Electronic Supplementary Material (ESI) for RSC Advances.

On the Mechanism of Retro-Diels-Alder Reaction of Partially Saturated 2-Pyrones to Produce Biorenewable Chemicals

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TABLES

Table S1. Frequency analysis of the transition states.

DHHP	DHHMP				HOPP			
TS_{1a}	TS_{2a}	TS_{2b}	TS_{2a}^{*}	TS_{2a}^{**}	TS_{3a}	TS_{3b}	TS_{3a}^{*}	TS_{3a}^{*}
469.91ι	146.94ι	267.63ι	175.05ι	251.2ι	201.73ι	267.51ι	196.45ι	341.76ι
98.82	88.84	39.21	82.29	61.84	9.68	30.71	20.64	44.11
262.95	122.34	65.4	106.97	86.7	28.07	45.12	41.69	62.52
287.11	179.73	115.27	148.05	147.85	71.77	59.6	76.31	74.22
372	193.19	142.91	178.12	171.3	121.1	91.18	97.31	137.64
384.15	266.82	184.36	249.87	228.76	144.4	104.94	139.33	151.3
452.07	337.78	199.1	314.07	344.44	150.59	116.85	146.33	152.43
571.94	373.72	244.79	350.9	355.98	174.96	129.02	173.57	173.47
607.55	412.04	302.41	392.88	399.07	219.81	147.45	253.97	221.56
665.18	476.78	391.29	427.51	431.18	307.07	210.63	297.25	313.7
691.33	502.91	468.52	496.75	496.9	342.96	303.38	354.74	329.44
850.59	510.48	483.59	510.77	511.84	388.34	332.51	397.01	370.23
911.92	593.37	517.54	565	562.11	425.77	356.2	410.26	401.03
952.59	619.36	541.26	609.46	598.6	437.42	401.73	441.79	430.86
980.16	731.07	623.99	669.83	677.23	461.77	442.31	461.48	472.53
1.01E+03	778.16	674.89	721.68	723.67	528.58	495.67	511.21	486.78
1.03E+03	800.54	810.5	805.44	799.6	573.79	536.24	524.5	527.49
1.05E+03	889.71	825.52	892.21	884.38	589.5	549.92	575.55	573.12
1.11E+03	895.25	885.78	904.35	907.85	608.66	574.64	588.51	584.1
1.19E+03	933.92	920.39	926.32	922.86	629.96	603.3	636.24	613.61
1.22E+03	967.37	957.43	969.21	957.85	721.99	666.9	694.04	685.25
1.28E+03	999.15	974.8	1.01E+03	994.91	762.14	673.7	718.4	706.78
1.40E+03	1.08E+03	1.00E+03	1.06E+03	1.06E+03	793.45	758.49	766.46	756.78
1.46E+03	1.13E+03	1.03E+03	1.11E+03	1.10E+03	813.55	819.86	794.47	801.71
1.52E+03	1.16E+03	1.13E+03	1.12E+03	1.13E+03	842.98	844.32	831.14	847.95
1.55E+03	1.17E+03	1.19E+03	1.18E+03	1.18E+03	873.31	855.51	890.62	871.27
1.80E+03	1.25E+03	1.23E+03	1.24E+03	1.23E+03	932.55	888.45	904.95	916.14
3.04E+03	1.25E+03	1.27E+03	1.27E+03	1.27E+03	948.77	951.1	940.42	934.86
3.15E+03	1.29E+03	1.29E+03	1.30E+03	1.28E+03	964.81	964.67	948.25	942.44
3.16E+03	1.34E+03	1.35E+03	1.36E+03	1.35E+03	1.01E+03	974.04	1.01E+03	1.01E+03
3.16E+03	1.38E+03	1.37E+03	1.38E+03	1.38E+03	1.05E+03	1.01E+03	1.07E+03	1.03E+03
3.17E+03	1.40E+03	1.39E+03	1.41E+03	1.42E+03	1.10E+03	1.03E+03	1.08E+03	1.06E+03
3.25E+03	1.44E+03	1.42E+03	1.45E+03	1.44E+03	1.15E+03	1.06E+03	1.11E+03	1.11E+03
	1.45E+03	1.44E+03	1.46E+03	1.46E+03	1.16E+03	1.16E+03	1.13E+03	1.16E+03
	1.50E+03	1.57E+03	1.52E+03	1.51E+03	1.17E+03	1.18E+03	1.18E+03	1.17E+03
	1.55E+03	1.66E+03	1.59E+03	1.58E+03	1.18E+03	1.20E+03	1.18E+03	1.18E+03

	1.62E+03	1.97E+03	1.73E+03	1.73E+03	1.23E+03	1.24E+03	1.23E+03	1.23E+03
	2.98E+03	3.00E+03	2.99E+03	2.99E+03	1.26E+03	1.24E+03	1.25E+03	1.24E+03
	3.03E+03	3.06E+03	3.07E+03	3.07E+03	1.27E+03	1.32E+03	1.28E+03	1.29E+03
	3.08E+03	3.10E+03	3.07E+03	3.08E+03	1.33E+03	1.32E+03	1.28E+03	1.32E+03
	3.12E+03	3.10E+03	3.11E+03	3.10E+03	1.34E+03	1.35E+03	1.35E+03	1.36E+03
	3.14E+03	3.13E+03	3.12E+03	3.12E+03	1.38E+03	1.36E+03	1.38E+03	1.40E+03
	3.16E+03	3.13E+03	3.16E+03	3.16E+03	1.41E+03	1.40E+03	1.41E+03	1.41E+03
	3.20E+03	3.23E+03	3.21E+03	3.17E+03	1.41E+03	1.41E+03	1.42E+03	1.43E+03
	3.63E+03	3.65E+03	3.65E+03	3.65E+03	1.42E+03	1.42E+03	1.44E+03	1.44E+03
					1.45E+03	1.44E+03	1.44E+03	1.46E+03
					1.51E+03	1.54E+03	1.50E+03	1.52E+03
					1.54E+03	1.64E+03	1.55E+03	1.54E+03
					1.62E+03	1.70E+03	1.70E+03	1.74E+03
					1.69E+03	1.89E+03	1.73E+03	1.75E+03
					3.02E+03	2.96E+03	3.02E+03	3.01E+03
					3.03E+03	3.01E+03	3.02E+03	3.02E+03
					3.06E+03	3.04E+03	3.04E+03	3.07E+03
					3.08E+03	3.08E+03	3.07E+03	3.08E+03
					3.09E+03	3.12E+03	3.09E+03	3.09E+03
					3.12E+03	3.13E+03	3.13E+03	3.11E+03
					3.12E+03	3.14E+03	3.14E+03	3.12E+03
					3.13E+03	3.14E+03	3.15E+03	3.13E+03
					3.15E+03	3.24E+03	3.18E+03	3.15E+03
					3.61E+03	3.64E+03	3.65E+03	3.66E+03

