Supporting information for

Basis set dependence of S=O stretching frequencies and its consequences for IR and VCD spectra predictions

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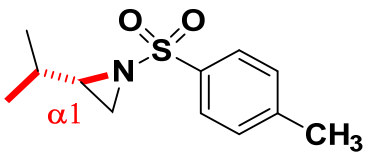
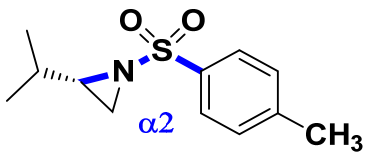
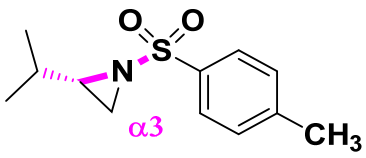
1. Conformational analysis

Conformational analysis of 1







	B3LYP / 6-311++G (2d,p)						
	α1	α2	α3	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	-78.8	159.6	137.7	0.00	0.00	45.6	46.4
c2	-79.8	-95.2	141.8	0.17	0.20	34.1	33.0
c3	167.3	161.6	134.6	1.18	1.21	6.2	6.0
c4	45.3	159.6	134.5	1.43	1.42	4.1	4.2
c5	168.0	-92.5	138.2	1.45	1.43	4.0	4.2
c6	-80.0	35.6	134.6	1.67	1.62	2.7	3.0
c7	44.4	-95.9	138.8	1.70	1.73	2.6	2.5
c8	166.4	37.5	131.6	2.84	2.80	0.4	0.4
c9	44.7	35.9	131.9	3.12	3.07	0.2	0.3
c10	-83.5	-167.5	-3.2	3.97	4.06	0.1	0.0
c11	-83.9	97.2	-6.8	5.47	5.52	0.0	0.0
c12	-82.3	-47.8	3.9	7.21	7.27	0.0	0.0
c13	51.7	178.1	-5.4	8.60	8.65	0.0	0.0
c14	65.7	106.7	-4.8	10.56	10.58	0.0	0.0

Referenced to E(c1)= -1070.8068 hartree and G(c1)= -1070.8248 hartree

	B3LYP / 6-311G (3df,2dp)[a]				B3LYP / 6-311++G (3df,2dp)[b]			
	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	0.00	0.00	50.7	48.4	0.00	0.00	45.6	45.8
c2	0.36	0.33	27.5	27.6	0.19	0.22	33.0	31.8
c3	1.32	1.27	5.5	5.7	1.24	1.26	5.6	5.5
c4	1.43	1.32	4.5	5.2	1.48	1.45	3.7	3.9
c5	1.55	1.46	3.7	4.1	1.50	1.47	3.6	3.8
c6	1.44	1.32	4.5	5.2	1.31	1.23	5	5.7
c7	1.78	1.74	2.5	2.6	1.77	1.78	2.3	2.3
c8	2.70	2.57	0.5	0.6	2.52	2.45	0.6	0.7
c9	2.78	2.67	0.5	0.5	2.77	2.71	0.4	0.5
c10	3.85	3.82	0.1	0.1	3.90	3.97	0.1	0.1
c11	5.27	5.25	0.0	0.0	5.28	5.30	0.0	0.0
c12	6.80	6.75	0.0	0.0	6.69	6.68	0.0	0.0
c13	8.23	8.22	0.0	0.0	8.40	8.45	0.0	0.0
c14	9.98	9.93	0.0	0.0	10.19	10.23	0.0	0.0

[a] Referenced to E(c1)= -1070.8563 hartree and G(c1)= -1070.8743 hartree

[b] Referenced to E(c1)= -1070.8627 hartree and G(c1)= -1070.8808 hartree

	B3PW91 / 6-311G (3df,2dp)[a]				B3PW91 / 6-311++G (3df,2dp)[b]			
	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	0.00	0.00	44.0	44.8	0.00	0.00	43.5	43.4
c2	0.27	0.32	28.1	26.0	0.21	0.23	30.4	29.2
c3	1.10	1.11	6.9	6.8	1.15	1.15	6.3	6.2
c4	1.27	1.24	5.2	5.6	1.40	1.38	4.1	4.2
c5	1.34	1.33	4.6	4.8	1.39	1.35	4.2	4.4
c6	1.11	1.06	6.8	7.5	1.06	0.99	7.3	8.1
c7	1.66	1.69	2.7	2.6	1.72	1.73	2.4	2.3
c8	2.22	2.17	1.0	1.1	2.15	2.08	1.1	1.3
c9	2.41	2.36	0.8	0.8	2.47	2.41	0.7	0.7
c10	3.77	3.82	0.1	0.1	3.92	3.98	0.1	0.1
c11	5.23	5.29	0.0	0.0	5.28	5.33	0.0	0.0
c12	6.55	6.56	0.0	0.0	6.49	6.48	0.0	0.0
c13	8.25	8.32	0.0	0.0	8.49	8.54	0.0	0.0
c14	10.12	10.15	0.0	0.0	10.40	10.41	0.0	0.0

[a] Referenced to E(c1)= -1070.5480 hartree and G(c1)= -1070.5661 hartree

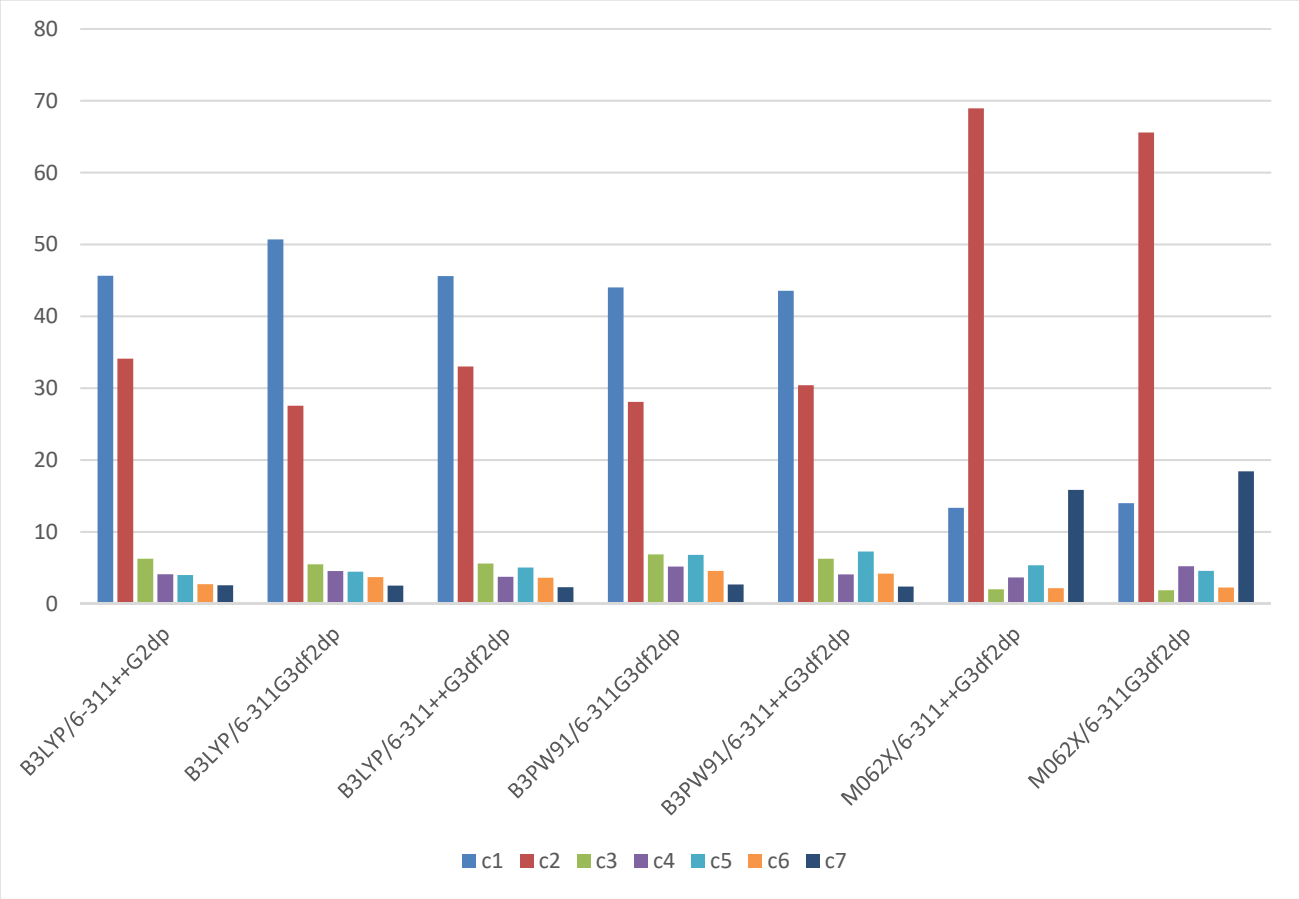
[b] Referenced to E(c1)= -1070.5536 hartree and G(c1)= -1070.5717 hartree

	M06-2X / 6-311G (3df,2dp)[a]				M06-2X / 6-311++G (3df,2dp)[b]			
	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	0.91	0.97	14.0	12.3	0.97	1.01	13.3	12.2
c2	0.00	0.00	65.6	63.6	0.00	0.00	68.9	67.5
c3	2.11	2.08	1.9	1.9	2.10	2.11	2.0	1.9
c4	1.50	1.51	5.2	5.0	1.74	1.73	3.7	3.7
c5	2.00	1.99	2.3	2.2	2.05	2.04	2.2	2.1
c6	1.58	1.61	4.6	4.2	1.52	1.57	5.3	4.7
c7	0.75	0.66	18.4	20.9	0.87	0.78	15.8	18.1
c8	2.85	2.81	0.5	0.5	2.78	2.75	0.6	0.6
c9	2.24	2.22	1.5	1.5	2.32	2.32	1.4	1.3
c10	4.09	4.17	0.1	0.1	4.29	4.39	0.0	0.0
c11	5.17	5.22	0.0	0.0	5.32	5.36	0.0	0.0
c12	5.69	5.70	0.0	0.0	5.66	5.66	0.0	0.0
c13	8.64	8.60	0.0	0.0	8.91	8.89	0.0	0.0
c14	10.20	10.17	0.0	0.0	10.31	10.30	0.0	0.0

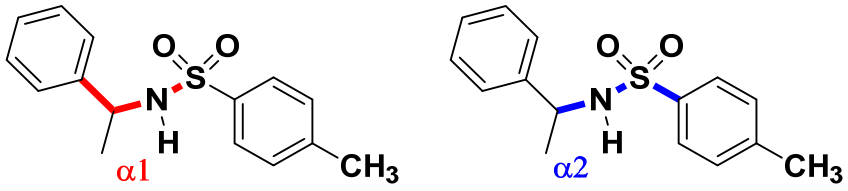
[a] Referenced to E(c2)= -1070.5320 hartree and G(c2)= -1070.5504 hartree

[b] Referenced to E(c2)= -1070.5375 hartree and G(c2)= -1070.5559 hartree

Comparison of the predicted conformational distributions



Conformational analysis of 2



	B3LYP / 6-311++G (2d,p)						
	α1	α2	α3	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	-150.2	60.1	-137.1	0.00	0.00	19.8	22.1
c2	-89.0	-61.7	139.3	0.01	0.08	19.5	19.3
c3	-86.1	73.6	-150.8	0.14	0.27	15.6	14.1
c4	-85.2	95.4	134.6	0.15	0.28	15.4	13.7
c5	-145.1	85.2	138.7	0.58	0.70	7.5	6.8
c6	-159.3	-95.5	-133.3	0.64	0.60	6.7	8.0
c7	-136.0	-68.4	146.1	0.68	0.69	6.3	6.9
c8	-82.6	-83.2	-140.6	0.88	0.99	4.5	4.2
c9	-74.0	-147.4	-136.1	1.42	1.50	1.8	1.8
c10	-161.8	147.3	135.8	1.46	1.47	1.7	1.9
c11	-142.6	-159.9	-129.3	1.79	1.81	1.0	1.0
c12	96.4	87.0	153.3	3.41	3.53	0.1	0.1
c13	62.9	-97.3	-141.3	3.78	3.85	0.0	0.0
c14	61.0	147.3	138.6	4.78	4.88	0.0	0.0
c15	80.5	-63.7	150.4	4.82	4.83	0.0	0.0

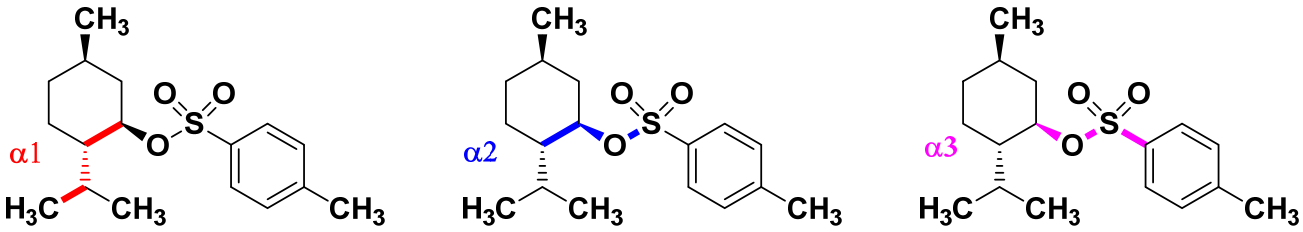
Referenced to E(c1)= -1185.1734 hartree and G(c1)= -1185.1907 hartree

	B3LYP / 6-311G (3df,2dp)[a]				B3PW91 / 6-311G (3df,2dp)[b]			
	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	0.15	0.02	18.0	21.8	0.22	0.12	23.0	26.8
c2	0.04	0.00	22.0	22.6	0.00	0.00	33.0	32.6
c3	0.00	0.00	23.3	22.6	0.10	0.14	27.7	25.7
c4	0.24	0.40	15.6	11.5	Converts to c3			
c5	0.68	0.70	7.4	7.0	0.79	0.87	8.8	7.5
c6	0.97	0.88	4.5	5.1	1.07	1.02	5.4	5.8
c7	0.68	0.62	7.5	7.9	Converts to c2			
c8	Converts to c2				Converts to c2			
c9	1.59	1.66	1.6	1.4	1.70	1.83	1.9	1.5
c10	Converts to c3				Converts to c1			
c11	Converts to c6				Converts to c6			
c12	3.05	3.10	0.1	0.1	3.05	3.19	0.2	0.1
c13	3.61	3.65	0.1	0.0	3.83	3.91	0.1	0.0
c14	Converts to c12				Converts to c1			
c15	4.61	4.56	0.0	0.0	4.82	4.83	0.0	0.0

[a] Referenced to E(c3)= -1185.2268 hartree and G(c3)= -1185.2440 hartree

[b] Referenced to E(c2)= -1184.8676 hartree and G(c2)= -1185.8849 hartree

Conformational analysis of 3



	B3LYP / 6-311++G (2d,p)						
	α1	α2	α3	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	-164.2	-134.7	-84.8	0.00	0.00	43.3	45.1
c2	-165.6	-154.0	153.4	0.17	0.24	32.3	29.9
c3	-161.6	-148.7	85.5	0.42	0.42	21.4	22.0
c4	44.1	-163.3	153.4	1.79	1.86	2.1	2.0
c5	-91.6	-131.1	-82.3	2.78	2.70	0.4	0.5
c6	-92.2	-146.7	79.9	3.05	2.97	0.3	0.3
c7	-167.9	82.9	-160.9	3.34	3.40	0.2	0.1
c8	-168.8	75.3	92.7	3.45	3.52	0.1	0.1
c9	-36.6	-157.6	163.3	3.94	3.90	0.1	0.1
c10	42.6	80.6	89.3	5.28	5.25	0.0	0.0
c11	-58.3	-134.1	75.6	5.31	5.32	0.0	0.0
c12	42.9	92.6	-167.2	5.48	5.52	0.0	0.0
c13	-59.3	-107.1	-175.0	5.82	5.79	0.0	0.0
c14	-70.5	77.6	91.0	7.04	7.01	0.0	0.0
c15	-60.5	86.0	-162.8	7.04	7.09	0.0	0.0
c16	-158.9	-133.4	74.1	7.94	7.86	0.0	0.0
c17	-159.1	-106.1	179.8	8.14	8.14	0.0	0.0
c18	53.7	-137.6	77.1	8.24	8.23	0.0	0.0
c19	54.5	-100.7	-167.7	8.63	8.61	0.0	0.0
c20	-161.6	79.2	92.1	10.46	10.49	0.0	0.0
c21	62.8	77.9	91.7	12.19	12.19	0.0	0.0
c22	-163.4	73.3	-162.8	16.70	16.68	0.0	0.0
c23	60.4	72.3	-162.2	16.82	16.83	0.0	0.0

Referenced to E(c1)= -1287.2174 hartree and G(c1)= -1287.2311 hartree

	B3LYP / 6-311G (2d,p)[a]				B3LYP / 6-311++G (3df,2dp)[b]			
	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	0.00	0.00	42.9	43.7	0.00	0.00	45.6	46.1
c2	0.24	0.28	28.5	27.4	0.32	0.34	26.8	26.1
c3	0.31	0.32	25.4	25.6	0.36	0.36	24.9	25.0
c4	1.82	1.83	2.0	2.0	1.94	1.99	1.7	1.6
c5	2.62	2.55	0.5	0.6	2.80	2.71	0.4	0.5
c6	2.90	2.83	0.3	0.4	3.03	2.95	0.3	0.3
c7	3.46	3.53	0.1	0.1	3.38	3.42	0.2	0.1
c8	3.40	3.47	0.1	0.1	3.42	3.48	0.1	0.1
c9	3.77	3.71	0.1	0.1	4.02	3.98	0.1	0.1
c10	4.96	4.93	0.0	0.0	5.28	5.25	0.0	0.0
c11	5.12	5.14	0.0	0.0	5.35	5.32	0.0	0.0
c12	5.30	4.78	0.0	0.0	5.52	5.55	0.0	0.0
c13	5.80	5.79	0.0	0.0	5.83	5.85	0.0	0.0
c14	6.76	6.74	0.0	0.0	7.02	6.99	0.0	0.0
c15	6.93	6.96	0.0	0.0	7.02	7.08	0.0	0.0
c16	7.83	7.76	0.0	0.0	7.94	7.89	0.0	0.0
c17	8.25	8.25	0.0	0.0	8.34	8.33	0.0	0.0
c18	8.02	8.03	0.0	0.0	8.29	8.27	0.0	0.0
c19	8.57	8.60	0.0	0.0	8.85	8.82	0.0	0.0
c20	10.36	10.40	0.0	0.0	10.43	10.47	0.0	0.0
c21	11.92	11.93	0.0	0.0	12.14	12.16	0.0	0.0
c22	16.66	16.61	0.0	0.0	16.77	16.72	0.0	0.0
c23	16.71	16.69	0.0	0.0	16.82	16.83	0.0	0.0

[a] Referenced to E(c1)= -1287.2082 hartree and G(c1)= -1287.2219 hartree

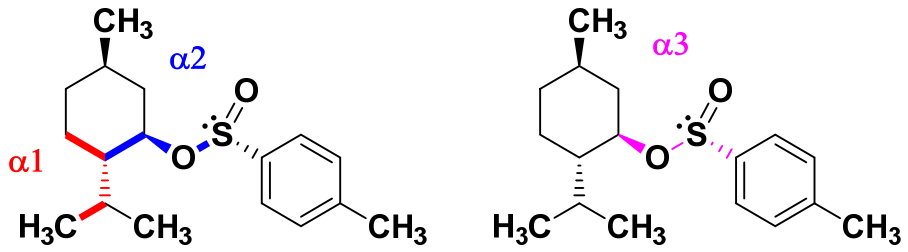
[b] Referenced to E(c1)= -1287.2846 hartree and G(c1)= -1287.2983 hartree

	B3PW91 / 6-311G (3df,2dp)[a]				B3LYP / 6-311G (3df,2dp)[b]			
	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	0.00	0.00	50.8	51.1	0.00	0.00	46.0	47.0
c2	0.57	0.56	19.5	19.8	0.37	0.39	24.8	24.3
c3	0.37	0.39	27.2	26.6	0.33	0.35	26.5	25.9
c4	2.19	2.25	1.3	1.1	2.01	2.04	1.5	1.5
c5	2.70	2.62	0.5	0.6	2.69	2.63	0.5	0.6
c6	2.99	2.90	0.3	0.4	2.95	2.89	0.3	0.4
c7	3.52	3.58	0.1	0.1	3.45	3.52	0.1	0.1
c8	3.31	3.38	0.2	0.2	3.35	3.45	0.2	0.1
c9	4.20	4.17	0.0	0.0	3.93	3.90	0.1	0.1
c10	5.05	5.03	0.0	0.0	5.00	5.00	0.0	0.0
c11	5.09	5.07	0.0	0.0	5.15	5.14	0.0	0.0
c12	5.65	5.67	0.0	0.0	5.44	5.48	0.0	0.0
c13	5.96	5.95	0.0	0.0	5.90	5.90	0.0	0.0
c14	6.79	6.77	0.0	0.0	6.76	6.74	0.0	0.0
c15	7.20	7.24	0.0	0.0	6.93	6.99	0.0	0.0
c16	7.95	7.35	0.0	0.0	7.87	7.81	0.0	0.0
c17	8.75	8.72	0.0	0.0	8.41	8.41	0.0	0.0
c18	8.42	8.38	0.0	0.0	8.11	8.12	0.0	0.0
c19	9.13	9.11	0.0	0.0	8.76	8.77	0.0	0.0
c20	10.19	10.21	0.0	0.0	10.36	10.40	0.0	0.0
c21	11.96	11.96	0.0	0.0	11.96	11.97	0.0	0.0
c22	17.11	17.06	0.0	0.0	16.64	16.58	0.0	0.0
c23	17.18	17.15	0.0	0.0	16.63	16.63	0.0	0.0

