7064429	1.4606504
	H	-0.0038890	2.3517702	0.8875314
	H	1.9195597	1.8652754	-0.2239194
	H	0.9540491	0.9453334	-1.3590134
	H	2.2463533	-0.1567192	1.1670542
	H	2.9162655	-0.2878136	-0.4581598
	H	-2.0624352	-1.0453191	1.1789157
	H	0.4790151	-1.4548640	0.3457379
g-G+TG+G-g-	C	2.2647242	-0.2083167	-0.4876980
	C	0.7510987	-0.2519783	-0.6072387
	C	0.0854559	0.9649366	0.0261242
	C	-1.4206903	1.0692850	-0.2016384
	C	-2.2506378	-0.0059637	0.4834306
	O	2.7190827	-0.2738846	0.8588899
	O	-2.1082105	-1.2997121	-0.0900499
	H	2.6533508	0.6912359	-0.9776506
	H	2.7055141	-1.0720860	-0.9812662
	H	0.4948441	-0.2890419	-1.6703847
	H	0.3772815	-1.1680526	-0.1539931
	H	0.5595985	1.8683322	-0.3707638
	H	0.2648900	0.9625599	1.1054782
	H	-1.6366670	1.0568963	-1.2747761
	H	-1.7685104	2.0363039	0.1714203
	H	-3.3033960	0.2904859	0.4879742
	H	-1.9340735	-0.1145479	1.5206853
	H	2.4522377	0.5341076	1.3014972
	H	-2.4564666	-1.2645227	-0.9837715
g+TG-G-G-g-	C	1.8372413	-0.0227359	0.3910352
	C	0.8730619	0.2692156	-0.7444615
	C	-0.2588220	1.2113966	-0.3412372
	C	-1.1249223	0.6949284	0.8076640
	C	-1.7162047	-0.6810509	0.5476741
	O	2.9065432	-0.8723691	-0.0009490
	O	-2.4464786	-0.7427950	-0.6710828
	H	1.3371495	-0.5545641	1.1983101
	H	2.2194314	0.9179131	0.8034488
	H	1.4332388	0.7263512	-1.5651041

	H	0.4719676	-0.6704560	-1.1256877
	H	-0.8930176	1.3838092	-1.2106236
	H	0.1597575	2.1800962	-0.0578402
	H	-1.9391545	1.4030236	0.9859561
	H	-0.5519492	0.6507802	1.7368695
	H	-2.3438121	-0.9821043	1.3908545
	H	-0.9281639	-1.4251073	0.4465774
	H	3.3550850	-0.4569235	-0.7411473
	H	-3.1989364	-0.1512541	-0.5943471
tTG-G-G-g-	C	1.8384100	-0.0040180	0.3793908
	C	0.8763438	0.2802723	-0.7529584
	C	-0.2652512	1.2093787	-0.3498769
	C	-1.1227942	0.6942708	0.8059000
	C	-1.7097233	-0.6855140	0.5572995
	O	2.9166363	-0.7656512	-0.1525197
	O	-2.4605954	-0.7539423	-0.6478489
	H	1.3409316	-0.5600670	1.1789601
	H	2.2016858	0.9399675	0.8002763
	H	1.4436812	0.7354861	-1.5658780
	H	0.4852534	-0.6634003	-1.1346423
	H	-0.9041344	1.3673309	-1.2185839
	H	0.1422509	2.1855774	-0.0763342
	H	-1.9399534	1.3987432	0.9866653
	H	-0.5442506	0.6574625	1.7322090
	H	-2.3208304	-0.9896132	1.4118135
	H	-0.9184428	-1.4243075	0.4425740
	H	3.5180265	-0.9802802	0.5635666
	H	-3.2041500	-0.1517076	-0.5666047

1-6 hexanediol calculated by MP2/6-31+G(d,p)

tG+TTTG-t	C	3.1501026	0.5091102	0.2608089
	C	1.7579104	0.8073818	-0.2596928
	C	0.6980461	-0.1566985	0.2661060
	C	-0.6980460	0.1566985	-0.2661060
	C	-1.7579102	-0.8073819	0.2596927
	C	-3.1501025	-0.5091102	-0.2608089
	O	3.5233942	-0.7936351	-0.2137422
	O	-3.5233941	0.7936350	0.2137426
	H	3.1531987	0.5307333	1.3568507
	H	3.8586466	1.2618980	-0.1005903
	H	1.4977089	1.8321921	0.0251844
	H	1.7835907	0.7728442	-1.3527427
	H	0.6837214	-0.1104503	1.3612721
	H	0.9786996	-1.1774789	-0.0043881
	H	-0.6837214	0.1104504	-1.3612722
	H	-0.9786995	1.1774789	0.0043882
	H	-1.7835905	-0.7728445	1.3527426
	H	-1.4977088	-1.8321921	-0.0251848
	H	-3.1531987	-0.5307329	-1.3568507
	H	-3.8586465	-1.2618981	0.1005902
	H	4.4019191	-1.0055340	0.1268841

H	-4.4019190	1.0055341	-0.1268836	
tG-TTTTt	C	-3.2943535	0.2224159	0.3323713
C	-1.9685612	0.8311443	-0.0800554	
C	-0.7700649	-0.0481921	0.2657091	
C	0.5580319	0.5642548	-0.1730186	
C	1.7596013	-0.3034635	0.1949481	
C	3.0724214	0.3037383	-0.2555772	
O	-3.4693229	-0.9854852	-0.4233713	
O	4.1261970	-0.5825771	0.1490078	
H	-4.1119720	0.9213380	0.1268663	
H	-3.2892875	0.0034580	1.4065473	
H	-1.9967403	1.0167461	-1.1577774	
H	-1.8691180	1.8039490	0.4130789	
H	-0.8962741	-1.0260654	-0.2041255	
H	-0.7480440	-0.2160552	1.3485988	
H	0.6687914	1.5542788	0.2841916	
H	0.5376700	0.7208184	-1.2572726	
H	1.6595309	-1.2923446	-0.2597943	
H	1.7985545	-0.4489347	1.2777546	
H	3.0733312	0.4284623	-1.3442832	
H	3.2058394	1.2906824	0.2019187	
H	-4.2965125	-1.4033654	-0.1516622	
H	4.9686690	-0.2125522	-0.1447899	
tG-TTTG-t	C	3.1932509	0.2314714	-0.3114769
C	1.7844720	0.7910019	-0.3019994	
C	0.7063227	-0.2891698	-0.2956329	
C	-0.7063227	0.2891709	-0.2956320	
C	-1.7844720	-0.7910008	-0.3020024	
C	-3.1932509	-0.2314704	-0.3114777	
O	3.3753107	-0.5102049	0.9046642	
O	-3.3753106	0.5102017	0.9046660	
H	3.9234808	1.0453427	-0.3729054	
H	3.3316316	-0.4224342	-1.1806332	
H	1.6729812	1.4325487	0.5768182	
H	1.6641998	1.4284009	-1.1846201	
H	0.8435913	-0.9248710	0.5821247	
H	0.8371181	-0.9305081	-1.1757270	
H	-0.8371180	0.9305121	-1.1757239	
H	-0.8435914	0.9248691	0.5821277	
H	-1.6729810	-1.4325508	0.5768129	
H	-1.6641998	-1.4283966	-1.1846253	
H	-3.3316319	0.4224382	-1.1806317	
H	-3.9234807	-1.0453416	-0.3729090	
H	4.2660991	-0.8832810	0.9076549	
H	-4.2660991	0.8832775	0.9076581	
tG-TTTTg+	C	-3.2945973	0.2262366	0.3235137
C	-1.9697195	0.8287725	-0.1006689	
C	-0.7701004	-0.0395490	0.2681975	
C	0.5575724	0.5662015	-0.1810005	
C	1.7624959	-0.2898733	0.2042779	
C	3.0799021	0.3110070	-0.2609074	

O	-3.4585930	-1.0066133	-0.3941336	
O	4.2193023	-0.4529992	0.1572885	
H	-4.1145904	0.9135894	0.0908620	
H	-3.2949755	0.0415654	1.4040844	
H	-1.9954523	0.9889947	-1.1824896	
H	-1.8735741	1.8129230	0.3699745	
H	-0.8935423	-1.0279763	-0.1801543	
H	-0.7505540	-0.1830090	1.3546421	
H	0.6692451	1.5637856	0.2587054	
H	0.5390676	0.7035119	-1.2678457	
H	1.6495162	-1.2893077	-0.2312524	
H	1.8023310	-0.4157346	1.2896598	
H	3.0773169	0.4293080	-1.3507529	
H	3.2257882	1.2965322	0.1815510	
H	-4.2917840	-1.4131131	-0.1233447	
H	4.1296922	-1.3429152	-0.2088357	
tG+TTTTg+	C	3.2937712	0.2198736	0.3352773
	C	1.9687329	0.8312233	-0.0757274
	C	0.7699628	-0.0507854	0.2622802
	C	-0.5579413	0.5684414	-0.1675408
	C	-1.7622636	-0.3043198	0.1805342
	C	-3.0801353	0.3167354	-0.2560219
	O	3.4626201	-0.9916296	-0.4162098
	O	-4.2088761	-0.5279394	0.0070904
	H	3.2913853	0.0049110	1.4103244
	H	4.1127265	0.9156110	0.1247676
	H	1.8683643	1.8007410	0.4236819
	H	1.9978019	1.0236396	-1.1521560
	H	0.7502138	-0.2307888	1.3434984
	H	0.8944351	-1.0233420	-0.2188686
	H	-0.5387862	0.7410171	-1.2491740
	H	-0.6704749	1.5513083	0.3043419
	H	-1.7863852	-0.4738012	1.2633762
	H	-1.6648797	-1.2837583	-0.2951841
	H	-3.2142266	1.2943795	0.2217446
	H	-3.0893180	0.4685297	-1.3353787
	H	4.2971789	-1.4026874	-0.1567758
	H	-4.2335880	-0.7021498	0.9573689
tG+TTTG-g+	C	3.1589876	0.4852756	0.2666780
	C	1.7611890	0.8228923	-0.2140738
	C	0.7031121	-0.1587276	0.2817837
	C	-0.6982259	0.1763526	-0.2240650
	C	-1.7613354	-0.7947275	0.2847390
	C	-3.1550426	-0.5208451	-0.2626339
	O	3.5045013	-0.7986645	-0.2735825
	O	-3.6858007	0.7418407	0.1615273
	H	3.1825287	0.4576103	1.3622741
	H	3.8697087	1.2453615	-0.0741223
	H	1.5165868	1.8346534	0.1263184
	H	1.7682119	0.8420790	-1.3077625
	H	0.6976441	-0.1594994	1.3776629

H	0.9752590	-1.1677800	-0.0354741	
H	-0.6949391	0.1676141	-1.3206386	
H	-0.9482621	1.1967192	0.0871757	
H	-1.8022179	-0.7582265	1.3770180	
H	-1.4786862	-1.8149433	0.0031185	
H	-3.1493058	-0.5834512	-1.3575049	
H	-3.8626440	-1.2601915	0.1110098	
H	4.3881188	-1.0364489	0.0354506	
H	-3.1608992	1.4433047	-0.2442954	
tG-TTTG+g+	C	3.1474357	-0.5182964	0.2580455
	C	1.7620858	-0.7965655	-0.2907857
	C	0.6958358	0.1471087	0.2586284
	C	-0.6944198	-0.1460056	-0.2997358
	C	-1.7601755	0.8070277	0.2334569
	C	-3.1611838	0.4929949	-0.2713903
	O	3.5234008	0.8030893	-0.1606270
	O	-3.6146550	-0.8098987	0.1242283
	H	3.8611388	-1.2554567	-0.1244972
	H	3.1380877	-0.5827085	1.3524635
	H	1.8013202	-0.7188119	-1.3811733
	H	1.4990748	-1.8320342	-0.0502376
	H	0.9789863	1.1771259	0.0288823
	H	0.6707395	0.0617307	1.3516070
	H	-0.9808289	-1.1744573	-0.0639272
	H	-0.6670166	-0.0716327	-1.3927347
	H	-1.5124795	1.8354328	-0.0519272
	H	-1.7623303	0.7832551	1.3301036
	H	-3.8688552	1.2592348	0.0633395
	H	-3.1775289	0.4741083	-1.3616007
	H	4.4018603	0.9990683	0.1895989
	H	-3.6794514	-0.8210480	1.0885327
tG+TTTG+g+	C	-3.1946846	-0.3451156	-0.1261898
	C	-1.7903546	-0.5207124	-0.6692288
	C	-0.7050415	-0.2239316	0.3618833
	C	0.7040276	-0.3974516	-0.1991619
	C	1.7911753	-0.1117167	0.8327354
	C	3.2029528	-0.2378379	0.2782879
	O	-3.3495396	1.0350616	0.2396839
	O	3.4621960	0.6777606	-0.7952575
	H	-3.3430870	-0.9896637	0.7481954
	H	-3.9319820	-0.6214491	-0.8871970
	H	-1.6881830	-1.5501326	-1.0287599
	H	-1.6700575	0.1366810	-1.5351026
	H	-0.8381118	-0.8882142	1.2242081
	H	-0.8321535	0.7977056	0.7278889
	H	0.8407015	0.2642008	-1.0583000
	H	0.8268211	-1.4214575	-0.5708165
	H	1.6907323	-0.8016218	1.6782382
	H	1.6553681	0.8972818	1.2404151
	H	3.9400875	-0.1049681	1.0777730
	H	3.3542885	-1.2263308	-0.1568734

H	-4.2398228	1.1624848	0.5916886	
H	3.3860712	1.5755484	-0.4451595	
tTTTTt	C	1.4025317	2.8693130	0.0000000
	C	1.4093156	1.3541218	0.0000000
	C	0.0010940	0.7636804	0.0000000
	C	-0.0010944	-0.7636801	0.0000000
	C	-1.4093158	-1.3541218	0.0000000
	C	-1.4025315	-2.8693130	0.0000000
	O	2.7675247	3.3108938	0.0000000
	O	-2.7675243	-3.3108943	0.0000000
	H	0.8788664	3.2418274	0.8875725
	H	0.8788664	3.2418274	-0.8875725
	H	1.9596104	1.0101820	-0.8797253
	H	1.9596104	1.0101820	0.8797253
	H	-0.5470248	1.1212303	-0.8783883
	H	-0.5470248	1.1212303	0.8783883
	H	0.5470244	-1.1212300	0.8783883
	H	0.5470244	-1.1212300	-0.8783883
	H	-1.9596107	-1.0101821	-0.8797253
	H	-1.9596107	-1.0101821	0.8797253
	H	-0.8788661	-3.2418272	-0.8875725
	H	-0.8788661	-3.2418272	0.8875725
	H	2.7784993	4.2767738	0.0000000
	H	-2.7784986	-4.2767743	0.0000000
tTTTTg+	C	-3.1538521	0.5034025	-0.0161972
	C	-1.9178984	-0.3726973	0.0124751
	C	-0.6251824	0.4396583	-0.0133018
	C	0.6252867	-0.4370588	0.0116310
	C	1.9212741	0.3707326	-0.0143473
	C	3.1598905	-0.5122263	0.0078293
	O	-4.2991199	-0.3596433	0.0162867
	O	4.3783466	0.2368119	-0.0867165
	H	-3.1591974	1.1144473	-0.9258143
	H	-3.1563191	1.1768594	0.8483425
	H	-1.9531775	-0.9920724	0.9125600
	H	-1.9523486	-1.0487992	-0.8457851
	H	-0.6024358	1.1199159	0.8452128
	H	-0.6033193	1.0670403	-0.9109543
	H	0.6042406	-1.1147039	-0.8484887
	H	0.6033525	-1.0673586	0.9071885
	H	1.9458438	1.0459639	0.8487794
	H	1.9572119	0.9952605	-0.9110300
	H	3.1625449	-1.1375532	0.9082039
	H	3.1694928	-1.1742236	-0.8580432
	H	-5.0963700	0.1851858	-0.0084372
	H	4.4202822	0.8339902	0.6718844
g+G+TTTG-g-	C	3.1582458	0.5043511	0.2679803
	C	1.7638341	0.7962676	-0.2678635
	C	0.6927086	-0.1362306	0.2903616
	C	-0.6927086	0.1362302	-0.2903617
	C	-1.7638342	-0.7962678	0.2678635

C	-3.1582459	-0.5043512	-0.2679802	
O	3.6139367	-0.8155696	-0.0617381	
O	-3.6139366	0.8155695	0.0617381	
H	3.1611495	0.5355303	1.3580812	
H	3.8708347	1.2540788	-0.0924682	
H	1.5119084	1.8353165	-0.0283050	
H	1.7797180	0.7271729	-1.3622714	
H	0.6567525	-0.0230950	1.3800196	
H	0.9805000	-1.1725014	0.0944479	
H	-0.6567525	0.0230946	-1.3800198	
H	-0.9804999	1.1725011	-0.0944481	
H	-1.7797179	-0.7271732	1.3622713	
H	-1.5119085	-1.8353167	0.0283049	
H	-3.1611498	-0.5355306	-1.3580810	
H	-3.8708348	-1.2540788	0.0924686	
H	3.7019417	-0.8682992	-1.0228144	
H	-3.7019414	0.8682993	1.0228144	
g+G-TTTTg-	C	-3.3045930	0.2205737	0.3368587
	C	-1.9714312	0.8227056	-0.0855687
	C	-0.7698314	-0.0662370	0.2264781
	C	0.5622946	0.5760773	-0.1560392
	C	1.7656412	-0.3084770	0.1641323
	C	3.0861955	0.3359956	-0.2304193
	O	-3.6338948	-0.9724381	-0.3854813
	O	4.2125608	-0.5189121	-0.0000770
	H	-4.1181991	0.9118028	0.1199684
	H	-3.3064292	0.0269783	1.4163373
	H	-2.0079501	1.0313031	-1.1584035
	H	-1.8525913	1.7823484	0.4295429
	H	-0.8609283	-1.0166766	-0.3094556
	H	-0.7611772	-0.3013540	1.2974846
	H	0.6615165	1.5336709	0.3664940
	H	0.5540106	0.8024127	-1.2274471
	H	1.6781101	-1.2650950	-0.3579065
	H	1.7795211	-0.5275441	1.2380454
	H	3.1029815	0.5401913	-1.3009005
	H	3.2135178	1.2895366	0.2952250
	H	-3.0197983	-1.6693742	-0.1221004
	H	4.2396521	-0.7295653	0.9426425
tTTTTG+g+	C	3.0710341	0.2991385	0.2749752
	C	1.7626805	-0.2931102	-0.2077739
	C	0.5568083	0.5588484	0.1822076
	C	-0.7668700	-0.0373965	-0.2914204
	C	-1.9718294	0.8236103	0.0760569
	C	-3.3015799	0.2086106	-0.3374940
	O	4.1276950	-0.5747425	-0.1469962
	O	-3.5515927	-1.0511950	0.3003955
	H	3.0612040	0.3893170	1.3671515
	H	3.2089199	1.3000939	-0.1494987
	H	1.8101391	-0.3990063	-1.2947107
	H	1.6611013	-1.2981975	0.2096278

H	0.6697920	1.5657442	-0.2355943	
H	0.5276152	0.6743995	1.2716500	
H	-0.8931735	-1.0356515	0.1346923	
H	-0.7369477	-0.1628461	-1.3793627	
H	-1.8839379	1.8072859	-0.3987322	
H	-1.9826857	1.0026463	1.1580652	
H	-4.1226972	0.9059968	-0.1392410	
H	-3.3013755	-0.0145663	-1.4049193	
H	4.9688765	-0.2094433	0.1562927	
H	-3.6406973	-0.8925711	1.2495988	
tG-TTTG-g+	C	3.1962304	0.1863712	-0.3461381
	C	1.7896531	0.7513501	-0.3763355
	C	0.7100997	-0.3208609	-0.2583173
	C	-0.7029109	0.2569771	-0.2914385
	C	-1.7865067	-0.8140763	-0.1871900
	C	-3.2023528	-0.2657259	-0.2953855
	O	3.3828834	-0.4409142	0.9309253
	O	-3.5523908	0.6027303	0.7899932
	H	3.9286414	0.9879881	-0.4878152
	H	3.3245706	-0.5444954	-1.1531423
	H	1.6903529	1.4718082	0.4407602
	H	1.6620737	1.3041273	-1.3131584
	H	0.8568567	-0.8764164	0.6704448
	H	0.8240516	-1.0377167	-1.0796698
	H	-0.8424980	0.8232300	-1.2207151
	H	-0.8036614	0.9689648	0.5348804
	H	-1.6887414	-1.3465239	0.7628784
	H	-1.6441002	-1.5481169	-0.9880890
	H	-3.3343518	0.2502268	-1.2542942
	H	-3.9291056	-1.0760846	-0.2488975
	H	4.2733199	-0.8132994	0.9657643
	H	-3.0017129	1.3940336	0.7360386
g+G+TTTTg+	C	3.3009562	0.2058633	0.3402611
	C	1.9722989	0.8238698	-0.0723492
	C	0.7667946	-0.0386401	0.2898835
	C	-0.5567177	0.5630859	-0.1772709
	C	-1.7651763	-0.2934074	0.1959822
	C	-3.0782391	0.3107947	-0.2778037
	O	3.5461520	-1.0556817	-0.2962184
	O	-4.2093174	-0.5236486	0.0040383
	H	3.3016005	-0.0159412	1.4080110
	H	4.1237265	0.9006059	0.1400665
	H	1.8844065	1.8053268	0.4070057
	H	1.9838671	1.0075693	-1.1534440
	H	0.7388497	-0.1727955	1.3770656
	H	0.8915684	-1.0334520	-0.1445949
	H	-0.5286792	0.6908760	-1.2651516
	H	-0.6716585	1.5649226	0.2518613
	H	-1.7989025	-0.4182895	1.2844372
	H	-1.6653350	-1.2917699	-0.2380885
	H	-3.2170395	1.3057907	0.1612003

H	-3.0754688	0.4220303	-1.3621854
H	3.6430596	-0.8979936	-1.2448443
H	-4.2490961	-0.6575485	0.9603193
g+G+TTTG-g+ C	-3.1701083	0.4693358	-0.2763269
C	-1.7652055	0.8214009	0.1931981
C	-0.7002841	-0.1484136	-0.3104057
C	0.6959418	0.1712290	0.2194072
C	1.7646773	-0.7840661	-0.3071569
C	3.1525501	-0.5259808	0.2625356
O	-3.5977816	-0.8221180	0.1764930
O	3.6864724	0.7489861	-0.1178518
H	-3.2022431	0.4083707	-1.3645621
H	-3.8821809	1.2394448	0.0390992
H	-1.5325582	1.8370317	-0.1459406
H	-1.7512968	0.8496951	1.2894357
H	-0.6833174	-0.1229467	-1.4054396
H	-0.9762627	-1.1664991	-0.0249841
H	0.6825344	0.1306115	1.3154548
H	0.9484979	1.2003254	-0.0588082
H	1.8165839	-0.7146370	-1.3972585
H	1.4800708	-1.8125730	-0.0596167
H	3.1361131	-0.6220754	1.3549400
H	3.8641332	-1.2534615	-0.1263885
H	-3.6743142	-0.7912057	1.1394294
H	3.1601751	1.4382839	0.3065147
g-G+TTTG+g- C	-3.2052666	0.2466692	-0.3197261
C	-1.7866295	0.7968104	-0.2629450
C	-0.7087650	-0.2845941	-0.2597132
C	0.7087650	0.2845943	-0.2597132
C	1.7866294	-0.7968103	-0.2629449
C	3.2052666	-0.2466694	-0.3197260
O	-3.5587240	-0.5097986	0.8445758
O	3.5587240	0.5097985	0.8445758
H	-3.3397434	-0.3581032	-1.2246349
H	-3.9267937	1.0622247	-0.3527827
H	-1.6394838	1.4493809	-1.1306954
H	-1.6899245	1.4178027	0.6320320
H	-0.8369030	-0.9275943	-1.1385863
H	-0.8233389	-0.9217756	0.6232800
H	0.8233389	0.9217757	0.6232801
H	0.8369031	0.9275945	-1.1385863
H	1.6394836	-1.4493809	-1.1306952
H	1.6899243	-1.4178025	0.6320321
H	3.9267936	-1.0622250	-0.3527824
H	3.3397437	0.3581028	-1.2246349
H	-3.0437781	-1.3264708	0.8477210
H	3.0437783	1.3264708	0.8477208
g+G-TTTG-g- C	3.2053881	-0.3668691	0.0902565
C	1.7891722	-0.7964416	-0.2665847
C	0.7043973	0.0517655	0.3935520
C	-0.7076670	-0.4316758	0.0699681

C	-1.7923910	0.4119651	0.7331768	
C	-3.2041869	-0.0332236	0.3769508	
O	3.5292715	0.9463422	-0.3847286	
O	-3.4706291	0.0415130	-1.0294907	
H	3.9328338	-1.0229555	-0.3863835	
H	3.3566322	-0.4283083	1.1748034	
H	1.6756418	-0.7589709	-1.3534879	
H	1.6634789	-1.8412703	0.0380336	
H	0.7969711	1.0926981	0.0648621	
H	0.8506590	0.0456199	1.4806435	
H	-0.8157682	-1.4721999	0.3955029	
H	-0.8568615	-0.4254162	-1.0123929	
H	-1.6669161	1.4640376	0.4502763	
H	-1.6822217	0.3688735	1.8225484	
H	-3.3463917	-1.0837618	0.6323682	
H	-3.9412592	0.5521990	0.9370771	
H	2.9929393	1.5862201	0.1001626	
H	-3.4399708	0.9713340	-1.2914509	
tTTTG-G-t	C	2.7239740	-0.3863313	0.4682516
	C	1.6435565	0.2626453	-0.3723136
	C	0.2782725	0.2392347	0.3119881
	C	-0.8126484	0.8747688	-0.5476262
	C	-2.1628313	1.0128382	0.1575883
	C	-2.7446396	-0.3047493	0.6348433
	O	3.9577983	-0.2956576	-0.2584950
	O	-2.8312491	-1.1774886	-0.5008424
	H	2.4692884	-1.4344689	0.6618470
	H	2.8088796	0.1286676	1.4320419
	H	1.9401392	1.2937647	-0.5818538
	H	1.5880677	-0.2589375	-1.3312770
	H	0.3419526	0.7692938	1.2701331
	H	0.0096336	-0.7969232	0.5384784
	H	-0.9433787	0.2847080	-1.4573050
	H	-0.4818443	1.8707496	-0.8586098
	H	-2.8806152	1.4799175	-0.5217816
	H	-2.0636923	1.6730721	1.0259080
	H	-2.1108550	-0.7501851	1.4084833
	H	-3.7370824	-0.1366222	1.0658245
	H	4.6537414	-0.7158685	0.2630556
	H	-3.2605046	-1.9982721	-0.2271745
tG+G+TTTg+	C	2.7449996	-0.2875933	0.6336237
	C	2.1665148	1.0193469	0.1239076
	C	0.8118973	0.8672636	-0.5698652
	C	-0.2746249	0.2537718	0.3109349
	C	-1.6429815	0.2482959	-0.3681487
	C	-2.7227639	-0.3809656	0.4984646
	O	2.8098578	-1.1955410	-0.4759433
	O	-4.0221602	-0.3297188	-0.1049451
	H	2.1186116	-0.7045663	1.4287771
	H	3.7442030	-0.1139669	1.0460819
	H	2.0751551	1.7035709	0.9741889

H	2.8816978	1.4647064	-0.5725084	
H	0.9373415	0.2547839	-1.4655373	
H	0.4808899	1.8559539	-0.9030556	
H	-0.3423167	0.8136971	1.2513597	
H	-0.0013698	-0.7732442	0.5704707	
H	-1.5731835	-0.3030414	-1.3128614	
H	-1.9457567	1.2697764	-0.6137577	
H	-2.4549365	-1.4153999	0.7437429	
H	-2.8266237	0.1679594	1.4345621	
H	3.2455719	-2.0069508	-0.1849914	
H	-3.9742367	-0.7931831	-0.9516181	
tG-G-TTTg+	C	-2.7452753	-0.2962517	0.6347992
	C	-2.1605328	1.0188868	0.1538810
	C	-0.8114063	0.8740602	-0.5522380
	C	0.2787592	0.2412011	0.3102130
	C	1.6415360	0.2354742	-0.3801741
	C	2.7286359	-0.3913151	0.4790404
	O	-2.8299456	-1.1721925	-0.4984973
	O	3.9968931	-0.4582485	-0.1863482
	H	-3.7384563	-0.1250339	1.0626942
	H	-2.1141842	-0.7399612	1.4116093
	H	-2.8771891	1.4856975	-0.5268253
	H	-2.0590151	1.6816136	1.0199647
	H	-0.4793313	1.8677509	-0.8698135
	H	-0.9448810	0.2783636	-1.4578169
	H	0.0039742	-0.7893566	0.5530666
	H	0.3539185	0.7839794	1.2602730
	H	1.9280170	1.2645673	-0.6266226
	H	1.5802969	-0.3154871	-1.3223353
	H	2.8219480	0.1530025	1.4262169
	H	2.4792702	-1.4265351	0.7119307
	H	-3.2560565	-1.9938659	-0.2225887
	H	4.2506036	0.4411797	-0.4323719
tTTTG+G+g+	C	-2.7239429	-0.4019186	0.4504279
	C	-1.6449916	0.2763171	-0.3689921
	C	-0.2789271	0.2283926	0.3124582
	C	0.8115119	0.8903300	-0.5277129
	C	2.1590412	1.0101325	0.1859925
	C	2.7368131	-0.3202099	0.6515036
	O	-3.9593850	-0.2802186	-0.2683888
	O	2.8322773	-1.2842453	-0.4053299
	H	-2.8042937	0.0764293	1.4333463
	H	-2.4706114	-1.4569584	0.6030289
	H	-1.5913530	-0.2122282	-1.3453564
	H	-1.9423549	1.3139967	-0.5421460
	H	-0.0104583	-0.8145290	0.5036997
	H	-0.3398613	0.7277535	1.2870233
	H	0.4799871	1.8927209	-0.8164477
	H	0.9397612	0.3218585	-1.4522397
	H	2.0597732	1.6609803	1.0620696
	H	2.8796922	1.4973534	-0.4805229

H	3.7162041	-0.1618975	1.1158674	
H	2.0925511	-0.7867794	1.3953684	
H	-4.6524049	-0.7296817	0.2322770	
H	3.4546399	-0.9482872	-1.0642922	
tG-TTG-G-t	C	-2.8194599	-0.6875817	0.1592408
	C	-1.6625383	-0.0197599	0.8753555
	C	-0.4185790	0.1278684	0.0031970
	C	0.7468645	0.7592313	0.7614139
	C	1.9620894	1.0718673	-0.1132926
	C	2.5390197	-0.1413685	-0.8181021
	O	-3.1875652	0.1477773	-0.9491520
	O	2.8564411	-1.1183279	0.1852100
	H	-3.6676465	-0.8091707	0.8413170
	H	-2.5177753	-1.6800166	-0.1957775
	H	-1.9921413	0.9630595	1.2248029
	H	-1.4204824	-0.6143635	1.7626330
	H	-0.6680215	0.7335584	-0.8723070
	H	-0.1286017	-0.8624236	-0.3620743
	H	1.0537088	0.0975027	1.5750046
	H	0.4056392	1.6923724	1.2215317
	H	2.7480049	1.5200282	0.5005016
	H	1.6892735	1.8075311	-0.8773241
	H	1.8184760	-0.5517324	-1.5325947
	H	3.4397531	0.1449403	-1.3710199
	H	-3.9262884	-0.2654466	-1.4141768
	H	3.2799632	-1.8727952	-0.2440560
tG-TG+TTt	C	2.9162873	-0.7992809	0.1701934
	C	1.4789714	-0.5624926	-0.2508533
	C	0.8592054	0.6629069	0.4170712
	C	-0.5452666	0.9935006	-0.0918863
	C	-1.5692543	-0.1125627	0.1594561
	C	-2.9755387	0.3126930	-0.2106581
	O	3.6907238	0.3290932	-0.2641626
	O	-3.8477052	-0.7991891	0.0398706
	H	3.2965596	-1.7189160	-0.2862924
	H	2.9750488	-0.9052311	1.2597502
	H	1.4545092	-0.4439623	-1.3387183
	H	0.9063757	-1.4623461	-0.0097294
	H	1.5147579	1.5195193	0.2488388
	H	0.8196448	0.5000345	1.5004754
	H	-0.4950674	1.2092030	-1.1649892
	H	-0.8864031	1.9137268	0.3942023
	H	-1.5605356	-0.3961501	1.2160987
	H	-1.3250339	-1.0066914	-0.4175161
	H	-3.2763868	1.1783365	0.3899701
	H	-3.0142553	0.5994833	-1.2676220
	H	4.6078748	0.1963801	0.0078736
	H	-4.7483849	-0.5435099	-0.1976360
tG+TTG-G-t	C	-2.9664165	-0.0932083	0.0910971
	C	-1.7278241	-0.7116726	-0.5266800
	C	-0.4514402	-0.4112220	0.2545627

C	0.7756760	-1.0843385	-0.3564593	
C	2.0569861	-0.8964488	0.4576633	
C	2.4860443	0.5518808	0.6014277	
O	-2.7942939	1.3317874	0.0863419	
O	2.6694568	1.0802146	-0.7201757	
H	-3.0943340	-0.4576700	1.1173862	
H	-3.8551552	-0.3708648	-0.4856233	
H	-1.8811405	-1.7947087	-0.5843077	
H	-1.6290483	-0.3443525	-1.5521637	
H	-0.5767199	-0.7534957	1.2897377	
H	-0.3143328	0.6704401	0.2902701	
H	0.9364112	-0.6996100	-1.3662349	
H	0.5817163	-2.1580776	-0.4515427	
H	2.8742232	-1.4485949	-0.0142039	
H	1.9239461	-1.3130202	1.4620360	
H	1.7281731	1.1287726	1.1404478	
H	3.4219033	0.6066733	1.1677839	
H	-3.5810147	1.7381932	0.4717535	
H	2.9112256	2.0124965	-0.6492118	
tTTG-TTt	C	2.9928052	0.0496719	-0.2585429
	C	1.5456136	-0.0618026	0.1766664
	C	0.7136383	1.1369421	-0.2761375
	C	-0.7136379	1.1369418	0.2761375
	C	-1.5456133	-0.0618033	-0.1766650
	C	-2.9928052	0.0496707	0.2585437
	O	3.6792215	-1.1192659	0.2104257
	O	-3.6792216	-1.1192672	-0.2104246
	H	3.4435805	0.9544043	0.1648643
	H	3.0516909	0.1171472	-1.3508118
	H	1.1402362	-0.9909586	-0.2279516
	H	1.5183991	-0.1439262	1.2672322
	H	0.6731533	1.1631502	-1.3706718
	H	1.2125442	2.0591266	0.0401358
	H	-1.2125438	2.0591260	-0.0401369
	H	-0.6731528	1.1631511	1.3706718
	H	-1.1402357	-0.9909587	0.2279540
	H	-1.5183988	-0.1439279	-1.2672307
	H	-3.0516912	0.1171461	1.3508126
	H	-3.4435803	0.9544030	-0.1648637
	H	4.6002971	-1.0719219	-0.0764685
	H	-4.6002996	-1.0719185	0.0764609
tTTTG-Tt	C	2.8567474	-0.6401363	0.2130578
	C	1.8313790	0.4138296	-0.1521766
	C	0.4068672	-0.0091120	0.2002423
	C	-0.6269533	1.0568069	-0.1648029
	C	-2.0481068	0.7439664	0.3067943
	C	-2.6288115	-0.5112713	-0.3147878
	O	4.1466888	-0.1443458	-0.1714124
	O	-4.0008732	-0.5947464	0.0975052
	H	2.6347177	-1.5772197	-0.3101104
	H	2.8258713	-0.8347903	1.2910247

H	2.0856892	1.3406958	0.3685228	
H	1.9076594	0.6148569	-1.2241024	
H	0.3407922	-0.2156931	1.2747612	
H	0.1755388	-0.9470652	-0.3140708	
H	-0.6248013	1.2037487	-1.2505534	
H	-0.3163141	2.0093135	0.2746866	
H	-2.7117436	1.5746490	0.0546908	
H	-2.0679231	0.6377988	1.3949433	
H	-2.5600553	-0.4511766	-1.4077055	
H	-2.0812688	-1.3993231	0.0148340	
H	4.8135089	-0.8001115	0.0701775	
H	-4.3771158	-1.4143273	-0.2485433	
tTTTG-Tg+	C	2.8590429	-0.6361683	0.2058598
	C	1.8305451	0.4194681	-0.1458567
	C	0.4080088	-0.0104382	0.2061588
	C	-0.6287274	1.0546026	-0.1527202
	C	-2.0479023	0.7289560	0.3187616
	C	-2.6317366	-0.5199085	-0.3262384
	O	4.1474319	-0.1289120	-0.1680914
	O	-3.9729529	-0.7829072	0.1048628
	H	2.6417109	-1.5659008	-0.3319247
	H	2.8265468	-0.8472328	1.2806723
	H	2.0845607	1.3413203	0.3838518
	H	1.9035669	0.6315768	-1.2158500
	H	0.3439176	-0.2221949	1.2796099
	H	0.1786141	-0.9462103	-0.3123662
	H	-0.6288719	1.2068572	-1.2377582
	H	-0.3209236	2.0058199	0.2915849
	H	-2.7033193	1.5760036	0.0872499
	H	-2.0649407	0.6022569	1.4048494
	H	-2.5890608	-0.4317076	-1.4189423
	H	-2.0730248	-1.4093262	-0.0405744
	H	4.8154967	-0.7901534	0.0544069
	H	-4.5133121	-0.0125065	-0.1153487
g+TTTG-G-g-	C	2.7306260	-0.4053653	0.4616309
	C	1.6445974	0.2475974	-0.3796003
	C	0.2806649	0.2283753	0.3080676
	C	-0.8099543	0.8815618	-0.5385917
	C	-2.1539542	1.0176800	0.1786960
	C	-2.7388135	-0.3049960	0.6573461
	O	4.0012663	-0.4426943	-0.2008698
	O	-2.8401046	-1.2775730	-0.3904691
	H	2.4843613	-1.4491288	0.6560531
	H	2.8175558	0.1051434	1.4280449
	H	1.9303245	1.2845422	-0.5919047
	H	1.5869509	-0.2730556	-1.3391304
	H	0.3514715	0.7453009	1.2726826
	H	0.0079223	-0.8090642	0.5207234
	H	-0.9447547	0.2985330	-1.4530422
	H	-0.4761450	1.8781576	-0.8449179
	H	-2.8732411	1.5035399	-0.4901955

H	-2.0472874	1.6758620	1.0483667	
H	-2.0968246	-0.7681631	1.4050688	
H	-3.7167558	-0.1366107	1.1209810	
H	4.2559529	0.4665195	-0.4066573	
H	-3.4686126	-0.9496939	-1.0474542	
tTG+TTG-t	C	-2.3759998	0.6049554	-0.2257386
	C	-1.9547270	-0.7875245	0.2014738
	C	-0.5671857	-1.1844377	-0.3061812
	C	0.5662109	-0.3033206	0.2182987
	C	1.9435221	-0.8183751	-0.1904362
	C	3.0787470	0.0442110	0.3246864
	O	-3.7403862	0.7824026	0.1857010
	O	2.9327708	1.3481396	-0.2586247
	H	-2.2892756	0.7023759	-1.3145207
	H	-1.7400369	1.3644220	0.2378113
	H	-1.9848151	-0.8434931	1.2931775
	H	-2.7025870	-1.4895684	-0.1755629
	H	-0.5602996	-1.1664353	-1.4019016
	H	-0.3743971	-2.2218413	-0.0145801
	H	0.5091382	-0.2596010	1.3127130
	H	0.4570581	0.7194959	-0.1456325
	H	2.0137211	-0.8674181	-1.2810223
	H	2.0861105	-1.8357795	0.1889227
	H	3.0341512	0.1088844	1.4181149
	H	4.0431207	-0.3920045	0.0442306
	H	-4.0064404	1.6882386	-0.0184113
	H	3.6505678	1.9104607	0.0598091
tG-TG-TG-t	C	2.9536977	-0.5837289	-0.2211369
	C	1.4410527	-0.6063470	-0.3156103
	C	0.7614739	0.0726438	0.8720214
	C	-0.7614742	-0.0726449	0.8720212
	C	-1.4410525	0.6063464	-0.3156106
	C	-2.9536974	0.5837297	-0.2211373
	O	3.3693340	0.7909776	-0.2335058
	O	-3.3693350	-0.7909764	-0.2335058
	H	3.3944895	-1.1215888	-1.0672259
	H	3.2791282	-1.0712515	0.7053410
	H	1.1533182	-0.1247272	-1.2528194
	H	1.1169651	-1.6511102	-0.3753936
	H	1.0343987	1.1308580	0.8838799
	H	1.1587203	-0.3629744	1.7955676
	H	-1.1587207	0.3629734	1.7955673
	H	-1.0343992	-1.1308591	0.8838795
	H	-1.1533182	0.1247263	-1.2528197
	H	-1.1169639	1.6511093	-0.3753939
	H	-3.2791275	1.0712528	0.7053405
	H	-3.3944887	1.1215898	-1.0672263
	H	4.3325658	0.8217538	-0.1696824
	H	-4.3325668	-0.8217517	-0.1696806
tG-TTG+Tg+	C	-3.0887208	-0.0332385	0.3195492
	C	-1.9456128	0.8180862	-0.1969861

C	-0.5737389	0.2971356	0.2228039	
C	0.5661797	1.1778976	-0.2884138	
C	1.9520831	0.7674811	0.2156652	
C	2.3973841	-0.6046235	-0.2701728	
O	-2.9428970	-1.3442676	-0.2462567	
O	3.7571178	-0.8930525	0.0870433	
H	-4.0486855	0.4040594	0.0259738	
H	-3.0533628	-0.0841950	1.4141511	
H	-2.0096021	0.8585912	-1.2882087	
H	-2.0835690	1.8394206	0.1734881	
H	-0.4642090	-0.7250256	-0.1419819	
H	-0.5275592	0.2512796	1.3177883	
H	0.3771539	2.2131253	0.0133609	
H	0.5649316	1.1717488	-1.3841899	
H	1.9572361	0.7812111	1.3120859	
H	2.6980621	1.4942577	-0.1157937	
H	1.7349950	-1.3906917	0.1038230	
H	2.3792701	-0.6417654	-1.3599368	
H	-3.6690014	-1.8987772	0.0670009	
H	3.8171929	-0.8897171	1.0515633	
tTTG-TTg+	C	2.9925773	0.0543735	-0.2503104
	C	1.5422782	-0.0604774	0.1735924
	C	0.7139011	1.1454605	-0.2663814
	C	-0.7162522	1.1394820	0.2789074
	C	-1.5489378	-0.0539776	-0.1876502
	C	-3.0011018	0.0483536	0.2541612
	O	3.6686591	-1.1301055	0.1942656
	O	-3.8050175	-1.0361771	-0.2268526
	H	3.4455482	0.9458394	0.1978300
	H	3.0584304	0.1479203	-1.3402113
	H	1.1397577	-0.9829399	-0.2492552
	H	1.5076419	-0.1601858	1.2625563
	H	0.6794456	1.1875775	-1.3605138
	H	1.2115839	2.0625839	0.0658352
	H	-1.2162182	2.0623725	-0.0328470
	H	-0.6822559	1.1572064	1.3737770
	H	-1.1264094	-0.9837634	0.2054752
	H	-1.5233698	-0.1250320	-1.2790893
	H	-3.0601160	0.1149509	1.3469016
	H	-3.4625052	0.9448038	-0.1601754
	H	4.5940559	-1.0777261	-0.0777492
	H	-3.4412136	-1.8575965	0.1290249
tG-TTG-Tg+	C	-3.0162777	-0.2105804	0.5582479
	C	-1.8992436	0.7844161	0.3125226
	C	-0.5545325	0.1190155	0.0313766
	C	0.5617817	1.1384322	-0.1940618
	C	1.8964991	0.5190782	-0.6155054
	C	2.4966915	-0.4014909	0.4372474
	O	-3.1777500	-0.9835104	-0.6399338
	O	3.7716920	-0.9262742	0.0446164
	H	-3.9453478	0.3160204	0.8004374

H	-2.7597113	-0.8623584	1.4015744	
H	-2.1825193	1.4211976	-0.5305255	
H	-1.8156643	1.4308035	1.1927443	
H	-0.6500246	-0.5210994	-0.8491197	
H	-0.3045269	-0.5343060	0.8734791	
H	0.7064243	1.7295922	0.7178519	
H	0.2425733	1.8417822	-0.9693384	
H	2.6135696	1.3219561	-0.8212923	
H	1.7738106	-0.0438735	-1.5447407	
H	2.5782079	0.1281905	1.3946999	
H	1.8743025	-1.2806953	0.5926061	
H	-3.8826645	-1.6286325	-0.4995373	
H	4.3571959	-0.1791766	-0.1369410	
tG-TG+TG-t	C	2.9905565	0.5378893	-0.3155225
	C	1.5492437	0.6257042	0.1477869
	C	0.7099249	-0.5748980	-0.2842902
	C	-0.7099248	-0.5748980	0.2842903
	C	-1.5492438	0.6257039	-0.1477871
	C	-2.9905563	0.5378890	0.3155230
	O	3.5866562	-0.6011149	0.3235110
	O	-3.5866563	-0.6011149	-0.3235108
	H	3.5316302	1.4505611	-0.0444567
	H	3.0269877	0.4262756	-1.4055355
	H	1.5445528	0.7088173	1.2393373
	H	1.1272149	1.5533218	-0.2496310
	H	1.2224064	-1.4865749	0.0290355
	H	0.6584205	-0.6009735	-1.3792502
	H	-0.6584203	-0.6009732	1.3792502
	H	-1.2224062	-1.4865752	-0.0290350
	H	-1.5445533	0.7088165	-1.2393375
	H	-1.1272148	1.5533217	0.2496301
	H	-3.0269872	0.4262748	1.4055359
	H	-3.5316300	1.4505610	0.0444577
	H	4.4976249	-0.6863973	0.0143041
	H	-4.4976256	-0.6863961	-0.0143054
tG+TTG+G+g+C		2.8221149	-0.7100784	0.0272480
	C	1.6617198	-0.1986886	0.8578158
	C	0.4240505	0.1221789	0.0241260
	C	-0.7437873	0.6029792	0.8822868
	C	-1.9517515	1.0766181	0.0721738
	C	-2.5296218	0.0177642	-0.8578457
	O	3.2028005	0.3369059	-0.8784806
	O	-2.8568005	-1.2014218	-0.1763269
	H	2.5188350	-1.6044625	-0.5293630
	H	3.6637280	-0.9764237	0.6754451
	H	1.4145056	-0.9593756	1.6059509
	H	1.9903362	0.6935067	1.3990310
	H	0.1313639	-0.7769250	-0.5266530
	H	0.6816823	0.8849355	-0.7157282
	H	-0.4050916	1.4296692	1.5152100
	H	-1.0519248	-0.2029122	1.5539874

H	-1.6730653	1.9446858	-0.5356906	
H	-2.7382060	1.4168033	0.7557648	
H	-3.4095330	0.4136462	-1.3765892	
H	-1.8041595	-0.2734978	-1.6160011	
H	3.9300334	0.0193421	-1.4289085	
H	-3.5501600	-1.0074636	0.4688533	
tG+TTG-Tg+	C	3.0805935	-0.0380308	0.3271908
C	1.9430591	0.8257034	-0.1812319	
C	0.5673962	0.3013983	0.2215723	
C	-0.5681488	1.1785608	-0.3047542	
C	-1.9530429	0.7749527	0.2070476	
C	-2.3801449	-0.6189207	-0.2301662	
O	2.9431246	-1.3331878	-0.2759377	
O	-3.6942005	-0.9577526	0.2334114	
H	3.0312246	-0.1181822	1.4193815	
H	4.0438626	0.4073650	0.0574802	
H	2.0813772	1.8403070	0.2070914	
H	2.0146456	0.8840470	-1.2712764	
H	0.5069230	0.2549398	1.3155630	
H	0.4646360	-0.7208113	-0.1454324	
H	-0.5630205	1.1569159	-1.4004362	
H	-0.3779259	2.2173603	-0.0163199	
H	-2.6939076	1.4944650	-0.1597201	
H	-1.9791251	0.8215183	1.2994033	
H	-2.3246244	-0.7024403	-1.3224879	
H	-1.7324232	-1.3822587	0.1965234	
H	3.6517881	-1.9030070	0.0495109	
H	-4.3100607	-0.2972421	-0.1106772	
tTG-TTG-t	C	2.4839643	-0.4030759	0.4236968
C	1.9008253	0.5520832	-0.5993635	
C	0.5616823	1.1557952	-0.1719106	
C	-0.5506843	0.1288371	0.0395448	
C	-1.9038553	0.7839415	0.3034638	
C	-3.0139496	-0.2180358	0.5521570	
O	3.8054584	-0.7485218	-0.0188616	
O	-3.1546724	-1.0129822	-0.6346802	
H	1.8679233	-1.3028121	0.5111775	
H	2.5253529	0.0828027	1.4063320	
H	2.6314517	1.3484379	-0.7617803	
H	1.7866770	0.0225998	-1.5490194	
H	0.2410871	1.8662151	-0.9401216	
H	0.7003597	1.7375487	0.7468065	
H	-0.3065828	-0.5223632	0.8854956	
H	-0.6303803	-0.5128552	-0.8415347	
H	-2.1859011	1.4095310	-0.5482325	
H	-1.8328199	1.4402243	1.1774831	
H	-2.7608870	-0.8536786	1.4089326	
H	-3.9509203	0.3029676	0.7751779	
H	4.1600938	-1.4253674	0.5719219	
H	-3.8661097	-1.6513492	-0.4960930	
tG+G+TTG+g+C		-2.5539075	-0.0224126	-0.8223393

C	-1.9543684	1.0890599	0.0187066	
C	-0.7410841	0.6543419	0.8425667	
C	0.4132408	0.1051973	0.0072350	
C	1.6522492	-0.1889977	0.8481805	
C	2.8191659	-0.7337886	0.0374521	
O	-2.8764970	-1.1085815	0.0593085	
O	3.2650141	0.1778455	-0.9768771	
H	-1.8454446	-0.3527967	-1.5884365	
H	-3.4549004	0.3407226	-1.3276017	
H	-1.6737604	1.9070335	-0.6532385	
H	-2.7298948	1.4720466	0.6872917	
H	-1.0553512	-0.0990698	1.5687446	
H	-0.3859919	1.5182345	1.4143962	
H	0.6746994	0.8156345	-0.7824472	
H	0.1043135	-0.8203444	-0.4878972	
H	1.4033221	-0.9186651	1.6266888	
H	1.9719456	0.7219117	1.3688191	
H	3.6505875	-1.0034450	0.6978725	
H	2.5187418	-1.6298975	-0.5064061	
H	-3.3114335	-1.8017543	-0.4536449	
H	3.6003649	0.9704522	-0.5370168	
tG+TG-TG-t	C	-2.9125957	-0.4604591	0.5040984
	C	-1.4252878	-0.5715641	0.2305627
	C	-0.7657232	0.7806602	-0.0324720
	C	0.7147086	0.6798539	-0.4043259
	C	1.5938413	0.1117713	0.7079958
	C	3.0714169	0.1496584	0.3710834
	O	-3.5362025	0.0808517	-0.6706024
	O	3.2765653	-0.6956346	-0.7710161
	H	-3.0873658	0.1963487	1.3645002
	H	-3.3286275	-1.4469618	0.7338984
	H	-0.9643355	-1.0641352	1.0914875
	H	-1.2796371	-1.2274369	-0.6330831
	H	-0.8752395	1.4126371	0.8574938
	H	-1.3071857	1.2774894	-0.8398345
	H	1.0829036	1.6790426	-0.6621077
	H	0.8277022	0.0655200	-1.3007776
	H	1.3246775	-0.9248492	0.9235737
	H	1.4384512	0.6861618	1.6283408
	H	3.3781984	1.1774604	0.1447458
	H	3.6637688	-0.2080705	1.2200050
	H	-4.4854417	0.1545532	-0.5084769
	H	4.2112523	-0.6666854	-1.0124731
tG-TG-TTt	C	3.0359575	-0.1126214	0.5195723
	C	1.5367873	0.0259370	0.6970038
	C	0.8792647	0.8225948	-0.4277850
	C	-0.6000389	1.1250125	-0.1802067
	C	-1.4716642	-0.1253295	-0.0681192
	C	-2.9467803	0.2120951	0.0079651
	O	3.2628503	-0.8239774	-0.7062652
	O	-3.6700569	-1.0191747	0.1495517

H	3.4680608	-0.6599786	1.3639368
H	3.5018503	0.8789998	0.4762272
H	1.1070656	-0.9760691	0.7611473
H	1.3515113	0.5214364	1.6568067
H	0.9907421	0.2759310	-1.3669079
H	1.4187980	1.7682710	-0.5495867
H	-0.9724865	1.7476970	-1.0006975
H	-0.6998119	1.7223302	0.7335292
H	-1.2109717	-0.7017071	0.8216751
H	-1.3067048	-0.7737902	-0.9332237
H	-3.1376516	0.8686990	0.8645901
H	-3.2587598	0.7374631	-0.9016306
H	4.2148477	-0.9301663	-0.8296920
H	-4.6142561	-0.8188825	0.1869862
g+TTTG+G+g+C	-2.7306255	-0.3467715	0.5109304
C	-1.6444201	0.2290536	-0.3845986
C	-0.2794083	0.2652924	0.3003024
C	0.8122093	0.8362745	-0.6025431
C	2.1603053	1.0226063	0.0956202
C	2.7387794	-0.2596422	0.6802016
O	-4.0266589	-0.3242858	-0.1017208
O	2.8272500	-1.3173815	-0.2838918
H	-2.8369791	0.2550307	1.4135877
H	-2.4681548	-1.3663738	0.8158175
H	-1.5733755	-0.3740829	-1.2969841
H	-1.9420063	1.2366807	-0.6872916
H	-0.0080699	-0.7482911	0.6087741
H	-0.3502445	0.8697807	1.2123734
H	0.4833727	1.8053065	-0.9909452
H	0.9399245	0.1767380	-1.4647313
H	2.0616269	1.7515702	0.9077782
H	2.8796055	1.4463064	-0.6142297
H	3.7207600	-0.0610051	1.1226944
H	2.0980894	-0.6542557	1.4673455
H	-3.9809173	-0.8492901	-0.9117492
H	3.4557631	-1.0499376	-0.9678313
tG-G-TTG+g+ C	2.4769747	0.5167012	0.6176191
C	2.0830647	-0.9277281	0.3705861
C	0.7783225	-1.0856397	-0.4120830
C	-0.4333827	-0.4503423	0.2657911
C	-1.7334586	-0.7299669	-0.4826925
C	-2.9487372	-0.0600612	0.1427408
O	2.5530574	1.1692898	-0.6587479
O	-2.8367532	1.3692625	0.1826662
H	3.4467636	0.5544586	1.1246665
H	1.7405229	1.0150793	1.2555083
H	2.8951929	-1.4179531	-0.1727687
H	1.9974872	-1.4262395	1.3420260
H	0.5885027	-2.1545861	-0.5557903
H	0.9060475	-0.6494643	-1.4056429
H	-0.2994739	0.6300644	0.3413916

H	-0.5239894	-0.8322635	1.2900537	
H	-1.9168125	-1.8096305	-0.5208170	
H	-1.6360767	-0.3963117	-1.5228290	
H	-3.8614216	-0.3551832	-0.3865727	
H	-3.0542273	-0.3600350	1.1859217	
H	2.8302294	2.0839946	-0.5197716	
H	-2.7743214	1.6878206	-0.7278276	
tTTG+TTg+	C	2.9905930	0.0497416	0.2608039
	C	1.5438071	-0.0591834	-0.1766283
	C	0.7129098	1.1405397	0.2750538
	C	-0.7150793	1.1408800	-0.2751892
	C	-1.5459031	-0.0650071	0.1620347
	C	-3.0038323	0.0603923	-0.2547326
	O	3.6717675	-1.1265403	-0.1963657
	O	-3.7786962	-1.0985810	0.0758474
	H	3.0474513	0.1263943	1.3526581
	H	3.4461892	0.9488338	-0.1691990
	H	1.5173655	-0.1425437	-1.2670011
	H	1.1368038	-0.9876254	0.2282973
	H	1.2112627	2.0623148	-0.0430244
	H	0.6746871	1.1688441	1.3697862
	H	-0.6781701	1.1762428	-1.3693453
	H	-1.2174601	2.0581410	0.0497762
	H	-1.4928590	-0.1641182	1.2532180
	H	-1.1479400	-0.9875998	-0.2646682
	H	-3.4480438	0.9584741	0.1902387
	H	-3.0822140	0.1512971	-1.3382011
	H	4.5959636	-1.0752140	0.0798083
	H	-3.7425146	-1.2178518	1.0341653
tG-TG+TTg+	C	2.9160105	-0.8050987	0.1608751
	C	1.4820581	-0.5584133	-0.2662573
	C	0.8591788	0.6553310	0.4196676
	C	-0.5455219	0.9916046	-0.0847669
	C	-1.5757257	-0.1112815	0.1570425
	C	-2.9844785	0.3224627	-0.2193693
	O	3.6921112	0.3354508	-0.2356589
	O	-3.9485672	-0.7282927	-0.0720349
	H	3.3009327	-1.7117548	-0.3172028
	H	2.9655380	-0.9408218	1.2477164
	H	1.4650742	-0.4192948	-1.3517036
	H	0.9068264	-1.4621622	-0.0464526
	H	1.5128986	1.5155927	0.2639603
	H	0.8208759	0.4775434	1.5009606
	H	-0.4980690	1.2124497	-1.1567952
	H	-0.8850212	1.9097964	0.4061797
	H	-1.5595327	-0.3948640	1.2166490
	H	-1.3326008	-1.0063270	-0.4192014
	H	-3.2802046	1.1990346	0.3686238
	H	-3.0276249	0.5977924	-1.2731829
	H	4.6097603	0.1912242	0.0288006
	H	-3.9583893	-0.9943517	0.8569011

tG-TG-TTg+	C	3.0433606	-0.1052865	0.5035344
	C	1.5485861	0.0512925	0.7033244
	C	0.8791557	0.8304699	-0.4267051
	C	-0.6015763	1.1255664	-0.1776267
	C	-1.4754178	-0.1256595	-0.0902308
	C	-2.9545197	0.2110392	0.0223183
	O	3.2403014	-0.8594879	-0.7013966
	O	-3.7906058	-0.9534342	0.0426646
	H	3.4870671	-0.6277259	1.3576149
	H	3.5157415	0.8803942	0.4184471
	H	1.1134366	-0.9464261	0.7948963
	H	1.3831454	0.5679767	1.6554920
	H	0.9913938	0.2757122	-1.3609501
	H	1.4109600	1.7789964	-0.5591193
	H	-0.9755913	1.7577711	-0.9896937
	H	-0.7055260	1.7096478	0.7441638
	H	-1.1856945	-0.7277996	0.7768524
	H	-1.3262351	-0.7478139	-0.9772719
	H	-3.1354399	0.8279601	0.9105105
	H	-3.2830963	0.7768501	-0.8494490
	H	4.1889735	-0.9680396	-0.8467663
	H	-3.5294031	-1.4936794	0.7999348
tG+TG+TG+g+	C	2.9466754	0.6110419	-0.1710376
	C	1.4326061	0.6472451	-0.2385606
	C	0.7684791	-0.1621805	0.8738240
	C	-0.7559393	-0.0327398	0.9031030
	C	-1.4498082	-0.6317879	-0.3181545
	C	-2.9678275	-0.5457601	-0.2463693
	O	3.3553164	-0.7519428	-0.3604146
	O	-3.4448611	0.8059175	-0.1830042
	H	3.2874107	0.9796501	0.8034068
	H	3.3763870	1.2489726	-0.9505813
	H	1.1119934	1.6928744	-0.1719282
	H	1.1309312	0.2771418	-1.2211274
	H	1.1703007	0.1766994	1.8349755
	H	1.0508051	-1.2128139	0.7705961
	H	-1.0368668	1.0196309	0.9997998
	H	-1.1385179	-0.5374685	1.7965886
	H	-1.1687531	-1.6864404	-0.4185016
	H	-1.1141862	-0.1351611	-1.2347079
	H	-3.4203393	-1.0688326	-1.0958828
	H	-3.3330843	-1.0125975	0.6689519
	H	4.3188017	-0.7953756	-0.3092380
	H	-3.1880842	1.2495019	-1.0025185
tTG-TTTg+	C	-2.6284846	-0.5116102	-0.3078199
	C	-2.0468345	0.7518711	0.2962120
	C	-0.6252943	1.0569723	-0.1792990
	C	0.4066691	-0.0058035	0.1998926
	C	1.8330219	0.4019714	-0.1644407
	C	2.8585066	-0.6541802	0.2188463
	O	-4.0008622	-0.5859477	0.1043659