4HDMP				**4HMTHP**			**DTMP**		
4a	**4b**	**4a***	**4a****	**5a**	**5a***	**5a****	**6a**	**6a***	**6a****
82.36ι	238.45ι	144.88ι	206.75ι	137.06ι	294.77ι	355.74ι	86.21ι	209.52ι	277.71ι
68.53	15.36	65.97	86.74	38.84	81.14	79.28	27.36	93.33	81.26
105.27	19.05	125.45	130.27	80.86	133.12	102.07	35.26	138.44	121.3
109.21	27.67	128.03	155.07	180.04	199.05	193.32	92.81	146.41	130.57
165.06	57.88	174.05	170.96	239.98	217.39	212.97	108.55	155.81	163.14
176.49	94.43	188.08	193.62	283.86	325.21	335.06	153.86	219.11	186.6
216.87	130.49	224.36	213.68	337.79	346.79	348.11	171	226	221.5
231.35	182.47	252.64	246.65	399.91	380.84	375.43	220.79	235.14	222.14
269.13	209.45	277.66	265.65	445.67	424.53	420.16	272.14	306.63	297.23
312.68	213.53	311.37	331.58	472.5	480.11	484.09	322.83	336.49	321.13
358.01	259.22	339.04	349.66	588.44	598.28	596.94	341.72	343.73	337.11
398.61	291.33	375.13	394.53	621.74	619.41	629.42	395.26	352.17	351.96
483.75	371.93	444.61	446.59	704.5	707.66	705.2	423.07	420.53	414.26
533.26	461.16	493.52	502.49	768.75	779.93	780.68	448.38	455.31	452.07

576.76	490.42	539.76	541.47	872.35	883.02	873.74	493.55	473.31	461.61
640.82	504.49	599.27	593.24	909.19	893.52	886.78	561.73	572.68	564.53
705.92	553.18	659.22	672.36	934.8	929.07	931.25	580.44	598.88	591.85
745.37	625.8	700.86	708.49	983.92	983.51	974.1	672.7	647.31	631.22
759.25	659.71	728.39	726.69	1.00E+03	1.00E+03	989.46	721.98	719.25	715.08
812.38	789.15	798.22	796.49	1.03E+03	1.03E+03	1.03E+03	812.17	811.1	805.68
834.32	818.38	833.63	832.67	1.07E+03	1.06E+03	1.05E+03	820.51	823.88	815.78
902.99	921.68	886.58	893.39	1.12E+03	1.09E+03	1.08E+03	857.2	867.52	858.17
933.92	944.2	944.36	930.97	1.18E+03	1.18E+03	1.17E+03	902.15	931.98	930.43
990.78	952.66	989.52	994.23	1.20E+03	1.19E+03	1.19E+03	932.89	938.05	939.74
1.01E+03	1.02E+03	1.01E+03	1.02E+03	1.24E+03	1.23E+03	1.22E+03	936.61	953.11	949.75
1.05E+03	1.03E+03	1.05E+03	1.05E+03	1.29E+03	1.28E+03	1.27E+03	985.5	996.85	984.92
1.07E+03	1.05E+03	1.07E+03	1.07E+03	1.32E+03	1.32E+03	1.32E+03	1.00E+03	1.02E+03	1.02E+03
1.13E+03	1.09E+03	1.12E+03	1.11E+03	1.33E+03	1.35E+03	1.34E+03	1.03E+03	1.04E+03	1.04E+03
1.18E+03	1.11E+03	1.14E+03	1.14E+03	1.39E+03	1.42E+03	1.43E+03	1.05E+03	1.04E+03	1.05E+03
1.21E+03	1.18E+03	1.17E+03	1.17E+03	1.43E+03	1.43E+03	1.44E+03	1.08E+03	1.09E+03	1.08E+03
1.25E+03	1.21E+03	1.23E+03	1.23E+03	1.45E+03	1.46E+03	1.46E+03	1.15E+03	1.12E+03	1.12E+03
1.26E+03	1.23E+03	1.25E+03	1.25E+03	1.51E+03	1.50E+03	1.51E+03	1.18E+03	1.17E+03	1.17E+03
1.29E+03	1.31E+03	1.29E+03	1.28E+03	1.57E+03	1.55E+03	1.55E+03	1.24E+03	1.23E+03	1.22E+03
1.32E+03	1.33E+03	1.31E+03	1.32E+03	1.67E+03	1.73E+03	1.76E+03	1.29E+03	1.29E+03	1.29E+03
1.34E+03	1.35E+03	1.36E+03	1.36E+03	2.98E+03	3.00E+03	3.00E+03	1.33E+03	1.34E+03	1.34E+03
1.35E+03	1.37E+03	1.37E+03	1.38E+03	3.04E+03	3.06E+03	3.04E+03	1.33E+03	1.35E+03	1.36E+03
1.40E+03	1.40E+03	1.41E+03	1.42E+03	3.05E+03	3.06E+03	3.06E+03	1.33E+03	1.36E+03	1.37E+03
1.41E+03	1.41E+03	1.43E+03	1.43E+03	3.12E+03	3.11E+03	3.11E+03	1.35E+03	1.36E+03	1.37E+03
1.43E+03	1.42E+03	1.45E+03	1.45E+03	3.13E+03	3.13E+03	3.15E+03	1.39E+03	1.41E+03	1.41E+03
1.45E+03	1.43E+03	1.46E+03	1.46E+03	3.15E+03	3.15E+03	3.15E+03	1.40E+03	1.42E+03	1.43E+03
1.45E+03	1.45E+03	1.47E+03	1.47E+03	3.16E+03	3.15E+03	3.17E+03	1.41E+03	1.43E+03	1.44E+03
1.49E+03	1.55E+03	1.50E+03	1.51E+03	3.17E+03	3.17E+03	3.18E+03	1.42E+03	1.44E+03	1.44E+03
1.57E+03	1.65E+03	1.60E+03	1.59E+03				1.43E+03	1.44E+03	1.45E+03
1.62E+03	1.96E+03	1.71E+03	1.73E+03				1.44E+03	1.45E+03	1.46E+03
3.00E+03	2.99E+03	3.00E+03	3.00E+03				1.45E+03	1.47E+03	1.47E+03
3.05E+03	3.01E+03	3.03E+03	3.02E+03				1.48E+03	1.49E+03	1.49E+03
3.07E+03	3.05E+03	3.07E+03	3.06E+03				1.55E+03	1.55E+03	1.55E+03
3.09E+03	3.09E+03	3.09E+03	3.09E+03				1.66E+03	1.71E+03	1.75E+03
3.12E+03	3.10E+03	3.11E+03	3.09E+03				3.00E+03	2.99E+03	2.99E+03
3.12E+03	3.12E+03	3.11E+03	3.10E+03				3.00E+03	3.00E+03	3.00E+03
3.14E+03	3.12E+03	3.12E+03	3.11E+03				3.00E+03	3.00E+03	3.00E+03
3.14E+03	3.15E+03	3.13E+03	3.12E+03				3.05E+03	3.06E+03	3.06E+03
3.21E+03	3.19E+03	3.26E+03	3.24E+03				3.05E+03	3.06E+03	3.06E+03
3.60E+03	3.64E+03	3.66E+03	3.65E+03				3.06E+03	3.09E+03	3.08E+03
							3.07E+03	3.09E+03	3.09E+03