[a] Referenced to E(c1)= -1287.8881 hartree and G(c1)= -1287.9019 hartree

[b] Referenced to E(c1)= -1287.2778 hartree and G(c1)= -1287.2917 hartree

Conformational analysis of 4



	B3LYP / 6-311++G (2d,p)						
	α1	α2	α3	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	-55.3	-146.8	-161.0	0.00	0.00	47.9	49.9
c2	-56.9	-140.9	166.3	0.05	0.10	44.1	42.2
c3	152.4	-155.1	-161.7	1.49	1.52	3.9	3.8
c4	150.7	-146.7	168.6	2.00	2.05	1.6	1.6
c5	-58.7	67.0	155.4	2.37	2.41	0.9	0.9
c6	-57.2	76.1	-154.8	2.56	2.64	0.6	0.6
c7	21.5	-145.7	-161.8	2.61	2.57	0.6	0.7
c8	20.5	-139.6	168.1	2.98	2.96	0.3	0.3
c9	152.2	97.4	169.3	4.47	4.49	0.0	0.0
c10	151.5	84.8	-162.0	5.13	5.15	0.0	0.0
c11	55.1	84.6	167.7	6.02	6.05	0.0	0.0
c12	146.2	61.3	-174.2	6.40	6.39	0.0	0.0
c13	74.0	80.6	-154.4	6.46	6.52	0.0	0.0
c14	-59.6	97.3	-58.0	6.77	6.87	0.0	0.0
c15	152.7	82.1	82.7	7.17	7.15	0.0	0.0
c16	38.3	80.5	84.7	8.84	8.82	0.0	0.0

Referenced to E(c1)= -1211.9716 hartree and G(c1)= -1211.9858 hartree

	B3LYP / 6-311G (2d,p)[a]				B3LYP / 6-311++G (3df,2dp)[b]			
	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	0.00	0.15	55.0	39.3	0.00	0.00	52.9	74.2
c2	0.33	0.00	31.5	50.6	0.16	0.72	40.2	22.0
c3	1.06	1.15	9.2	7.2	1.64	2.21	3.3	1.8
c4	2.08	2.76	1.6	0.5	2.13	2.69	1.5	0.8
c5	2.32	2.32	1.1	1.0	2.56	3.12	0.7	0.4
c6	3.21	3.14	0.2	0.3	2.62	3.24	0.6	0.3
c7	2.45	2.43	0.9	0.8	2.77	3.25	0.5	0.3
c8	3.09	3.32	0.3	0.2	3.15	3.62	0.3	0.2
c9	4.07	4.53	0.1	0.0	4.57	5.12	0.0	0.0
c10	5.47	6.15	0.0	0.0	5.19	5.75	0.0	0.0
c11	5.45	5.34	0.0	0.0	6.14	6.65	0.0	0.0
c12	5.47	29.99	0.0	0.0	6.60	7.10	0.0	0.0
c13	6.89	31.39	0.0	0.0	6.47	7.05	0.0	0.0
c14	6.39	6.99	0.0	0.0	6.56	7.16	0.0	0.0
c15	6.43	7.55	0.0	0.0	7.13	7.65	0.0	0.0
c16	8.12	9.02	0.0	0.0	8.79	9.33	0.0	0.0

[a] Referenced to E(c1)= -1211.9619 hartree and G(c2)= -1212.0153 hartree

[b] Referenced to E(c1)= -1211.0242 hartree and G(c1)= -1211.0393 hartree

	B3PW91 / 6-311G (3df,2dp)[a]				B3LYP / 6-311G (3df,2dp)[b]			
	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	0.00	0.00	53.5	56.2	0.00	0.00	53.6	55.3
c2	0.23	0.31	36.5	33.3	0.25	0.32	35.1	32.5
c3	1.32	1.32	5.8	6.1	1.18	1.16	7.3	7.8
c4	2.13	2.16	1.5	1.5	2.06	2.03	1.7	1.8
c5	2.25	2.26	1.2	1.2	2.44	2.43	0.9	0.9
c6	2.69	2.79	0.6	0.5	2.94	3.04	0.4	0.3
c7	2.54	2.51	0.7	0.8	2.53	2.45	0.7	0.9
c8	3.10	3.09	0.3	0.3	3.03	2.98	0.3	0.4
c9	4.00	4.05	0.1	0.1	4.08	4.10	0.1	0.1
c10	5.18	5.23	0.0	0.0	5.28	5.30	0.0	0.0
c11	5.61	5.63	0.0	0.0	5.62	5.58	0.0	0.0
c12	6.54	6.54	0.0	0.0	6.53	6.55	0.0	0.0
c13	6.51	6.56	0.0	0.0	6.54	6.62	0.0	0.0
c14	6.14	6.24	0.0	0.0	6.07	5.58	0.0	0.0
c15	6.53	6.53	0.0	0.0	6.48	6.45	0.0	0.0
c16	8.18	8.21	0.0	0.0	8.15	8.14	0.0	0.0

[a] Referenced to E(c1)= -1211.6536 hartree and G(c1)= -1211.6678 hartree

[b] Referenced to E(c1)= -1211.0175 hartree and G(c1)= -1211.0317 hartree

Comparison with crystal structure data

Compound 2	C-S		S=O		S=O		S-N		N-C		C-C		MAD
Exptl. from X-ray structure	1.767		1.432		1.442		1.616		1.478		1.521		
B3LYP / 6-31+G(2d,p)	1.785	(0.018)	1.453	(0.021)	1.451	(0.009)	1.663	(0.047)	1.493	(0.015)	1.537	(0.013)	0.018
B3LYP / 6-311G(2d,p)	1.786	(0.019)	1.449	(0.017)	1.446	(0.004)	1.663	(0.047)	1.48	(0.002)	1.534	(0.012)	0.017
B3LYP / 6-311G(3df,2dp)	1.778	(0.011)	1.44	(0.008)	1.439	(-0.003)	1.637	(0.021)	1.471	(-0.007)	1.533	(0.012)	0.009
B3LYP / 6-311++G(2d,p)	1.787	(0.020)	1.452	(0.020)	1.449	(0.007)	1.663	(0.047)	1.481	(0.003)	1.534	(0.013)	0.018
B3LYP / 6-311G++(3df,2dp)	1.779	(0.012)	1.436	(0.004)	1.43	(-0.012)	1.643	(0.027)	1.476	(-0.002)	1.533	(0.012)	0.011
B3PW91 / 6-311G(2d,p)	1.776	(0.009)	1.446	(0.014)	1.443	(0.001)	1.653	(0.037)	1.472	(-0.006)	1.528	(0.007)	0.011
B3PW91 / 6-311G(3df,2dp)	1.769	(0.002)	1.436	(0.004)	1.436	(-0.006)	1.63	(0.014)	1.464	(-0.014)	1.527	(0.006)	0.005
B3PW91 / 6-311G++(2d,p)	1.776	(0.009)	1.447	(0.015)	1.444	(0.002)	1.653	(0.037)	1.472	(-0.006)	1.528	(0.007)	0.012
B3PW91 / 6-311G++(3df,2dp)	1.770	(0.003)	1.435	(0.003)	1.438	(-0.004)	1.636	(0.020)	1.469	(-0.009)	1.527	(0.007)	0.006
M062X / 6-311G(2d,p)	1.768	(0.001)	1.442	(0.010)	1.437	(-0.005)	1.656	(0.040)	1.475	(-0.003)	1.527	(0.006)	0.010
M062X / 6-311G(3df,2dp)	1.764	(-0.003)	1.429	(-0.003)	1.433	(-0.009)	1.643	(0.027)	1.473	(-0.005)	1.526	(0.005)	0.008
M062X / 6-311G++(2d,p)	1.769	(0.002)	1.443	(0.011)	1.438	(-0.004)	1.657	(0.041)	1.476	(-0.002)	1.527	(0.006)	0.011
M062X / 6-311G++(3df,2dp)	1.764	(-0.003)	1.43	(-0.002)	1.435	(-0.007)	1.643	(0.027)	1.474	(-0.004)	1.526	(0.005)	0.007

Compound 3	C-S		S=O		S=O		S-O		O-C		C-C		MAD
Exptl. from X-ray structure	1.761		1.430		1.431		1.574		1.486		1.542		
B3LYP / 6-31+G(2d,p)	1.775	(0.014)	1.445	(0.015)	1.449	(0.018)	1.608	(0.034)	1.478	(-0.008)	1.532	(-0.010)	0.015
B3LYP / 6-311G(2d,p)	1.777	(0.016)	1.443	(0.013)	1.447	(0.016)	1.605	(0.031)	1.478	(-0.008)	1.529	(-0.013)	0.015
B3LYP / 6-311G(3df,2dp)	1.769	(0.008)	1.433	(0.003)	1.438	(0.007)	1.587	(0.013)	1.476	(-0.010)	1.528	(-0.014)	0.007
B3LYP / 6-311++G(2d,p)	1.778	(0.017)	1.445	(0.015)	1.448	(0.017)	1.606	(0.032)	1.480	(-0.006)	1.530	(-0.012)	0.016
B3LYP / 6-311G++(3df,2dp)	1.770	(0.009)	1.435	(0.005)	1.439	(0.008)	1.586	(0.012)	1.478	(-0.008)	1.529	(-0.013)	0.008
B3PW91 / 6-311G(2d,p)	1.767	(0.006)	1.439	(0.009)	1.443	(0.012)	1.597	(0.023)	1.468	(-0.018)	1.524	(-0.018)	0.011
B3PW91 / 6-311G(3df,2dp)	1.760	(-0.001)	1.430	(0.000)	1.434	(0.003)	1.579	(0.005)	1.466	(-0.020)	1.523	(-0.019)	0.005
B3PW91 / 6-311G++(2d,p)	1.767	(0.006)	1.440	(0.010)	1.444	(0.013)	1.597	(0.023)	1.469	(-0.017)	1.524	(-0.018)	0.012
B3PW91 / 6-311G++(3df,2dp)	1.760	(-0.001)	1.432	(0.002)	1.435	(0.004)	1.579	(0.005)	1.467	(-0.019)	1.523	(-0.019)	0.005
M062X / 6-311G(2d,p)	1.759	(-0.002)	1.433	(0.003)	1.436	(0.005)	1.586	(0.012)	1.462	(-0.024)	1.524	(-0.018)	0.007
M062X / 6-311G(3df,2dp)	1.756	(-0.005)	1.424	(-0.006)	1.429	(-0.002)	1.571	(-0.003)	1.459	(-0.027)	1.523	(-0.019)	0.006
M062X / 6-311G++(2d,p)	1.760	(-0.001)	1.434	(0.004)	1.438	(0.007)	1.586	(0.012)	1.463	(-0.023)	1.524	(-0.018)	0.007
M062X / 6-311G++(3df,2dp)	1.756	(-0.005)	1.426	(-0.004)	1.43	(-0.001)	1.571	(-0.003)	1.461	(-0.025)	1.523	(-0.019)	0.005

Compound 4	C-S		S=O		S-O		O-C		C-C		MAD
Exptl. from X-ray structure	1.794		1.473		1.631		1.474		1.525		
B3LYP / 6-311G(2d,p)	1.807	(0.013)	1.483	(0.010)	1.673	(0.042)	1.463	(-0.011)	1.530	(0.005)	0.014
B3LYP / 6-311G(3df,2dp)	1.798	(0.004)	1.473	(0.000)	1.652	(0.021)	1.461	(-0.013)	1.528	(0.003)	0.006
B3LYP / 6-311++G(2d,p)	1.807	(0.013)	1.487	(0.014)	1.673	(0.042)	1.467	(-0.007)	1.530	(0.005)	0.015
B3LYP / 6-311G++(3df,2dp)	1.799	(0.005)	1.475	(0.002)	1.648	(0.017)	1.464	(-0.010)	1.529	(0.004)	0.006
B3PW91 / 6-311G(3df,2dp)	1.789	(-0.005)	1.469	(-0.004)	1.640	(0.009)	1.454	(-0.020)	1.523	(-0.002)	0.004

2. Additional spectra plots

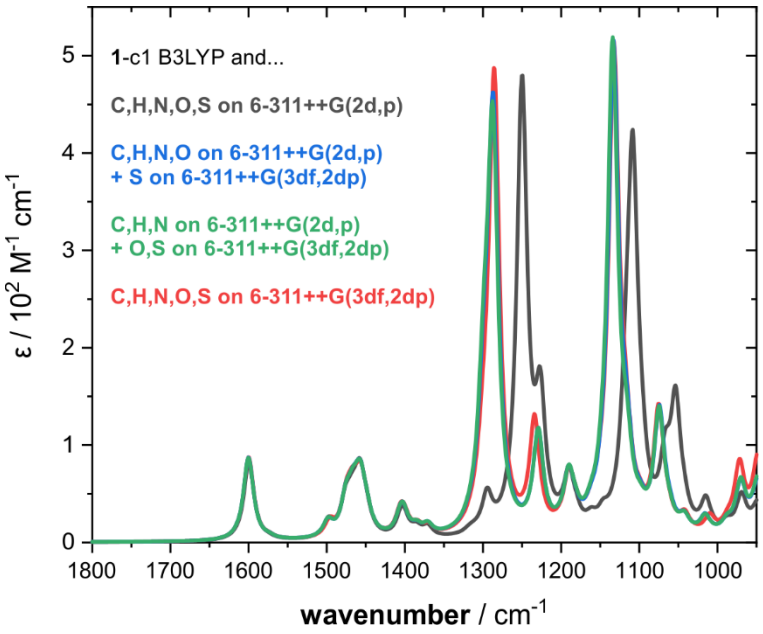


Figure S1. Effect of different basis sets on only S or S+O.

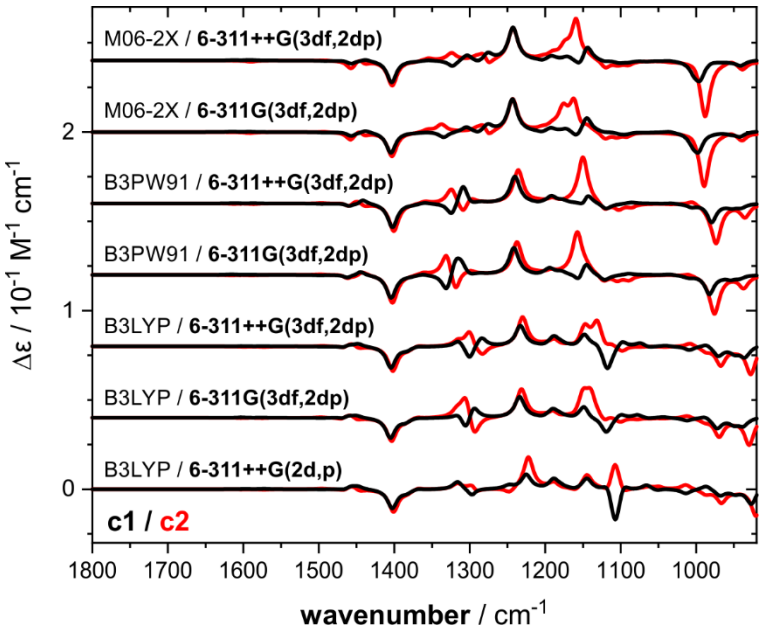


Figure S2. Comparison of single conformer spectra **1**-c1 and -c2.

3. Data for thio-menthol

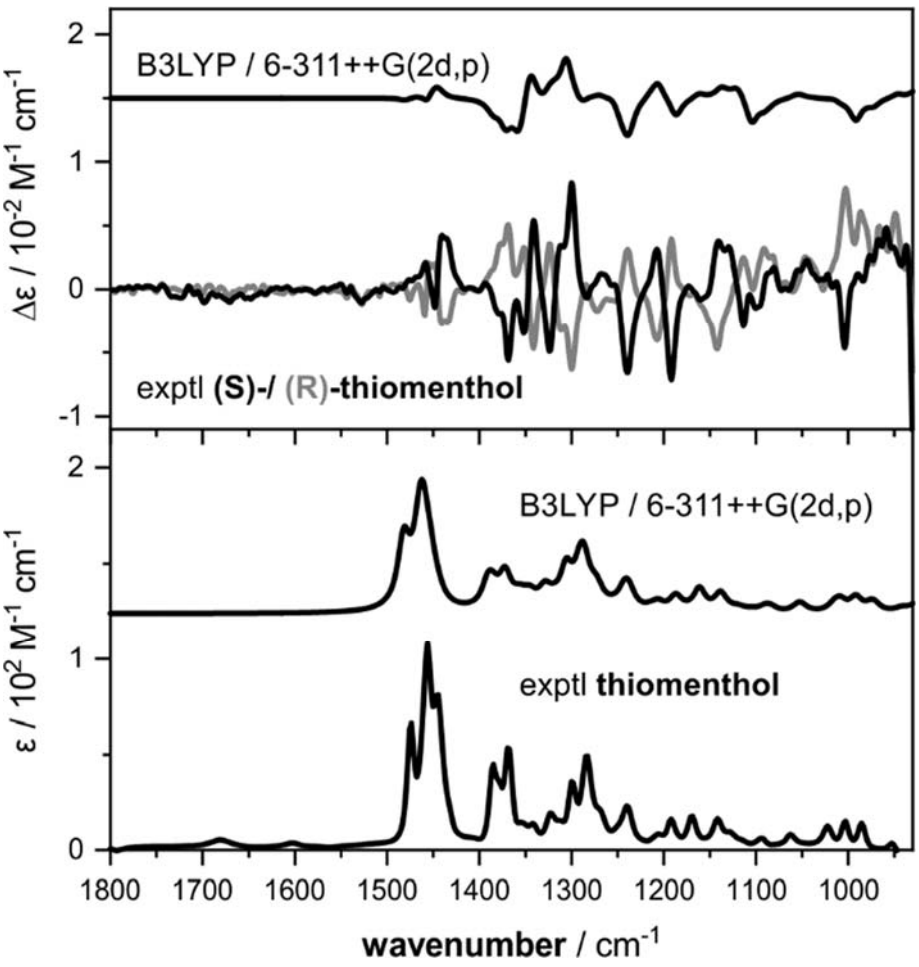
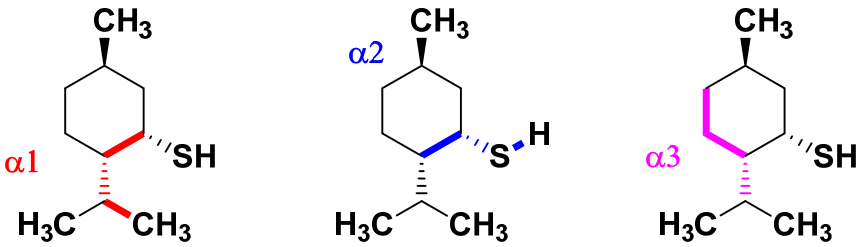


Figure S3. Comparison of the experimental and computed spectra of thiomenthol.