O	4.1890697	-0.3120844	-0.1891070	
H	-2.0828749	-1.3955990	0.0354940	
H	-2.5584234	-0.4677225	-1.4014086	
H	-2.7096505	1.5794340	0.0320254	
H	-2.0672108	0.6611626	1.3857317	
H	-0.3140597	2.0150953	0.2478678	
H	-0.6227861	1.1893845	-1.2668788	
H	0.1732627	-0.9509781	-0.2996169	
H	0.3438529	-0.1964509	1.2774678	
H	2.0805243	1.3431516	0.3398113	
H	1.9083711	0.5848679	-1.2397694	
H	2.8237979	-0.8398822	1.2987101	
H	2.6428894	-1.5946512	-0.2883524	
H	-4.3768942	-1.4128493	-0.2241034	
H	4.4298875	0.5172525	0.2445183	
tG+TTG+Tg+	C	3.0228499	-0.1861186	0.5555730
	C	1.9064337	0.7984369	0.2689668
	C	0.5571390	0.1239565	0.0357421
	C	-0.5606231	1.1344890	-0.2220576
	C	-1.8997659	0.5058407	-0.6151108
	C	-2.5026077	-0.3743514	0.4701995
	O	3.1631280	-1.0296364	-0.5972520
	O	-3.8328757	-0.8047405	0.1476350
	H	2.7766654	-0.7861890	1.4393633
	H	3.9576734	0.3489969	0.7523208
	H	1.8331920	1.4895229	1.1154185
	H	2.1825940	1.3902071	-0.6084768
	H	0.3170829	-0.4904236	0.9093751
	H	0.6415868	-0.5555574	-0.8161791
	H	-0.2444961	1.8100560	-1.0229641
	H	-0.7029588	1.7579401	0.6681976
	H	-1.7666505	-0.0868432	-1.5275846
	H	-2.6242416	1.2909271	-0.8460383
	H	-1.8666400	-1.2411492	0.6727013
	H	-2.6074200	0.1897140	1.3978127
	H	3.8791391	-1.6572840	-0.4353258
	H	-3.7886597	-1.3132598	-0.6730277
tTTTG+Tg+	C	-2.8628549	-0.6400117	0.2007359
	C	-1.8334112	0.4174164	-0.1427169
	C	-0.4108723	-0.0171695	0.2035272
	C	0.6264064	1.0514159	-0.1438707
	C	2.0491173	0.7247163	0.3164274
	C	2.6391861	-0.5109807	-0.3482151
	O	-4.1516687	-0.1250710	-0.1604713
	O	4.0268391	-0.6897736	-0.0327180
	H	-2.8258646	-0.8644561	1.2727949
	H	-2.6502549	-1.5635499	-0.3495047
	H	-1.9071592	0.6395691	-1.2105422
	H	-2.0856313	1.3347010	0.3957128
	H	-0.1825077	-0.9475589	-0.3249482
	H	-0.3474898	-0.2404156	1.2750181

H	0.3194785	1.9976117	0.3116972	
H	0.6258525	1.2166909	-1.2268173	
H	2.0561064	0.5877457	1.4042678	
H	2.7103124	1.5666657	0.0967188	
H	2.0746980	-1.4098496	-0.0820772	
H	2.6091445	-0.4051850	-1.4333293	
H	-4.8194642	-0.7912913	0.0474980	
H	4.1035804	-0.7901058	0.9254588	
tG+TG-TTg+	C	-2.9193504	-0.7946452	0.1848344
	C	-1.4789424	-0.5714441	-0.2339922
	C	-0.8595720	0.6671553	0.4096638
	C	0.5456681	0.9890111	-0.1029559
	C	1.5750802	-0.1067181	0.1727337
	C	2.9850513	0.3153925	-0.2115733
	O	-3.6867434	0.3259031	-0.2797852
	O	3.9662883	-0.6867749	0.0863160
	H	-2.9839496	-0.8755492	1.2761830
	H	-3.3000738	-1.7233611	-0.2526097
	H	-0.9106492	-1.4675848	0.0309362
	H	-1.4489888	-0.4775402	-1.3241890
	H	-0.8226700	0.5272073	1.4962663
	H	-1.5146723	1.5199842	0.2219527
	H	0.8862705	1.9180149	0.3660344
	H	0.4982744	1.1842641	-1.1800512
	H	1.3174913	-1.0139985	-0.3831494
	H	1.5694407	-0.3681272	1.2351545
	H	3.0226645	0.5853761	-1.2734189
	H	3.2912175	1.1878602	0.3655156
	H	-4.6054415	0.2051557	-0.0072807
	H	3.7451786	-1.4792481	-0.4203182
tTG+TTTg+	C	-2.6269765	-0.5114936	0.3106375
	C	-2.0475661	0.7490012	-0.3016998
	C	-0.6255607	1.0582267	0.1696200
	C	0.4053101	-0.0093038	-0.1991445
	C	1.8337386	0.4073113	0.1465322
	C	2.8572784	-0.6574352	-0.2176684
	O	-4.0022108	-0.5854227	-0.0916886
	O	4.2056981	-0.2425880	0.0339987
	H	-2.5495612	-0.4639904	1.4036860
	H	-2.0848000	-1.3973526	-0.0333133
	H	-2.0693921	0.6521920	-1.3905869
	H	-2.7106985	1.5774814	-0.0412431
	H	-0.6229879	1.2022204	1.2559248
	H	-0.3134699	2.0111744	-0.2678835
	H	0.3391650	-0.2134119	-1.2738801
	H	0.1734971	-0.9482881	0.3130205
	H	1.9002753	0.6181031	1.2202215
	H	2.0922245	1.3309380	-0.3781244
	H	2.6375593	-1.5909559	0.3135895
	H	2.8228449	-0.8661796	-1.2869355
	H	-4.3747185	-1.4149129	0.2342184

H	4.2865299	-0.0476227	0.9770610
g+G+TTG-G-g-C	2.9724743	-0.0786223	-0.0963986
C	1.7321294	-0.7081810	0.5222475
C	0.4556255	-0.4372969	-0.2688707
C	-0.7734996	-1.0809352	0.3692126
C	-2.0574300	-0.9020160	-0.4423728
C	-2.4778572	0.5509061	-0.6251422
O	2.8751456	1.3463198	-0.2128502
O	-2.6168723	1.2460630	0.6217142
H	3.1080207	-0.4325627	-1.1190957
H	3.8648079	-0.3550148	0.4762821
H	1.8995724	-1.7882448	0.6023355
H	1.6134131	-0.3366015	1.5471844
H	0.5803914	-0.8207926	-1.2888417
H	0.3180158	0.6419517	-0.3520022
H	-0.9194847	-0.6612211	1.3682032
H	-0.5896419	-2.1524763	0.5001802
H	-2.8742103	-1.4470747	0.0446095
H	-1.9359726	-1.3497552	-1.4352498
H	-1.7232608	1.1121328	-1.1738003
H	-3.4103726	0.6020021	-1.1974420
H	2.7808153	1.7140582	0.6761451
H	-3.3373145	0.8332083	1.1165348
tG-TTG+G+g+ C	-2.9852045	-0.1052724	-0.0709756
C	-1.7351562	-0.7147566	0.5325270
C	-0.4686501	-0.3923395	-0.2560940
C	0.7685184	-1.0675474	0.3324335
C	2.0348385	-0.8720166	-0.5025240
C	2.4894579	0.5775077	-0.6151041
O	-2.8249981	1.3203843	-0.0607183
O	2.7178391	1.1852168	0.6630188
H	-3.8657350	-0.3942981	0.5126833
H	-3.1190150	-0.4668088	-1.0975188
H	-1.6330454	-0.3554269	1.5604334
H	-1.8755856	-1.7999977	0.5809085
H	-0.3384417	0.6903741	-0.2766056
H	-0.6007336	-0.7206484	-1.2946699
H	0.5775981	-2.1416877	0.4282420
H	0.9402591	-0.6853692	1.3422100
H	1.8748256	-1.2599397	-1.5150024
H	2.8514137	-1.4627662	-0.0713213
H	3.3912986	0.6391961	-1.2340857
H	1.7240986	1.1941218	-1.0835885
H	-3.6161754	1.7230071	-0.4411315
H	3.4359050	0.7063626	1.0981711
tTTG-TG+g+ C	2.9714102	0.3179900	-0.2233203
C	1.5695726	-0.1133613	0.1569064
C	0.5423252	0.9958652	-0.0648028
C	-0.8549587	0.6550979	0.4566638
C	-1.4772361	-0.5706724	-0.2076112
C	-2.9348560	-0.7805357	0.1795374

O	3.8439914	-0.8005063	-0.0097285	
O	-3.7779160	0.3107332	-0.2146028	
H	3.2818174	1.1699103	0.3919000	
H	2.9959608	0.6281956	-1.2742166	
H	1.3183072	-0.9981259	-0.4315383	
H	1.5730694	-0.4143472	1.2086650	
H	0.4792945	1.2266999	-1.1343872	
H	0.8884170	1.9096708	0.4296499	
H	-1.5169157	1.5104160	0.3035936	
H	-0.8045696	0.4866876	1.5383271	
H	-0.9227827	-1.4755794	0.0584657	
H	-1.4093065	-0.4739445	-1.2986689	
H	-3.3090709	-1.7207560	-0.2392998	
H	-3.0356296	-0.8333792	1.2641296	
H	4.7442137	-0.5382111	-0.2417727	
H	-3.7935332	0.3414337	-1.1804284	
g+TTTG-Tg+	C	2.8616963	-0.6491264	0.2120598
	C	1.8323558	0.4080942	-0.1583405
	C	0.4080279	-0.0075908	0.2050729
	C	-0.6269822	1.0546144	-0.1670861
	C	-2.0465607	0.7367520	0.3085983
	C	-2.6322274	-0.5196951	-0.3201482
	O	4.1902053	-0.2972305	-0.1935228
	O	-3.9732818	-0.7746660	0.1153463
	H	2.6486316	-1.5843576	-0.3056413
	H	2.8286791	-0.8473612	1.2897110
	H	2.0785214	1.3449149	0.3546063
	H	1.9050620	0.6015897	-1.2319756
	H	0.3469312	-0.2045646	1.2814554
	H	0.1769292	-0.9502239	-0.2996648
	H	-0.6269352	1.1929679	-1.2539604
	H	-0.3184420	2.0112896	0.2653079
	H	-2.7007197	1.5816557	0.0661876
	H	-2.0638090	0.6240550	1.3962104
	H	-2.5898287	-0.4458624	-1.4138971
	H	-2.0747670	-1.4061304	-0.0230646
	H	4.4320865	0.5233178	0.2558929
	H	-4.5143187	-0.0091822	-0.1198644
g+TG+TTG-g-	C	2.3951538	-0.6144117	-0.2464989
	C	1.9562185	0.7777879	0.1852284
	C	0.5648405	1.1669688	-0.3204264
	C	-0.5688598	0.3043615	0.2343009
	C	-1.9477705	0.8137975	-0.1753383
	C	-3.0870313	-0.0550899	0.3388864
	O	3.7601489	-0.8865918	0.1007417
	O	-3.0211464	-1.4014685	-0.1500127
	H	2.3599597	-0.6990409	-1.3333261
	H	1.7392860	-1.3833480	0.1721210
	H	1.9739852	0.8389932	1.2796935
	H	2.6982155	1.4890908	-0.1860876
	H	0.5536369	1.1200645	-1.4153894

H	0.3765103	2.2124375	-0.0562708	
H	-0.5066871	0.2894627	1.3288896	
H	-0.4643476	-0.7296629	-0.0987795	
H	-2.0087847	0.8754624	-1.2685053	
H	-2.0936088	1.8326687	0.2005091	
H	-3.0318188	-0.1495377	1.4238891	
H	-4.0537923	0.3949637	0.0890248	
H	3.8346924	-0.8509511	1.0635874	
H	-3.1598174	-1.3798986	-1.1062510	
tG+TTG-G-g+	C	-2.9365857	-0.0763440	0.1372377
	C	-1.7303436	-0.7592149	-0.4769822
	C	-0.4311385	-0.4562403	0.2647522
	C	0.7845422	-1.1029324	-0.3969351
	C	2.0932119	-0.9159744	0.3743271
	C	2.4850535	0.5387988	0.6029772
	O	-2.7258386	1.3406063	0.0369259
	O	2.6481717	1.2680811	-0.6207797
	H	-3.0427546	-0.3726902	1.1871871
	H	-3.8480079	-0.3642792	-0.3965510
	H	-1.9100461	-1.8392060	-0.4858709
	H	-1.6470964	-0.4372731	-1.5191964
	H	-0.5143204	-0.8149484	1.2976880
	H	-0.3124805	0.6279029	0.3199179
	H	0.8994077	-0.7112325	-1.4130543
	H	0.5988922	-2.1756636	-0.5113690
	H	2.9046119	-1.4091073	-0.1672983
	H	2.0127890	-1.4032836	1.3526796
	H	1.7610900	1.0411422	1.2522400
	H	3.4571877	0.5892641	1.0927718
	H	-3.4839444	1.7947731	0.4267370
	H	1.7744610	1.4201794	-1.0039597
tTG+TTG+g+	C	2.4935964	-0.3969524	-0.4162527
	C	1.8969218	0.5563753	0.6006211
	C	0.5583986	1.1528874	0.1621520
	C	-0.5466936	0.1201494	-0.0601002
	C	-1.9015232	0.7634169	-0.3420940
	C	-3.0183786	-0.2478099	-0.5581859
	O	3.8139494	-0.7308429	0.0364108
	O	-3.2281916	-1.0945725	0.5795398
	H	2.5378507	0.0866960	-1.3995764
	H	1.8850177	-1.3012356	-0.5056600
	H	1.7791653	0.0277535	1.5503104
	H	2.6216983	1.3569655	0.7675286
	H	0.7015656	1.7356558	-0.7551304
	H	0.2278532	1.8624753	0.9272744
	H	-0.6290708	-0.5245260	0.8191922
	H	-0.2907542	-0.5312584	-0.9017881
	H	-1.8327142	1.3960862	-1.2342676
	H	-2.1741213	1.4275692	0.4869123
	H	-3.9483548	0.2631875	-0.8301289
	H	-2.7617370	-0.9300237	-1.3692592

H	4.1768688	-1.4098555	-0.5467084
H	-3.5289795	-0.5413111	1.3126712
tG+TG-TG+g+ C	2.9850681	0.5360716	0.3399737
C	1.5503502	0.6289549	-0.1426471
C	0.7081646	-0.5813238	0.2554934
C	-0.7060237	-0.5677649	-0.3270666
C	-1.5508291	0.6227540	0.1210829
C	-3.0066281	0.5207914	-0.3138419
O	3.5888283	-0.5970954	-0.3015641
O	-3.6752304	-0.6204924	0.2405088
H	3.0065364	0.4140586	1.4292947
H	3.5295598	1.4512698	0.0851691
H	1.1198696	1.5484201	0.2647544
H	1.5604906	0.7308394	-1.2324471
H	0.6466832	-0.6307653	1.3494383
H	1.2240337	-1.4859703	-0.0720035
H	-1.2216460	-1.4880642	-0.0434669
H	-0.6449362	-0.5690766	-1.4213546
H	-1.1449448	1.5566747	-0.2801047
H	-1.5122661	0.7118576	1.2144509
H	-3.5466743	1.4386948	-0.0574961
H	-3.0711117	0.3840967	-1.3937826
H	4.4996604	-0.6786897	0.0091441
H	-3.7047625	-0.5110328	1.2002749
tG-TG+TG-g+ C	-2.9991166	0.5573477	0.2654309
C	-1.5529830	0.6201856	-0.1876139
C	-0.7216043	-0.5552721	0.3216238
C	0.7092330	-0.5804641	-0.2209183
C	1.5617068	0.6126855	0.2070157
C	2.9941963	0.5528163	-0.3067721
O	-3.5791292	-0.6322431	-0.2896813
O	3.7422706	-0.5430242	0.2355005
H	-3.5418109	1.4425570	-0.0820476
H	-3.0475589	0.5309096	1.3603127
H	-1.5356913	0.6396922	-1.2818240
H	-1.1351323	1.5687723	0.1608541
H	-1.2277486	-1.4817788	0.0442932
H	-0.6890451	-0.5266157	1.4169206
H	0.6771310	-0.6297527	-1.3160463
H	1.1839876	-1.5045896	0.1238012
H	1.5867930	0.6729581	1.2994183
H	1.1172295	1.5422563	-0.1613546
H	2.9996648	0.5135754	-1.4027823
H	3.5438995	1.4425762	-0.0015344
H	-4.4986197	-0.6915039	-0.0001563
H	3.3766798	-1.3649218	-0.1150940
tG-G-TTG-g+ C	-2.5390823	-0.2347554	0.7917905
C	-1.9740749	1.0540316	0.2238496
C	-0.7520658	0.8504217	-0.6729534
C	0.4200507	0.1542287	0.0159706
C	1.6694567	0.1114901	-0.8618208

	C	2.8258189	-0.6612861	-0.2441355
	O	-2.8197957	-1.1086529	-0.3110886
	O	3.3288224	-0.0546690	0.9539653
	H	-3.4532726	-0.0215752	1.3552232
	H	-1.8230186	-0.7037770	1.4745747
	H	-2.7615297	1.5545592	-0.3454349
	H	-1.7160113	1.7094159	1.0625327
	H	-0.4189399	1.8292757	-1.0320805
	H	-1.0463078	0.2718143	-1.5513669
	H	0.1366852	-0.8705124	0.2782871
	H	0.6427925	0.6809227	0.9515983
	H	2.0047499	1.1297871	-1.0781645
	H	1.4171606	-0.3591147	-1.8184000
	H	2.5248987	-1.6977315	-0.0490638
	H	3.6770653	-0.6823511	-0.9237770
	H	-3.2542547	-1.9022945	0.0269050
	H	2.6390243	-0.0981523	1.6281599
g+TTTG-Tg-	C	2.8672636	-0.6486162	0.2150910
	C	1.8352749	0.4046116	-0.1591819
	C	0.4121653	-0.0127370	0.2071823
	C	-0.6247508	1.0505532	-0.1571386
	C	-2.0474682	0.7308552	0.3082064
	C	-2.6407760	-0.5101754	-0.3439389
	O	4.1944034	-0.2973197	-0.1949250
	O	-4.0280396	-0.6825695	-0.0245371
	H	2.6546833	-1.5872711	-0.2966318
	H	2.8366872	-0.8404432	1.2940779
	H	2.0796578	1.3442917	0.3493885
	H	1.9061638	0.5935441	-1.2336788
	H	0.3557036	-0.2131393	1.2835047
	H	0.1801816	-0.9539243	-0.2997059
	H	-0.6241455	1.1986312	-1.2425594
	H	-0.3183138	2.0040720	0.2837059
	H	-2.7074328	1.5716609	0.0807095
	H	-2.0535626	0.6048928	1.3973357
	H	-2.6123291	-0.4142037	-1.4299832
	H	-2.0776423	-1.4077312	-0.0707339
	H	4.4332988	0.5300623	0.2434676
	H	-4.1029905	-0.7846403	0.9335791
tG-TG-TG+g+	C	-3.0703770	-0.2811589	0.2334170
	C	-1.5998616	-0.4607024	0.5557502
	C	-0.7096991	-0.4167696	-0.6843716
	C	0.7639929	-0.7093979	-0.3973965
	C	1.4252817	0.3121320	0.5255567
	C	2.9323286	0.1269700	0.6392218
	O	-3.2312405	1.0273970	-0.3349174
	O	3.6092097	0.2812419	-0.6157672
	H	-3.6728046	-0.3774593	1.1428688
	H	-3.3949792	-1.0487427	-0.4787669
	H	-1.3132028	0.3189673	1.2654178
	H	-1.4756071	-1.4238565	1.0634486

H	-0.8040309	0.5637066	-1.1576679	
H	-1.0826931	-1.1499583	-1.4078899	
H	1.3163947	-0.7359260	-1.3394492	
H	0.8591913	-1.7065241	0.0485885	
H	1.0018782	0.2533649	1.5329315	
H	1.2164745	1.3256930	0.1610926	
H	3.3461145	0.8185163	1.3811059	
H	3.1678312	-0.8885491	0.9594544	
H	-4.1618174	1.1535601	-0.5606649	
H	3.4810101	1.1920779	-0.9125333	
tG+TG-TG-g+	C	2.9260105	0.6652523	-0.1028594
	C	1.4356877	0.5216549	-0.3434598
	C	0.7659410	-0.4343767	0.6411889
	C	-0.7122846	-0.6879486	0.3381693
	C	-1.5886513	0.5613508	0.4215458
	C	-3.0776482	0.2619361	0.3185361
	O	3.5267348	-0.6227696	-0.3046029
	O	-3.4514715	-0.2751213	-0.9569668
	H	3.1090397	1.0151957	0.9198499
	H	3.3510912	1.3962088	-0.7982601
	H	0.9878718	1.5171837	-0.2785307
	H	1.2846507	0.1647396	-1.3669388
	H	0.8603867	-0.0309894	1.6562843
	H	1.3059136	-1.3830040	0.6257818
	H	-1.0933561	-1.4335381	1.0458208
	H	-0.7891392	-1.1301998	-0.6611129
	H	-1.3277638	1.2668129	-0.3705199
	H	-1.4081047	1.0626843	1.3798412
	H	-3.3819079	-0.4188180	1.1228146
	H	-3.6595015	1.1778455	0.4166977
	H	4.4781838	-0.5458633	-0.1575391
	H	-3.0457188	-1.1464597	-1.0502543
g+TG-TTG+g+	C	2.3819743	-0.6240996	0.2108107
	C	1.9568966	0.7839917	-0.1807866
	C	0.5667443	1.1675082	0.3322518
	C	-0.5629635	0.3076421	-0.2342114
	C	-1.9445202	0.8193365	0.1636622
	C	-3.0796461	-0.0587035	-0.3444739
	O	3.7014683	-0.9439491	-0.2489424
	O	-3.0182002	-1.3957285	0.1701161
	H	1.7407266	-1.3725894	-0.2507426
	H	2.3140226	-0.7466168	1.2989731
	H	2.6928226	1.4911848	0.2182695
	H	1.9928181	0.8694705	-1.2704020
	H	0.3768815	2.2152518	0.0784761
	H	0.5525865	1.1084710	1.4266989
	H	-0.4629597	-0.7267265	0.0996620
	H	-0.4901072	0.2932548	-1.3278776
	H	-2.0906991	1.8332558	-0.2252989
	H	-2.0108844	0.8940618	1.2558198
	H	-4.0483273	0.3959991	-0.1110225

H	-3.0150497	-0.1731563	-1.4269612
H	4.3121755	-0.2940038	0.1232887
H	-3.1671556	-1.3562735	1.1242001
tG-TG+TG+g+ C	2.9109715	-0.4528575	0.5135484
C	1.4186446	-0.5579702	0.2646177
C	0.7684273	0.7917880	-0.0328250
C	-0.7110990	0.6939560	-0.4097199
C	-1.6010493	0.1442891	0.7026466
C	-3.0819285	0.1603265	0.3502764
O	3.5218143	0.0327772	-0.6909168
O	-3.3880862	-0.6400849	-0.7994389
H	3.3195214	-1.4338789	0.7777213
H	3.1044199	0.2361007	1.3441816
H	1.2572659	-1.2395948	-0.5763818
H	0.9656034	-1.0184204	1.1473354
H	1.3163673	1.2659535	-0.8493041
H	0.8783883	1.4432049	0.8426531
H	-0.8214456	0.0741992	-1.3033520
H	-1.0742405	1.6909632	-0.6807301
H	-1.4600542	0.7381064	1.6137072
H	-1.3129257	-0.8819315	0.9547175
H	-3.6818357	-0.1615022	1.2087178
H	-3.3972869	1.1683181	0.0791357
H	4.4731171	0.1119053	-0.5441900
H	-3.1667713	-1.5575217	-0.5909102
tTTG+TG-g+ C	-2.9823172	0.2993819	-0.2110836
C	-1.5739687	-0.1044980	0.1767585
C	-0.5556370	0.9933258	-0.1261447
C	0.8591365	0.6774775	0.3662718
C	1.4910430	-0.5402049	-0.3047773
C	2.9161401	-0.8162493	0.1563192
O	-3.8511131	-0.7952929	0.1101123
O	3.8346328	0.2266893	-0.1947998
H	-3.0259028	0.5228861	-1.2830340
H	-3.2798249	1.1996262	0.3383504
H	-1.5638750	-0.3381914	1.2453477
H	-1.3275508	-1.0234269	-0.3581121
H	-0.8887904	1.9264604	0.3399974
H	-0.5235578	1.1779723	-1.2054798
H	0.8360575	0.5236961	1.4517047
H	1.4851564	1.5560646	0.1818621
H	1.4980267	-0.3986010	-1.3897772
H	0.8961070	-1.4338813	-0.0954588
H	2.9347810	-0.9935365	1.2383517
H	3.3054123	-1.7074873	-0.3345242
H	-4.7515539	-0.5616210	-0.1500535
H	3.6328175	1.0048495	0.3395231
tG+G+TTG-g+ C	-2.4911350	0.5383723	0.6079508
C	-2.0670250	-0.9098237	0.4473006
C	-0.7794464	-1.0922340	-0.3580254
C	0.4371668	-0.3876667	0.2391928

C	1.7267747	-0.7102454	-0.5135326	
C	2.9701214	-0.0864928	0.1041014	
O	-2.5941393	1.1070585	-0.7051213	
O	2.9643065	1.3465814	0.0563921	
H	-1.7598860	1.0925615	1.2057598	
H	-3.4552778	0.5865382	1.1246192	
H	-1.9460107	-1.3407807	1.4469104	
H	-2.8792148	-1.4537533	-0.0418305	
H	-0.9403103	-0.7299760	-1.3756907	
H	-0.5662511	-2.1635388	-0.4302046	
H	0.5502802	-0.6813042	1.2908738	
H	0.2657031	0.6925367	0.2200821	
H	1.6418288	-0.3717725	-1.5498640	
H	1.8677538	-1.7965647	-0.5357972	
H	3.0907724	-0.4324164	1.1380409	
H	3.8598673	-0.3789228	-0.4524315	
H	-2.9290855	2.0095074	-0.6261164	
H	2.2305330	1.6643090	0.5975735	
tTTTG-G-g+	C	2.7408682	-0.3335650	0.4910029
	C	1.6476875	0.2390713	-0.3886201
	C	0.2882766	0.2604890	0.3074600
	C	-0.8136404	0.8407109	-0.5794252
	C	-2.1655798	1.0046861	0.1195879
	C	-2.7685774	-0.2923649	0.6440865
	O	3.9602890	-0.3103336	-0.2624865
	O	-3.0251858	-1.2471749	-0.3941480
	H	2.4891692	-1.3594868	0.7830854
	H	2.8405080	0.2664655	1.4026170
	H	1.9332434	1.2525699	-0.6817487
	H	1.5913868	-0.3567325	-1.3036115
	H	0.3564024	0.8543957	1.2261116
	H	0.0300607	-0.7579123	0.6168012
	H	-0.9298301	0.2189491	-1.4735738
	H	-0.4898672	1.8203768	-0.9429305
	H	-2.8783267	1.4566002	-0.5749280
	H	-2.0542193	1.6936071	0.9643489
	H	-2.1334859	-0.7335790	1.4195907
	H	-3.7432080	-0.0966011	1.0898395
	H	4.6696967	-0.6682339	0.2868291
	H	-2.1797369	-1.5329307	-0.7635365
tTTTG+G-t	C	2.6569580	0.5411287	0.2731836
	C	1.6218555	-0.4537528	-0.2097448
	C	0.2223852	-0.1326231	0.3103488
	C	-0.8163169	-1.1480350	-0.1663757
	C	-2.2380603	-0.9165925	0.3539214
	C	-2.9964195	0.2142081	-0.3157727
	O	3.9279050	0.1517652	-0.2701500
	O	-2.3895777	1.4651612	0.0462695
	H	2.6936029	0.5416317	1.3683624
	H	2.3906769	1.5500939	-0.0605490
	H	1.6249869	-0.4518643	-1.3032830

H	1.9265424	-1.4538676	0.1112336	
H	-0.0777716	0.8681711	-0.0026471	
H	0.2318292	-0.1272635	1.4062274	
H	-0.4915731	-2.1462053	0.1456691	
H	-0.8347748	-1.1606561	-1.2624120	
H	-2.2202653	-0.7333798	1.4324815	
H	-2.8257974	-1.8267046	0.1959005	
H	-2.9729551	0.0824322	-1.4039897	
H	-4.0421527	0.1978049	0.0091148	
H	4.5958350	0.7808322	0.0316721	
H	-2.9001684	2.1792824	-0.3573859	
tTG-TTG-g+	C	2.4927356	-0.3943725	0.4273531
	C	1.9053837	0.5611046	-0.5930160
	C	0.5635979	1.1586661	-0.1665600
	C	-0.5547359	0.1319741	0.0174807
	C	-1.9111442	0.7831866	0.2793168
	C	-3.0285519	-0.2150813	0.5468747
	O	3.8029716	-0.7545348	-0.0327965
	O	-3.3164256	-1.0478809	-0.5834922
	H	1.8697962	-1.2880638	0.5291979
	H	2.5514798	0.0964964	1.4062189
	H	2.6317040	1.3615929	-0.7523907
	H	1.7963417	0.0345039	-1.5449949
	H	0.2488439	1.8836289	-0.9230623
	H	0.6919567	1.7213138	0.7649421
	H	-0.3170695	-0.5380635	0.8509724
	H	-0.6081317	-0.4859104	-0.8858546
	H	-2.1936420	1.4023499	-0.5766758
	H	-1.8303333	1.4460001	1.1481365
	H	-2.7847342	-0.8295429	1.4219293
	H	-3.9623426	0.3061637	0.7546259
	H	4.1772946	-1.4025099	0.5778629
	H	-2.5627075	-1.6325580	-0.7321933
g+G-TG-TTg-	C	3.0412581	-0.1311419	0.5293093
	C	1.5323937	-0.0042919	0.6865294
	C	0.8750734	0.8037814	-0.4311271
	C	-0.6016369	1.1186538	-0.1811937
	C	-1.4845730	-0.1229765	-0.0615607
	C	-2.9627848	0.2289661	0.0165663
	O	3.4194495	-0.8574700	-0.6472952
	O	-3.7969695	-0.9181701	0.2177447
	H	3.4635632	-0.6995392	1.3572188
	H	3.5061965	0.8619435	0.5305011
	H	1.1073269	-1.0091724	0.7319527
	H	1.3300283	0.4806572	1.6486985
	H	0.9593332	0.2613373	-1.3788721
	H	1.4194239	1.7474355	-0.5539942
	H	-0.9728040	1.7444348	-0.9996812
	H	-0.6915619	1.7155136	0.7329789
	H	-1.2253847	-0.7008613	0.8275416
	H	-1.3155766	-0.7724272	-0.9289605

H	-3.1550449	0.8705093	0.8766519	
H	-3.2697923	0.7741027	-0.8835770	
H	3.2033365	-0.3203137	-1.4199006	
H	-3.6694417	-1.5152679	-0.5313189	
tTTG-TG-g+	C	-2.9544708	0.2191213	0.0312818
	C	-1.4832051	-0.1274485	-0.0758952
	C	-0.6018911	1.1181400	-0.1514227
	C	0.8743028	0.8090672	-0.4114412
	C	1.5298843	-0.0340319	0.6815347
	C	3.0413167	-0.1391149	0.5344401
	O	-3.6852989	-1.0121557	0.1119358
	O	3.4400398	-0.8232627	-0.6601495
	H	-3.2692868	0.7957199	-0.8457844
	H	-3.1318616	0.8299986	0.9237344
	H	-1.2157540	-0.7398922	0.7871090
	H	-1.3367090	-0.7437737	-0.9675497
	H	-0.6884850	1.6859691	0.7816637
	H	-0.9708565	1.7711844	-0.9493587
	H	1.4204031	1.7551678	-0.5048539
	H	0.9568419	0.2959919	-1.3754975
	H	1.1144039	-1.0438510	0.6860587
	H	1.3142125	0.4134497	1.6589629
	H	3.4941318	0.8590836	0.5712955
	H	3.4631452	-0.7284238	1.3479019
	H	-4.6266544	-0.8083126	0.1850820
	H	3.1970603	-0.2781455	-1.4191527
tG-G+TTTg+	C	-2.9993922	0.2133891	-0.3132465
	C	-2.2376634	-0.9199431	0.3480931
	C	-0.8165230	-1.1446460	-0.1771694
	C	0.2224799	-0.1370838	0.3158020
	C	1.6240106	-0.4474371	-0.2060645
	C	2.6624784	0.5442946	0.2947575
	O	-2.3821672	1.4615767	0.0399965
	O	3.9924635	0.2267784	-0.1397036
	H	-4.0410406	0.2012643	0.0244097
	H	-2.9898767	0.0807106	-1.4016314
	H	-2.2169321	-0.7436446	1.4276687
	H	-2.8241306	-1.8300897	0.1858925
	H	-0.8363160	-1.1395514	-1.2734330
	H	-0.4920095	-2.1477563	0.1187685
	H	0.2350816	-0.1508181	1.4113735
	H	-0.0772586	0.8691899	0.0206360
	H	1.6148659	-0.4318578	-1.3025435
	H	1.9303669	-1.4528065	0.0969267
	H	2.3919913	1.5611952	-0.0117405
	H	2.7114390	0.5259366	1.3834762
	H	-2.9026753	2.1789442	-0.3447892
	H	3.9951570	0.2255997	-1.1060445
tG+G-TTTg+	C	2.9954510	0.2104475	-0.3148638
	C	2.2366545	-0.9246604	0.3470368
	C	0.8140304	-1.1496641	-0.1737722

C	-0.2209198	-0.1324371	0.3075331
C	-1.6229221	-0.4410888	-0.2139618
C	-2.6579545	0.5590599	0.2770329
O	2.3874602	1.4579196	0.0560913
O	-3.9664558	0.3168351	-0.2593255
H	2.9725834	0.0862692	-1.4040003
H	4.0409144	0.1915857	0.0105345
H	2.8224981	-1.8346291	0.1815579
H	2.2199775	-0.7494576	1.4269249
H	0.4869179	-2.1485066	0.1344359
H	0.8321119	-1.1577302	-1.2698584
H	0.0809804	0.8685820	-0.0025532
H	-0.2308210	-0.1296036	1.4033544
H	-1.9202019	-1.4484752	0.1018889
H	-1.6277718	-0.4346220	-1.3076104
H	-2.6889883	0.5634919	1.3727939
H	-2.4004461	1.5651529	-0.0533301
H	2.8990397	2.1762958	-0.3386914
H	-4.2339650	-0.5733630	0.0049536
g+G-TTG-G-g- C	2.8296422	-0.6476738	-0.2676616
C	1.6717431	0.1394070	-0.8643545
C	0.4219527	0.1515172	0.0135011
C	-0.7515983	0.8657300	-0.6541840
C	-1.9674793	1.0481247	0.2553378
C	-2.5249737	-0.2552425	0.8128757
O	3.3239565	-0.0769178	0.9516090
O	-2.8095345	-1.2191744	-0.2093570
H	3.6832712	-0.6413603	-0.9446348
H	2.5339321	-1.6913692	-0.1080092
H	2.0043201	1.1647626	-1.0494409
H	1.4228344	-0.3036640	-1.8349790
H	0.6433168	0.6504561	0.9642814
H	0.1398512	-0.8810031	0.2435191
H	-1.0458650	0.3040041	-1.5443679
H	-0.4204203	1.8511818	-0.9965848
H	-2.7585336	1.5668132	-0.2976591
H	-1.7067761	1.6945867	1.1008398
H	-1.7993181	-0.7444513	1.4610013
H	-3.4197958	-0.0554374	1.4119688
H	2.6453314	-0.1775826	1.6309708
H	-3.5171941	-0.8685120	-0.7665439
g+G+TG-TG-g-C	2.9258392	0.3091765	0.5877291
C	1.4188916	0.4485688	0.4167882
C	0.7674471	-0.7936618	-0.1874746
C	-0.7070057	-0.6054707	-0.5495572
C	-1.6100170	-0.3247496	0.6491302
C	-3.0823476	-0.2171500	0.2769460
O	3.6107035	0.1011011	-0.6543160
O	-3.3453883	0.8546113	-0.6389964
H	3.1597086	-0.5719894	1.1860813
H	3.3331013	1.1847990	1.1047074

H	0.9892354	0.6723895	1.3981476
H	1.2116933	1.3184013	-0.2193488
H	0.8670975	-1.6268595	0.5179849
H	1.3246192	-1.0765598	-1.0833322
H	-1.0683635	-1.5102847	-1.0494721
H	-0.8059776	0.2064452	-1.2751054
H	-1.3077088	0.6007379	1.1509143
H	-1.5004830	-1.1276131	1.3877728
H	-3.4090051	-1.1166182	-0.2458098
H	-3.6969655	-0.1081160	1.1771494
H	3.4982475	0.8947027	-1.1942829
H	-3.1367771	1.6859015	-0.1922909
g+G+TG-TTg+ C	-2.9374941	-0.7784138	0.1902175
C	-1.4797863	-0.5764295	-0.2020509
C	-0.8551754	0.6577925	0.4443013
C	0.5435443	0.9895609	-0.0796683
C	1.5774344	-0.1075702	0.1722668
C	2.9815371	0.3178599	-0.2300971
O	-3.7776574	0.3115583	-0.2123546
O	3.9676935	-0.6838238	0.0502570
H	-3.0354879	-0.8204231	1.2754870
H	-3.3152667	-1.7216205	-0.2185973
H	-0.9273175	-1.4789951	0.0768555
H	-1.4132198	-0.4949458	-1.2944821
H	-0.8074790	0.5069165	1.5285707
H	-1.5151819	1.5116910	0.2762116
H	0.8872582	1.9139884	0.3958181
H	0.4848821	1.1968500	-1.1542745
H	1.3114187	-1.0110226	-0.3860439
H	1.5875276	-0.3765344	1.2326773
H	3.0039418	0.5922795	-1.2913424
H	3.2943508	1.1885513	0.3461041
H	-3.8026861	0.3289247	-1.1783118
H	3.7407235	-1.4754723	-0.4550721
tG-TG-TG-g+ C	2.9668642	-0.5130009	-0.3355645
C	1.4551100	-0.5283961	-0.4473152
C	0.7625950	-0.1275034	0.8534078
C	-0.7599370	-0.2736106	0.8058898
C	-1.4343355	0.6250743	-0.2304589
C	-2.9523352	0.6363733	-0.1209823
O	3.3638194	0.8328996	-0.0327047
O	-3.5411206	-0.6430836	-0.3923283
H	3.4191590	-0.8414092	-1.2771633
H	3.2918222	-1.1940776	0.4597368
H	1.1676409	0.1427668	-1.2595123
H	1.1431910	-1.5385315	-0.7351338
H	1.0247463	0.9048597	1.0961198
H	1.1545049	-0.7499853	1.6652434
H	-1.1668538	-0.0365281	1.7960260
H	-1.0061552	-1.3220446	0.6033500
H	-1.1671520	0.3106757	-1.2416736

H	-1.0748655	1.6524977	-0.1019668	
H	-3.2566796	0.9925661	0.8706032	
H	-3.3840860	1.3054183	-0.8645902	
H	4.3269500	0.8632547	0.0330483	
H	-3.2821507	-1.2509413	0.3118848	
g+G+G+TG-G-g-	C	2.6727346	-0.3046132	-0.5561757
C	1.6185046	-1.0954960	0.2072556	
C	0.3806411	-0.2865730	0.6010374	
C	-0.3778890	0.2912093	-0.5914214	
C	-1.6185261	1.0960002	-0.1979496	
C	-2.6763010	0.2985392	0.5536758	
O	3.0816574	0.8847717	0.1334110	
O	-3.0830480	-0.8839626	-0.1489169	
H	2.2863473	0.0475179	-1.5111834	
H	3.5387800	-0.9418555	-0.7654803	
H	1.3199646	-1.9501799	-0.4099299	
H	2.0777787	-1.5134387	1.1104267	
H	0.6785477	0.5288794	1.2665143	
H	-0.2795539	-0.9433518	1.1726460	
H	-0.6727728	-0.5235765	-1.2590882	
H	0.2817208	0.9508800	-1.1603426	
H	-2.0735538	1.5203015	-1.1003121	
H	-1.3240031	1.9463701	0.4270957	
H	-2.2942446	-0.0629912	1.5069086	
H	-3.5428472	0.9343265	0.7653287	
H	3.4865094	0.6214163	0.9707427	
H	-3.4835594	-0.6123539	-0.9857042	
tG-G-TG-G-t	C	-2.3972205	0.3312809	-0.5486436
C	-1.9604177	-0.9520069	0.1339799	
C	-0.4970970	-0.9431815	0.5803954	
C	0.4970969	-0.9431814	-0.5803954	
C	1.9604176	-0.9520067	-0.1339799	
C	2.3972202	0.3312811	0.5486437	
O	-2.2307575	1.3992462	0.3968415	
O	2.2307571	1.3992464	-0.3968413	
H	-3.4468815	0.2520149	-0.8509824	
H	-1.7974019	0.5199848	-1.4440181	
H	-2.6091752	-1.1077832	1.0000976	
H	-2.1359478	-1.7854968	-0.5546799	
H	-0.3142693	-1.8292345	1.1979604	
H	-0.3406943	-0.0721606	1.2189605	
H	0.3406941	-0.0721606	-1.2189605	
H	0.3142693	-1.8292345	-1.1979605	
H	2.6091752	-1.1077828	-1.0000976	
H	2.1359478	-1.7854967	0.5546798	
H	1.7974016	0.5199848	1.4440182	
H	3.4468812	0.2520151	0.8509826	
H	-2.4361125	2.2339311	-0.0432403	
H	2.4361143	2.2339311	0.0432399	
g+TTTG-G-g+	C	2.7454616	-0.3542719	0.4920876
C	1.6491580	0.2241083	-0.3905011	

C	0.2905040	0.2560478	0.3075466	
C	-0.8110992	0.8455569	-0.5735819	
C	-2.1610711	1.0082249	0.1291691	
C	-2.7709812	-0.2918902	0.6381048	
O	4.0053173	-0.4552166	-0.1810614	
O	-3.0372519	-1.2297106	-0.4125889	
H	2.4996818	-1.3758670	0.7825259	
H	2.8447824	0.2396360	1.4083226	
H	1.9267130	1.2414173	-0.6890292	
H	1.5889403	-0.3723751	-1.3049775	
H	0.3660492	0.8454189	1.2285247	
H	0.0293406	-0.7622914	0.6138553	
H	-0.9313109	0.2300171	-1.4714014	
H	-0.4855880	1.8271756	-0.9308120	
H	-2.8721433	1.4716673	-0.5593843	
H	-2.0456422	1.6867302	0.9818231	
H	-2.1373233	-0.7480418	1.4058631	
H	-3.7427275	-0.0947106	1.0894945	
H	4.2746724	0.4338712	-0.4475285	
H	-2.1950280	-1.5391283	-0.7699440	
g+G+G+TTG-g+ C	-2.4795132	0.5284036	0.6438180	
C	-2.0748128	-0.9228200	0.4192890	
C	-0.7818812	-1.0931424	-0.3799861	
C	0.4267799	-0.3919532	0.2370683	
C	1.7321605	-0.7431654	-0.4743379	
C	2.9598774	-0.0800439	0.1342099	
O	-2.5426642	1.2819840	-0.5732860	
O	2.9655161	1.3442383	-0.0207952	
H	-1.7424960	1.0484846	1.2541398	
H	-3.4366082	0.5734330	1.1744953	
H	-1.9718259	-1.4006544	1.4000537	
H	-2.8892407	-1.4452359	-0.0949363	
H	-0.9288250	-0.7139522	-1.3943219	
H	-0.5670171	-2.1627243	-0.4701695	
H	0.5094301	-0.6677911	1.2961312	
H	0.2647325	0.6888431	0.1944525	
H	1.6673534	-0.4566798	-1.5277832	
H	1.8787167	-1.8283968	-0.4395414	
H	3.0467889	-0.3498361	1.1939814	
H	3.8639605	-0.4170801	-0.3717007	
H	-3.2478365	0.9133556	-1.1219199	
H	2.2092220	1.7073476	0.4572261	
g+TTTG+G-g- C	2.6461003	0.5797383	0.2342743	
C	1.6270121	-0.4745763	-0.1699113	
C	0.2084898	-0.1100490	0.2637421	
C	-0.8114686	-1.1789642	-0.1288317	
C	-2.2440770	-0.9193563	0.3428581	
C	-2.9564601	0.2384332	-0.3463001	
O	3.9903280	0.2160655	-0.1081132	
O	-2.4295121	1.5307088	-0.0131543	
H	2.6563625	0.7015622	1.3174636	

H	2.3852142	1.5471254	-0.2097711	
H	1.6524507	-0.5981587	-1.2589838	
H	1.9257370	-1.4311616	0.2681327	
H	-0.0816040	0.8494671	-0.1674327	
H	0.1884645	0.0167993	1.3526661	
H	-0.4813071	-2.1408300	0.2773977	
H	-0.8148259	-1.2907522	-1.2192660	
H	-2.2564376	-0.7562744	1.4271500	
H	-2.8426603	-1.8189305	0.1620692	
H	-2.8399645	0.1602292	-1.4281183	
H	-4.0280977	0.2023146	-0.1226018	
H	4.0324668	0.1060056	-1.0672303	
H	-2.6152473	1.6982140	0.9202340	
g+G-TG-TTg+	C	3.0459667	-0.1411110	0.5251298
	C	1.5367307	-0.0252398	0.6883942
	C	0.8744199	0.8188766	-0.3995963
	C	-0.6034805	1.1192871	-0.1375821
	C	-1.4873167	-0.1267624	-0.0959026
	C	-2.9630001	0.2180703	0.0391555
	O	3.4250715	-0.8383958	-0.6684175
	O	-3.8078870	-0.9388195	0.0092830
	H	3.4729827	-0.7266652	1.3386186
	H	3.5059132	0.8541575	0.5486260
	H	1.1168264	-1.0333562	0.6995257
	H	1.3341923	0.4260584	1.6669229
	H	0.9592286	0.3115635	-1.3663760
	H	1.4151946	1.7683094	-0.4882360
	H	-0.9728180	1.7871274	-0.9226724
	H	-0.6954026	1.6670888	0.8068665
	H	-1.1969214	-0.7665508	0.7432021
	H	-1.3507459	-0.7132163	-1.0091301
	H	-3.1343634	0.7955510	0.9552188
	H	-3.2899726	0.8260305	-0.8044170
	H	3.1945099	-0.2899633	-1.4290320
	H	-3.5629053	-1.5071283	0.7513308
tTTTG-G+g+	C	-2.6361437	0.5833180	0.1928426
	C	-1.6266396	-0.4913931	-0.1547142
	C	-0.2059977	-0.1067269	0.2527312
	C	0.8109415	-1.1860889	-0.1176481
	C	2.2462048	-0.9181921	0.3402428
	C	2.9445197	0.2459506	-0.3529025
	O	-3.9311358	0.1154625	-0.2123627
	O	2.4298008	1.5353208	0.0097344
	H	-2.3846875	1.5146967	-0.3261566
	H	-2.6203327	0.7775451	1.2713455
	H	-1.9249760	-1.4198115	0.3401077
	H	-1.6710209	-0.6719746	-1.2321873
	H	-0.1705283	0.0580784	1.3362504
	H	0.0771436	0.8381939	-0.2141758
	H	0.8082773	-1.3239046	-1.2048988
	H	0.4817556	-2.1377836	0.3127311

H	2.8478514	-1.8142865	0.1525663	
H	2.2688376	-0.7562600	1.4246652	
H	4.0212955	0.2050760	-0.1561071	
H	2.8011486	0.1817422	-1.4323772	
H	-4.5810142	0.8027779	-0.0168778	
H	2.6251102	1.6823726	0.9445658	
g+G-TG+TG+g+	C	2.9078316	-0.5468166	0.4424292
C	1.4194843	-0.5996416	0.1223933	
C	0.7659861	0.7783157	0.0302603	
C	-0.7215937	0.7405489	-0.3294712	
C	-1.6022900	0.0892637	0.7340199	
C	-3.0829130	0.1170184	0.3783714	
O	3.6851954	0.0707412	-0.5902027	
O	-3.3734284	-0.5791118	-0.8399360	
H	3.3117218	-1.5548749	0.5296340	
H	3.0690726	-0.0363744	1.3997403	
H	1.2858012	-1.1322802	-0.8239478	
H	0.9353488	-1.1936237	0.9033270	
H	1.2816767	1.3686647	-0.7335692	
H	0.8975259	1.3066539	0.9825368	
H	-0.8537941	0.2187445	-1.2804941	
H	-1.0745480	1.7649650	-0.4875157	
H	-1.4700344	0.6087765	1.6903699	
H	-1.3016762	-0.9500566	0.9014500	
H	-3.6797722	-0.2891154	1.2021937	
H	-3.4114067	1.1412970	0.1993318	
H	3.4635519	1.0098480	-0.6205597	
H	-3.1612226	-1.5129856	-0.7096142	
g+G-TG-TG-g-	C	-2.9595910	0.6025384	0.0118295
C	-1.4400787	0.6273240	-0.0775879	
C	-0.7653241	-0.4414234	0.7818130	
C	0.7567770	-0.3031222	0.8629977	
C	1.4645230	-0.4915081	-0.4765370	
C	2.9814791	-0.4330151	-0.3608453	
O	-3.5284241	-0.6055448	-0.5100775	
O	3.4502038	0.8259116	0.1410171	
H	-3.3905145	1.3989372	-0.5941188	
H	-3.2792204	0.7577411	1.0493231	
H	-1.1595652	0.5105621	-1.1267632	
H	-1.0961373	1.6167896	0.2460789	
H	-1.0073971	-1.4368567	0.3933394	
H	-1.1769821	-0.3870498	1.7963813	
H	1.1451366	-1.0467526	1.5668469	
H	1.0139777	0.6759725	1.2751854	
H	1.1370221	0.2672710	-1.1947246	
H	1.1897300	-1.4625039	-0.9051657	
H	3.3366713	-1.1698492	0.3604984	
H	3.4465299	-0.6557506	-1.3272173	
H	-3.2886109	-1.3333519	0.0774976	
H	3.2278528	1.5071458	-0.5076760	
g+G+TTG-G-g+	C	2.9392131	-0.0589091	-0.1684927

C	1.7401706	-0.7544495	0.4614076	
C	0.4284665	-0.4538641	-0.2586634	
C	-0.7816249	-1.0762103	0.4368459	
C	-2.0943948	-0.9301458	-0.3361980	
C	-2.4998762	0.5106360	-0.6215446	
O	2.8274377	1.3704264	-0.1333552	
O	-2.6783698	1.2826667	0.5737111	
H	3.0086897	-0.3087234	-1.2278986	
H	3.8675418	-0.3816253	0.3146459	
H	1.9241271	-1.8345078	0.4614513	
H	1.6635600	-0.4530786	1.5130291	
H	0.4911893	-0.8346754	-1.2847741	
H	0.3173632	0.6302217	-0.3385192	
H	-0.8938152	-0.6427840	1.4364298	
H	-0.5898032	-2.1420245	0.5961200	
H	-2.8999404	-1.4084525	0.2269358	
H	-2.0119955	-1.4553929	-1.2944897	
H	-1.7771926	0.9964233	-1.2848859	
H	-3.4693417	0.5325371	-1.1185824	
H	2.9114118	1.6555079	0.7862410	
H	-1.8086485	1.4606299	0.9545041	
g+G-TG+TTg-	C	2.9187317	-0.8119598	0.1711246
C	1.4914269	-0.5481423	-0.2911942	
C	0.8582017	0.6799343	0.3592976	
C	-0.5564987	0.9883303	-0.1380494	
C	-1.5803500	-0.0995180	0.1838933	
C	-2.9923789	0.3038721	-0.2152840	
O	3.8336338	0.2233753	-0.2082548	
O	-3.9712730	-0.6807408	0.1365979	
H	3.3069830	-1.7140915	-0.3003073	
H	2.9414171	-0.9640926	1.2568715	
H	1.4959502	-0.4266028	-1.3786682	
H	0.8998093	-1.4398253	-0.0635986	
H	1.4838341	1.5554485	0.1601510	
H	0.8356285	0.5445677	1.4470995	
H	-0.5256962	1.1556352	-1.2201678	
H	-0.8903555	1.9283664	0.3130093	
H	-1.5725818	-0.3162334	1.2561235	
H	-1.3213245	-1.0278175	-0.3345260	
H	-3.2951556	1.2043618	0.3189787	
H	-3.0337088	0.5210416	-1.2890572	
H	3.6400370	1.0112664	0.3147278	
H	-3.7521654	-1.4997467	-0.3270942	
g+G+TG+TG-g+	C	-3.0824917	0.1062529	0.3823799
C	-1.6018266	0.0693594	0.7365424	
C	-0.7214890	0.7474831	-0.3104015	
C	0.7660232	0.7771984	0.0505115	
C	1.4201816	-0.6023717	0.1082832	
C	2.9087562	-0.5569856	0.4278754	
O	-3.3733477	-0.5583031	-0.8538868	
O	3.6851983	0.0833243	-0.5920572	

H	-3.4111652	1.1347483	0.2297362
H	-3.6792341	-0.3213297	1.1953634
H	-1.4689996	0.5642732	1.7058110
H	-1.3011742	-0.9739664	0.8771674
H	-1.0751917	1.7752597	-0.4431719
H	-0.8530879	0.2491500	-1.2740425
H	0.8970750	1.2817174	1.0157117
H	1.2815135	1.3867619	-0.6983267
H	1.2859418	-1.1115523	-0.8508567
H	0.9366943	-1.2156127	0.8746928
H	3.0713013	-0.0677158	1.3959242
H	3.3128579	-1.5666921	0.4920337
H	-3.1607525	-1.4951838	-0.7474787
H	3.4618249	1.0224934	-0.6025738
g+TTTG-G+g+ C	-2.6413980	0.5927131	0.2083270
C	-1.6267608	-0.4738572	-0.1739543
C	-0.2068796	-0.1082787	0.2544816
C	0.8090325	-1.1846296	-0.1279135
C	2.2431239	-0.9251313	0.3391592
C	2.9498262	0.2381916	-0.3467645
O	-3.9667109	0.2906052	-0.2488590
O	2.4298283	1.5276338	0.0077614
H	-2.3902362	1.5421629	-0.2639095
H	-2.6372389	0.7460279	1.2939006
H	-1.9163241	-1.4259544	0.2868254
H	-1.6670724	-0.6169919	-1.2573154
H	-0.1806974	0.0363353	1.3411364
H	0.0821911	0.8440925	-0.1927837
H	0.8099980	-1.3069062	-1.2170049
H	0.4770823	-2.1419229	0.2881799
H	2.8418433	-1.8231540	0.1512396
H	2.2601271	-0.7670738	1.4241775
H	4.0240932	0.1974007	-0.1369104
H	2.8194664	0.1722055	-1.4277868
H	-4.2301362	-0.5528202	0.1422596
H	2.6293361	1.6848626	0.9401048
g+G-TG+TG-g-C	-2.9893457	0.5467512	0.3356404
C	-1.5617339	0.6177774	-0.1906560
C	-0.7071810	-0.5873578	0.1972347
C	0.7177520	-0.5488882	-0.3597162
C	1.5528633	0.6215923	0.1538219
C	3.0125277	0.5406287	-0.2741873
O	-3.7435970	-0.5348168	-0.2248476
O	3.6714132	-0.6351129	0.2137727
H	-3.5403945	1.4443150	0.0569466
H	-2.9841462	0.4821635	1.4305346
H	-1.5969872	0.7069683	-1.2806743
H	-1.1118756	1.5365106	0.1978566
H	-1.1867756	-1.5017448	-0.1657718
H	-0.6645604	-0.6642300	1.2906912
H	0.6746197	-0.5046437	-1.4536699