							3.11E+03	3.10E+03	3.10E+03
							3.12E+03	3.11E+03	3.11E+03
							3.12E+03	3.11E+03	3.11E+03
							3.13E+03	3.16E+03	3.15E+03
							3.17E+03	3.16E+03	3.16E+03

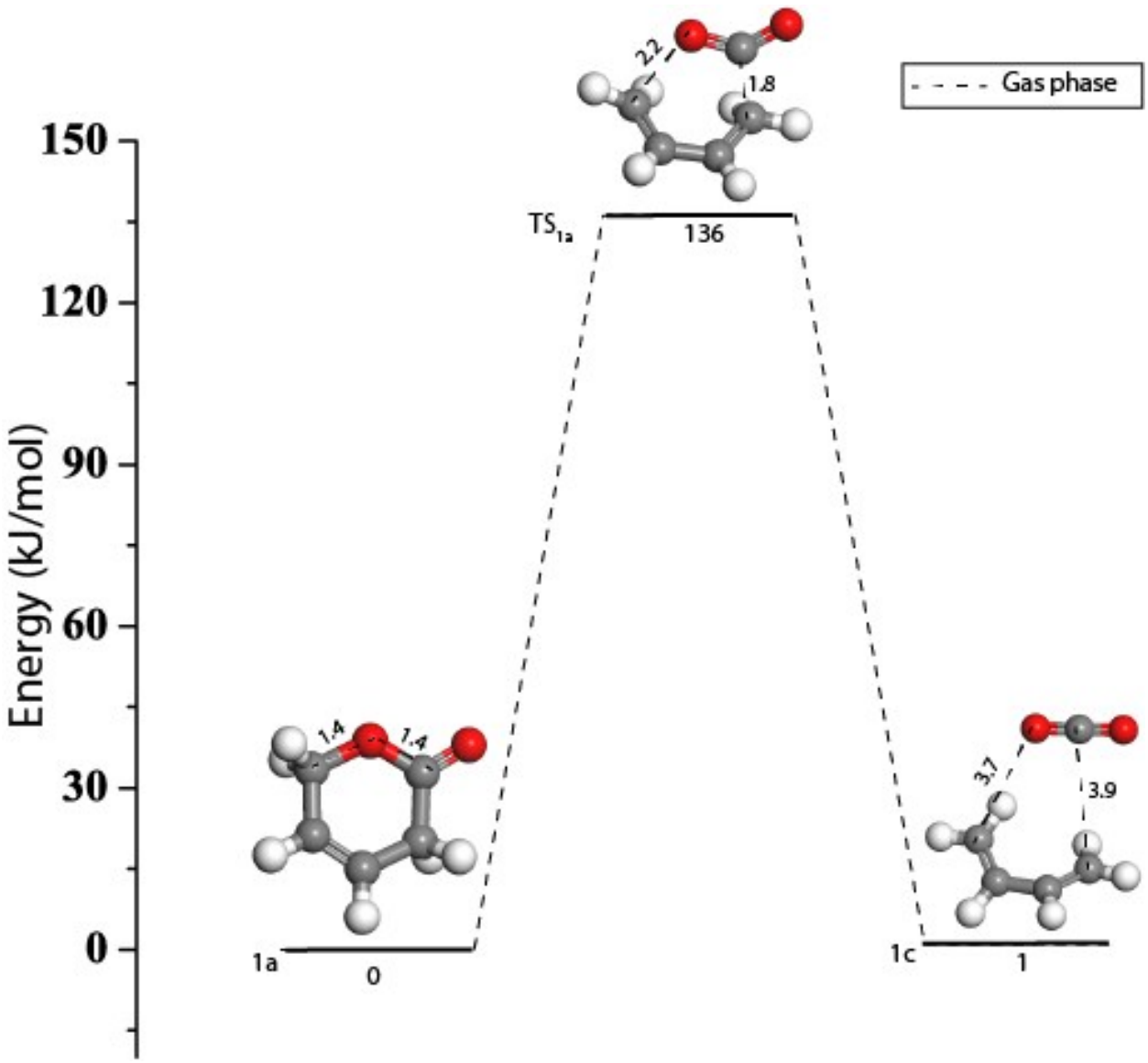

Figure S1. Reaction diagram for rDA reaction of DHHP in gas phase.