	B3LYP / 6-311++G (2d,p)						
	α1	α2	α3	ΔE_{ZPC}	ΔG_{298K}	popΔE	popΔG
c1	52.8	-75.5	176.4	0.00	0.00	33.0	33.2
c2	50.7	64.4	175.6	0.00	0.02	33.0	32.3
c3	50.8	-178.4	176.0	0.07	0.04	29.5	31.0
c4	142.8	179.7	171.7	2.00	2.07	1.1	1.0
c5	140.4	66.0	171.7	2.00	2.15	1.1	0.9
c6	140.6	-75.1	172.3	2.10	2.28	1.0	0.7
c7	-79.1	172.6	168.3	2.36	2.54	0.6	0.5
c8	-81.3	59.5	167.9	2.66	2.88	0.4	0.3
c9	-80.7	-82.6	168.1	2.84	2.94	0.3	0.2
c10	158.0	78.9	-85.2	6.75	6.80	0.0	0.0
c11	158.4	-163.8	-85.7	6.88	6.88	0.0	0.0
c12	157.2	-56.2	-85.0	7.10	7.06	0.0	0.0
c13	67.7	-157.2	-67.9	7.15	6.96	0.0	0.0
c14	88.8	-58.5	-71.9	7.54	7.45	0.0	0.0
c15	-37.6	78.1	-80.0	9.41	9.77	0.0	0.0
c16	-35.5	-59.9	-79.5	9.42	9.82	0.0	0.0

Referenced to E(c1)= -791.1847 hartree and G(c1)= -791.2232 hartree

4. Crystal structure of 1

The single crystal was analyzed on a *Rigaku* Synergy dual source device, with Co micro focus sealed tube (Cu K_α) using mirror monochromators and a HyPix-6000HE: Hybrid photon counting X-ray detector. The Crystal were mounted in *Hampton* CrypLoops using *GE/Bayer* silicone grease. Data was recorded and reduced using the CrysalisPro[i] Software. The structure was solved using WinGX[ii] in combination with ShelXT[iii] and refined with shelXle[iv] and ShelXL. Tables for the publication were generated using a modified version of Ciftab. The Picture was generated with Diamond 4.[v]

Compound	**(S)-2-Isopropyl-1-tosylaziridine (1)**
CCDC-Number	2035537
Empirical formula	C12 H17 N O2 S
Formula weight [g/mol]	239.32
Crystal system	Orthorhombic
Space group	P212121 (19)
Lattice parameters [Å]	
a	6.27149(10)
b	13.8374(3)
c	14.1502(2)
α	90
β	90
γ	90
Density [g/cm^3]	1.295
Crystal size [mm^3]	0.309 x 0.258 x 0.141
Volume [Å^3]	1227.97(4)
Z	4
Temperature [K]	170.00(10)
Diffraction Device	XtaLAB Synergy, Dualflex, HyPix
Radiation Type	1.54184 Å (Cu K/ micro-focus sealed X-ray tube)
F(000)	512
Absorption coefficient [mm^{-1}]	2.228
Absorption correction	Semi-empirical from equivalents
Measurement range	4.5 - 66.5
Index range	-7 < h < 7
	-14 < k < 16
	-16 < l < 16
Measured reflexes	17363
Independent	2170
Observed	2108
R(int)	0.0591
Completeness (%) / theta (°)	99.9 / 66.489
Transmission (min / max)	0.38717 / 1.00000
R1 (observed/all)	0.0315 / 0.0325
wR2 (observed/all)	0.0833 / 0.0840
GooF = S	1.073
Rest electron density max./min. [e-/Å^3]	-0.436 / 0.373

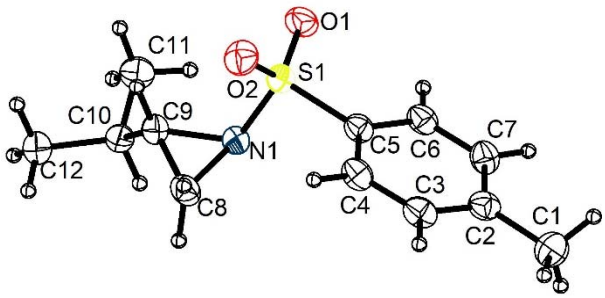


Figure S*n*: Asymmetric unit of compound **1.**

[i] Meyer, M.; Paciorek, W.; Kowalski, A.; Muszynski, A.; Wisniewski, A.; Pol, M.; Przewozniczek, M.; Stec, P.; Bujnik, D.; Kulza, H. *et al. CrysAlisPro*; Rigaku Oxford Diffraction (1995-2018), 2018.
[ii] Farrugia, L. J. WinGX suite for small-molecule single-crystal crystallography. *J. Appl. Crystallogr.* **1999**, *32*, 837–838, DOI: 10.1107/S0021889899006020.
[iii] Sheldrick, G. M. A short history of SHELX. *Acta Crystallogr A Found Crystallogr* **2008**, *64*, 112–122, DOI: 10.1107/S0108767307043930.
[iv] Hübschle, C. B.; Sheldrick, G. M.; Dittrich, B. ShelXle: a Qt graphical user interface for SHELXL. *J. Appl. Crystallogr.* **2011**, *44*, 1281–1284, DOI: 10.1107/S0021889811043202.
[v] Putz, H.; Brandenburg, K. *Diamond*; Crystal Impact: Bonn, Deutschland, 2014.

Atomic coordinates and equivalent isotropic displacement parameters [Å^2] for compound **1**.

	x	y	z	U(eq)
S(1)	0.32103(9)	0.53940(4)	0.57600(4)	0.02889(19)
O(1)	0.0919(3)	0.54158(14)	0.57357(12)	0.0364(4)
N(1)	0.4010(3)	0.63288(15)	0.51105(14)	0.0287(5)
C(1)	0.6088(5)	0.6641(2)	0.96553(19)	0.0425(7)
C(10)	0.3555(4)	0.68158(18)	0.33890(16)	0.0301(5)
C(11)	0.1145(4)	0.6734(2)	0.3317(2)	0.0374(6)
C(12)	0.4646(5)	0.6640(2)	0.24369(18)	0.0385(6)
C(2)	0.5385(4)	0.62981(19)	0.86958(18)	0.0319(5)
O(2)	0.4263(3)	0.45129(13)	0.54928(13)	0.0395(5)
C(3)	0.6786(4)	0.58474(19)	0.80734(17)	0.0336(6)
C(4)	0.6172(4)	0.55630(19)	0.71764(18)	0.0326(6)
C(6)	0.2635(4)	0.61727(18)	0.75016(17)	0.0312(5)
C(5)	0.4079(4)	0.57347(18)	0.68928(17)	0.0284(5)
C(7)	0.3274(4)	0.64444(19)	0.83955(17)	0.0337(5)
C(9)	0.4396(4)	0.60978(18)	0.40936(17)	0.0292(5)
C(8)	0.6232(4)	0.6279(2)	0.47266(17)	0.0346(6)
H(1A)	0.510848	0.63915	1.013693	0.064
H(1B)	0.607922	0.73488	0.967045	0.064
H(1C)	0.753243	0.64052	0.978375	0.064
H(10)	0.392315	0.74814	0.361074	0.036
H(11A)	0.050274	0.68822	0.393122	0.056
H(11B)	0.075919	0.60744	0.312985	0.056
H(11C)	0.06175	0.71912	0.284255	0.056
H(12A)	0.619289	0.67045	0.251138	0.058
H(12B)	0.41359	0.7115	0.197585	0.058
H(12C)	0.430736	0.5987	0.221394	0.058
H(3)	0.821134	0.57312	0.827089	0.04
H(4)	0.715676	0.52572	0.676289	0.039
H(6)	0.12092	0.62848	0.730251	0.037
H(7)	0.227487	0.6734	0.88132	0.04
H(9)	0.417226	0.5405	0.391885	0.035
H(8A)	0.702049	0.68933	0.464796	0.042
H(8AB)	0.712229	0.57185	0.491074	0.042

Anisotropic displacement parameters [Å^2] forcompound (1)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	0.0277(3)	0.0291(3)	0.0298(3)	0.0010(2)	0.0007(2)	-0.0015(2)
O(1)	0.0254(9)	0.0483(10)	0.0354(10)	0.0039(10)	-0.0022(7)	-0.0064(8)
N(1)	0.0272(10)	0.0320(11)	0.0269(10)	-0.0012(8)	0.0021(8)	-0.0020(8)
C(1)	0.0424(15)	0.0490(17)	0.0360(14)	0.0011(12)	-0.0054(12)	-0.0023(13)
C(10)	0.0338(14)	0.0280(12)	0.0284(12)	0.0001(10)	0.0010(10)	-0.0037(10)
C(11)	0.0325(14)	0.0381(14)	0.0416(14)	0.0015(12)	-0.0026(11)	0.0013(11)
C(12)	0.0431(15)	0.0423(15)	0.0301(13)	-0.0018(11)	0.0045(11)	-0.0046(12)
C(2)	0.0324(12)	0.0304(12)	0.0329(13)	0.0073(10)	-0.0021(10)	-0.0031(10)
O(2)	0.0481(11)	0.0294(10)	0.0411(10)	-0.0020(8)	0.0020(8)	0.0030(8)
C(3)	0.0257(11)	0.0370(13)	0.0382(13)	0.0082(10)	-0.0021(11)	0.0016(11)
C(4)	0.0272(12)	0.0345(14)	0.0359(13)	0.0046(10)	0.0034(10)	0.0045(10)
C(6)	0.0229(11)	0.0365(13)	0.0340(12)	0.0037(11)	0.0024(9)	0.0011(10)
C(5)	0.0269(11)	0.0296(12)	0.0287(12)	0.0050(9)	0.0003(9)	-0.0007(10)
C(7)	0.0307(12)	0.0387(14)	0.0317(12)	0.0014(10)	0.0035(11)	0.0042(11)
C(9)	0.0300(12)	0.0307(12)	0.0269(12)	-0.0020(10)	0.0029(9)	0.0006(9)
C(8)	0.0251(12)	0.0467(15)	0.0321(12)	0.0024(11)	0.0028(10)	-0.0026(11)

5. Selected Cartesian coordinates

(1S)-**1**-c1 B3LYP / 6-31G (d,p)

C	2.57793800	-0.01328300	-0.56757100
C	1.54518300	-0.35008800	-1.58018200
H	2.84986000	1.04216900	-0.53009500
H	1.50660600	-1.34277800	-2.01993600
H	1.16998500	0.46055200	-2.19886800
N	1.19051100	-0.33174100	-0.14070400
C	3.65708100	-0.97849200	-0.11577500
H	3.23883400	-1.99086700	-0.19071000
C	4.03921200	-0.71682800	1.34760100
H	3.16248400	-0.77707200	1.99890000
H	4.77614200	-1.44886300	1.69301400
H	4.47823500	0.28085700	1.46513500
C	4.87220300	-0.87951500	-1.05082400
H	5.31337800	0.12343200	-1.01739200
H	5.64639600	-1.59280300	-0.75146300
H	4.59866800	-1.09277900	-2.08928000
S	0.25671500	0.98685800	0.42236600
O	0.43145100	2.17391700	-0.43718300
O	0.54936900	1.09732800	1.85850200
C	-1.39864900	0.35883200	0.19743400
C	-2.19577200	0.87371400	-0.82472600
C	-1.87549800	-0.63505300	1.05713900
C	-3.48867100	0.37769400	-0.98767000
H	-1.80975600	1.65172000	-1.47323500
C	-3.16707700	-1.11901600	0.87589600
H	-1.24710700	-1.01857700	1.85326600
C	-3.99391400	-0.62136900	-0.14470100
H	-4.11410900	0.77516300	-1.78184300
H	-3.54261100	-1.89375000	1.53832500
C	-5.40342400	-1.13378000	-0.30818600
H	-5.46602600	-2.20394900	-0.09099300
H	-6.08435600	-0.62225400	0.38281800
H	-5.77588200	-0.96459800	-1.32173300

(1S)-**1**-c1 B3LYP / 6-31G (2d,p)

C	2.57067000	0.26706400	-0.49893200
C	1.54222900	0.47543500	-1.54859100
H	2.84487800	1.16502900	0.05315800
H	1.50636400	-0.17616600	-2.41632600
H	1.17275100	1.48597900	-1.69122600
N	1.17914700	-0.20634400	-0.28705600
C	3.63674200	-0.80649100	-0.56817000
H	3.21039900	-1.65023300	-1.12566300
C	4.00446300	-1.29012600	0.84055100
H	3.11751300	-1.63438700	1.37995500
H	4.72288300	-2.11439800	0.79313200
H	4.46062000	-0.48216000	1.42442200
C	4.86232200	-0.28397500	-1.33125700
H	5.31095700	0.57277600	-0.81530400
H	5.62705300	-1.06294900	-1.40788400
H	4.59863600	0.03389600	-2.34502300
S	0.26100200	0.66231100	0.83548700
O	0.43141400	2.09885700	0.66379100
O	0.55425700	0.06062400	2.12206100
C	-1.38512800	0.22500200	0.34152900
C	-2.16368700	1.14249800	-0.35855200
C	-1.88645200	-1.03492100	0.67666900
C	-3.45776700	0.78753500	-0.73305800
H	-1.76344000	2.12103000	-0.59401700
C	-3.17721600	-1.37221000	0.29330400

H	-1.27317500	-1.73148100	1.23570700
C	-3.98283300	-0.46892000	-0.41650100
H	-4.06858700	1.50132600	-1.27665100
H	-3.57121100	-2.35042900	0.55160800
C	-5.38729100	-0.84858600	-0.81127900
H	-5.40336200	-1.80896600	-1.33676300
H	-6.02620300	-0.95616400	0.07267800
H	-5.83780600	-0.09495400	-1.46131600

(1S)-**1**-c1 B3LYP / 6-31G (3df,2pd)

C	2.57406300	0.17692300	-0.53347600
C	1.54896400	0.20229700	-1.60428900
H	2.86596300	1.15338000	-0.15593800
H	1.50514500	-0.59706900	-2.33352400
H	1.19409400	1.16999100	-1.93617200
N	1.17529500	-0.22331800	-0.23944000
C	3.62261600	-0.90895900	-0.41356800
H	3.18628500	-1.82378300	-0.82706600
C	3.97981600	-1.16331600	1.05545600
H	3.09393400	-1.42750500	1.63393600
H	4.70031000	-1.97864800	1.14149800
H	4.42535700	-0.27401100	1.50832200
C	4.85667700	-0.53584700	-1.24614600
H	5.31752300	0.38235900	-0.87378200
H	5.60588200	-1.32748700	-1.19547100
H	4.59976000	-0.38164000	-2.29581500
S	0.25746100	0.82089500	0.69639800
O	0.42015400	2.19586800	0.26999500
O	0.55227800	0.48132000	2.06770100
C	-1.38067400	0.29188700	0.29630700
C	-2.16048700	1.05016100	-0.57330600
C	-1.87849300	-0.88259800	0.86658100
C	-3.45035800	0.62247200	-0.87591300
H	-1.76634100	1.96358400	-0.99461200
C	-3.16560700	-1.29329500	0.55237800
H	-1.26704800	-1.45447000	1.54999500
C	-3.97127300	-0.55043400	-0.32306200
H	-4.05967900	1.21220500	-1.54867200
H	-3.55552600	-2.20155500	0.99454300
C	-5.36976400	-1.00940100	-0.64515200
H	-5.36679700	-2.02668500	-1.04225300
H	-5.99371000	-1.01736000	0.25162200
H	-5.84393800	-0.35925000	-1.37931800

(1S)-**1**-c1 B3LYP / 6-31++G (d,p)

C	2.59370200	0.01245000	-0.55762000
C	1.57045300	-0.25786200	-1.60195100
H	2.88620600	1.05908600	-0.46349500
H	1.52226200	-1.22998000	-2.08524600
H	1.21783700	0.58599900	-2.18902500
N	1.19315600	-0.29777900	-0.16801800
C	3.64950200	-0.99608200	-0.14310400
H	3.21460900	-1.99547400	-0.27717700
C	4.02305300	-0.82184200	1.33631700
H	3.14208000	-0.91434800	1.97881400
H	4.75221000	-1.57986800	1.64155700
H	4.46951800	0.16409900	1.51413600
C	4.87679000	-0.86894600	-1.06081500
H	5.33744900	0.12185600	-0.96652300
H	5.63304000	-1.61438200	-0.79376400
H	4.60976500	-1.01901800	-2.11252600
S	0.25218500	0.99238400	0.44749800
O	0.41579400	2.21666800	-0.36498700
O	0.55135500	1.05304700	1.88774600

C	-1.40367800	0.36358500	0.20771700
C	-2.16941000	0.82901500	-0.86288600
C	-1.90706000	-0.58907300	1.09894800
C	-3.45897400	0.32487200	-1.04057700
H	-1.76740500	1.57679000	-1.53726700
C	-3.19571900	-1.08095300	0.90307500
H	-1.30290700	-0.93564800	1.93020000
C	-3.99253800	-0.63260300	-0.16462700
H	-4.05868200	0.68548500	-1.87157600
H	-3.59081200	-1.82219000	1.59220300
C	-5.39937100	-1.14896800	-0.34376400
H	-5.47758700	-2.20064700	-0.05270600
H	-6.10027500	-0.58373600	0.28293100
H	-5.73203900	-1.05099000	-1.38071700

(1S)-**1**-c1 B3LYP / 6-31++G (2d,p)

C	2.58251400	0.05631400	-0.55322300
C	1.55484000	-0.15390900	-1.60477500
H	2.86721200	1.09542300	-0.39194100
H	1.51278400	-1.09485700	-2.14497800
H	1.19148000	0.72064600	-2.13537100
N	1.18549700	-0.28357000	-0.17624800
C	3.64419200	-0.96994100	-0.21160800
H	3.21173700	-1.96098700	-0.40032000
C	4.03407600	-0.88275400	1.27016400
H	3.16115500	-1.01427000	1.91676100
H	4.76796400	-1.65563100	1.52188000
H	4.48142000	0.09177500	1.50066900
C	4.86074100	-0.78370400	-1.13185700
H	5.31882000	0.20174500	-0.98403300
H	5.62251100	-1.54009300	-0.91660500
H	4.58377500	-0.87235800	-2.18785100
S	0.25425100	0.94442600	0.51468600
O	0.41638700	2.20910200	-0.19555400
O	0.54449000	0.90131800	1.93826600
C	-1.39026800	0.33942600	0.22606300
C	-2.17655000	0.91970800	-0.76678300
C	-1.88312000	-0.70507200	1.01335000
C	-3.47027200	0.44129100	-0.97519200
H	-1.78600400	1.73806000	-1.35957000
C	-3.17367500	-1.17007800	0.79029500
H	-1.26586400	-1.14051700	1.79035500
C	-3.98856100	-0.60563700	-0.20469300
H	-4.08438300	0.89485000	-1.74697000
H	-3.55840800	-1.98127800	1.40123800
C	-5.39296900	-1.11145000	-0.41913000
H	-5.40803300	-2.20128800	-0.52561900
H	-6.03130000	-0.86234600	0.43671700
H	-5.84405800	-0.67321800	-1.31297000

(1S)-**1**-c1 B3LYP / 6-31++G (3df,2pd)

C	2.57839300	0.03365800	-0.55535400
C	1.55206100	-0.22237700	-1.59507200
H	2.86981000	1.07494000	-0.44559300
H	1.50742400	-1.18564600	-2.08815000
H	1.19500100	0.62372000	-2.16890900
N	1.17955500	-0.27702200	-0.16417400
C	3.63252200	-0.98103600	-0.16375100
H	3.19338100	-1.97389400	-0.30417600
C	4.02223700	-0.82503400	1.31128000
H	3.15129700	-0.92048700	1.96148900
H	4.74942500	-1.58681100	1.59968700
H	4.47332100	0.15424200	1.49364500
C	4.84955400	-0.84868300	-1.09067500
H	5.31219300	0.13699000	-0.99146800

H	5.60412300	-1.59642700	-0.83926800
H	4.57303100	-0.98731100	-2.13803800
S	0.25462400	0.96969600	0.46875800
O	0.41551400	2.19307300	-0.29285400
O	0.54335200	0.99537000	1.88393300
C	-1.38374100	0.35258500	0.21214900
C	-2.16403500	0.86597900	-0.82300100
C	-1.88189800	-0.64160700	1.05814500
C	-3.45421700	0.37467800	-1.00981600
H	-1.77143300	1.64266600	-1.46369600
C	-3.17068900	-1.12071500	0.85589400
H	-1.27184700	-1.02745800	1.86292100
C	-3.97809400	-0.62107900	-0.17706000
H	-4.06081800	0.77461100	-1.81296700
H	-3.55753300	-1.89196700	1.51062700
C	-5.38570900	-1.12648500	-0.36333900
H	-5.45796000	-2.19140900	-0.13821800
H	-6.07329600	-0.60512500	0.30882900
H	-5.73622500	-0.96347600	-1.38265000

(1S)-**1**-c1 B3LYP / 6-311G (d,p)

C	2.57891300	-0.01309300	-0.56366900
C	1.54405800	-0.34712500	-1.57362100
H	2.85850100	1.03833900	-0.53100500
H	1.50172800	-1.34067100	-2.00524700
H	1.17855700	0.46143600	-2.19680700
N	1.18887600	-0.31495900	-0.13582000
C	3.64876100	-0.98592200	-0.11135900
H	3.22335300	-1.99335400	-0.18561200
C	4.03654500	-0.72915400	1.35038800
H	3.16424000	-0.79352200	2.00468800
H	4.77358000	-1.46236900	1.68847700
H	4.47511600	0.26692800	1.46930900
C	4.86219400	-0.89691100	-1.04860000
H	5.31241700	0.10038200	-1.01401900
H	5.62810300	-1.61798000	-0.75194500
H	4.58449100	-1.10637800	-2.08520500
S	0.25494900	1.00170100	0.41608800
O	0.42464200	2.18015300	-0.44626900
O	0.54665000	1.12468300	1.84517100
C	-1.40017200	0.36284000	0.19399100
C	-2.20123500	0.87275200	-0.82335800
C	-1.86537100	-0.63529600	1.05073600
C	-3.49039700	0.37078600	-0.98133100
H	-1.82481400	1.65379400	-1.47088100
C	-3.15258000	-1.12513900	0.87413000
H	-1.23362600	-1.01703900	1.84249200
C	-3.98535400	-0.63135500	-0.14050300
H	-4.11915700	0.76641200	-1.77125900
H	-3.51892600	-1.90253800	1.53563200
C	-5.39111200	-1.15256200	-0.29868900
H	-5.43871200	-2.22770500	-0.11201200
H	-6.06350800	-0.66778900	0.41696500
H	-5.77849200	-0.95807900	-1.30015700