H	1.2297603	-1.4794031	-0.1051460	
H	1.5039506	0.6574651	1.2494308	
H	1.1494293	1.5724653	-0.2069609	
H	3.0850324	0.4715286	-1.3600709	
H	3.5524998	1.4393201	0.0424892	
H	-3.3828128	-1.3654277	0.1096192	
H	3.7252185	-0.5708181	1.1765310	
tG+TG+TG-g+ C	-3.0711693	0.0383341	0.4160753	
C	-1.5919198	-0.0694331	0.7322250	
C	-0.7246890	0.7600129	-0.2121912	
C	0.7626732	0.7547342	0.1493841	
C	1.4287293	-0.6138593	0.0163620	
C	2.9156465	-0.6009652	0.3457128	
O	-3.2690790	-0.4834092	-0.9054377	
O	3.6899692	0.1875653	-0.5665888	
H	-3.3899632	1.0861765	0.4650191	
H	-3.6558664	-0.5339705	1.1438898	
H	-1.4377226	0.2664431	1.7638191	
H	-1.3132621	-1.1245582	0.6892763	
H	-1.0883398	1.7932523	-0.1995764	
H	-0.8541526	0.3950505	-1.2335085	
H	0.8899187	1.1220826	1.1753618	
H	1.2716093	1.4672055	-0.5076292	
H	1.2995115	-0.9860830	-1.0040934	
H	0.9478339	-1.3313141	0.6877367	
H	3.0703180	-0.2549194	1.3750755	
H	3.3297815	-1.6054206	0.2655161	
H	-4.2063970	-0.4154014	-1.1282158	
H	3.4467918	1.1146220	-0.4509294	
g+G+TG-TG-g+ C	2.9440551	0.4918212	-0.4197797	
C	1.4400989	0.2889604	-0.5458137	
C	0.7616852	0.0244259	0.7961778	
C	-0.7114617	-0.3702565	0.6738735	
C	-1.5901686	0.7012651	0.0298539	
C	-3.0772187	0.3820634	0.0954310	
O	3.6174054	-0.6579544	0.1101625	
O	-3.4284675	-0.7897507	-0.6518345	
H	3.1609808	1.2929645	0.2876308	
H	3.3732942	0.7721534	-1.3874840	
H	1.0172747	1.1783265	-1.0226534	
H	1.2492833	-0.5491168	-1.2277104	
H	0.8434447	0.9214819	1.4204776	
H	1.3075355	-0.7675392	1.3138199	
H	-1.1005751	-0.5927944	1.6743238	
H	-0.7752568	-1.2981662	0.0948238	
H	-1.3175892	0.8403898	-1.0187570	
H	-1.4242959	1.6569508	0.5410361	
H	-3.3952499	0.2780226	1.1397170	
H	-3.6603222	1.1852916	-0.3538220	
H	3.5400914	-1.3731112	-0.5352597	
H	-3.0439637	-1.5579978	-0.2110691	

tG+G-TTG-g+	C	2.8728811	0.2458377	-0.1716031
	C	2.0868145	-0.7958420	0.6027567
	C	0.7658002	-1.2294972	-0.0386899
	C	-0.3666602	-0.2061745	0.0497592
	C	-1.6797199	-0.7433801	-0.5149608
	C	-2.8008976	0.2866106	-0.5227420
	O	2.1597786	1.4924861	-0.1370436
	O	-3.1705932	0.7212489	0.7918751
	H	3.0077911	-0.0853214	-1.2081484
	H	3.8626594	0.3684580	0.2804084
	H	2.7352267	-1.6723663	0.7019052
	H	1.9086516	-0.4166500	1.6134251
	H	0.4337164	-2.1531963	0.4468218
	H	0.9447537	-1.4823103	-1.0903452
	H	-0.0769533	0.7059501	-0.4755690
	H	-0.5000904	0.0635101	1.1029438
	H	-2.0069404	-1.6140536	0.0610889
	H	-1.5204932	-1.0773577	-1.5467268
	H	-2.5161285	1.1458747	-1.1416936
	H	-3.7110174	-0.1416011	-0.9418390
	H	2.7004523	2.1651700	-0.5714758
	H	-2.4263224	1.2079534	1.1685502
tG+G+TG+G+g+	C	-2.3296068	0.4211023	0.5718042
	C	-1.9763582	-0.9463504	0.0142325
	C	-0.5516358	-1.0264562	-0.5374560
	C	0.5253856	-1.0077334	0.5481019
	C	1.9471511	-0.9404963	-0.0127515
	C	2.3097632	0.4234736	-0.5882134
	O	-2.2488963	1.3573243	-0.5132301
	O	2.2357742	1.4685814	0.3928687
	H	-1.6397303	0.7057299	1.3719330
	H	-3.3437461	0.4052779	0.9849626
	H	-2.1171611	-1.6927486	0.8034407
	H	-2.6934870	-1.1765227	-0.7781473
	H	-0.4116642	-0.1964060	-1.2321761
	H	-0.4447406	-1.9488593	-1.1174819
	H	0.4215060	-1.9096269	1.1602785
	H	0.3807682	-0.1550890	1.2152017
	H	2.0763042	-1.6959526	-0.7960561
	H	2.6696747	-1.1850975	0.7743156
	H	3.3097168	0.3905780	-1.0339670
	H	1.6084213	0.7229322	-1.3654353
	H	-2.2911942	2.2527881	-0.1544896
	H	2.9020571	1.2885232	1.0697029
tG-G+TTG-g+	C	-2.7539230	0.4091402	-0.2844704
	C	-2.1748499	-0.8597192	0.3139232
	C	-0.8004765	-1.2681431	-0.2237648
	C	0.3661111	-0.4151392	0.2737687
	C	1.7123280	-0.8897648	-0.2678568
	C	2.8884757	-0.0676161	0.2403932
	O	-1.9833091	1.5361665	0.1658210

O	2.8558809	1.2918365	-0.2128820	
H	-3.7963769	0.5205645	0.0312946	
H	-2.7309318	0.3478595	-1.3788244	
H	-2.1364277	-0.7451347	1.4013560	
H	-2.8889707	-1.6625404	0.1040101	
H	-0.8239862	-1.2444073	-1.3194638	
H	-0.6138302	-2.3102793	0.0566826	
H	0.3863522	-0.4452071	1.3698292	
H	0.1823403	0.6218576	-0.0085101	
H	1.7079967	-0.8492982	-1.3611963	
H	1.8750778	-1.9351373	0.0184560	
H	2.9259958	-0.1029548	1.3360925	
H	3.8284731	-0.4659856	-0.1403032	
H	-2.3888591	2.3405667	-0.1838845	
H	2.0599476	1.7084678	0.1423582	
tG+G+TG-G-T+	C	2.6721665	0.3104267	0.5221891
C	1.6108476	1.1084019	-0.2118408	
C	0.3707986	0.2982403	-0.5969356	
C	-0.3707981	-0.2982412	0.5969348	
C	-1.6108477	-1.1084020	0.2118401	
C	-2.6721665	-0.3104258	-0.5221889	
O	3.0241094	-0.8098008	-0.3047273	
O	-3.0241084	0.8098014	0.3047284	
H	2.2980979	-0.0354943	1.4907623	
H	3.5487377	0.9412910	0.7034035	
H	1.3186629	1.9499631	0.4252010	
H	2.0634182	1.5289718	-1.1138915	
H	0.6669166	-0.5013363	-1.2812532	
H	-0.3001334	0.9624999	-1.1479062	
H	-0.6669154	0.5013353	1.2812528	
H	0.3001337	-0.9625014	1.1479050	
H	-2.0634182	-1.5289721	1.1138908	
H	-1.3186638	-1.9499631	-0.4252023	
H	-2.2980983	0.0354956	-1.4907620	
H	-3.5487381	-0.9412896	-0.7034032	
H	3.7250970	-1.3077098	0.1351950	
H	-3.7250982	1.3077093	-0.1351919	
g+G+TG+TG+g+	C	2.9624997	0.5814576	-0.2056601
C	1.4425882	0.6398808	-0.2729546	
C	0.7625636	-0.0630321	0.8998772	
C	-0.7625634	0.0630334	0.8998766	
C	-1.4425875	-0.6398797	-0.2729554	
C	-2.9624992	-0.5814591	-0.2056604	
O	3.4679541	-0.7601498	-0.2339095	
O	-3.4679556	0.7601477	-0.2339088	
H	3.3167138	0.9926245	0.7401623	
H	3.4033759	1.1718775	-1.0163104	
H	1.1406815	1.6936985	-0.2939780	
H	1.1180679	0.2053769	-1.2245625	
H	1.1529712	0.3654589	1.8289229	
H	1.0476167	-1.1185259	0.9046937	

H	-1.0476166	1.1185273	0.9046927	
H	-1.1529715	-0.3654573	1.8289223	
H	-1.1406792	-1.6936970	-0.2939797	
H	-1.1180685	-0.2053745	-1.2245630	
H	-3.4033750	-1.1718792	-1.0163107	
H	-3.3167123	-0.9926269	0.7401620	
H	3.2340859	-1.1490470	-1.0872904	
H	-3.2340888	1.1490454	-1.0872900	
tG-G-TG+G+g+	C	2.6746659	-0.3080440	0.5350083
C	1.6254339	-1.1055000	-0.2169727	
C	0.3820356	-0.3009646	-0.6025498	
C	-0.3690198	0.2845472	0.5909019	
C	-1.6054460	1.0962170	0.1978935	
C	-2.6739731	0.3004612	-0.5400630	
O	3.0119137	0.8340306	-0.2674665	
O	-3.0960004	-0.8646727	0.1827803	
H	3.5593407	-0.9305767	0.7048423	
H	2.2949669	0.0127041	1.5102640	
H	2.0870294	-1.5108172	-1.1212330	
H	1.3356558	-1.9579402	0.4065092	
H	-0.2820061	-0.9654471	-1.1609034	
H	0.6763272	0.5058839	-1.2788683	
H	0.2965446	0.9423581	1.1557580	
H	-0.6673264	-0.5250339	1.2636310	
H	-1.3071189	1.9373835	-0.4377460	
H	-2.0529269	1.5332111	1.0982322	
H	-3.5324880	0.9439282	-0.7613600	
H	-2.2970729	-0.0817836	-1.4871465	
H	3.7187514	1.3219032	0.1743566	
H	-3.4882906	-0.5731722	1.0167759	
g+G-TG-TG-g-	C	-2.9450276	0.6579503	-0.0501016
C	-1.4258484	0.6501857	-0.1465219	
C	-0.7663185	-0.3771812	0.7732408	
C	0.7573201	-0.2536233	0.8496646	
C	1.4645980	-0.5248534	-0.4758432	
C	2.9816696	-0.4662680	-0.3630646	
O	-3.5369684	-0.5706948	-0.4920712	
O	3.4555418	0.8191241	0.0612746	
H	-3.3649436	1.4217858	-0.7037781	
H	-3.2568757	0.8841886	0.9765156	
H	-1.1524131	0.4650971	-1.1875958	
H	-1.0629257	1.6509146	0.1154620	
H	-1.0208607	-1.3895241	0.4405593	
H	-1.1785064	-0.2606036	1.7823876	
H	1.1355354	-0.9616176	1.5946061	
H	1.0260613	0.7437808	1.2068603	
H	1.1409450	0.1914952	-1.2378457	
H	1.1852245	-1.5181465	-0.8460441	
H	3.3334937	-1.1590843	0.4020464	
H	3.4461766	-0.7493517	-1.3137356	
H	-3.3086770	-1.2631835	0.1409937	

H	3.2370092	1.4600758	-0.6284404
g+G-G-TTG-g- C	2.5783190	0.0254013	-0.8212848
C	1.9511814	1.0745668	0.0879968
C	0.7383876	0.5829051	0.8823685
C	-0.4237184	0.0965444	0.0168353
C	-1.6611430	-0.2559556	0.8379114
C	-2.8359663	-0.7172328	-0.0137674
O	3.0613388	-1.1170861	-0.1015086
O	-3.2683857	0.2814306	-0.9465066
H	3.4582740	0.4374472	-1.3140822
H	1.8766478	-0.2843029	-1.6025768
H	2.7180124	1.4294865	0.7814146
H	1.6541111	1.9271814	-0.5327476
H	0.3851285	1.4028479	1.5154514
H	1.0446613	-0.2106706	1.5729409
H	-0.1288420	-0.7869315	-0.5598765
H	-0.6848354	0.8667165	-0.7139502
H	-1.9680638	0.6121284	1.4332960
H	-1.4196993	-1.0509585	1.5527036
H	-2.5466701	-1.5688100	-0.6307532
H	-3.6691992	-1.0318840	0.6237701
H	2.3027626	-1.5936668	0.2595819
H	-3.6336302	1.0224130	-0.4447743
tG+TTG+G-t C	2.7929208	0.4134964	-0.4845412
C	1.6452341	-0.5549448	-0.6925265
C	0.3742633	-0.1480857	0.0480318
C	-0.7468331	-1.1716590	-0.1298642
C	-2.0522440	-0.8329824	0.5972172
C	-2.9288184	0.1920595	-0.0973858
O	3.1555108	0.3660315	0.9045525
O	-2.2607777	1.4638357	-0.0919208
H	2.4826725	1.4270111	-0.7633999
H	3.6477877	0.1295653	-1.1077191
H	1.4427795	-0.6193510	-1.7672689
H	1.9728325	-1.5471549	-0.3667520
H	0.0370131	0.8281494	-0.3043170
H	0.6009623	-0.0431223	1.1118899
H	-0.3884378	-2.1406706	0.2336234
H	-0.9584034	-1.3043784	-1.1980528
H	-1.8378251	-0.4820725	1.6109813
H	-2.6540431	-1.7424016	0.6959393
H	-3.1250112	-0.1274443	-1.1278593
H	-3.8879753	0.2699656	0.4257199
H	3.8440548	1.0236397	1.0658625
H	-2.8431705	2.1149223	-0.5047324
tTG-TG-G-t C	2.2590069	0.5930795	0.1175756
C	1.7461168	-0.7335261	-0.4072832
C	0.2281861	-0.7593111	-0.5973411
C	-0.5572337	-0.5633403	0.6997025
C	-2.0562101	-0.8320744	0.5577893
C	-2.7407993	0.0575435	-0.4632985

O	3.6940959	0.5309487	0.1043247	
O	-2.4776575	1.4207095	-0.0972794	
H	-2.3605826	-0.1446120	-1.4696730	
H	1.9053647	1.4087689	-0.5238256	
H	2.2441274	-0.9268834	-1.3606866	
H	2.0526876	-1.5260775	0.2809414	
H	-0.0501936	-1.7211161	-1.0417595	
H	-0.0532703	0.0127249	-1.3202236	
H	-0.4221677	0.4535096	1.0721030	
H	-0.1546584	-1.2391849	1.4619920	
H	-2.5460247	-0.6873794	1.5242663	
H	-2.2213233	-1.8741984	0.2641276	
H	1.8986902	0.7761377	1.1337099	
H	-3.8180619	-0.1378482	-0.4619983	
H	4.0389784	1.3372299	0.5090089	
H	-2.9619640	1.9995106	-0.6999484	
g-G+TG+TG+g-	C	2.9675514	0.5814931	-0.2466153
C	1.4494488	0.5686352	-0.3588294	
C	0.7610265	-0.0814675	0.8405010	
C	-0.7610266	0.0814677	0.8405011	
C	-1.4494488	-0.5686351	-0.3588294	
C	-2.9675513	-0.5814932	-0.2466154	
O	3.5368102	-0.7344162	-0.2388885	
O	-3.5368103	0.7344161	-0.2388883	
H	3.2760206	1.1358472	0.6479284	
H	3.4088004	1.0720717	-1.1134566	
H	1.1058082	1.6053361	-0.4529055	
H	1.1790304	0.0506434	-1.2812969	
H	1.1632323	0.3575667	1.7610489	
H	0.9951546	-1.1510116	0.8676529	
H	-0.9951548	1.1510119	0.8676528	
H	-1.1632325	-0.3575664	1.7610489	
H	-1.1058080	-1.6053361	-0.4529052	
H	-1.1790301	-0.0506436	-1.2812970	
H	-3.4088000	-1.0720715	-1.1134569	
H	-3.2760205	-1.1358475	0.6479281	
H	3.2947122	-1.1668617	0.5898629	
H	-3.2947126	1.1668613	0.5898634	
tG+G+TG+Tg+ C	2.7384477	0.0623675	-0.4733910	
C	2.0624563	-0.8521531	0.5315597	
C	0.5657509	-0.5829079	0.6960108	
C	-0.2327307	-0.7479015	-0.5974670	
C	-1.7498661	-0.7132867	-0.3949250	
C	-2.2628543	0.6253611	0.1160784	
O	2.4785974	1.4151248	-0.0700337	
O	-3.6971045	0.6806906	0.1510527	
H	2.3491490	-0.1145935	-1.4811883	
H	3.8155235	-0.1336757	-0.4868256	
H	2.2219762	-1.8868797	0.2099609	
H	2.5619701	-0.7328034	1.4964638	
H	0.4370500	0.4249592	1.0933653	

H	0.1701539	-1.2761221	1.4464922	
H	0.0358147	-1.7020330	-1.0639774	
H	0.0450076	0.0371518	-1.3074971	
H	-2.0404881	-1.5036008	0.3074350	
H	-2.2569695	-0.9236993	-1.3400317	
H	-1.8532921	0.8549627	1.1039618	
H	-1.9667846	1.4254686	-0.5629232	
H	2.9522831	2.0106091	-0.6648615	
H	-4.0051104	-0.0107637	0.7517828	
g-G+TTG+G+g-	C	-2.8424763	0.7003952	0.0377843
C	-1.6766216	0.1648514	0.8574072	
C	-0.4329395	-0.1436925	0.0262105	
C	0.7480682	-0.6020913	0.8821880	
C	1.9679437	-1.0630337	0.0805889	
C	2.5640865	0.0010829	-0.8321819	
O	-3.3485088	-0.2550303	-0.9027965	
O	3.0301638	1.1520182	-0.1157562	
H	-2.5513751	1.6250964	-0.4752169	
H	-3.6876155	0.9301084	0.6856997	
H	-1.4253983	0.9090987	1.6214773	
H	-2.0034087	-0.7386562	1.3794098	
H	-0.1627954	0.7491097	-0.5498004	
H	-0.6602675	-0.9315040	-0.7003831	
H	0.4172733	-1.4291689	1.5172011	
H	1.0356663	0.2008096	1.5695222	
H	1.6896335	-1.9241611	-0.5372257	
H	2.7470710	-1.3978746	0.7700663	
H	3.4474335	-0.3916034	-1.3345455	
H	1.8487800	0.2977077	-1.6068281	
H	-2.6892839	-0.3816091	-1.5967914	
H	2.2680318	1.6037208	0.2689544	
tTG+TG+G+g+C		-2.2648298	0.6041451	0.0949068
C	-1.7563814	-0.7467756	-0.3689925	
C	-0.2406045	-0.7824656	-0.5745084	
C	0.5603662	-0.5481728	0.7069090	
C	2.0553866	-0.8312774	0.5528065	
C	2.7401563	0.0306174	-0.5001498	
O	-3.6985216	0.5307545	0.1286887	
O	2.5377361	1.4336829	-0.2827625	
H	-1.9366787	1.3839079	-0.6019784	
H	-1.8765591	0.8471853	1.0882295	
H	-2.0554511	-1.5041329	0.3609310	
H	-2.2638861	-0.9871509	-1.3063785	
H	0.0352589	-0.0358049	-1.3252176	
H	0.0311060	-1.7592538	-0.9890445	
H	0.1618246	-1.1928449	1.4976158	
H	0.4317129	0.4825030	1.0437368	
H	2.2092975	-1.8826377	0.2849351	
H	2.5565033	-0.6801303	1.5155898	
H	3.8100333	-0.2005367	-0.5378892	
H	2.3275877	-0.1597186	-1.4896480	

H	-4.0405997	1.3702614	0.4620053
H	2.9723636	1.6754316	0.5459552
tG+G+G+TTg+ C	2.1459960	-0.9194646	0.3541268
C	1.6601298	0.3580832	1.0123117
C	0.9531912	1.3165200	0.0504594
C	-0.2408899	0.7160955	-0.6948851
C	-1.3527133	0.2036453	0.2197828
C	-2.5751703	-0.2559716	-0.5601165
O	2.9936692	-0.5473958	-0.7427878
O	-3.5943199	-0.8143870	0.2798986
H	1.3012403	-1.5167711	-0.0052056
H	2.7007712	-1.5223034	1.0804420
H	0.9998896	0.0844369	1.8403901
H	2.5223195	0.8673993	1.4505656
H	1.6804472	1.6753924	-0.6801498
H	0.6148497	2.1897673	0.6179326
H	0.1012481	-0.0943769	-1.3455754
H	-0.6525469	1.4838507	-1.3583974
H	-1.6478111	1.0011829	0.9126721
H	-1.0056351	-0.6347352	0.8280795
H	-2.9787117	0.5722915	-1.1538312
H	-2.3068230	-1.0587453	-1.2471325
H	3.3530585	-1.3509805	-1.1402726
H	-3.8743950	-0.1298476	0.9018038
tTG-G-TG-t	C	-1.9947917	-0.5629454
	C	-1.6956198	0.7316280
	C	-0.6635362	1.6054438
	C	0.6805253	0.9230795
	C	1.3834965	0.4230901
	C	2.7259730	-0.2170938
	O	-3.0716887	-1.2066678
	O	2.4792229	-1.3742290
	H	-1.1149898	-1.2127176
	H	-2.2862062	-0.3493503
	H	-2.6337089	1.2834078
	H	-1.3659228	0.4929498
	H	-0.4928616	2.5063859
	H	-1.0857168	1.9445738
	H	1.3380118	1.6381948
	H	0.5506782	0.0879993
	H	0.7683289	-0.3142342
	H	1.5411005	1.2579885
	H	3.3744867	0.4905419
	H	3.2204081	-0.5076920
	H	-3.2093582	-2.0799222
	H	3.3246028	-1.7942668
tG-G-TG-Tg+	C	-2.7391750	0.0554027
	C	-2.0572111	-0.8397984
	C	-0.5588629	-0.5702633
	C	0.2283851	-0.7497602
	C	1.7460891	-0.7288553

C	2.2651773	0.5964827	0.1397140	
O	-2.4707146	1.4162333	-0.0972480	
O	3.6917203	0.6048540	0.2872072	
H	-3.8170599	-0.1366165	-0.4670682	
H	-2.3598726	-0.1450335	-1.4751103	
H	-2.5492692	-0.7011179	1.5165484	
H	-2.2206333	-1.8803596	0.2502015	
H	-0.1569541	-1.2543722	1.4542024	
H	-0.4257075	0.4422927	1.0830196	
H	-0.0485038	0.0341979	-1.3108353	
H	-0.0506368	-1.7043805	-1.0584178	
H	2.2375617	-0.9281847	-1.3586325	
H	2.0482634	-1.5270023	0.2844971	
H	1.9404375	1.4182256	-0.5100799	
H	1.8839058	0.7917930	1.1401055	
H	-2.9566574	1.9996147	-0.6943455	
H	4.0807739	0.4176708	-0.5774905	
g+G+G-TTG-g+	C	2.7931360	0.3025595	-0.2275568
C	2.1118388	-0.7956425	0.5809809	
C	0.7679579	-1.2706910	0.0252762	
C	-0.3497687	-0.2283131	0.0387088	
C	-1.6846775	-0.8064844	-0.4258659	
C	-2.7844423	0.2380662	-0.5541794	
O	2.1543500	1.5835389	-0.1193783	
O	-3.1090861	0.8628224	0.6948312	
H	2.7615701	0.0621685	-1.2913209	
H	3.8454638	0.3846229	0.0643832	
H	2.7975274	-1.6491662	0.6175200	
H	1.9903894	-0.4550427	1.6159816	
H	0.4406843	-2.1414873	0.6031766	
H	0.9170682	-1.6221713	-1.0022034	
H	-0.0693144	0.6191986	-0.5911856	
H	-0.4514990	0.1570279	1.0593032	
H	-2.0168153	-1.5836131	0.2687171	
H	-1.5527292	-1.2804785	-1.4052580	
H	-2.4992981	0.9941304	-1.2952009	
H	-3.7136349	-0.2238620	-0.8866368	
H	2.2906348	1.9096497	0.7797747	
H	-2.3590671	1.4094602	0.9615484	
tTTG-G-Tg+	C	-2.6338082	-0.2027745	0.4582420
C	-1.3432391	0.1271531	-0.2643242	
C	-0.4678026	1.0922792	0.5326628	
C	0.7805740	1.5571389	-0.2247520	
C	1.7110264	0.4309023	-0.6841580	
C	2.2391252	-0.4213426	0.4602579	
O	-3.3784595	-1.1023496	-0.3740167	
O	3.1379117	-1.4440455	0.0123503	
H	-3.2065300	0.7133337	0.6418491	
H	-2.4128742	-0.6678325	1.4257563	
H	-0.8158450	-0.8089902	-0.4594184	
H	-1.5928428	0.5648873	-1.2352656	

H	-0.1798452	0.6290626	1.4817143	
H	-1.0576296	1.9769393	0.7943708	
H	1.3437934	2.2482859	0.4111062	
H	0.4658138	2.1312754	-1.1014044	
H	2.5649273	0.8759972	-1.2071257	
H	1.2103653	-0.2202406	-1.4039195	
H	2.7246241	0.2155808	1.2101807	
H	1.4332790	-0.9626480	0.9537642	
H	-4.1917204	-1.3473564	0.0860071	
H	3.8627694	-1.0162445	-0.4625541	
tTTG-G-G-t	C	2.5766593	-0.2105443	-0.5469375
	C	1.3467917	0.1999440	0.2366378
	C	0.2421875	0.7456621	-0.6669752
	C	-0.9571574	1.3138259	0.0947972
	C	-1.6625906	0.3180010	1.0188444
	C	-2.1397549	-0.9377582	0.3146129
	O	3.5316760	-0.7404333	0.3844288
	O	-2.9891448	-0.5330621	-0.7698421
	H	2.9932802	0.6560130	-1.0722665
	H	2.3099395	-0.9672142	-1.2936660
	H	0.9991610	-0.6708769	0.7969399
	H	1.6390457	0.9573852	0.9698841
	H	-0.0960142	-0.0361691	-1.3540741
	H	0.6563529	1.5419409	-1.2945059
	H	-1.6835077	1.6967103	-0.6245103
	H	-0.6237543	2.1662765	0.6954888
	H	-2.5290692	0.8067957	1.4718128
	H	-1.0036444	0.0188882	1.8389639
	H	-1.2910192	-1.5165017	-0.0647896
	H	-2.6916680	-1.5694747	1.0183454
	H	4.3299280	-0.9876769	-0.1000731
	H	-3.3465383	-1.3247364	-1.1922775
tG+G-TTG+g+	C	-2.7767660	0.4094302	0.2815206
	C	-2.1825229	-0.8672889	-0.2834038
	C	-0.7983069	-1.2384828	0.2570434
	C	0.3606575	-0.4045637	-0.2894851
	C	1.7099435	-0.8836444	0.2384294
	C	2.8901131	-0.0708621	-0.2746373
	O	-2.0154347	1.5280518	-0.1977842
	O	2.8308742	1.3080028	0.1154999
	H	-2.7548981	0.3752622	1.3774978
	H	-3.8206653	0.5008094	-0.0372503
	H	-2.8832708	-1.6747111	-0.0467575
	H	-2.1508943	-0.7825798	-1.3737712
	H	-0.6095632	-2.2921774	0.0230810
	H	-0.8135749	-1.1669732	1.3514963
	H	0.2132357	0.6460602	-0.0456505
	H	0.3629070	-0.4718508	-1.3834149
	H	1.8702010	-1.9317548	-0.0405819
	H	1.7099450	-0.8554319	1.3355393
	H	3.8333715	-0.5186972	0.0579492

H	2.8933767	-0.0514813	-1.3649490	
H	-2.4178785	2.3401241	0.1370156	
H	2.8301534	1.3422457	1.0814449	
tG-TG-G-G-t	C	-2.7400907	0.0221412	0.0781185
	C	-1.4382593	-0.6896992	0.3898222
	C	-0.4326106	-0.6155633	-0.7569220
	C	0.8946232	-1.3192777	-0.4670598
	C	1.6734526	-0.7529364	0.7242225
	C	1.9380481	0.7374961	0.6257264
	O	-2.4394373	1.4195744	-0.0699266
	O	2.6491168	0.9703885	-0.6000595
	H	-3.4596956	-0.1257528	0.8900389
	H	-3.1748796	-0.3743648	-0.8465564
	H	-1.0271291	-0.2442340	1.2992569
	H	-1.6612915	-1.7378074	0.6181762
	H	-0.2527150	0.4295863	-1.0137132
	H	-0.8828949	-1.0754913	-1.6434966
	H	1.5266772	-1.2564673	-1.3549223
	H	0.7075669	-2.3832546	-0.2850356
	H	2.6344590	-1.2686612	0.7999888
	H	1.1404038	-0.9414242	1.6606030
	H	0.9986783	1.2991566	0.6328865
	H	2.5375219	1.0648350	1.4819001
	H	-3.2514454	1.8863121	-0.3059924
	H	2.7922982	1.9207820	-0.6948104
tTTG-G-Tt	C	-2.6323530	-0.2007890	0.4501160
	C	-1.3364777	0.1264764	-0.2638603
	C	-0.4689741	1.0971643	0.5351641
	C	0.7809266	1.5666094	-0.2168605
	C	1.7172096	0.4477906	-0.6793942
	C	2.2312145	-0.4135227	0.4571392
	O	-3.3575579	-1.1286982	-0.3682494
	O	3.2076664	-1.3084127	-0.0952547
	H	-3.2167830	0.7131686	0.6050874
	H	-2.4187161	-0.6400992	1.4314632
	H	-0.8056526	-0.8098384	-0.4486747
	H	-1.5774238	0.5572318	-1.2399977
	H	-0.1831015	0.6354506	1.4859448
	H	-1.0645608	1.9787723	0.7946840
	H	1.3392565	2.2583219	0.4226164
	H	0.4674156	2.1423596	-1.0928695
	H	2.5840427	0.8857818	-1.1802041
	H	1.2237209	-0.1945114	-1.4117732
	H	2.6848286	0.2189350	1.2299950
	H	1.4159155	-0.9819604	0.9157884
	H	-4.1891942	-1.3453342	0.0727684
	H	3.4932749	-1.9181092	0.5974013
tTG-G-TTg+	C	2.2402520	-0.3999440	0.4521386
	C	1.7139762	0.4499782	-0.6873959
	C	0.7765817	1.5693485	-0.2279371
	C	-0.4726557	1.1025776	0.5274522

C	-1.3458731	0.1316897	-0.2658646	
C	-2.6336416	-0.2143917	0.4663344	
O	3.1831830	-1.3254504	-0.1078887	
O	-3.4929375	-1.0715269	-0.2953963	
H	1.4265514	-0.9432433	0.9435683	
H	2.7254063	0.2381906	1.2004175	
H	2.5744366	0.8860926	-1.2004895	
H	1.2171006	-0.2012627	-1.4097262	
H	0.4617925	2.1412432	-1.1059117	
H	1.3345474	2.2645157	0.4079866	
H	-1.0694598	1.9840658	0.7835181	
H	-0.1871209	0.6441350	1.4797602	
H	-0.7959039	-0.7936589	-0.4664449	
H	-1.6036638	0.5666557	-1.2358882	
H	-2.4050796	-0.6661241	1.4390448	
H	-3.2225130	0.6849765	0.6465584	
H	3.5169751	-1.8915174	0.6001653	
H	-3.0109839	-1.8879496	-0.4824864	
g+G+TTG+G-g-	C	2.7960710	0.3590563	-0.5061439
C	1.6608585	-0.6492007	-0.6129728	
C	0.3567529	-0.1544952	0.0060048	
C	-0.7506966	-1.2065713	-0.0520503	
C	-2.0681164	-0.8021957	0.6153071	
C	-2.9023725	0.2172728	-0.1503548	
O	3.1409156	0.6628005	0.8538030	
O	-2.2941813	1.5114489	-0.2608872	
H	2.4972938	1.3144905	-0.9381110	
H	3.6776116	0.0027979	-1.0501458	
H	1.5035154	-0.8789480	-1.6729550	
H	1.9708928	-1.5875237	-0.1360531	
H	0.0314052	0.7502406	-0.5106572	
H	0.5395932	0.1225812	1.0484555	
H	-0.3859471	-2.1203773	0.4299540	
H	-0.9502985	-1.4699846	-1.0975060	
H	-1.8710759	-0.4241276	1.6257499	
H	-2.6932601	-1.6934637	0.7392884	
H	-3.0427031	-0.1118112	-1.1808964	
H	-3.8925884	0.3058060	0.3103936	
H	3.4832449	-0.1446155	1.2600645	
H	-2.2000618	1.8756939	0.6295045	
tG+TG+G+Tg+C	-2.7496133	-0.2241364	0.2961470	
C	-1.4267053	0.4362699	0.6325577	
C	-0.6838751	0.9336053	-0.6051893	
C	0.6584642	1.6027432	-0.2930995	
C	1.6803316	0.7085810	0.4166650	
C	2.0166096	-0.5595702	-0.3554859	
O	-2.4531899	-1.4034469	-0.4668968	
O	3.1078363	-1.2807191	0.2351602	
H	-3.3768042	0.4610432	-0.2859534	
H	-3.2864846	-0.4891700	1.2129896	
H	-1.6174271	1.2748717	1.3112003	

H	-0.8246112	-0.2917577	1.1818423	
H	-1.3202282	1.6587815	-1.1240376	
H	-0.5444328	0.1005124	-1.2962233	
H	0.4814077	2.4907475	0.3224524	
H	1.0992479	1.9613842	-1.2290083	
H	1.3186992	0.4374368	1.4140528	
H	2.6091955	1.2656544	0.5630248	
H	1.1415836	-1.2098695	-0.4492118	
H	2.3570999	-0.3089414	-1.3611841	
H	-3.2834816	-1.8242940	-0.7244649	
H	2.8315169	-1.5675307	1.1157129	
tTG+TG-Tt	C	2.7198350	-0.3863476	-0.2236431
	C	1.8087071	0.7733637	0.1300867
	C	0.3623083	0.5854731	-0.3336936
	C	-0.3623085	-0.5854737	0.3336942
	C	-1.8087074	-0.7733642	-0.1300857
	C	-2.7198347	0.3863480	0.2236428
	O	4.0550563	0.0014522	0.1325974
	O	-4.0550562	-0.0014518	-0.1325970
	H	2.6556352	-0.5954010	-1.2982610
	H	2.4330228	-1.2912292	0.3197383
	H	1.8389223	0.9259263	1.2125040
	H	2.2287327	1.6710310	-0.3301973
	H	0.3414468	0.4470094	-1.4210189
	H	-0.1782555	1.5136741	-0.1324020
	H	-0.3414467	-0.4470101	1.4210195
	H	0.1782551	-1.5136747	0.1324022
	H	-2.2287334	-1.6710307	0.3301996
	H	-1.8389230	-0.9259281	-1.2125028
	H	-2.6556348	0.5954028	1.2982604
	H	-2.4330223	1.2912288	-0.3197398
	H	4.6447064	-0.7478707	-0.0219259
	H	-4.6447056	0.7478726	0.0219222
tG+TG+G+G+g+	C	2.7639729	0.0204711	0.0594962
	C	1.4609032	-0.6775938	0.3973823
	C	0.4471288	-0.6221977	-0.7431778
	C	-0.8790186	-1.3173445	-0.4282071
	C	-1.6475168	-0.7196419	0.7542104
	C	-1.9360359	0.7692200	0.6134318
	O	2.4695482	1.4163570	-0.0995208
	O	-2.6325444	1.0842068	-0.5998590
	H	3.1830271	-0.3907479	-0.8662754
	H	3.4936779	-0.1246759	0.8631990
	H	1.6793907	-1.7217006	0.6473702
	H	1.0607911	-0.2084969	1.2997311
	H	0.8887746	-1.1029674	-1.6228288
	H	0.2683834	0.4175773	-1.0211543
	H	-0.6936432	-2.3774959	-0.2241338
	H	-1.5131423	-1.2748907	-1.3166436
	H	-1.0995236	-0.8730811	1.6889850
	H	-2.5966539	-1.2554416	0.8697773

H	-2.5018796	1.1241716	1.4818959
H	-1.0131104	1.3453030	0.5632794
H	3.2743104	1.8751511	-0.3726831
H	-3.4928428	0.6444230	-0.5739748
tTG+G+TTg+ C	-2.2345404	-0.4117336	0.4479216
C	-1.7142807	0.4556834	-0.6812230
C	-0.7776048	1.5701139	-0.2091950
C	0.4694485	1.0943954	0.5436038
C	1.3386355	0.1225694	-0.2529593
C	2.6390574	-0.2051233	0.4656476
O	-3.2036009	-1.3064970	-0.1168615
O	3.4258489	-1.1829522	-0.2252418
H	-2.6959192	0.2162330	1.2197079
H	-1.4214459	-0.9799127	0.9107091
H	-1.2190489	-0.1839709	-1.4149134
H	-2.5780322	0.8978222	-1.1836187
H	-1.3361806	2.2589808	0.4329632
H	-0.4612328	2.1513285	-1.0807618
H	0.1815023	0.6272070	1.4908120
H	1.0672413	1.9724806	0.8097036
H	1.5691541	0.5614463	-1.2312695
H	0.8082617	-0.8136799	-0.4400596
H	3.2207391	0.7093147	0.6307285
H	2.4321397	-0.6487511	1.4398572
H	-3.4940457	-1.9199621	0.5704677
H	3.6402246	-0.8303974	-1.0991298
tG-G+TTG+g+ C	-2.9350440	0.1789507	-0.0888669
C	-2.0492438	-0.8580026	0.5759182
C	-0.7418110	-1.1639088	-0.1621171
C	0.3697670	-0.1342326	0.0411405
C	1.6429168	-0.5035203	-0.7145135
C	2.7966837	0.4568787	-0.4624674
O	-2.2730859	1.4527142	-0.0532444
O	3.2130919	0.4771675	0.9103384
H	-3.8922082	0.2375169	0.4402767
H	-3.1340428	-0.1156066	-1.1262248
H	-1.8365583	-0.5335043	1.5988092
H	-2.6424674	-1.7753393	0.6495315
H	-0.9535754	-1.2693212	-1.2331370
H	-0.3739277	-2.1396585	0.1737614
H	0.5951072	-0.0521418	1.1078175
H	0.0223121	0.8477886	-0.2828798
H	1.4416830	-0.5226200	-1.7918329
H	1.9603276	-1.5185066	-0.4431050
H	3.6450450	0.2137223	-1.1118881
H	2.4916313	1.4815538	-0.6763321
H	-2.8611174	2.1135831	-0.4418303
H	3.5335811	-0.4064383	1.1353920
tG+TTG-G+g+ C	-2.8849320	-0.0831875	0.2774035
C	-1.7115104	-0.9043710	-0.2199965
C	-0.3602406	-0.3749250	0.2534017

C	0.7973343	-1.2453229	-0.2359446
C	2.1801258	-0.8565680	0.2939577
C	2.7735086	0.4182335	-0.2934117
O	-2.7590313	1.2357702	-0.2718980
O	2.0703678	1.6138380	0.0664191
H	-2.8754484	-0.0438526	1.3732354
H	-3.8279036	-0.5401817	-0.0416593
H	-1.8482604	-1.9357882	0.1235840
H	-1.7422733	-0.9220309	-1.3134404
H	-0.3516832	-0.3553379	1.3506363
H	-0.2287651	0.6515128	-0.0850480
H	0.8218744	-1.2302262	-1.3316430
H	0.5988122	-2.2836431	0.0524484
H	2.8849118	-1.6659744	0.0733276
H	2.1476103	-0.7695314	1.3869327
H	3.8279569	0.5011009	-0.0061627
H	2.7267070	0.3855747	-1.3826979
H	-3.4916240	1.7762442	0.0504524
H	2.1258644	1.7172123	1.0256221
tG+TG-G-G-t	C	2.5718453	-0.7284100
			0.3744108
	C	1.3208704	0.0809519
			0.6576691
	C	0.4460035	0.2781510
			-0.5783800
	C	-0.7568961	1.1944978
			-0.3455740
	C	-1.7306215	0.7258849
			0.7391779
	C	-2.2938688	-0.6620266
			0.4993064
	O	3.3674705	0.0100481
			-0.5646907
	O	-2.9302690	-0.6570288
			-0.7870643
	H	2.2987132	-1.7051268
			-0.0423703
	H	3.1336966	-0.8936363
			1.2997960
	H	0.7648324	-0.4320594
			1.4485443
	H	1.6235391	1.0540135
			1.0573806
	H	0.1049082	-0.6967418
			-0.9425502
	H	1.0622360	0.7038432
			-1.3726499
	H	-1.3065399	1.3013038
			-1.2827325
	H	-0.3938570	2.1918268
			-0.0760797
	H	-2.5666847	1.4279423
			0.7963312
	H	-1.2475571	0.7313351
			1.7208584
	H	-1.4973105	-1.4135767
			0.5247514
	H	-3.0173804	-0.9093849
			1.2833792
	H	4.1593770	-0.5035789
			-0.7689829
	H	-3.3258462	-1.5249823
			-0.9383949
tTG-TG-Tt	C	2.5360030	-0.5433911
			-0.2043000
	C	1.8824250	0.5944466
			0.5554046
	C	0.3641335	0.4499417
			0.6732344
	C	-0.3641334	0.4499415
			-0.6732341
	C	-1.8824249	0.5944466
			-0.5554046
	C	-2.5360030	-0.5433906
			0.2043005
	O	3.9561716	-0.3655138
			-0.0989246
	O	-3.9561717	-0.3655140
			0.0989239
	H	2.2311548	-0.5360863
			-1.2549217
	H	2.2372967	-1.5036253
			0.2336286

H	2.3308391	0.6278001	1.5513394	
H	2.1317936	1.5365417	0.0596537	
H	-0.0190632	1.2778064	1.2786889	
H	0.1356128	-0.4675884	1.2252090	
H	-0.1356129	-0.4675889	-1.2252083	
H	0.0190634	1.2778059	-1.2786889	
H	-2.3308388	0.6277996	-1.5513395	
H	-2.1317935	1.5365420	-0.0596542	
H	-2.2372961	-1.5036251	-0.2336271	
H	-2.2311557	-0.5360849	1.2549224	
H	4.3914851	-1.0319511	-0.6461277	
H	-4.3914854	-1.0319525	0.6461252	
g+G+G+TG+Tg-	C	2.7409836	0.0274217	-0.4886898
C	2.0530957	-0.8357066	0.5613577	
C	0.5572175	-0.5537909	0.7097879	
C	-0.2320055	-0.7556118	-0.5841857	
C	-1.7492501	-0.7339984	-0.3826292	
C	-2.2695673	0.5998656	0.1336003	
O	2.5212109	1.4292701	-0.2835836	
O	-3.6954964	0.6079251	0.2862127	
H	2.3415833	-0.1738473	-1.4815928	
H	3.8134268	-0.1934308	-0.5133286	
H	2.2094019	-1.8865436	0.2927986	
H	2.5489141	-0.6852978	1.5268311	
H	0.4262218	0.4690681	1.0682522	
H	0.1514468	-1.2154554	1.4824816	
H	0.0487105	-1.7172019	-1.0274338	
H	0.0432162	0.0170535	-1.3083249	
H	-2.0497752	-1.5206103	0.3152652	
H	-2.2407528	-0.9505751	-1.3377791	
H	-1.8861223	0.8135386	1.1295202	
H	-1.9483975	1.4102741	-0.5315921	
H	2.9428375	1.6827013	0.5484192	
H	-4.0875326	0.4121379	-0.5751152	
tTTG+G+Tg+	C	2.6383391	-0.1764655	0.4411584
C	1.3318754	0.1265856	-0.2642045	
C	0.4694399	1.1157679	0.5171496	
C	-0.7882126	1.5626479	-0.2361948	
C	-1.7217453	0.4296243	-0.6723125	
C	-2.2300662	-0.4197940	0.4831659	
O	3.3491928	-1.1326935	-0.3568514	
O	-3.2353205	-1.3558423	0.0706017	
H	2.4394306	-0.5816666	1.4399262	
H	3.2254230	0.7416566	0.5552646	
H	1.5578690	0.5282641	-1.2562847	
H	0.8040001	-0.8180118	-0.4126432	
H	1.0646763	2.0056172	0.7470786	
H	0.1937478	0.6785560	1.4818848	
H	-0.4845382	2.1264816	-1.1234326	
H	-1.3499606	2.2593948	0.3944615	
H	-1.2167389	-0.2146879	-1.3993319	

H	-2.5910726	0.8537319	-1.1809031	
H	-1.4073458	-0.9464761	0.9774388	
H	-2.7199399	0.2088377	1.2279822	
H	4.1861238	-1.3385175	0.0793623	
H	-2.8434621	-1.9393464	-0.5929221	
g+G+G+TG-Tg+	C	2.8487726	0.0681424	0.5081784
C	1.8812744	1.0832832	-0.0870229	
C	0.5198388	0.5032219	-0.4767891	
C	-0.2302562	-0.1433906	0.6875590	
C	-1.6154153	-0.6748677	0.3079787	
C	-2.6128831	0.4144397	-0.0603986	
O	3.0268380	-1.0835210	-0.3264357	
O	-3.9043918	-0.1144071	-0.3870088	
H	2.4727479	-0.3272501	1.4504288	
H	3.8125432	0.5465305	0.7131573	
H	1.7470985	1.8913127	0.6410238	
H	2.3442198	1.5380031	-0.9700401	
H	0.6563452	-0.2435796	-1.2635064	
H	-0.0789276	1.3097159	-0.9078076	
H	-0.3289905	0.5788470	1.5073190	
H	0.3593350	-0.9779537	1.0733789	
H	-2.0231402	-1.2399740	1.1536756	
H	-1.5320182	-1.3734370	-0.5291020	
H	-2.6912667	1.1411369	0.7578140	
H	-2.3028367	0.9506580	-0.9552992	
H	3.4293660	-0.7952744	-1.1566369	
H	-4.2165460	-0.6262872	0.3710938	
g+TG+TG+G+g+	C	-2.2703354	0.6279742	0.1141648
C	-1.7541184	-0.7155868	-0.3808054	
C	-0.2371902	-0.7490899	-0.5843171	
C	0.5625717	-0.5612754	0.7055622	
C	2.0559108	-0.8496578	0.5440611	
C	2.7427073	0.0271982	-0.4953148	
O	-3.7039787	0.6792130	0.1523847	
O	2.5363707	1.4265044	-0.2613695	
H	-1.9777673	1.4204736	-0.5750848	
H	-1.8592539	0.8705187	1.0986525	
H	-2.0427816	-1.4981105	0.3311456	
H	-2.2604845	-0.9386426	-1.3232748	
H	0.0385800	0.0248331	-1.3067044	
H	0.0337971	-1.7102834	-1.0344896	
H	0.1597427	-1.2286981	1.4752712	
H	0.4395432	0.4587232	1.0746329	
H	2.2041314	-1.8968404	0.2571609	
H	2.5584763	-0.7180544	1.5088376	
H	3.8129827	-0.2021538	-0.5327007	
H	2.3336895	-0.1518286	-1.4885061	
H	-4.0093005	-0.0124562	0.7543015	
H	2.9727063	1.6618615	0.5683194	
g+G-TTG+G-g-C		2.8633382	-0.0310159	0.2778607
C	1.7132822	-0.9212082	-0.1725794	

C	0.3422818	-0.3954806	0.2456619
C	-0.7980920	-1.3026415	-0.2140373
C	-2.1941564	-0.8702415	0.2387703
C	-2.6748628	0.4593482	-0.3321025
O	2.8571470	1.2536986	-0.3563555
O	-2.0099880	1.6041248	0.2242243
H	3.8200934	-0.4731111	0.0016433
H	2.8465935	0.0812771	1.3689979
H	1.7571984	-1.0186378	-1.2613319
H	1.8660521	-1.9206260	0.2503357
H	0.1775078	0.6053920	-0.1559846
H	0.3100368	-0.3028018	1.3383153
H	-0.6109803	-2.3176185	0.1525600
H	-0.7864061	-1.3638987	-1.3081808
H	-2.2361554	-0.8250802	1.3334583
H	-2.9148895	-1.6374108	-0.0644556
H	-2.4678845	0.5074614	-1.4021256
H	-3.7572317	0.5557514	-0.1972250
H	2.0499484	1.7172754	-0.0978496
H	-2.2831917	1.6884034	1.1472351
tTG+TG-Tg+ C	2.7212718	0.3865178	0.2328897
C	1.8094242	-0.7661481	-0.1416246
C	0.3643865	-0.5884830	0.3303517
C	-0.3643822	0.5899444	-0.3190777
C	-1.8122173	0.7594161	0.1501695
C	-2.7253867	-0.3937437	-0.2422627
O	4.0539104	0.0103930	-0.1436959
O	-4.0785380	-0.1857314	0.1818753
H	2.6651835	0.5689147	1.3128000
H	2.4283827	1.3040630	-0.2857393
H	1.8364641	-0.8969142	-1.2269421
H	2.2306279	-1.6728733	0.2991599
H	0.3472912	-0.4642922	1.4193316
H	-0.1751748	-1.5146377	0.1187835
H	-0.3448787	0.4676564	-1.4084032
H	0.1726955	1.5171663	-0.1043702
H	-2.2196190	1.6806781	-0.2811194
H	-1.8449480	0.8771530	1.2369675
H	-2.6821854	-0.5528126	-1.3267812
H	-2.4261415	-1.3201649	0.2440203
H	4.6456625	0.7527014	0.0348562
H	-4.3937340	0.6352829	-0.2189111
tTG-TG+G+g+ C	-2.5970612	0.3573451	-0.1440752
C	-1.6118094	-0.6730790	0.3727011
C	-0.2523406	-0.0861463	0.7593345
C	0.5050857	0.5454429	-0.4086483
C	1.8891497	1.0795403	-0.0328194
C	2.8655495	0.0144610	0.4502123
O	-3.8634928	-0.3027049	-0.2922593
O	3.0212068	-1.0592149	-0.4870203
H	-2.2703231	0.7645059	-1.1053555

H	-2.6792518	1.1855086	0.5704491	
H	-2.0661766	-1.1527382	1.2431382	
H	-1.4805319	-1.4482062	-0.3869983	
H	0.3487662	-0.8903773	1.1895228	
H	-0.3884583	0.6609198	1.5506163	
H	-0.0751569	1.3754900	-0.8209408	
H	0.6092833	-0.1951236	-1.2065276	
H	1.7950102	1.8379556	0.7527360	
H	2.3267645	1.5872811	-0.8999875	
H	3.8354485	0.4720672	0.6732777	
H	2.5106921	-0.4628073	1.3621122	
H	-4.4875529	0.3161223	-0.6930228	
H	3.4016589	-0.6973852	-1.2986342	
tTTG+G+G+g+ C	-2.5794376	-0.1918753	-0.5484085	
C	-1.3459102	0.1922310	0.2430102	
C	-0.2465085	0.7691752	-0.6471729	
C	0.9556694	1.3120717	0.1286483	
C	1.6550339	0.2862357	1.0240200	
C	2.1195980	-0.9633074	0.2886267	
O	-3.5355373	-0.7370373	0.3726918	
O	2.9525715	-0.6661270	-0.8402422	
H	-2.3182684	-0.9321509	-1.3130523	
H	-2.9918022	0.6895045	-1.0521723	
H	-1.6357080	0.9236925	1.0032878	
H	-0.9954528	-0.6973390	0.7712515	
H	-0.6639535	1.5869572	-1.2439693	
H	0.0898910	0.0126816	-1.3625321	
H	0.6296099	2.1519333	0.7506273	
H	1.6793202	1.7110640	-0.5857216	
H	0.9965917	-0.0238035	1.8413352	
H	2.5218961	0.7608377	1.4976273	
H	2.6381612	-1.6353477	0.9810160	
H	1.2746532	-1.5104798	-0.1273233	
H	-4.3261758	-0.9931105	-0.1196450	
H	3.7567432	-0.2390970	-0.5161205	
tTG+TG-G-t	C	2.5886722	0.3467032	-0.1516834
C	1.6021592	-0.6664697	0.3957413	
C	0.2437901	-0.0650446	0.7637164	
C	-0.5038154	0.5481297	-0.4201029	
C	-1.8922740	1.0876025	-0.0684462	
C	-2.8622842	0.0310993	0.4276566	
O	3.8577517	-0.3154763	-0.2682561	
O	-2.9455680	-0.9865376	-0.5811238	
H	2.6653599	1.2002921	0.5329681	
H	2.2666008	0.7178503	-1.1287706	
H	1.4695046	-1.4629366	-0.3413306	
H	2.0563306	-1.1207811	1.2799594	
H	0.3802825	0.6954797	1.5421728	
H	-0.3637544	-0.8577393	1.2069182	
H	-0.6032037	-0.1996613	-1.2108906	
H	0.0793590	1.3749173	-0.8350925	

H	-2.3294321	1.5612225	-0.9514306	
H	-1.8076001	1.8606953	0.7029541	
H	-2.5210585	-0.3993034	1.3743640	
H	-3.8447966	0.4839643	0.5968890	
H	4.4783857	0.2847165	-0.7012710	
H	-3.5842494	-1.6524069	-0.2954864	
tG-TTG+G-g+	C	2.8372175	0.0086584	0.3399603
C	1.7228892	-0.9395611	-0.0573105	
C	0.3332575	-0.3563651	0.1853973	
C	-0.7842957	-1.3061703	-0.2456349	
C	-2.1965866	-0.8892968	0.1740793	
C	-2.6617305	0.4700889	-0.3399497	
O	2.7074667	1.1886384	-0.4677589	
O	-2.1895818	1.5774872	0.4392374	
H	3.8118851	-0.4615922	0.1746061	
H	2.7521947	0.2633600	1.4027338	
H	1.8403098	-1.1908895	-1.1154212	
H	1.8390059	-1.8675772	0.5118880	
H	0.2713089	0.5827430	-0.3699311	
H	0.2242364	-0.1188766	1.2498835	
H	-0.5806049	-2.2980180	0.1718847	
H	-0.7518954	-1.4193376	-1.3351497	
H	-2.2798188	-0.8812876	1.2649636	
H	-2.8991351	-1.6453709	-0.1924315	
H	-2.3848009	0.5936067	-1.3943760	
H	-3.7471463	0.5386427	-0.2731340	
H	3.4135286	1.8043338	-0.2325672	
H	-1.2363235	1.6589928	0.3140879	
tG-G-G-TTg+	C	-2.1489155	-0.9469663	0.2789596
C	-1.6614309	0.2751954	1.0344471	
C	-0.9515068	1.3042433	0.1507488	
C	0.2459740	0.7637993	-0.6345257	
C	1.3616260	0.1970204	0.2430590	
C	2.5848420	-0.2052375	-0.5670035	
O	-2.9989199	-0.4905781	-0.7830957	
O	3.6615167	-0.6838833	0.2493560	
H	-2.7013138	-1.6056806	0.9571750	
H	-1.3044769	-1.5138388	-0.1288224	
H	-2.5236457	0.7501677	1.5096445	
H	-1.0031490	-0.0621876	1.8404846	
H	-0.6150541	2.1312166	0.7842622	
H	-1.6767712	1.7175942	-0.5524680	
H	0.6562230	1.5802538	-1.2376810	
H	-0.0918345	0.0029675	-1.3448589	
H	1.0030953	-0.6791571	0.7940957	
H	1.6665761	0.9387203	0.9872743	
H	2.3102060	-0.9553648	-1.3181830	
H	2.9931948	0.6580908	-1.0922304	
H	-3.3622280	-1.2599591	-1.2403272	
H	3.3450435	-1.4552343	0.7378581	
tG+G+TG-Tg+	C	2.8572263	0.0340348	0.4439368

C	1.8936236	1.0879873	-0.0697722
C	0.5086051	0.5471386	-0.4324824
C	-0.2371749	-0.0882784	0.7404367
C	-1.6019731	-0.6689477	0.3593998
C	-2.5994565	0.3728516	-0.1260510
O	2.9336314	-1.0019176	-0.5465014
O	-3.8832637	-0.1951206	-0.4201773
H	2.5136234	-0.3775696	1.3982007
H	3.8424573	0.4835722	0.6053825
H	1.8020590	1.8663637	0.6954125
H	2.3384941	1.5555518	-0.9519805
H	0.6133225	-0.1893025	-1.2328880
H	-0.0774287	1.3764411	-0.8372851
H	-0.3661202	0.6536747	1.5379702
H	0.3673449	-0.8957917	1.1602040
H	-2.0307125	-1.1728230	1.2332793
H	-1.4812842	-1.4285945	-0.4177090
H	-2.6961196	1.1740388	0.6173182
H	-2.2783016	0.8222099	-1.0636834
H	3.5830288	-1.6563699	-0.2585701
H	-4.2023776	-0.6358950	0.3785615
g+TTG+G+Tg+C	2.6431146	-0.1949123	0.4729725
C	1.3434851	0.1219263	-0.2520372
C	0.4703780	1.1037550	0.5274927
C	-0.7801303	1.5587291	-0.2329310
C	-1.7161508	0.4321477	-0.6803747
C	-2.2432262	-0.4143777	0.4690727
O	3.4316442	-1.1791235	-0.2071769
O	-3.2517327	-1.3414994	0.0446848
H	2.4349514	-0.6285960	1.4512144
H	3.2230300	0.7219623	0.6291741
H	1.5748415	0.5452272	-1.2369836
H	0.8163233	-0.8191035	-0.4244602
H	1.0637531	1.9902568	0.7743680
H	0.1866192	0.6539059	1.4838290
H	-0.4683456	2.1262504	-1.1151946
H	-1.3430964	2.2548768	0.3971959
H	-1.2082854	-0.2153522	-1.4026526
H	-2.5771337	0.8623938	-1.1978221
H	-1.4304768	-0.9478442	0.9723674
H	-2.7361473	0.2180541	1.2084977
H	3.6699446	-0.8242697	-1.0738514
H	-2.8533400	-1.9399956	-0.6012569
g-G+G+TG-G-t C	2.6868184	-0.3169101	-0.5119457
C	1.6094144	-1.0962311	0.2309270
C	0.3683132	-0.2802306	0.6048301
C	-0.3746565	0.3070742	-0.5942152
C	-1.6237244	1.1087834	-0.2201142
C	-2.6764904	0.3042922	0.5200717
O	3.1991080	0.7868457	0.2477096
O	-2.9935837	-0.8387180	-0.2877127