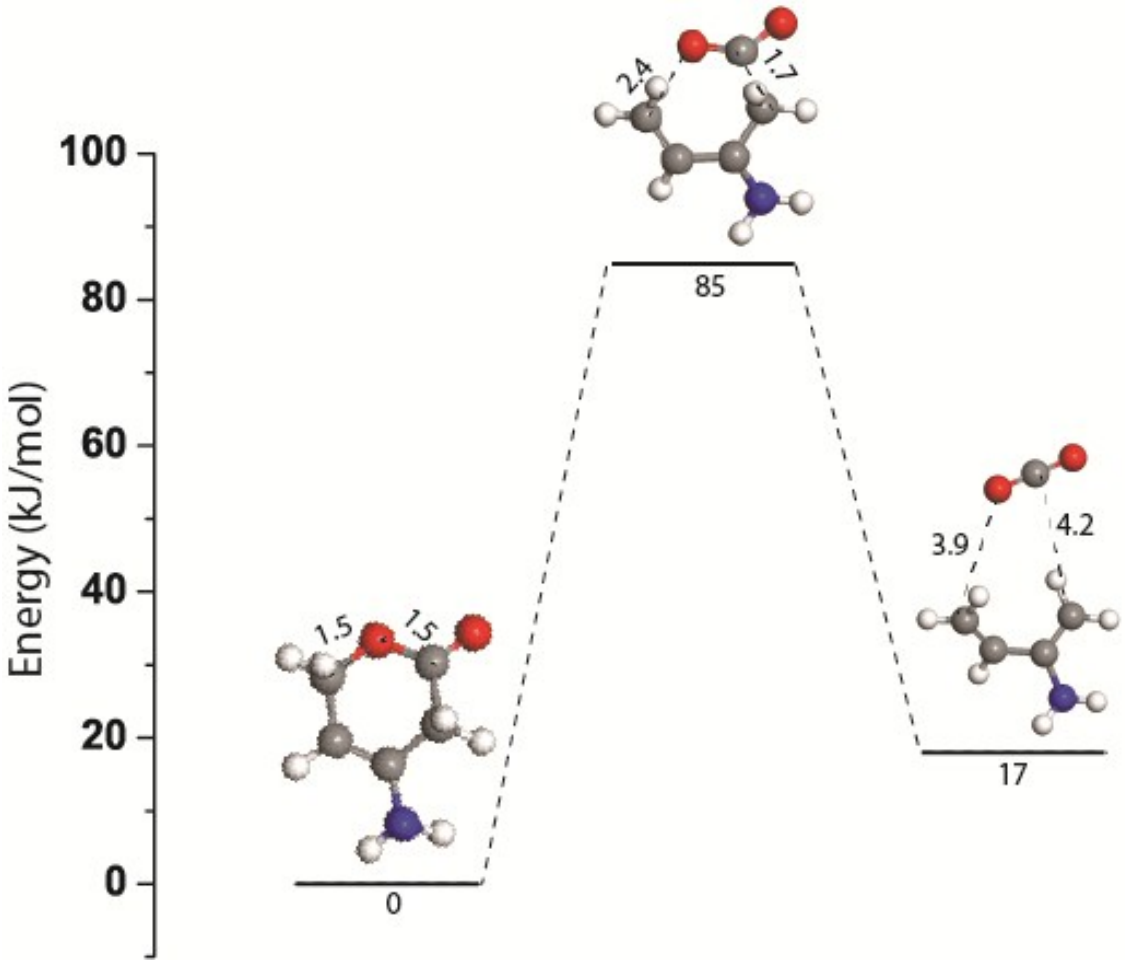

Figure S2. Reaction diagram for rDA reaction of 4-NH_2-DHHP.

XYZ coordinates for 1a

ATOM	1	C	MOL	-0.864	-1.267	-0.099	1.00	0.00	C
ATOM	2	C	MOL	0.650	-1.202	-0.055	1.00	0.00	C
ATOM	3	C	MOL	1.244	0.163	-0.184	1.00	0.00	C
ATOM	4	C	MOL	0.493	1.257	-0.047	1.00	0.00	C
ATOM	5	C	MOL	-0.968	1.185	0.223	1.00	0.00	C
ATOM	6	O	MOL	-1.582	-0.111	0.013	1.00	0.00	O
ATOM	7	O	MOL	-1.464	-2.312	-0.236	1.00	0.00	O
ATOM	8	H	MOL	1.011	-1.884	-0.837	1.00	0.00	H
ATOM	9	H	MOL	0.960	-1.675	0.892	1.00	0.00	H
ATOM	10	H	MOL	2.313	0.240	-0.381	1.00	0.00	H
ATOM	11	H	MOL	0.923	2.256	-0.120	1.00	0.00	H