(1S)-**1**-c1 B3LYP / 6-311G (2d,p)

C	2.57018700	0.02061500	-0.55871100
C	1.53983800	-0.26243000	-1.58440200
H	2.84144600	1.06887600	-0.46312600
H	1.50754900	-1.23021600	-2.07027500
H	1.16341500	0.57474800	-2.15910600
N	1.18238600	-0.31437400	-0.14857600
C	3.64504400	-0.96761500	-0.16334700
H	3.22533500	-1.97121600	-0.29014100
C	4.03398500	-0.78704900	1.30740200

H	3.16344900	-0.88615500	1.95811900
H	4.77263300	-1.53401300	1.60637100
H	4.46992700	0.20178000	1.47687800
C	4.85509600	-0.82236700	-1.09442900
H	5.29885300	0.17356700	-1.00787200
H	5.62550200	-1.55247300	-0.83770000
H	4.57738700	-0.97771300	-2.13951600
S	0.25738000	0.96229600	0.46531600
O	0.42755100	2.17597800	-0.32030200
O	0.54261500	1.00275700	1.88640300
C	-1.38988100	0.34512700	0.20672400
C	-2.19646800	0.92229000	-0.76445900
C	-1.86049300	-0.69947800	1.00051000
C	-3.48918700	0.44266300	-0.94442000
H	-1.81997700	1.74134600	-1.36171800
C	-3.14890500	-1.16702500	0.80496000
H	-1.22676300	-1.13253000	1.76284300
C	-3.98443100	-0.60544500	-0.16898800
H	-4.12138400	0.89521100	-1.69940200
H	-3.51765800	-1.97916400	1.42121400
C	-5.38541000	-1.12376900	-0.36051700
H	-5.37969500	-2.19327800	-0.58535800
H	-5.97836700	-0.98987500	0.54804600
H	-5.89401800	-0.60798100	-1.17503000

(1S)-**1**-c1 B3LYP / 6-311G (3df,2pd)

C	2.57544200	0.13748000	-0.54165600
C	1.55824200	0.09199400	-1.61592800
H	2.87178700	1.13601000	-0.23482600
H	1.51385200	-0.75646100	-2.28562600
H	1.21070400	1.03423800	-2.01753900
N	1.17608900	-0.23143700	-0.22818500
C	3.61945200	-0.93761000	-0.34069500
H	3.18367800	-1.87952900	-0.68495900
C	3.97603400	-1.08155100	1.14098800
H	3.09244900	-1.30584000	1.73765700
H	4.69956000	-1.88436300	1.28609700
H	4.41738400	-0.16013200	1.52647700
C	4.85388700	-0.62892500	-1.19474900
H	5.31498500	0.31269900	-0.88974600
H	5.60107800	-1.41501700	-1.08425700
H	4.59978300	-0.55176300	-2.25256900
S	0.25620200	0.87465500	0.62806000
O	0.40899000	2.21269900	0.10300800
O	0.55218700	0.64075900	2.01774800
C	-1.38143300	0.30891500	0.26950400
C	-2.18104500	1.02492200	-0.61146800
C	-1.85735200	-0.84709500	0.88548400
C	-3.46840000	0.57528500	-0.87791200
H	-1.80358900	1.92610000	-1.07106600
C	-3.14143300	-1.28126100	0.60667600
H	-1.23122500	-1.39134900	1.57716200
C	-3.96839300	-0.57944800	-0.27794800
H	-4.09292900	1.13483400	-1.56177500
H	-3.51250000	-2.17841800	1.08531400
C	-5.36662100	-1.05918100	-0.55628600
H	-5.37069200	-2.11096500	-0.84467700
H	-5.99191800	-0.96878800	0.33405700
H	-5.83396400	-0.48448800	-1.35350000

(1S)-**1**-c1 B3LYP / 6-311++G (d,p)

C	2.58855300	0.02810400	-0.55745400
C	1.56711700	-0.21292000	-1.60798800
H	2.87858500	1.07037000	-0.43627500
H	1.51964800	-1.16949100	-2.11618600

H	1.21609200	0.64573800	-2.16989100
N	1.18847500	-0.29067300	-0.17764000
C	3.64313200	-0.98885700	-0.17006400
H	3.20826800	-1.98291700	-0.32575200
C	4.02012100	-0.84857900	1.31037900
H	3.14180900	-0.95171100	1.95175900
H	4.74592900	-1.61434800	1.59709800
H	4.46966700	0.13009800	1.50819800
C	4.86666000	-0.84127100	-1.08693400
H	5.32685700	0.14551500	-0.97192400
H	5.62217400	-1.59132600	-0.83906200
H	4.59736500	-0.96790100	-2.13918600
S	0.25292800	0.97870600	0.47446600
O	0.41208600	2.22067600	-0.29948600
O	0.55669400	0.99947900	1.90813900
C	-1.40403900	0.35638200	0.21975300
C	-2.18007300	0.87430800	-0.81392600
C	-1.89218600	-0.64480400	1.05936900
C	-3.46640100	0.37620700	-1.00550200
H	-1.78829600	1.65826600	-1.44906400
C	-3.17774400	-1.12970900	0.85065800
H	-1.27970800	-1.03284600	1.86335500
C	-3.98510200	-0.62826000	-0.18043700
H	-4.07488900	0.77818700	-1.80820500
H	-3.56159200	-1.90861400	1.50048100
C	-5.39000500	-1.13949600	-0.37345500
H	-5.46525000	-2.19949900	-0.12194700
H	-6.08716000	-0.59919400	0.27591500
H	-5.72611200	-1.00279000	-1.40292500

(1S)-**1**-c1 B3LYP / 6-311++G (2d,p)

C	2.58023000	-0.14974300	0.52797600
C	1.55971000	-0.13369400	1.60152900
H	2.86105700	-1.14003300	0.17839200
H	1.52555600	0.68987100	2.30472600
H	1.19623700	-1.08735300	1.96416900
N	1.18329600	0.25762600	0.22349800
C	3.64422700	0.91624200	0.38321100
H	3.22131100	1.85147500	0.76537900
C	4.02331800	1.11995800	-1.08710400
H	3.15169100	1.39165300	-1.68523700
H	4.76654700	1.91443500	-1.18584100
H	4.45155300	0.20660400	-1.51026400
C	4.86371200	0.54747200	1.23807800
H	5.31433200	-0.38845800	0.89524400
H	5.62604800	1.32671400	1.17229700
H	4.59455200	0.42642400	2.29005100
S	0.25362900	-0.83829800	-0.67108400
O	0.41880300	-2.20374500	-0.18823900
O	0.54209500	-0.55107600	-2.06482900
C	-1.39421800	-0.29416100	-0.28270800
C	-2.17122200	-1.02938500	0.60286100
C	-1.89220400	0.85996600	-0.88461400
C	-3.46180300	-0.59789000	0.89146100
H	-1.77624200	-1.93082400	1.05128300
C	-3.17907500	1.27624500	-0.58392800
H	-1.28222400	1.41779400	-1.58256200
C	-3.98504200	0.55635100	0.30745100
H	-4.07029100	-1.17293700	1.57959200
H	-3.56855200	2.17312800	-1.05219600
C	-5.38543600	1.01845400	0.61202600
H	-5.38984400	2.05545100	0.95641700
H	-6.01268400	0.97367600	-0.28246500
H	-5.85053900	0.40145100	1.38097500

(1S)-**1**-c1 B3LYP / 6-311++G (3df,2pd)

C	2.57515000	0.04259600	-0.55451700
C	1.55292800	-0.18987400	-1.59921800
H	2.86835400	1.07978700	-0.42409400
H	1.50764500	-1.14166100	-2.11129100
H	1.20026900	0.66715800	-2.15688600
N	1.17746700	-0.27079300	-0.17366500
C	3.62667600	-0.97806300	-0.18142100
H	3.18941600	-1.96728600	-0.34177600
C	4.01324900	-0.85133900	1.29448300
H	3.14229100	-0.95946300	1.94022300
H	4.73896500	-1.61774700	1.56835400
H	4.46356300	0.12281000	1.49666800
C	4.84373800	-0.82710000	-1.10114800
H	5.30486400	0.15544500	-0.98153300
H	5.59697500	-1.57830100	-0.86280500
H	4.56992500	-0.94508000	-2.15023300
S	0.25438300	0.96063400	0.48466100
O	0.41315900	2.19692100	-0.25095100
O	0.54432100	0.95895300	1.89720100
C	-1.38494700	0.34916600	0.21814400
C	-2.16769900	0.88918500	-0.79419700
C	-1.87740300	-0.66662600	1.03556600
C	-3.45567000	0.40374400	-0.98768200
H	-1.77997700	1.68387800	-1.41372700
C	-3.16219500	-1.13872100	0.82687100
H	-1.26449700	-1.07354900	1.82638600
C	-3.97287700	-0.61346800	-0.18616700
H	-4.06645200	0.82687000	-1.77411300
H	-3.54539900	-1.92666300	1.46220300
C	-5.37189800	-1.12849200	-0.38655900
H	-5.38309200	-2.21674900	-0.45566600
H	-6.00931800	-0.85369000	0.45610500
H	-5.82007900	-0.72339200	-1.29167000

(1S)-**1**-c1 B3LYP / 6-311++G with C,N,H,O= (2d,p) and S= (3df,2dp)

C	2.57900600	0.15041900	-0.53098900
C	1.55777400	0.13089100	-1.60410500
H	2.86949700	1.14199900	-0.19285000
H	1.51622000	-0.70136000	-2.29653300
H	1.20249300	1.08312900	-1.97868200
N	1.17760500	-0.23834200	-0.22137700
C	3.63245700	-0.92411200	-0.37382300
H	3.20092800	-1.85897300	-0.74709100
C	4.00747900	-1.11639900	1.09907400
H	3.13268800	-1.37535900	1.69822100
H	4.74417600	-1.91576500	1.20677000
H	4.44227300	-0.20240500	1.51406800
C	4.85648300	-0.57535000	-1.23063600
H	5.31548900	0.35968500	-0.89660400
H	5.61128300	-1.36105300	-1.15580400
H	4.58994200	-0.46245600	-2.28418800
S	0.25441300	0.84737500	0.66171500
O	0.41350400	2.20332000	0.17550400
O	0.54226200	0.57425800	2.05003500
C	-1.38630400	0.29971200	0.28161500
C	-2.16421400	1.02008400	-0.61690200
C	-1.88586200	-0.84739600	0.89768000
C	-3.45360100	0.58296400	-0.90181600
H	-1.77014900	1.91571600	-1.07779000
C	-3.17171700	-1.26934800	0.60110900
H	-1.27632600	-1.39489500	1.60430700
C	-3.97686400	-0.56316600	-0.30195100
H	-4.06143000	1.14712800	-1.59951500
H	-3.56107700	-2.15995500	1.08137400

C	-5.37639000	-1.03073400	-0.60207100
H	-5.38037500	-2.07489900	-0.92398400
H	-6.00701100	-0.96617900	0.28888100
H	-5.83808500	-0.42997000	-1.38579900

(1S)-**1**-c1 B3LYP / 6-311++G with C,N,H,= (2d,p) and S,O= (3df,2dp)

C	2.57867200	0.15020200	-0.53084500
C	1.55773000	0.13103300	-1.60435600
H	2.86989900	1.14175400	-0.19319500
H	1.51600600	-0.70121600	-2.29677200
H	1.20327000	1.08350500	-1.97918500
N	1.17703600	-0.23730300	-0.22183300
C	3.63155000	-0.92483900	-0.37303900
H	3.19952100	-1.85961900	-0.74594100
C	4.00635900	-1.11675600	1.09996400
H	3.13132600	-1.37458700	1.69926500
H	4.74229300	-1.91677900	1.20807500
H	4.44209500	-0.20299400	1.51448900
C	4.85594700	-0.57727700	-1.22981400
H	5.31547400	0.35766200	-0.89620900
H	5.61029400	-1.36337400	-1.15448500
H	4.58963300	-0.46475700	-2.28346600
S	0.25463900	0.84886500	0.66132000
O	0.41345500	2.20220400	0.17473100
O	0.54302700	0.57622300	2.04717300
C	-1.38593400	0.30061900	0.28189700
C	-2.16403200	1.01932700	-0.61787500
C	-1.88546500	-0.84618900	0.89865900
C	-3.45332600	0.58168400	-0.90249800
H	-1.77012400	1.91447700	-1.07989500
C	-3.17118900	-1.26887200	0.60237500
H	-1.27595200	-1.39292900	1.60593500
C	-3.97642000	-0.56395200	-0.30155400
H	-4.06111000	1.14485100	-1.60105200
H	-3.56030500	-2.15918700	1.08339700
C	-5.37604100	-1.03180400	-0.60090900
H	-5.38112700	-2.07851800	-0.91431100
H	-6.00844200	-0.95889800	0.28817100
H	-5.83518400	-0.43658100	-1.39035800

(1S)-**1**-c1 B3PW91 / 6-311G (2d,p)

C	2.55314600	-0.01905300	0.55255100
C	1.51958700	0.27142100	1.56836900
H	2.81873000	-1.07054800	0.46200600
H	1.49048200	1.24160700	2.05168700
H	1.13540300	-0.56473600	2.14166000
N	1.17519000	0.32078500	0.13666000
C	3.63082200	0.96279000	0.16623200
H	3.21239800	1.96798800	0.29341500
C	4.02655900	0.78395000	-1.29700200
H	3.16039100	0.88893400	-1.95360300
H	4.77140300	1.52779700	-1.59037300
H	4.45883300	-0.20714100	-1.46600300
C	4.82943900	0.80990900	1.10161000
H	5.27018000	-0.18788700	1.01391900
H	5.60529900	1.53784800	0.85289400
H	4.54565600	0.96205600	2.14611300
S	0.25991400	-0.95487000	-0.46538700
O	0.43397800	-2.15966900	0.32576800
O	0.54124600	-1.00278300	-1.88290700
C	-1.37903600	-0.34428400	-0.20752100
C	-2.18188100	-0.92189400	0.76370100
C	-1.85136000	0.69699600	-1.00103900
C	-3.47339000	-0.44543900	0.94429000
H	-1.80062000	-1.74067100	1.36075600

C	-3.13865200	1.16169300	-0.80466800
H	-1.21744400	1.13002000	-1.76501900
C	-3.97077700	0.59990900	0.16947500
H	-4.10528500	-0.89855000	1.70076600
H	-3.51036700	1.97332800	-1.42157900
C	-5.36796400	1.11317000	0.36151800
H	-5.36476300	2.18464700	0.57911100
H	-5.96295600	0.97156700	-0.54515700
H	-5.87304200	0.60074900	1.18099500

(1S)-**1**-c1 B3PW91 / 6-311++G (2d,p)

C	2.56103300	0.13861400	-0.52580200
C	1.53552000	0.09473300	-1.58955700
H	2.83541000	1.13933500	-0.19735800
H	1.50436700	-0.74284500	-2.27773500
H	1.16333900	1.04116100	-1.96568600
N	1.17506800	-0.27142500	-0.20836500
C	3.62924800	-0.91536200	-0.37159000
H	3.20755100	-1.85890400	-0.73725700
C	4.01734300	-1.09306100	1.09388200
H	3.15105500	-1.36207100	1.70198300
H	4.76750500	-1.88071500	1.20081900
H	4.44170700	-0.16996400	1.50078900
C	4.83572200	-0.55242900	-1.23714700
H	5.28300900	0.39153900	-0.91057300
H	5.60455300	-1.32559800	-1.16586400
H	4.55873300	-0.44756300	-2.28940200
S	0.25666100	0.84009700	0.65826100
O	0.42732800	2.19021000	0.14825300
O	0.54058900	0.58074600	2.05369300
C	-1.38267600	0.29752200	0.27925700
C	-2.15749000	1.02294800	-0.61311200
C	-1.88063300	-0.84718300	0.89422200
C	-3.44668300	0.59063000	-0.89552400
H	-1.75876500	1.91950000	-1.07125700
C	-3.16613100	-1.26472200	0.59922500
H	-1.26894900	-1.39702400	1.59904000
C	-3.97024300	-0.55474500	-0.29876700
H	-4.05625900	1.15853600	-1.59045900
H	-3.55749800	-2.15649900	1.07809800
C	-5.36696400	-1.01601300	-0.59588300
H	-5.37508900	-2.06099300	-0.91671400
H	-5.99596200	-0.94879200	0.29666300
H	-5.82838000	-0.41394200	-1.37949800

(1S)-**1**-c1 B3PW91 / 6-311G (3df,2pd)

C	2.55402400	0.04383500	-0.55326500
C	1.52560700	-0.19480800	-1.58614300
H	2.83909200	1.08548100	-0.42581700
H	1.48489700	-1.14636800	-2.10178300
H	1.16113300	0.66423300	-2.13602900
N	1.16929000	-0.28119800	-0.16425500
C	3.61093900	-0.96820200	-0.19065900
H	3.17595200	-1.95993100	-0.35107900
C	4.00116400	-0.84071000	1.27835600
H	3.13196200	-0.95063300	1.92746600
H	4.73108500	-1.60460000	1.55135900
H	4.44906600	0.13579300	1.47863800
C	4.81756300	-0.80728200	-1.11253800
H	5.27288300	0.17874000	-0.99186700
H	5.57855200	-1.55392000	-0.88073700
H	4.53950300	-0.92322400	-2.16155800
S	0.25860300	0.94986800	0.49057100
O	0.42078000	2.17931200	-0.24549000
O	0.54642100	0.94650100	1.89785800

C	-1.37228500	0.34430600	0.22190000
C	-2.16807100	0.92068400	-0.75772600
C	-1.84879600	-0.70350300	1.00272700
C	-3.45333800	0.43925400	-0.95486700
H	-1.78492000	1.74184300	-1.34789600
C	-3.13232400	-1.17265100	0.79010300
H	-1.22157700	-1.13944700	1.76876800
C	-3.95567500	-0.61080600	-0.18875500
H	-4.07682700	0.88950000	-1.71821800
H	-3.50561500	-1.99001800	1.39580000
C	-5.35537800	-1.10961000	-0.38773100
H	-5.42068400	-2.18523500	-0.22276900
H	-6.03717900	-0.63114800	0.32037900

(1S)-**1**-c1 B3PW91 / 6-311++G (3df,2pd)

C	2.55649400	0.01954100	-0.55102700
C	1.52809300	-0.26216900	-1.57298900
H	2.84310200	1.06501000	-0.46659200
H	1.48623600	-1.23567300	-2.04570500
H	1.16417900	0.57169500	-2.16070800
N	1.17042300	-0.28649200	-0.14818600
C	3.61353700	-0.97804000	-0.14990600
H	3.17903900	-1.97535000	-0.27214800
C	4.00794500	-0.79565400	1.31229300
H	3.14176200	-0.88695600	1.96844000
H	4.74237300	-1.54617500	1.60929000
H	4.45220500	0.18934900	1.47589300
C	4.81818800	-0.85176000	-1.08034500
H	5.27400500	0.13795600	-0.99743500
H	5.57929400	-1.58963600	-0.82228500
H	4.53764900	-1.00684400	-2.12366100
S	0.25715100	0.97040700	0.45125500
O	0.42148600	2.16880900	-0.33647300
O	0.54208800	1.02950300	1.85950000
C	-1.37438400	0.35568300	0.20705000
C	-2.15561200	0.86251900	-0.82182300
C	-1.86437800	-0.63231700	1.05488300
C	-3.44082100	0.37197900	-0.99923700
H	-1.76415500	1.63700700	-1.46700100
C	-3.14780600	-1.11094900	0.86107400
H	-1.24841000	-1.01451200	1.85783800
C	-3.95738400	-0.61821100	-0.16554900
H	-4.05256700	0.76790800	-1.80110400
H	-3.53116000	-1.88143300	1.51949600
C	-5.35710800	-1.12458900	-0.34378600
H	-5.42431300	-2.19021900	-0.12359600
H	-6.03980600	-0.60928200	0.33703300
H	-5.71598900	-0.95660100	-1.35859100

(1S)-**1**-c1 M06 / 6-311G (2d,p)

C	2.51068700	-0.39664500	-0.41195500
C	1.45391300	-1.29480000	-0.90016500
H	2.78361500	0.41603700	-1.08874100
H	1.42595700	-2.32608600	-0.55956200
H	1.03790200	-1.09901100	-1.88465800
N	1.15785100	-0.32025700	0.15777500
C	3.58600100	-0.83593900	0.53711800
H	3.16446200	-1.64239800	1.15465900
C	3.97831100	0.32344900	1.43493800
H	3.10710800	0.71992600	1.96520500
H	4.72677000	0.01892600	2.17224800
H	4.40704600	1.13797200	0.83814800
C	4.77246900	-1.37166800	-0.24466200
H	5.19126900	-0.58974400	-0.88957800
H	5.56620400	-1.70543900	0.42978100