H	2.3224700	0.0271565	-1.4850695	
H	3.5506451	-0.9560003	-0.6919632	
H	1.3066336	-1.9414424	-0.3969799	
H	2.0544928	-1.5103847	1.1394628	
H	0.6475912	0.5214586	1.2989627	
H	-0.3050162	-0.9360162	1.1616837	
H	-0.6613551	-0.5014989	-1.2709624	
H	0.2886634	0.9686689	-1.1596421	
H	-2.0777944	1.5125033	-1.1287609	
H	-1.3464584	1.9624013	0.4079501	
H	-2.3066433	-0.0133829	1.5000338	
H	-3.5670496	0.9211470	0.6786243	
H	2.4937982	1.4387430	0.3496916	
H	-3.6999386	-1.3356489	0.1447745	
tTG-TG-Tg+	C	-2.5328776	-0.5507439	0.1894414
	C	-1.8849259	0.6153744	-0.5315332
	C	-0.3670113	0.4781482	-0.6630446
	C	0.3683232	0.4393229	0.6790330
	C	1.8863679	0.5878869	0.5512836
	C	2.5405472	-0.5451406	-0.2262806
	O	-3.9534436	-0.3666868	0.1051434
	O	3.9646074	-0.4052594	-0.3055445
	H	2.2078843	-0.5549772	-1.2626872
	H	-2.2394260	-1.4932503	-0.2887431
	H	-2.3382775	0.6843205	-1.5232952
	H	-2.1332345	1.5382943	-0.0003172
	H	0.0107403	1.3253633	-1.2443845
	H	-0.1391887	-0.4209202	-1.2441936
	H	0.1450196	-0.4944282	1.2053279
	H	-0.0120358	1.2488943	1.3104208
	H	2.3292035	0.6213000	1.5530552
	H	2.1319048	1.5349738	0.0628538
	H	2.2733820	-1.5099236	0.2228897
	H	-2.2181125	-0.5849134	1.2368738
	H	-4.3854301	-1.0663006	0.6119816
	H	4.3112083	-0.3695454	0.5959337
tTG-TG-Tg+	C	-2.5329289	-0.5507109	0.1894129
	C	-1.8849148	0.6153904	-0.5315334
	C	-0.3670052	0.4780974	-0.6630286
	C	0.3683083	0.4391806	0.6790595
	C	1.8863501	0.5877986	0.5513442
	C	2.5405775	-0.5451677	-0.2262701
	O	-3.9534812	-0.3665454	0.1051626
	O	3.9646208	-0.4051760	-0.3055983
	H	-2.2181341	-0.5849452	1.2368348
	H	-2.2395583	-1.4932200	-0.2888176
	H	-2.3382500	0.6843801	-1.5233001
	H	-2.1331873	1.5383112	-0.0003008
	H	0.0107910	1.3253218	-1.2443261
	H	-0.1392127	-0.4209542	-1.2442152
	H	0.1450193	-0.4946186	1.2052751

H	-0.0120798	1.2486908	1.3105086	
H	2.3291687	0.6211759	1.5531250	
H	2.1318630	1.5349189	0.0629648	
H	2.2735055	-1.5099781	0.2228990	
H	2.2078636	-0.5550145	-1.2626608	
H	-4.3855072	-1.0661562	0.6119735	
H	4.3112608	-0.3694110	0.5958621	
tG+TG-G-Tg+	C	2.5173263	-0.9604377	0.0672614
	C	1.2569915	-0.2745657	0.5579143
	C	0.6508157	0.6636159	-0.4830065
	C	-0.5521448	1.4586942	0.0342015
	C	-1.7119026	0.6088165	0.5625031
	C	-2.2878337	-0.3413249	-0.4766049
	O	3.4949776	0.0575059	-0.1944863
	O	-3.3840516	-1.1125093	0.0332589
	H	2.3032942	-1.5276872	-0.8461982
	H	2.8875117	-1.6570603	0.8263741
	H	0.5418422	-1.0526695	0.8410250
	H	1.4999838	0.2862885	1.4658476
	H	0.3682077	0.0839646	-1.3682741
	H	1.4214184	1.3648597	-0.8086898
	H	-0.9212087	2.1053245	-0.7688910
	H	-0.2145074	2.1252001	0.8338169
	H	-2.5112304	1.2774755	0.9014048
	H	-1.4043785	0.0269647	1.4344123
	H	-2.5935551	0.2179577	-1.3693657
	H	-1.5519493	-1.0825312	-0.7847936
	H	4.3043543	-0.3657495	-0.5083693
	H	-4.0613963	-0.4969655	0.3435364
tG-TG-G-G-g+	C	-2.7471526	-0.0080495	0.0981191
	C	-1.4279427	-0.6909045	0.4018984
	C	-0.4364215	-0.5951024	-0.7551398
	C	0.8954107	-1.3024057	-0.4888616
	C	1.6890916	-0.7620760	0.7052438
	C	1.9658849	0.7346305	0.6454263
	O	-2.4689237	1.3874361	-0.0958138
	O	2.7194549	1.1109984	-0.5160995
	H	-3.4462873	-0.1451625	0.9293292
	H	-3.1953289	-0.4370391	-0.8055806
	H	-1.0154043	-0.2351703	1.3051062
	H	-1.6251419	-1.7435980	0.6319751
	H	-0.2756635	0.4594864	-0.9912550
	H	-0.8949346	-1.0389669	-1.6454875
	H	1.5189214	-1.2431002	-1.3861856
	H	0.7071647	-2.3690076	-0.3288515
	H	2.6469632	-1.2859919	0.7580427
	H	1.1600707	-0.9739787	1.6396399
	H	1.0353287	1.3086104	0.6979726
	H	2.5856282	1.0324012	1.4908597
	H	-3.2973956	1.8449115	-0.2890978
	H	2.1412658	1.0462868	-1.2869731

g-TG-TG+Tt	C	-2.7300818	-0.3866182	-0.2691448
	C	-1.8128923	0.7579126	0.1395967
	C	-0.3600437	0.5829235	-0.3122707
	C	0.3691588	-0.5830507	0.3592205
	C	1.8118398	-0.7741765	-0.1143780
	C	2.7222839	0.3944891	0.2108073
	O	-4.1061201	-0.1114184	0.0269823
	O	4.0557133	0.0025405	-0.1453360
	H	-2.4259331	-1.3268851	0.2001140
	H	-2.6978450	-0.5256192	-1.3503568
	H	-2.2238267	1.6757702	-0.2881549
	H	-1.8420343	0.8730584	1.2296369
	H	0.1730489	1.5147474	-0.1076946
	H	-0.3338999	0.4458654	-1.3995634
	H	-0.1728287	-1.5128629	0.1713892
	H	0.3582641	-0.4338268	1.4454030
	H	1.8326964	-0.9457737	-1.1940747
	H	2.2385003	-1.6624594	0.3576993
	H	2.4298563	1.2876975	-0.3487940
	H	2.6637615	0.6249583	1.2814986
	H	-4.1873331	0.0054925	0.9828869
	H	4.6446602	0.7566505	-0.0129359
tG+G+G+TG+g+	C	-1.9694335	0.7620994	0.5927930
	C	-1.6557965	-0.7115438	0.7722821
	C	-0.8849727	-1.3240888	-0.4011074
	C	0.4356638	-0.6287228	-0.7393667
	C	1.4721699	-0.6782386	0.3806971
	C	2.7688039	0.0355711	0.0238822
	O	-2.7106976	0.9007813	-0.6274111
	O	2.5814991	1.4418547	-0.1920159
	H	-1.0474697	1.3518383	0.5454091
	H	-2.5592148	1.1221750	1.4426596
	H	-1.1003984	-0.8300277	1.7074207
	H	-2.5996930	-1.2486554	0.8976199
	H	-1.5285633	-1.3060852	-1.2824671
	H	-0.6879498	-2.3773008	-0.1739774
	H	0.2536564	0.4095269	-1.0235411
	H	0.8644720	-1.1123291	-1.6233784
	H	1.7049365	-1.7225533	0.6200424
	H	1.0741391	-0.2343869	1.2999226
	H	3.5256654	-0.1321429	0.7978116
	H	3.1639817	-0.3417874	-0.9198195
	H	-2.9055220	1.8366008	-0.7663269
	H	2.3304115	1.8404449	0.6517952
g-TG-TG+G+t	C	-2.6089447	0.3663177	-0.1282739
	C	-1.5998231	-0.6351377	0.4149801
	C	-0.2340979	-0.0260389	0.7454231
	C	0.5121461	0.5202132	-0.4716135
	C	1.8992924	1.0820085	-0.1512672
	C	2.8616011	0.0643408	0.4331943
	O	-3.9206820	-0.2014571	-0.2607140

O	2.9328973	-1.0394058	-0.4818660	
H	-2.2812577	0.7790152	-1.0868556	
H	-2.7313896	1.1949525	0.5703904	
H	-2.0319182	-1.0827266	1.3137159	
H	-1.4651750	-1.4438553	-0.3127551	
H	0.3712802	-0.7987092	1.2252897	
H	-0.3648644	0.7729712	1.4851723	
H	-0.0719784	1.3189727	-0.9360748	
H	0.6152634	-0.2734944	-1.2158677	
H	1.8111898	1.9124247	0.5574569	
H	2.3432447	1.4853432	-1.0651151	
H	3.8484206	0.5213659	0.5598471	
H	2.5195933	-0.2780325	1.4148922	
H	-3.8602966	-0.9438357	-0.8766191	
H	3.5815379	-1.6732973	-0.1496490	
g-G+TG-TG+g-C	0.2631126	3.0018595	0.5692817	
C	-0.2305036	1.5613592	0.6069147	
C	0.2611807	0.7196959	-0.5687919	
C	-0.2611805	-0.7196959	-0.5687919	
C	0.2305035	-1.5613593	0.6069148	
C	-0.2631125	-3.0018596	0.5692818	
O	-0.2421116	3.7403350	-0.5503479	
O	0.2421113	-3.7403350	-0.5503481	
H	1.3593427	3.0256526	0.5800684	
H	-0.0912111	3.5449164	1.4447179	
H	0.1040938	1.1213684	1.5509333	
H	-1.3246105	1.5702637	0.6196136	
H	1.3575217	0.7024187	-0.5719834	
H	-0.0523898	1.1932427	-1.5042414	
H	0.0523902	-1.1932427	-1.5042414	
H	-1.3575216	-0.7024188	-0.5719836	
H	-0.1040942	-1.1213684	1.5509333	
H	1.3246104	-1.5702635	0.6196140	
H	0.0912116	-3.5449166	1.4447178	
H	-1.3593426	-3.0256528	0.5800689	
H	0.1810354	3.4097217	-1.3525002	
H	-0.1810358	-3.4097213	-1.3525003	
tTG+G+TG-t	C	2.2920120	-0.3258354	-0.4701952
C	1.7140277	0.6231943	0.5605707	
C	0.5495941	1.4619632	0.0270585	
C	-0.6518449	0.6621124	-0.4866768	
C	-1.2576608	-0.2699765	0.5598411	
C	-2.5118596	-0.9682273	0.0710836	
O	3.4394353	-0.9535794	0.1221020	
O	-3.4946276	0.0405474	-0.2059696	
H	2.5806075	0.2312560	-1.3695573	
H	1.5568434	-1.0834471	-0.7599004	
H	1.4089674	0.0452570	1.4357725	
H	2.5187761	1.2854152	0.8891685	
H	0.9152725	2.1075923	-0.7783804	
H	0.2095686	2.1303766	0.8240389	

H	-0.3674348	0.0763663	-1.3677130
H	-1.4235923	1.3592442	-0.8186597
H	-1.5072420	0.2978785	1.4615182
H	-0.5386637	-1.0405526	0.8536940
H	-2.2906133	-1.5437867	-0.8356531
H	-2.8813941	-1.6592390	0.8357454
H	3.8052701	-1.5847975	-0.5109837
H	-4.3021858	-0.3914918	-0.5124324
tTG+G+TG+g+ C	2.0293739	-0.5280299	-0.3467704
C	1.6779200	0.7278535	0.4266145
C	0.6569909	1.6150237	-0.2917669
C	-0.6821161	0.9406039	-0.6081054
C	-1.4312977	0.4435759	0.6257171
C	-2.7507441	-0.2340871	0.2821377
O	3.0656816	-1.2019597	0.3827112
O	-2.5686494	-1.4193490	-0.5062312
H	2.3773002	-0.2615290	-1.3520435
H	1.1565775	-1.1805776	-0.4513462
H	1.3171478	0.4389158	1.4162465
H	2.6012343	1.2908377	0.5837898
H	1.0981774	1.9779241	-1.2258999
H	0.4724493	2.5010185	0.3239608
H	-0.5388314	0.1086092	-1.3008529
H	-1.3193852	1.6619708	-1.1305378
H	-1.6355282	1.2859814	1.2968086
H	-0.8162389	-0.2618680	1.1944048
H	-3.3123007	-0.4657120	1.1932867
H	-3.3668831	0.4204081	-0.3351843
H	3.2944279	-2.0137686	-0.0882480
H	-2.1288789	-2.0788006	0.0467857
g+TG-G-TG-g- C	-2.0203517	-0.5549048	-0.3393007
C	-1.6823737	0.7199739	0.4186119
C	-0.6615343	1.6050064	-0.3036122
C	0.6802015	0.9282116	-0.6022575
C	1.4086045	0.4232340	0.6403619
C	2.7545342	-0.2118592	0.3186590
O	-2.9861610	-1.3605866	0.3488948
O	2.6312836	-1.3602707	-0.5308413
H	-1.1476471	-1.1983933	-0.4384564
H	-2.3712274	-0.3114031	-1.3495121
H	-2.6045155	1.2938799	0.5622572
H	-1.3287999	0.4485030	1.4157874
H	-0.4834474	2.4991193	0.3022672
H	-1.0975569	1.9544180	-1.2453311
H	1.3261169	1.6506979	-1.1120225
H	0.5453517	0.1010420	-1.3019815
H	0.7969114	-0.3097673	1.1769845
H	1.5744356	1.2550631	1.3350536
H	3.3801780	0.4841724	-0.2412954
H	3.2838760	-0.4739373	1.2410344
H	-3.7827931	-0.8283567	0.4754242

H	2.1723885	-2.0518375	-0.0353444
g-TG-TG-Tt	C	2.5408436	-0.5598142
			-0.2392990
C	1.8869455	0.5472893	0.5750398
C	0.3674877	0.4036946	0.6911272
C	-0.3707767	0.5120407	-0.6456414
C	-1.8882601	0.6434666	-0.5040467
C	-2.5346772	-0.5543102	0.1642765
O	3.9731453	-0.5020214	-0.1884143
O	-3.9553523	-0.3686218	0.0866229
H	2.2002014	-0.5386839	-1.2789389
H	2.2846526	-1.5344968	0.1779287
H	2.3380933	0.5378763	1.5703954
H	2.1254308	1.5175097	0.1236591
H	-0.0084346	1.1822809	1.3629552
H	0.1414223	-0.5538236	1.1712434
H	-0.1449693	-0.3555983	-1.2734450
H	0.0055310	1.3885103	-1.1835190
H	-2.3442506	0.7577151	-1.4904212
H	-2.1350321	1.5411657	0.0693963
H	-2.2396033	-1.4743343	-0.3546109
H	-2.2207252	-0.6340701	1.2092063
H	4.2497596	0.3479076	-0.5562079
H	-4.3867496	-1.0872082	0.5668843
g+TG-TG-Tg+	C	2.5370727	-0.5487875
			-0.2164777
C	1.8869154	0.6054530	0.5329472
C	0.3693168	0.4618993	0.6704269
C	-0.3693169	0.4618994	-0.6704268
C	-1.8869155	0.6054528	-0.5329472
C	-2.5370727	-0.5487877	0.2164777
O	3.9607303	-0.4125050	-0.3043179
O	-3.9607304	-0.4125050	0.3043184
H	2.2011282	-0.5852623	-1.2513181
H	2.2700070	-1.5011362	0.2584247
H	2.3327891	0.6653216	1.5319802
H	2.1319900	1.5388853	0.0185986
H	-0.0083248	1.2899693	1.2788304
H	0.1465516	-0.4554772	1.2243622
H	-0.1465515	-0.4554770	-1.2243623
H	0.0083246	1.2899696	-1.2788301
H	-2.3327892	0.6653214	-1.5319802
H	-2.1319903	1.5388851	-0.0185986
H	-2.2700073	-1.5011363	-0.2584249
H	-2.2011279	-0.5852626	1.2513180
H	4.3118533	-0.3631404	0.5947425
H	-4.3118536	-0.3631397	-0.5947420
tG-G-G-TG+g+	C	-2.3060735	-0.6477386
			0.5101281
C	-1.7209392	0.7328798	0.7412164
C	-0.7506075	1.1832237	-0.3542916
C	0.4400051	0.2509946	-0.5878439
C	1.3221417	0.0518841	0.6424811
C	2.5913395	-0.7369081	0.3482648

O	-2.9508961	-0.6365857	-0.7716771
O	3.4409461	-0.0901960	-0.6083343
H	-3.0272825	-0.8815899	1.3003953
H	-1.5206178	-1.4111082	0.5326239
H	-2.5461094	1.4472642	0.8032527
H	-1.2288769	0.7343211	1.7185485
H	-0.3747481	2.1786130	-0.0943002
H	-1.3059140	1.2897049	-1.2879765
H	1.0537197	0.6593776	-1.3938495
H	0.0864565	-0.7231696	-0.9404800
H	0.7755795	-0.4756594	1.4311706
H	1.5982943	1.0285150	1.0603511
H	3.1422553	-0.9327632	1.2748238
H	2.3437247	-1.6979182	-0.1042729
H	-3.3577254	-1.4999695	-0.9202036
H	3.7419760	0.7439233	-0.2238015
g+TTG-G-Tg- C	-2.6514677	-0.1836129	0.4505104
C	-1.3441526	0.1192876	-0.2666471
C	-0.4735501	1.1045779	0.5116479
C	0.7812008	1.5549576	-0.2445268
C	1.7222053	0.4271057	-0.6780744
C	2.2363329	-0.4163864	0.4791558
O	-3.5048179	-1.0592922	-0.2964848
O	3.2545370	-1.3403484	0.0709578
H	-3.2320621	0.7294017	0.5818506
H	-2.4498768	-0.5988692	1.4449440
H	-0.8044411	-0.8206930	-0.4235854
H	-1.5769917	0.5232278	-1.2562508
H	-0.1954674	0.6661707	1.4751199
H	-1.0699929	1.9926984	0.7442432
H	1.3394717	2.2562020	0.3840810
H	0.4739639	2.1151581	-1.1327325
H	2.5885664	0.8563304	-1.1873816
H	1.2221227	-0.2221362	-1.4045670
H	2.7154268	0.2177850	1.2260757
H	1.4180194	-0.9529120	0.9706965
H	-3.0444887	-1.9010704	-0.4107114
H	2.8804581	-1.9137013	-0.6113281
g+TTG-G-G-g- C	2.5907589	-0.1686570	-0.5613892
C	1.3538986	0.1834850	0.2513146
C	0.2481699	0.7882368	-0.6130939
C	-0.9531084	1.3038454	0.1826726
C	-1.6572584	0.2476622	1.0380715
C	-2.1264653	-0.9711249	0.2550535
O	3.6595904	-0.6809651	0.2455289
O	-2.9536386	-0.6276991	-0.8643092
H	2.9999340	0.7235434	-1.0351291
H	2.3324890	-0.8808016	-1.3537400
H	0.9934090	-0.7223116	0.7507171
H	1.6445444	0.8868545	1.0373348
H	-0.0879783	0.0576171	-1.3548465

H	0.6661131	1.6262677	-1.1803388
H	-1.6749680	1.7311820	-0.5168947
H	-0.6254907	2.1190433	0.8357441
H	-2.5223089	0.7075709	1.5289505
H	-1.0009937	-0.0959319	1.8438923
H	-1.2829111	-1.5065741	-0.1793804
H	-2.6503198	-1.6661952	0.9201650
H	3.3493208	-1.4905238	0.6722139
H	-3.7592938	-0.2134532	-0.5272568
tG-G-G-TG-g+ C	1.9959683	0.6775062	0.6761023
C	1.7009251	-0.8106236	0.6626958
C	0.8872660	-1.2663414	-0.5516927
C	-0.4340613	-0.5213378	-0.7531097
C	-1.4066146	-0.6448533	0.4184399
C	-2.7653970	-0.0174913	0.1403846
O	2.6413053	1.0041731	-0.5643151
O	-2.6915128	1.4024801	-0.0500051
H	2.6482300	0.9172191	1.5221118
H	1.0727632	1.2556457	0.7867163
H	2.6510263	-1.3508727	0.6751012
H	1.1820974	-1.0619881	1.5922031
H	0.6805565	-2.3367611	-0.4497007
H	1.5004016	-1.1449317	-1.4465430
H	-0.9180574	-0.9157273	-1.6541403
H	-0.2167809	0.5319203	-0.9535843
H	-0.9938989	-0.1743633	1.3142390
H	-1.5593588	-1.7055355	0.6501710
H	-3.2315957	-0.4946765	-0.7298964
H	-3.4309987	-0.1506329	0.9926198
H	2.8903254	1.9372238	-0.5440025
H	-2.2221702	1.5723480	-0.8767031
g+TG+TG-Tg+ C	-2.7318589	0.3918445	-0.2611145
C	-1.8127160	-0.7537128	0.1402079
C	-0.3642883	-0.5822783	-0.3268763
C	0.3691479	0.5908455	0.3273369
C	1.8163663	0.7576368	-0.1448645
C	2.7279210	-0.3976635	0.2453179
O	-4.1057491	0.1187410	0.0460356
O	4.0791912	-0.1955003	-0.1861736
H	-2.7081980	0.5308418	-1.3425709
H	-2.4227360	1.3317924	0.2058265
H	-1.8309936	-0.8672822	1.2306077
H	-2.2288614	-1.6716538	-0.2820823
H	-0.3485031	-0.4539695	-1.4152394
H	0.1715267	-1.5116000	-0.1195936
H	0.3533875	0.4618447	1.4161352
H	-0.1657232	1.5205908	0.1196464
H	2.2261742	1.6779615	0.2859147
H	1.8467315	0.8758311	-1.2315982
H	2.6896388	-0.5539919	1.3305180
H	2.4229733	-1.3242757	-0.2371538

H	-4.1787063	-0.0037053	1.0019176	
H	4.3990476	0.6265922	0.2087097	
tG+TG-G-G-g+ C	2.5673823	-0.7079098	0.4010916	
C	1.3153691	0.1067244	0.6636369	
C	0.4461606	0.2743001	-0.5804175	
C	-0.7620558	1.1909093	-0.3669850	
C	-1.7441346	0.7385092	0.7186571	
C	-2.3006305	-0.6642411	0.5141626	
O	3.3511279	-0.0008644	-0.5710291	
O	-3.0260286	-0.8037540	-0.7143305	
H	2.2958842	-1.7008135	0.0234680	
H	3.1354053	-0.8357986	1.3282670	
H	0.7561421	-0.3875322	1.4634380	
H	1.6147262	1.0901463	1.0391369	
H	0.1209619	-0.7156446	-0.9216771	
H	1.0636903	0.6853052	-1.3811994	
H	-1.2995632	1.3044498	-1.3139473	
H	-0.4011657	2.1925783	-0.1140749	
H	-2.5833027	1.4381448	0.7521068	
H	-1.2626505	0.7744853	1.7008996	
H	-1.5027505	-1.4129080	0.5708098	
H	-3.0251833	-0.8972882	1.2938283	
H	4.1542926	-0.5072389	-0.7479244	
H	-2.4098522	-0.6780342	-1.4475503	
g+G+G+TG-G-g+ C	-2.6739296	0.3058939	-0.5433082	
C	-1.6214668	1.0970016	0.2233421	
C	-0.3795772	0.2874753	0.6039302	
C	0.3756523	-0.2838223	-0.5953610	
C	1.6223242	-1.0909238	-0.2208257	
C	2.6953187	-0.3056643	0.5221818	
O	-3.0647215	-0.8951931	0.1345804	
O	3.2063258	0.7972668	-0.2390036	
H	-2.2905640	-0.0299272	-1.5053641	
H	-3.5467647	0.9379032	-0.7388591	
H	-1.3325913	1.9594629	-0.3882169	
H	-2.0784444	1.5033548	1.1326504	
H	-0.6731417	-0.5350474	1.2617252	
H	0.2779285	0.9359641	1.1906218	
H	0.6504019	0.5267953	-1.2808347	
H	-0.2884968	-0.9413629	-1.1605095	
H	2.0697318	-1.5015170	-1.1296588	
H	1.3248831	-1.9391494	0.4055248	
H	2.3281187	0.0402374	1.4937875	
H	3.5606161	-0.9415415	0.7061511	
H	-3.4957145	-0.6473317	0.9635230	
H	2.4959404	1.4407784	-0.3573238	
g+TG+TG-G-g-C	2.6131313	0.3640113	-0.1600981	
C	1.6139533	-0.6219536	0.4280946	
C	0.2524598	-0.0054899	0.7617559	
C	-0.5104033	0.5125256	-0.4576983	
C	-1.8972089	1.0698202	-0.1285415	

C	-2.8657298	0.0454695	0.4492798
O	3.9242190	-0.2042523	-0.2920584
O	-3.0126526	-1.1095030	-0.3875814
H	2.7424478	1.2148791	0.5100405
H	2.2715708	0.7453915	-1.1270000
H	1.4698432	-1.4529269	-0.2722187
H	2.0594831	-1.0416824	1.3335415
H	0.3922589	0.8121293	1.4789038
H	-0.3455596	-0.7662551	1.2685125
H	-0.6133845	-0.2990023	-1.1836015
H	0.0639435	1.3039784	-0.9460424
H	-2.3385803	1.4948978	-1.0371068
H	-1.8069294	1.8961939	0.5855410
H	-2.5077170	-0.3448980	1.4004258
H	-3.8390921	0.5136838	0.6307065
H	3.8566950	-0.9718915	-0.8754681
H	-3.4088874	-0.8274573	-1.2228981
g+TG+TG+Tg+C	2.5410483	-0.5688684	0.2035936
C	1.8915984	0.5958946	-0.5304426
C	0.3731082	0.4608885	-0.6684374
C	-0.3731080	0.4608879	0.6684371
C	-1.8915981	0.5958945	0.5304425
C	-2.5410485	-0.5688685	-0.2035932
O	3.9731953	-0.5074104	0.1643978
O	-3.9731955	-0.5074104	-0.1643968
H	2.2868848	-1.5100142	-0.2856661
H	2.1949274	-0.6241603	1.2402533
H	2.1260719	1.5297807	-0.0060910
H	2.3496863	0.6608685	-1.5204933
H	0.1508658	-0.4540176	-1.2262489
H	0.0017603	1.2920167	-1.2771565
H	-0.0017598	1.2920152	1.2771572
H	-0.1508659	-0.4540190	1.2262475
H	-2.1260714	1.5297805	0.0060907
H	-2.3496859	0.6608688	1.5204933
H	-2.1949280	-0.6241606	-1.2402532
H	-2.2868849	-1.5100143	0.2856664
H	4.2484313	0.3101662	0.6001517
H	-4.2484316	0.3101655	-0.6001520
tTTTG+G-g+ C	-2.6201330	0.6318974	-0.0985439
C	-1.6380592	-0.5078514	0.0825505
C	-0.1896797	-0.0747884	-0.1369346
C	0.8000695	-1.2166001	0.1031902
C	2.2458890	-0.9408284	-0.3187512
C	2.9163978	0.2463087	0.3664401
O	-3.9358032	0.1086077	0.1252281
O	2.6048545	1.5125272	-0.2318056
H	-2.5358415	1.0418312	-1.1113608
H	-2.3998432	1.4343415	0.6148204
H	-1.7580289	-0.9135074	1.0905805
H	-1.8968072	-1.3045428	-0.6193844

H	0.0264562	0.7554639	0.5460603	
H	-0.0720858	0.3030808	-1.1585725	
H	0.4446869	-2.0977184	-0.4402430	
H	0.7799228	-1.4827085	1.1657191	
H	2.3015878	-0.7803205	-1.3995111	
H	2.8389863	-1.8350001	-0.1003982	
H	2.6735634	0.2551541	1.4364673	
H	3.9988900	0.1669520	0.2740098	
H	-4.5770082	0.8197854	-0.0020649	
H	1.6644819	1.6878771	-0.1089811	
g+TG+TG-Tg-	C	-2.7332041	-0.3976807	0.2527414
C	-1.8164342	0.7588356	-0.1218515	
C	-0.3672800	0.5790251	0.3398705	
C	0.3672803	-0.5790248	-0.3398707	
C	1.8164344	-0.7588355	0.1218516	
C	2.7332046	0.3976805	-0.2527414	
O	-4.1081587	-0.1180825	-0.0432457	
O	4.1081589	0.1180825	0.0432471	
H	-2.7063473	-0.5640648	1.3303097	
H	-2.4244735	-1.3250859	-0.2387284	
H	-1.8355192	0.8983239	-1.2091425	
H	-2.2341577	1.6656344	0.3224522	
H	-0.3515994	0.4268494	1.4254777	
H	0.1670384	1.5134384	0.1526139	
H	0.3515999	-0.4268490	-1.4254779	
H	-0.1670381	-1.5134380	-0.1526143	
H	2.2341578	-1.6656345	-0.3224518	
H	1.8355191	-0.8983235	1.2091426	
H	2.7063488	0.5640637	-1.3303099	
H	2.4244735	1.3250861	0.2387274	
H	-4.1851753	0.0231949	-0.9962110	
H	4.1851746	-0.0231946	0.9962125	
tG-TG+G+G+g+	C	-2.5743794	-0.7846227	0.2241111
C	-1.3126288	-0.0622431	0.6561961	
C	-0.4487858	0.3793619	-0.5230548	
C	0.7520845	1.2385353	-0.1225816	
C	1.7220496	0.5746514	0.8584621	
C	2.2788476	-0.7579819	0.3761611	
O	-3.3737027	0.1435192	-0.5242598	
O	2.9052185	-0.6669126	-0.9103161	
H	-3.1266344	-1.1395034	1.1006136	
H	-2.3153658	-1.6513785	-0.3951435	
H	-1.6023966	0.8086345	1.2528516	
H	-0.7545439	-0.7331560	1.3166762	
H	-1.0729308	0.9512824	-1.2123229	
H	-0.1056854	-0.5015992	-1.0750877	
H	0.3900192	2.1704144	0.3239428	
H	1.2985068	1.5160008	-1.0269254	
H	1.2386206	0.4105430	1.8268445	
H	2.5577156	1.2571299	1.0515277	
H	2.9799891	-1.1613736	1.1151511	

H	1.4833025	-1.4905583	0.2444173	
H	-4.1654966	-0.3129867	-0.8363037	
H	3.6541743	-0.0603177	-0.8364877	
g+G-TG-G-G-g-	C	-2.7666318	-0.0127932	0.1254444
C	-1.4136270	-0.6463885	0.4180951	
C	-0.4348827	-0.5434498	-0.7500447	
C	0.8869311	-1.2807002	-0.5250218	
C	1.6892885	-0.7943271	0.6850084	
C	1.9697544	0.7025406	0.6772970	
O	-2.6851710	1.4067305	-0.0593131	
O	2.5828319	1.1446790	-0.5416449	
H	-3.4417953	-0.1455212	0.9701998	
H	-3.2249773	-0.4868502	-0.7507809	
H	-1.0036012	-0.1667664	1.3103760	
H	-1.5741831	-1.7031639	0.6621509	
H	-0.2184968	0.5053805	-0.9723038	
H	-0.9122964	-0.9587468	-1.6449634	
H	1.5008301	-1.1744366	-1.4221480	
H	0.6857297	-2.3502596	-0.4049989	
H	2.6416056	-1.3352140	0.7188671	
H	1.1696145	-1.0383145	1.6166825	
H	1.0458838	1.2751068	0.7470718	
H	2.5899950	0.9729012	1.5384986	
H	-2.2016758	1.5808721	-0.8770211	
H	3.4543717	0.7322961	-0.6077271	
g-G-G-G-TG+g-	C	-2.2489479	-0.6800369	0.5292832
C	-1.7398844	0.7414847	0.7277260	
C	-0.7748794	1.2141668	-0.3627662	
C	0.4443360	0.3138046	-0.5774798	
C	1.3275606	0.1527843	0.6579387	
C	2.5587854	-0.7100942	0.4136663	
O	-2.8331507	-0.8853631	-0.7640093	
O	3.4696940	-0.1348820	-0.5318341	
H	-2.9638220	-0.9369176	1.3183735	
H	-1.4323185	-1.3994990	0.5808869	
H	-2.5967389	1.4236827	0.7618769	
H	-1.2685512	0.8003581	1.7136827	
H	-0.4328199	2.2235648	-0.1128091	
H	-1.3194393	1.2909306	-1.3064899	
H	1.0364905	0.7525522	-1.3865713	
H	0.1175644	-0.6701681	-0.9299439	
H	0.7586965	-0.3072711	1.4724870	
H	1.6553740	1.1367185	1.0073426	
H	3.1376262	-0.8136899	1.3309334	
H	2.2568151	-1.7137431	0.0908754	
H	-3.6165993	-0.3232927	-0.8327663	
H	3.0608599	-0.1645752	-1.4059624	
tG+G-G-TTg+	C	2.5186310	0.6376638	0.0358300
C	1.9312222	-0.5474703	0.7810738	
C	1.1021617	-1.5103209	-0.0743627	
C	-0.1438478	-0.9184322	-0.7395375	

C	-1.1529547	-0.3423731	0.2508625	
C	-2.4208857	0.1354958	-0.4388040	
O	1.4698394	1.5892413	-0.2186590	
O	-3.3879496	0.6613974	0.4811442	
H	2.9672252	0.3042601	-0.9076668	
H	3.3020204	1.1044471	0.6415061	
H	2.7660420	-1.1090448	1.2122482	
H	1.3467766	-0.1653192	1.6215380	
H	0.7963650	-2.3510004	0.5573066	
H	1.7523077	-1.9297483	-0.8500368	
H	-0.6269092	-1.7121665	-1.3200689	
H	0.1502003	-0.1379179	-1.4442307	
H	-0.7027180	0.5030588	0.7772392	
H	-1.4249361	-1.0948886	0.9977170	
H	-2.1721055	0.8831524	-1.2008479	
H	-2.9267006	-0.6935618	-0.9343519	
H	1.8564818	2.3561281	-0.6617527	
H	-2.9728593	1.3955715	0.9531323	
tG+G+G+TG-g+ C	2.2681281	-0.5544226	0.6354260	
C	1.7466087	0.8689398	0.5736435	
C	0.7777068	1.1212392	-0.5846707	
C	-0.4411121	0.1957706	-0.6225388	
C	-1.3332363	0.2850023	0.6141220	
C	-2.5560946	-0.6204166	0.5475699	
O	2.8663019	-0.8536436	-0.6343864	
O	-3.4668418	-0.2616681	-0.4992253	
H	1.4545436	-1.2574407	0.8455929	
H	3.0068590	-0.6436597	1.4385873	
H	1.2738535	1.1005000	1.5324305	
H	2.6011446	1.5430196	0.4728200	
H	1.3259041	1.0202115	-1.5231512	
H	0.4319382	2.1584142	-0.5280102	
H	-0.1136895	-0.8394820	-0.7670680	
H	-1.0267440	0.4616473	-1.5082775	
H	-1.6700383	1.3171783	0.7509826	
H	-0.7661918	0.0083387	1.5088001	
H	-2.2435222	-1.6663647	0.4392311	
H	-3.1400105	-0.5392086	1.4639021	
H	3.2585221	-1.7351821	-0.5903375	
H	-3.0377093	-0.4313178	-1.3473546	
tG-TG+G+Tg+ C	-2.5243106	-0.9630170	0.0372327	
C	-1.2578638	-0.2985291	0.5422369	
C	-0.6534796	0.6709562	-0.4705410	
C	0.5506010	1.4509312	0.0671076	
C	1.7181094	0.5945803	0.5675566	
C	2.2938240	-0.3301581	-0.4944387	
O	-3.5004021	0.0665347	-0.1773818	
O	3.4925588	-0.9862422	-0.0565795	
H	-2.8902364	-1.6866990	0.7729081	
H	-2.3193089	-1.4962227	-0.8985642	
H	-1.4928062	0.2320386	1.4702824	

H	-0.5444281	-1.0891317	0.7944744	
H	-1.4254169	1.3815069	-0.7720333	
H	-0.3734821	0.1185296	-1.3737528	
H	0.2141519	2.0952146	0.8852619	
H	0.9180451	2.1196015	-0.7182126	
H	1.4056974	-0.0005721	1.4324076	
H	2.5240977	1.2469243	0.9129984	
H	1.5552226	-1.0728307	-0.8133234	
H	2.5917619	0.2425045	-1.3735537	
H	-4.3119653	-0.3407582	-0.5064355	
H	3.2799283	-1.4923814	0.7388498	
tTTG+G+G-t	C	-2.4222812	0.2329419	0.4311007
	C	-1.1714679	-0.3124290	-0.2265350
	C	-0.1611808	-0.8182811	0.8004419
	C	1.0603107	-1.4961691	0.1723174
	C	1.9020154	-0.6310894	-0.7703960
	C	2.5735986	0.5657811	-0.1219607
	O	-3.3188339	0.6519247	-0.6093439
	O	1.5765828	1.5656557	0.1484585
	H	-2.1630765	1.0787468	1.0775265
	H	-2.8922927	-0.5408753	1.0492765
	H	-1.4628159	-1.1248656	-0.8997538
	H	-0.7321189	0.4813209	-0.8315873
	H	-0.6503533	-1.5476212	1.4558671
	H	0.1622981	0.0146144	1.4274659
	H	0.7220039	-2.3767805	-0.3841101
	H	1.7106070	-1.8688483	0.9715870
	H	1.3052854	-0.2736515	-1.6127921
	H	2.6940230	-1.2585139	-1.1917840
	H	3.0688195	0.2604987	0.8079532
	H	3.3338615	0.9721175	-0.7969284
	H	-4.0983444	1.0497860	-0.2006017
	H	2.0197664	2.3537313	0.4892731
tTG-G-TG+g+	C	-2.3077065	-0.3179241	-0.4555073
	C	-1.7057204	0.6299870	0.5626582
	C	-0.5428120	1.4571465	0.0084767
	C	0.6454898	0.6438622	-0.5145571
	C	1.2544206	-0.2926381	0.5257896
	C	2.5325129	-0.9656925	0.0437891
	O	-3.4484991	-0.9352129	0.1593283
	O	3.5725610	-0.0285196	-0.2665176
	H	-1.5830256	-1.0815231	-0.7556725
	H	-2.6079870	0.2385741	-1.3513498
	H	-2.4997487	1.2998462	0.9016145
	H	-1.3915215	0.0522025	1.4348255
	H	-0.1882474	2.1283556	0.7971016
	H	-0.9136534	2.1005219	-0.7962761
	H	1.4198099	1.3318094	-0.8613753
	H	0.3472791	0.0575884	-1.3901138
	H	0.5436056	-1.0776556	0.8031812
	H	1.4698494	0.2669722	1.4446929

H	2.8834312	-1.6926388	0.7840196	
H	2.3508110	-1.4992796	-0.8899268	
H	-3.8299482	-1.5665266	-0.4644153	
H	3.8342964	0.4093728	0.5543483	
tTG-TG+G-t	C	-2.5882717	0.3312769	0.1835148
	C	-1.5665381	-0.7431144	-0.1336123
	C	-0.1682438	-0.4483142	0.4132792
	C	0.4719980	0.8111965	-0.1753341
	C	1.9087642	1.0770043	0.2866923
	C	2.9731153	0.2127805	-0.3641091
	O	-3.8702432	-0.1567398	-0.2426071
	O	2.8221680	-1.1419108	0.0888401
	H	-2.3510603	1.2642102	-0.3362362
	H	-2.5948011	0.5306573	1.2618718
	H	-1.9352254	-1.6808618	0.2894047
	H	-1.5249967	-0.8781212	-1.2182491
	H	0.4806476	-1.3007092	0.2157806
	H	-0.2180864	-0.3442834	1.5035150
	H	-0.1320158	1.6839166	0.0896778
	H	0.4548038	0.7474213	-1.2703375
	H	1.9823803	0.9616970	1.3723432
	H	2.1678676	2.1162925	0.0596230
	H	2.8737351	0.2617742	-1.4548927
	H	3.9654955	0.5888533	-0.0933550
	H	-4.5265856	0.5367306	-0.0966926
	H	3.5172627	-1.6781044	-0.3149465
g+G-G+TTG-g-C		2.6567976	0.4726438	0.3567161
	C	2.1991114	-0.8975278	-0.1358053
	C	0.7767105	-1.3003935	0.2624890
	C	-0.3280575	-0.3551678	-0.2099843
	C	-1.7255736	-0.9282919	0.0088629
	C	-2.8331681	0.0473141	-0.3640078
	O	2.2192722	1.5612467	-0.4669027
	O	-2.7855008	1.2548235	0.4089417
	H	3.7442326	0.5324772	0.3240510
	H	2.3471080	0.6261869	1.3981889
	H	2.3060787	-0.9146332	-1.2244028
	H	2.8905449	-1.6473716	0.2629652
	H	0.7218797	-1.3916997	1.3533831
	H	0.5767537	-2.2995886	-0.1387689
	H	-0.1958257	-0.1370158	-1.2755943
	H	-0.2725159	0.5955990	0.3271323
	H	-1.8435320	-1.2227385	1.0585000
	H	-1.8487124	-1.8399919	-0.5858291
	H	-2.7191309	0.3730441	-1.3984630
	H	-3.8138675	-0.4300223	-0.2674489
	H	1.2634310	1.6570363	-0.3763299
	H	-3.0134691	1.0359679	1.3222727
tTTG-G-G-g+	C	2.5834334	-0.1810058	-0.5518690
	C	1.3500368	0.1915427	0.2459423
	C	0.2470912	0.7758131	-0.6346433

C	-0.9558962	1.3012412	0.1553577	
C	-1.6644083	0.2604743	1.0279283	
C	-2.1546049	-0.9653332	0.2690066	
O	3.5368901	-0.7400737	0.3617151	
O	-3.1094022	-0.6441026	-0.7518681	
H	2.9961002	0.7077067	-1.0423074	
H	2.3218452	-0.9096049	-1.3278104	
H	1.0016255	-0.7032820	0.7656896	
H	1.6379724	0.9174380	1.0117899	
H	-0.0744145	0.0202380	-1.3601689	
H	0.6588496	1.6023316	-1.2230898	
H	-1.6781329	1.7429117	-0.5386242	
H	-0.6219538	2.1228338	0.7961559	
H	-2.5257909	0.7308684	1.5089766	
H	-0.9977553	-0.0757887	1.8276900	
H	-1.3145401	-1.5237765	-0.1580168	
H	-2.6839280	-1.6360799	0.9447825	
H	4.3304554	-0.9855877	-0.1313770	
H	-2.6634408	-0.1279616	-1.4356114	
g+TG+G+TG+g+ C	2.0461426	-0.5576301	-0.3466959	
C	1.6893724	0.7077717	0.4190633	
C	0.6562713	1.5853009	-0.2949017	
C	-0.6814926	0.9038955	-0.6011124	
C	-1.4123736	0.3918599	0.6372046	
C	-2.7798121	-0.1963988	0.3169620	
O	3.1487962	-1.2600688	0.2442874	
O	-2.7036493	-1.3165641	-0.5749534	
H	2.3790295	-0.3088186	-1.3549805	
H	1.1810643	-1.2227910	-0.4354406	
H	1.3295086	0.4356028	1.4171478	
H	2.6095375	1.2791465	0.5646165	
H	1.0921915	1.9437485	-1.2330451	
H	0.4712441	2.4743310	0.3164181	
H	-0.5421232	0.0810484	-1.3049118	
H	-1.3286817	1.6267837	-1.1087663	
H	-1.5489308	1.2128045	1.3510960	
H	-0.8157409	-0.3690595	1.1523436	
H	-3.3015005	-0.4764916	1.2384451	
H	-3.3943030	0.5363412	-0.2070634	
H	2.9103047	-1.4754051	1.1557599	
H	-2.2626628	-2.0407190	-0.1110871	
tG+G-TG-Tg+ C	2.7866784	0.2309840	-0.5625705	
C	2.0599602	-1.0238593	-0.1166213	
C	0.5345196	-0.9718518	-0.2482487	
C	-0.1739300	-0.1644012	0.8421147	
C	-1.6999012	-0.2634556	0.7755221	
C	-2.2926758	0.3562914	-0.4816977	
O	2.4570495	1.3053437	0.3320515	
O	-3.7255905	0.2928755	-0.5034529	
H	2.4898663	0.4864168	-1.5867025	
H	3.8671170	0.0524863	-0.5531918	

H	2.4428428	-1.8447518	-0.7314987
H	2.3415629	-1.2424833	0.9177927
H	0.1488434	-1.9970166	-0.2205939
H	0.2852353	-0.5765839	-1.2384781
H	0.1390501	0.8795363	0.7889750
H	0.1595849	-0.5340056	1.8167802
H	-2.1275891	0.2492568	1.6446674
H	-2.0192561	-1.3082611	0.8346264
H	-1.9527308	1.3944437	-0.5810345
H	-1.9819919	-0.1845733	-1.3738581
H	2.9611168	2.0866436	0.0690830
H	-4.0527576	0.7344384	0.2915517
g+TTG-G-G-g+C	2.5937636	-0.1587199	-0.5660125
C	1.3600250	0.1829808	0.2566571
C	0.2504660	0.8005271	-0.5934104
C	-0.9528178	1.2893440	0.2197555
C	-1.6649525	0.2101160	1.0412155
C	-2.1606236	-0.9756019	0.2237466
O	3.6636483	-0.6815973	0.2297248
O	-3.1142326	-0.6025249	-0.7791085
H	3.0013807	0.7396768	-1.0294162
H	2.3316459	-0.8598192	-1.3672939
H	1.0001073	-0.7278441	0.7458831
H	1.6529748	0.8774838	1.0493345
H	-0.0694226	0.0772683	-1.3517038
H	0.6620828	1.6522360	-1.1444104
H	-1.6733714	1.7641973	-0.4536155
H	-0.6187663	2.0796828	0.8985084
H	-2.5239112	0.6597008	1.5457384
H	-0.9994008	-0.1673299	1.8235830
H	-1.3225320	-1.5159567	-0.2306184
H	-2.6918448	-1.6764697	0.8667689
H	3.3596029	-1.5021239	0.6396288
H	-2.6688510	-0.0526271	-1.4364918
tG-TG+G+G-t	2.3431976	0.7934322	0.2674368
C	1.0915576	0.0220160	0.6345711
C	0.3886615	-0.5737481	-0.5816900
C	-0.8017767	-1.4664675	-0.2230313
C	-1.9330880	-0.8042573	0.5696358
C	-2.6250861	0.3504599	-0.1326434
O	3.2809584	-0.1308351	-0.3100118
O	-1.7746309	1.5088321	-0.0647225
H	2.7751643	1.2608086	1.1586472
H	2.0954358	1.5831363	-0.4511630
H	1.3707570	-0.7727757	1.3343900
H	0.4180017	0.7062787	1.1554202
H	1.1091517	-1.1688947	-1.1473084
H	0.0579145	0.2414874	-1.2297869
H	-0.4357042	-2.3215176	0.3555277
H	-1.2249149	-1.8804277	-1.1451392
H	-1.5780961	-0.4465856	1.5394360

H	-2.6935990	-1.5637890	0.7776602	
H	-2.8281677	0.0878464	-1.1778332	
H	-3.5798301	0.5648099	0.3585667	
H	4.0718170	0.3580290	-0.5711196	
H	-2.2318694	2.2466588	-0.4893164	
tTG-TG-G-g+	C	2.2765506	0.5910235	0.1197043
C	1.7534394	-0.7351295	-0.3970888	
C	0.2362109	-0.7537633	-0.5919320	
C	-0.5562054	-0.5426915	0.7003830	
C	-2.0546871	-0.8214854	0.5628031	
C	-2.7658057	0.0535910	-0.4617120	
O	3.7086345	0.5160171	0.1087838	
O	-2.6861143	1.4506660	-0.1493122	
H	1.9150781	0.7844485	1.1339316	
H	1.9314996	1.4053988	-0.5296059	
H	2.2523254	-0.9397979	-1.3473964	
H	2.0512955	-1.5246546	0.2980435	
H	-0.0478890	-1.7185991	-1.0241972	
H	-0.0353582	0.0033875	-1.3359324	
H	-0.4128722	0.4746983	1.0768734	
H	-0.1489838	-1.2041200	1.4719554	
H	-2.5403839	-0.6777190	1.5313236	
H	-2.2031946	-1.8688297	0.2769548	
H	-2.3828914	-0.1342613	-1.4699415	
H	-3.8317418	-0.1714124	-0.4677807	
H	4.0631951	1.3168378	0.5161799	
H	-1.7737587	1.7408762	-0.2749913	
tG+TTG+G-g+	C	2.7793457	0.1688106	-0.5342485
C	1.6969777	-0.8694618	-0.3144556	
C	0.3256136	-0.2541773	-0.0463008	
C	-0.7712499	-1.3108238	0.0874286	
C	-2.1325945	-0.7872566	0.5547762	
C	-2.7352140	0.3165905	-0.3105146	
O	2.8663224	0.9593710	0.6602095	
O	-2.2621510	1.6308005	0.0146691	
H	2.5240069	0.8014371	-1.3926100	
H	3.7368095	-0.3204867	-0.7405347	
H	1.6480600	-1.5097536	-1.2015180	
H	1.9867538	-1.5034469	0.5281196	
H	0.0920724	0.4209316	-0.8790376	
H	0.3822323	0.3484892	0.8636827	
H	-0.4327855	-2.0751936	0.7944450	
H	-0.8951110	-1.8170265	-0.8767970	
H	-2.0634389	-0.4105914	1.5794742	
H	-2.8339151	-1.6278850	0.5732356	
H	-2.5682951	0.0988525	-1.3733644	
H	-3.8112135	0.3740699	-0.1502743	
H	3.5640996	1.6174887	0.5462726	
H	-1.3044346	1.6517066	-0.1011267	
g-G+G+TG-Tt	C	2.8832608	0.0251245	0.4126380
C	1.8966570	1.0761733	-0.0813138	

C	0.5042296	0.5398403	-0.4260227	
C	-0.2485876	-0.0611906	0.7623744	
C	-1.6113760	-0.6570209	0.4016890	
C	-2.5974034	0.3590491	-0.1420985	
O	3.1383467	-0.9970576	-0.5587153	
O	-3.8595073	-0.3089659	-0.2771852	
H	2.5481710	-0.4190811	1.3553126	
H	3.8534159	0.4861423	0.5950121	
H	1.8058064	1.8483722	0.6909133	
H	2.3265348	1.5530042	-0.9658357	
H	0.5821161	-0.2066602	-1.2246893	
H	-0.0765883	1.3630089	-0.8492163	
H	-0.3775086	0.7088040	1.5316403	
H	0.3523169	-0.8502964	1.2226004	
H	-2.0618627	-1.1090122	1.2886073	
H	-1.4896865	-1.4553745	-0.3357850	
H	-2.6828525	1.2034667	0.5525915	
H	-2.2684499	0.7442618	-1.1115109	
H	2.3379919	-1.5268035	-0.6654219	
H	-4.4839650	0.2934226	-0.7017935	
g+G+TG-G-G-g+ C	2.5868424	-0.7214377	0.3679887	
C	1.3159787	0.0691976	0.6496947	
C	0.4406337	0.2470691	-0.5882603	
C	-0.7541467	1.1803565	-0.3720203	
C	-1.7326632	0.7461827	0.7238306	
C	-2.3159650	-0.6467946	0.5261603	
O	3.4285280	-0.0907643	-0.6063472	
O	-3.0555423	-0.7734649	-0.6950027	
H	2.3409671	-1.6927953	-0.0626458	
H	3.1415458	-0.8956282	1.2960084	
H	0.7662144	-0.4470379	1.4430387	
H	1.5879946	1.0533057	1.0512597	
H	0.1014570	-0.7397928	-0.9234825	
H	1.0578488	0.6436233	-1.3973534	
H	-1.2978389	1.2948880	-1.3151326	
H	-0.3793409	2.1792726	-0.1273800	
H	-2.5593234	1.4601281	0.7644034	
H	-1.2409736	0.7747370	1.7013622	
H	-1.5319157	-1.4102321	0.5767308	
H	-3.0371387	-0.8650087	1.3131902	
H	3.7632637	0.7319497	-0.2254383	
H	-2.4405605	-0.6893145	-1.4350855	
g+TTTG+G-g+ C	-2.6203824	0.6531328	-0.0976535	
C	-1.6405771	-0.4971665	0.0802909	
C	-0.1886645	-0.0722840	-0.1347522	
C	0.7966698	-1.2195536	0.0970033	
C	2.2439440	-0.9437586	-0.3199016	
C	2.9146094	0.2388229	0.3733571	
O	-3.9866766	0.2411500	0.0216411	
O	2.6135610	1.5076285	-0.2238269	
H	-2.5387100	1.0684835	-1.1021600	

H	-2.3967823	1.4548066	0.6162079	
H	-1.7506746	-0.9126845	1.0885453	
H	-1.9037947	-1.2899965	-0.6245906	
H	0.0313665	0.7538998	0.5517466	
H	-0.0731673	0.3105191	-1.1546046	
H	0.4397272	-2.0948692	-0.4547334	
H	0.7746138	-1.4946441	1.1573977	
H	2.3023168	-0.7772932	-1.3995339	
H	2.8347238	-1.8403223	-0.1053195	
H	2.6647420	0.2457637	1.4418616	
H	3.9972973	0.1545691	0.2882723	
H	-4.1125181	-0.1263815	0.9065315	
H	1.6744329	1.6914469	-0.1040281	
tG+G+TG-G+g+ C	2.7084397	0.1161537	-0.4565295	
C	1.6163965	-0.9266685	-0.6077135	
C	0.2932716	-0.5603128	0.0678157	
C	-0.3293744	0.7314464	-0.4610701	
C	-1.6624730	1.1153820	0.1870616	
C	-2.8523467	0.2336774	-0.1736086	
O	2.8880187	0.3598820	0.9469687	
O	-2.7900771	-1.0931961	0.3680958	
H	2.4357267	1.0437908	-0.9699116	
H	3.6375395	-0.2548713	-0.9018069	
H	1.4537005	-1.0922215	-1.6783658	
H	1.9833882	-1.8683286	-0.1910031	
H	0.4623983	-0.4599150	1.1433498	
H	-0.4094495	-1.3824825	-0.0704100	
H	-0.4752799	0.6505712	-1.5455204	
H	0.3682151	1.5583749	-0.3016077	
H	-1.9208093	2.1364464	-0.1151650	
H	-1.5490581	1.1397694	1.2775928	
H	-3.7818488	0.7213694	0.1408898	
H	-2.9009636	0.0909615	-1.2541062	
H	3.6223492	0.9769798	1.0599007	
H	-2.7964006	-1.0221237	1.3319375	
tG+G-TG+Tg+ C	2.9738590	0.2097362	0.3822607	
C	1.9222562	1.0655940	-0.2993516	
C	0.4806386	0.8142281	0.1573259	
C	-0.1761454	-0.4206739	-0.4652606	
C	-1.5667247	-0.7308381	0.0950172	
C	-2.6019559	0.3514393	-0.1748259	
O	2.7970623	-1.1583773	-0.0169150	
O	-3.9247478	-0.0476418	0.2141581	
H	2.8769930	0.3024868	1.4704683	
H	3.9720447	0.5580344	0.0963969	
H	2.1863730	2.1080254	-0.0945291	
H	2.0040975	0.9243020	-1.3812182	
H	-0.1112418	1.7017795	-0.0825969	
H	0.4644127	0.7199464	1.2502829	
H	0.4732528	-1.2816677	-0.3106701	
H	-0.2495063	-0.2758177	-1.5492770	

H	-1.4921695	-0.8952589	1.1770033	
H	-1.9393146	-1.6607337	-0.3422513	
H	-2.3338801	1.2887706	0.3222682	
H	-2.6713449	0.5474986	-1.2455616	
H	3.4859053	-1.6910194	0.4019403	
H	-3.9030509	-0.2618521	1.1562745	
tG-G+G+TTg+ C	2.5636382	0.5736156	-0.1165163	
C	1.9077320	-0.6297774	-0.7695345	
C	1.0656200	-1.5009202	0.1674267	
C	-0.1552743	-0.8267831	0.8009419	
C	-1.1661408	-0.3057114	-0.2182314	
C	-2.4241011	0.2290827	0.4484374	
O	1.5549448	1.5655887	0.1366372	
O	-3.3668763	0.7669627	-0.4891347	
H	3.3295106	0.9830649	-0.7831918	
H	3.0491481	0.2747824	0.8205391	
H	1.3141616	-0.2764937	-1.6161358	
H	2.7071089	-1.2514589	-1.1853593	
H	1.7154049	-1.8787721	0.9644819	
H	0.7278539	-2.3784865	-0.3944059	
H	0.1678907	0.0015820	1.4338053	
H	-0.6461810	-1.5596055	1.4510718	
H	-1.4434744	-1.1166736	-0.9041980	
H	-0.7273467	0.4968697	-0.8121041	
H	-2.8950413	-0.5537694	1.0551221	
H	-2.1763100	1.0608587	1.1077568	
H	1.9840663	2.3566668	0.4884141	
H	-3.5943471	0.0656659	-1.1138765	
g+G-G-G-TG-g- C	1.9726451	0.7513438	0.6286528	
C	1.6844892	-0.7404625	0.7336990	
C	0.8945938	-1.3134492	-0.4474416	
C	-0.4356066	-0.6140950	-0.7426965	
C	-1.4407875	-0.6787018	0.4042293	
C	-2.7601174	0.0035714	0.0697675	
O	2.7355342	1.0902740	-0.5358548	
O	-2.5991048	1.4010063	-0.2121347	
H	2.5867852	1.0726408	1.4695762	
H	1.0444765	1.3320420	0.6567249	
H	2.6384207	-1.2684439	0.8094667	
H	1.1488847	-0.9195534	1.6712942	
H	0.7043134	-2.3744865	-0.2571410	
H	1.5220944	-1.2829884	-1.3434962	
H	-0.8867906	-1.0832477	-1.6232817	
H	-0.2743444	0.4328376	-1.0121921	
H	-1.0277909	-0.2180231	1.3078301	
H	-1.6445033	-1.7258587	0.6565401	
H	-3.1859887	-0.4178706	-0.8414417	
H	-3.4836910	-0.1418996	0.8788263	
H	2.1769556	0.9664114	-1.3140781	
H	-2.3427249	1.8447809	0.6072921	
tG-G+TG+Tg+ C	2.7907343	-0.2229391	-0.5648040	