ATOM 12 H MOL 1.525 1.871 -0.430 1.00 0.00 H

ATOM 13 H MOL -1.192 1.480 1.261 1.00 0.00 H

XYZ coordinates for TS_{1a}

ATOM 1 C MOL -1.008 -1.297 -0.448 1.00 0.00 C

ATOM 2 C MOL 0.619 -1.073 0.230 1.00 0.00 C

ATOM 3 C MOL 1.196 0.119 -0.278 1.00 0.00 C

ATOM 4 C MOL 0.558 1.356 -0.152 1.00 0.00 C

ATOM 5 C MOL -0.630 1.418 0.544 1.00 0.00 C

ATOM 6 O MOL -1.710 -0.266 -0.386 1.00 0.00 O

ATOM 7 O MOL -1.164 -2.456 -0.797 1.00 0.00 O

ATOM 8 H MOL 1.148 -1.999 0.008 1.00 0.00 H

ATOM 9 H MOL 0.265 -1.043 1.267 1.00 0.00 H

ATOM 10 H MOL 2.031 0.040 -0.975 1.00 0.00 H

ATOM 11 H MOL 0.849 2.171 -0.813 1.00 0.00 H

ATOM 12 H MOL -1.332 2.235 0.388 1.00 0.00 H

ATOM 13 H MOL -0.822 0.796 1.412 1.00 0.00 H

XYZ coordinates for 1b

ATOM 1 C MOL -2.390 -2.006 -0.472 1.00 0.00 C

ATOM 2 C MOL 1.296 -0.893 0.249 1.00 0.00 C

ATOM 3 C MOL 1.383 0.253 -0.447 1.00 0.00 C

ATOM 4 C MOL 0.777 1.530 -0.073 1.00 0.00 C

ATOM 5 C MOL -0.373 1.686 0.601 1.00 0.00 C

ATOM 6 O MOL -2.793 -0.902 -0.474 1.00 0.00 O

ATOM 7 O MOL -1.995 -3.113 -0.467 1.00 0.00 O

ATOM 8 H MOL 1.764 -1.810 -0.105 1.00 0.00 H

ATOM 9 H MOL 0.777 -0.937 1.208 1.00 0.00 H

ATOM 10 H MOL 1.977 0.259 -1.364 1.00 0.00 H

ATOM 11 H MOL 1.311 2.424 -0.404 1.00 0.00 H

ATOM 12 H MOL -0.749 2.675 0.856 1.00 0.00 H

ATOM 13 H MOL -0.985 0.833 0.894 1.00 0.00 H

XYZ coordinates for 2a

ATOM	1	C	MOL	-1.873	0.318	0.085	1.00	0.00	C
ATOM	2	C	MOL	-1.103	-0.953	-0.050	1.00	0.00	C
ATOM	3	C	MOL	0.217	-0.944	-0.272	1.00	0.00	C
ATOM	4	C	MOL	0.954	0.347	-0.429	1.00	0.00	C
ATOM	5	C	MOL	-1.033	1.501	0.501	1.00	0.00	C
ATOM	6	C	MOL	2.377	0.290	0.091	1.00	0.00	C
ATOM	7	O	MOL	-1.891	-2.063	0.081	1.00	0.00	O
ATOM	8	O	MOL	0.298	1.465	0.295	1.00	0.00	O
ATOM	9	O	MOL	-1.518	2.497	1.022	1.00	0.00	O
ATOM	10	H	MOL	-2.682	0.211	0.818	1.00	0.00	H
ATOM	11	H	MOL	-2.360	0.577	-0.869	1.00	0.00	H
ATOM	12	H	MOL	0.787	-1.866	-0.383	1.00	0.00	H
ATOM	13	H	MOL	0.964	0.673	-1.481	1.00	0.00	H
ATOM	14	H	MOL	2.939	-0.459	-0.481	1.00	0.00	H
ATOM	15	H	MOL	2.391	0.005	1.150	1.00	0.00	H
ATOM	16	H	MOL	2.873	1.260	-0.032	1.00	0.00	H
ATOM	17	H	MOL	-1.341	-2.858	-0.048	1.00	0.00	H

XYZ coordinates for TS_{2a}

ATOM	1	C	MOL	-1.800	0.190	-0.158	1.00	0.00	C
ATOM	2	C	MOL	-1.008	-1.019	0.086	1.00	0.00	C
ATOM	3	C	MOL	0.377	-0.997	-0.022	1.00	0.00	C
ATOM	4	C	MOL	0.987	0.133	-0.541	1.00	0.00	C
ATOM	5	C	MOL	-1.317	1.416	0.745	1.00	0.00	C
ATOM	6	C	MOL	2.432	0.415	-0.408	1.00	0.00	C
ATOM	7	O	MOL	-1.667	-2.052	0.612	1.00	0.00	O1+
ATOM	8	O	MOL	-0.069	1.647	0.775	1.00	0.00	O1-
ATOM	9	O	MOL	-2.235	2.057	1.300	1.00	0.00	O
ATOM	10	H	MOL	-2.865	0.014	0.000	1.00	0.00	H
ATOM	11	H	MOL	-1.653	0.544	-1.188	1.00	0.00	H