H	4.48718000	-2.21571700	-0.88075200
S	0.27354400	1.03065800	-0.30440200
O	0.47167400	1.34064100	-1.70074500
O	0.56333300	2.03401300	0.68454800
C	-1.36396400	0.42265700	-0.08800200
C	-2.12161100	0.08380600	-1.19458200
C	-1.86383400	0.27847000	1.19907200
C	-3.40395700	-0.40364300	-1.00613400
H	-1.70973000	0.21209500	-2.18977700
C	-3.14204400	-0.21057900	1.36806100
H	-1.25133200	0.55268100	2.05178700
C	-3.93113100	-0.55605100	0.27052400
H	-4.00921500	-0.66960900	-1.86818200
H	-3.54648500	-0.32782000	2.37000700
C	-5.32072100	-1.06414000	0.47784000
H	-5.34209700	-1.85724100	1.23089500
H	-5.97608900	-0.26456500	0.83904000
H	-5.74900200	-1.45548300	-0.44726600

(1S)-**1**-c1 M06 / 6-311++G (2d,p)

C	2.51661300	-0.45363800	-0.33247500
C	1.46442100	-1.42317600	-0.67198200
H	2.79990000	0.23262100	-1.13353800
H	1.43268300	-2.38027300	-0.15867400
H	1.05822100	-1.40126900	-1.67947100
N	1.15641600	-0.28161900	0.19998900
C	3.58170700	-0.73367900	0.68655100
H	3.15055500	-1.42545500	1.42465700
C	3.98089500	0.55320900	1.38552300
H	3.11495500	1.03419000	1.85024400
H	4.73085800	0.36548000	2.15948800
H	4.41192200	1.25974500	0.66558800
C	4.76862000	-1.39893500	0.01130500
H	5.20016400	-0.73493400	-0.74730000
H	5.55372400	-1.62637200	0.73801200
H	4.47993300	-2.33221900	-0.48282600
S	0.26958800	0.96624400	-0.49170400
O	0.46511900	1.02555000	-1.92288100
O	0.56189800	2.13131800	0.30232800
C	-1.36777900	0.40788600	-0.16668900
C	-2.10453900	-0.18000200	-1.17955200
C	-1.88550300	0.54662000	1.11379800
C	-3.38386500	-0.63353500	-0.90263700
H	-1.68069200	-0.27139900	-2.17399800
C	-3.16072100	0.08754800	1.37206000
H	-1.29010400	1.01286100	1.89203300
C	-3.92860400	-0.50654400	0.36989900
H	-3.97230900	-1.09321600	-1.69165800
H	-3.57848000	0.19077400	2.37006200
C	-5.31360200	-0.97950800	0.66948600
H	-5.33058500	-1.60331900	1.56798300
H	-5.98051800	-0.13167800	0.85789400
H	-5.73054100	-1.55652100	-0.15846000

(1S)-**1**-c1 M06 / 6-311G (3df,2pd)

C	2.52130400	-0.43874100	-0.36569000
C	1.48474100	-1.39313900	-0.78361400
H	2.81901500	0.28917200	-1.12093300
H	1.44636900	-2.37631200	-0.32868700
H	1.10634800	-1.31733300	-1.79689400
N	1.15185800	-0.30570100	0.13517400
C	3.56300200	-0.75872400	0.66472800
H	3.12377500	-1.49285700	1.35163900
C	3.91855600	0.49551600	1.44066800
H	3.03264500	0.93487100	1.90252800

H	4.64842000	0.28098900	2.22319300
H	4.35439700	1.24455400	0.77237900
C	4.77893600	-1.36794800	-0.00915600
H	5.21846000	-0.66001400	-0.71811900
H	5.54552100	-1.61959000	0.72541400
H	4.52092100	-2.27651300	-0.55758400
S	0.27241600	0.97416600	-0.45951000
O	0.45178300	1.11808900	-1.87581800
O	0.57747800	2.08198500	0.39084400
C	-1.35967400	0.41212300	-0.15095800
C	-2.10603700	-0.12548200	-1.18434900
C	-1.87070200	0.49104200	1.13713800
C	-3.38435600	-0.58544600	-0.92155000
H	-1.69052300	-0.17026100	-2.18263200
C	-3.14581600	0.02790700	1.38004700
H	-1.27103200	0.91719600	1.93126200
C	-3.92124500	-0.51594000	0.35721300
H	-3.97818500	-1.00474400	-1.72561900
H	-3.55728700	0.08699300	2.38166700
C	-5.30546600	-0.99667900	0.64334700
H	-5.31589000	-1.67595600	1.49754800
H	-5.96086900	-0.16007700	0.89586200
H	-5.73727800	-1.51439300	-0.21223600

(1S)-**1**-c1 M06 / 6-311++G (3df,2pd)

C	2.52047700	-0.44988000	-0.34607500
C	1.47795600	-1.41641800	-0.71845100
H	2.81910800	0.24439800	-1.13169500
H	1.43704700	-2.37813200	-0.21991200
H	1.09483800	-1.38421300	-1.73230900
N	1.15289700	-0.28817700	0.15411100
C	3.56607400	-0.73587200	0.69069300
H	3.12312300	-1.43203600	1.41360700
C	3.94742400	0.54660700	1.40616500
H	3.07231600	1.02222500	1.85281200
H	4.67840200	0.35504400	2.19358300
H	4.39217600	1.25633200	0.70182600
C	4.76711200	-1.39318700	0.03484000
H	5.21018900	-0.72499700	-0.70952000
H	5.53633900	-1.62203100	0.77410700
H	4.49093200	-2.32213000	-0.46882300
S	0.26995700	0.96432500	-0.49079800
O	0.45232800	1.05602600	-1.91254300
O	0.56898500	2.10726800	0.31667400
C	-1.36158900	0.40980600	-0.16545200
C	-2.09980300	-0.17854800	-1.17697800
C	-1.87931100	0.54531700	1.11535300
C	-3.37779000	-0.63219200	-0.89914600
H	-1.67989000	-0.26906500	-2.17040900
C	-3.15380000	0.08711100	1.37306200
H	-1.28612800	1.01012600	1.89256100
C	-3.92160300	-0.50746900	0.37267700
H	-3.96539700	-1.09033100	-1.68631300
H	-3.57037500	0.19011300	2.36895800
C	-5.30337100	-0.98514000	0.67526000
H	-5.30572900	-1.65266700	1.53887800
H	-5.95741700	-0.14576000	0.92147600
H	-5.74028700	-1.51599000	-0.16957600

(1S)-**1**-c1 M06-2X / 6-311G (2d,p)

C	2.51970800	-0.51129600	-0.24530700
C	1.45866300	-1.53453700	-0.37962600
H	2.78340400	0.00166500	-1.16728600
H	1.43082400	-2.37031500	0.30739500
H	1.04770500	-1.69799900	-1.36797400

N	1.16375400	-0.24351000	0.26073900
C	3.60212200	-0.58355700	0.79972300
H	3.18977000	-1.12379500	1.65764700
C	3.98979900	0.82495500	1.24079600
H	3.11768500	1.36865200	1.60693700
H	4.73852200	0.79092500	2.03344800
H	4.41040900	1.38393900	0.40082600
C	4.79849200	-1.35578100	0.24883500
H	5.21528400	-0.84442300	-0.62254900
H	5.58482600	-1.43111900	1.00098600
H	4.51420000	-2.36543200	-0.05298400
S	0.27266800	0.84310800	-0.64608400
O	0.47406700	0.62656000	-2.06162500
O	0.55315100	2.14147100	-0.08908900
C	-1.36849800	0.35769100	-0.23074800
C	-2.11130100	-0.38388800	-1.13377100
C	-1.88530100	0.72488700	1.00629200
C	-3.39946000	-0.76811800	-0.78602600
H	-1.68883000	-0.64263700	-2.09567400
C	-3.16891600	0.33229300	1.33569500
H	-1.28663900	1.31388600	1.68904500
C	-3.94302800	-0.41853800	0.44639600
H	-3.99068900	-1.34555300	-1.48632400
H	-3.58495100	0.61312100	2.29623700
C	-5.34199900	-0.82149700	0.82187500
H	-5.35345000	-1.31604800	1.79416200
H	-5.98535300	0.05755100	0.89508100
H	-5.77111100	-1.49750300	0.08411200

(1S)-**1**-c1 M06-2X / 6-311++G (2d,p)

C	-2.52657200	-0.52879200	0.18818800
C	-1.47243200	-1.56776500	0.22246800
H	-2.79592000	-0.11278600	1.15632600
H	-1.44421500	-2.32561500	-0.54993500
H	-1.06975700	-1.83942700	1.19031500
N	-1.16404800	-0.21819400	-0.27558200
C	-3.60164000	-0.49059500	-0.86653200
H	-3.18501200	-0.94465000	-1.77105500
C	-3.98558600	0.95505400	-1.16887600
H	-3.11359900	1.53059400	-1.48329100
H	-4.73527600	0.99804800	-1.96043400
H	-4.40511400	1.43158800	-0.27891700
C	-4.80325500	-1.31068100	-0.40232300
H	-5.22769900	-0.88469000	0.51039400
H	-5.58277000	-1.31213100	-1.16540400
H	-4.52253900	-2.34525500	-0.19641200
S	-0.27001200	0.76354300	0.74155300
O	-0.46853200	0.39487300	2.12718500
O	-0.55354600	2.11641000	0.33167700
C	1.37165100	0.33117800	0.27274500
C	2.10142700	-0.53894800	1.06528200
C	1.90089000	0.86615000	-0.89610500
C	3.38917200	-0.88278700	0.67383400
H	1.67118100	-0.92910400	1.97831300
C	3.18389400	0.51142700	-1.27069900
H	1.31340900	1.55285200	-1.49198500
C	3.94503800	-0.36671200	-0.49341400
H	3.97020200	-1.55897600	1.28917000
H	3.60922600	0.92358100	-2.17838400
C	5.34090200	-0.72966900	-0.91741500
H	5.34009600	-1.14943400	-1.92469500
H	5.97807800	0.15651000	-0.93363900
H	5.78392400	-1.45785800	-0.23994900

(1S)-**1**-c1 M06-2X / 6-311G (3df,2pd)

C	2.52511600	-0.51193300	-0.25202700
C	1.47409200	-1.54086000	-0.40701200
H	2.80340500	0.00350600	-1.16697600
H	1.43948900	-2.37774100	0.27616900
H	1.08165900	-1.70711900	-1.40101600
N	1.16084000	-0.25573400	0.22513800
C	3.58986600	-0.57668300	0.81080300
H	3.16722800	-1.11874900	1.66020500
C	3.96073400	0.83386400	1.25657600
H	3.08151400	1.37187900	1.60886400
H	4.69710400	0.80489300	2.05866600
H	4.38950000	1.39381900	0.42360000
C	4.79986100	-1.33963700	0.27994800
H	5.22627200	-0.82530800	-0.58284900
H	5.57292000	-1.40939200	1.04382200
H	4.52837100	-2.34952700	-0.02668200
S	0.27233100	0.83398200	-0.65599100
O	0.46199800	0.63278000	-2.06680400
O	0.56057600	2.12132100	-0.09891700
C	-1.36454000	0.35700700	-0.23393800
C	-2.11259800	-0.38808000	-1.13016700
C	-1.87709500	0.72715800	1.00416800
C	-3.39923600	-0.76922800	-0.77621900
H	-1.69553600	-0.65096700	-2.09169400
C	-3.15975000	0.33805700	1.33899300
H	-1.27661200	1.31633100	1.68293400
C	-3.93816100	-0.41476400	0.45617900
H	-3.99301400	-1.34816300	-1.47092400
H	-3.57115600	0.62211500	2.29898300
C	-5.33576100	-0.81285200	0.83743300
H	-5.34765600	-1.28894400	1.81694900
H	-5.97905500	0.06540400	0.89480100
H	-5.76336700	-1.50072100	0.11238300

(1S)-**1**-c1 M06-2X / 6-311++G (3df,2pd)

C	2.52614900	-0.51794800	-0.22790300
C	1.47329900	-1.55068300	-0.33890200
H	2.80661300	-0.04141300	-1.16295300
H	1.43707400	-2.35598600	0.38112700
H	1.08022900	-1.76074300	-1.32437800
N	1.16133900	-0.23790400	0.23669900
C	3.59140800	-0.54566600	0.83633700
H	3.16713800	-1.05282500	1.70625900
C	3.97312900	0.87792200	1.22833700
H	3.09992300	1.43438000	1.56686300
H	4.71384400	0.87227500	2.02700000
H	4.40125900	1.40438700	0.37342800
C	4.79599900	-1.33597200	0.33300800
H	5.22538700	-0.85618500	-0.54809600
H	5.56872700	-1.38261700	1.09901900
H	4.51759000	-2.35464500	0.06378700
S	0.27050300	0.81030500	-0.69127300
O	0.46217500	0.54832900	-2.09327400
O	0.55550500	2.12379700	-0.19266500
C	-1.36653600	0.34994300	-0.25092500
C	-2.10194500	-0.45867600	-1.10162300
C	-1.89070100	0.79537600	0.95733500
C	-3.38823900	-0.82729100	-0.73135000
H	-1.67747000	-0.78193800	-2.04125400
C	-3.17286900	0.41757700	1.30864100
H	-1.30003600	1.43239400	1.60057600
C	-3.93891100	-0.39863300	0.47220400
H	-3.97227400	-1.45494000	-1.39096600
H	-3.59303500	0.76073400	2.24513700
C	-5.33346800	-0.78820100	0.87283400

H	-5.33299100	-1.26150200	1.85406700
H	-5.97151600	0.09313100	0.93683300
H	-5.77321400	-1.47756500	0.15656500

(S)-**2**-c1 B3LYP / 6-31+G (2d,p)

C	2.47797300	0.44406400	0.41250500
C	3.46440100	-0.54576500	0.35319300
C	4.71714600	-0.26588600	-0.19273300
C	5.00107100	1.00947500	-0.68647500
C	4.02152000	2.00174700	-0.63279100
C	2.76836800	1.71713300	-0.08719500
H	3.24424100	-1.54303000	0.71954800
H	5.47039600	-1.04639100	-0.23774500
H	5.97446300	1.22499300	-1.11556000
H	4.22758500	2.99393800	-1.02206100
H	2.00697600	2.49228700	-0.05619900
C	1.13071400	0.18767300	1.07224400
C	1.22189900	0.33584600	2.59905500
H	0.23392400	0.23333200	3.06086600
H	1.89259300	-0.42003100	3.02149000
H	1.62033500	1.32097100	2.85333700
N	0.61255400	-1.16667800	0.77536700
H	0.23448200	-1.65803700	1.57916400
H	0.42193500	0.94023700	0.70477100
S	-0.34705100	-1.44223300	-0.55123000
C	-1.83977600	-0.48440200	-0.35367600
C	-2.85658600	-0.95976100	0.48085200
C	-1.98154400	0.73079000	-1.02179000
C	-4.01186700	-0.20457200	0.64603800
H	-2.74975100	-1.91531100	0.98173500
C	-3.14847000	1.47580300	-0.84522000
H	-1.19739900	1.07976800	-1.68281900
C	-4.17818200	1.02479200	-0.01247100
H	-4.80248400	-0.57853300	1.28995000
H	-3.25772300	2.41973600	-1.37039100
C	-5.44597000	1.82204000	0.16527000
H	-6.29918500	1.30384900	-0.28801700
H	-5.68017300	1.96068500	1.22616000
H	-5.36666100	2.80799800	-0.29959600
O	-0.70215800	-2.84871800	-0.46601500
O	0.35805700	-0.91476300	-1.70315500

(S)-**2**-c1 B3LYP / 6-311G (2d,p)

C	2.44994500	0.44498800	0.41821900
C	3.41950400	-0.54722700	0.27794500
C	4.65602800	-0.25126600	-0.28407800
C	4.94017400	1.04143200	-0.71424500
C	3.97713800	2.03577700	-0.58173100
C	2.74040500	1.73634400	-0.01981300
H	3.19552700	-1.55814600	0.59477800
H	5.39790000	-1.03394000	-0.39215600
H	5.90251000	1.26979700	-1.15682300
H	4.18461000	3.04343300	-0.92245400
H	1.99038500	2.51506900	0.07354400
C	1.12015000	0.16970800	1.10132700
C	1.24225600	0.30099100	2.62461100
H	0.26847500	0.17782800	3.10511300
H	1.93048500	-0.44901200	3.02067400
H	1.63045200	1.28596000	2.88301000
N	0.60975800	-1.18687900	0.80261700
H	0.20082300	-1.65803500	1.60188100
H	0.39976500	0.91945400	0.75787000
S	-0.33541000	-1.45812300	-0.53838600
C	-1.82181400	-0.48508700	-0.35159700
C	-2.83468700	-0.93795600	0.49297400

C	-1.95987800	0.71255700	-1.04167800
C	-3.98245100	-0.17819600	0.64512600
H	-2.73074800	-1.88356900	1.00889600
C	-3.11935600	1.46359600	-0.87777800
H	-1.17644600	1.04168600	-1.71051300
C	-4.14427700	1.03559400	-0.03468000
H	-4.77225700	-0.53492900	1.29666100
H	-3.22734000	2.39506800	-1.42123600
C	-5.40192900	1.84555300	0.14078200
H	-6.28052800	1.27567200	-0.17246000
H	-5.55122600	2.11486800	1.18956500
H	-5.36914600	2.76490200	-0.44393500
O	-0.70619900	-2.85679300	-0.45479400
O	0.38341900	-0.93931000	-1.68131600

(S)-**2**-c1 B3LYP / 6-311G (3df,2dp)

C	2.49062100	0.45677100	0.39927600
C	3.44157400	-0.56081600	0.35299700
C	4.69982400	-0.32642900	-0.18745700
C	5.02478300	0.92901100	-0.68973600
C	4.08081000	1.94794700	-0.65101400
C	2.82218700	1.71031300	-0.11075100
H	3.18913400	-1.54400000	0.72541200
H	5.42601700	-1.12783300	-0.22184600
H	6.00296900	1.10874300	-1.11517500
H	4.31964700	2.92550300	-1.04847400
H	2.08804500	2.50673700	-0.09216300
C	1.13300700	0.24979400	1.04990000
C	1.20389400	0.45897700	2.56660900
H	0.21232600	0.38671800	3.01483300
H	1.85519500	-0.28518900	3.02650200
H	1.61020700	1.44378500	2.78768500
N	0.58983000	-1.09938600	0.79660100
H	0.26040500	-1.59710100	1.61262400
H	0.44641100	0.99563000	0.64116300
S	-0.34109800	-1.42205800	-0.51883600
C	-1.84557800	-0.48886200	-0.34438600
C	-2.84475500	-0.94856200	0.51267600
C	-2.01407800	0.69741300	-1.04783100
C	-4.00577100	-0.20986300	0.66271500
H	-2.71929500	-1.88201200	1.04249700
C	-3.18635900	1.42675200	-0.88610500
H	-1.24352900	1.03427900	-1.72492000
C	-4.19718200	0.98998400	-0.03169900
H	-4.78155200	-0.57202300	1.32517500
H	-3.31541900	2.34829200	-1.43851900
C	-5.47338600	1.77006200	0.12964200
H	-6.30947300	1.24621000	-0.33815400
H	-5.72548500	1.89986400	1.18255800
H	-5.39896300	2.75456800	-0.32823500
O	-0.67295800	-2.81875100	-0.41656100
O	0.35227800	-0.90730800	-1.66778900

(S)-**2**-c1 B3LYP / 6-311++G (2d,p)

C	2.46326400	0.44044100	0.41871300
C	3.44885000	-0.54107600	0.31613900
C	4.68816700	-0.24244200	-0.24010400
C	4.95937800	1.04316200	-0.70138100
C	3.98064700	2.02710800	-0.60525300
C	2.74105700	1.72424800	-0.04923500
H	3.23855400	-1.54742400	0.65692900
H	5.44208700	-1.01699400	-0.31907800
H	5.92330400	1.27342300	-1.13941000
H	4.17759300	3.02837800	-0.97007000
H	1.97953600	2.49469300	0.01476000

C	1.12907000	0.16298600	1.09231100
C	1.24021500	0.28637300	2.61715800
H	0.26206700	0.16694800	3.08949500
H	1.92166400	-0.46836600	3.01639200
H	1.63165800	1.26845900	2.88219900
N	0.61463300	-1.18994400	0.78083600
H	0.22913400	-1.68316900	1.57861700
H	0.41259500	0.91576700	0.74817100
S	-0.34416500	-1.45312300	-0.55174800
C	-1.83225000	-0.48306000	-0.35360300
C	-2.85208000	-0.95180200	0.47382700
C	-1.96137400	0.73187200	-1.01565400
C	-3.99865700	-0.19061000	0.63712800
H	-2.75495100	-1.90810800	0.97127900
C	-3.11946300	1.48349000	-0.84114600
H	-1.17350900	1.07684900	-1.67126800
C	-4.15269700	1.03900700	-0.01573400
H	-4.79247800	-0.55958800	1.27681800
H	-3.21918200	2.42882000	-1.36183800
C	-5.41349300	1.84383000	0.15896000
H	-6.25881800	1.35077500	-0.32952700
H	-5.66964800	1.95064500	1.21547300
H	-5.31308600	2.84027600	-0.27177000
O	-0.71071900	-2.85574700	-0.47236300
O	0.36620300	-0.92837400	-1.69986200