C	2.0600211	1.0304610	-0.1209498	
C	0.5347840	0.9734554	-0.2527860	
C	-0.1709845	0.1596473	0.8349249	
C	-1.6979182	0.2478726	0.7747669	
C	-2.2960135	-0.3825610	-0.4746593	
O	2.4666401	-1.2950007	0.3336308	
O	-3.7296160	-0.4359079	-0.4298378	
H	3.8704491	-0.0398611	-0.5580564	
H	2.4931692	-0.4822635	-1.5878038	
H	2.3404871	1.2509722	0.9133890	
H	2.4406062	1.8519029	-0.7365477	
H	0.2867216	0.5820297	-1.2447861	
H	0.1467751	1.9979799	-0.2205829	
H	0.1629802	0.5261412	1.8106293	
H	0.1445903	-0.8831467	0.7782619	
H	-2.0090751	1.2983947	0.8322420	
H	-2.1306831	-0.2605221	1.6401540	
H	-1.9700370	0.1436082	-1.3772144	
H	-1.9778676	-1.4222323	-0.5589728	
H	2.9690272	-2.0772816	0.0703452	
H	-4.0557275	0.4683879	-0.3303250	
g+G+TG-G-G-g-	C	2.5931223	-0.7929364	0.1879473
C	1.3118008	-0.1008735	0.6340763	
C	0.4423297	0.3555203	-0.5349926	
C	-0.7444085	1.2286356	-0.1225854	
C	-1.7123235	0.5744056	0.8667878	
C	-2.2958206	-0.7461514	0.3824148	
O	3.4459783	0.0613763	-0.5860910	
O	-2.9333847	-0.6361481	-0.8966212	
H	2.3618547	-1.6288659	-0.4730635	
H	3.1355122	-1.1875195	1.0539647	
H	0.7629378	-0.7947733	1.2793897	
H	1.5728986	0.7615853	1.2607386	
H	0.0848890	-0.5204755	-1.0850227	
H	1.0659500	0.9185762	-1.2329172	
H	-1.2961952	1.5141056	-1.0210420	
H	-0.3675132	2.1558064	0.3222489	
H	-2.5345233	1.2688327	1.0740508	
H	-1.2194570	0.3964528	1.8280175	
H	-1.5139550	-1.4908778	0.2379949	
H	-2.9954645	-1.1425770	1.1264559	
H	3.7434754	0.7820251	-0.0149365	
H	-3.6801250	-0.0287584	-0.8087842	
g+TG-TG-G-g+C	2.2793042	0.6014493	0.1240342	
C	1.7603669	-0.7412862	-0.3701183	
C	0.2449832	-0.7651204	-0.5843385	
C	-0.5598315	-0.5541867	0.7003687	
C	-2.0574195	-0.8289766	0.5452583	
C	-2.7583785	0.0582901	-0.4757388	
O	3.7016540	0.6120428	0.2909511	
O	-2.6955427	1.4498457	-0.1393016	

H	1.8856197	0.8370733	1.1111026
H	1.9669742	1.3982150	-0.5631137
H	2.2597970	-0.9786859	-1.3159377
H	2.0512506	-1.5142920	0.3463889
H	-0.0336287	-1.7308214	-1.0182157
H	-0.0195902	-0.0086614	-1.3314421
H	-0.4165556	0.4613890	1.0811871
H	-0.1627380	-1.2186146	1.4743954
H	-2.5519035	-0.6948595	1.5106161
H	-2.2043452	-1.8730674	0.2470205
H	-2.3584765	-0.1102440	-1.4809297
H	-3.8222296	-0.1746948	-0.5025402
H	4.1044031	0.3895705	-0.5588838
H	-1.7801236	1.7458822	-0.2215678
tTG+G+TG-g+ C	2.2758574	-0.3346247	-0.4783351
C	1.7230883	0.6170064	0.5640999
C	0.5627255	1.4730410	0.0508128
C	-0.6525180	0.6890100	-0.4574192
C	-1.2711945	-0.2389631	0.5855575
C	-2.5031561	-0.9796618	0.0829062
O	3.4297914	-0.9673904	0.0931934
O	-3.6007858	-0.1087904	-0.2190424
H	2.5505133	0.2213236	-1.3829407
H	1.5311039	-1.0882848	-0.7541758
H	1.4242210	0.0404598	1.4420174
H	2.5394611	1.2696953	0.8825549
H	0.9264603	2.1206971	-0.7537298
H	0.2371288	2.1376990	0.8565731
H	-0.3811597	0.1065599	-1.3451666
H	-1.4020719	1.4170765	-0.7833335
H	-1.5490224	0.3382223	1.4726237
H	-0.5396174	-0.9886870	0.9026075
H	-2.2457157	-1.5874297	-0.7932406
H	-2.8829224	-1.6493651	0.8536785
H	3.7776597	-1.6062175	-0.5424498
H	-3.3717188	0.4138919	-0.9976913
tTG+TG+G-t C	2.2966571	0.3564610	-0.4618236
C	1.6979815	-0.2589822	0.7878269
C	0.1721149	-0.1624164	0.8405667
C	-0.5304093	-0.9598164	-0.2611385
C	-2.0557030	-1.0242876	-0.1330341
C	-2.7913721	0.2289942	-0.5684431
O	3.7245329	0.3378683	-0.3088985
O	-2.4676034	1.2988743	0.3330326
H	1.9373038	1.3860795	-0.5758350
H	2.0074374	-0.2085326	-1.3530604
H	2.0165940	-1.3035959	0.8516348
H	2.1295602	0.2595740	1.6475432
H	-0.1418688	0.8815564	0.7961533
H	-0.1674202	-0.5415013	1.8094431
H	-0.1380025	-1.9828441	-0.2463981

H	-0.2824037	-0.5502149	-1.2461855	
H	-2.3369949	-1.2544108	0.8989535	
H	-2.4322135	-1.8421995	-0.7559197	
H	-2.4980161	0.4938038	-1.5913519	
H	-3.8705753	0.0429128	-0.5590786	
H	4.1246972	0.6740281	-1.1212125	
H	-2.9835763	2.0763534	0.0822325	
tG+G-G-TG+g+	C	2.6319336	0.3389904	-0.1245283
C	1.9276222	-0.8113089	0.5729061	
C	0.7968969	-1.4646505	-0.2279750	
C	-0.3830308	-0.5612791	-0.5950030	
C	-1.0882218	0.0478433	0.6128468	
C	-2.3544132	0.8045492	0.2391792	
O	1.7873669	1.5015853	-0.0608949	
O	-3.3492520	-0.0312356	-0.3728655	
H	2.8401202	0.0754618	-1.1684581	
H	3.5847731	0.5470189	0.3730124	
H	2.6809418	-1.5764848	0.7861495	
H	1.5681959	-0.4509301	1.5401463	
H	0.4203641	-2.3171718	0.3481796	
H	1.2228040	-1.8821805	-1.1470814	
H	-1.1047339	-1.1489990	-1.1679402	
H	-0.0416537	0.2492739	-1.2428016	
H	-0.4177453	0.7439662	1.1229824	
H	-1.3445201	-0.7403667	1.3334068	
H	-2.7727024	1.3066388	1.1184108	
H	-2.1316912	1.5663605	-0.5084331	
H	2.2463306	2.2356754	-0.4901847	
H	-3.6152559	-0.6960755	0.2761807	
g+G-G-TG+Tg+	C	-2.8834536	0.0556479	0.4278465
C	-1.8984176	1.0690163	-0.1416332	
C	-0.5131718	0.5050607	-0.4707628	
C	0.2439678	-0.0448464	0.7396080	
C	1.6144433	-0.6399321	0.4029777	
C	2.6157060	0.3775118	-0.1268306	
O	-3.1519732	-1.0254105	-0.4746028	
O	3.9321969	-0.1751304	-0.2588459	
H	-3.8502356	0.5309804	0.5899068	
H	-2.5405043	-0.3295216	1.3933926	
H	-2.3365702	1.4933741	-1.0485340	
H	-1.7939948	1.8864920	0.5805408	
H	0.0704979	1.3013425	-0.9385783	
H	-0.6050842	-0.2792885	-1.2309452	
H	-0.3513391	-0.8201241	1.2300471	
H	0.3693545	0.7539291	1.4795408	
H	1.4912419	-1.4425426	-0.3339617	
H	2.0490430	-1.0932764	1.2972834	
H	2.2871244	0.7979739	-1.0818542	
H	2.7258815	1.1993727	0.5816893	
H	-2.3549514	-1.5649327	-0.5535481	
H	3.8900447	-0.8972829	-0.8997314	

g+TG-G-TG+g-C	-2.2750920	-0.3463435	-0.4851177	
C	-1.7209605	0.6017135	0.5680187	
C	-0.5651454	1.4684958	0.0599485	
C	0.6519587	0.6896843	-0.4516986	
C	1.2723947	-0.2419122	0.5868857	
C	2.5114134	-0.9702437	0.0831080	
O	-3.3698847	-1.1300756	0.0057095	
O	3.6009018	-0.0875094	-0.2149343	
H	-1.5288458	-1.0793464	-0.7884266	
H	-2.5738936	0.2164544	-1.3781616	
H	-2.5299822	1.2609797	0.9015733	
H	-1.4183083	0.0173125	1.4395671	
H	-0.2417633	2.1310409	0.8683799	
H	-0.9322573	2.1174436	-0.7420677	
H	1.3998807	1.4217020	-0.7717408	
H	0.3826324	0.1120796	-1.3428775	
H	0.5456265	-0.9997458	0.8956833	
H	1.5435941	0.3309617	1.4788644	
H	2.8957510	-1.6383910	0.8529251	
H	2.2607120	-1.5781168	-0.7945561	
H	-4.0625725	-0.5238923	0.3001785	
H	3.3806743	0.4137748	-1.0099423	
g+TG+G+TG-g-C	2.3119182	-0.3233553	-0.4780356	
C	1.7101019	0.5996052	0.5711089	
C	0.5443499	1.4444954	0.0479825	
C	-0.6471232	0.6513110	-0.4982577	
C	-1.2585363	-0.3161146	0.5117830	
C	-2.5482547	-0.9560887	0.0147926	
O	3.5088599	-0.9663428	-0.0172815	
O	-3.5784420	0.0044466	-0.2514174	
H	2.6197167	0.2494781	-1.3535290	
H	1.5859086	-1.0736564	-0.8074654	
H	1.3878953	0.0045861	1.4324570	
H	2.5047309	1.2595845	0.9279571	
H	0.9175552	2.1092112	-0.7378706	
H	0.1934906	2.0936974	0.8565237	
H	-0.3527906	0.0934166	-1.3929924	
H	-1.4197648	1.3531849	-0.8196786	
H	-1.4605085	0.2104631	1.4530281	
H	-0.5555995	-1.1203723	0.7526940	
H	-2.3793049	-1.4560075	-0.9395791	
H	-2.9021419	-1.7063654	0.7298421	
H	3.2852770	-1.4832349	0.7681308	
H	-3.8366105	0.4072389	0.5882615	
tG-G+TG+G+g+C	-2.5100278	0.4349544	-0.4727529	
C	-1.9168239	-0.9577558	-0.3600219	
C	-0.3885965	-1.0215649	-0.4261809	
C	0.3307002	-0.4314240	0.7861402	
C	1.8383853	-0.6877788	0.7757237	
C	2.5605500	-0.1267338	-0.4428383	
O	-2.2642091	1.1459193	0.7513423	

O	2.2988759	1.2671585	-0.6544170	
H	-3.5884031	0.3618005	-0.6496723	
H	-2.0569441	0.9646711	-1.3188150	
H	-2.2774159	-1.4107553	0.5684739	
H	-2.3278419	-1.5498188	-1.1841943	
H	-0.0604999	-0.5106912	-1.3369795	
H	-0.0943468	-2.0724207	-0.5337626	
H	-0.0926776	-0.8664156	1.6969418	
H	0.1342454	0.6381799	0.8403288	
H	2.0378745	-1.7649584	0.8176473	
H	2.2844684	-0.2572395	1.6797580	
H	3.6382485	-0.3031599	-0.3537080	
H	2.2230153	-0.6133001	-1.3568006	
H	-2.6493406	2.0285327	0.6723404	
H	2.5870327	1.7485175	0.1327300	
tG+G-TG+G+g+ C		-2.8684403	-0.2835529	0.2081567
C	-1.6703058	-1.1079911	-0.2241263	
C	-0.3318484	-0.6929567	0.3962526	
C	0.3173064	0.5258268	-0.2601383	
C	1.5841765	0.9990606	0.4544081	
C	2.6813571	-0.0516814	0.5654244	
O	-2.7362313	1.0505801	-0.3093020	
O	3.0363462	-0.6225372	-0.7011843	
H	-2.9253216	-0.2601427	1.3028564	
H	-3.7868302	-0.7428549	-0.1728935	
H	-1.8879148	-2.1442608	0.0541233	
H	-1.6015759	-1.0811211	-1.3157142	
H	0.3533473	-1.5416063	0.3233956	
H	-0.4799242	-0.5001990	1.4665206	
H	-0.4013430	1.3445119	-0.2922072	
H	0.5597933	0.2738532	-1.2963053	
H	1.3353531	1.3345968	1.4678708	
H	1.9865162	1.8750302	-0.0676614	
H	3.5644887	0.3788021	1.0504224	
H	2.3559323	-0.8977042	1.1686727	
H	-3.5173676	1.5565703	-0.0495660	
H	3.3528352	0.0900809	-1.2723081	
tG-G+G+TG-g+ C		-2.6105459	0.3825353	-0.1182243
C	-1.9458891	-0.8018804	0.5599914	
C	-0.8256390	-1.4694973	-0.2435136	
C	0.3879391	-0.5934946	-0.5706585	
C	1.1129762	-0.0613222	0.6628245	
C	2.3343041	0.7817703	0.3257256	
O	-1.7185544	1.5093113	-0.0548157	
O	3.3746295	0.0390705	-0.3280200	
H	-3.5481444	0.6230917	0.3931615	
H	-2.8417867	0.1379977	-1.1619133	
H	-1.5876903	-0.4760439	1.5394013	
H	-2.7225017	-1.5507451	0.7455590	
H	-1.2517499	-1.8484655	-1.1790066	
H	-0.4814161	-2.3467637	0.3144046	

H	0.0781813	0.2499903	-1.1922168	
H	1.0769875	-1.2049350	-1.1634034	
H	1.4293553	-0.8959152	1.2969136	
H	0.4310009	0.5644673	1.2435948	
H	2.0368668	1.6408164	-0.2871178	
H	2.7966991	1.1628664	1.2357191	
H	-2.1666395	2.2748356	-0.4382526	
H	3.0517481	-0.2303452	-1.1970667	
g+G+TTG+G-g+	C	2.7843321	0.1948623	-0.5393705
C	1.6964189	-0.8513010	-0.3422322	
C	0.3222833	-0.2468658	-0.0652634	
C	-0.7668005	-1.3100999	0.0813448	
C	-2.1270193	-0.7949951	0.5604902	
C	-2.7486709	0.3010131	-0.3014933	
O	2.9405083	1.0513926	0.5991237	
O	-2.2851374	1.6197303	0.0158352	
H	2.5219248	0.8653968	-1.3585345	
H	3.7354765	-0.2862510	-0.7911773	
H	1.6514264	-1.4771218	-1.2405680	
H	1.9774530	-1.5141594	0.4844722	
H	0.0795528	0.4235318	-0.8985905	
H	0.3770233	0.3640780	0.8397329	
H	-0.4172931	-2.0712505	0.7868087	
H	-0.8957465	-1.8199182	-0.8801839	
H	-2.0505321	-0.4134920	1.5829059	
H	-2.8210124	-1.6413837	0.5895916	
H	-2.5930894	0.0818845	-1.3657134	
H	-3.8231183	0.3480375	-0.1282755	
H	3.2711754	0.5181099	1.3342571	
H	-1.3360639	1.6659796	-0.1518019	
g-G+TG+G+G+g-	C	2.7894906	0.0355065	-0.1327647
C	1.4158912	0.6253258	-0.4218952	
C	0.4460253	0.5041650	0.7520111	
C	-0.8765615	1.2489315	0.5418012	
C	-1.6912655	0.7921977	-0.6724422	
C	-2.0398716	-0.6905724	-0.6724500	
O	2.7515475	-1.3824008	0.0745697	
O	-2.8364554	-1.0737245	0.4569984	
H	3.2431890	0.5366142	0.7306558	
H	3.4507297	0.1765859	-0.9870536	
H	1.5436983	1.6846227	-0.6735435	
H	1.0128109	0.1275250	-1.3067269	
H	0.9281589	0.9045006	1.6512627	
H	0.2472095	-0.5538761	0.9535832	
H	-0.6633340	2.3170926	0.4370222	
H	-1.4908480	1.1571948	1.4429822	
H	-1.1484976	1.0161168	-1.5957874	
H	-2.6233780	1.3619444	-0.7056820	
H	-2.6535405	-0.9285768	-1.5405451	
H	-1.1362731	-1.3069193	-0.7292011	
H	2.3301620	-1.5572861	0.9254740	

H	-2.2936787	-1.0052394	1.2527432
tTTG-G-G+g+ C	2.4200826	0.1794735	0.4368647
C	1.1778505	-0.3563323	-0.2442957
C	0.1495881	-0.8738458	0.7585452
C	-1.0853016	-1.4978217	0.1017461
C	-1.9252915	-0.5651954	-0.7757716
C	-2.5432410	0.6216969	-0.0459137
O	3.3068109	0.6572870	-0.5870224
O	-1.5940669	1.6323597	0.3286901
H	2.9017040	-0.6132841	1.0202602
H	2.1487314	0.9924523	1.1190698
H	0.7561242	0.4482080	-0.8489150
H	1.4742175	-1.1561709	-0.9298100
H	-0.1567155	-0.0575198	1.4154752
H	0.6204226	-1.6379595	1.3867033
H	-1.7343758	-1.9035120	0.8853748
H	-0.7667066	-2.3515220	-0.5059934
H	-2.7472629	-1.1485020	-1.2051599
H	-1.3403802	-0.1990335	-1.6256989
H	-3.3369346	1.0649127	-0.6568412
H	-2.9910206	0.2956153	0.8942123
H	4.0959698	1.0204714	-0.1646442
H	-1.2676176	2.0495402	-0.4794649
tG-G+TG-G-g+ C	2.8729346	-0.2521518	0.1853279
C	1.6822646	-1.1146914	-0.1919483
C	0.3495699	-0.7100668	0.4474479
C	-0.3073979	0.5264757	-0.1696958
C	-1.6053447	0.9490822	0.5243690
C	-2.7198890	-0.0888592	0.4926732
O	2.7165108	1.0479005	-0.4036977
O	-3.1429772	-0.4124193	-0.8384580
H	3.7931848	-0.7203791	-0.1794883
H	2.9397860	-0.1697252	1.2766639
H	1.5911287	-1.1213776	-1.2823865
H	1.9256223	-2.1375098	0.1130781
H	0.5058925	-0.5386741	1.5194525
H	-0.3306220	-1.5644916	0.3749092
H	-0.4960691	0.3414209	-1.2335767
H	0.3987515	1.3554290	-0.1407633
H	-1.9801075	1.8641904	0.0584138
H	-1.3919894	1.1854002	1.5731874
H	-2.4258350	-0.9973638	1.0289060
H	-3.6115987	0.3047537	0.9795623
H	3.4990920	1.5748922	-0.1948764
H	-2.3924732	-0.7958570	-1.3104661
tTG-TG-G+g+ C	2.3140708	-0.3120177	-0.4816365
C	1.6892309	0.1980067	0.8024022
C	0.1632284	0.0891458	0.8177875
C	-0.5245864	0.9702220	-0.2279624
C	-2.0507940	1.0274338	-0.1203145
C	-2.7813939	-0.2284534	-0.5790647

O	3.7383969	-0.2932596	-0.3007351
O	-2.5408878	-1.3798175	0.2417472
H	2.0350648	0.3196650	-1.3302863
H	1.9663488	-1.3320298	-0.6828474
H	2.1088322	-0.3857646	1.6253627
H	1.9985987	1.2359568	0.9557501
H	-0.1945953	0.3866025	1.8094030
H	-0.1384891	-0.9508577	0.6797011
H	-0.2645795	0.6335601	-1.2369144
H	-0.1308798	1.9883342	-0.1321068
H	-2.4209484	1.8537570	-0.7371313
H	-2.3423825	1.2605955	0.9109171
H	-3.8570620	-0.0302606	-0.6426058
H	-2.4373852	-0.5193308	-1.5725919
H	4.1561483	-0.5758282	-1.1245138
H	-2.9091778	-1.2050305	1.1180930
tG-TG-G-G+g- C	2.4019638	-0.0979468	0.1726546
C	1.1612385	-0.8691677	0.5811414
C	0.2606336	-1.1811193	-0.6160139
C	-1.1770520	-1.5460794	-0.2442987
C	-1.9682379	-0.4444887	0.4739957
C	-1.9409129	0.9317466	-0.1984477
O	1.9444942	1.1312517	-0.4276576
O	-0.8769951	1.7762064	0.2492416
H	2.9954539	-0.6634569	-0.5534908
H	3.0258031	0.1177154	1.0441728
H	1.4636181	-1.7973466	1.0753873
H	0.6275799	-0.2692570	1.3203467
H	0.7014282	-2.0050564	-1.1867700
H	0.2470875	-0.3262218	-1.2959486
H	-1.1774380	-2.4474062	0.3780728
H	-1.7092562	-1.8092836	-1.1642893
H	-1.6202897	-0.3120645	1.5012889
H	-3.0094376	-0.7760780	0.5434012
H	-1.9250495	0.8245685	-1.2905699
H	-2.8474721	1.4789715	0.0609950
H	2.6739489	1.7624736	-0.4707162
H	-0.0256218	1.5090491	-0.1319422
tG-G+TG-G-t C	2.8651501	-0.2916073	0.2267543
C	1.6659280	-1.1142053	-0.2062232
C	0.3256025	-0.6849489	0.4010898
C	-0.3204526	0.5203562	-0.2829204
C	-1.5853604	1.0171678	0.4194355
C	-2.6800582	-0.0254435	0.5501401
O	2.7420504	1.0385825	-0.3019309
O	-2.9796824	-0.5132286	-0.7668347
H	3.7839105	-0.7582715	-0.1446582
H	2.9150751	-0.2599705	1.3216481
H	1.6047125	-1.0970804	-1.2983791
H	1.8773965	-2.1486568	0.0838172
H	0.4709133	-0.4714139	1.4679211

H	-0.3601435	-1.5348061	0.3441722	
H	-0.5684365	0.2504971	-1.3123853	
H	0.4014382	1.3355554	-0.3294813	
H	-1.9904108	1.8724409	-0.1279622	
H	-1.3360158	1.3698765	1.4263565	
H	-2.3565090	-0.8493577	1.1943959	
H	-3.5701451	0.4261944	1.0009846	
H	3.5217135	1.5445594	-0.0379844	
H	-3.7130832	-1.1383266	-0.7023916	
g+G-G-TG+G-g-	C	-2.7293362	0.1189816	-0.4338645
C	-1.6195481	-0.9103578	-0.6054958	
C	-0.2892090	-0.5470104	0.0605137	
C	0.3417697	0.7393515	-0.4754365	
C	1.6772344	1.1212714	0.1693954	
C	2.8527050	0.2115964	-0.1694765	
O	-3.0787666	0.3388148	0.9396024	
O	2.7669226	-1.0986339	0.4082552	
H	-3.6463576	-0.2403075	-0.8996228	
H	-2.4654242	1.0666400	-0.9147841	
H	-1.9733311	-1.8619847	-0.2004535	
H	-1.4563156	-1.0579827	-1.6790771	
H	0.4104767	-1.3716140	-0.0746437	
H	-0.4304512	-0.4573585	1.1445138	
H	-0.3485930	1.5774964	-0.3377213	
H	0.4876414	0.6429040	-1.5578294	
H	1.5647535	1.1719936	1.2591916	
H	1.9491881	2.1310734	-0.1569990	
H	2.8959441	0.0402059	-1.2459777	
H	3.7906534	0.6917328	0.1297096	
H	-2.3107397	0.7098725	1.3926054	
H	2.8512783	-1.0103828	1.3668847	
g+TTG+G+G-g-	C	-2.4140887	0.2384590	0.4510637
C	-1.1893596	-0.3552342	-0.2273330	
C	-0.1522943	-0.8474639	0.7796800	
C	1.0733953	-1.4993558	0.1324980	
C	1.9167085	-0.5971377	-0.7733439	
C	2.5509371	0.6000270	-0.0748744	
O	-3.3662487	0.7641809	-0.4848426	
O	1.6120750	1.6241517	0.2884910	
H	-2.1268361	1.0886962	1.0692983	
H	-2.8876477	-0.5065694	1.1008936	
H	-1.5015163	-1.1886929	-0.8691942	
H	-0.7645032	0.4103573	-0.8788537	
H	-0.6218088	-1.5860374	1.4385055	
H	0.1633812	-0.0098293	1.4041852	
H	0.7450139	-2.3669803	-0.4501636	
H	1.7231609	-1.8894292	0.9233831	
H	1.3298394	-0.2445055	-1.6275814	
H	2.7297316	-1.1991175	-1.1938903	
H	3.0060897	0.2892413	0.8668965	
H	3.3416381	1.0245707	-0.7024943	

H	-3.6639961	0.0355039	-1.0453508	
H	1.3074128	2.0541759	-0.5213694	
g+TG+G+TG-g+	C	2.2771050	-0.3380243	-0.5034393
C	1.7278860	0.5874576	0.5720654	
C	0.5649058	1.4614129	0.0930826	
C	-0.6542707	0.6984238	-0.4374446	
C	-1.2733493	-0.2629764	0.5741926	
C	-2.5160171	-0.9731556	0.0532855	
O	3.4793259	-1.0019829	-0.0902937	
O	-3.6056647	-0.0799026	-0.2082998	
H	2.5621013	0.2356635	-1.3862393	
H	1.5279044	-1.0751131	-0.8105870	
H	1.4221977	-0.0069123	1.4393088	
H	2.5459359	1.2298650	0.9070776	
H	0.9305393	2.1314693	-0.6918085	
H	0.2441459	2.1023855	0.9197951	
H	-0.3883167	0.1472478	-1.3460884	
H	-1.4028616	1.4399011	-0.7331692	
H	-1.5394693	0.2818819	1.4850306	
H	-0.5471288	-1.0320341	0.8563337	
H	-2.2707097	-1.5512464	-0.8458310	
H	-2.8971183	-1.6664568	0.8023013	
H	3.2752585	-1.5263039	0.6955654	
H	-3.3890764	0.4490798	-0.9862358	
tTG+TG-G+g+	C	2.5854009	0.3041881	0.2570434
C	1.5757770	-0.7078640	-0.2490208	
C	0.1536754	-0.4770689	0.2668402	
C	-0.4666419	0.8413099	-0.2004954	
C	-1.9027997	1.0847398	0.2714907	
C	-2.9598559	0.1738394	-0.3427462	
O	3.8828531	-0.1351576	-0.1731137	
O	-2.8936954	-1.1877810	0.1043514	
H	2.5429223	0.3554490	1.3518276	
H	2.3759768	1.3014383	-0.1410232	
H	1.5845625	-0.6963418	-1.3425840	
H	1.9212008	-1.6972269	0.0607271	
H	0.1570786	-0.5014512	1.3635505	
H	-0.4798015	-1.3030721	-0.0561594	
H	-0.4449681	0.8775439	-1.2962692	
H	0.1459730	1.6788842	0.1455961	
H	-2.1838404	2.1143240	0.0238396	
H	-1.9540291	1.0084582	1.3643473	
H	-3.9579809	0.5819228	-0.1497684	
H	-2.8266526	0.1195308	-1.4241111	
H	4.5340912	0.5296781	0.0854909	
H	-3.1152829	-1.2051382	1.0447936	
g+G-G-TG-G-g-	C	2.1112543	0.4571494	0.4664728
C	1.9204610	-0.9191996	-0.1740982	
C	0.4744844	-1.1974411	-0.5883545	
C	-0.5138433	-1.2146934	0.5821432	
C	-1.9565214	-0.8853193	0.1900267	

C	-2.0997541	0.4803235	-0.4774349	
O	1.5799290	1.5163410	-0.3305473	
O	-1.3597061	1.5136055	0.2013540	
H	3.1772369	0.6627562	0.5739841	
H	1.6760827	0.4825647	1.4709248	
H	2.5575067	-0.9770902	-1.0605097	
H	2.2741432	-1.6822711	0.5290321	
H	0.4229030	-2.1516078	-1.1209844	
H	0.1966282	-0.4316842	-1.3138489	
H	-0.2029098	-0.4948803	1.3409770	
H	-0.4900393	-2.1941740	1.0685805	
H	-2.5875375	-0.9182246	1.0847311	
H	-2.3536605	-1.6389645	-0.4984575	
H	-1.6884714	0.4741228	-1.4845322	
H	-3.1534911	0.7635475	-0.5529980	
H	0.6267281	1.5875580	-0.1544343	
H	-1.7504171	1.6582384	1.0740845	
tG+G-TG-G-t	C	2.5094211	0.4403566	-0.4726589
	C	1.9061551	-0.9517470	-0.4155294
	C	0.3766101	-0.9999650	-0.4538848
	C	-0.3164944	-0.3960463	0.7670888
	C	-1.8225041	-0.6610939	0.8004549
	C	-2.5716355	-0.1283350	-0.4067924
	O	2.3358035	1.0700059	0.8059886
	O	-2.2937791	1.2764152	-0.5121789
	H	2.0188465	1.0271452	-1.2584264
	H	3.5762104	0.3709120	-0.7111424
	H	2.2953050	-1.5114274	-1.2723681
	H	2.2802622	-1.4475285	0.4853097
	H	0.0718124	-2.0489099	-0.5524736
	H	0.0378184	-0.4911825	-1.3623923
	H	-0.1322335	0.6759077	0.8061392
	H	0.1315582	-0.8173462	1.6723015
	H	-2.2507668	-0.2070356	1.6980228
	H	-2.0123014	-1.7385981	0.8627366
	H	-2.2545835	-0.6456541	-1.3181001
	H	-3.6463017	-0.2961602	-0.2796384
	H	2.7004268	1.9634370	0.7591871
	H	-2.8233255	1.6392980	-1.2338124
tG+TG-G-G+g+	C	-2.3640096	0.7836407	0.2783472
	C	-1.1242868	-0.0061033	0.6506221
	C	-0.3903634	-0.5611189	-0.5665270
	C	0.7951353	-1.4614785	-0.2108206
	C	1.9388176	-0.8019731	0.5658864
	C	2.6153406	0.3579964	-0.1564037
	O	-3.2904269	-0.1221891	-0.3420266
	O	1.8384797	1.5671415	-0.1615060
	H	-2.0963595	1.5904185	-0.4132566
	H	-2.8134355	1.2287089	1.1725627
	H	-0.4673888	0.6556157	1.2212259
	H	-1.4238723	-0.8232914	1.3150915

H	-0.0502469	0.2731878	-1.1846703	
H	-1.0991731	-1.1416265	-1.1609823	
H	1.2111717	-1.8764890	-1.1353833	
H	0.4274911	-2.3151526	0.3688120	
H	2.7035461	-1.5619166	0.7608190	
H	1.5981019	-0.4588565	1.5485262	
H	3.6001154	0.5527936	0.2813102	
H	2.7627977	0.1135906	-1.2094615	
H	-4.0596726	0.3804431	-0.6390971	
H	1.8362024	1.9204316	0.7375379	
g-G+G+TG+G+t	C	2.1542495	0.4698434	-0.4482821
C	1.9561820	-0.8840461	0.2373598	
C	0.4962454	-1.1634566	0.6003408	
C	-0.4533247	-1.1718410	-0.6006119	
C	-1.9209495	-0.9272108	-0.2407039	
C	-2.1497874	0.4006111	0.4659262	
O	1.5137611	1.5403109	0.2493434	
O	-1.4368903	1.4260917	-0.2597490	
H	1.8061406	0.4333931	-1.4855006	
H	3.2157623	0.7185528	-0.4729300	
H	2.3466788	-1.6677471	-0.4218471	
H	2.5544265	-0.9038944	1.1521097	
H	0.1916977	-0.4014076	1.3196375	
H	0.4269143	-2.1206593	1.1259010	
H	-0.3704758	-2.1285449	-1.1247131	
H	-0.1623667	-0.4063590	-1.3207990	
H	-2.2972790	-1.7230053	0.4104327	
H	-2.5201088	-0.9474291	-1.1545518	
H	-3.2176053	0.6337298	0.4884834	
H	-1.7867864	0.3681477	1.4964332	
H	0.5627057	1.5043325	0.0496819	
H	-1.7663800	2.2884283	0.0281751	
tG-G+G+TG+C+	C	-2.0446635	0.8710654	-0.1313873
C	-1.9282024	-0.4924645	0.5306240	
C	-1.1340681	-1.5383206	-0.2617387	
C	0.2825651	-1.1208191	-0.6602729	
C	1.2127079	-0.8785730	0.5293003	
C	2.4429538	-0.0589705	0.1645744	
O	-0.8474216	1.6353415	0.1378774	
O	2.0910287	1.2362360	-0.3374395	
H	-2.9048266	1.4094256	0.2762619	
H	-2.1842861	0.7639911	-1.2128839	
H	-1.5085704	-0.3426212	1.5280034	
H	-2.9420447	-0.8767028	0.6782947	
H	-1.6976296	-1.7805123	-1.1691087	
H	-1.0918977	-2.4602223	0.3281701	
H	0.2338216	-0.2177949	-1.2708198	
H	0.7149658	-1.8995141	-1.2966616	
H	1.5308779	-1.8347927	0.9575191	
H	0.6829313	-0.3425632	1.3215800	
H	3.0896862	0.0513165	1.0412704	

H	3.0209320	-0.5539631	-0.6200300	
H	-0.9762012	2.5256500	-0.2180156	
H	1.1889227	1.4299092	-0.0364658	
tG+G+TG+G-g+	C	2.6039729	-0.1635591	-0.3803120
C	1.8154588	-0.6030327	0.8395390	
C	0.3184646	-0.3039894	0.7385207	
C	-0.3591184	-0.9804301	-0.4545438	
C	-1.8902162	-0.9635116	-0.4298577	
C	-2.5310974	0.4209041	-0.4599841	
O	2.3433710	1.2337650	-0.5801104	
O	-2.5690234	1.0731557	0.8160615	
H	2.3028438	-0.7358930	-1.2634068	
H	3.6721826	-0.3345731	-0.2128764	
H	1.9700024	-1.6782228	0.9780546	
H	2.2292873	-0.1005047	1.7175308	
H	0.2056882	0.7811442	0.6712937	
H	-0.1656297	-0.6315657	1.6638480	
H	-0.0290342	-2.0247614	-0.4968156	
H	-0.0191542	-0.5081072	-1.3815465	
H	-2.2616903	-1.4889291	0.4551568	
H	-2.2519918	-1.5165175	-1.3033612	
H	-2.0287190	1.0540094	-1.2019217	
H	-3.5782058	0.3368287	-0.7495660	
H	2.8863619	1.5477299	-1.3147506	
H	-1.6655393	1.2858515	1.0794066	
tG+G-TG-G-g+ C	-2.2685303	0.5620074	0.2825606	
C	-1.9489401	-0.9014505	0.0383154	
C	-0.5198977	-1.2797011	0.4485432	
C	0.4997714	-1.1059031	-0.6857456	
C	1.9391569	-0.8959463	-0.2115018	
C	2.1253008	0.3869984	0.5971389	
O	-1.3137676	1.3815891	-0.4245074	
O	1.6373186	1.5444894	-0.0819865	
H	-2.2105957	0.7786462	1.3546980	
H	-3.2794338	0.7933514	-0.0650539	
H	-2.6793258	-1.4797410	0.6123727	
H	-2.1133716	-1.1381504	-1.0167228	
H	-0.4940244	-2.3180392	0.7910703	
H	-0.2398096	-0.6724592	1.3145735	
H	0.2127420	-0.2617509	-1.3135657	
H	0.4579526	-1.9879186	-1.3318321	
H	2.5955635	-0.8528250	-1.0845453	
H	2.2675890	-1.7442765	0.4003003	
H	1.6517249	0.2955099	1.5813067	
H	3.1868350	0.5694038	0.7659898	
H	-1.5983185	2.3037532	-0.3603844	
H	0.6744421	1.4531790	-0.1800360	
tG-G+G+G-G-g+ C	2.2215430	-0.4014927	0.0140263	
C	1.4005263	0.5570544	0.8578112	
C	0.6004787	1.6048709	0.0714054	
C	-0.5164551	1.1243005	-0.8688393	

C	-1.8586650	0.7844646	-0.2103913	
C	-1.8795155	-0.4297138	0.7128113	
O	1.3321569	-1.3556114	-0.6000253	
O	-1.4762590	-1.6341883	0.0654767	
H	2.9424632	-0.9286426	0.6453472	
H	2.7704563	0.1449922	-0.7605721	
H	0.7642832	-0.0335220	1.5187136	
H	2.1032792	1.0921683	1.5049724	
H	1.3231414	2.1759418	-0.5222076	
H	0.1720518	2.3156551	0.7869034	
H	-0.1705148	0.2788177	-1.4650528	
H	-0.7100951	1.9353002	-1.5774631	
H	-2.5902659	0.6063285	-1.0035986	
H	-2.2093674	1.6531489	0.3601671	
H	-1.2775423	-0.2473686	1.6099883	
H	-2.9021830	-0.6079771	1.0481136	
H	1.8496084	-2.0494731	-1.0299043	
H	-0.5322404	-1.5682785	-0.1567581	
tTG-G+TTg+	C	1.9152461	-0.7564711	0.1010770
	C	2.0301035	0.7449518	-0.0771121
	C	0.8175740	1.5492930	0.4001014
	C	-0.5008262	1.2313775	-0.3237748
	C	-1.3418274	0.1460549	0.3507840
	C	-2.6121207	-0.1698182	-0.4242280
	O	3.1882959	-1.3161995	-0.2519094
	O	-3.3856172	-1.2130261	0.1813302
	H	1.1325859	-1.1676548	-0.5434331
	H	1.6663817	-0.9967458	1.1415547
	H	2.9182786	1.0704498	0.4704258
	H	2.2155055	0.9530821	-1.1344619
	H	1.0557205	2.6068493	0.2607885
	H	0.6815094	1.4082946	1.4781311
	H	-0.2850105	0.9405932	-1.3583233
	H	-1.1073208	2.1402900	-0.3842953
	H	-1.6119294	0.4832679	1.3582070
	H	-0.7764025	-0.7794729	0.4690656
	H	-3.2166300	0.7365342	-0.5464528
	H	-2.3671994	-0.5430900	-1.4187385
	H	3.1188589	-2.2793410	-0.2254453
	H	-3.6421739	-0.9197469	1.0657594
g-G+G+TG+G+g-	C	2.4610401	0.3036873	-0.5530282
	C	1.9620968	-0.9416986	0.1690991
	C	0.4895673	-0.8900562	0.5877444
	C	-0.4901923	-0.8905663	-0.5874087
	C	-1.9627508	-0.9413647	-0.1687737
	C	-2.4611893	0.3045684	0.5527595
	O	2.4657903	1.4681899	0.2827827
	O	-2.4646424	1.4688694	-0.2833309
	H	1.8811615	0.4897748	-1.4633084
	H	3.5012070	0.1713996	-0.8477498
	H	2.1167385	-1.8052382	-0.4868555

H	2.5884438	-1.0899905	1.0523329	
H	0.3205524	-0.0209046	1.2323020	
H	0.2752075	-1.7604813	1.2154398	
H	-0.2760642	-1.7617483	-1.2141319	
H	-0.3209420	-0.0221769	-1.2329226	
H	-2.1178040	-1.8045087	0.4876073	
H	-2.5890983	-1.0898325	-1.0519772	
H	-3.5016154	0.1730852	0.8469298	
H	-1.8816888	0.4904475	1.4633216	
H	1.5636697	1.6406800	0.5806443	
H	-1.5622011	1.6407557	-0.5805696	
g+G-TG+G+G-g-	C	2.3482274	0.7627834	0.3493029
C	1.1520899	-0.1184799	0.6827050	
C	0.3902270	-0.5950439	-0.5514002	
C	-0.8268949	-1.4674653	-0.2283566	
C	-1.9557063	-0.7892065	0.5536433	
C	-2.5938995	0.4019227	-0.1520903	
O	3.3632438	0.0749655	-0.3948638	
O	-1.7666524	1.5771212	-0.1613632	
H	2.8461142	1.0900115	1.2617791	
H	2.0148327	1.6550146	-0.1933403	
H	1.5021302	-0.9810109	1.2587124	
H	0.4876720	0.4605217	1.3306016	
H	1.0621404	-1.1928685	-1.1758612	
H	0.0776444	0.2727580	-1.1373136	
H	-0.4903215	-2.3447693	0.3342130	
H	-1.2468068	-1.8469090	-1.1661688	
H	-1.6121082	-0.4748204	1.5444385	
H	-2.7427701	-1.5308378	0.7288250	
H	-2.7660381	0.1701456	-1.2043701	
H	-3.5636313	0.6336507	0.3005637	
H	3.0196292	-0.1067403	-1.2786598	
H	-1.7465289	1.9342490	0.7359934	
tTG-G-G-G-t	C	2.3489557	0.0277062	0.3151986
C	1.3035606	0.2709748	-0.7550353	
C	0.1701380	1.1932910	-0.2984494	
C	-0.6239444	0.7016902	0.9165260	
C	-1.2414852	-0.6896916	0.7584683	
C	-2.1745080	-0.8121080	-0.4317149	
O	3.4002251	-0.7460529	-0.2831332	
O	-3.1924653	0.1898961	-0.2896805	
H	1.9204591	-0.5135020	1.1644814	
H	2.7376060	0.9857581	0.6804871	
H	1.8090878	0.7136901	-1.6169262	
H	0.9146921	-0.6954877	-1.0847471	
H	-0.5149548	1.3526751	-1.1351969	
H	0.5875968	2.1780007	-0.0633674	
H	-1.4245814	1.4155363	1.1193016	
H	0.0173532	0.6981195	1.8028926	
H	-1.8067651	-0.9336479	1.6618310	
H	-0.4621320	-1.4512267	0.6576961	

H	-1.6283215	-0.6679049	-1.3696620	
H	-2.6208183	-1.8118534	-0.4501846	
H	4.0609127	-0.9417500	0.3938434	
H	-3.8143570	0.1026658	-1.0235487	
g+G+TG-G-G+g+ C	-2.3835749	0.7936491	0.2490461	
C	-1.1243380	0.0246204	0.6251523	
C	-0.3850630	-0.5344309	-0.5865769	
C	0.7827826	-1.4557780	-0.2254577	
C	1.9244946	-0.8195853	0.5732542	
C	2.6285244	0.3340858	-0.1330566	
O	-3.3602385	-0.0240257	-0.4113263	
O	1.8672433	1.5529730	-0.1438654	
H	-2.1449267	1.5794238	-0.4680908	
H	-2.8221304	1.2657689	1.1351961	
H	-0.4739945	0.7007913	1.1872741	
H	-1.3959819	-0.7915331	1.3076458	
H	-0.0268275	0.3000549	-1.1934504	
H	-1.0945160	-1.0976546	-1.1977418	
H	1.2050257	-1.8673387	-1.1486447	
H	0.3959294	-2.3103875	0.3406894	
H	2.6742741	-1.5926094	0.7747439	
H	1.5737144	-0.4763089	1.5522104	
H	3.6091473	0.5131137	0.3201557	
H	2.7887084	0.0914525	-1.1847900	
H	-3.6482660	-0.7040455	0.2121293	
H	1.8881854	1.9239962	0.7477591	
tG-G-G+TTg+ C	1.9743695	0.7790707	0.6962385	
C	2.2237727	-0.6677880	0.3167150	
C	1.1491125	-1.3008752	-0.5722745	
C	-0.2599968	-1.3217356	0.0415551	
C	-1.1245453	-0.1184582	-0.3409734	
C	-2.4781053	-0.1350998	0.3507892	
O	1.8537234	1.5352441	-0.5170847	
O	-3.2794479	1.0108105	0.0314856	
H	2.8115372	1.1499783	1.2964163	
H	1.0633637	0.8719851	1.2974205	
H	3.1895735	-0.7238486	-0.1925504	
H	2.3140810	-1.2461805	1.2424079	
H	1.4659571	-2.3260317	-0.7827444	
H	1.1221976	-0.7790340	-1.5318887	
H	-0.1828779	-1.3871305	1.1336302	
H	-0.7799713	-2.2304832	-0.2775266	
H	-1.2753646	-0.1271890	-1.4266684	
H	-0.6193061	0.8188927	-0.1088211	
H	-3.0178049	-1.0587609	0.1098116	
H	-2.3536692	-0.0960421	1.4334003	
H	1.7939034	2.4728231	-0.2921203	
H	-3.3953321	1.0327117	-0.9277197	
tG+G-G-G+G-g+ C	-2.1749985	-0.4991332	0.0770101	
C	-1.3691456	0.5175160	0.8645646	
C	-0.7203617	1.6220618	0.0242376	

C	0.5373040	1.2350482	-0.7651123	
C	1.7456314	0.8413186	0.1111446	
C	2.1696803	-0.6190465	-0.0075242	
O	-1.2880931	-1.2524785	-0.7796910	
O	1.2258085	-1.5357382	0.5450589	
H	-2.9266458	0.0069853	-0.5377389	
H	-2.6858604	-1.1799769	0.7638743	
H	-2.0679658	0.9806230	1.5688486	
H	-0.6207825	-0.0084833	1.4613331	
H	-0.4571310	2.4491798	0.6916619	
H	-1.4705447	2.0170950	-0.6702840	
H	0.8085854	2.0965537	-1.3816229	
H	0.2971897	0.4287207	-1.4610796	
H	1.5399292	1.0509091	1.1654018	
H	2.6112659	1.4534419	-0.1619026	
H	2.3704769	-0.8590261	-1.0594385	
H	3.0917975	-0.7836528	0.5515583	
H	-1.7836187	-1.9783889	-1.1823310	
H	0.4164679	-1.5197956	0.0053313	
tG+G+G+G+G+g+ C	2.3237398	0.6665296	0.2637379	
C	1.2877618	0.5821209	-0.8416486	
C	0.3850588	-0.6507728	-0.7507066	
C	-0.3755821	-0.8005207	0.5690416	
C	-1.2727074	0.3845346	0.9351637	
C	-2.3219083	0.7189059	-0.1169592	
O	3.0979962	-0.5410661	0.2270127	
O	-3.1539441	-0.4007203	-0.4471632	
H	1.8409771	0.7775423	1.2405510	
H	2.9665195	1.5385541	0.1031431	
H	0.6952089	1.5022345	-0.8197188	
H	1.8122928	0.5700731	-1.8007337	
H	1.0007032	-1.5405059	-0.8952655	
H	-0.3261501	-0.6294021	-1.5808248	
H	0.3342698	-0.9723604	1.3830449	
H	-0.9917342	-1.7003826	0.5059911	
H	-0.6747945	1.2845401	1.1133773	
H	-1.7808620	0.1694087	1.8824436	
H	-2.9334042	1.5637990	0.2187968	
H	-1.8557530	1.0044497	-1.0590903	
H	3.7891091	-0.4842736	0.8993406	
H	-3.6313632	-0.6647468	0.3507602	
g+G+G-TG-G-g+ C	-2.2306476	0.6017313	0.3140140	
C	-1.9659901	-0.8728751	0.0388342	
C	-0.5469041	-1.3050958	0.4275684	
C	0.4848134	-1.1188353	-0.6940776	
C	1.9176673	-0.9166103	-0.1994248	
C	2.1045532	0.3729070	0.6001709	
O	-1.2969951	1.4892943	-0.3321737	
O	1.6599786	1.5316352	-0.1054348	
H	-2.1080144	0.8072059	1.3777460	
H	-3.2524431	0.8744887	0.0336723	

H	-2.7100435	-1.4372236	0.6106391	
H	-2.1523005	-1.0973880	-1.0173523	
H	-0.5486344	-2.3554911	0.7317162	
H	-0.2513992	-0.7377310	1.3151394	
H	0.2187052	-0.2597773	-1.3107126	
H	0.4471202	-1.9894884	-1.3556919	
H	2.5891591	-0.8859741	-1.0614950	
H	2.2289169	-1.7629620	0.4241262	
H	1.6044061	0.3033713	1.5723385	
H	3.1656783	0.5315673	0.7953177	
H	-1.4867893	1.4970480	-1.2804578	
H	0.6881300	1.5521109	-0.0874171	
tG+G-TG+G-t	C	2.8170754	-0.3882221	-0.2565750
C	1.6113372	-1.0922389	0.3379032	
C	0.2523077	-0.6822666	-0.2376700	
C	-0.2523075	0.6822663	0.2376723	
C	-1.6113364	1.0922391	-0.3379018	
C	-2.8170752	0.3882218	0.2565746	
O	2.8116047	0.9895170	0.1545928	
O	-2.8116030	-0.9895174	-0.1545930	
H	2.7832726	-0.4568126	-1.3503846	
H	3.7352554	-0.8752703	0.0892029	
H	1.7575292	-2.1633649	0.1633720	
H	1.6241196	-0.9446351	1.4223545	
H	-0.4869424	-1.4411057	0.0196472	
H	0.3164082	-0.6786004	-1.3325720	
H	0.4869431	1.4411052	-0.0196439	
H	-0.3164090	0.6785996	1.3325744	
H	-1.6241178	0.9446363	-1.4223532	
H	-1.7575286	2.1633650	-0.1633696	
H	-2.7832742	0.4568124	1.3503843	
H	-3.7352548	0.8752694	-0.0892049	
H	3.5999988	1.4166583	-0.2053895	
H	-3.6000029	-1.4166565	0.2053792	
g+TG-G-G-G-g-	C	2.3505748	0.0077675	0.3393627
C	1.3107638	0.2742417	-0.7388544	
C	0.1811869	1.2012594	-0.2805149	
C	-0.6241710	0.6944978	0.9209498	
C	-1.2406337	-0.6939178	0.7361434	
C	-2.1604746	-0.8053772	-0.4727252	
O	3.4072845	-0.8468731	-0.1175493	
O	-3.2034538	0.1783680	-0.4677304	
H	1.9157232	-0.5234674	1.1846517	
H	2.7563558	0.9562251	0.7121499	
H	1.8126690	0.7316075	-1.5988610	
H	0.9180271	-0.6850529	-1.0848976	
H	-0.4967661	1.3805502	-1.1187127	
H	0.6059827	2.1774545	-0.0243464	
H	-1.4237230	1.4113535	1.1205480	
H	0.0059927	0.6815423	1.8148192	
H	-1.8084625	-0.9531250	1.6368329	

H	-0.4602820	-1.4560641	0.6420568	
H	-1.6154482	-0.6265703	-1.3987030	
H	-2.5842824	-1.8137923	-0.5294160	
H	3.8235518	-0.4237279	-0.8803161	
H	-3.7717188	0.0101605	0.2958596	
g+G+G-TG-G-g-	C	2.4692451	0.4591687	-0.4850392
C	1.8884884	-0.9486812	-0.4080217	
C	0.3598852	-1.0181287	-0.4219615	
C	-0.3194236	-0.3968656	0.7971822	
C	-1.8298876	-0.6371244	0.8349354	
C	-2.5722055	-0.1388645	-0.3991117	
O	2.3149661	1.2189119	0.7230844	
O	-2.2727105	1.2257628	-0.7193832	
H	1.9495074	1.0395163	-1.2483849	
H	3.5281416	0.4112829	-0.7616751	
H	2.2733315	-1.5085854	-1.2674389	
H	2.2811998	-1.4494207	0.4852676	
H	0.0606621	-2.0701141	-0.5005059	
H	0.0044102	-0.5218213	-1.3300775	
H	-0.1119380	0.6722928	0.8222665	
H	0.1217180	-0.8174120	1.7074054	
H	-2.2496933	-0.1503488	1.7226528	
H	-2.0394766	-1.7076730	0.9424135	
H	-2.2788651	-0.7008199	-1.2846521	
H	-3.6513447	-0.2730369	-0.2659573	
H	2.8420286	0.7925821	1.4115919	
H	-2.5134522	1.7742091	0.0393525	
tG+TG-G+Tg+	C	2.4884870	-0.9761174	-0.1264164
C	1.2678675	-0.3561656	0.5259552	
C	0.6900739	0.8103016	-0.2764144	
C	-0.5713755	1.4326349	0.3438927	
C	-1.8994527	0.8619878	-0.1659630	
C	-2.1049235	-0.6241410	0.0885140	
O	3.4983170	0.0395880	-0.2156121	
O	-3.4336896	-1.0503359	-0.2463981	
H	2.2316296	-1.3472390	-1.1258207	
H	2.8479206	-1.8197291	0.4718949	
H	0.5233771	-1.1442619	0.6639953	
H	1.5507482	-0.0047523	1.5224563	
H	0.4704183	0.4774029	-1.2982445	
H	1.4696899	1.5683328	-0.3641797	
H	-0.5801054	2.5065799	0.1409267	
H	-0.5282618	1.3315041	1.4339962	
H	-1.9741236	1.0486726	-1.2441073	
H	-2.7298333	1.3936240	0.3066772	
H	-1.3721039	-1.2221123	-0.4623846	
H	-1.9969068	-0.8500662	1.1500049	
H	4.2844789	-0.3417011	-0.6270687	
H	-3.5849007	-0.8438018	-1.1785221	
tTG+G+G+G+g+	C	-2.3493771	0.0277797	0.3262611
C	-1.3114010	0.2660538	-0.7523716	

C	-0.1792906	1.1970205	-0.3110339	
C	0.6238098	0.7180831	0.9034199	
C	1.2358034	-0.6764719	0.7531332	
C	2.1634128	-0.8182965	-0.4466224	
O	-3.3977610	-0.7604835	-0.2571965	
O	3.2159549	0.1553285	-0.4506121	
H	-2.7427547	0.9873737	0.6824273	
H	-1.9127073	-0.5003590	1.1798322	
H	-0.9208719	-0.7013933	-1.0772803	
H	-1.8233014	0.6999057	-1.6148252	
H	-0.5993243	2.1815376	-0.0802347	
H	0.5003244	1.3526778	-1.1525622	
H	-0.0074630	0.7284133	1.7968715	
H	1.4256960	1.4366537	1.0874949	
H	0.4523631	-1.4366443	0.6690373	
H	1.7966677	-0.9194335	1.6628869	
H	2.5781659	-1.8315174	-0.4818245	
H	1.6268874	-0.6509100	-1.3795556	
H	-4.0585360	-0.9451037	0.4228387	
H	3.7740141	-0.0025494	0.3226483	
tG-G+TG+G-t	C	-2.5350044	-0.5204225	0.3725799
	C	-1.8402650	0.7848807	0.7130076
	C	-0.3099474	0.7315983	0.6996565
	C	0.3099472	0.7315984	-0.6996564
	C	1.8402648	0.7848805	-0.7130076
	C	2.5350040	-0.5204229	-0.3725801
	O	-2.3183425	-0.8220916	-1.0167270
	O	2.3183420	-0.8220922	1.0167267
	H	-3.6085257	-0.4288659	0.5699618
	H	-2.1363848	-1.3256195	1.0007124
	H	-2.2035650	1.5598890	0.0304917
	H	-2.1751712	1.0646922	1.7173596
	H	0.0326129	-0.1429890	1.2559152
	H	0.0709483	1.6042451	1.2415532
	H	-0.0709483	1.6042454	-1.2415528
	H	-0.0326132	-0.1429886	-1.2559153
	H	2.2035651	1.5598886	-0.0304917
	H	2.1751710	1.0646920	-1.7173597
	H	2.1363843	-1.3256198	-1.0007128
	H	3.6085254	-0.4288665	-0.5699619
	H	-2.7972523	-1.6340510	-1.2285298
	H	2.7972547	-1.6340497	1.2285305
tG-G-G-G-G-t	C	2.3292264	0.6901697	-0.1836095
	C	1.2824779	0.4893648	0.8962795
	C	0.3795289	-0.7250864	0.6645617
	C	-0.3795285	-0.7250865	-0.6645614
	C	-1.2824776	0.4893646	-0.8962791
	C	-2.3292261	0.6901694	0.1836099
	O	3.1137188	-0.5094045	-0.2559535
	O	-3.1137189	-0.5094048	0.2559533
	H	2.9630858	1.5468653	0.0689317