ATOM 12 H MOL 0.963 -1.751 0.506 1.00 0.00 H

ATOM 13 H MOL 0.456 0.724 -1.283 1.00 0.00 H

ATOM 14 H MOL 2.960 0.005 -1.286 1.00 0.00 H

ATOM 15 H MOL 2.867 -0.036 0.489 1.00 0.00 H

ATOM 16 H MOL 2.615 1.495 -0.418 1.00 0.00 H

ATOM 17 H MOL -1.042 -2.784 0.790 1.00 0.00 H

XYZ coordinates for 2b

ATOM 1 C MOL -1.835 -0.011 -0.254 1.00 0.00 C

ATOM 2 C MOL -0.850 -0.877 0.330 1.00 0.00 C

ATOM 3 C MOL 0.565 -0.763 0.171 1.00 0.00 C

ATOM 4 C MOL 1.160 0.158 -0.628 1.00 0.00 C

ATOM 5 C MOL -1.997 1.325 0.755 1.00 0.00 C

ATOM 6 C MOL 2.620 0.331 -0.765 1.00 0.00 C

ATOM 7 O MOL -1.326 -1.800 1.157 1.00 0.00 O1+

ATOM 8 O MOL -1.245 2.266 0.446 1.00 0.00 O1-

ATOM 9 O MOL -2.857 1.167 1.640 1.00 0.00 O

ATOM 10 H MOL -2.818 -0.482 -0.290 1.00 0.00 H

ATOM 11 H MOL -1.534 0.387 -1.222 1.00 0.00 H

ATOM 12 H MOL 1.183 -1.452 0.752 1.00 0.00 H

ATOM 13 H MOL 0.534 0.834 -1.213 1.00 0.00 H

ATOM 14 H MOL 2.910 0.227 -1.822 1.00 0.00 H

ATOM 15 H MOL 3.191 -0.376 -0.155 1.00 0.00 H

ATOM 16 H MOL 2.896 1.360 -0.488 1.00 0.00 H

ATOM 17 H MOL -0.596 -2.295 1.585 1.00 0.00 H

XYZ coordinates for TS_{2b}

ATOM 1 C MOL -1.829 -0.311 -0.312 1.00 0.00 C

ATOM 2 C MOL -0.771 -0.958 0.312 1.00 0.00 C

ATOM 3 C MOL 0.638 -0.661 0.144 1.00 0.00 C

ATOM 4 C MOL 1.140 0.256 -0.709 1.00 0.00 C

ATOM 5 C MOL -2.160 1.225 0.977 1.00 0.00 C

ATOM 6 C MOL 2.584 0.561 -0.864 1.00 0.00 C

ATOM 7 O MOL -1.092 -1.912 1.209 1.00 0.00 O

ATOM 8 O MOL -1.576 2.187 0.529 1.00 0.00 O

ATOM 9 O MOL -2.886 0.807 1.853 1.00 0.00 O

ATOM 10 H MOL -2.804 -0.791 -0.257 1.00 0.00 H

ATOM 11 H MOL -1.619 0.260 -1.211 1.00 0.00 H

ATOM 12 H MOL 1.325 -1.239 0.768 1.00 0.00 H

ATOM 13 H MOL 0.456 0.830 -1.337 1.00 0.00 H

ATOM 14 H MOL 2.892 0.418 -1.910 1.00 0.00 H

ATOM 15 H MOL 3.213 -0.060 -0.215 1.00 0.00 H

ATOM 16 H MOL 2.774 1.621 -0.637 1.00 0.00 H

ATOM 17 H MOL -0.287 -2.234 1.659 1.00 0.00 H

XYZ coordinates for 2c

ATOM 1 C MOL -1.799 -0.556 -0.489 1.00 0.00 C

ATOM 2 C MOL -0.853 -1.137 0.274 1.00 0.00 C

ATOM 3 C MOL 0.595 -1.062 0.061 1.00 0.00 C

ATOM 4 C MOL 1.249 -0.044 -0.527 1.00 0.00 C

ATOM 5 C MOL -2.334 2.853 0.920 1.00 0.00 C

ATOM 6 C MOL 2.721 -0.004 -0.759 1.00 0.00 C

ATOM 7 O MOL -1.253 -1.906 1.355 1.00 0.00 O

ATOM 8 O MOL -1.507 3.347 0.248 1.00 0.00 O

ATOM 9 O MOL -3.163 2.367 1.594 1.00 0.00 O

ATOM 10 H MOL -2.853 -0.644 -0.234 1.00 0.00 H

ATOM 11 H MOL -1.521 -0.005 -1.383 1.00 0.00 H

ATOM 12 H MOL 1.174 -1.916 0.430 1.00 0.00 H

ATOM 13 H MOL 0.673 0.822 -0.863 1.00 0.00 H

ATOM 14 H MOL 2.946 0.056 -1.834 1.00 0.00 H

ATOM 15 H MOL 3.220 -0.891 -0.350 1.00 0.00 H

ATOM 16 H MOL 3.168 0.892 -0.302 1.00 0.00 H

ATOM 17 H MOL -0.462 -2.171 1.858 1.00 0.00 H

XYZ coordinates for 3a

ATOM	1	C	MOL	-2.642	-0.662	0.092	1.00	0.00 C
ATOM	2	C	MOL	-2.089	-2.047	-0.110	1.00	0.00 C
ATOM	3	C	MOL	-0.607	-2.158	-0.022	1.00	0.00 C
ATOM	4	C	MOL	0.172	-1.132	0.334	1.00	0.00 C
ATOM	5	C	MOL	-0.376	0.212	0.679	1.00	0.00 C
ATOM	6	O	MOL	-1.821	0.355	0.435	1.00	0.00 O
ATOM	7	O	MOL	-3.831	-0.413	-0.049	1.00	0.00 O
ATOM	8	O	MOL	-0.169	-3.416	-0.341	1.00	0.00 O
ATOM	9	C	MOL	0.283	1.352	-0.094	1.00	0.00 C
ATOM	10	C	MOL	1.704	1.654	0.333	1.00	0.00 C
ATOM	11	C	MOL	2.473	2.588	-0.556	1.00	0.00 C
ATOM	12	O	MOL	2.193	1.168	1.353	1.00	0.00 O
ATOM	13	H	MOL	-2.569	-2.703	0.632	1.00	0.00 H
ATOM	14	H	MOL	-2.447	-2.402	-1.087	1.00	0.00 H
ATOM	15	H	MOL	1.253	-1.242	0.408	1.00	0.00 H
ATOM	16	H	MOL	-0.261	0.410	1.754	1.00	0.00 H
ATOM	17	H	MOL	0.804	-3.442	-0.262	1.00	0.00 H
ATOM	18	H	MOL	-0.293	2.277	0.064	1.00	0.00 H
ATOM	19	H	MOL	0.256	1.158	-1.175	1.00	0.00 H
ATOM	20	H	MOL	2.666	2.089	-1.516	1.00	0.00 H
ATOM	21	H	MOL	3.423	2.869	-0.092	1.00	0.00 H
ATOM	22	H	MOL	1.878	3.483	-0.782	1.00	0.00 H

XYZ coordinates for TS_{3a}

ATOM	1	C	MOL	-2.640	-0.201	-0.308	1.00	0.00 C
ATOM	2	C	MOL	-1.616	-1.246	-0.968	1.00	0.00 C
ATOM	3	C	MOL	-0.833	-1.996	0.015	1.00	0.00 C
ATOM	4	C	MOL	-0.164	-1.378	1.071	1.00	0.00 C
ATOM	5	C	MOL	0.029	-0.011	1.154	1.00	0.00 C
ATOM	6	O	MOL	-2.209	0.524	0.637	1.00	0.00 O1-