(S)-**2**-c1 B3LYP / 6-311++G (3df,2dp)

C	-2.49825600	-0.45488100	0.39790200
C	-3.45849700	0.55498200	0.37458700
C	-4.71938800	0.31847800	-0.16036100
C	-5.03761400	-0.93237400	-0.68008700
C	-4.08430500	-1.94404800	-0.66389200
C	-2.82332300	-1.70343100	-0.12859900
H	-3.21364500	1.53491200	0.76051500
H	-5.45236100	1.11402500	-0.17685600
H	-6.01715700	-1.11376500	-1.10130400
H	-4.31742800	-2.91730300	-1.07462700
H	-2.08268100	-2.49383100	-0.12797500
C	-1.13750400	-0.24668900	1.04173700
C	-1.20154200	-0.45344800	2.55932000
H	-0.20758700	-0.38387200	3.00258200
H	-1.84845500	0.29328800	3.02134000
H	-1.60999300	-1.43668700	2.78336800
N	-0.59303200	1.10194000	0.78324100
H	-0.27405200	1.60696100	1.59903700
H	-0.45313000	-0.99321300	0.63121300
S	0.34810400	1.42315500	-0.52491100
C	1.85114200	0.48718800	-0.34576400
C	2.85285100	0.95265800	0.50558700
C	2.01533400	-0.70608100	-1.03874000
C	4.01327700	0.21273200	0.65968000
H	2.73113100	1.89029600	1.02866500
C	3.18714100	-1.43628000	-0.87237900
H	1.24421300	-1.05068900	-1.71127000
C	4.20097500	-0.99423600	-0.02382000
H	4.79064000	0.57987000	1.31732000
H	3.31264300	-2.36300800	-1.41664200
C	5.47529500	-1.77618600	0.14316600
H	6.31474900	-1.25053400	-0.31629700
H	5.71913200	-1.91044700	1.19750400
H	5.40295800	-2.75868600	-0.31921200
O	0.68117300	2.82171400	-0.41672300
O	-0.34003800	0.91557600	-1.68221400

(S)-**2**-c1 B3PW91 / 6-311G (2d,p)

C	2.44086200	0.45177000	0.40279400
C	3.39826500	-0.55154200	0.28299900
C	4.64385700	-0.27500500	-0.26441100
C	4.94838300	1.00905600	-0.69999200
C	3.99671100	2.01450300	-0.58783500
C	2.75125900	1.73464500	-0.04047400
H	3.15609100	-1.55788500	0.60533200
H	5.37832800	-1.06798000	-0.35708300
H	5.91980300	1.22287100	-1.13231300
H	4.22079000	3.01777500	-0.93415200
H	2.00818700	2.52325500	0.03738700
C	1.10362600	0.19769900	1.06955300
C	1.20356100	0.38345100	2.58312300
H	0.22309300	0.27693600	3.05518800
H	1.88767600	-0.35151300	3.01503300
H	1.58878200	1.37752900	2.81194600
N	0.60424700	-1.16209300	0.80986900
H	0.20392700	-1.61906000	1.62100900
H	0.38670300	0.93414400	0.68692400
S	-0.33724400	-1.46495000	-0.51465700
C	-1.81486200	-0.49478300	-0.34475000
C	-2.82289100	-0.92903000	0.51200400
C	-1.95457300	0.68654300	-1.05851100
C	-3.96757100	-0.16610700	0.65348300
H	-2.71639600	-1.86560600	1.04622400
C	-3.11068000	1.44105500	-0.90494700
H	-1.17251900	0.99850400	-1.73931800
C	-4.13055900	1.03249300	-0.04901500
H	-4.75626900	-0.50899100	1.31538500
H	-3.22158800	2.36175200	-1.46802900
C	-5.38036500	1.84680000	0.11752900
H	-6.26695200	1.25859700	-0.13432100
H	-5.49713900	2.17560300	1.15409500
H	-5.36813700	2.73218000	-0.51902900
O	-0.70459100	-2.85822500	-0.39858100
O	0.37479800	-0.96971900	-1.66743900

(S)-**2**-c1 B3PW91 / 6-311G (3df,2dp)

C	2.47236800	0.46026200	0.38668500
C	3.41340400	-0.56330200	0.33736000
C	4.67557700	-0.33440800	-0.19219800
C	5.01353700	0.92133800	-0.67970400
C	4.07872000	1.94656500	-0.63742700
C	2.81656300	1.71463000	-0.10818000
H	3.14824900	-1.54856500	0.69980600
H	5.39625600	-1.14247700	-0.22968200
H	5.99707100	1.09731200	-1.09777600
H	4.32853500	2.92705200	-1.02452000
H	2.08744400	2.51761700	-0.08593000
C	1.11352200	0.26000700	1.02630200
C	1.17333800	0.51011400	2.53172700
H	0.17924800	0.44340400	2.97736400
H	1.82830700	-0.21766500	3.01449200
H	1.57288000	1.50369700	2.72895500
N	0.58603500	-1.09222000	0.80450500
H	0.25751800	-1.57386300	1.63035100
H	0.42417400	0.99104200	0.59065100
S	-0.34162800	-1.43722500	-0.49791900
C	-1.83332600	-0.49914200	-0.33844800
C	-2.82946200	-0.93679400	0.52989200
C	-1.99592100	0.67457300	-1.06130400
C	-3.98389300	-0.18871400	0.67129800
H	-2.70569400	-1.86270600	1.07640400
C	-3.16067000	1.41321900	-0.90770400
H	-1.22331200	0.99292600	-1.74771600

C	-4.17002500	0.99809900	-0.04265100
H	-4.76009000	-0.53299600	1.34486300
H	-3.28639700	2.32786100	-1.47502600
C	-5.43860600	1.78422000	0.10174900
H	-6.24517500	1.32244800	-0.47359200
H	-5.76570000	1.82099000	1.14150300
H	-5.31872800	2.80513800	-0.25887100
O	-0.67693000	-2.82728000	-0.36778600
O	0.34923800	-0.94697700	-1.65477300

(S)-**2**-c1 B3PW91 / 6-311++G (2d,p)

C	2.45060600	0.44817800	0.40400100
C	3.41739400	-0.54893200	0.30608000
C	4.66432500	-0.27082200	-0.23896600
C	4.96089400	1.00900700	-0.69386000
C	4.00006200	2.00842500	-0.60265400
C	2.75328900	1.72659400	-0.05765100
H	3.18424100	-1.55297800	0.64283000
H	5.40583900	-1.05913500	-0.31477900
H	5.93290500	1.22381100	-1.12457900
H	4.21758100	3.00794800	-0.96392300
H	2.00371600	2.51063300	0.00322000
C	1.11079000	0.19354000	1.06551200
C	1.20456700	0.37354200	2.58031900
H	0.22125000	0.27093200	3.04734600
H	1.88320300	-0.36556100	3.01417100
H	1.59352100	1.36530000	2.81358000
N	0.60642600	-1.16320200	0.79723800
H	0.22096200	-1.63433800	1.60773600
H	0.39719600	0.93320200	0.68321500
S	-0.34326400	-1.46061700	-0.52265500
C	-1.82264100	-0.49348100	-0.34669200
C	-2.83814400	-0.94172600	0.49410400
C	-1.95364100	0.70249100	-1.03787700
C	-3.98198200	-0.17767000	0.64269100
H	-2.73838000	-1.88793800	1.01279600
C	-3.10916900	1.45742300	-0.87777000
H	-1.16683900	1.02775100	-1.70711400
C	-4.13710500	1.03486500	-0.03778200
H	-4.77555200	-0.53134500	1.29316900
H	-3.21248600	2.38978100	-1.42301700
C	-5.38878700	1.84584500	0.12960300
H	-6.26105700	1.29489300	-0.23385600
H	-5.56982200	2.07498600	1.18327500
H	-5.33133800	2.78675500	-0.41888400
O	-0.70663400	-2.85719700	-0.41002500
O	0.36407900	-0.96106400	-1.67844000

(S)-**2**-c1 B3PW91 / 6-311++G (3df,2dp)

C	-2.47738900	-0.45874000	0.38728600
C	-3.42514400	0.55936000	0.35342000
C	-4.68853800	0.32886600	-0.17364200
C	-5.02075700	-0.92377700	-0.67440200
C	-4.07909000	-1.94384400	-0.64753000
C	-2.81599700	-1.70959000	-0.12019600
H	-3.16612400	1.54259000	0.72576200
H	-5.41419900	1.13274900	-0.19894100
H	-6.00466800	-1.10099900	-1.09076200
H	-4.32404000	-2.92129500	-1.04488900
H	-2.08202300	-2.50823500	-0.11020300
C	-1.11698500	-0.25751700	1.02331700
C	-1.17347900	-0.50326300	2.52978700
H	-0.17799000	-0.43845700	2.97257500
H	-1.82522900	0.22755600	3.01240100
H	-1.57543300	-1.49519900	2.73037400

N	-0.58739300	1.09364600	0.79600300
H	-0.26454800	1.58066200	1.62104100
H	-0.42944800	-0.99043000	0.58836600
S	0.34556100	1.43622700	-0.50296200
C	1.83680000	0.49722200	-0.34087100
C	2.83594800	0.94166900	0.52128600
C	1.99625400	-0.68223200	-1.05478600
C	3.99041000	0.19398900	0.66528400
H	2.71509500	1.87174200	1.06119100
C	3.16187400	-1.42027900	-0.89817800
H	1.22306900	-1.00807500	-1.73701900
C	4.17360000	-0.99968200	-0.03887300
H	4.76867600	0.54436800	1.33320000
H	3.28557300	-2.33899000	-1.45912000
C	5.43958100	-1.78812300	0.11532300
H	6.27570400	-1.27291300	-0.36379700
H	5.70034100	-1.91329600	1.16736100
H	5.35263000	-2.77501200	-0.33708000
O	0.68121000	2.82808600	-0.37059100
O	-0.34335300	0.94987800	-1.66421400

(S)-**2**-c1 M06-2X / 6-311G (2d,p)

C	2.01689800	0.38220400	0.57318300
C	3.14155500	-0.21682500	0.01189900
C	4.07824600	0.54989000	-0.66228800
C	3.90239600	1.92484100	-0.78202800
C	2.78353700	2.52673100	-0.22590700
C	1.84359900	1.75487200	0.44833100
H	3.26527100	-1.29049500	0.08898600
H	4.94647900	0.07539700	-1.10216700
H	4.63373500	2.52141800	-1.31256400
H	2.63701400	3.59549400	-0.31948700
H	0.96373700	2.22331400	0.87717600
C	1.02316100	-0.42983700	1.37361600
C	1.59425500	-0.78891000	2.74351100
H	0.86272300	-1.34006000	3.33781200
H	2.49099600	-1.39897400	2.62791500
H	1.85883300	0.12257200	3.27811900
N	0.67712200	-1.69565300	0.69978400
H	0.22369400	-2.35246000	1.32878900
H	0.12259800	0.17745800	1.52084500
S	-0.19102300	-1.66148300	-0.71057300
C	-1.52741700	-0.53558800	-0.44191300
C	-2.66272900	-0.97803300	0.22522800
C	-1.40193000	0.78293700	-0.85160400
C	-3.68472900	-0.08016300	0.47933500
H	-2.74361900	-2.01506900	0.52547400
C	-2.43576200	1.67042600	-0.58687000
H	-0.50678200	1.10049500	-1.37127100
C	-3.58661100	1.25394700	0.07814200
H	-4.57700000	-0.41643300	0.99436700
H	-2.34714600	2.70235000	-0.90511900
C	-4.71802100	2.20921900	0.33912500
H	-5.51464200	2.06235300	-0.39360400
H	-5.14725500	2.04526800	1.32771200
H	-4.38524400	3.24389100	0.26980500
O	-0.72618900	-2.99369500	-0.84145100
O	0.64299400	-1.10099000	-1.73763400

(12S)-**2**-c1 M06-2X / 6-311G (3df,2dp)

C	2.02346400	0.38177600	0.57817000
C	3.14841400	-0.22196800	0.02433400
C	4.08760400	0.53832100	-0.65209100
C	3.91397500	1.91189800	-0.78181500
C	2.79513000	2.51867600	-0.23315200

C	1.85282200	1.75307000	0.44362500
H	3.27086900	-1.29386900	0.10850900
H	4.95523900	0.06014500	-1.08556100
H	4.64660700	2.50297800	-1.31373100
H	2.65035900	3.58552600	-0.33422300
H	0.97369900	2.22514700	0.86612600
C	1.02368500	-0.42417800	1.37665400
C	1.59217700	-0.79657100	2.74312600
H	0.85695500	-1.34379800	3.33309700
H	2.48188800	-1.41307800	2.62331900
H	1.86509100	0.10760600	3.28252100
N	0.65587200	-1.67779900	0.69662400
H	0.23920400	-2.36149600	1.31949100
H	0.13157900	0.19236800	1.52800600
S	-0.18633800	-1.64632400	-0.71327000
C	-1.53113000	-0.53555100	-0.44892200
C	-2.66380600	-0.98515500	0.21856800
C	-1.41468400	0.78616300	-0.85089400
C	-3.69008500	-0.09449400	0.47668700
H	-2.73957800	-2.02199500	0.51627500
C	-2.45278400	1.66651700	-0.58174900
H	-0.52353800	1.11159400	-1.36948000
C	-3.60029200	1.24163800	0.08198000
H	-4.57874400	-0.43739200	0.99064900
H	-2.36993300	2.69906300	-0.89463600
C	-4.73624800	2.18835100	0.34805400
H	-5.53361100	2.03640700	-0.38033600
H	-5.16029300	2.02080700	1.33642800
H	-4.41181800	3.22381600	0.27796500
O	-0.70305700	-2.97387000	-0.86703300
O	0.64641600	-1.07350600	-1.72345700

(S)-**2**-c1 M06-2X / 6-311++G (2d,p)

C	2.03130600	0.37911300	0.57222400
C	3.16039200	-0.22196000	0.02153500
C	4.10131900	0.54199400	-0.65141200
C	3.92525000	1.91664400	-0.78010600
C	2.80243400	2.52085400	-0.23302900
C	1.85864800	1.75147000	0.43972500
H	3.28644300	-1.29506700	0.10510200
H	4.97250700	0.06553800	-1.08346400
H	4.65928100	2.51084500	-1.30973800
H	2.65578100	3.58911700	-0.33292900
H	0.97653600	2.22261400	0.86108000
C	1.03076700	-0.42863100	1.36899800
C	1.59481700	-0.79184300	2.74089500
H	0.85703900	-1.33653100	3.33350900
H	2.48750000	-1.40875300	2.62905800
H	1.86476100	0.11814200	3.27558000
N	0.67688000	-1.69193200	0.69360500
H	0.23266900	-2.35454500	1.32353300
H	0.13318400	0.18360100	1.51430700
S	-0.19855800	-1.65554400	-0.71265900
C	-1.53733300	-0.53274500	-0.43931800
C	-2.67243100	-0.97789300	0.22693000
C	-1.41366900	0.78654600	-0.84734800
C	-3.69614200	-0.08132500	0.48212600
H	-2.75311700	-2.01519800	0.52706100
C	-2.44945100	1.67253900	-0.58218200
H	-0.51977500	1.10733500	-1.36742800
C	-3.60030500	1.25374900	0.08207600
H	-4.58795000	-0.42024600	0.99633900
H	-2.36180100	2.70488800	-0.89951700
C	-4.73325800	2.20680800	0.34331100
H	-5.52852800	2.05946300	-0.39089000

H	-5.16348500	2.04061900	1.33112900
H	-4.40194700	3.24211800	0.27562900
O	-0.72997100	-2.99083800	-0.84619400
O	0.63192200	-1.09086700	-1.74225700

(S)-**2**-c1 M06-2X / 6-311++G (3df,2dp)

C	2.02479000	0.38065700	0.58003800
C	3.15843000	-0.21458000	0.03465300
C	4.09349200	0.55161600	-0.64186200
C	3.90713100	1.92331800	-0.77904400
C	2.77991800	2.52189900	-0.23714300
C	1.84218900	1.74989100	0.43942500
H	3.29221500	-1.28474000	0.12403900
H	4.96724600	0.07972100	-1.06961400
H	4.63587300	2.51885400	-1.31110900
H	2.62519200	3.58672700	-0.34359600
H	0.95675000	2.21562200	0.85556700
C	1.02709200	-0.43153800	1.37505500
C	1.59572200	-0.80997700	2.73994400
H	0.86052700	-1.35991400	3.32748700
H	2.48566100	-1.42577300	2.61766900
H	1.86815400	0.09213800	3.28303800
N	0.66016200	-1.68301300	0.68891900
H	0.24830200	-2.37166700	1.30969600
H	0.13374800	0.18231200	1.52937300
S	-0.18752900	-1.64714800	-0.71784800
C	-1.53101700	-0.53523600	-0.44944900
C	-2.66285000	-0.98511500	0.21979400
C	-1.41405500	0.78662600	-0.85087900
C	-3.68815600	-0.09349800	0.48072200
H	-2.73928800	-2.02161600	0.51845900
C	-2.45156100	1.66747300	-0.57881400
H	-0.52358400	1.11395400	-1.36948400
C	-3.59821600	1.24323100	0.08713400
H	-4.57566100	-0.43640500	0.99647700
H	-2.36803900	2.70023500	-0.89053500
C	-4.73288300	2.19051500	0.35645900
H	-5.53333400	2.03600100	-0.36799000
H	-5.15184800	2.02499400	1.34734400
H	-4.40876100	3.22577700	0.28224800
O	-0.70562500	-2.97621000	-0.87250200
O	0.64387700	-1.07534500	-1.73151500

(3R,4S,6S)-**3**-c1 B3LYP / 6-31+G (2d,p)

C	4.26164800	-0.64471500	-1.04280300
C	3.79135100	0.73576900	-0.56865100
C	2.25591800	0.89273000	-0.62159000
C	1.62154100	-0.24542800	0.18992400
C	2.08580600	-1.62881300	-0.26224200
C	3.61655800	-1.77221700	-0.22436200
H	4.14177500	0.89339700	0.45960200
H	4.25667200	1.51827200	-1.17705000
H	4.00621600	-0.77938200	-2.10431200
H	5.35447400	-0.70940000	-0.97266800
H	1.81552200	-0.10316600	1.25782800
H	1.61245400	-2.39068800	0.36451100
H	1.73209800	-1.78902100	-1.29021400
H	3.94239700	-1.65573000	0.82067900
H	1.94247700	0.73081000	-1.66407600
C	1.75298500	2.30528400	-0.21649300
H	0.66249100	2.23096500	-0.13765800
C	2.05173800	3.33897600	-1.31461300
H	1.64170300	3.02454400	-2.28131600
H	1.60520800	4.30710400	-1.06166100
H	3.12842100	3.50091400	-1.44259900

C	2.27741000	2.79738500	1.14244700
H	1.77931200	3.73349000	1.41793600
H	2.08508700	2.08041100	1.94686800
H	3.35443100	2.99702800	1.11414900
O	0.15458900	-0.17237000	-0.01689100
C	4.05418900	-3.16069100	-0.70233700
H	5.14328000	-3.26977900	-0.64911300
H	3.60640000	-3.95200000	-0.09067500
H	3.75143800	-3.33017600	-1.74323800
S	-0.80583400	-0.39665100	1.25723800
C	-2.36650100	-0.27150400	0.43201400
C	-3.01373000	0.96271100	0.36997900
C	-2.94068000	-1.41463800	-0.12494000
C	-4.24736100	1.04751600	-0.26969800
H	-2.56411000	1.83686600	0.82546200
C	-4.17435300	-1.30980400	-0.76099500
H	-2.43524500	-2.37024600	-0.05119900
C	-4.84440300	-0.08123900	-0.84840200
H	-4.75656700	2.00543200	-0.31298500
H	-4.62673300	-2.19892700	-1.18934600
C	-6.16835100	0.02680500	-1.56186100
H	-6.71720200	-0.91843700	-1.52968900
H	-6.79573200	0.80742400	-1.12236800
H	-6.01754900	0.28356500	-2.61777200
O	-0.61877600	-1.74190700	1.76836600
O	-0.64055700	0.71357500	2.17638000

(3R,4S,6S)-**3**-c1 B3LYP / 6-311G (2d,p)