H	1.8552537	0.8926177	-1.1498753
H	1.7987007	0.3748765	1.8533105
H	0.6901267	1.4071920	0.9663186
H	-0.3331837	-0.7958307	1.4911458
H	0.9941989	-1.6261153	0.7108801
H	-0.9941981	-1.6261155	-0.7108800
H	0.3331842	-0.7958304	-1.4911455
H	-1.7987005	0.3748763	-1.8533101
H	-0.6901266	1.4071919	-0.9663182
H	-1.8552535	0.8926168	1.1498759
H	-2.9630853	1.5468652	-0.0689310
H	3.7961617	-0.3906908	-0.9290216
H	-3.7961647	-0.3906892	0.9290181
tG-TG+G-Tg+ C	2.5196780	-0.8796662	0.3819294
C	1.1125232	-0.4834298	-0.0219371
C	0.8081128	0.9847492	0.2648202
C	-0.5587095	1.4615515	-0.2343333
C	-1.7576335	0.7114863	0.3705752
C	-2.2702336	-0.4209416	-0.5104813
O	3.4341852	-0.1151525	-0.4181450
O	-3.3224579	-1.1698129	0.1112485
H	2.6721918	-1.9507777	0.2148263
H	2.6769477	-0.6705543	1.4465715
H	0.9924387	-0.6901084	-1.0898817
H	0.4162581	-1.1318053	0.5180134
H	1.5883335	1.5963528	-0.1928358
H	0.8669720	1.1534243	1.3464862
H	-0.5905367	1.3828744	-1.3274288
H	-0.6472326	2.5270747	-0.0078458
H	-2.5868064	1.4080058	0.5340236
H	-1.4973909	0.3022619	1.3512536
H	-2.6047629	-0.0165760	-1.4730916
H	-1.4893375	-1.1512309	-0.7117004
H	4.3361494	-0.3530043	-0.1677871
H	-4.0460170	-0.5598550	0.3078090
g+G+G+G+G+G+g+ C	-2.3164902	0.7087835	-0.2076270
C	-1.2807021	0.4883085	0.8869608
C	-0.3837435	-0.7311989	0.6621683
C	0.3837435	-0.7311991	-0.6621674
C	1.2807018	0.4883085	-0.8869604
C	2.3164908	0.7087835	0.2076266
O	-3.1380450	-0.4431534	-0.4361862
O	3.1380459	-0.4431534	0.4361850
H	-1.8381818	0.9016957	-1.1670954
H	-2.9365429	1.5794539	0.0329351
H	-0.6824432	1.4013811	0.9742943
H	-1.7991096	0.3773820	1.8462464
H	-1.0013924	-1.6314590	0.6951524
H	0.3211941	-0.8123981	1.4938653
H	-0.3211941	-0.8123988	-1.4938643
H	1.0013926	-1.6314590	-0.6951511

H	0.6824426	1.4013810	-0.9742934	
H	1.7991086	0.3773822	-1.8462464	
H	2.9365431	1.5794540	-0.0329360	
H	1.8381831	0.9016955	1.1670954	
H	-3.6287406	-0.6279494	0.3758258	
H	3.6287394	-0.6279503	-0.3758281	
tTTG+G-G-t	C	2.6911335	0.1274047	-0.0110398
	C	1.1822606	-0.0048964	-0.0547948
	C	0.4887953	1.3536974	-0.1440850
	C	-1.0236690	1.2929684	-0.3779569
	C	-1.8171398	0.5816027	0.7274712
	C	-2.0622268	-0.8961662	0.4740016
	O	3.2390645	-1.1901694	0.1420828
	O	-2.8912758	-0.9923449	-0.6960252
	H	2.9873115	0.7657392	0.8292617
	H	3.0539442	0.5887739	-0.9362330
	H	0.9133838	-0.6233321	-0.9157577
	H	0.8697589	-0.5410643	0.8438098
	H	0.9406659	1.9283131	-0.9601634
	H	0.6844375	1.9169602	0.7756917
	H	-1.2353252	0.8076067	-1.3343482
	H	-1.3872671	2.3199254	-0.4696824
	H	-2.7999399	1.0471415	0.8361986
	H	-1.3073918	0.6939534	1.6907239
	H	-1.1236361	-1.4328991	0.3167089
	H	-2.5725864	-1.3398754	1.3355338
	H	4.2027551	-1.1241423	0.1493941
	H	-3.0081807	-1.9259625	-0.9139559
tTTG+G-Tt	C	-2.6949627	-0.0403169	-0.2038805
	C	-1.2177957	0.0247418	0.1276875
	C	-0.6277970	1.4074019	-0.1418330
	C	0.8246868	1.5809770	0.3118833
	C	1.8252575	0.6327270	-0.3683515
	C	2.1208673	-0.6151600	0.4432215
	O	-3.1420882	-1.3756921	0.0704306
	O	3.0500060	-1.4053510	-0.3128069
	H	-2.8535029	0.2091274	-1.2591749
	H	-3.2488829	0.6821839	0.4060479
	H	-1.0908219	-0.2411110	1.1812032
	H	-0.7060871	-0.7356503	-0.4658932
	H	-1.2420074	2.1617008	0.3619599
	H	-0.6889783	1.6228386	-1.2142815
	H	0.8786262	1.4576732	1.3999123
	H	1.1180282	2.6146460	0.1120842
	H	2.7775416	1.1408912	-0.5351217
	H	1.4558698	0.3308470	-1.3526225
	H	2.5581548	-0.3298274	1.4071372
	H	1.2074389	-1.1831264	0.6379351
	H	-4.0796332	-1.4391848	-0.1533239
	H	3.2282521	-2.2202058	0.1744881
g-G-G+TG-G+tC		-2.8059100	0.3100745	0.2412038

C	-1.6113039	1.1167576	-0.2542195	
C	-0.2511657	0.7125297	0.3195798	
C	0.2395588	-0.6720761	-0.1096538	
C	1.6199680	-1.0486901	0.4392692	
C	2.8014891	-0.4259581	-0.2806133	
O	-2.8574053	-1.0331875	-0.2638331	
O	2.8026778	0.9925967	-0.0488491	
H	-3.7370653	0.8336058	-0.0027062	
H	-2.7613434	0.1983765	1.3254184	
H	-1.5825718	1.0755151	-1.3501909	
H	-1.8008551	2.1643474	0.0046094	
H	-0.3107881	0.7424197	1.4141264	
H	0.4919949	1.4567781	0.0322131	
H	0.2676772	-0.7215476	-1.2056145	
H	-0.4864030	-1.4211241	0.2092301	
H	1.7468607	-2.1337113	0.3657790	
H	1.6852867	-0.7945026	1.5017031	
H	3.7329953	-0.8655464	0.0919220	
H	2.7301118	-0.6330561	-1.3549032	
H	-2.9624905	-0.9848396	-1.2232026	
H	3.5754970	1.3715706	-0.4877171	
tG+TG+G-G-t	C	2.4797865	-0.2259752	-0.3743677
	C	1.1203947	0.2211853	-0.8716842
	C	0.4681499	1.2674599	0.0357746
	C	-1.0294202	1.4685704	-0.2421431
	C	-1.9426543	0.6293151	0.6572626
	C	-1.7027619	-0.8669551	0.5991646
	O	2.2700916	-0.9408014	0.8566872
	O	-1.9232912	-1.2956310	-0.7553524
	H	3.1289996	0.6410866	-0.2035707
	H	2.9609779	-0.8779689	-1.1106538
	H	1.2345034	0.6365105	-1.8782580
	H	0.4795239	-0.6560270	-0.9699134
	H	0.9997645	2.2151501	-0.0980753
	H	0.6130421	0.9787813	1.0806722
	H	-1.2449414	1.2434316	-1.2900037
	H	-1.2949404	2.5183760	-0.0890987
	H	-2.9877838	0.8196642	0.3977876
	H	-1.8054642	0.9451124	1.6970658
	H	-0.6838971	-1.1111080	0.9158481
	H	-2.4006505	-1.3736777	1.2740200
	H	3.1299136	-1.1898222	1.2195148
	H	-1.8572766	-2.2589188	-0.7848316
tG+G+G-TTg+	C	2.0766166	-0.9007211	0.4557901
	C	1.8043333	0.5657423	0.7444879
	C	1.0163929	1.2909437	-0.3561297
	C	-0.4975637	1.3443245	-0.1307128
	C	-1.1931869	-0.0150988	-0.0661386
	C	-2.7079611	0.1200400	-0.0188349
	O	2.9233503	-0.9525873	-0.7029617
	O	-3.3790607	-1.1463906	0.0117516

H	1.1477165	-1.4461660	0.2693452	
H	2.5800611	-1.3604923	1.3130897	
H	1.2778792	0.6447518	1.7021496	
H	2.7774086	1.0435317	0.8820486	
H	1.2353088	0.8200791	-1.3180339	
H	1.3771268	2.3200401	-0.4320271	
H	-0.9473677	1.9269779	-0.9418705	
H	-0.7011053	1.8954627	0.7947165	
H	-0.8652018	-0.5639053	0.8229056	
H	-0.9267799	-0.6200864	-0.9374685	
H	-3.0063119	0.7337220	0.8393849	
H	-3.0729988	0.6093409	-0.9218070	
H	3.0685436	-1.8777789	-0.9390062	
H	-3.1105157	-1.6067161	0.8177852	
tG-TG-G+Tg+	C	2.6901465	-0.2982643	0.3677405
	C	1.3975646	0.3737898	0.7862025
	C	0.7108219	1.1089699	-0.3656099
	C	-0.6857957	1.6473442	-0.0161643
	C	-1.8397476	0.7096039	-0.3869677
	C	-1.8116426	-0.6479812	0.3006544
	O	2.3517983	-1.3158559	-0.5876906
	O	-2.9992122	-1.4085146	0.0319137
	H	3.1854829	-0.7426048	1.2370804
	H	3.3703925	0.4354672	-0.0805222
	H	0.7428431	-0.3906861	1.2089498
	H	1.6187822	1.0838926	1.5896368
	H	0.6440386	0.4422833	-1.2293288
	H	1.3582723	1.9392009	-0.6657887
	H	-0.8518166	2.5939217	-0.5371625
	H	-0.7335436	1.8787937	1.0541197
	H	-1.8319371	0.5546251	-1.4722513
	H	-2.7929291	1.1847550	-0.1402994
	H	-0.9258716	-1.2196081	0.0097651
	H	-1.7975309	-0.5261973	1.3844981
	H	3.1627862	-1.7584064	-0.8693697
	H	-3.0329805	-1.5776624	-0.9190149
tTG-G+TG-t	C	-2.2904562	-0.3909774	-0.4993607
	C	-1.7529852	0.7177308	0.3862536
	C	-0.5592660	1.4619098	-0.2356031
	C	0.8118139	0.9868986	0.2533119
	C	1.1117438	-0.4827614	-0.0299329
	C	2.5150861	-0.8850588	0.3810171
	O	-3.3429073	-1.0483449	0.2213355
	O	3.4370573	-0.1322401	-0.4213415
	H	-1.5012085	-1.1036668	-0.7553921
	H	-2.6751245	0.0391330	-1.4311789
	H	-2.5775466	1.4070223	0.5801306
	H	-1.4732832	0.2871966	1.3521477
	H	-0.6450119	2.5286433	-0.0143405
	H	-0.5995612	1.3788207	-1.3281948
	H	0.8790375	1.1583322	1.3340628

H	1.5899123	1.5957305	-0.2116829	
H	0.9956232	-0.6907852	-1.0981501	
H	0.4094180	-1.1264778	0.5079377	
H	2.6698117	-0.6695739	1.4447881	
H	2.6621252	-1.9583911	0.2220372	
H	-3.7262037	-1.7295798	-0.3461443	
H	4.3366975	-0.3634776	-0.1567923	
g-G+TG+G+G-g-	C	2.4353306	-0.0511801	0.0461289
C	1.2680899	-0.9358336	0.4653496	
C	0.2490695	-1.1417540	-0.6613563	
C	-1.1487758	-1.5336747	-0.1774233	
C	-1.9001049	-0.4488640	0.6023532	
C	-2.0572940	0.8731114	-0.1421913	
O	2.0689065	1.3300663	-0.0341132	
O	-0.8580114	1.6715548	-0.1517513	
H	2.8389072	-0.3956659	-0.9144624	
H	3.2389908	-0.0949286	0.7815789	
H	1.6476510	-1.9100072	0.7902357	
H	0.8016469	-0.4724303	1.3383532	
H	0.6224752	-1.9230579	-1.3303594	
H	0.1690183	-0.2370159	-1.2676718	
H	-1.0777938	-2.4320057	0.4450864	
H	-1.7576412	-1.8085659	-1.0452908	
H	-1.4189902	-0.2519205	1.5653353	
H	-2.9016333	-0.8248237	0.8363418	
H	-2.2891363	0.6983199	-1.1938419	
H	-2.8770291	1.4571513	0.2865485	
H	1.1925016	1.3924585	-0.4467747	
H	-0.7191475	2.0192014	0.7402379	
g-G+G+G+G+G+t	C	2.3389320	0.6940095	0.2041297
C	1.2808288	0.5252626	-0.8786724	
C	0.3728825	-0.6937392	-0.6883507	
C	-0.3820201	-0.7463646	0.6436116	
C	-1.2854571	0.4582669	0.9194361	
C	-2.3264329	0.6993365	-0.1578652	
O	3.2405070	-0.4179015	0.2795601	
O	-3.0897941	-0.5074130	-0.2989560	
H	1.8746162	0.8741355	1.1796886	
H	2.9721305	1.5514925	-0.0216913	
H	0.6829809	1.4419679	-0.9137921	
H	1.7897776	0.4427468	-1.8426697	
H	0.9708276	-1.6050351	-0.7906135	
H	-0.3458840	-0.7324786	-1.5108983	
H	0.3249890	-0.8407806	1.4743755	
H	-0.9948635	-1.6495561	0.6586707	
H	-0.6929910	1.3714410	1.0300709	
H	-1.8055289	0.3027283	1.8682247	
H	-2.9747192	1.5318111	0.1345972	
H	-1.8490301	0.9601758	-1.1083092	
H	2.7434908	-1.1935299	0.5699703	
H	-3.7831090	-0.3589859	-0.9548550	

g+G+G+TG+G-g+	C	-2.1304532	0.3364666	0.6019000
	C	-1.9274644	-0.8924334	-0.2791330
	C	-0.4724347	-1.0988996	-0.7054233
	C	0.5122296	-1.2768268	0.4587261
	C	1.9503386	-0.8872714	0.0949972
	C	2.2344957	0.6023866	0.2759746
	O	-1.4548630	1.5039902	0.0956790
	O	1.4327169	1.4558641	-0.5415810
	H	-1.7067894	0.1880837	1.5932021
	H	-3.1962917	0.5477029	0.7282362
	H	-2.3002512	-1.7645488	0.2696138
	H	-2.5516915	-0.7993600	-1.1743402
	H	-0.1605962	-0.2526961	-1.3169211
	H	-0.4144227	-1.9784349	-1.3533452
	H	0.4757952	-2.3165111	0.7972614
	H	0.2075740	-0.6733821	1.3198588
	H	2.1652274	-1.1740783	-0.9387591
	H	2.6580660	-1.4287668	0.7317313
	H	2.1117917	0.8655932	1.3344036
	H	3.2675992	0.8177783	-0.0003574
	H	-1.8676235	1.7625395	-0.7403453
	H	0.5310432	1.4959722	-0.1795115
g+G+G-TG+G-G-	C	2.7887981	-0.3564606	-0.2841064
	C	1.6138994	-1.0822606	0.3611130
	C	0.2278484	-0.7098646	-0.1714529
	C	-0.2278482	0.7098649	0.1714522
	C	-1.6138996	1.0822606	-0.3611130
	C	-2.7887979	0.3564603	0.2841070
	O	2.8844141	1.0331798	0.0642598
	O	-2.8844143	-1.0331799	-0.0642601
	H	2.6856720	-0.3647904	-1.3701967
	H	3.7252009	-0.8672638	-0.0340609
	H	1.7721561	-2.1545010	0.2010687
	H	1.6503700	-0.9287930	1.4466769
	H	-0.5020568	-1.4231674	0.2136305
	H	0.2291270	-0.8302268	-1.2620659
	H	0.5020567	1.4231678	-0.2136317
	H	-0.2291262	0.8302274	1.2620653
	H	-1.6503707	0.9287929	-1.4466768
	H	-1.7721565	2.1545009	-0.2010686
	H	-2.6856709	0.3647894	1.3701972
	H	-3.7252009	0.8672637	0.0340626
	H	3.0668881	1.0901036	1.0115296
	H	-3.0668889	-1.0901031	-1.0115297
tG+G-G-G-Tg+ C		2.5488583	-0.1539149	-0.4684880
	C	1.3739331	0.7234225	-0.8597148
	C	0.6263998	1.3732765	0.3085833
	C	-0.1207730	0.4201570	1.2502184
	C	-1.1346996	-0.4962557	0.5609428
	C	-2.2167824	0.2550494	-0.1994049
	O	2.0481392	-1.3592362	0.1332302

O	-3.1743290	-0.6248414	-0.8059854	
H	3.1973832	0.3820187	0.2349989	
H	3.1370547	-0.3984280	-1.3590654	
H	1.7675749	1.5210127	-1.4981535	
H	0.6961771	0.1328000	-1.4814802	
H	-0.0771611	2.1038768	-0.1019453	
H	1.3450522	1.9518744	0.8994654	
H	-0.6383489	1.0250815	2.0032445	
H	0.5995595	-0.2034147	1.7801312	
H	-1.6186130	-1.1139840	1.3264889	
H	-0.6263407	-1.1830149	-0.1175905	
H	-2.7208907	0.9669256	0.4663550	
H	-1.7983299	0.8180178	-1.0326697	
H	2.7978107	-1.9371711	0.3268787	
H	-3.5283773	-1.1976789	-0.1127136	
tTTG-G+Tg+	C	2.6963497	-0.0379040	-0.1965736
	C	1.2191974	0.0323340	0.1346146
	C	0.6293858	1.4117936	-0.1503684
	C	-0.8271482	1.5833292	0.2906305
	C	-1.8173873	0.6181067	-0.3832105
	C	-2.1409829	-0.6053057	0.4659001
	O	3.1346617	-1.3781033	0.0656613
	O	-3.1065012	-1.4628267	-0.1563317
	H	3.2532138	0.6764577	0.4199941
	H	2.8574049	0.2200783	-1.2495491
	H	0.7082503	-0.7350581	-0.4511206
	H	1.0898438	-0.2237217	1.1899366
	H	0.6990039	1.6196452	-1.2239434
	H	1.2377866	2.1710860	0.3525654
	H	-1.1258294	2.6128860	0.0784166
	H	-0.8884755	1.4693334	1.3791174
	H	-1.4175604	0.2941519	-1.3513589
	H	-2.7627878	1.1234121	-0.5922746
	H	-1.2352149	-1.1659434	0.7139137
	H	-2.6060615	-0.2928945	1.4012630
	H	4.0787335	-1.4384560	-0.1298033
	H	-2.7182511	-1.8070938	-0.9716722
tG-G+G+G+G+g+	C	-2.5914225	0.1968229	-0.1908059
	C	-1.3510558	0.9769633	-0.5875937
	C	-0.3105047	1.1601113	0.5215824
	C	0.3407081	-0.1160537	1.0636155
	C	1.0381089	-0.9754505	0.0074151
	C	2.0869723	-0.2361286	-0.8107749
	O	-2.2507508	-1.1974359	-0.1003262
	O	3.0855808	0.3993746	0.0020709
	H	-3.3742952	0.3384279	-0.9431605
	H	-2.9702859	0.5602342	0.7719675
	H	-0.9147124	0.4935144	-1.4658296
	H	-1.6812789	1.9692719	-0.9116693
	H	-0.7890445	1.6843161	1.3561905
	H	0.4715170	1.8319370	0.1565114

H	-0.4118549	-0.7314501	1.5591631	
H	1.0698886	0.1800179	1.8223171	
H	0.2972063	-1.4025556	-0.6735623	
H	1.5183779	-1.8263119	0.5051084	
H	2.5577302	-0.9214110	-1.5244534	
H	1.6409878	0.5765781	-1.3832361	
H	-3.0500114	-1.6921835	0.1235425	
H	3.5270401	-0.2875696	0.5194605	
g+G-G-G-G-G-g-	C	-2.3360237	0.6747286	0.2667611
C	-1.2858762	0.5844590	-0.8330585	
C	-0.3803294	-0.6474595	-0.7412926	
C	0.3824866	-0.8011065	0.5786203	
C	1.2793214	0.3849935	0.9417329	
C	2.3163856	0.7228669	-0.1214929	
O	-3.2427039	-0.4354647	0.2642669	
O	3.1325256	-0.4012434	-0.4750143	
H	-2.9665395	1.5495842	0.1112330	
H	-1.8645502	0.7783851	1.2501594	
H	-1.8011234	0.5749617	-1.7970212	
H	-0.6856812	1.4998505	-0.8048841	
H	0.3331719	-0.6268463	-1.5687212	
H	-0.9812472	-1.5474610	-0.9063364	
H	0.9983854	-1.7007746	0.5135256	
H	-0.3172661	-0.9691310	1.4038221	
H	1.7966106	0.1643408	1.8822193	
H	0.6799771	1.2814557	1.1301904	
H	1.8395416	1.0235467	-1.0535481	
H	2.9388267	1.5590264	0.2147799	
H	-2.7458400	-1.2354519	0.4788068	
H	3.6538682	-0.6504672	0.2998227	
tG+TG+G+G-t	C	2.5754825	-0.1485420	0.3662256
C	1.1237933	-0.5031217	0.6211305	
C	0.3486175	-0.7739349	-0.6659361	
C	-1.0036408	-1.4548477	-0.4370213	
C	-2.0017180	-0.7092280	0.4545855	
C	-2.4230066	0.6581909	-0.0539665	
O	2.6060106	1.0435192	-0.4340970	
O	-1.3638075	1.5851558	0.2275263	
H	3.0744822	-0.9706546	-0.1613559	
H	3.0971398	0.0174445	1.3151449	
H	1.1066849	-1.3934525	1.2614440	
H	0.6547429	0.3139449	1.1715894	
H	0.9481634	-1.4271581	-1.3107722	
H	0.2167373	0.1655713	-1.2019234	
H	-0.8283376	-2.4426349	0.0038955	
H	-1.4782853	-1.6341748	-1.4083242	
H	-1.6065502	-0.5836429	1.4660789	
H	-2.9030615	-1.3238921	0.5449900	
H	-2.6208726	0.6141370	-1.1317886	
H	-3.3417791	0.9774056	0.4495351	
H	3.5287923	1.2684820	-0.6096142	

H	-1.5839655	2.4405448	-0.1637395	
g+TG-G+TG-g-C	2.2592061	-0.4336697	0.5126208	
C	1.7654324	0.7185774	-0.3534832	
C	0.5573939	1.4599543	0.2436336	
C	-0.8017718	0.9879825	-0.2804191	
C	-1.1172718	-0.4812474	-0.0129176	
C	-2.5400329	-0.8590938	-0.4037176	
O	3.3235267	-1.1692801	-0.1030528	
O	-3.5300427	-0.1356172	0.3401914	
H	1.4742189	-1.1680345	0.6804690	
H	2.5732867	-0.0509510	1.4910028	
H	2.5989935	1.4162935	-0.4861969	
H	1.5225677	0.3312025	-1.3473211	
H	0.6479377	2.5280334	0.0305813	
H	0.5753913	1.3690139	1.3363678	
H	-0.8439320	1.1643883	-1.3611947	
H	-1.5892098	1.6000100	0.1656290	
H	-0.9711085	-0.7072958	1.0506404	
H	-0.4320884	-1.1289277	-0.5689215	
H	-2.7288208	-0.5996215	-1.4460071	
H	-2.6924617	-1.9377333	-0.2922288	
H	4.0515007	-0.5561942	-0.2717512	
H	-3.4692333	-0.4115919	1.2644376	
C+G+TG+G-Tg+ C	-2.6929339	-0.2925005	0.3761554	
C	-1.3911189	0.3636293	0.7910647	
C	-0.7084529	1.1088549	-0.3567305	
C	0.6874269	1.6461480	-0.0024874	
C	1.8393391	0.7139309	-0.3922632	
C	1.8054788	-0.6565676	0.2683037	
O	-2.3705909	-1.2994604	-0.5946681	
O	2.9290046	-1.4636727	-0.1113251	
H	-3.3713706	0.4525984	-0.0558078	
H	-3.1835886	-0.7435441	1.2448234	
H	-1.5989131	1.0649552	1.6059024	
H	-0.7386706	-0.4118011	1.1973447	
H	-1.3568984	1.9413308	-0.6482453	
H	-0.6414838	0.4498813	-1.2261477	
H	0.7354840	1.8623363	1.0711569	
H	0.8505373	2.6003303	-0.5103207	
H	2.7882591	1.1976963	-0.1321772	
H	1.8439972	0.5700186	-1.4762638	
H	1.7629915	-0.5514332	1.3594902	
H	-3.1861291	-1.7354510	-0.8735703	
H	0.9356047	-1.2273500	-0.0519443	
H	3.7331328	-0.9786820	0.1170670	
g+TG+G+G+G+g+ C	-2.3591701	0.0287639	0.3425059	
C	-1.3200000	0.2406395	-0.7485297	
C	-0.1825274	1.1803333	-0.3373146	
C	0.6257256	0.7356392	0.8866799	
C	1.2454715	-0.6586919	0.7715928	
C	2.1653466	-0.8298779	-0.4304893	

O	-3.5013149	-0.7033123	-0.1246198
O	3.2063443	0.1539666	-0.4755293
H	-2.7571016	0.9881669	0.6752542
H	-1.9222653	-0.4728811	1.2120256
H	-0.9191048	-0.7320863	-1.0548217
H	-1.8331486	0.6535719	-1.6206589
H	-0.6052888	2.1688011	-0.1303882
H	0.4932946	1.3160723	-1.1854062
H	-0.0024797	0.7664359	1.7813670
H	1.4246661	1.4626490	1.0484775
H	0.4665084	-1.4264346	0.7162983
H	1.8133454	-0.8721773	1.6841847
H	2.5906869	-1.8394034	-0.4361634
H	1.6196556	-0.6985625	-1.3640736
H	-3.1936929	-1.5620420	-0.4440004
H	3.7736662	0.0280587	0.2968663
tG-G+G-TTg+	C	2.1222332	0.9559052
			0.2863984
	C	2.3415810	-0.5076639
			-0.0522309
	C	1.2176930	-1.4828932
			0.3129325
	C	-0.1290461	-1.2517268
			-0.3909964
	C	-1.0950267	-0.3728216
			0.4031474
	C	-2.3467483	-0.0365188
			-0.3900183
	O	1.1750743	1.5157518
			-0.6406405
	O	-3.3007480	0.7185422
			0.3715894
	H	3.0737616	1.4907700
			0.2080237
	H	1.7559583	1.0602677
			1.3148512
	H	2.5543693	-0.5729086
			-1.1232512
	H	3.2494932	-0.8253818
			0.4709993
	H	1.0657516	-1.4701289
			1.3982804
	H	1.5801665	-2.4861456
			0.0711551
	H	-0.6124824	-2.2183426
			-0.5642716
	H	0.0475012	-0.8050155
			-1.3736090
	H	-0.5974353	0.5587152
			0.6806065
	H	-1.3909789	-0.8841221
			1.3238579
	H	-2.0731697	0.5026549
			-1.3038610
	H	-2.8752564	-0.9452147
			-0.6801908
	H	1.2089877	2.4784166
			-0.5654945
	H	-2.8677621	1.5350476
			0.6538085
tTG+G-TTg+	C	-2.1380048	-0.5900609
			0.4600530
	C	-1.8130411	0.6274336
			-0.3859881
	C	-0.8245999	1.5895969
			0.2932035
	C	0.6332315	1.4103127
			-0.1418702
	C	1.2183285	0.0278274
			0.1406861
	C	2.7000784	-0.0498426
			-0.1964247
	O	-3.0014108	-1.4329219
			-0.3149461
	O	3.2725467	-1.3261089
			0.1132152
	H	-2.6380898	-0.2717814
			1.3818201
	H	-1.2273663	-1.1286264
			0.7370480
	H	-1.4162256	0.2881301
			-1.3470990
	H	-2.7556978	1.1348700
			-0.6007983
	H	-0.8906462	1.4813763
			1.3820435

H	-1.1169658	2.6197936	0.0758487
H	1.2456281	2.1624702	0.3666190
H	0.7085359	1.6211501	-1.2141824
H	0.6861861	-0.7298393	-0.4435803
H	1.0929597	-0.2283812	1.1966914
H	2.8612727	0.1985374	-1.2519418
H	3.2635727	0.6640403	0.4042907
H	-3.2601881	-2.1907181	0.2252779
H	2.8168752	-1.9941839	-0.4158430
tTG+TG+G-g+ C	-2.4046687	-0.0104384	-0.5406238
C	-1.6534348	-0.2931523	0.7456076
C	-0.1355414	-0.3502233	0.5617749
C	0.4732059	0.9629589	0.0604871
C	1.9951357	1.0703221	0.1908248
C	2.7965957	0.0268236	-0.5814427
O	-3.8039262	-0.1252930	-0.2468748
O	2.9056361	-1.2364726	0.0878885
H	-2.1135839	-0.7366210	-1.3094637
H	-2.1770039	0.9927583	-0.9128988
H	-1.9096740	0.4760055	1.4790200
H	-2.0162694	-1.2454742	1.1394625
H	0.0934507	-1.1624088	-0.1391131
H	0.3204864	-0.6146302	1.5206357
H	0.0210235	1.7868357	0.6232502
H	0.2004295	1.1207271	-0.9881096
H	2.2898200	1.0119158	1.2428326
H	2.2986517	2.0588294	-0.1695819
H	2.3786563	-0.1042769	-1.5876974
H	3.8278309	0.3598665	-0.6931500
H	-4.3059620	0.1156918	-1.0361649
H	2.0288389	-1.6346992	0.1421939
tTG+G-TG+g+ C	-2.2810938	-0.4052112	0.5017275
C	-1.7604779	0.7237794	-0.3683525
C	-0.5572496	1.4581378	0.2464555
C	0.8063806	0.9881508	-0.2675058
C	1.1179951	-0.4819441	-0.0011447
C	2.5359530	-0.8680586	-0.4011362
O	-3.3501562	-1.0416560	-0.2120797
O	3.5358487	-0.1488389	0.3331365
H	-2.6441750	0.0028621	1.4520600
H	-1.4884957	-1.1260028	0.7226467
H	-1.4976148	0.3154507	-1.3484393
H	-2.5895971	1.4154470	-0.5316763
H	-0.5839014	1.3622137	1.3386999
H	-0.6447157	2.5275024	0.0392157
H	1.5914856	1.5987637	0.1845873
H	0.8564655	1.1658937	-1.3477168
H	0.4255196	-1.1261659	-0.5522459
H	0.9773658	-0.7067102	1.0636093
H	2.6835219	-1.9474526	-0.2881952
H	2.7182872	-0.6123045	-1.4455063

H	-3.7238849	-1.7361598	0.3456016	
H	3.4709722	-0.4110797	1.2611067	
tTTG-G+G+g+ C	-2.6932089	0.1249985	-0.0224946	
C	-1.1837896	-0.0056108	-0.0574783	
C	-0.4929464	1.3553964	-0.1269591	
C	1.0204948	1.2964529	-0.3542318	
C	1.8020490	0.5581099	0.7419331	
C	2.0563109	-0.9173499	0.4480994	
O	-3.2412267	-1.1946704	0.0991776	
O	2.8239416	-1.1101954	-0.7478014	
H	-3.0482743	0.6056801	-0.9408265	
H	-2.9963342	0.7462595	0.8281644	
H	-0.8759356	-0.5517744	0.8367058	
H	-0.9083546	-0.6137035	-0.9233765	
H	-0.6933728	1.9088590	0.7975721	
H	-0.9400679	1.9383595	-0.9394635	
H	1.3872000	2.3239873	-0.4270644	
H	1.2318507	0.8249806	-1.3181146	
H	1.2800949	0.6415070	1.7022324	
H	2.7765760	1.0370977	0.8879946	
H	2.5574509	-1.3869904	1.3016513	
H	1.1278846	-1.4546282	0.2689260	
H	-4.2049922	-1.1302920	0.0970959	
H	3.6915369	-0.7049063	-0.6159567	
tTG+G-TG-t C	-1.7702814	-0.6432547	0.2738559	
C	-1.8388459	0.7254376	-0.3747560	
C	-0.6926038	1.6689474	0.0019746	
C	0.7045442	1.1399387	-0.3594178	
C	1.4008864	0.4053339	0.7875775	
C	2.6616305	-0.3133064	0.3499451	
O	-2.9685396	-1.3437833	-0.0968317	
O	2.2610027	-1.3690062	-0.5384107	
H	-1.7134539	-0.5427737	1.3645741	
H	-0.8893526	-1.1922831	-0.0699513	
H	-1.8548593	0.5876235	-1.4592990	
H	-2.7946661	1.1769459	-0.0962937	
H	-0.7338871	1.8926701	1.0742411	
H	-0.8676233	2.6180986	-0.5110720	
H	1.3470050	1.9727998	-0.6627620	
H	0.6328854	0.4737838	-1.2231821	
H	0.7367980	-0.3338866	1.2400675	
H	1.6603258	1.1217597	1.5736601	
H	3.3361702	0.3827861	-0.1623895	
H	3.1859493	-0.7268877	1.2176504	
H	-2.8774886	-2.2667751	0.1723673	
H	3.0523003	-1.8078583	-0.8762260	
g+G+TG+G+G-g+ C	2.4062852	-0.1232980	0.1188651	
C	1.1798931	-0.9146014	0.5505796	
C	0.2341320	-1.1777300	-0.6233103	
C	-1.2025853	-1.5193576	-0.2233867	
C	-1.9636354	-0.4186226	0.5259458	

C	-1.9827864	0.9480720	-0.1578520
O	2.0451040	1.2027350	-0.3154641
O	-0.8288287	1.7497640	0.1229538
H	2.8823907	-0.5890854	-0.7450241
H	3.1453591	-0.0664853	0.9227461
H	1.4992825	-1.8650712	0.9906028
H	0.6731638	-0.3543780	1.3402760
H	0.6385806	-2.0016456	-1.2201366
H	0.2302564	-0.3128555	-1.2924581
H	-1.1991649	-2.4264892	0.3903567
H	-1.7614321	-1.7669255	-1.1319684
H	-1.5654153	-0.2774501	1.5337531
H	-2.9991319	-0.7533441	0.6481412
H	-2.1214508	0.8341445	-1.2400217
H	-2.8215994	1.5326582	0.2201982
H	1.9523082	1.7615508	0.4686728
H	-0.0705513	1.4422130	-0.3964761
tTTG+G-Tg+ C	-2.6984695	-0.0325685	-0.2075459
C	-1.2207276	0.0257742	0.1239356
C	-0.6258077	1.4058289	-0.1481081
C	0.8245367	1.5782608	0.3128422
C	1.8256934	0.6235999	-0.3584974
C	2.1092157	-0.6344559	0.4537353
O	-3.1516667	-1.3648490	0.0680500
O	2.9975822	-1.5325841	-0.2224772
H	-2.8558129	0.2170934	-1.2630284
H	-3.2482432	0.6936460	0.4018305
H	-1.0950215	-0.2383397	1.1779387
H	-0.7128057	-0.7385822	-0.4677914
H	-1.2396943	2.1636098	0.3506945
H	-0.6811420	1.6184922	-1.2214041
H	0.8736071	1.4555079	1.4011062
H	1.1210384	2.6109311	0.1121293
H	2.7785883	1.1408896	-0.5128104
H	1.4678258	0.3285022	-1.3491963
H	2.5170287	-0.3564227	1.4329348
H	1.2030887	-1.2120647	0.6226987
H	-4.0895623	-1.4245699	-0.1552100
H	3.8288435	-1.0659042	-0.3819996
tG+TG+G-Tg+ C	-2.6452681	-0.5476713	0.5129809
C	-1.1655939	-0.2220911	0.5768548
C	-0.8301643	1.1204805	-0.0675918
C	0.6300870	1.5536027	0.0896186
C	1.6493531	0.5865001	-0.5370372
C	2.2570803	-0.3818915	0.4699775
O	-3.0115345	-0.6237025	-0.8723398
O	3.1411197	-1.3306045	-0.1393043
H	-3.2237816	0.2348282	1.0181455
H	-2.8439479	-1.5010743	1.0134563
H	-0.8647460	-0.2160714	1.6304828
H	-0.6206245	-1.0315367	0.0853065

H	-1.4739101	1.8901342	0.3727039	
H	-1.0809415	1.0749740	-1.1297348	
H	0.8590170	1.6865164	1.1540929	
H	0.7401751	2.5408413	-0.3661142	
H	2.4688173	1.1542479	-0.9903384	
H	1.1845142	0.0111978	-1.3426744	
H	2.7798777	0.1806855	1.2527877	
H	1.4895843	-0.9848007	0.9510181	
H	-3.9484290	-0.8505743	-0.9322532	
H	3.8376066	-0.8390323	-0.5948104	
g+TG+G-TG+g+	C	-2.2758050	-0.4232015	0.5153432
	C	-1.7713835	0.7177182	-0.3593424
	C	-0.5551575	1.4543697	0.2277426
	C	0.8027964	0.9771190	-0.2944379
	C	1.1239585	-0.4865351	-0.0044968
	C	2.5479341	-0.8668492	-0.3894610
	O	-3.4480306	-1.0492068	-0.0224543
	O	3.5355532	-0.1273790	0.3406353
	H	-2.5864867	-0.0362929	1.4861228
	H	-1.4922778	-1.1669446	0.6877138
	H	-1.5218117	0.3303129	-1.3545956
	H	-2.6064408	1.4084192	-0.4959642
	H	-0.5709596	1.3711594	1.3209283
	H	-0.6438491	2.5210740	0.0074878
	H	1.5905993	1.5970722	0.1396893
	H	0.8418979	1.1376495	-1.3779525
	H	0.4410166	-1.1458013	-0.5501171
	H	0.9769540	-0.6968900	1.0619780
	H	2.7038078	-1.9429977	-0.2590077
	H	2.7353839	-0.6251576	-1.4363037
	H	-3.2247946	-1.4005340	-0.8946187
	H	3.4752971	-0.3849774	1.2702319
g+TG-TG-G+g-C		2.4098261	0.0000892	-0.5481310
	C	1.6574743	-0.2854974	0.7436485
	C	0.1389931	-0.3544031	0.5605421
	C	-0.4742696	0.9604213	0.0686191
	C	-1.9957126	1.0647259	0.2070924
	C	-2.8013901	0.0318397	-0.5746290
	O	3.8289912	0.0385189	-0.3568875
	O	-2.8975160	-1.2439851	0.0738305
	H	2.1590258	0.9839456	-0.9406215
	H	2.1437162	-0.7442295	-1.3092427
	H	2.0139273	-1.2381595	1.1506303
	H	1.9098268	0.4876654	1.4744257
	H	-0.3172062	-0.6293107	1.5162544
	H	-0.0832217	-1.1624150	-0.1472973
	H	-0.2059454	1.1249039	-0.9797966
	H	-0.0213189	1.7816530	0.6343862
	H	-2.3006192	2.0575348	-0.1400071
	H	-2.2855127	0.9932964	1.2596348
	H	-3.8350862	0.3627851	-0.6680042

H	-2.3949113	-0.0797694	-1.5877082	
H	4.1064387	-0.8163123	-0.0014644	
H	-2.0218106	-1.6474512	0.0934094	
tG-TG+G-G-t	C	2.3325574	-0.8359652	0.3090889
	C	1.0561183	-0.4238296	-0.3957150
	C	0.5272771	0.9332803	0.0705988
	C	-0.8354514	1.3055418	-0.5344215
	C	-2.0407568	0.9456533	0.3398068
	C	-2.1723170	-0.5259448	0.6803906
	O	3.3334713	0.1531494	0.0228447
	O	-2.2522272	-1.2609331	-0.5500162
	H	2.6591183	-1.8201104	-0.0437951
	H	2.1600310	-0.8983509	1.3907020
	H	1.2508959	-0.3829337	-1.4712728
	H	0.3062118	-1.2034767	-0.2458326
	H	1.2692393	1.6894650	-0.1905514
	H	0.4600675	0.9426876	1.1658523
	H	-0.9455931	0.8305301	-1.5125571
	H	-0.8733524	2.3844731	-0.7077570
	H	-2.9599482	1.2626898	-0.1602537
	H	-1.9793182	1.5002216	1.2824872
	H	-1.3141576	-0.8649498	1.2714485
	H	-3.0754439	-0.6843165	1.2787330
	H	4.1529624	-0.1003080	0.4666204
	H	-2.5077496	-2.1707112	-0.3500477
g-TG-G-G-Tt	C	-2.3135504	-0.1172847	-0.3621867
	C	-1.3329890	0.0728070	0.7860880
	C	-0.4440214	1.3105618	0.6340679
	C	0.4400538	1.3255313	-0.6203768
	C	1.3328970	0.0951096	-0.7966551
	C	2.3020764	-0.1160801	0.3497363
	O	-3.2392953	-1.1839702	-0.1159422
	O	3.1333651	-1.2322830	0.0015470
	H	-1.7874695	-0.2860844	-1.3070791
	H	-2.9337084	0.7723791	-0.4789297
	H	-1.9135922	0.1542715	1.7083644
	H	-0.7157109	-0.8267384	0.8832074
	H	0.1813549	1.4048429	1.5260944
	H	-1.0808085	2.2010749	0.6213983
	H	1.0691506	2.2211136	-0.5903596
	H	-0.1863202	1.4314401	-1.5098623
	H	1.9197547	0.2000227	-1.7123062
	H	0.7321271	-0.8098572	-0.9146991
	H	2.9089676	0.7856030	0.4949021
	H	1.7668608	-0.3211816	1.2821875
	H	-2.7331299	-2.0021976	-0.0231126
	H	3.7355416	-1.4095943	0.7358755
tTG-G-G-Tg+	C	2.3098758	-0.1134774	0.3590402
	C	1.3385140	0.0799522	-0.7889461
	C	0.4392079	1.3069426	-0.6217498
	C	-0.4417687	1.2983590	0.6344678

C	-1.3342803	0.0629750	0.7833934	
C	-2.3155374	-0.1162870	-0.3659787	
O	3.1784242	-1.1974194	0.0019567	
O	-3.1608051	-1.2593646	-0.1899926	
H	1.7774708	-0.3461370	1.2866865	
H	2.8874067	0.8054753	0.5171861	
H	1.9258649	0.1839754	-1.7044191	
H	0.7440616	-0.8296833	-0.9012050	
H	-0.1898976	1.4029794	-1.5105652	
H	1.0636943	2.2059877	-0.5998612	
H	-1.0723935	2.1934943	0.6232885	
H	0.1866099	1.3876278	1.5249012	
H	-1.9050095	0.1539618	1.7143912	
H	-0.7347818	-0.8459985	0.8735212	
H	-2.9175249	0.7925187	-0.4900314	
H	-1.7945916	-0.3020520	-1.3038482	
H	3.7582475	-1.3882427	0.7507153	
H	-3.6342531	-1.1551674	0.6460792	
tG+G-G-G-G-t	C	2.5883374	0.2096665	-0.1925287
	C	1.3438469	0.9766569	-0.6026121
	C	0.2994011	1.1668452	0.5020021
	C	-0.3392795	-0.1059244	1.0658928
	C	-1.0374550	-0.9887102	0.0296908
	C	-2.0954215	-0.2686754	-0.7837898
	O	2.2604059	-1.1874408	-0.1053400
	O	-3.0462780	0.2996696	0.1320668
	H	2.9533666	0.5777645	0.7738511
	H	3.3778287	0.3586558	-0.9366861
	H	1.6680336	1.9666304	-0.9401253
	H	0.9132326	0.4768329	-1.4745334
	H	-0.4888906	1.8246005	0.1240410
	H	0.7710266	1.7115166	1.3275528
	H	-1.0682033	0.1902998	1.8235882
	H	0.4230994	-0.7080235	1.5630382
	H	-1.5160887	-1.8265560	0.5441089
	H	-0.3002464	-1.4157771	-0.6545476
	H	-1.6455619	0.5203171	-1.3964028
	H	-2.5911753	-0.9763267	-1.4567908
	H	3.0575613	-1.6726393	0.1453116
	H	-3.7479121	0.7230617	-0.3791038
tTG+G+G+G-t	C	2.2158274	0.2455120	-0.1765259
	C	1.1366274	-0.5199478	0.5631742
	C	0.1160368	0.3838553	1.2576303
	C	-0.6174850	1.3630085	0.3322731
	C	-1.3649286	0.7439406	-0.8527309
	C	-2.5530401	-0.1257700	-0.4841674
	O	3.1878034	-0.7097399	-0.6302551
	O	-2.0687236	-1.3532997	0.0828905
	H	2.6840433	0.9766787	0.4942307
	H	1.7963461	0.7870824	-1.0307064
	H	0.6350099	-1.1980356	-0.1288351

H	1.6310751	-1.1443271	1.3117577	
H	0.6247707	0.9683599	2.0324577	
H	-0.6126240	-0.2504293	1.7629024	
H	0.0950219	2.0956803	-0.0595104	
H	-1.3344927	1.9368726	0.9299163	
H	-0.6909027	0.1533811	-1.4786426	
H	-1.7437433	1.5569784	-1.4806552	
H	-3.1927541	0.4009549	0.2344144	
H	-3.1461939	-0.3367139	-1.3801728	
H	3.8489895	-0.2458368	-1.1600606	
H	-2.8258915	-1.9236726	0.2700701	
g+G+TG-G+G+g+ C	-2.6090839	-0.5551834	0.5303747	
C	-1.1077004	-0.4130432	0.3153250	
C	-0.6875003	1.0231916	0.0103561	
C	0.7626540	1.1942923	-0.4505473	
C	1.8255160	0.7697138	0.5721362	
C	2.2754380	-0.6841479	0.4629853	
O	-3.3726612	-0.1949045	-0.6282216	
O	2.8364007	-0.9913478	-0.8206626	
H	-2.9479380	0.1269546	1.3111153	
H	-2.8534937	-1.5754521	0.8450880	
H	-0.6064713	-0.7796851	1.2166640	
H	-0.8015628	-1.0734789	-0.5050142	
H	-0.8551395	1.6361591	0.9038623	
H	-1.3504218	1.4165509	-0.7640135	
H	0.9098579	2.2500408	-0.6946070	
H	0.9233809	0.6392268	-1.3793987	
H	1.4626453	0.9488777	1.5911342	
H	2.7167000	1.3969621	0.4569076	
H	2.9961144	-0.9104421	1.2566677	
H	1.4393574	-1.3715055	0.5669500	
H	-3.1588400	-0.8212779	-1.3326835	
H	3.6239842	-0.4442603	-0.9427901	
g-G+G+G+G+Tt C	2.1890076	-0.8226766	-0.4334997	
C	1.2435173	-0.6893615	0.7535607	
C	0.6213165	0.7009927	0.9112051	
C	-0.1768154	1.1954367	-0.3019295	
C	-1.3122029	0.2721675	-0.7504736	
C	-2.3510085	0.0280803	0.3266239	
O	3.3130994	0.0629716	-0.3521439	
O	-3.4087054	-0.7340323	-0.2713577	
H	1.6551140	-0.6756595	-1.3782238	
H	2.6217733	-1.8222897	-0.4537072	
H	0.4583519	-1.4450092	0.6495560	
H	1.8006390	-0.9331596	1.6617733	
H	1.4109243	1.4253733	1.1346910	
H	-0.0202096	0.6979029	1.7965722	
H	0.4952629	1.3512239	-1.1513913	
H	-0.5907824	2.1813416	-0.0668150	
H	-0.9235460	-0.6924857	-1.0842599	
H	-1.8233190	0.7163162	-1.6080053	

H	-1.9193844	-0.5215169	1.1689517	
H	-2.7313274	0.9858761	0.7015791	
H	2.9965071	0.9701604	-0.4490772	
H	-4.0542731	-0.9556530	0.4122829	
tG+G+G-TG+g+	C	2.2044599	-0.5086174	0.6731314
C	2.0534193	0.9554703	0.3091134	
C	0.8238706	1.2901460	-0.5409912	
C	-0.5219980	0.9216669	0.1034381	
C	-1.0517512	-0.4505082	-0.3136136	
C	-2.3576464	-0.8256921	0.3702104	
O	2.2469291	-1.2665252	-0.5458707	
O	-3.4192190	0.1005768	0.0974087	
H	1.3689720	-0.8416582	1.2986895	
H	3.1278741	-0.6508842	1.2434843	
H	2.0132337	1.5282422	1.2418320	
H	2.9561541	1.2688325	-0.2221469	
H	0.9139635	0.7960160	-1.5118004	
H	0.8501729	2.3656841	-0.7364011	
H	-1.2740157	1.6686352	-0.1581923	
H	-0.4329943	0.9592578	1.1960356	
H	-0.3126219	-1.2290821	-0.1110057	
H	-1.2010399	-0.4603466	-1.4000760	
H	-2.6580366	-1.8405082	0.0866193	
H	-2.2416567	-0.8017415	1.4546090	
H	2.5312932	-2.1662384	-0.3393018	
H	-3.5882596	0.0845834	-0.8541419	
g+G-G+TG-G-g-	C	-2.8112237	0.1155343	0.0816444
C	-1.7206452	0.9742468	-0.5537837	
C	-0.3883828	1.0095593	0.2018961	
C	0.2686026	-0.3532742	0.4276026	
C	1.6669840	-0.2648019	1.0449760	
C	2.7200252	0.3337790	0.1204291	
O	-2.7363032	-1.2724357	-0.2720007	
O	2.8390132	-0.3832858	-1.1146806	
H	-3.7910807	0.4285848	-0.2767209	
H	-2.8022949	0.2361577	1.1725709	
H	-1.5654865	0.6194740	-1.5768018	
H	-2.0955144	2.0001794	-0.6283752	
H	-0.5420720	1.4904098	1.1750740	
H	0.2961248	1.6529096	-0.3567108	
H	0.3335540	-0.8939641	-0.5209455	
H	-0.3507681	-0.9460959	1.1093995	
H	1.9964541	-1.2663646	1.3428733	
H	1.6298454	0.3338710	1.9620483	
H	2.4590860	1.3494109	-0.1725466	
H	3.6857686	0.3762594	0.6351438	
H	-1.8863896	-1.6194466	0.0241872	
H	3.1692663	-1.2703662	-0.9187903	
g+TG-TG+G-g+	C	2.5452323	0.1819036	-0.4468551
C	1.6077582	-0.5909630	0.4715295	
C	0.1331037	-0.4899099	0.0678157	

C	-0.4777415	0.8922151	0.3136323
C	-1.8865276	1.0970438	-0.2516522
C	-2.9505504	0.1275014	0.2549274
O	3.9147504	0.0756628	-0.0404932
O	-2.9747006	-1.1247977	-0.4444613
H	2.3342714	1.2492868	-0.4227010
H	2.4217326	-0.1621155	-1.4808671
H	1.9105853	-1.6436347	0.4607701
H	1.7434889	-0.2314392	1.4953075
H	-0.4180019	-1.2369880	0.6483588
H	0.0263175	-0.7601586	-0.9891716
H	0.1713612	1.6580423	-0.1185021
H	-0.4930940	1.0780951	1.3934425
H	-1.8693050	1.0347328	-1.3437658
H	-2.2079357	2.1124897	0.0021770
H	-2.8369275	-0.0344896	1.3342342
H	-3.9424973	0.5451337	0.0868821
H	4.1609300	-0.8587755	-0.0586891
H	-2.1555422	-1.5986343	-0.2587757
tTG-G-G-G+g+ C	-2.2428454	0.2490782	-0.1560515
C	-1.1449921	-0.5028730	0.5695513
C	-0.1135312	0.4067998	1.2401928
C	0.6205445	1.3650513	0.2936647
C	1.3790793	0.7175077	-0.8684825
C	2.5662711	-0.1475845	-0.4613999
O	-3.1759405	-0.7261648	-0.6473376
O	2.2018788	-1.3686664	0.1979711
H	-1.8355103	0.8304669	-0.9894041
H	-2.7393883	0.9418481	0.5337619
H	-1.6180604	-1.1325195	1.3270709
H	-0.6627974	-1.1801523	-0.1380979
H	0.6151273	-0.2213787	1.7533089
H	-0.6165462	1.0061975	2.0069822
H	1.3348142	1.9516763	0.8816265
H	-0.0897973	2.0886824	-0.1180424
H	1.7681872	1.5147829	-1.5115854
H	0.7020370	0.1279137	-1.4960745
H	3.1857441	-0.3660224	-1.3381032
H	3.1876729	0.3849942	0.2601780
H	-3.8778127	-0.2659027	-1.1254773
H	1.7566113	-1.9359708	-0.4450532
g+TTG+G-Tg- C	-2.7071515	-0.0347693	-0.2131310
C	-1.2251091	0.0279682	0.1264331
C	-0.6290103	1.4075935	-0.1467199
C	0.8249070	1.5796542	0.3027255
C	1.8226223	0.6224159	-0.3711527
C	2.1367001	-0.6120430	0.4652598
O	-3.2571857	-1.3481079	-0.0541731
O	3.1136342	-1.4585853	-0.1528664
H	-2.8663174	0.2116676	-1.2630836
H	-3.2641931	0.6913943	0.3901007

H	-1.0895654	-0.2272012	1.1841557	
H	-0.7138456	-0.7393445	-0.4592001	
H	-1.2413665	2.1650534	0.3541063	
H	-0.6937711	1.6171007	-1.2200979	
H	0.8819097	1.4608697	1.3910595	
H	1.1211844	2.6112372	0.0972617	
H	2.7703830	1.1305136	-0.5618107	
H	1.4341738	0.3115264	-1.3481797	
H	2.5858142	-0.3121056	1.4124671	
H	1.2283968	-1.1785456	0.6905410	
H	-3.1664857	-1.6001752	0.8743736	
H	2.7489569	-1.7741252	-0.9905020	
tTG-G+TG+g+ C	2.2746605	-0.3337782	0.4654812	
C	1.6289810	0.5645795	-0.5729167	
C	0.6323517	1.5655354	0.0367758	
C	-0.8347555	1.1432769	-0.0837564	
C	-1.1770886	-0.1680447	0.6178733	
C	-2.6546663	-0.5244137	0.5246747	
O	3.0957012	-1.2813010	-0.2313622	
O	-3.0998949	-0.6910245	-0.8277417	
H	1.5144569	-0.8514518	1.0582048	
H	2.8817335	0.2721584	1.1476585	
H	2.4306169	1.0880008	-1.0978447	
H	1.1306292	-0.0650794	-1.3154909	
H	0.7468510	2.5349369	-0.4542498	
H	0.8767391	1.7339595	1.0926838	
H	-1.0992140	1.0614095	-1.1409634	
H	-1.4678107	1.9343549	0.3324975	
H	-0.9072749	-0.1046036	1.6787524	
H	-0.5926562	-0.9920904	0.1946181	
H	-2.8665494	-1.4259304	1.1099347	
H	-3.2672944	0.2855538	0.9221842	
H	3.5692436	-1.8168866	0.4181869	
H	-2.6307206	-1.4468575	-1.2059820	
tG-G+G-G-G+g+ C	2.2956374	-0.3302098	0.0217541	
C	1.5730138	0.9865001	0.2231237	
C	0.4061136	1.2108608	-0.7597319	
C	-0.9200744	1.5546549	-0.0695525	
C	-1.5079114	0.4528895	0.8183146	
C	-2.1629228	-0.7072506	0.0760344	
O	1.3839764	-1.3958748	0.3693417	
O	-1.2740047	-1.4320166	-0.7764938	
H	3.1777692	-0.3877019	0.6658512	
H	2.6127663	-0.4385765	-1.0203084	
H	1.2252587	1.0166023	1.2591138	
H	2.3118780	1.7866676	0.1250681	
H	0.2618303	0.3280459	-1.3823641	
H	0.6605665	2.0302445	-1.4375546	
H	-1.6596597	1.8223299	-0.8314445	
H	-0.7675193	2.4522504	0.5399036	
H	-2.2766218	0.8915348	1.4637317	

H	-0.7399958	0.0534784	1.4880011	
H	-2.6212957	-1.3845571	0.8071195	
H	-2.9581649	-0.3356609	-0.5739155	
H	1.8421437	-2.2408614	0.2629467	
H	-0.4235044	-1.5255063	-0.3139551	
g+TG-G-G-G-g+	C	2.3543053	0.0050513	0.3384034
C	1.3137152	0.2799979	-0.7375393	
C	0.1817462	1.1994467	-0.2704013	
C	-0.6216535	0.6751964	0.9265476	
C	-1.2506868	-0.7069384	0.7290300	
C	-2.1895854	-0.8044168	-0.4665008	
O	3.4141049	-0.8366947	-0.1306909	
O	-3.3102644	0.0835741	-0.3697242	
H	1.9218418	-0.5404440	1.1756841	
H	2.7543353	0.9507160	0.7246915	
H	1.8143848	0.7487003	-1.5919507	
H	0.9221875	-0.6755438	-1.0937803	
H	-0.4867287	1.3832754	-1.1170690	
H	0.6017648	2.1754361	-0.0062787	
H	-1.4076120	1.3979462	1.1671455	
H	0.0172402	0.6448516	1.8129505	
H	-1.8143517	-0.9701199	1.6276276	
H	-0.4696212	-1.4648362	0.6116237	
H	-1.6494127	-0.6355536	-1.4041801	
H	-2.6264125	-1.8012805	-0.5154705	
H	3.8306560	-0.4013114	-0.8863689	
H	-2.9886792	0.9922534	-0.4282693	
g+TTG+G-G-g-C	2.6934838	0.1351508	-0.0160388	
C	1.1779902	0.0001854	-0.0368944	
C	0.4819948	1.3572806	-0.1370162	
C	-1.0273710	1.2967689	-0.3897638	
C	-1.8389010	0.5951127	0.7079161	
C	-2.0510308	-0.8998276	0.4865757	
O	3.3600320	-1.1191296	0.1698705	
O	-2.7293552	-1.1810885	-0.7449992	
H	3.0087504	0.7494767	0.8276081	
H	3.0408907	0.6226429	-0.9343040	
H	0.8857470	-0.6239325	-0.8893889	
H	0.8768201	-0.5272386	0.8705805	
H	0.9423848	1.9290133	-0.9500736	
H	0.6693456	1.9228523	0.7826437	
H	-1.2221803	0.8018128	-1.3453497	
H	-1.3872856	2.3238550	-0.4955648	
H	-2.8283957	1.0592208	0.7846351	
H	-1.3619719	0.7411474	1.6840299	
H	-1.1056256	-1.4308193	0.4069104	
H	-2.6036404	-1.3251959	1.3314055	
H	3.1146048	-1.6983745	-0.5637279	
H	-3.6127747	-0.7915001	-0.6979293	
g-G+G-TG-G+ttC	2.5422330	-0.3726216	-0.5338583	
C	1.7898166	-0.8421170	0.7080285	