ATOM 7 O MOL -3.768 -0.181 -0.848 1.00 0.00 O

ATOM 8 O MOL -1.024 -3.315 -0.010 1.00 0.00 O1+

ATOM 9 C MOL 0.495 0.940 0.108 1.00 0.00 C

ATOM 10 C MOL 1.943 1.376 0.362 1.00 0.00 C

ATOM 11 C MOL 2.509 2.324 -0.653 1.00 0.00 C

ATOM 12 O MOL 2.585 0.974 1.328 1.00 0.00 O

ATOM 13 H MOL -2.178 -1.924 -1.614 1.00 0.00 H

ATOM 14 H MOL -0.977 -0.613 -1.596 1.00 0.00 H

ATOM 15 H MOL -0.024 -1.968 1.979 1.00 0.00 H

ATOM 16 H MOL 0.164 0.372 2.167 1.00 0.00 H

ATOM 17 H MOL -0.538 -3.746 0.724 1.00 0.00 H

ATOM 18 H MOL -0.114 1.854 0.121 1.00 0.00 H

ATOM 19 H MOL 0.447 0.544 -0.912 1.00 0.00 H

ATOM 20 H MOL 2.518 1.845 -1.642 1.00 0.00 H

ATOM 21 H MOL 3.527 2.616 -0.376 1.00 0.00 H

ATOM 22 H MOL 1.869 3.212 -0.739 1.00 0.00 H

XYZ coordinates for 3b

ATOM 1 C MOL 1 -4.594 1.396 -2.025 1.00 0.00 C

ATOM 2 C MOL 1 -1.246 -1.464 -0.811 1.00 0.00 C

ATOM 3 C MOL 1 -1.055 -1.814 0.477 1.00 0.00 C

ATOM 4 C MOL 1 0.227 -1.882 1.185 1.00 0.00 C

ATOM 5 C MOL 1 1.301 -1.084 1.040 1.00 0.00 C

ATOM 6 O MOL 1 -3.712 2.120 -2.304 1.00 0.00 O

ATOM 7 O MOL 1 -5.475 0.671 -1.746 1.00 0.00 O

ATOM 8 O MOL 1 -2.156 -2.194 1.226 1.00 0.00 O

ATOM 9 C MOL 1 1.448 0.073 0.113 1.00 0.00 C

ATOM 10 C MOL 1 2.378 1.168 0.612 1.00 0.00 C

ATOM 11 C MOL 1 2.401 2.426 -0.210 1.00 0.00 C

ATOM 12 O MOL 3.069 1.035 1.621 1.00 0.00 O

ATOM 13 H MOL -2.246 -1.456 -1.242 1.00 0.00 H

ATOM 14 H MOL -0.402 -1.240 -1.455 1.00 0.00 H

ATOM 15 H MOL 0.279 -2.664 1.949 1.00 0.00 H

ATOM 16 H MOL 2.165 -1.281 1.676 1.00 0.00 H

ATOM 17 H MOL -1.879 -2.302 2.153 1.00 0.00 H

ATOM 18 H MOL 0.478 0.517 -0.155 1.00 0.00 H

ATOM 19 H MOL 1.870 -0.252 -0.855 1.00 0.00 H

ATOM 20 H MOL 2.479 2.193 -1.279 1.00 0.00 H

ATOM 21 H MOL 3.223 3.077 0.102 1.00 0.00 H

ATOM 22 H MOL 1.447 2.956 -0.073 1.00 0.00 H

XYZ coordinates for TS_{3b}

ATOM 1 C MOL -2.745 0.407 -0.497 1.00 0.00 C

ATOM 2 C MOL -1.645 -1.107 -0.950 1.00 0.00 C

ATOM 3 C MOL -1.351 -1.757 0.256 1.00 0.00 C

ATOM 4 C MOL -0.185 -1.592 1.095 1.00 0.00 C

ATOM 5 C MOL 0.857 -0.740 0.955 1.00 0.00 C

ATOM 6 O MOL -2.106 1.428 -0.691 1.00 0.00 O

ATOM 7 O MOL -3.845 0.007 -0.157 1.00 0.00 O

ATOM 8 O MOL -2.281 -2.626 0.680 1.00 0.00 O

ATOM 9 C MOL 1.077 0.322 -0.061 1.00 0.00 C

ATOM 10 C MOL 2.229 1.266 0.268 1.00 0.00 C

ATOM 11 C MOL 2.291 2.513 -0.561 1.00 0.00 C

ATOM 12 O MOL 3.047 1.012 1.147 1.00 0.00 O

ATOM 13 H MOL -2.367 -1.630 -1.575 1.00 0.00 H

ATOM 14 H MOL -0.815 -0.658 -1.483 1.00 0.00 H

ATOM 15 H MOL -0.139 -2.283 1.939 1.00 0.00 H

ATOM 16 H MOL 1.659 -0.831 1.690 1.00 0.00 H

ATOM 17 H MOL -2.040 -2.990 1.555 1.00 0.00 H

ATOM 18 H MOL 0.170 0.907 -0.267 1.00 0.00 H

ATOM 19 H MOL 1 1.344 -0.132 -1.034 1.00 0.00 H

ATOM 20 H MOL 1 2.176 2.273 -1.626 1.00 0.00 H

ATOM 21 H MOL 1 3.228 3.052 -0.389 1.00 0.00 H

ATOM 22 H MOL 1 1.441 3.157 -0.293 1.00 0.00 H

XYZ coordinates for 3c

ATOM 1 C MOL -4.594 1.396 -2.025 1.00 0.00 C

ATOM 2 C MOL -1.246 -1.464 -0.811 1.00 0.00 C

ATOM 3 C MOL -1.055 -1.814 0.477 1.00 0.00 C

ATOM 4 C MOL 0.227 -1.882 1.185 1.00 0.00 C

ATOM 5 C MOL 1.301 -1.084 1.040 1.00 0.00 C

ATOM 6 O MOL -3.712 2.120 -2.304 1.00 0.00 O

ATOM 7 O MOL -5.475 0.671 -1.746 1.00 0.00 O

ATOM 8 O MOL -2.156 -2.194 1.226 1.00 0.00 O

ATOM 9 C MOL 1.448 0.073 0.113 1.00 0.00 C

ATOM 10 C MOL 2.378 1.168 0.612 1.00 0.00 C

ATOM 11 C MOL 2.401 2.426 -0.210 1.00 0.00 C

ATOM 12 O MOL 3.069 1.035 1.621 1.00 0.00 O

ATOM 13 H MOL -2.246 -1.456 -1.242 1.00 0.00 H

ATOM 14 H MOL -0.402 -1.240 -1.455 1.00 0.00 H

ATOM 15 H MOL 0.279 -2.664 1.949 1.00 0.00 H

ATOM 16 H MOL 2.165 -1.281 1.676 1.00 0.00 H

ATOM 17 H MOL -1.879 -2.302 2.153 1.00 0.00 H

ATOM 18 H MOL 0.478 0.517 -0.155 1.00 0.00 H

ATOM 19 H MOL 1.870 -0.252 -0.855 1.00 0.00 H

ATOM 20 H MOL 2.479 2.193 -1.279 1.00 0.00 H

ATOM 21 H MOL 3.223 3.077 0.102 1.00 0.00 H

ATOM 22 H MOL 1.447 2.956 -0.073 1.00 0.00 H

XYZ coordinates for 3a*

ATOM 1 C MOL -2.905 -0.800 -0.247 1.00 0.00 C

ATOM 2 C MOL -2.088 -1.974 0.571 1.00 0.00 C

ATOM 3 C MOL -0.755 -2.167 0.033 1.00 0.00 C

ATOM 4 C MOL 0.153 -1.117 -0.082 1.00 0.00 C

ATOM 5 C MOL -0.180 0.133 0.409 1.00 0.00 C

ATOM 6 O MOL -2.261 0.277 -0.445 1.00 0.00 O1-

ATOM 7 O MOL -4.071 -1.106 -0.518 1.00 0.00 O

ATOM 8 O MOL -0.531 -3.342 -0.581 1.00 0.00 O1+

ATOM 9 C MOL 0.518 1.362 -0.062 1.00 0.00 C

ATOM 10 C MOL 1.922 1.631 0.520 1.00 0.00 C

ATOM 11 C MOL 2.739 2.619 -0.278 1.00 0.00 C

ATOM 12 O MOL 2.339 1.094 1.533 1.00 0.00 O

ATOM 13 H MOL -2.079 -1.579 1.595 1.00 0.00 H

ATOM 14 H MOL -2.689 -2.884 0.535 1.00 0.00 H

ATOM 15 H MOL 0.975 -1.214 -0.795 1.00 0.00 H

ATOM 16 H MOL -0.792 0.221 1.301 1.00 0.00 H

ATOM 17 H MOL 0.342 -3.315 -1.018 1.00 0.00 H

ATOM 18 H MOL -0.081 2.252 0.181 1.00 0.00 H

ATOM 19 H MOL 0.614 1.350 -1.155 1.00 0.00 H

ATOM 20 H MOL 3.100 2.124 -1.192 1.00 0.00 H

ATOM 21 H MOL 3.602 2.964 0.300 1.00 0.00 H

ATOM 22 H MOL 2.130 3.471 -0.604 1.00 0.00 H

XYZ coordinates for 3a[**]