C	4.35812900	-0.15472900	-0.95170400
C	3.68145200	1.10176500	-0.39645000
C	2.14616300	1.05364100	-0.52692200
C	1.64308000	-0.22301600	0.15474700
C	2.30479100	-1.48460000	-0.38918800
C	3.83520500	-1.42837000	-0.27774200
H	3.95695700	1.21646000	0.65706400
H	4.06188300	1.98553700	-0.91300300
H	4.17892300	-0.22255700	-2.03201000
H	5.44191600	-0.08152000	-0.81927500
H	1.78000400	-0.15127400	1.23535300
H	1.91464400	-2.35531600	0.14118000
H	2.01972500	-1.59479600	-1.44170300
H	4.09362700	-1.37170100	0.78809000
H	1.90923100	0.94225200	-1.59328300
C	1.42775500	2.34134100	-0.04635500
H	0.35687300	2.13031100	-0.11287600
C	1.70790900	3.52083800	-0.98732900
H	1.47522600	3.26703900	-2.02497800
H	1.09680800	4.38345800	-0.71058600
H	2.75340100	3.83715600	-0.94564500
C	1.72840200	2.72739300	1.40829200
H	1.12342300	3.59056400	1.69700000
H	1.49357700	1.92102400	2.10537300
H	2.77634500	3.00510900	1.54619900
O	0.18674500	-0.30870200	-0.10311900
C	4.47823200	-2.69191300	-0.85175500
H	5.56553200	-2.66273000	-0.74501600
H	4.11496500	-3.58839600	-0.34316900
H	4.24977500	-2.79628500	-1.91668800
S	-0.75298900	-0.89731700	1.06321800
C	-2.32387700	-0.49911100	0.34718700
C	-2.92855600	0.71569500	0.65336200
C	-2.94277600	-1.41755200	-0.49302900
C	-4.16467900	1.01114500	0.09840700
H	-2.44269700	1.40918300	1.32615400
C	-4.17886900	-1.10389600	-1.04018300

H	-2.46743200	-2.36578600	-0.70420800
C	-4.80675900	0.11228300	-0.75889900
H	-4.64242300	1.95347800	0.34039100
H	-4.66691700	-1.81991000	-1.69104900
C	-6.13659300	0.45626700	-1.37595800
H	-6.68986900	-0.44082800	-1.65583500
H	-6.75176800	1.04271900	-0.69172400
H	-5.99715800	1.05369500	-2.28215300
O	-0.59625200	-2.33485100	1.12887100
O	-0.54434100	-0.12556200	2.27124900

(3R,4S,6S)-**3**-c1 B3LYP / 6-311G (3df,2dp)

C	4.32337600	-0.27975200	-1.00016700
C	3.70288000	1.01041000	-0.46022400
C	2.16517600	1.01197600	-0.55415200
C	1.63767400	-0.23018400	0.16912600
C	2.24231600	-1.52464900	-0.36126000
C	3.77467500	-1.51793000	-0.28467600
H	4.00627200	1.14013000	0.58193900
H	4.09932000	1.86723400	-1.00547500
H	4.11659700	-0.36634700	-2.07237500
H	5.41010700	-0.24043900	-0.89470200
H	1.80685600	-0.13967600	1.24248800
H	1.83514600	-2.36810100	0.19605400
H	1.93175800	-1.64658600	-1.40337000
H	4.05881000	-1.44561400	0.77176100
H	1.89909800	0.88410600	-1.60992300
C	1.50394700	2.33355000	-0.08764300
H	0.42643600	2.16250100	-0.12917600
C	1.80792400	3.48171700	-1.05755300
H	1.54863500	3.21526000	-2.08375700
H	1.23276900	4.36907300	-0.78928200
H	2.86243000	3.76177500	-1.04049600
C	1.84719700	2.73705700	1.35127900
H	1.27949000	3.62499800	1.63351100
H	1.59851500	1.95518500	2.06815200
H	2.90500500	2.97977800	1.46254600
O	0.17427500	-0.27769800	-0.04682500
C	4.36096800	-2.81440700	-0.84237000
H	5.44894500	-2.82003800	-0.76030000
H	3.98005800	-3.68469500	-0.30588700
H	4.10559700	-2.93493800	-1.89758000
S	-0.76775300	-0.76404800	1.13763700
C	-2.32821700	-0.44236000	0.38141700
C	-2.94757800	0.78655500	0.58213500
C	-2.92924400	-1.42752900	-0.39497000
C	-4.17749400	1.02714100	-0.01111600
H	-2.47900500	1.53397300	1.20493200
C	-4.15859600	-1.16794900	-0.98075800
H	-2.44627400	-2.38446700	-0.52628900
C	-4.80017800	0.06035700	-0.80398800
H	-4.66487600	1.97969300	0.15039000
H	-4.63116200	-1.93545000	-1.57967000
C	-6.12122200	0.34101600	-1.46605600
H	-6.70572300	-0.56962300	-1.58856600
H	-6.70979100	1.05529000	-0.89232600
H	-5.96882400	0.76709100	-2.46049100
O	-0.60320900	-2.17983200	1.33116300
O	-0.58153600	0.10184900	2.27210700

(3R,4S,6S)-**3**-c1 B3LYP / 6-311++G (2d,p)

C	-2.78622300	2.72485300	-0.12385000
C	-3.43224400	1.38199300	0.22707600
C	-2.69295500	0.18559900	-0.40479800
C	-1.22175600	0.24489700	0.02491600

C	-0.56312900	1.57683300	-0.31833200
C	-1.31177100	2.77080600	0.29219900
H	-3.44819900	1.27059100	1.31633300
H	-4.47463800	1.37601300	-0.09881200
H	-2.85843400	2.89778200	-1.20492400
H	-3.33461500	3.53891500	0.36007700
H	-1.12843800	0.02592500	1.08912600
H	0.47542900	1.57207400	0.02111000
H	-0.54306500	1.68015400	-1.40920200
H	-1.27043100	2.67189200	1.38522100
H	-2.69777100	0.33308800	-1.49269500
C	-3.36801500	-1.18523000	-0.13901800
H	-2.68613400	-1.94302200	-0.53466500
C	-4.68040700	-1.32075500	-0.92355700
H	-4.52795000	-1.13350100	-1.98989700
H	-5.08515400	-2.33033500	-0.81782100
H	-5.44420000	-0.62504300	-0.56575400
C	-3.59293600	-1.50116400	1.34613300
H	-3.96926200	-2.52117600	1.45653500
H	-2.67120700	-1.43277100	1.92730600
H	-4.33071300	-0.83147600	1.79547100
O	-0.50415100	-0.82247300	-0.70817500
C	-0.64476900	4.09426500	-0.08699000
H	-1.16281600	4.94019300	0.37197100
H	0.39802300	4.12252400	0.23964100
H	-0.65955600	4.24189700	-1.17114000
S	0.53727600	-1.79396800	0.03324700
C	2.07481000	-0.90148400	0.02933800
C	2.76948900	-0.74476800	-1.16893300
C	2.57515600	-0.38408400	1.21677300
C	3.96922300	-0.05223000	-1.16738600
H	2.37883000	-1.16374800	-2.08683400
C	3.78355300	0.30518800	1.19992500
H	2.03183000	-0.52428200	2.14120400
C	4.49701200	0.48420800	0.01437900
H	4.51008800	0.07083700	-2.09881800
H	4.17602400	0.70593400	2.12720200
C	5.80969400	1.22156700	-0.00292000
H	6.02711900	1.67147800	0.96588500
H	6.63162700	0.54489200	-0.25263300
H	5.80507700	2.01365800	-0.75544000
O	0.12206100	-1.99254200	1.40640500
O	0.65130700	-2.91898000	-0.86574800

(3R,4S,6S)-**3**-c1 B3LYP / 6-311++G (3df,2dp)

C	4.28260700	-0.46231000	-1.04464000
C	3.74202800	0.87327400	-0.53047500
C	2.20413200	0.95223400	-0.58433900
C	1.63063300	-0.23977500	0.18713200
C	2.16093600	-1.57866700	-0.31183600
C	3.69336000	-1.64638700	-0.27209000
H	4.07974200	1.01724300	0.49904500
H	4.16558700	1.69326700	-1.11103800
H	4.04127700	-0.57355000	-2.10727700
H	5.37241300	-0.47429300	-0.96920700
H	1.81957400	-0.12463800	1.25497700
H	1.72725400	-2.38264600	0.28242300
H	1.81996300	-1.71823400	-1.34215500
H	4.00867100	-1.55250200	0.77366500
H	1.90252000	0.80787800	-1.62818900
C	1.62934300	2.32110200	-0.13899700
H	0.54571700	2.19710700	-0.09486500
C	1.90930900	3.40783900	-1.18446200
H	1.54795600	3.11255000	-2.17108100
H	1.40836700	4.33772000	-0.91127700

H	2.97520100	3.62628900	-1.26928700
C	2.09361100	2.77764700	1.24952000
H	1.56142500	3.68468200	1.53957400
H	1.89665800	2.02963200	2.01728400
H	3.15994500	3.00757700	1.26366300
O	0.16074100	-0.22849800	-0.00898000
C	4.19976700	-2.98939300	-0.79781000
H	5.28804200	-3.04589400	-0.74363600
H	3.79190400	-3.82044000	-0.22040700
H	3.90963000	-3.13336200	-1.84107800
S	-0.78953100	-0.58321300	1.21328000
C	-2.34663800	-0.35846100	0.41506700
C	-2.97268300	0.88191300	0.47126800
C	-2.93687500	-1.42811200	-0.25115500
C	-4.19989400	1.04752100	-0.15464000
H	-2.51255800	1.69897500	1.00665500
C	-4.16313600	-1.24272200	-0.87109300
H	-2.44897800	-2.39126600	-0.27315200
C	-4.81231000	-0.00531500	-0.83800600
H	-4.69222400	2.00966800	-0.10480500
H	-4.62694900	-2.07535100	-1.38348900
C	-6.12967900	0.18982800	-1.53705100
H	-6.74147700	-0.71003400	-1.48792900
H	-6.69213100	1.01474600	-1.10304600
H	-5.97206200	0.41857900	-2.59361600
O	-0.61673000	-1.96778100	1.57065300
O	-0.62026500	0.40582900	2.24675200

(3R,4S,6S)-**3**-c1 B3PW91 / 6-311G (2d,p)

C	-2.72612300	2.73179600	-0.10055000
C	-3.38976900	1.40032200	0.23545900
C	-2.67319000	0.20780500	-0.41241500
C	-1.20868900	0.23620600	0.02199700
C	-0.53154600	1.55544300	-0.31110400
C	-1.25616500	2.74929100	0.31302300
H	-3.40137800	1.27346000	1.32416000
H	-4.43483200	1.41397000	-0.08446200
H	-2.79506900	2.91636300	-1.18072300
H	-3.26128500	3.55113800	0.39062000
H	-1.12726400	0.01503500	1.08882700
H	0.50935300	1.52989100	0.02275200
H	-0.51512800	1.66874900	-1.40199700
H	-1.21539500	2.63493700	1.40548900
H	-2.67212200	0.37282800	-1.49918400
C	-3.36677800	-1.15039000	-0.17064400
H	-2.70195700	-1.91000000	-0.59438100
C	-4.68741200	-1.24125500	-0.93553300
H	-4.54897600	-1.02475700	-1.99875800
H	-5.10854800	-2.24676000	-0.85294300
H	-5.43428800	-0.54389200	-0.54490700
C	-3.57410900	-1.49327200	1.30458400
H	-3.98327000	-2.50271500	1.39917200
H	-2.63902600	-1.47053900	1.86867300
H	-4.28093500	-0.81000700	1.78384500
O	-0.51460400	-0.83457100	-0.70303800
C	-0.57145300	4.06132300	-0.05120200
H	-1.07530400	4.91134700	0.41689300
H	0.47272300	4.06995500	0.27343100
H	-0.58565500	4.22021200	-1.13424000
S	0.51498000	-1.79654000	0.04867700
C	2.04298200	-0.91029000	0.03080900
C	2.71221100	-0.73192600	-1.17634500
C	2.57064600	-0.42371200	1.21713800
C	3.91277200	-0.04624600	-1.18506700
H	2.29993100	-1.13398600	-2.09368300

C	3.77922200	0.25882100	1.18983400
H	2.04431400	-0.58814000	2.14878300
C	4.46532000	0.46315200	-0.00538100
H	4.43818400	0.09190600	-2.12432500
H	4.19717500	0.63414300	2.11791500
C	5.76290100	1.21630100	-0.03670600
H	6.16322500	1.36440700	0.96689800
H	6.51129600	0.68754500	-0.63158600
H	5.62698200	2.20198200	-0.49233900
O	0.10354700	-1.97224100	1.42049300
O	0.62513800	-2.92851900	-0.83247500

(3R,4S,6S)-**3**-c1 B3PW91 / 6-311G (3df,2dp)

C	-2.71511300	2.73247700	-0.10777600
C	-3.37696800	1.40467600	0.24094600
C	-2.66729000	0.20850500	-0.40532500
C	-1.20048200	0.23849600	0.01873300
C	-0.52522400	1.55449700	-0.32817400
C	-1.24359000	2.75059600	0.29613300
H	-3.37964100	1.28407200	1.32886200
H	-4.42315900	1.41697900	-0.07006900
H	-2.79031500	2.90976200	-1.18723300
H	-3.24548000	3.55459500	0.38069900
H	-1.11284700	0.02667600	1.08590000
H	0.51735600	1.53008500	-0.00482500
H	-0.52032400	1.66281400	-1.41817000
H	-1.19560900	2.64084400	1.38723000
H	-2.67367400	0.36697600	-1.49154600
C	-3.36139200	-1.14554300	-0.14955200
H	-2.70253000	-1.91012800	-0.56998600
C	-4.68541700	-1.23917300	-0.90607900
H	-4.55277100	-1.03116700	-1.97011300
H	-5.10751600	-2.24175000	-0.81369500
H	-5.42748200	-0.53837600	-0.51690900
C	-3.56292100	-1.47546400	1.32819500
H	-3.96895000	-2.48351600	1.43267200
H	-2.62813000	-1.44567700	1.88928800
H	-4.26907300	-0.79051200	1.80235400
O	-0.50944100	-0.83688400	-0.69856800
C	-0.56089700	4.05926800	-0.07913500
H	-1.05963900	4.91073200	0.38817800
H	0.48430300	4.06840800	0.23682500
H	-0.58346100	4.21284400	-1.16123700
S	0.51017600	-1.80074000	0.02660200
C	2.03419900	-0.92023900	0.02580600
C	2.72195500	-0.74609700	-1.17161200
C	2.54293600	-0.42101600	1.21561100
C	3.91921400	-0.05540000	-1.16686000
H	2.32689400	-1.15589800	-2.09173300
C	3.74801600	0.26632500	1.20156100
H	2.00532000	-0.58131500	2.13992400
C	4.45166700	0.46493200	0.01621400
H	4.45793100	0.07741700	-2.09774500
H	4.14986600	0.64942300	2.13200500
C	5.74414000	1.22425900	-0.00052000
H	6.14441800	1.35347900	1.00410200
H	6.49340700	0.71425300	-0.60747100
H	5.60210600	2.21768700	-0.43344400
O	0.10039100	-1.99781200	1.38687200
O	0.62394900	-2.91698500	-0.85936600

(3R,4S,6S)-**3**-c1 B3PW91 / 6-311++G (2d,p)

C	-2.73364900	2.72809500	-0.11956900
C	-3.39496900	1.39857300	0.22802900
C	-2.67725100	0.20026300	-0.40834200

C	-1.21169300	0.23426400	0.02331300
C	-0.53750600	1.55345800	-0.31694500
C	-1.26481100	2.75078000	0.29757900
H	-3.40649000	1.28208800	1.31791900
H	-4.44027100	1.40668700	-0.09196100
H	-2.80072100	2.90300400	-1.20155200
H	-3.27131300	3.55081000	0.36345400
H	-1.12750500	0.01568000	1.09068100
H	0.50344200	1.53281300	0.01742700
H	-0.52096900	1.65991600	-1.40861100
H	-1.22655600	2.64473200	1.39103500
H	-2.67761800	0.35400600	-1.49674400
C	-3.37061100	-1.15504300	-0.14870100
H	-2.69467100	-1.92361800	-0.53722800
C	-4.67318000	-1.27074300	-0.94129200
H	-4.50845200	-1.09268800	-2.00798000
H	-5.09926600	-2.27192400	-0.83312000
H	-5.42719300	-0.55805300	-0.59396600
C	-3.61230800	-1.46066700	1.32981000
H	-3.99784500	-2.47756700	1.44298700
H	-2.69594800	-1.39546200	1.92130200
H	-4.35040000	-0.78253900	1.76764200
O	-0.51520900	-0.83762500	-0.70125000
C	-0.58056900	4.06107800	-0.07472100
H	-1.08609600	4.91376500	0.38703700
H	0.46322400	4.07314800	0.25150300
H	-0.59324400	4.21292900	-1.15891500
S	0.52198700	-1.79620400	0.04468000
C	2.04974600	-0.90770600	0.03203700
C	2.73550300	-0.74947500	-1.16890100
C	2.55785400	-0.39522300	1.21608600
C	3.93395900	-0.05904700	-1.17361500
H	2.33679300	-1.16712200	-2.08548800
C	3.76489900	0.29160200	1.19296000
H	2.01811800	-0.53901100	2.14368900
C	4.46926900	0.47307700	0.00450400
H	4.46975400	0.06615400	-2.10897700
H	4.16543600	0.68984300	2.11925000
C	5.77750200	1.20764000	-0.01950300
H	6.00559400	1.64941900	0.95118100
H	6.59659400	0.53235400	-0.28405600
H	5.76567300	2.00622400	-0.76584200
O	0.11055000	-1.98154200	1.41633100
O	0.63653900	-2.92481800	-0.84282200

(3R,4S,6S)-**3**-c1 B3PW91 / 6-311++G (3df,2dp)

C	-2.71436100	2.73265200	-0.12218100
C	-3.37886500	1.40764400	0.23166000
C	-2.66817900	0.20549600	-0.40275600
C	-1.20211100	0.23638800	0.02426800
C	-0.52492300	1.55128500	-0.32379300
C	-1.24538200	2.75115600	0.29110000
H	-3.38604200	1.29457500	1.32029200
H	-4.42384800	1.41792100	-0.08364300
H	-2.78263200	2.90341200	-1.20312000
H	-3.24682500	3.55806000	0.35828300
H	-1.11576100	0.02427100	1.09161300
H	0.51606100	1.52788900	0.00463900
H	-0.51493900	1.65521900	-1.41415600
H	-1.20435400	2.64686000	1.38294800
H	-2.67089500	0.35459600	-1.49018600
C	-3.36617600	-1.14457000	-0.13489100
H	-2.69565300	-1.91840600	-0.51800500
C	-4.66883100	-1.25860900	-0.92539000
H	-4.50400400	-1.08869900	-1.99164500

H	-5.09930300	-2.25528000	-0.81015000
H	-5.41727600	-0.54055000	-0.58234900
C	-3.60936200	-1.43854600	1.34451900
H	-3.99560000	-2.45255200	1.46447100
H	-2.69535700	-1.36965200	1.93612300
H	-4.34616200	-0.75703500	1.77496200
O	-0.50952800	-0.84022300	-0.69265200
C	-0.55839400	4.05722100	-0.08636300
H	-1.05932900	4.91138200	0.37366400
H	0.48474900	4.06667300	0.23637000
H	-0.57401400	4.20522800	-1.16940200
S	0.51445800	-1.80290500	0.02700300
C	2.03805800	-0.92088900	0.02866900
C	2.72833400	-0.75127500	-1.16815400
C	2.54364700	-0.41627900	1.21776500
C	3.92575100	-0.06005200	-1.16358900
H	2.33582000	-1.16483200	-2.08764200
C	3.74884100	0.27160100	1.20308100
H	2.00493200	-0.57022300	2.14253700
C	4.45496400	0.46631400	0.01837100
H	4.46605600	0.06896000	-2.09397500
H	4.14801700	0.65888000	2.13283600
C	5.74598100	1.22810300	0.00121200
H	6.14406000	1.36181400	1.00610700
H	6.49710600	0.71714300	-0.60258700
H	5.60198200	2.21949900	-0.43570900
O	0.10605000	-2.01087800	1.38684900
O	0.62947100	-2.91571300	-0.86613400

(3R,4S,6S)-**3**-c1 M06-2X / 6-311G (2d,p)

C	-2.34706200	2.85697900	-0.09031800
C	-3.00655200	1.59657600	0.46423700
C	-2.54659000	0.33213200	-0.27327100
C	-1.02512400	0.25699000	-0.19093600
C	-0.34572200	1.50571500	-0.72864100
C	-0.82381100	2.76717200	-0.00958500
H	-2.75423400	1.50687400	1.52615600
H	-4.09349900	1.67992500	0.40538600
H	-2.63769400	2.99571900	-1.13856300
H	-2.69595600	3.73671700	0.45645700
H	-0.72104300	0.07111800	0.84364200
H	0.73898700	1.40178000	-0.63731200
H	-0.57745300	1.58650400	-1.79688900
H	-0.54738700	2.67980000	1.04916300
H	-2.78781100	0.45306300	-1.33778500
C	-3.23952400	-0.95510100	0.21474300
H	-2.70484300	-1.79318900	-0.23979000
C	-4.68652800	-1.01686600	-0.27447600
H	-4.74162000	-0.92952400	-1.36140200
H	-5.14500300	-1.96516500	0.01172000
H	-5.28918700	-0.21688000	0.16196200
C	-3.18665100	-1.13909800	1.73179400
H	-3.55705300	-2.13095200	1.99658100
H	-2.17054100	-1.05736700	2.12033700
H	-3.81576400	-0.40459700	2.24007600
O	-0.58010500	-0.86719300	-1.01222600
C	-0.15050500	4.00720000	-0.58503100
H	-0.47496200	4.90782700	-0.06068900
H	0.93626000	3.93945300	-0.50613400
H	-0.40561400	4.12181700	-1.64183600
S	0.34985700	-1.96442700	-0.34424000
C	1.83649400	-1.07792300	-0.02828200
C	2.67836100	-0.78346200	-1.09475200
C	2.11333200	-0.63578200	1.25445400
C	3.80991400	-0.02491100	-0.86150400