C	0.2645886	-0.7224399	0.6404882	
C	-0.2632814	0.7047378	0.4664526	
C	-1.7742844	0.8593285	0.6715723	
C	-2.6336214	0.3706176	-0.4789783	
O	2.7648058	1.0449788	-0.5795671	
O	-2.4964620	-1.0538799	-0.5903567	
H	2.0235511	-0.7095061	-1.4401616	
H	3.5447992	-0.7987439	-0.5477563	
H	2.0381700	-1.8962929	0.8700647	
H	2.1820153	-0.2896117	1.5677307	
H	-0.1541218	-1.1280755	1.5670301	
H	-0.1209954	-1.3510443	-0.1636813	
H	-0.0264838	1.0774671	-0.5381880	
H	0.2491073	1.3583668	1.1807467	
H	-2.0076947	1.9194826	0.8127400	
H	-2.0814325	0.3403214	1.5841511	
H	-3.6797150	0.6355788	-0.2929582	
H	-2.3177152	0.8565381	-1.4099764	
H	1.9086608	1.4876158	-0.6153643	
H	-3.0872022	-1.3642524	-1.2892093	
tG+TG-G+G+g+ C	-2.3153934	-0.8385403	0.2811632	
C	-1.0507975	-0.4031802	-0.4296868	
C	-0.5162155	0.9395594	0.0720479	
C	0.8464926	1.3185670	-0.5290354	
C	2.0487066	0.9323796	0.3385092	
C	2.1482436	-0.5450703	0.6880410	
O	-3.3178970	0.1652627	0.0527391	
O	2.1741200	-1.3955595	-0.4671923	
H	-2.1242591	-0.9444007	1.3559474	
H	-2.6516822	-1.8064617	-0.1048408	
H	-0.2987460	-1.1873550	-0.3204359	
H	-1.2647163	-0.3246358	-1.4997080	
H	-0.4438925	0.9203415	1.1667166	
H	-1.2543752	1.7068929	-0.1659719	
H	0.8917548	2.3996902	-0.6863231	
H	0.9463123	0.8592887	-1.5165367	
H	2.0110017	1.4941654	1.2786198	
H	2.9735043	1.2382169	-0.1648581	
H	3.0317011	-0.7232771	1.3105521	
H	1.2773092	-0.8706655	1.2559741	
H	-4.1314387	-0.1067526	0.4964160	
H	2.9474912	-1.1575246	-0.9963055	
g+TTG+G-Tg+ C	-2.7095545	-0.0270669	-0.2071772	
C	-1.2230360	0.0212666	0.1154234	
C	-0.6264455	1.4038126	-0.1430613	
C	0.8238633	1.5779765	0.3170709	
C	1.8265431	0.6262691	-0.3558346	
C	2.1098788	-0.6312802	0.4570241	
O	-3.2681168	-1.3378362	-0.0607469	
O	2.9937219	-1.5338333	-0.2176646	
H	-2.8795151	0.2361491	-1.2513487	

H	-3.2536954	0.6942757	0.4137123	
H	-1.0783187	-0.2496843	1.1682408	
H	-0.7212561	-0.7382814	-0.4878529	
H	-1.2426669	2.1569092	0.3599037	
H	-0.6847352	1.6212787	-1.2150442	
H	0.8748636	1.4547692	1.4053842	
H	1.1173632	2.6116790	0.1176352	
H	2.7786977	1.1448688	-0.5095309	
H	1.4690617	0.3313457	-1.3466579	
H	2.5190764	-0.3525843	1.4355851	
H	1.2020767	-1.2059696	0.6276450	
H	-3.1486937	-1.6131052	0.8578948	
H	3.8243926	-1.0692117	-0.3863404	
g+G-G+G+TG-g-	C	2.6580931	-0.3397477	-0.1024337
C	1.9143150	0.8026846	0.5795556	
C	0.7912582	1.4540244	-0.2343161	
C	-0.4089545	0.5714055	-0.5921104	
C	-1.0916599	-0.0690515	0.6132580	
C	-2.3734362	-0.8043980	0.2469851	
O	1.9444401	-1.5862244	-0.0989138	
O	-3.3582431	0.0515022	-0.3491831	
H	3.5789125	-0.5521036	0.4404002	
H	2.9327006	-0.0580228	-1.1260515	
H	1.5409259	0.4405552	1.5407694	
H	2.6535587	1.5787395	0.8064581	
H	1.2190663	1.8598128	-1.1576142	
H	0.4186744	2.3149515	0.3308059	
H	-0.1173455	-0.2104934	-1.3031583	
H	-1.1410144	1.1817984	-1.1260837	
H	-1.3239793	0.7066243	1.3536326	
H	-0.4189481	-0.7784861	1.1029036	
H	-2.1725672	-1.5654427	-0.5083340	
H	-2.7878110	-1.3076993	1.1267160	
H	1.2556891	-1.5463598	-0.7728725	
H	-3.6499637	0.6833017	0.3214958	
tTG-G+TG-g+	C	-2.3009010	-0.3855367	-0.4947402
C	-1.7493820	0.7142065	0.3939869	
C	-0.5648426	1.4644812	-0.2372410	
C	0.8124876	0.9852017	0.2324155	
C	1.1147891	-0.4809822	-0.0663695	
C	2.5134624	-0.9100564	0.3581905	
O	-3.3496061	-1.0391120	0.2324940	
O	3.5518574	-0.2505717	-0.3767618	
H	-1.5180160	-1.1009168	-0.7623824	
H	-2.6911057	0.0531031	-1.4202160	
H	-2.5698078	1.4030272	0.6052952	
H	-1.4573788	0.2744804	1.3518800	
H	-0.6484763	2.5294859	-0.0074450	
H	-0.6163220	1.3876259	-1.3294635	
H	0.8958475	1.1536455	1.3126194	
H	1.5691226	1.6151692	-0.2463304	

H	1.0058204	-0.6722449	-1.1381945	
H	0.3995900	-1.1217176	0.4585200	
H	2.6460461	-0.7509932	1.4351023	
H	2.6602008	-1.9706262	0.1569059	
H	-3.7352311	-1.7239123	-0.3291022	
H	3.5721917	0.6777584	-0.1129191	
g+TG+TG-G+g-	C	-2.5488955	0.1534952	-0.4606945
C	-1.6051294	-0.5878602	0.4771622	
C	-0.1304530	-0.4848732	0.0736831	
C	0.4794431	0.9007870	0.3021516	
C	1.8902943	1.0977937	-0.2607454	
C	2.9503358	0.1306237	0.2592407	
O	-3.9258855	-0.0666726	-0.1290178	
O	2.9795508	-1.1251408	-0.4328537	
H	-2.4403233	-0.2262658	-1.4770513	
H	-2.3316888	1.2256887	-0.4779845	
H	-1.7289647	-0.2044973	1.4967169	
H	-1.9147594	-1.6355633	0.4911625	
H	-0.0254126	-0.7680325	-0.9799450	
H	0.4228215	-1.2240952	0.6621444	
H	0.4924691	1.1006830	1.3797760	
H	-0.1683474	1.6607377	-0.1423832	
H	2.2129413	2.1152220	-0.0165402	
H	1.8763155	1.0241329	-1.3521548	
H	3.9436576	0.5470978	0.0965215	
H	2.8285084	-0.0250993	1.3386698	
H	-4.0793273	0.2818733	0.7591764	
H	2.1572956	-1.5967557	-0.2549887	
tG+G+G-TG-g+	C	1.8573028	-0.7773355	0.6663784
C	1.9709237	0.7338075	0.6056287	
C	0.9888446	1.4191002	-0.3488942	
C	-0.4926626	1.1606769	-0.0288282	
C	-1.1023403	-0.0027710	-0.8129072	
C	-2.5426361	-0.3066578	-0.4306347	
O	2.0638078	-1.2851040	-0.6596099	
O	-2.6699068	-0.8127148	0.9072450	
H	0.8742107	-1.0793679	1.0429302	
H	2.6159147	-1.1735016	1.3493623	
H	1.8193606	1.1214045	1.6189106	
H	2.9936784	0.9878221	0.3147360	
H	1.2010130	1.1029794	-1.3730379	
H	1.1875961	2.4933972	-0.3054443	
H	-1.0773983	2.0603200	-0.2490199	
H	-0.5943199	0.9871467	1.0492362	
H	-0.5057043	-0.9069685	-0.6890074	
H	-1.0752040	0.2458797	-1.8794751	
H	-3.1697869	0.5837697	-0.5604628	
H	-2.9464033	-1.0950292	-1.0650485	
H	2.0847632	-2.2501755	-0.6200278	
H	-2.4624711	-0.0979740	1.5221285	
tG-G+G+G+Tg+	C	-2.5306354	-0.2400357	-0.4185702

C	-1.3889450	0.6127308	-0.9417696	
C	-0.6387301	1.4236334	0.1191049	
C	0.1140680	0.6179703	1.1854414	
C	1.1356639	-0.3847288	0.6431984	
C	2.2049526	0.2406980	-0.2391529	
O	-1.9800199	-1.3773072	0.2663936	
O	3.2388384	-0.6932289	-0.5868536	
H	-3.1538804	-0.5752819	-1.2540636	
H	-3.1567983	0.3495821	0.2617288	
H	-0.7072199	-0.0361771	-1.4980995	
H	-1.8132898	1.3132449	-1.6681604	
H	-1.3584706	2.0775598	0.6237447	
H	0.0599258	2.0911789	-0.3939768	
H	-0.6027722	0.0746793	1.8023932	
H	0.6286491	1.3270931	1.8432662	
H	0.6147807	-1.1724243	0.0914720	
H	1.6407041	-0.8695993	1.4828668	
H	1.7677749	0.6664632	-1.1484735	
H	2.7186746	1.0435703	0.2917060	
H	-2.7095751	-1.9297069	0.5769222	
H	2.8155278	-1.4557189	-1.0037363	
tG-G-G+TG+g+	C	-1.7981858	-0.8396235	0.6076545
C	-1.9709184	0.6664588	0.6382810	
C	-1.0067970	1.4464954	-0.2605875	
C	0.4794024	1.2108762	0.0529708	
C	1.1338547	0.1461117	-0.8286022	
C	2.5395343	-0.2164027	-0.3752600	
O	-1.9515955	-1.2806158	-0.7510831	
O	2.5576810	-0.8356075	0.9213143	
H	-2.5525212	-1.3075981	1.2478934	
H	-0.8107765	-1.1223180	0.9890422	
H	-3.0010394	0.8987161	0.3549709	
H	-1.8386446	0.9937046	1.6750959	
H	-1.2416885	2.5079062	-0.1431833	
H	-1.2081835	1.1983274	-1.3059927	
H	0.6021214	0.9369702	1.1051011	
H	1.0345787	2.1445055	-0.0828294	
H	1.1853351	0.5153274	-1.8589799	
H	0.5159998	-0.7553569	-0.8659697	
H	3.0262659	-0.8658469	-1.1108354	
H	3.1508668	0.6800600	-0.2633651	
H	-2.0950006	-2.2356990	-0.7510611	
H	2.1068868	-1.6870369	0.8455753	
tTG-G-G-Tt	C	0.1976054	2.3238547	-0.1163709
C	-0.8809724	1.2762421	0.0776701	
C	-0.6571423	0.3959330	1.3094207	
C	0.6571423	-0.3959330	1.3094209	
C	0.8809726	-1.2762423	0.0776705	
C	-0.1976052	-2.3238551	-0.1163704	
O	-0.2145345	3.1601595	-1.2066225	
O	0.2145344	-3.1601595	-1.2066224	

H	1.1604898	1.8555555	-0.3424739	
H	0.3112151	2.9160648	0.7997386	
H	-1.8356351	1.7991984	0.1739451	
H	-0.9458163	0.6709888	-0.8294507	
H	-1.5007819	-0.2932602	1.4039476	
H	-0.6842236	1.0242241	2.2057720	
H	0.6842235	-1.0242238	2.2057724	
H	1.5007819	0.2932603	1.4039476	
H	1.8356353	-1.7991986	0.1739459	
H	0.9458166	-0.6709894	-0.8294504	
H	-0.3112144	-2.9160654	0.7997390	
H	-1.1604897	-1.8555559	-0.3424728	
H	0.4982161	3.7810699	-1.4056304	
H	-0.4982173	-3.7810680	-1.4056321	
g+TG-G+TG-g+	C	-2.2885242	-0.4067475	-0.5090923
C	-1.7505554	0.7046702	0.3840057	
C	-0.5661616	1.4637511	-0.2377674	
C	0.8097378	0.9861722	0.2373715	
C	1.1167972	-0.4789881	-0.0618520	
C	2.5155048	-0.9032463	0.3666855	
O	-3.3206121	-1.1713450	0.1249322	
O	3.5534542	-0.2446003	-0.3709430	
H	-1.5123096	-1.1301658	-0.7502870	
H	-2.6504036	0.0203842	-1.4518184	
H	-2.5716618	1.4003268	0.5854397	
H	-1.4660464	0.2723901	1.3477481	
H	-0.6538202	2.5280172	-0.0055575	
H	-0.6139744	1.3883175	-1.3302781	
H	0.8883409	1.1541810	1.3181076	
H	1.5666670	1.6186238	-0.2375963	
H	1.0123673	-0.6697831	-1.1342017	
H	0.4023446	-1.1234717	0.4594675	
H	2.6471763	-0.7383873	1.4428134	
H	2.6643991	-1.9643775	0.1706120	
H	-4.0482826	-0.5723917	0.3393091	
H	3.5777759	0.6830421	-0.1050325	
g-G+G+TG-G+g-	C	-2.7290589	0.3067257	0.1293735
C	-1.6721075	-0.3106959	1.0374384	
C	-0.2656993	-0.3738743	0.4332669	
C	0.3825109	0.9968620	0.2265376	
C	1.7097655	0.9869598	-0.5383064	
C	2.8140545	0.1274649	0.0719075	
O	-2.9357612	-0.4484844	-1.0709858	
O	2.7399431	-1.2563206	-0.2962712	
H	-2.4888207	1.3471760	-0.1107290	
H	-3.6944847	0.3018657	0.6342371	
H	-1.6389325	0.2646513	1.9693995	
H	-2.0016059	-1.3210088	1.2921030	
H	-0.2971669	-0.9227855	-0.5143976	
H	0.3524624	-0.9671496	1.1149400	
H	0.5384093	1.4586814	1.2080524	

H	-0.3098268	1.6526044	-0.3090994	
H	2.0748678	2.0174053	-0.5978606	
H	1.5538218	0.6473274	-1.5666782	
H	3.7851834	0.4508787	-0.3007285	
H	2.8239114	0.2378538	1.1635945	
H	-2.1708246	-0.3295487	-1.6481525	
H	1.9415921	-1.6377749	0.0877607	
g+G+TG+G-G-g- C	-2.5021243	-0.1856257	0.3367082	
C	-1.1395972	0.2600964	0.8446093	
C	-0.4543529	1.2575259	-0.0928198	
C	1.0352529	1.4702885	0.2211993	
C	1.9753380	0.6191980	-0.6385182	
C	1.7113265	-0.8784194	-0.5912826	
O	-2.4064888	-0.9451289	-0.8794835	
O	1.7595309	-1.4186565	0.7379953	
H	-3.1212783	0.6752623	0.0806368	
H	-3.0293582	-0.7638334	1.1027604	
H	-1.2654441	0.7209464	1.8307836	
H	-0.5064362	-0.6174030	1.0006437	
H	-0.9859604	2.2114463	-0.0222368	
H	-0.5721409	0.9205638	-1.1270213	
H	1.2176388	1.2622936	1.2794267	
H	1.3039498	2.5182653	0.0629780	
H	3.0139274	0.8074717	-0.3422922	
H	1.8906346	0.9350159	-1.6842552	
H	0.7080163	-1.1037100	-0.9509861	
H	2.4202349	-1.4041308	-1.2396994	
H	-1.9670906	-1.7798347	-0.6680371	
H	2.6492697	-1.2760569	1.0883237	
g-G+G-TG+G-t C	2.7833671	0.2406977	0.2099521	
C	1.5993887	1.1465709	-0.1172124	
C	0.2555116	0.7309090	0.4880488	
C	-0.2263771	-0.6690724	0.0967290	
C	-1.6524727	-0.9969420	0.5562429	
C	-2.7525438	-0.4585355	-0.3397378	
O	2.8947884	-0.9040010	-0.6489994	
O	-2.7399574	0.9757702	-0.2869997	
H	2.7439554	-0.0707096	1.2616266	
H	3.7195518	0.7771139	0.0594095	
H	1.8349847	2.1530199	0.2442387	
H	1.5198528	1.2147773	-1.2065658	
H	-0.5046311	1.4541047	0.1933848	
H	0.3271799	0.7780152	1.5809301	
H	0.4395830	-1.4167257	0.5424246	
H	-0.1657701	-0.7911337	-0.9913974	
H	-1.8125239	-0.6262348	1.5730295	
H	-1.7807527	-2.0834494	0.5898464	
H	-2.5911521	-0.8017007	-1.3682875	
H	-3.7211998	-0.8394826	0.0007169	
H	2.1078019	-1.4497080	-0.5345619	
H	-3.4458893	1.3099805	-0.8558520	

tTTG+G-G-g+	C	2.5185792	0.1816961	0.2809502
	C	1.1087673	0.0823896	-0.2672447
	C	0.2697458	1.3206267	0.0547877
	C	-1.1447829	1.3123350	-0.5454965
	C	-2.2292906	0.6642876	0.3218198
	C	-2.0187938	-0.8029317	0.6706114
	O	3.2120586	-1.0132453	-0.1009610
	O	-1.9523683	-1.6490556	-0.4824107
	H	2.4907074	0.2794340	1.3720298
	H	3.0183166	1.0661231	-0.1298698
	H	1.1752399	-0.0439584	-1.3520123
	H	0.6614461	-0.8248424	0.1423964
	H	0.8067581	2.1947337	-0.3267329
	H	0.2038425	1.4530679	1.1408892
	H	-1.1203605	0.8346712	-1.5305452
	H	-1.4552654	2.3444485	-0.7284323
	H	-3.1890522	0.7530861	-0.1941657
	H	-2.3150852	1.2239661	1.2602432
	H	-1.1308355	-0.9334432	1.2979231
	H	-2.8730719	-1.1707429	1.2387250
	H	4.1091563	-0.9789428	0.2556525
	H	-1.1218005	-1.4757801	-0.9444321
g+TTG+G+G-g+	C	2.4618152	-0.1457609	0.4388061
	C	1.1594533	0.2714711	-0.2290589
	C	0.1744862	0.8877799	0.7631215
	C	-1.0668662	1.5053069	0.1094621
	C	-1.9099164	0.5847136	-0.7787718
	C	-2.5738982	-0.5942756	-0.0753131
	O	3.3667956	-0.7913706	-0.4632241
	O	-1.6953886	-1.7038899	0.1622380
	H	2.2702019	-0.8831047	1.2191037
	H	2.9406489	0.7214685	0.9088213
	H	1.3800678	1.0063336	-1.0128029
	H	0.7250089	-0.6022283	-0.7175732
	H	0.6833687	1.6754971	1.3290436
	H	-0.1142794	0.1409359	1.5113043
	H	-0.7385627	2.3568443	-0.4953169
	H	-1.7100765	1.9182586	0.8940915
	H	-1.3189592	0.1958971	-1.6116786
	H	-2.7081486	1.1918042	-1.2192841
	H	-3.0406133	-0.2647899	0.8610006
	H	-3.3597789	-1.0029873	-0.7099397
	H	3.5653265	-0.1744984	-1.1801311
	H	-1.1113531	-1.4857760	0.8978436
g+TTG-G+G+g+	C	2.4236360	-0.1243818	0.4165964
	C	1.1289953	-0.1944157	-0.3764978
	C	0.2237204	-1.3411845	0.0807035
	C	-1.1729399	-1.3141797	-0.5613001
	C	-2.2412821	-0.6210878	0.2901849
	C	-1.9260275	0.8147413	0.6838352
	O	3.3255591	0.8715984	-0.0828782

O	-1.6694807	1.6642140	-0.4427630	
H	2.9722817	-1.0639632	0.3435689	
H	-1.0177121	0.8631523	1.2840524	
H	0.6000730	0.7588988	-0.3019304	
H	1.3763159	-0.3297412	-1.4330494	
H	0.1237219	-1.3266288	1.1728799	
H	0.7198907	-2.2855208	-0.1619501	
H	-1.5137943	-2.3364336	-0.7460128	
H	-1.1099574	-0.8274990	-1.5382669	
H	-2.3944732	-1.1919341	1.2129442	
H	-3.1980317	-0.6389844	-0.2443721	
H	-2.7412745	1.2228241	1.2907363	
H	2.2070673	0.0544644	1.4769910	
H	2.8576271	1.7175008	-0.0856609	
H	-2.4688790	1.6944444	-0.9856692	
g+TG+G-TG+g-	C	2.3116266	-0.3901557	-0.5108078
C	1.7531511	0.6987970	0.3969850	
C	0.5658827	1.4574187	-0.2209583	
C	-0.8118309	0.9786459	0.2473304	
C	-1.1238681	-0.4809652	-0.0723702	
C	-2.5224784	-0.9091550	0.3534056	
O	3.4500936	-1.0482807	0.0586287	
O	-3.5602362	-0.2379564	-0.3717879	
H	2.6788909	0.0525627	-1.4368883	
H	1.5393208	-1.1193589	-0.7737207	
H	1.4526052	0.2560422	1.3541264	
H	2.5730808	1.3854689	0.6179554	
H	0.6152574	1.3881337	-1.3136194	
H	0.6538948	2.5202200	0.0172660	
H	-1.5666542	1.6189534	-0.2201870	
H	-0.8917058	1.1330617	1.3301426	
H	-0.4093341	-1.1351010	0.4374089	
H	-1.0208208	-0.6567594	-1.1472551	
H	-2.6741951	-1.9670077	0.1418464	
H	-2.6510512	-0.7600025	1.4323095	
H	3.1703791	-1.4725677	0.8806000	
H	-3.5805962	0.6865272	-0.0946271	
g-G+G+G+G+G+g-	C	-2.3418171	0.6991708	-0.1832186
C	-1.2872194	0.4909467	0.8961972	
C	-0.3803869	-0.7213838	0.6656831	
C	0.3803864	-0.7213842	-0.6656817	
C	1.2872186	0.4909463	-0.8961968	
C	2.3418175	0.6991703	0.1832179	
O	-3.2423167	-0.4098398	-0.3007865	
O	3.2423179	-0.4098399	0.3007838	
H	-1.8766287	0.9175387	-1.1503284	
H	-2.9746474	1.5476431	0.0748631	
H	-0.6882894	1.4042816	0.9689153	
H	-1.8001142	0.3712108	1.8538764	
H	-0.9797076	-1.6347659	0.7309966	
H	0.3263314	-0.7853197	1.4987980	

H	-0.3263319	-0.7853210	-1.4987966
H	0.9797073	-1.6347662	-0.7309946
H	0.6882885	1.4042812	-0.9689141
H	1.8001125	0.3712105	-1.8538765
H	2.9746469	1.5476433	-0.0748639
H	1.8766302	0.9175371	1.1503285
H	-2.7605961	-1.1590577	-0.6739038
H	2.7605984	-1.1590582	0.6739014
tG-G-G+TG-g+ C	-2.3083758	-0.7126487	0.4063941
C	-1.7683641	0.6788063	0.6891483
C	-0.7675999	1.1910121	-0.3577191
C	0.7047921	0.9839881	0.0112277
C	1.1279438	-0.4720645	0.1934459
C	2.6153145	-0.6397001	0.4780042
O	-3.0584709	-0.6337445	-0.8151117
O	3.4476331	-0.2473027	-0.6198547
H	-2.9564385	-1.0342244	1.2287679
H	-1.4960821	-1.4375683	0.3050352
H	-2.6319970	1.3463507	0.7376542
H	-1.3119662	0.6837575	1.6850339
H	-0.9264991	2.2617618	-0.5091302
H	-0.9813924	0.7137277	-1.3175896
H	0.9239470	1.5356024	0.9337719
H	1.3121737	1.4377266	-0.7787896
H	0.8788638	-1.0468431	-0.7034710
H	0.5827264	-0.9159987	1.0320691
H	2.8900140	-0.0854239	1.3838121
H	2.8524334	-1.6899908	0.6445077
H	-3.3710271	-1.5183667	-1.0443110
H	3.3764162	0.7089431	-0.7316024
tG-TG+G-G-g+ C	2.3988446	-0.7785516	0.3772344
C	1.0357749	-0.4805339	-0.2184308
C	0.5256988	0.9186315	0.1320734
C	-0.8178820	1.2913851	-0.5139306
C	-2.0639405	0.9448609	0.3097977
C	-2.2423283	-0.5283582	0.6478179
O	3.3314826	0.1550590	-0.1849858
O	-2.3694158	-1.3608827	-0.5106366
H	2.6964541	-1.8051328	0.1402023
H	2.3616956	-0.6731451	1.4678376
H	1.1138828	-0.5778434	-1.3061151
H	0.3480767	-1.2547541	0.1319591
H	1.2892703	1.6308494	-0.1842396
H	0.4466884	1.0132277	1.2217065
H	-0.8852154	0.8347544	-1.5078404
H	-0.8400998	2.3695506	-0.6918983
H	-2.9533633	1.2806134	-0.2302267
H	-2.0285697	1.5025810	1.2521851
H	-1.4254541	-0.8806970	1.2871699
H	-3.1714978	-0.6741458	1.1980767
H	4.2042156	-0.0135447	0.1927747

H	-1.5697167	-1.2633276	-1.0438895	
tG+TG+G-G-g+	C	2.5557966	-0.2981028	-0.4521094
C	1.0953556	-0.0567236	-0.7813703	
C	0.5082371	1.1381920	-0.0283157	
C	-0.9737285	1.4144188	-0.3270093	
C	-1.9640771	0.7285775	0.6216553	
C	-1.8967422	-0.7916955	0.6565219	
O	2.6282497	-0.6337155	0.9410355	
O	-2.1995743	-1.3939715	-0.6091246	
H	3.1418880	0.6047585	-0.6599016	
H	2.9513942	-1.1157262	-1.0632931	
H	1.0109953	0.1155770	-1.8601232	
H	0.5522757	-0.9764818	-0.5526194	
H	1.0991031	2.0193118	-0.2989822	
H	0.6497375	0.9906417	1.0452229	
H	-1.1997379	1.1451265	-1.3652728	
H	-1.1573670	2.4900960	-0.2619998	
H	-2.9818691	1.0181087	0.3461666	
H	-1.7861465	1.0957516	1.6383319	
H	-0.9218251	-1.1302586	1.0219335	
H	-2.6544454	-1.1807343	1.3360600	
H	3.5509016	-0.8012195	1.1725487	
H	-1.5332384	-1.1082158	-1.2473136	
g+G+G-TG-G+g-	C	2.6253490	-0.3692124	-0.4880882
C	1.7661772	-0.8594543	0.6708662	
C	0.2555082	-0.6962379	0.4782737	
C	-0.2504024	0.7472236	0.5570337	
C	-1.7716846	0.8931483	0.6556472	
C	-2.5628008	0.3476463	-0.5300029	
O	2.5755360	1.0485344	-0.6947338	
O	-2.7991398	-1.0669668	-0.4702070	
H	2.2702433	-0.7995553	-1.4256440	
H	3.6618354	-0.6932289	-0.3439144	
H	1.9937634	-1.9217789	0.8109497	
H	2.0764190	-0.3544999	1.5933222	
H	-0.2563565	-1.2922651	1.2413781	
H	0.0005660	-1.1326741	-0.4953661	
H	0.1181706	1.3085024	-0.3036727	
H	0.1950873	1.2161852	1.4413933	
H	-2.0030684	1.9594315	0.7489513	
H	-2.1463547	0.4071056	1.5619145	
H	-3.5611741	0.7834172	-0.5439132	
H	-2.0681973	0.6161505	-1.4716710	
H	2.9738811	1.4786625	0.0736681	
H	-1.9521508	-1.5230198	-0.5392616	
g+G-G+TG+G-g-	C	2.5627649	0.3476836	-0.5300526
C	1.7716718	0.8931877	0.6556155	
C	0.2503877	0.7472513	0.5570286	
C	-0.2554865	-0.6962226	0.4782566	
C	-1.7661452	-0.8595102	0.6708628	
C	-2.6253506	-0.3692909	-0.4880743	

O	2.7991494	-1.0669240	-0.4702396	
O	-2.5755651	1.0484592	-0.6947234	
H	3.5611259	0.7834818	-0.5440047	
H	2.0681215	0.6161558	-1.4717090	
H	2.1463630	0.4071457	1.5618741	
H	2.0030554	1.9594716	0.7489113	
H	-0.1182003	1.3085223	-0.3036765	
H	-0.1950983	1.2162051	1.4413934	
H	0.2564122	-1.2922470	1.2413404	
H	-0.0005403	-1.1326207	-0.4953994	
H	-2.0764033	-0.3545863	1.5933299	
H	-1.9936783	-1.9218485	0.8109297	
H	-2.2702586	-0.7996295	-1.4256375	
H	-3.6618294	-0.6933224	-0.3438763	
H	1.9521712	-1.5230038	-0.5392555	
H	-2.9739171	1.4785779	0.0736796	
tG+TG-G+G-t	C	2.2511245	-0.8570248	0.0233787
	C	1.0385196	-0.1649785	0.6106334
	C	0.4365547	0.8778049	-0.3293253
	C	-0.8467094	1.5261032	0.2131812
	C	-2.1676587	0.8683638	-0.2002635
	C	-2.3985764	-0.5622235	0.2527182
	O	3.2649183	0.1378801	-0.1980515
	O	-1.5977246	-1.4436858	-0.5541326
	H	1.9784986	-1.3410348	-0.9210062
	H	2.6206811	-1.6246030	0.7120400
	H	0.2967655	-0.9313038	0.8406867
	H	1.3337547	0.3142924	1.5494249
	H	0.2299561	0.4113910	-1.2972744
	H	1.1885731	1.6498338	-0.5016981
	H	-0.8930733	2.5644930	-0.1278712
	H	-0.7950154	1.5718299	1.3074383
	H	-2.2683538	0.8914402	-1.2893698
	H	-2.9879024	1.4696943	0.2059621
	H	-2.1398471	-0.6743799	1.3126067
	H	-3.4568696	-0.8143921	0.1321121
	H	4.0245743	-0.2862828	-0.6170500
	H	-1.8771770	-2.3521837	-0.3807706
g+G+G-G-G-G-g-	C	2.6097908	0.1840356	-0.1578626
	C	1.3762039	0.9731285	-0.5823919
	C	0.3140481	1.1395301	0.5082489
	C	-0.3396561	-0.1469059	1.0214705
	C	-1.0688938	-0.9650180	-0.0459038
	C	-2.1334089	-0.1932458	-0.8140991
	O	2.3777555	-1.2276461	-0.0279640
	O	-3.1039328	0.4226710	0.0436709
	H	2.9406615	0.5078434	0.8302411
	H	3.4316245	0.3627169	-0.8593556
	H	1.7133309	1.9700476	-0.8872576
	H	0.9506386	0.5118827	-1.4804682
	H	-0.4631547	1.8182667	0.1458372

H	0.7814920	1.6482722	1.3582499	
H	-1.0542773	0.1309519	1.8002288	
H	0.4149276	-0.7848668	1.4843878	
H	-1.5385966	-1.8322472	0.4326500	
H	-0.3543664	-1.3730785	-0.7669392	
H	-1.6948027	0.6335745	-1.3722419	
H	-2.6268546	-0.8529860	-1.5366387	
H	2.2871265	-1.5977190	-0.9156196	
H	-3.5475671	-0.2766838	0.5424771	
g+G-G-G+G+G-g-	C	-1.8232688	-0.4788277	0.6816166
C	-1.8055289	0.8403276	-0.0835368	
C	-0.5028953	1.1865525	-0.8144812	
C	0.6657130	1.6644380	0.0600488	
C	1.5051157	0.6129313	0.7970075	
C	2.1401262	-0.4339117	-0.1131871	
O	-1.6032208	-1.6047732	-0.1654421	
O	1.2452847	-1.5225080	-0.4314109	
H	-2.8096133	-0.6291673	1.1223049	
H	-1.0993614	-0.4660929	1.5038075	
H	-2.6112067	0.7920330	-0.8212128	
H	-2.0542709	1.6518312	0.6106876	
H	-0.7333940	2.0003873	-1.5080541	
H	-0.1920007	0.3468603	-1.4418267	
H	0.2850441	2.3860062	0.7908840	
H	1.3569885	2.2220946	-0.5813304	
H	0.9287093	0.0991877	1.5695492	
H	2.3123571	1.1394865	1.3176054	
H	2.4184513	0.0074736	-1.0715114	
H	3.0473200	-0.8400663	0.3411199	
H	-0.6820838	-1.5556985	-0.4724808	
H	1.3552995	-2.2079732	0.2411479	
tG-G-G-G-G+g+	C	-2.1450168	-0.2071781	-0.7883779
C	-1.0767058	-0.9827143	-0.0406870	
C	-0.3406671	-0.1673629	1.0244026	
C	0.3035235	1.1253383	0.5151427	
C	1.3565499	0.9748264	-0.5869389	
C	2.6110806	0.2119180	-0.1772062	
O	-3.0611408	0.3223341	0.1818706	
O	2.4065757	-1.2003559	-0.0155185	
H	-2.6678006	-0.8720461	-1.4842470	
H	-1.6988501	0.6068044	-1.3702501	
H	-1.5507197	-1.8441730	0.4371076	
H	-0.3701151	-1.3814469	-0.7740969	
H	0.4228380	-0.8044162	1.4733461	
H	-1.0526978	0.0965363	1.8092295	
H	0.7752207	1.6316085	1.3644358	
H	-0.4802710	1.8028297	0.1637195	
H	1.6730193	1.9764008	-0.8994723	
H	0.9285019	0.5031029	-1.4784663	
H	3.4130088	0.3909837	-0.9016300	
H	2.9595765	0.5586732	0.7967738	

H	-3.7714230	0.7812251	-0.2847288	
H	2.2636001	-1.5829902	-0.8908633	
g+G-TG+G-G-g-	C	2.6098674	-0.6411206	0.4718052
C	1.1225440	-0.4693539	0.1891726	
C	0.7012301	0.9889646	0.0223851	
C	-0.7701159	1.1994538	-0.3489823	
C	-1.7723519	0.6705889	0.6874695	
C	-2.2979575	-0.7311331	0.3933018	
O	3.4431259	-0.2312437	-0.6188467	
O	-2.9940637	-0.8015476	-0.8575039	
H	2.8459247	-1.6940965	0.6214192	
H	2.8843269	-0.1017942	1.3867138	
H	0.8716084	-1.0344378	-0.7131045	
H	0.5782313	-0.9218081	1.0238052	
H	1.3098532	1.4504294	-0.7619672	
H	0.9179009	1.5315447	0.9508190	
H	-0.9775897	0.7302142	-1.3147215	
H	-0.9287292	2.2721377	-0.4886456	
H	-2.6367180	1.3412461	0.7432451	
H	-1.3244501	0.6766348	1.6879829	
H	-1.4854613	-1.4478203	0.2952043	
H	-2.9464814	-1.0668224	1.2100901	
H	3.3791830	0.7275970	-0.7103431	
H	-3.7718388	-0.2303187	-0.8018359	
g+G-G-TG-G+g-	C	-2.6380321	-0.1671752	-0.3247758
C	-1.7994507	-0.5364773	0.8925153	
C	-0.3041949	-0.2482674	0.7395772	
C	0.3511855	-0.9891965	-0.4289207	
C	1.8824981	-0.9735926	-0.4326118	
C	2.5232325	0.4105953	-0.4916759	
O	-2.5551654	1.2269707	-0.6498005	
O	2.6204178	1.0611430	0.7814984	
H	-3.6922157	-0.3472373	-0.1163059	
H	-2.3643223	-0.7787758	-1.1902179	
H	-2.1867970	0.0119583	1.7546982	
H	-1.9424433	-1.6037352	1.0948941	
H	0.2000253	-0.5280923	1.6695380	
H	-0.1750245	0.8339914	0.6262914	
H	-0.0017831	-0.5761200	-1.3805452	
H	0.0161496	-2.0317635	-0.4090287	
H	2.2275470	-1.5425675	-1.3020403	
H	2.2678781	-1.4845557	0.4545530	
H	3.5555464	0.3273148	-0.8292835	
H	1.9903604	1.0460426	-1.2111091	
H	-1.7064690	1.3948887	-1.0784294	
H	1.7313551	1.2572635	1.1000421	
tG+G-G+TG-g+	C	2.3691438	-0.5972976	0.2289888
C	2.1714971	0.8446042	-0.2022129	
C	0.8761585	1.5312302	0.2432840	
C	-0.4293743	0.9111629	-0.2810884	
C	-1.0490058	-0.1110623	0.6720677	

C	-2.2179723	-0.8691538	0.0633112
O	1.5123871	-1.4386645	-0.5625619
O	-3.3224831	-0.0195560	-0.2845812
H	2.1401900	-0.7131841	1.2951863
H	3.4140325	-0.8830032	0.0719651
H	3.0144594	1.4196404	0.1948247
H	2.2516416	0.8782213	-1.2927265
H	0.9398757	2.5713039	-0.0892199
H	0.8428554	1.5660860	1.3382358
H	-0.2420723	0.4370083	-1.2499379
H	-1.1523508	1.7156638	-0.4464063
H	-1.3915814	0.3987428	1.5778573
H	-0.2943871	-0.8448291	0.9613514
H	-1.8780916	-1.4310990	-0.8141797
H	-2.6296470	-1.5790640	0.7804385
H	1.7533281	-2.3600331	-0.3990673
H	-3.0443495	0.5524409	-1.0111437
g+TTG-G+G-g-C	2.3514185	-0.0735320	0.3894431
C	1.0811284	-0.3747355	-0.3888465
C	0.1186788	-1.2605382	0.4021966
C	-1.2378947	-1.4814840	-0.2845623
C	-2.3396052	-0.4705796	0.0500662
C	-2.0785926	0.9818647	-0.3302142
O	3.2874619	0.7110987	-0.3623349
O	-1.1257093	1.6400430	0.5208357
H	2.8845252	-0.9935236	0.6321243
H	2.0995199	0.4300093	1.3298350
H	0.5962577	0.5711648	-0.6346254
H	1.3536925	-0.8695893	-1.3254873
H	-0.0419448	-0.8301258	1.3957563
H	0.5987613	-2.2319959	0.5578404
H	-1.6184824	-2.4700344	-0.0115327
H	-1.0912253	-1.5031199	-1.3703242
H	-2.5632645	-0.5149031	1.1226398
H	-3.2554528	-0.7821022	-0.4642915
H	-1.6568282	1.0466317	-1.3341239
H	-3.0199336	1.5412738	-0.3295120
H	2.8505733	1.5420684	-0.5926191
H	-1.5205573	1.7230380	1.3991155
tG+G+G-G-G-t C	-2.2094302	0.4242643	0.3215410
C	-1.9114285	-0.9535663	-0.2384233
C	-0.4388179	-1.2352621	-0.5513633
C	0.5290548	-1.1485992	0.6362790
C	1.0674441	0.2456332	0.9824089
C	1.8061061	0.9185309	-0.1586158
O	-1.6360749	1.3999244	-0.5637787
O	2.8692240	0.0421848	-0.5694459
H	-1.7917042	0.5329608	1.3274917
H	-3.2929854	0.5644449	0.3919968
H	-2.2779507	-1.6906938	0.4844051
H	-2.4966628	-1.0845576	-1.1528433

H	-0.1116682	-0.5755367	-1.3564069	
H	-0.3898634	-2.2500443	-0.9567591	
H	1.3920530	-1.7826914	0.4252321	
H	0.0463713	-1.5705501	1.5253894	
H	1.7572786	0.1494268	1.8259629	
H	0.2679376	0.9187576	1.2956358	
H	1.1249643	1.1172430	-0.9896756	
H	2.2152518	1.8753900	0.1839501	
H	-1.9774916	2.2705618	-0.3213780	
H	3.3274413	0.4473258	-1.3167971	
g+TTG+G-G-g+	C	2.5268515	0.1758965	0.2929050
C	1.1144751	0.0716069	-0.2656922	
C	0.2739301	1.3113265	0.0496013	
C	-1.1398671	1.3078982	-0.5529682	
C	-2.2285799	0.6708440	0.3176581	
C	-2.0248912	-0.7953715	0.6734968	
O	3.3054201	-1.0019591	0.0538764	
O	-1.9650955	-1.6470210	-0.4769137	
H	2.4974844	0.2785224	1.3777167	
H	3.0289811	1.0608662	-0.1148125	
H	1.1730363	-0.0514712	-1.3541717	
H	0.6656782	-0.8362353	0.1415651	
H	0.8148954	2.1844036	-0.3287984	
H	0.2073252	1.4414517	1.1357519	
H	-1.1179226	0.8255700	-1.5361543	
H	-1.4441261	2.3407603	-0.7418912	
H	-3.1877893	0.7624000	-0.1988259	
H	-2.3105300	1.2362049	1.2527640	
H	-1.1355193	-0.9277814	1.2983695	
H	-2.8792386	-1.1577640	1.2445258	
H	3.4008131	-1.1110563	-0.9015512	
H	-1.1520969	-1.4507966	-0.9600851	
tG+TG+G-G+g+	C	-2.5075964	-0.0582747	0.4363743
C	-1.1006241	0.3422366	0.8339347	
C	-0.4078646	1.1757419	-0.2428021	
C	1.0616169	1.5170924	0.0536964	
C	2.1157048	0.5515313	-0.5034556	
C	2.2773473	-0.7963906	0.1867697	
O	-2.4098950	-0.8813601	-0.7397693	
O	1.1586304	-1.6793895	0.0503595	
H	-3.1135618	0.8308024	0.2231843	
H	-2.9853580	-0.6153939	1.2487078	
H	-1.1593174	0.9223136	1.7615243	
H	-0.5276958	-0.5623374	1.0358651	
H	-0.9687181	2.1095121	-0.3609520	
H	-0.4778913	0.6543550	-1.2006576	
H	1.2059501	1.6236998	1.1352619	
H	1.2797519	2.4986349	-0.3773463	
H	3.0936362	1.0427747	-0.4469785	
H	1.9235767	0.3846654	-1.5704927	
H	3.1845442	-1.2846139	-0.1874199	

H	2.3945979	-0.6580067	1.2629940	
H	-3.2987378	-1.1672917	-0.9868472	
H	0.9311518	-1.7521375	-0.8865036	
tG-G+G+G+G-tC	-2.4145541	0.3745498	-0.2624555	
C	-1.1087842	1.1294820	-0.0966106	
C	-0.2617134	0.7204511	1.1107009	
C	0.2617131	-0.7204519	1.1107006	
C	1.1087845	-1.1294819	-0.0966108	
C	2.4145541	-0.3745490	-0.2624546	
O	-2.1286296	-0.9552878	-0.7328736	
O	2.1286295	0.9552887	-0.7328721	
H	-3.0517462	0.8929552	-0.9867342	
H	-2.9495008	0.3305085	0.6943212	
H	-0.5297077	1.0420390	-1.0176437	
H	-1.3615490	2.1895197	0.0119544	
H	-0.8586755	0.8651232	2.0190636	
H	0.5825565	1.4091944	1.1733039	
H	-0.5825568	-1.4091953	1.1733029	
H	0.8586749	-0.8651245	2.0190633	
H	0.5297084	-1.0420384	-1.0176442	
H	1.3615495	-2.1895196	0.0119537	
H	2.9495002	-0.3305080	0.6943225	
H	3.0517469	-0.8929539	-0.9867330	
H	-2.9674830	-1.4121483	-0.8785305	
H	2.9674829	1.4121468	-0.8785361	
tG+G-G-G-G+g+ C	-2.4218937	-0.3387240	-0.2323285	
C	-1.1401883	-1.1388462	-0.0851821	
C	-0.2537316	-0.7490827	1.1003293	
C	0.2568266	0.6956650	1.1180466	
C	1.1188922	1.1215949	-0.0721755	
C	2.4219722	0.3496426	-0.2372160	
O	-2.0973690	0.9456868	-0.7944524	
O	2.2459836	-0.9910506	-0.7250730	
H	-2.9055093	-0.2163059	0.7444021	
H	-3.1166106	-0.8658245	-0.8944940	
H	-1.4182665	-2.1910854	0.0320484	
H	-0.5896683	-1.0689086	-1.0258277	
H	0.5962935	-1.4334796	1.1239827	
H	-0.8238668	-0.9176833	2.0212511	
H	0.8444305	0.8334981	2.0331230	
H	-0.5922322	1.3789679	1.1830204	
H	1.3802158	2.1777344	0.0585973	
H	0.5382986	1.0690308	-0.9977347	
H	3.1014336	0.8972215	-0.8996522	
H	2.9214744	0.2321037	0.7259729	
H	-2.9165715	1.4464732	-0.9040663	
H	1.8883817	-0.9314662	-1.6208625	
C-G-TG-G+G-t C	-2.3940095	-0.0348868	0.2647172	
C	-1.1211268	-0.7234946	0.7383316	
C	-0.3006715	-1.3260284	-0.4064983	
C	1.1785956	-1.5375750	-0.0602573	

C	2.0987759	-0.3449496	-0.3466988	
C	1.8636956	0.9340426	0.4398925	
O	-2.1191515	1.0363462	-0.6437822	
O	0.7330278	1.6485278	-0.1069962	
H	-2.9524349	0.3456293	1.1270605	
H	-3.0388414	-0.7393368	-0.2669037	
H	-0.5256457	0.0114931	1.2842199	
H	-1.3839200	-1.5069904	1.4564210	
H	-0.3731143	-0.6849831	-1.2880065	
H	-0.7507087	-2.2834161	-0.6852655	
H	1.5667965	-2.3796797	-0.6404610	
H	1.2736282	-1.8262296	0.9930031	
H	2.0553714	-0.0925717	-1.4102640	
H	3.1278840	-0.6554484	-0.1382591	
H	1.6910626	0.7136757	1.4990466	
H	2.7494491	1.5703820	0.3630686	
H	-1.2034822	1.3204446	-0.4898329	
H	0.7603437	2.5554551	0.2277714	
g+G-G+TG-G+g+ C		-2.7769275	0.2801317	0.2547032
C	-1.5996169	1.1262754	-0.2217705	
C	-0.2273850	0.7417220	0.3400906	
C	0.2026805	-0.7017834	0.0674857	
C	1.6371268	-1.0372565	0.4881658	
C	2.7319424	-0.4134432	-0.3710322	
O	-2.9585284	-0.9348667	-0.4879581	
O	2.8725245	1.0048070	-0.2050600	
H	-3.7105400	0.8219365	0.1076611	
H	-2.6827217	0.0653225	1.3268912	
H	-1.5832010	1.0923269	-1.3153564	
H	-1.7974254	2.1666037	0.0569266	
H	-0.2276678	0.9044457	1.4247686	
H	0.5227666	1.4154946	-0.0747664	
H	0.0907913	-0.9230497	-1.0006690	
H	-0.4597747	-1.3865916	0.6095169	
H	1.7720631	-2.1233326	0.4407245	
H	1.7943692	-0.7535480	1.5354338	
H	3.6874173	-0.9097294	-0.1702469	
H	2.5025521	-0.5503395	-1.4287519	
H	-2.1810825	-1.4912143	-0.3609463	
H	3.2256932	1.1697147	0.6791246	
tG-G+G-TG+g+ C		-2.4162480	-0.5493926	0.2657972
C	-2.1718951	0.8784301	-0.1887574	
C	-0.8398173	1.5193714	0.2152722	
C	0.4302613	0.8579416	-0.3433774	
C	1.0358842	-0.1915472	0.5861226	
C	2.2546516	-0.8829258	-0.0047875	
O	-1.6221891	-1.4385037	-0.5385593	
O	3.3266243	0.0244378	-0.3042526	
H	-3.4767104	-0.7915148	0.1447037	
H	-2.1597989	-0.6622939	1.3262719	
H	-2.2795699	0.9036072	-1.2770679	

H	-2.9815536	1.4896154	0.2238465	
H	-0.7781103	1.5592059	1.3093948	
H	-0.8773420	2.5597314	-0.1208122	
H	1.1850879	1.6241101	-0.5326419	
H	0.2075221	0.3916485	-1.3073027	
H	0.2931460	-0.9587763	0.8126928	
H	1.3174013	0.2809017	1.5361311	
H	2.6069790	-1.6744008	0.6662681	
H	1.9999059	-1.3405663	-0.9607761	
H	-1.9201088	-2.3434824	-0.3783809	
H	3.6045287	0.4364795	0.5246270	
g+G+G-G-G-G-g+ C	-2.6174070	-0.1969974	-0.1742471	
C	-1.3699138	-0.9618001	-0.6012904	
C	-0.3149865	-1.1326306	0.4957708	
C	0.3396279	0.1545725	1.0109722	
C	1.0845817	0.9728634	-0.0474437	
C	2.1661343	0.2078034	-0.7981146	
O	-2.3980319	1.2085901	0.0203866	
O	3.2071682	-0.2774432	0.0605333	
H	-2.9700552	-0.5637932	0.7909852	
H	-3.4199493	-0.3526426	-0.9027852	
H	-1.6931589	-1.9576366	-0.9239746	
H	-0.9404523	-0.4819391	-1.4868849	
H	0.4538893	-1.8200564	0.1272631	
H	-0.7865924	-1.6426810	1.3426602	
H	1.0344281	-0.1094853	1.8156001	
H	-0.4215557	0.7918451	1.4621414	
H	1.5496397	1.8354037	0.4368585	
H	0.3742050	1.3683193	-0.7792392	
H	1.7342410	-0.6185155	-1.3736395	
H	2.6725603	0.8677175	-1.5019452	
H	-2.2905377	1.6188950	-0.8475188	
H	2.8181541	-0.9019120	0.6863678	
tTTG-G+G-t C	2.3187214	-0.0243360	0.3870182	
C	1.0806634	-0.3987445	-0.3992177	
C	0.1060628	-1.2373405	0.4272757	
C	-1.2378072	-1.4830416	-0.2770726	
C	-2.3492897	-0.4740377	0.0307785	
C	-2.0823174	0.9738391	-0.3401123	
O	3.1926344	0.7045027	-0.4902278	
O	-1.1750092	1.5326576	0.6243177	
H	2.8178584	-0.9267353	0.7592510	
H	2.0363111	0.5930738	1.2464325	
H	0.6017361	0.5203211	-0.7339987	
H	1.3884615	-0.9584069	-1.2872717	
H	-0.0740441	-0.7494569	1.3892095	
H	0.5781490	-2.2012966	0.6424686	
H	-1.6176146	-2.4688403	0.0067672	
H	-1.0746990	-1.5223163	-1.3601444	
H	-2.5890634	-0.5020930	1.0978710	
H	-3.2517322	-0.7870140	-0.5043441	

H	-1.6591745	1.0386312	-1.3495101	
H	-3.0234357	1.5331346	-0.3285362	
H	3.9757033	0.9698012	0.0091906	
H	-1.0395493	2.4658095	0.4122929	
g+G-G-G+TG-g-	C	-2.2622880	-0.5258171	0.6252600
C	-2.0739074	0.9465183	0.2884958	
C	-0.8122499	1.2897253	-0.5125745	
C	0.5198754	0.9150336	0.1556781	
C	1.0310537	-0.4905411	-0.1655159	
C	2.4177725	-0.7621454	0.4050928	
O	-2.3563072	-1.3610731	-0.5347783	
O	3.4139190	0.1299252	-0.1102585	
H	-3.2069539	-0.6697310	1.1487705	
H	-1.4647234	-0.8771418	1.2888445	
H	-2.9514581	1.2835311	-0.2697652	
H	-2.0557687	1.5058882	1.2303377	
H	-0.8286283	2.3681893	-0.6898988	
H	-0.8647507	0.8332589	-1.5075797	
H	0.4284021	1.0245524	1.2425524	
H	1.2915825	1.6210934	-0.1569158	
H	1.0688328	-0.6230160	-1.2544437	
H	0.3573687	-1.2597790	0.2229663	
H	2.4222419	-0.5949355	1.4826926	
H	2.7058975	-1.8030666	0.2246548	
H	-1.5333907	-1.2795859	-1.0340891	
H	3.5354874	-0.0652220	-1.0489799	
tG+G-G+TTg+	C	-2.0868467	0.9667527	0.3422922
C	-2.3512725	-0.4815804	-0.0288102	
C	-1.2357312	-1.4871465	0.2757730	
C	0.1063022	-1.2301485	-0.4282935	
C	1.0785827	-0.3883713	0.3987161	
C	2.3008335	0.0295460	-0.4013662	
O	-1.1730934	1.5224652	-0.6170380	
O	3.2231004	0.8201172	0.3631140	
H	-1.6702898	1.0328997	1.3546133	
H	-3.0279155	1.5258710	0.3246640	
H	-3.2522282	-0.7977782	0.5067870	
H	-2.5915307	-0.5093522	-1.0957154	
H	-1.6101522	-2.4736461	-0.0125991	
H	-1.0732260	-1.5304688	1.3589373	
H	-0.0763698	-0.7357611	-1.3861030	
H	0.5845122	-2.1891634	-0.6516206	
H	1.3992367	-0.9675336	1.2734401	
H	0.5890809	0.5141750	0.7624132	
H	2.8059537	-0.8508675	-0.8168726	
H	2.0007529	0.6681363	-1.2316894	
H	-1.0474998	2.4596597	-0.4167570	
H	3.5196937	0.2865329	1.1120518	
g+TG+G+G-G-g-	C	-2.1934393	-0.1342031	-0.3756938
C	-1.1326109	-0.2992365	0.7034098	
C	-0.1709234	-1.4593786	0.4134149	

C	0.8582518	-1.1847901	-0.6958889	
C	2.1838170	-0.6011114	-0.1981569	
C	2.0674364	0.7219122	0.5457915	
O	-3.0716492	0.9665667	-0.1092576	
O	1.3677533	1.7257700	-0.2051023	
H	-2.8403641	-1.0115989	-0.4119769	
H	-1.7299167	-0.0175412	-1.3607774	
H	-0.5811392	0.6391579	0.7865468	
H	-1.6450380	-0.4658992	1.6543777	
H	-0.7683769	-2.3369405	0.1448577	
H	0.3593212	-1.7333663	1.3315708	
H	0.4306111	-0.5136139	-1.4438924	
H	1.0870737	-2.1179453	-1.2180196	
H	2.8595769	-0.4688343	-1.0508713	
H	2.6701380	-1.3193864	0.4714904	
H	1.4924738	0.6046521	1.4633318	
H	3.0622495	1.0829160	0.8268187	
H	-2.5290893	1.7653379	-0.0586585	
H	1.8899072	1.9310980	-0.9924486	
tG+G+G+G+G-g+ C	2.0886212	-0.2909243	-0.7837535	
C	1.0346724	-0.9841474	0.0587783	
C	0.3629183	-0.0573684	1.0750823	
C	-0.3045487	1.1871071	0.4792475	
C	-1.3517038	0.9587591	-0.6164696	
C	-2.5959336	0.1837986	-0.1959426	
O	3.0448463	0.2971116	0.1116165	
O	-2.4055418	-1.2376372	-0.1301264	
H	1.6356724	0.4812365	-1.4144545	
H	2.5750689	-1.0206963	-1.4389678	
H	0.2930029	-1.4230386	-0.6137117	
H	1.5140596	-1.8094058	0.5921524	
H	1.1167720	0.2738114	1.7922493	
H	-0.3619803	-0.6330179	1.6615330	
H	0.4773871	1.8405485	0.0822908	
H	-0.7748068	1.7483410	1.2940838	
H	-0.9152502	0.4522299	-1.4815792	
H	-1.6847235	1.9415910	-0.9679796	
H	-2.9749365	0.5655154	0.7599587	
H	-3.3809296	0.3160507	-0.9401494	
H	3.7490975	0.7005473	-0.4120855	
H	-1.8649229	-1.4380273	0.6431273	
tG-G-G+G+Tg+ C	2.1033171	0.6975751	0.5271092	
C	2.1795043	-0.6241439	-0.2131135	
C	0.8344696	-1.1789070	-0.6914999	
C	-0.1818866	-1.4355726	0.4339803	
C	-1.1344895	-0.2648417	0.7088887	
C	-2.2233429	-0.1460998	-0.3483140	
O	1.4534409	1.6529862	-0.3280300	
O	-3.0976716	0.9652882	-0.1100288	
H	3.1140829	1.0357665	0.7751658	
H	1.5456771	0.5885294	1.4634093	

H	2.8418985	-0.4960638	-1.0733192	
H	2.6539987	-1.3521647	0.4537501	
H	1.0382914	-2.1152063	-1.2182146	
H	0.4137912	-0.4956364	-1.4320796	
H	0.3568062	-1.6941125	1.3515490	
H	-0.7853755	-2.3159053	0.1888097	
H	-0.5752967	0.6729417	0.7364320	
H	-1.6210124	-0.3898207	1.6796668	
H	-1.7852133	-0.0749071	-1.3490028	
H	-2.8697914	-1.0241736	-0.3271333	
H	1.6145681	2.5380289	0.0239520	
H	-2.5645907	1.7701394	-0.1570964	
g+G+TG-G+G-g-	C	2.2858688	-0.8536054	-0.0174793
C	1.0225223	-0.2205186	0.5456855	
C	0.4321498	0.8494262	-0.3707057	
C	-0.8400817	1.5158467	0.1747625	
C	-2.1746272	0.8548231	-0.1862239	
C	-2.4039772	-0.5629620	0.3234702	
O	3.3422018	0.0946804	-0.2376250	
O	-1.6592232	-1.5630559	-0.3894588	
H	2.0871672	-1.2828490	-0.9998271	
H	2.6319888	-1.6599678	0.6381131	
H	0.2954764	-1.0171053	0.7106482	
H	1.2518286	0.2247291	1.5223232	
H	0.2251979	0.4054995	-1.3499268	
H	1.1936714	1.6150311	-0.5345398	
H	-0.8862397	2.5441215	-0.1960183	
H	-0.7668375	1.5926250	1.2659553	
H	-2.3016203	0.8580708	-1.2754225	
H	-2.9817506	1.4780114	0.2147856	
H	-2.0822188	-0.6553753	1.3617964	
H	-3.4717913	-0.8028859	0.2845094	
H	3.5881588	0.4665247	0.6198850	
H	-1.9888913	-1.5870501	-1.2976312	
g+G+TG+G-G-g+	C	2.5644320	-0.2678426	-0.4250990
C	1.1106229	-0.0028237	-0.7924390	
C	0.4989607	1.1537019	-0.0003549	
C	-0.9844658	1.4216931	-0.3014056	
C	-1.9708653	0.7062577	0.6298951	
C	-1.8725991	-0.8120395	0.6448007	
O	2.7218575	-0.6588543	0.9450547	
O	-2.1589423	-1.4087536	-0.6260210	
H	3.1526962	0.6449521	-0.5259992	
H	2.9959650	-1.0226930	-1.0907319	
H	1.0631346	0.2253040	-1.8637731	
H	0.5444827	-0.9278564	-0.6441071	
H	1.0809077	2.0511069	-0.2321813	
H	0.6350897	0.9711708	1.0689776	
H	-1.2010213	1.1715870	-1.3467280	
H	-1.1813091	2.4934866	-0.2174872	
H	-2.9923392	0.9807989	0.3529815	

H	-1.8053951	1.0621900	1.6524266	
H	-0.8882749	-1.1299431	1.0061233	
H	-2.6184576	-1.2281269	1.3213015	
H	2.3250813	-1.5333121	1.0551580	
H	-1.5674124	-1.0207198	-1.2838378	
g+G+G-G-G+G-g- C	-2.1360914	-0.6360760	0.0538648	
C	-1.4303421	0.4477741	0.8648711	
C	-0.8300228	1.5951746	0.0487192	
C	0.4506316	1.2758181	-0.7332851	
C	1.6657543	0.9106242	0.1447157	
C	2.1898777	-0.5029996	-0.0668681	
O	-1.3049315	-1.3075385	-0.8920046	
O	1.2717190	-1.5238639	0.3774294	
H	-2.9426218	-0.1897399	-0.5314606	
H	-2.5906815	-1.3586700	0.7435406	
H	-2.1745623	0.8597353	1.5554794	
H	-0.6610624	-0.0129194	1.4917791	
H	-0.6196128	2.4320164	0.7239380	
H	-1.5895103	1.9526179	-0.6546009	
H	0.6989176	2.1574114	-1.3304130	
H	0.2438577	0.4712854	-1.4396214	
H	1.4333740	1.0438210	1.2073932	
H	2.4966209	1.5917740	-0.0643837	
H	2.3338166	-0.7012689	-1.1286517	
H	3.1507764	-0.6412033	0.4374743	
H	-0.4804739	-1.5619940	-0.4420150	
H	1.2854018	-1.5403768	1.3438820	
g+G+G-G-G-G+g+ C	-2.4544456	-0.3561495	-0.2255634	
C	-1.1446841	-1.1283411	-0.1190867	
C	-0.2482633	-0.7248235	1.0537439	
C	0.2482636	0.7248226	1.0537445	
C	1.1446844	1.1283414	-0.1190858	
C	2.4544455	0.3561494	-0.2255641	
O	-2.2955475	0.9900575	-0.7037768	
O	2.2955466	-0.9900574	-0.7037777	
H	-2.9135667	-0.2515963	0.7587094	
H	-3.1603778	-0.8955292	-0.8661898	
H	-1.3946767	-2.1891414	-0.0078792	
H	-0.6034840	-1.0471602	-1.0672593	
H	0.6071169	-1.4021546	1.0804038	
H	-0.8129330	-0.8883090	1.9786568	
H	0.8129332	0.8883074	1.9786576	
H	-0.6071166	1.4021536	1.0804048	
H	1.3946777	2.1891413	-0.0078766	
H	0.6034840	1.0471625	-1.0672583	
H	3.1603771	0.8955292	-0.8661912	
H	2.9135677	0.2515959	0.7587082	
H	-2.0460685	0.9457160	-1.6359328	
H	2.0460672	-0.9457157	-1.6359335	
g+G+G+G-G-G-g- C	2.3257103	-0.3349645	0.4834556	
C	1.9825251	0.9804902	-0.2005406	

C	0.5166706	1.1282318	-0.6187901	
C	-0.4844570	1.0091840	0.5415722	
C	-1.0471746	-0.4022589	0.7471874	
C	-2.0690624	-0.7979980	-0.3107076	
O	1.9651577	-1.4830649	-0.2982346	
O	-3.2119321	0.0705645	-0.3350142	
H	1.7727588	-0.4454319	1.4156290	
H	3.3925126	-0.3628417	0.7297329	
H	2.2486976	1.7926674	0.4853454	
H	2.6242824	1.0988018	-1.0813237	
H	0.2861987	0.3862507	-1.3871127	
H	0.4066506	2.1046852	-1.0979243	
H	-1.3271539	1.6821933	0.3688534	
H	-0.0047541	1.3502981	1.4654118	
H	-1.5283302	-0.4657903	1.7303580	
H	-0.2479916	-1.1466047	0.7326573	
H	-1.6438314	-0.7252164	-1.3110762	
H	-2.3829306	-1.8359740	-0.1583688	
H	2.4796628	-1.4630215	-1.1165017	
H	-3.6647523	-0.0107740	0.5150383	
tG-G-G+G+G+g+ C	2.3293987	0.3320138	0.4709577	
C	1.9800651	-0.9840794	-0.1967199	
C	0.5135964	-1.1276405	-0.6147242	
C	-0.4906970	-1.0137352	0.5432783	
C	-1.0505689	0.3975577	0.7538191	
C	-2.0670166	0.8017237	-0.3063437	
O	1.9697572	1.3947475	-0.4261643	
O	-3.2168117	-0.0570569	-0.3310178	
H	3.4023999	0.3610469	0.6852586	
H	1.7936568	0.4403369	1.4203784	
H	2.6196367	-1.1012212	-1.0756298	
H	2.2381192	-1.7894897	0.4994352	
H	0.4048810	-2.1040972	-1.0941526	
H	0.2903491	-0.3845934	-1.3833226	
H	-0.0153407	-1.3604474	1.4673067	
H	-1.3348797	-1.6834728	0.3646587	
H	-0.2462622	1.1365685	0.7430748	
H	-1.5339490	0.4605688	1.7361235	
H	-2.3733556	1.8424374	-0.1553596	
H	-1.6395447	0.7243907	-1.3051793	
H	2.3675163	2.2151727	-0.1072357	
H	-3.6648113	0.0216974	0.5218223	
tTG+G-G-Tg+ C	-1.6856521	-0.7500351	0.3102661	
C	-1.6903702	0.7197936	-0.0706368	
C	-0.5561178	1.5371660	0.5688912	
C	0.6946472	1.6935081	-0.3059728	
C	1.3914375	0.3929620	-0.7135331	
C	1.9758695	-0.3763979	0.4617417	
O	-2.8192639	-1.3544571	-0.3287760	
O	2.5553466	-1.6263859	0.0652209	
H	-1.7653325	-0.8464108	1.3995675	

H	-0.7643670	-1.2437761	-0.0090542	
H	-1.6491386	0.8008372	-1.1606308	
H	-2.6591946	1.1209454	0.2351780	
H	-0.2913853	1.1065460	1.5402349	
H	-0.9256130	2.5426176	0.7859426	
H	1.4142846	2.3320097	0.2179781	
H	0.4099294	2.2336754	-1.2137610	
H	2.2057932	0.6343791	-1.4059201	
H	0.7070680	-0.2595026	-1.2603287	
H	2.7149691	0.2434107	0.9834586	
H	1.2061725	-0.6484727	1.1820102	
H	-2.8027243	-2.3034424	-0.1490326	
H	3.2429078	-1.4422233	-0.5887169	
g+G+G+G+G+G-g+ C	2.0794700	-0.2584359	-0.8072670	
C	1.0366164	-0.9714720	0.0430013	
C	0.3651246	-0.0645347	1.0768225	
C	-0.3166400	1.1810773	0.4989017	
C	-1.3567988	0.9568736	-0.6040318	
C	-2.5992658	0.1713483	-0.1994986	
O	3.0840020	0.3970735	-0.0204426	
O	-2.3965967	-1.2485711	-0.1278758	
H	1.6273385	0.5373309	-1.3977646	
H	2.5399169	-0.9657318	-1.5051621	
H	0.2908398	-1.4126408	-0.6242699	
H	1.5187059	-1.8075022	0.5626175	
H	1.1191874	0.2711035	1.7927528	
H	-0.3481427	-0.6535174	1.6638829	
H	0.4582988	1.8500976	0.1151487	
H	-0.7963177	1.7228701	1.3213022	
H	-0.9125246	0.4634280	-1.4726385	
H	-1.6939338	1.9414138	-0.9464100	
H	-2.9953909	0.5509395	0.7501565	
H	-3.3745471	0.2956656	-0.9551310	
H	3.5808992	-0.2808837	0.4568211	
H	-1.8850955	-1.4446329	0.6658985	
tG+G+G-G-Tg+ C	1.5960683	-0.9060429	0.6340271	
C	1.8775237	0.5681764	0.3839336	
C	0.9608407	1.2589137	-0.6344975	
C	-0.3639434	1.8049897	-0.0859272	
C	-1.3215612	0.7787582	0.5273388	
C	-1.7088955	-0.3372624	-0.4316661	
O	1.6685067	-1.5800619	-0.6330649	
O	-2.5366091	-1.3297402	0.1946335	
H	0.6145003	-1.0631639	1.0863447	
H	2.3518002	-1.3045463	1.3190683	
H	1.8399029	1.0957862	1.3436617	
H	2.9090757	0.6350342	0.0283321	
H	0.7851071	0.5790388	-1.4704378	
H	1.5057169	2.1109840	-1.0510142	
H	-0.8817511	2.3228496	-0.9006093	
H	-0.1438717	2.5676441	0.6680904	

H	-2.2322144	1.2986879	0.8466571	
H	-0.8928624	0.3357122	1.4284510	
H	-2.2117664	0.0830197	-1.3109751	
H	-0.8337506	-0.8830326	-0.7778537	
H	1.5052542	-2.5214511	-0.4886346	
H	-3.3320820	-0.8901816	0.5236472	
tTG+G-G-Tt	C	-1.6781761	-0.7631081	0.3063286
C	-1.6978798	0.7118631	-0.0532382	
C	-0.5604850	1.5293151	0.5799015	
C	0.6822323	1.6941456	-0.3049706	
C	1.3896186	0.4042811	-0.7253668	
C	1.9846064	-0.3651336	0.4372037	
O	-2.8299133	-1.3617393	-0.3047255	
O	2.5932723	-1.5483174	-0.1006013	
H	-1.7239870	-0.8754246	1.3963023	
H	-0.7657796	-1.2484036	-0.0494108	
H	-1.6734165	0.8082558	-1.1423848	
H	-2.6650293	1.1011854	0.2729028	
H	-0.2872380	1.0948157	1.5472451	
H	-0.9322222	2.5322745	0.8049544	
H	1.3997998	2.3402042	0.2125931	
H	0.3847898	2.2325558	-1.2097376	
H	2.2028158	0.6462034	-1.4141203	
H	0.7086412	-0.2512111	-1.2723532	
H	2.7306418	0.2551105	0.9475736	
H	1.2147481	-0.6370866	1.1659814	
H	-2.7834280	-2.3182238	-0.1781813	
H	3.0155369	-2.0329201	0.6206228	
g-G-G+G-TG+g-	C	-2.3609397	-0.6024344	0.2684751
C	-2.1732908	0.8368237	-0.1954761	
C	-0.8700692	1.5298524	0.2152243	
C	0.4322078	0.9000159	-0.3042283	
C	1.0362869	-0.1461433	0.6326227	
C	2.2452159	-0.8549934	0.0414956	
O	-1.5516993	-1.5480697	-0.4491296	
O	3.3476586	0.0268867	-0.2226166	
H	-3.4159763	-0.8843967	0.1889345	
H	-2.0686703	-0.7106788	1.3138247	
H	-2.2759083	0.8667765	-1.2866918	
H	-3.0094292	1.4208465	0.2048231	
H	-0.8259422	1.5877870	1.3086070	
H	-0.9334242	2.5628623	-0.1389998	
H	1.1633858	1.7015213	-0.4480395	
H	0.2541086	0.4488448	-1.2865862	
H	0.2917285	-0.9088885	0.8645642	
H	1.3353812	0.3375808	1.5675164	
H	2.6382631	-1.5881732	0.7449758	
H	1.9547150	-1.3867264	-0.8720432	
H	-1.8923703	-1.6050566	-1.3516001	
H	3.0925213	0.6244601	-0.9366741	
tTG-G-G+Tg+	C	-1.9911605	-0.3672328	-0.4426736

C	-1.3916559	0.3973893	0.7209088	
C	-0.6855083	1.6893951	0.3060591	
C	0.5603166	1.5280372	-0.5744922	
C	1.6985426	0.7117370	0.0616268	
C	1.7004089	-0.7619378	-0.3279294	
O	-2.6410731	-1.5247986	0.1017418	
O	2.8383020	-1.4596956	0.1946636	
H	-1.2188878	-0.6696625	-1.1564076	
H	-2.7123013	0.2682172	-0.9701841	
H	-2.2037567	0.6356483	1.4123211	
H	-0.7103154	-0.2624059	1.2630530	
H	-0.3931531	2.2285881	1.2122437	
H	-1.4029220	2.3335906	-0.2136737	
H	0.9299644	2.5311927	-0.8019667	
H	0.2913007	1.0884249	-1.5407868	
H	1.6491815	0.8001428	1.1533488	
H	2.6669492	1.1177184	-0.2394308	
H	0.7771815	-1.2603667	-0.0196473	
H	1.7874133	-0.8575652	-1.4109174	
H	-3.0182142	-2.0375224	-0.6250721	
H	2.7781756	-1.4486803	1.1591841	
tG+G+G-G-G-g+ C	-2.2204562	0.4142032	0.3346524	
C	-1.9160980	-0.9638845	-0.2215362	
C	-0.4423521	-1.2308037	-0.5423761	
C	0.5264819	-1.1367254	0.6460540	
C	1.0692819	0.2580692	0.9843005	
C	1.8224037	0.9325630	-0.1549660	
O	-1.6572772	1.3841891	-0.5615859	
O	2.9559584	0.1716389	-0.6016548	
H	-1.7973762	0.5308843	1.3374590	
H	-3.3044151	0.5470364	0.4105410	
H	-2.2707141	-1.7038820	0.5038400	
H	-2.5035123	-1.1017282	-1.1332872	
H	-0.1322638	-0.5593512	-1.3458632	
H	-0.3871058	-2.2436822	-0.9522892	
H	1.3845840	-1.7882251	0.4543115	
H	0.0432473	-1.5549024	1.5358979	
H	1.7511091	0.1633366	1.8342562	
H	0.2640376	0.9297910	1.2875559	
H	1.1496941	1.1497026	-0.9884187	
H	2.2393265	1.8789419	0.1892267	
H	-1.9802686	2.2595114	-0.3109194	
H	2.6326090	-0.5927139	-1.0951954	
tG-TG-G+G-t C	2.4937387	-0.1464267	0.5719332	
C	1.0267867	0.1481873	0.8171810	
C	0.4243049	1.0760869	-0.2362129	
C	-0.9971103	1.5625242	0.0856034	
C	-2.1630597	0.6945373	-0.4000278	
C	-2.2747060	-0.7048204	0.1790795	
O	2.6065494	-0.8269635	-0.6867611	
O	-1.3168908	-1.5461893	-0.4791461	

H	2.8927422	-0.7712350	1.3788666	
H	3.0644660	0.7903348	0.5494546	
H	0.4793628	-0.7940562	0.8399196	
H	0.9440993	0.6156802	1.8054312	
H	0.4412615	0.5773520	-1.2070164	
H	1.0752750	1.9539038	-0.3192654	
H	-1.1361811	2.5486425	-0.3679927	
H	-1.0909766	1.7145121	1.1677610	
H	-2.1267680	0.5978114	-1.4889930	
H	-3.0926517	1.2209513	-0.1592956	
H	-2.0944279	-0.6863690	1.2612715	
H	-3.2857755	-1.0896749	0.0095691	
H	3.5426045	-0.9837912	-0.8660889	
H	-1.4538204	-2.4586107	-0.1922788	
tTG-G-G+G+g+ C	-1.7142921	-0.3572543	-0.4320881	
C	-1.3410709	0.7596700	0.5229054	
C	-0.3911283	1.7921046	-0.0885478	
C	0.9400497	1.2610476	-0.6359373	
C	1.8629503	0.5902527	0.3895113	
C	1.6018086	-0.8920129	0.6465565	
O	-2.6672200	-1.1925036	0.2463226	
O	1.6197369	-1.6727664	-0.5581702	
H	-0.8372167	-0.9412498	-0.7210387	
H	-2.1587914	0.0674071	-1.3405690	
H	-2.2635888	1.2598006	0.8293719	
H	-0.9161600	0.3246569	1.4298417	
H	-0.1782619	2.5573543	0.6648484	
H	-0.9121860	2.3050777	-0.9040176	
H	1.4729519	2.1145134	-1.0651623	
H	0.7656467	0.5687583	-1.4631748	
H	1.8129066	1.1220443	1.3468173	
H	2.8995996	0.6843438	0.0462736	
H	2.3401335	-1.2762436	1.3585016	
H	0.6165322	-1.0649880	1.0712788	
H	-2.7984084	-1.9921304	-0.2795425	
H	2.5067295	-1.6187123	-0.9393039	
tTTG+G-G+g+ C	2.3384816	0.0209904	0.3963758	
C	1.0827621	0.3597680	-0.3790356	
C	0.1193911	1.2194622	0.4390870	
C	-1.2205083	1.4879224	-0.2640936	
C	-2.3472272	0.4897001	0.0201907	
C	-2.0863576	-0.9620574	-0.3627051	
O	3.2357817	-0.6565981	-0.4966959	
O	-1.1739043	-1.6321705	0.5212457	
H	2.0847599	-0.6213226	1.2465153	
H	2.8045846	0.9360286	0.7813020	
H	1.3738407	0.8996946	-1.2847904	
H	0.6082376	-0.5730191	-0.6797864	
H	0.6071827	2.1774239	0.6464469	
H	-0.0648808	0.7461788	1.4084848	
H	-1.0521634	1.5362048	-1.3458167	

H	-1.5872614	2.4761304	0.0287764	
H	-3.2400775	0.8182977	-0.5232382	
H	-2.6082488	0.5259449	1.0846342	
H	-3.0327102	-1.5118792	-0.4029951	
H	-1.6261730	-1.0242722	-1.3495508	
H	3.9913897	-0.9768623	0.0124398	
H	-1.6107301	-1.7285873	1.3778850	
tTG-G+G+G+g+	C	-1.8997985	-0.6237464	-0.3195665
C	-1.6015570	0.8425868	-0.0664349	
C	-0.2386461	1.3082264	-0.6059780	
C	0.8966974	1.3098495	0.4236194	
C	1.2619873	-0.0503329	1.0204485	
C	1.7847713	-1.0582757	0.0050389	
O	-3.1976791	-0.8947741	0.2279393	
O	2.9347766	-0.5816189	-0.7054141	
H	-1.1511960	-1.2678416	0.1503016	
H	-1.8895273	-0.8195537	-1.3979654	
H	-2.4065487	1.4127030	-0.5352902	
H	-1.6700098	1.0325423	1.0086086	
H	-0.3391257	2.3321277	-0.9743914	
H	0.0451168	0.7108043	-1.4785660	
H	0.6171189	1.9816391	1.2414001	
H	1.7885091	1.7358079	-0.0424020	
H	0.4035087	-0.4873405	1.5400204	
H	2.0309252	0.0963167	1.7878156	
H	2.0085153	-2.0089646	0.5018655	
H	1.0473978	-1.2583946	-0.7709795	
H	-3.4192610	-1.8189431	0.0548965	
H	3.6458369	-0.4416562	-0.0656777	
g+TG+G-G-Tg+	C	1.7217824	-0.7533068	-0.3313819
C	1.6954696	0.7159911	0.0737484	
C	0.5531807	1.5235145	-0.5662752	
C	-0.6930855	1.6786091	0.3142812	
C	-1.3964772	0.3790821	0.7128968	
C	-1.9966260	-0.3752501	-0.4646399	
O	2.8538360	-1.4438771	0.2112222	
O	-2.6180493	-1.6029579	-0.0666497	
H	1.8356340	-0.8363937	-1.4126081	
H	0.7959383	-1.2645161	-0.0523758	
H	1.6320732	0.7913910	1.1657345	
H	2.6615797	1.1388157	-0.2104977	
H	0.2862478	1.0804064	-1.5311983	
H	0.9155779	2.5287596	-0.7952125	
H	-1.4116294	2.3249066	-0.2011276	
H	-0.4019558	2.2106448	1.2250698	
H	-2.2040595	0.6203738	1.4130624	
H	-0.7151581	-0.2866682	1.2480163	
H	-2.7115096	0.2669816	-0.9930409	
H	-1.2306905	-0.6746028	-1.1779108	
H	2.7773113	-1.4333166	1.1745285	
H	-3.3156710	-1.3930169	0.5684844	

tG+G+G+G-Tg+	C	1.7915951	-1.0464126	0.0241040
	C	1.2673684	-0.0496776	
	C	0.8904442	1.3074658	
	C	-0.2278520	1.3012098	
	C	-1.5984920	0.8294825	
	C	-1.8748020	-0.6532027	
	O	2.9341198	-0.4534716	
	O	-3.1494698	-1.0534150	
	H	1.0277225	-1.2852035	
	H	2.0730196	-1.9765531	
	H	0.4154788	-0.4955764	
	H	2.0469740	0.1021647	
	H	1.7854036	1.7451561	
	H	0.5888072	1.9700541	
	H	0.0700949	0.7025103	
	H	-0.3262608	2.3246136	
	H	-2.3893233	1.3855850	
	H	-1.7028678	1.0547990	
	H	-1.8025468	-0.8907218	
	H	-1.1572367	-1.2761374	
	H	3.3084352	-1.0929128	
	H	-3.8262599	-0.5044452	
g+G-G+G-G-G+g-	C	-2.1429891	-0.6617129	0.0155482
	C	-1.7657736	0.8105783	
	C	-0.5702542	1.2575894	
	C	0.6936521	1.6244757	
	C	1.3379245	0.5117506	
	C	2.1582986	-0.4996268	
	O	-1.1776227	-1.5593933	
	O	1.3589260	-1.3077568	
	H	-3.0626111	-0.8581137	
	H	-2.3365864	-0.8915526	
	H	-1.5681146	1.0142007	
	H	-2.6498919	1.3973308	
	H	-0.3474542	0.4838682	
	H	-0.8547799	2.1416890	
	H	1.4438958	2.0306210	
	H	0.4291325	2.4462697	
	H	2.0253482	0.9688435	
	H	0.5824237	-0.0219835	
	H	2.6340398	-1.2040020	
	H	2.9460219	0.0032659	
	H	-0.3805827	-1.5523308	
	H	1.4150083	-0.9375003	
tG+G+G+G-G-g+	C	2.0384956	-0.8563943	-0.2043684
	C	1.0813563	-0.3312022	
	C	0.5063274	1.0528637	
	C	-0.4895748	1.0991231	
	C	-1.9627519	0.9657400	
	C	-2.3295699	-0.3274756	
	O	3.1250760	0.0739472	

O	-2.1369918	-1.4914285	-0.3402449	
H	1.5384101	-0.9562638	-1.1745560	
H	2.4048748	-1.8451042	0.0904262	
H	0.2879078	-1.0706244	0.9921112	
H	1.6291563	-0.2801918	1.7958036	
H	1.3502692	1.7118015	0.3164750	
H	0.0188206	1.4521578	1.4216271	
H	-0.2381871	0.3376302	-1.3902946	
H	-0.3815721	2.0515988	-1.1691522	
H	-2.5925633	1.0544385	-1.1279753	
H	-2.2199441	1.7994374	0.4239793	
H	-1.7771845	-0.4225362	1.4154284	
H	-3.3917791	-0.3323530	0.7168138	
H	3.7557853	-0.2541809	-0.9566252	
H	-1.2151086	-1.5104663	-0.6275994	
tG-G-G-G+Tg+ C	-1.8019383	-1.0469529	0.0280479	
C	-1.2680626	-0.0546686	1.0445598	
C	-0.8871876	1.3016425	0.4477905	
C	0.2241989	1.2928876	-0.6072501	
C	1.6035143	0.8306212	-0.1067741	
C	1.8875091	-0.6519751	-0.3120101	
O	-2.9456192	-0.4473650	-0.5975037	
O	3.2236995	-1.0076438	0.0665315	
H	-2.0842231	-1.9773779	0.5320280	
H	-1.0426725	-1.2864558	-0.7231427	
H	-2.0424597	0.0989657	1.8008566	
H	-0.4154499	-0.5073831	1.5591416	
H	-0.5782562	1.9619456	1.2647672	
H	-1.7832662	1.7438114	0.0078133	
H	0.3171861	2.3147499	-0.9836246	
H	-0.0778253	0.6895611	-1.4696658	
H	1.7070214	1.0756390	0.9573533	
H	2.3932345	1.3751217	-0.6298680	
H	1.1667720	-1.2758489	0.2240550	
H	1.8216081	-0.9001501	-1.3717621	
H	-3.3198457	-1.0787214	-1.2254029	
H	3.3421804	-0.7715851	0.9962915	
tG+G+G-G-G+g+ C	1.8913660	-0.4506969	0.6622802	
C	1.8846949	0.7254499	-0.2966613	
C	0.5208989	1.1480083	-0.8552104	
C	-0.5357036	1.5739656	0.1753877	
C	-1.3001939	0.4742839	0.9256579	
C	-2.2220522	-0.3952137	0.0765935	
O	1.1918311	-1.5543838	0.0496685	
O	-1.5465156	-1.2079689	-0.8848472	
H	1.4152274	-0.1890026	1.6110137	
H	2.9233305	-0.7444800	0.8736109	
H	2.3422511	1.5708688	0.2294048	
H	2.5400890	0.4820470	-1.1373469	
H	0.1212744	0.3632037	-1.4955133	
H	0.7099468	2.0071414	-1.5062047	

H	-1.2812153	2.1883396	-0.3407678
H	-0.0615492	2.2339030	0.9119153
H	-1.9293026	0.9590780	1.6805804
H	-0.6200789	-0.1785901	1.4761965
H	-2.8216669	-1.0271025	0.7432822
H	-2.9128355	0.2331150	-0.4909976
H	1.4204738	-2.3659431	0.5226885
H	-0.6843814	-1.4648286	-0.5161980
tTG-G+G+Tg+ C	1.7421344	-0.7289285	0.3414346
C	1.6974794	0.7270196	-0.0842396
C	0.5530364	1.5261799	0.5614171
C	-0.6975420	1.6678559	-0.3159481
C	-1.4013857	0.3664654	-0.7093586
C	-2.0045842	-0.3831355	0.4692590
O	2.8321946	-1.3446538	-0.3569259
O	-2.7723921	-1.5222002	0.0573061
H	0.8036415	-1.2381314	0.1024497
H	1.8949212	-0.7902842	1.4250080
H	2.6621890	1.1655347	0.1793683
H	1.6232439	0.7693395	-1.1745647
H	0.9085114	2.5351673	0.7844961
H	0.2922869	1.0867299	1.5298624
H	-0.4118954	2.1970308	-1.2299403
H	-1.4191410	2.3118456	0.1979810
H	-0.7083084	-0.2894278	-1.2471796
H	-2.2137338	0.5935865	-1.4044066
H	-1.2338742	-0.6878759	1.1842590
H	-2.7121821	0.2569207	0.9973870
H	2.9205896	-2.2569419	-0.0518135
H	-2.1945916	-2.1004616	-0.4584453
tTG-G+G+G-t C	-1.6727647	-0.5863662	0.1820622
C	-1.5293306	0.8149577	-0.3831841
C	-0.1161067	1.2192957	-0.8181882
C	0.8949641	1.4841578	0.3060439
C	1.5233807	0.2799480	1.0174718
C	2.3725034	-0.6211734	0.1388291
O	-3.0851055	-0.8600521	0.2502403
O	1.5020028	-1.4266319	-0.6759126
H	-1.2370642	-0.6612212	1.1816149
H	-1.1669866	-1.3073388	-0.4658848
H	-2.1868300	0.8622823	-1.2555422
H	-1.9187897	1.5353237	0.3427674
H	-0.2138443	2.1506252	-1.3843323
H	0.2819653	0.4720932	-1.5070351
H	0.4175067	2.1196456	1.0603024
H	1.7180563	2.0762055	-0.1101399
H	0.7711857	-0.3391933	1.5082418
H	2.1741896	0.6636299	1.8102057
H	3.0332159	-0.0159955	-0.4931484
H	2.9951067	-1.2678492	0.7656067
H	-3.2036812	-1.7437875	0.6213039

H	2.0475603	-2.0179884	-1.2115194	
g+TG-G+G+G+g+ C	-1.8782421	-0.6480443	-0.3085203	
C	-1.6018178	0.8318323	-0.0732304	
C	-0.2374734	1.3129160	-0.5953228	
C	0.8895928	1.3078316	0.4432330	
C	1.2628337	-0.0567498	1.0252439	
C	1.7830954	-1.0521532	-0.0039573	
O	-3.1437242	-1.0583831	0.2228230	
O	2.9184950	-0.5563546	-0.7251677	
H	-1.1516076	-1.2782465	0.1994179	
H	-1.8218835	-0.8687034	-1.3811868	
H	-2.3984719	1.3948675	-0.5714216	
H	-1.6957229	1.0405392	0.9965990	
H	-0.3403788	2.3408824	-0.9518541	
H	0.0548144	0.7262145	-1.4722912	
H	0.6005782	1.9680490	1.2672115	
H	1.7805518	1.7457913	-0.0129146	
H	0.4105106	-0.5026526	1.5470764	
H	2.0361835	0.0871899	1.7885005	
H	2.0232823	-2.0037494	0.4826600	
H	1.0381391	-1.2555239	-0.7717556	
H	-3.8297165	-0.5148205	-0.1874797	
H	3.6425468	-0.4324743	-0.0968550	
tTG+G+G-Tg+ C	-1.9896120	-0.3621461	0.4420693	
C	-1.3920725	0.4014838	-0.7233703	
C	-0.6759618	1.6877258	-0.3073292	
C	0.5631387	1.5184080	0.5811164	
C	1.7001426	0.7002388	-0.0533576	
C	1.6816733	-0.7808389	0.3061311	
O	-2.6780966	-1.4964208	-0.1023364	
O	2.7512180	-1.5040524	-0.3142735	
H	-2.6851132	0.2846166	0.9901521	
H	-1.2123284	-0.6912976	1.1386155	
H	-0.7199594	-0.2592369	-1.2751821	
H	-2.2082619	0.6498822	-1.4062692	
H	-1.3897751	2.3393548	0.2080997	
H	-0.3734665	2.2222711	-1.2127500	
H	0.2862855	1.0770956	1.5445101	
H	0.9351490	2.5196838	0.8132256	
H	2.6634412	1.1046379	0.2758129	
H	1.6776010	0.7974269	-1.1426139	
H	1.7232382	-0.8955492	1.3963314	
H	0.7767575	-1.2701669	-0.0477292	
H	-3.0263169	-2.0259996	0.6267050	
H	3.5845282	-1.0997839	-0.0373735	
g+G+G+G+G-G-g+ C	2.0749680	-0.8372552	-0.2567601	
C	1.0853038	-0.3558551	0.7986477	
C	0.5102532	1.0349427	0.5066333	
C	-0.5070928	1.0912087	-0.6454312	
C	-1.9724092	0.9742732	-0.2078943	
C	-2.3405068	-0.3208466	0.5015875	

O	3.2059169	0.0320381	-0.3881490	
O	-2.1883664	-1.4793808	-0.3282292	
H	1.6210296	-0.8486571	-1.2478517	
H	2.3996953	-1.8580366	-0.0288363	
H	0.2908709	-1.1023578	0.8949787	
H	1.5985544	-0.3409981	1.7667423	
H	1.3508896	1.6949274	0.2833137	
H	0.0408436	1.4284691	1.4138265	
H	-0.2776002	0.3247017	-1.3935747	
H	-0.3988728	2.0405680	-1.1754319	
H	-2.6205809	1.0801624	-1.0819848	
H	-2.2024849	1.8052065	0.4677889	
H	-1.7646497	-0.4335154	1.4267994	
H	-3.3957994	-0.3115442	0.7722081	
H	3.7065008	0.0012800	0.4381823	
H	-1.2827951	-1.4970368	-0.6633573	
g+G-TG-G+G-g-	C	2.5287584	-0.0933429	0.5426242
C	1.0482292	0.1654218	0.7863754	
C	0.4221348	1.0826111	-0.2645705	
C	-1.0125717	1.5402875	0.0409490	
C	-2.1556341	0.6303934	-0.4218648	
C	-2.2744181	-0.7358292	0.2439194	
O	2.7865876	-0.8122601	-0.6713984	
O	-1.2956894	-1.6867558	-0.1952482	
H	2.9385732	-0.7238751	1.3310355	
H	3.0844538	0.8532820	0.5451840	
H	0.5208983	-0.7872567	0.8136308	
H	0.9534112	0.6400931	1.7702138	
H	0.4333365	0.5926658	-1.2443066	
H	1.0514237	1.9764442	-0.3518649	
H	-1.1719466	2.5113308	-0.4373238	
H	-1.1104228	1.7141689	1.1185456	
H	-2.0958572	0.4882964	-1.5078205	
H	-3.0971952	1.1598087	-0.2376718	
H	-2.1225320	-0.6504966	1.3210961	
H	-3.2801779	-1.1376319	0.0806864	
H	2.4990027	-0.2646758	-1.4128210	
H	-1.4482425	-1.8689013	-1.1322176	
g+G+G+G-G+G-t	C	-1.9618813	0.8490024	-0.0857744
C	-0.5181312	-0.9766566	0.3709017	
C	0.7638559	-1.6305585	-0.1129102	
C	2.0704741	-0.8754815	0.1511055	
C	2.1923611	0.5200905	-0.4817781	
C	1.7466928	1.6553053	0.4382956	
O	-3.1963749	0.1575659	-0.0747361	
O	-0.8731388	0.0750686	-0.5312480	
H	-2.0676282	1.6504607	-0.8106637	
H	0.7082611	1.5373844	0.7427985	
H	-0.3942305	-0.5658050	1.3844077	
H	-1.3209582	-1.7214482	0.3971744	
H	0.6506375	-1.8147785	-1.1850556	

H	0.8318103	-2.6110444	0.3693988	
H	2.8791617	-1.5100760	-0.2230256	
H	2.2274698	-0.7955321	1.2332026	
H	1.6173880	0.5501692	-1.4098810	
H	3.2380187	0.6925314	-0.7516630	
H	2.3654119	1.6830356	1.3379997	
H	1.8382759	2.6226261	-0.0589903	
H	-3.2760972	-0.3441479	0.7462093	
H	-1.7440765	1.2504776	0.9135372	
g+TG+G-G-G-g- C	1.8947954	-0.6460823	-0.3177163	
C	1.6072255	0.8320660	-0.0860157	
C	0.2353749	1.3028461	-0.5988083	
C	-0.8869198	1.3018971	0.4447813	
C	-1.2639895	-0.0610139	1.0282145	
C	-1.7956573	-1.0531156	0.0014147	
O	3.2234915	-1.0097425	0.0782088	
O	-2.9320650	-0.5503549	-0.7125560	
H	1.8483270	-0.8715061	-1.3834063	
H	1.1640127	-1.2812862	0.1911068	
H	1.6946801	1.0552249	0.9843969	
H	2.4042806	1.3877156	-0.5854752	
H	-0.0591543	0.7095734	-1.4703307	
H	0.3335543	2.3285751	-0.9628297	
H	-1.7786376	1.7427213	-0.0069381	
H	-0.5924725	1.9616720	1.2674477	
H	-2.0309255	0.0858417	1.7973999	
H	-0.4102247	-0.5135206	1.5423878	
H	-1.0555207	-1.2599687	-0.7700007	
H	-2.0383701	-2.0036386	0.4890183	
H	3.3245573	-0.7949285	1.0151331	
H	-3.6536124	-0.4269273	-0.0812937	
tG-G+G-G-G-t C	2.3295032	-0.3582857	-0.5368698	
C	1.9090872	1.0599135	-0.1938478	
C	0.4050924	1.3535259	-0.1659857	
C	-0.4203601	0.6074038	0.8946054	
C	-1.0095283	-0.7329366	0.4449034	
C	-2.0776018	-0.6114675	-0.6253252	
O	2.1104490	-1.1972395	0.6091116	
O	-3.1320090	0.2170561	-0.1088550	
H	3.3911175	-0.3686905	-0.8040796	
H	1.7583611	-0.7281716	-1.3977484	
H	2.3560495	1.3124222	0.7723103	
H	2.3683275	1.7204117	-0.9370648	
H	-0.0091787	1.1732378	-1.1636448	
H	0.2983577	2.4288078	0.0044801	
H	-1.2495846	1.2429429	1.2113188	
H	0.2049227	0.4331537	1.7738941	
H	-1.4593730	-1.2294479	1.3091792	
H	-0.2165530	-1.3889594	0.0821054	
H	-1.6682790	-0.1709875	-1.5409184	
H	-2.4636473	-1.6060609	-0.8734871	

H	2.5219201	-2.0556843	0.4440526	
H	-3.8302113	0.2750562	-0.7736052	
tG+G-G-G+Tg+	C	-2.3809864	-0.5938903	0.1622513
C	-1.5149151	0.3000018	1.0319194	
C	-0.8712636	1.4894642	0.3090980	
C	0.1141417	1.2007060	-0.8321565	
C	1.5301009	0.7761560	-0.4233490	
C	1.6687682	-0.6164738	0.1791046	
O	-1.5248570	-1.4059712	-0.6598799	
O	3.0452265	-1.0286030	0.2432967	
H	-3.0434539	0.0162959	-0.4632922	
H	-3.0022711	-1.2342575	0.7965697	
H	-2.1563550	0.6996238	1.8244090	
H	-0.7706115	-0.3282089	1.5229469	
H	-0.3690080	2.1165454	1.0546547	
H	-1.6873730	2.0987339	-0.0955024	
H	0.2147606	2.1246274	-1.4099488	
H	-0.3061887	0.4513889	-1.5047552	
H	1.9440802	1.5161775	0.2733719	
H	2.1652560	0.7930997	-1.3135183	
H	1.2241270	-0.6702238	1.1760213	
H	1.1719513	-1.3552810	-0.4468961	
H	-2.0760135	-2.0212081	-1.1616613	
H	3.5175744	-0.3954677	0.8001364	
tG+G-G+G+G+g+	C	-2.3848757	-0.3591608	-0.4897684
C	-1.9483840	1.0566709	-0.1597712	
C	-0.4429014	1.3406250	-0.1886021	
C	0.4077625	0.5887619	0.8491485	
C	1.0200712	-0.7191231	0.3409102	
C	2.1611973	-0.5211772	-0.6478254	
O	-2.0773498	-1.2126620	0.6244062	
O	3.2611022	0.2149291	-0.0926161	
H	-1.8756913	-0.7122926	-1.3951941	
H	-3.4629299	-0.3723221	-0.6794779	
H	-2.4326346	1.7180947	-0.8858785	
H	-2.3568677	1.3120544	0.8223999	
H	-0.3199376	2.4162618	-0.0338550	
H	-0.0652183	1.1446135	-1.1980333	
H	-0.2055513	0.3761614	1.7275800	
H	1.2254199	1.2349814	1.1767931	
H	0.2492174	-1.3403884	-0.1202601	
H	1.4004115	-1.2959555	1.1924665	
H	2.5057575	-1.4921100	-1.0215118	
H	1.8428582	0.0684423	-1.5075731	
H	-2.4813602	-2.0765342	0.4690053	
H	3.5971909	-0.2819097	0.6655762	
tG+G-G+G+Tg+	C	-2.1998089	-0.7687625	-0.5127619
C	-2.1401336	0.7416691	-0.3768941	
C	-0.7434053	1.3708445	-0.3555273	
C	0.1382175	0.9938044	0.8500473	
C	1.1280024	-0.1443628	0.5803427	

C	2.3220088	0.3014774	-0.2503347	
O	-1.7849499	-1.3608312	0.7278826	
O	3.2565575	-0.7611301	-0.4889755	
H	-1.5508192	-1.1011805	-1.3326457	
H	-3.2250344	-1.0734253	-0.7465705	
H	-2.6934732	1.1630878	-1.2224927	
H	-2.6864848	1.0190481	0.5293284	
H	-0.8816097	2.4556176	-0.3755714	
H	-0.2295859	1.1200328	-1.2899066	
H	-0.5030150	0.7176027	1.6888129	
H	0.7090089	1.8721133	1.1699883	
H	0.6102990	-0.9651653	0.0766042	
H	1.5052086	-0.5459512	1.5240413	
H	1.9966977	0.7374537	-1.2013666	
H	2.8925757	1.0612955	0.2844999	
H	-1.9321053	-2.3145525	0.6783897	
H	2.7770495	-1.4846755	-0.9136473	
tG-G+G-G-Tg+ C	2.1376087	-0.7820295	-0.5476648	
C	2.1293448	0.7274035	-0.3849227	
C	0.7554369	1.4022388	-0.3189591	
C	-0.1299863	0.9977303	0.8732678	
C	-1.1120426	-0.1391150	0.5714141	
C	-2.2974385	0.3134791	-0.2683792	
O	1.7875546	-1.3793962	0.7110332	
O	-3.1658084	-0.7709220	-0.6262097	
H	3.1373262	-1.1114453	-0.8487790	
H	1.4291536	-1.0852622	-1.3279873	
H	2.7054378	0.9680601	0.5134581	
H	2.6761937	1.1493879	-1.2342911	
H	0.2251314	1.2170105	-1.2591073	
H	0.9315657	2.4812650	-0.2844923	
H	-0.7057080	1.8680481	1.2067415	
H	0.5085126	0.7071876	1.7094631	
H	-1.4918157	-0.5480887	1.5145100	
H	-0.6028563	-0.9562361	0.0602760	
H	-2.8582491	1.0930471	0.2613434	
H	-1.9699502	0.7302727	-1.2202517	
H	1.8499322	-2.3396693	0.6224921	
H	-3.4650551	-1.1907324	0.1913620	
tTG+G+G-G-g+ C	1.8357880	-0.4049967	-0.4400914	
C	1.4058302	0.6852722	0.5214916	
C	0.5002986	1.7433020	-0.1125227	
C	-0.8620431	1.2581351	-0.6245833	
C	-1.7771057	0.6538513	0.4528262	
C	-1.6972498	-0.8620388	0.6060447	
O	2.7152868	-1.2797988	0.2779811	
O	-2.2232721	-1.5577536	-0.5328960	
H	2.3496861	0.0402114	-1.3002367	
H	0.9726530	-0.9651392	-0.8140972	
H	0.9228536	0.2236874	1.3852969	
H	2.3119995	1.1674059	0.8963108	

H	1.0376167	2.2188015	-0.9400593	
H	0.3219596	2.5301744	0.6266200	
H	-0.7236257	0.5496927	-1.4488727	
H	-1.3657497	2.1178210	-1.0739427	
H	-2.8194829	0.8903013	0.2256609	
H	-1.5514487	1.1167859	1.4198923	
H	-0.6759390	-1.1928926	0.8131853	
H	-2.3242278	-1.1832152	1.4371827	
H	2.9760160	-2.0046989	-0.3049368	
H	-1.6837338	-1.3360684	-1.3026128	
g+G-G+G+G-G-g-	C	2.1288011	-0.3272792	-0.2238887
C	1.4653747	0.6553943	0.7542704	
C	0.5570431	1.7005681	0.0901662	
C	-0.5932954	1.2015592	-0.7954646	
C	-1.8710353	0.7634740	-0.0727069	
C	-1.7858266	-0.5524329	0.6871376	
O	1.5517441	-1.6316379	-0.2273348	
O	-1.3060087	-1.6275902	-0.1392946	
H	3.1690414	-0.4907024	0.0569910	
H	2.1299145	0.1004088	-1.2355000	
H	0.9384861	0.0733698	1.5125119	
H	2.2452183	1.2044738	1.2907676	
H	1.2009051	2.3298343	-0.5326600	
H	0.1461085	2.3628960	0.8602266	
H	-0.2467412	0.3973881	-1.4508427	
H	-0.8731728	2.0228844	-1.4614452	
H	-2.6758163	0.6748178	-0.8117594	
H	-2.1849144	1.5446215	0.6283210	
H	-1.0774724	-0.5001397	1.5106715	
H	-2.7626856	-0.8135153	1.1050110	
H	0.5869616	-1.5784434	-0.3376779	
H	-1.9202550	-1.7506591	-0.8765071	
g+G+G+G-G-G-g+	C	1.9648000	-0.5040765	0.5890674
C	1.7806140	0.8864898	-0.0117769	
C	0.4867393	1.1015898	-0.8062550	
C	-0.7517820	1.4844902	0.0142294	
C	-1.2894990	0.4393277	0.9961191	
C	-1.6029899	-0.9122643	0.3652503	
O	1.8570420	-1.5470184	-0.3899409	
O	-2.5974576	-0.8095008	-0.6662790	
H	1.1949568	-0.7334573	1.3211468	
H	2.9320202	-0.5591893	1.0999459	
H	1.8530948	1.6261848	0.7939352	
H	2.6350397	1.0734311	-0.6721391	
H	0.2944743	0.2094337	-1.4091460	
H	0.6601250	1.9132611	-1.5187068	
H	-1.5555086	1.7458003	-0.6809070	
H	-0.5308054	2.4029488	0.5678593	
H	-2.2100790	0.8272245	1.4407438	
H	-0.5877206	0.2872469	1.8215206	
H	-0.7001110	-1.3908209	-0.0234031	

H	-2.0374904	-1.5768971	1.1121235	
H	2.5863835	-1.4496990	-1.0172389	
H	-2.1726909	-0.4724961	-1.4651407	
g+G-G+TG-G+g-	C	-2.7268131	0.3373272	0.3638596
C	-1.6150262	1.0957245	-0.3580194	
C	-0.1852128	0.7389106	0.0649246	
C	0.1852127	-0.7389105	-0.0649242	
C	1.6150260	-1.0957246	0.3580198	
C	2.7268130	-0.3373277	-0.3638595	
O	-3.0575041	-0.9186169	-0.2443049	
O	3.0575042	0.9186168	0.2443042	
H	-3.6544698	0.9060925	0.3175014	
H	-2.4739443	0.2010146	1.4227834	
H	-1.7438714	0.9320297	-1.4318420	
H	-1.7605838	2.1663777	-0.1825448	
H	-0.0268777	1.0569372	1.1017975	
H	0.4872068	1.3347458	-0.5612511	
H	0.0268776	-1.0569370	-1.1017972	
H	-0.4872071	-1.3347456	0.5612515	
H	1.7605833	-2.1663778	0.1825455	
H	1.7438714	-0.9320295	1.4318423	
H	3.6544697	-0.9060931	-0.3175008	
H	2.4739443	-0.2010158	-1.4227834	
H	-2.2975114	-1.5082448	-0.1734981	
H	2.2975115	1.5082448	0.1734967	
tG-G+G+G+G-g+	C	-2.4209183	0.3871816	-0.2753965
C	-1.1075154	1.1181000	-0.0672117	
C	-0.2973820	0.6546952	1.1478057	
C	0.2672634	-0.7709748	1.0910965	
C	1.1371907	-1.1195883	-0.1202968	
C	2.4308963	-0.3269439	-0.2675745	
O	-2.1403413	-0.9474322	-0.7276494	
O	2.2587314	0.9884184	-0.8209589	
H	-3.0200846	0.9170094	-1.0230242	
H	-2.9886492	0.3598538	0.6626974	
H	-0.5186289	1.0401338	-0.9835139	
H	-1.3482288	2.1780959	0.0655619	
H	-0.9333738	0.7343262	2.0367216	
H	0.5156293	1.3690659	1.3224949	
H	-0.5658392	-1.4745109	1.1168813	
H	0.8536033	-0.9371882	2.0022932	
H	0.5609859	-1.0312329	-1.0432693	
H	1.4159611	-2.1753297	-0.0292514	
H	2.9552463	-0.2694656	0.6945627	
H	3.0917055	-0.8288073	-0.9740194	
H	-2.9787223	-1.3852855	-0.9253347	
H	1.8226966	1.5412151	-0.1620984	
tTG+G-G-G+g+	C	1.7395974	-0.5709408	0.1901887
C	1.5659150	0.7804937	-0.4752489	
C	0.1220373	1.1742885	-0.8026749	
C	-0.7921692	1.4222075	0.4071247	

C	-1.4810196	0.2083755	1.0431856	
C	-2.4439606	-0.5356577	0.1235746	
O	3.1492990	-0.8473979	0.2134392	
O	-1.7886947	-1.3634941	-0.8512382	
H	1.2073784	-1.3394941	-0.3815211	
H	1.3469815	-0.5610416	1.2110357	
H	2.0260488	1.5431359	0.1599426	
H	2.1435514	0.7511866	-1.4028364	
H	-0.3260671	0.4270149	-1.4600664	
H	0.1723771	2.1053352	-1.3743965	
H	-1.5887091	2.1093208	0.1014270	
H	-0.2214465	1.9500227	1.1796537	
H	-2.0584026	0.5637429	1.9040499	
H	-0.7553141	-0.5057259	1.4414384	
H	-3.1385570	-1.1397783	0.7162351	
H	-3.0348797	0.1726988	-0.4587731	
H	3.2939051	-1.6696847	0.6991571	
H	-1.4241399	-2.1315090	-0.3922619	
tTG+G-G-G-g+ C	1.8909660	-0.6257722	-0.3141139	
C	1.5966465	0.8439305	-0.0745194	
C	0.2244508	1.3061915	-0.5919909	
C	-0.8955910	1.2994392	0.4560067	
C	-1.2722462	-0.0635675	1.0416198	
C	-1.8019634	-1.0647168	0.0223949	
O	3.2099537	-0.8786147	0.1887232	
O	-3.0067305	-0.6226273	-0.6163653	
H	1.8421913	-0.8400918	-1.3882377	
H	1.1641112	-1.2649238	0.1941821	
H	1.6860124	1.0497625	0.9959276	
H	2.3915619	1.4073714	-0.5680409	
H	-0.0599234	0.7076514	-1.4651482	
H	0.3171069	2.3314139	-0.9592136	
H	-1.7904439	1.7602281	0.0244025	
H	-0.5967347	1.9575043	1.2773909	
H	-2.0461307	0.0825797	1.7997793	
H	-0.4117120	-0.5049925	1.5535301	
H	-1.0424211	-1.3043694	-0.7290609	
H	-2.0759209	-1.9943336	0.5206848	
H	3.4218992	-1.8102209	0.0459746	
H	-2.7987902	0.1453481	-1.1638116	
g+TG+G+G-G-g+ C	1.8348987	-0.4137474	-0.4506746	
C	1.4050775	0.6658547	0.5319555	
C	0.4978989	1.7350167	-0.0837427	
C	-0.8606309	1.2630117	-0.6181796	
C	-1.7985103	0.6598000	0.4392524	
C	-1.7207586	-0.8551166	0.6019675	
O	2.8049781	-1.3073542	0.1078522	
O	-2.2125061	-1.5611980	-0.5432999	
H	2.3303290	0.0389616	-1.3103402	
H	0.9746045	-0.9797721	-0.8230583	
H	0.9169433	0.2031818	1.3957296	

H	2.3123698	1.1432535	0.9103737	
H	1.0433738	2.2233077	-0.8981597	
H	0.3152224	2.5091371	0.6678341	
H	-0.7169835	0.5608929	-1.4464503	
H	-1.3507918	2.1309592	-1.0664680	
H	-2.8357515	0.8920558	0.1859851	
H	-1.5980268	1.1278150	1.4095789	
H	-0.7035504	-1.1806653	0.8385057	
H	-2.3673867	-1.1724494	1.4195369	
H	2.4032994	-1.7510159	0.8668354	
H	-1.6479079	-1.3545329	-1.2993056	
tG+G+G+G-G+g+	C	2.0237751	-0.6464499	-0.6092312
C	1.0196910	-0.7243600	0.5246110	
C	0.4389474	0.6320133	0.9373095	
C	-0.3932978	1.3624694	-0.1280256	
C	-1.8905771	1.0401637	-0.1842551	
C	-2.2834856	-0.3762829	-0.5863720	
O	3.0707881	0.2566135	-0.2159932	
O	-2.0678718	-1.3571574	0.4390774	
H	1.5504511	-0.2925505	-1.5315397	
H	2.4335837	-1.6431571	-0.8034354	
H	0.2194563	-1.4113206	0.2457806	
H	1.5283246	-1.1618014	1.3885367	
H	1.2725430	1.2742636	1.2279826	
H	-0.1741891	0.4884059	1.8324651	
H	0.0378358	1.1981333	-1.1206981	
H	-0.3089886	2.4381874	0.0522471	
H	-2.3548739	1.7184282	-0.9089904	
H	-2.3529669	1.2697124	0.7835416	
H	-3.3341040	-0.3942378	-0.8962026	
H	-1.6833744	-0.7150742	-1.4325796	
H	3.7378498	0.2751157	-0.9141472	
H	-2.6279537	-1.1275656	1.1925267	
g+TG+G-G-G-g+	C	1.8941556	-0.6392594	-0.3245679
C	1.6028138	0.8373666	-0.0855981	
C	0.2253700	1.3044702	-0.5862153	
C	-0.8872490	1.2936906	0.4693356	
C	-1.2711199	-0.0720215	1.0434390	
C	-1.8143536	-1.0590742	0.0173108	
O	3.2308150	-0.9945902	0.0499204	
O	-3.0170821	-0.5968228	-0.6109312	
H	1.8335014	-0.8624051	-1.3902205	
H	1.1742825	-1.2793771	0.1929443	
H	1.6972539	1.0589797	0.9841281	
H	2.3932420	1.3974331	-0.5903843	
H	-0.0638570	0.7086362	-1.4594277	
H	0.3164589	2.3311226	-0.9498413	
H	-1.7818581	1.7632755	0.0476489	
H	-0.5795393	1.9428029	1.2948751	
H	-2.0401192	0.0734417	1.8066536	
H	-0.4126049	-0.5273949	1.5468322	

H	-1.0605532	-1.3010424	-0.7387139	
H	-2.0957976	-1.9897428	0.5092190	
H	3.3314510	-0.8265892	0.9963513	
H	-2.7975563	0.1488864	-1.1838921	
g+TG-G+G+G+g- C	-1.8803243	-0.6426828	-0.3188365	
C	-1.5990533	0.8348606	-0.0731420	
C	-0.2286289	1.3120474	-0.5825921	
C	0.8879617	1.2968072	0.4690049	
C	1.2694251	-0.0711401	1.0398090	
C	1.8069368	-1.0578804	0.0105016	
O	-3.1505116	-1.0490219	0.2026175	
O	3.0091603	-0.5988844	-0.6218312	
H	-1.1590269	-1.2783561	0.1895729	
H	-1.8183602	-0.8576697	-1.3925646	
H	-2.3889332	1.4057183	-0.5727948	
H	-1.6977226	1.0377650	0.9971685	
H	-0.3239747	2.3409724	-0.9387871	
H	0.0588718	0.7227604	-1.4610794	
H	0.5840631	1.9445791	1.2967585	
H	1.7817114	1.7658510	0.0445053	
H	0.4114358	-0.5232202	1.5465080	
H	2.0415860	0.0715328	1.8002962	
H	2.0871925	-1.9902194	0.4997609	
H	1.0505263	-1.2964909	-0.7442060	
H	-3.8346432	-0.5174760	-0.2261968	
H	2.7926441	0.1604786	-1.1777458	
g+TG+G-G-G+g+ C	1.6670776	-0.6568930	0.0084180	
C	1.4983926	0.8211058	-0.3188985	
C	0.1104616	1.2388907	-0.8268764	
C	-0.9461650	1.5220428	0.2495424	
C	-1.5433788	0.3374693	1.0159219	
C	-2.3181954	-0.6535775	0.1546096	
O	3.0351863	-0.9909434	0.2883042	
O	-1.4836648	-1.4683022	-0.6827859	
H	1.3960093	-1.2641121	-0.8542050	
H	1.0346386	-0.9576653	0.8476558	
H	1.7607485	1.4205234	0.5620692	
H	2.2424812	1.0512337	-1.0859918	
H	-0.2603982	0.4917982	-1.5314530	
H	0.2374145	2.1674272	-1.3909641	
H	-1.7798559	2.0485327	-0.2284093	
H	-0.5199989	2.2257513	0.9732563	
H	-2.2430244	0.7378063	1.7583395	
H	-0.7779621	-0.1982648	1.5840900	
H	-2.9487653	-1.2884761	0.7856645	
H	-2.9729847	-0.1171692	-0.5341337	
H	3.3329515	-0.4340243	1.0201230	
H	-1.0529282	-2.1294867	-0.1255536	
tTG-G-G+G-t C	-2.3102050	0.2929457	-0.2129615	
C	-1.0972647	-0.1647789	0.5729968	
C	-0.1261652	0.9822499	0.8723405	

C	0.7454900	1.4026276	-0.3247149
C	2.1230179	0.7367942	-0.4096151
C	2.1378034	-0.7736785	-0.5628998
O	-3.0931344	-0.8710213	-0.5216797
O	1.8153667	-1.3611571	0.7070700
H	-2.0057006	0.7985963	-1.1358156
H	-2.8962793	1.0007104	0.3846201
H	-1.4471942	-0.6152091	1.5047876
H	-0.5934562	-0.9532047	0.0139805
H	0.5221370	0.6935563	1.7012460
H	-0.7068321	1.8453948	1.2161063
H	0.9154979	2.4826429	-0.2849024
H	0.2062553	1.2199472	-1.2606328
H	2.7108805	0.9852873	0.4790026
H	2.6545331	1.1583986	-1.2689910
H	1.4166376	-1.0863407	-1.3275180
H	3.1336438	-1.1001366	-0.8804761
H	-3.8870644	-0.5903180	-0.9949532
H	1.8175399	-2.3227673	0.6112706