H	2.44205700	-1.14580700	-2.08700300
C	3.25386400	0.12652000	1.46965800
H	1.44741900	-0.89035800	2.06857900
C	4.11235800	0.44301900	0.42081800
H	4.47457000	0.21146800	-1.68413400
H	3.47909000	0.47761700	2.46933900
C	5.35662800	1.25398200	0.65300600
H	5.35962900	1.69908500	1.64664600
H	6.24337000	0.62356700	0.55995100
H	5.44343500	2.05083300	-0.08651000
O	-0.21941600	-2.36749000	0.91152400
O	0.56700200	-2.92248300	-1.38699600

(3R,4S,6S)-**3**-c1 M06-2X / 6-311G (3df,2dp)

C	-2.32491800	2.86176000	-0.10110700
C	-2.99747000	1.60864500	0.45187700
C	-2.54339100	0.33990400	-0.27986300
C	-1.02366800	0.25413900	-0.18509700
C	-0.33173000	1.49501500	-0.72429600
C	-0.80387000	2.76048900	-0.01035100
H	-2.75241900	1.51870800	1.51368100
H	-4.08171400	1.69953800	0.38652200
H	-2.60658700	2.99935600	-1.15018900
H	-2.66991400	3.74467100	0.43965400
H	-0.73100700	0.07530900	0.85261000
H	0.75026500	1.38375600	-0.62817500
H	-0.55884600	1.57538100	-1.79182800
H	-0.53507200	2.67274000	1.04842800
H	-2.77578200	0.46073200	-1.34458200
C	-3.24956700	-0.93972700	0.20582100
H	-2.72520000	-1.78206000	-0.24913300
C	-4.69604200	-0.98507900	-0.28360300
H	-4.75036200	-0.89272800	-1.36844800
H	-5.16353700	-1.92817700	-0.00133600
H	-5.28912100	-0.18181200	0.15551500
C	-3.19946200	-1.12547700	1.72154400
H	-3.58169600	-2.11120000	1.98541700
H	-2.18421000	-1.05608100	2.10996300
H	-3.81865900	-0.38449300	2.22878400
O	-0.57902000	-0.87983500	-0.98891100
C	-0.11837000	3.99334300	-0.58416000
H	-0.43813500	4.89616100	-0.06429200
H	0.96573600	3.91725500	-0.49995800
H	-0.36702200	4.10736600	-1.64081700
S	0.34455200	-1.97006100	-0.33526300
C	1.83219400	-1.09093900	-0.02449400
C	2.68120400	-0.81011200	-1.08915200
C	2.10022400	-0.62490700	1.25200500
C	3.80937900	-0.04607200	-0.86024700
H	2.45405300	-1.18795000	-2.07630500
C	3.23709400	0.14277700	1.46226400
H	1.43117300	-0.86693800	2.06538300
C	4.10203500	0.44438300	0.41500700
H	4.47816600	0.17816800	-1.68107200
H	3.45435000	0.51073700	2.45613400
C	5.34233800	1.26084500	0.64208700
H	5.33447900	1.72817600	1.62355600
H	6.22883000	0.62976100	0.57377400
H	5.43772100	2.03866900	-0.11390200
O	-0.21550200	-2.37296800	0.91652900
O	0.55524700	-2.92944700	-1.36694300

(3R,4S,6S)-**3**-c1 M06-2X / 6-311++G (2d,p)

C	-2.34996400	2.85529500	-0.10047400
C	-3.01296500	1.59703600	0.45468100

C	-2.55208000	0.32977300	-0.27782300
C	-1.03095000	0.25327100	-0.18840600
C	-0.34830100	1.49983700	-0.72732300
C	-0.82723500	2.76364700	-0.01279700
H	-2.76491300	1.50963500	1.51784200
H	-4.09968500	1.68097500	0.39139700
H	-2.63593300	2.99168900	-1.15039900
H	-2.70024100	3.73683300	0.44270800
H	-0.73247700	0.07022500	0.84836400
H	0.73613300	1.39533700	-0.63307100
H	-0.57753400	1.57872700	-1.79633700
H	-0.55544600	2.67863600	1.04740900
H	-2.78915800	0.44869100	-1.34350400
C	-3.24909400	-0.95450300	0.21230600
H	-2.71353500	-1.79579800	-0.23554300
C	-4.69354400	-1.01736300	-0.28491400
H	-4.74202100	-0.93718000	-1.37282100
H	-5.15515500	-1.96317700	0.00495500
H	-5.29755500	-0.21349100	0.14262000
C	-3.20530400	-1.13024400	1.73082500
H	-3.57273500	-2.12232700	1.99927800
H	-2.19228700	-1.04037700	2.12638300
H	-3.84127400	-0.39565100	2.23050800
O	-0.58269200	-0.87535400	-1.00369100
C	-0.14997200	4.00144900	-0.58887300
H	-0.47531700	4.90379400	-0.06778600
H	0.93656500	3.93262500	-0.50595000
H	-0.40119600	4.11388900	-1.64695700
S	0.35554100	-1.96538700	-0.33508600
C	1.84208500	-1.07542000	-0.02438000
C	2.69498400	-0.80408100	-1.08829600
C	2.10790200	-0.60836400	1.25227700
C	3.82703200	-0.04363400	-0.85899900
H	2.46792800	-1.18431700	-2.07615100
C	3.24890800	0.15521600	1.46347800
H	1.43444300	-0.84366300	2.06622300
C	4.11906200	0.44856400	0.41678400
H	4.49958000	0.17460500	-1.68031800
H	3.46497200	0.52522900	2.45844200
C	5.36390000	1.25929900	0.64561000
H	5.35367800	1.73229100	1.62632500
H	6.24813700	0.62128200	0.58514500
H	5.46731100	2.03414700	-0.11486800
O	-0.20952500	-2.36786300	0.92424800
O	0.57250000	-2.92742300	-1.37613000

(3R,4S,6S)-**3**-c1 M06-2X / 6-311++G (3df,2dp)

C	-2.31502500	2.86517100	-0.11021900
C	-2.99418500	1.61643200	0.44449700
C	-2.54347100	0.34315300	-0.28185500
C	-1.02439400	0.25113100	-0.18232400
C	-0.32545400	1.48791400	-0.72235000
C	-0.79471800	2.75763400	-0.01370500
H	-2.75233900	1.52889200	1.50720200
H	-4.07788600	1.71099900	0.37586100
H	-2.59250900	3.00085700	-1.16064400
H	-2.65802300	3.75097100	0.42701700
H	-0.73553500	0.07174500	0.85640200
H	0.75574800	1.37309100	-0.62249800
H	-0.54909000	1.56642400	-1.79075200
H	-0.53011400	2.67222600	1.04630800
H	-2.77231600	0.46154500	-1.34754800
C	-3.25692600	-0.93126400	0.20722600
H	-2.73194100	-1.77879900	-0.23724500
C	-4.69981800	-0.97600000	-0.29323400

H	-4.74464200	-0.89505200	-1.37944100
H	-5.17316800	-1.91427600	-0.00458200
H	-5.29284600	-0.16554800	0.13268800
C	-3.21954500	-1.10513400	1.72496900
H	-3.60301600	-2.08912200	1.99347200
H	-2.20787900	-1.03038800	2.12235200
H	-3.84393400	-0.36059000	2.22054100
O	-0.58223200	-0.88760800	-0.98297600
C	-0.10172500	3.98576400	-0.58916900
H	-0.41967200	4.89140500	-0.07303100
H	0.98180200	3.90527100	-0.50092800
H	-0.34648700	4.09724200	-1.64706500
S	0.34478800	-1.97544300	-0.33038100
C	1.83222600	-1.09530500	-0.02024600
C	2.68513800	-0.82303400	-1.08424600
C	2.09506600	-0.61820100	1.25342500
C	3.81249000	-0.05638500	-0.85752500
H	2.46181200	-1.20803000	-2.06948300
C	3.23140800	0.15176900	1.46124100
H	1.42291600	-0.85031500	2.06725900
C	4.10005400	0.44557200	0.41456700
H	4.48348400	0.16157300	-1.67813100
H	3.44415800	0.52846100	2.45270900
C	5.33741400	1.26741100	0.63823000
H	5.33613100	1.72450400	1.62451000
H	6.22695900	0.64274700	0.55366400
H	5.41935600	2.05382500	-0.11055300
O	-0.21410800	-2.38279300	0.92152900
O	0.55524100	-2.93489100	-1.36451200

(3R,4S,6S)-**4**-c1 B3LYP / 6-311G (2d,p)

C	4.07250500	-1.23684000	-0.76166200
C	3.80999800	0.26047900	-0.57695000
C	2.31541000	0.61720700	-0.68810900
C	1.52174400	-0.23732100	0.30902500
C	1.78856800	-1.73107700	0.14774800
C	3.27972700	-2.08159500	0.24288400
H	4.18867600	0.56615700	0.40404600
H	4.37710600	0.82983000	-1.31705600
H	3.79397200	-1.53762100	-1.77943200
H	5.14233600	-1.44251400	-0.65728200
H	1.76478900	0.07403600	1.33069400
H	1.22017200	-2.28111800	0.90407100
H	1.40202500	-2.04208200	-0.82974100
H	3.62633700	-1.81278600	1.24981000
H	1.97490200	0.30584200	-1.68468800
C	2.01198000	2.13343200	-0.57082300
H	0.92336600	2.21707400	-0.52608800
C	2.47515300	2.89454400	-1.81983700
H	2.05021400	2.46185200	-2.72950700
H	2.16022200	3.93990100	-1.77030800
H	3.56383700	2.88753900	-1.92212100
C	2.56855900	2.79139300	0.69888000
H	2.22214900	3.82569300	0.76442800
H	2.23470100	2.28382400	1.60595200
H	3.66137900	2.81207500	0.70180600
O	0.09845200	0.00666100	0.07350100
C	3.51354400	-3.58070700	0.04866900
H	4.57354900	-3.82938400	0.14401300
H	2.96389200	-4.16819600	0.78865500
H	3.18362000	-3.90137700	-0.94409100
S	-0.82186100	0.15327300	1.46328300
C	-2.38209600	-0.06617600	0.57757500
C	-3.21177500	1.02697600	0.38545900
C	-2.76461900	-1.33695500	0.16130100

C	-4.43225800	0.84792100	-0.25550000
H	-2.89627400	2.00004600	0.73993200
C	-3.98663100	-1.50185000	-0.47394000
H	-2.11728600	-2.19005300	0.32812300
C	-4.83741400	-0.41322700	-0.69682100
H	-5.08234300	1.70181200	-0.40979000
H	-4.28852800	-2.49098500	-0.79988400
C	-6.15204900	-0.60115800	-1.40880200
H	-6.83401200	0.22643500	-1.21040800
H	-6.00269900	-0.65418100	-2.49155200
H	-6.63973000	-1.52905400	-1.10404000
O	-0.79328600	1.56641200	1.91241800

(3R,4S,6S)-**4**-c1 B3LYP / 6-311G (3df,2dp)

C	4.11638600	-1.05277500	-0.81534200
C	3.77729300	0.42325400	-0.59493100
C	2.26580800	0.70186800	-0.68937600
C	1.53722900	-0.21068900	0.30460300
C	1.86704400	-1.68449300	0.09052900
C	3.37327400	-1.96385700	0.16708900
H	4.14603100	0.72854600	0.38805700
H	4.30676900	1.03481800	-1.32596200
H	3.85094300	-1.34108700	-1.83832200
H	5.19416500	-1.20452100	-0.71911800
H	1.79897300	0.08390700	1.32456200
H	1.33398000	-2.28602000	0.83021200
H	1.49056000	-1.98015300	-0.89365700
H	3.71165500	-1.70897300	1.17840000
H	1.93485200	0.38746500	-1.68645000
C	1.88233400	2.19708000	-0.55206900
H	0.79188400	2.22836600	-0.58274700
C	2.38805400	3.01635200	-1.74531300
H	2.07425400	2.57473000	-2.69300900
H	1.99133100	4.03187100	-1.70510100
H	3.47661700	3.09380600	-1.75654600
C	2.31712700	2.84181300	0.76920600
H	1.95585500	3.87021100	0.81719900
H	1.91042800	2.31916500	1.63440900
H	3.40338600	2.87418800	0.86832700
O	0.10180700	-0.00655700	0.12327600
C	3.67899800	-3.44182600	-0.07340200
H	4.74879200	-3.64009900	0.00896900
H	3.16473900	-4.07651300	0.65012100
H	3.35953400	-3.74818400	-1.07209000
S	-0.81351500	-0.17240000	1.48824200
C	-2.36311400	-0.21925600	0.57780900
C	-3.20779000	0.87908700	0.61701700
C	-2.73008300	-1.37704300	-0.09975200
C	-4.42332200	0.82473400	-0.05351600
H	-2.90834800	1.75743300	1.17115400
C	-3.94705900	-1.41750400	-0.76231600
H	-2.07495500	-2.23829100	-0.11274000
C	-4.81115500	-0.31785600	-0.75432500
H	-5.08332000	1.68238000	-0.02594100
H	-4.23501300	-2.31736600	-1.29087000
C	-6.11943000	-0.36644000	-1.49679200
H	-6.81547100	0.38428700	-1.12623600
H	-5.96695700	-0.17716700	-2.56189300
H	-6.59015700	-1.34525700	-1.40751800
O	-0.79728900	1.10357600	2.22425000

(3R,4S,6S)-**4**-c1 B3LYP / 6-311++G (2d,p)

C	4.02796200	-1.31556800	-0.72795600
C	3.82306800	0.19503500	-0.58323800
C	2.34300600	0.60842000	-0.70327100

C	1.52305800	-0.18618100	0.32198700
C	1.72757100	-1.69329800	0.19245100
C	3.20335200	-2.10196500	0.29772800
H	4.21519200	0.51262400	0.38872300
H	4.40999300	0.72153600	-1.33930900
H	3.73824300	-1.63223500	-1.73786800
H	5.08933500	-1.55876800	-0.61711200
H	1.78699000	0.14147600	1.33302800
H	1.13809000	-2.20577100	0.95890600
H	1.33106700	-2.00858100	-0.77980600
H	3.56105400	-1.82230400	1.29782300
H	1.98844700	0.28185100	-1.69007000
C	2.10612900	2.13950500	-0.63166400
H	1.02196800	2.27544400	-0.60516600
C	2.61499200	2.84389400	-1.89682900
H	2.18471900	2.40073700	-2.79909300
H	2.33986300	3.90160500	-1.88230800
H	3.70377400	2.79264200	-1.98403100
C	2.68062000	2.80905500	0.62428300
H	2.37409500	3.85734500	0.66118400
H	2.32707400	2.33835700	1.54403900
H	3.77352700	2.78846800	0.63181900
O	0.10733100	0.12065300	0.09355600
C	3.37535000	-3.61401100	0.14157100
H	4.42459600	-3.90305600	0.24334000
H	2.80303200	-4.15958000	0.89650200
H	3.03176700	-3.94628700	-0.84287900
S	-0.83598300	0.12632200	1.47549500
C	-2.38571500	-0.05507300	0.56325100
C	-3.30327000	0.98297400	0.57019700
C	-2.67756200	-1.26218600	-0.06679300
C	-4.52015000	0.81943800	-0.08633400
H	-3.06142900	1.90598000	1.08170200
C	-3.89452300	-1.41220100	-0.71436700
H	-1.96041800	-2.07453600	-0.06187500
C	-4.83516900	-0.37427200	-0.73663100
H	-5.23545400	1.63406500	-0.08829400
H	-4.12045400	-2.34902500	-1.21163200
C	-6.15426800	-0.55566900	-1.44164200
H	-6.76031400	0.34920600	-1.39075000
H	-6.00461300	-0.80499100	-2.49533400
H	-6.72818200	-1.37258200	-0.99597800
O	-0.84769900	1.49782600	2.04895100

(3R,4S,6S)-**4**-c1 B3LYP / 6-311++G (3df,2dp)

C	4.00021500	-1.34829400	-0.72484700
C	3.81336900	0.16414200	-0.58843100
C	2.33855800	0.59347500	-0.70232500
C	1.51626200	-0.18559100	0.33136800
C	1.70325400	-1.69479900	0.21010900
C	3.17399600	-2.11807500	0.31045700
H	4.21377500	0.48249500	0.37771500
H	4.40057100	0.67884300	-1.34959100
H	3.70062200	-1.66766200	-1.72893100
H	5.05757300	-1.60247700	-0.61934000
H	1.78813900	0.14344000	1.33814500
H	1.11293800	-2.19457900	0.98154900
H	1.29948600	-2.01121800	-0.75663500
H	3.53952500	-1.83551200	1.30477000
H	1.97458000	0.26603600	-1.68330000
C	2.12107900	2.12666300	-0.63818800
H	1.04086000	2.27734100	-0.60634800
C	2.63134100	2.81663600	-1.90920800
H	2.19188500	2.37382600	-2.80482900
H	2.36920100	3.87567600	-1.89947900

H	3.71703400	2.75178600	-2.00117600
C	2.71130100	2.79532500	0.60940700
H	2.41845100	3.84561800	0.64195500
H	2.35857500	2.33497700	1.53236700
H	3.80190800	2.76092900	0.60983100
O	0.10386300	0.13263200	0.11196600
C	3.32867900	-3.63168200	0.16391600
H	4.37351600	-3.93052700	0.26163700
H	2.75578800	-4.16475100	0.92449800
H	2.97650500	-3.96594200	-0.81466100
S	-0.83349300	0.18195700	1.46699600
C	-2.37547300	-0.02786500	0.56540200
C	-3.29863500	1.00530300	0.54437900
C	-2.66295500	-1.25153200	-0.03362600
C	-4.51328200	0.81869800	-0.10796500
H	-3.06496200	1.94091900	1.03213800
C	-3.87803200	-1.42338700	-0.67732200
H	-1.94449200	-2.05989400	-0.00568400
C	-4.82249500	-0.39139000	-0.72808300
H	-5.23228300	1.62741100	-0.12923000
H	-4.10013000	-2.37305500	-1.14719200
C	-6.13350500	-0.59118000	-1.43979800
H	-6.80510500	0.25018100	-1.27963900
H	-5.97952000	-0.69728800	-2.51548400
H	-6.63404400	-1.49737800	-1.09641900
O	-0.84343400	1.55997100	1.99427300

(3R,4S,6S)-**4**-c1 B3PW91 / 6-311G (3df,2dp)

C	4.03606500	-1.22044700	-0.75908800
C	3.78432200	0.27259500	-0.58320100
C	2.29904500	0.63530500	-0.69512200
C	1.51282000	-0.19887100	0.31442900
C	1.76430100	-1.68965600	0.15529500
C	3.24636800	-2.04742200	0.25231500
H	4.16260800	0.58141700	0.39648100
H	4.35406700	0.83636300	-1.32460900
H	3.74785200	-1.52694900	-1.77179100
H	5.10426700	-1.43361900	-0.66136500
H	1.77724900	0.11718700	1.33013200
H	1.19090900	-2.23526400	0.91006000
H	1.37951800	-1.99749600	-0.82336200
H	3.59625300	-1.77031900	1.25516600
H	1.95187000	0.31323600	-1.68579500
C	2.01165900	2.14803100	-0.59383800
H	0.92402900	2.24485700	-0.55054200
C	2.48097300	2.88661800	-1.84575600
H	2.05325300	2.44879200	-2.75045800
H	2.17792400	3.93498100	-1.80867200
H	3.56875700	2.86747600	-1.94618400
C	2.57851400	2.80834200	0.66152200
H	2.23829400	3.84379600	0.72472600
H	2.25494700	2.30822800	1.57554600
H	3.67051100	2.82490800	0.65242900
O	0.09913400	0.06706400	0.10346000
C	3.46828500	-3.54310000	0.06966800
H	4.52574100	-3.79869700	0.16323200
H	2.91715300	-4.12151100	0.81415400
H	3.13369600	-3.86785300	-0.91918700
S	-0.81445600	0.04168400	1.46509500
C	-2.35555800	-0.10981500	0.57017900
C	-3.24373100	0.95161600	0.57731300
C	-2.68044500	-1.30716800	-0.05559800
C	-4.46178100	0.82056600	-0.07478900
H	-2.97159800	1.86413500	1.09213900
C	-3.89992400	-1.42377300	-0.69953700

H	-1.98770700	-2.14016200	-0.04411000
C	-4.80874200	-0.36257600	-0.72356500
H	-5.15780900	1.65154000	-0.07374800
H	-4.15590800	-2.35572100	-1.19049100
C	-6.11836900	-0.49632700	-1.44262400
H	-6.82488600	0.27181600	-1.13014200
H	-5.97834600	-0.39760800	-2.52226800
H	-6.57080500	-1.47283000	-1.26509600
O	-0.81580300	1.38279000	2.06486600