ATOM 1 C MOL -2.615 0.382 0.431 1.00 0.00 C

ATOM 2 C MOL -2.015 -0.914 -0.484 1.00 0.00 C

ATOM 3 C MOL -1.213 -1.796 0.321 1.00 0.00 C

ATOM 4 C MOL -0.163 -1.331 1.124 1.00 0.00 C

ATOM 5 C MOL 0.306 -0.031 1.055 1.00 0.00 C

ATOM 6 O MOL -1.749 0.975 1.128 1.00 0.00 O1-

ATOM 7 O MOL -3.806 0.574 0.206 1.00 0.00 O

ATOM 8 O MOL -1.721 -3.033 0.501 1.00 0.00 O1+

ATOM 9 C MOL 0.695 0.758 -0.149 1.00 0.00 C

ATOM 10 C MOL 2.174 1.176 -0.106 1.00 0.00 C

ATOM 11 C MOL 2.735 1.668 -1.417 1.00 0.00 C

ATOM 12 O MOL 2.836 1.131 0.917 1.00 0.00 O

ATOM 13 H MOL -2.873 -1.413 -0.935 1.00 0.00 H

ATOM 14 H MOL -1.449 -0.358 -1.235 1.00 0.00 H

ATOM 15 H MOL 0.045 -1.893 2.038 1.00 0.00 H

ATOM 16 H MOL 0.770 0.355 1.965 1.00 0.00 H

ATOM 17 H MOL -1.200 -3.506 1.176 1.00 0.00 H

ATOM 18 H MOL 0.125 1.701 -0.180 1.00 0.00 H

ATOM 19 H MOL 0.502 0.238 -1.095 1.00 0.00 H

ATOM 20 H MOL 2.906 0.808 -2.080 1.00 0.00 H

ATOM 21 H MOL 3.686 2.180 -1.249 1.00 0.00 H

ATOM 22 H MOL 2.026 2.330 -1.930 1.00 0.00 H

XYZ coordinates for 4a

ATOM 1 C MOL -1.233 0.118 -0.008 1.00 0.00 C

ATOM 2 C MOL -0.664 -1.067 -0.256 1.00 0.00 C

ATOM 3 C MOL 0.825 -1.221 -0.328 1.00 0.00 C

ATOM 4 C MOL 1.511 0.066 -0.745 1.00 0.00 C

ATOM 5 C MOL -0.393 1.335 0.206 1.00 0.00 C

ATOM 6 O MOL 0.910 1.248 -0.501 1.00 0.00 O

ATOM 7 O MOL 2.610 0.072 -1.286 1.00 0.00 O

ATOM 8 C MOL 1.418 -1.732 1.005 1.00 0.00 C

ATOM 9 C MOL -1.047 2.611 -0.288 1.00 0.00 C

ATOM 10 O MOL -1.322 -2.250 -0.454 1.00 0.00 O

ATOM 11 H MOL -2.315 0.232 0.069 1.00 0.00 H

ATOM 12 H MOL 1.068 -1.952 -1.110 1.00 0.00 H

ATOM 13 H MOL -0.121 1.454 1.266 1.00 0.00 H

ATOM 14 H MOL 2.500 -1.875 0.910 1.00 0.00 H

ATOM 15 H MOL 0.959 -2.694 1.261 1.00 0.00 H

ATOM 16 H MOL 1.223 -1.026 1.821 1.00 0.00 H

ATOM 17 H MOL -1.976 2.779 0.269 1.00 0.00 H

ATOM 18 H MOL -1.288 2.532 -1.355 1.00 0.00 H

ATOM 19 H MOL -0.387 3.471 -0.128 1.00 0.00 H

ATOM 20 H MOL -2.280 -2.101 -0.348 1.00 0.00 H

XYZ coordinates for 4a*

ATOM 1 C MOL -1.282 0.157 -0.212 1.00 0.00 C

ATOM 2 C MOL -0.647 -1.085 -0.335 1.00 0.00 C

ATOM 3 C MOL 0.799 -1.334 -0.212 1.00 0.00 C

ATOM 4 C MOL 1.679 -0.307 -1.086 1.00 0.00 C

ATOM 5 C MOL -0.667 1.272 0.307 1.00 0.00 C

ATOM 6 O MOL 1.433 0.927 -0.989 1.00 0.00 O1-

ATOM 7 O MOL 2.585 -0.876 -1.745 1.00 0.00 O

ATOM 8 C MOL 1.371 -1.353 1.221 1.00 0.00 C

ATOM 9 C MOL -1.190 2.638 0.119 1.00 0.00 C

ATOM 10 O MOL -1.328 -2.134 -0.797 1.00 0.00 O1+

ATOM 11 H MOL -2.251 0.267 -0.705 1.00 0.00 H

ATOM 12 H MOL 0.972 -2.323 -0.649 1.00 0.00 H

ATOM 13 H MOL 0.171 1.166 0.989 1.00 0.00 H

ATOM 14 H MOL 2.430 -1.628 1.166 1.00 0.00 H

ATOM 15 H MOL 0.852 -2.111 1.818 1.00 0.00 H

ATOM 16 H MOL 1.291 -0.387 1.725 1.00 0.00 H

ATOM 17 H MOL -1.678 2.978 1.047 1.00 0.00 H

ATOM 18 H MOL -1.907 2.707 -0.707 1.00 0.00 H

ATOM 19 H MOL -0.356 3.333 -0.049 1.00 0.00 H

ATOM 20 H MOL -2.277 -1.908 -0.906 1.00 0.00 H

XYZ coordinates for 4b

ATOM 1 C MOL -1.207 0.213 -0.277 1.00 0.00 C

ATOM 2 C MOL -0.538 -1.033 -0.487 1.00 0.00 C

ATOM 3 C MOL 0.782 -1.442 -0.058 1.00 0.00 C

ATOM 4 C MOL 1.840 -0.796 -1.220 1.00 0.00 C

ATOM 5 C MOL -0.633 1.340 0.217 1.00 0.00 C

ATOM 6 O MOL 2.330 0.301 -0.901 1.00 0.00 O1-

ATOM 7 O MOL 1.979 -1.541 -2.207 1.00 0.00 O

ATOM 8 C MOL 1.249 -1.093 1.353 1.00 0.00 C

ATOM 9 C MOL -1.336 2.630 0.366 1.00 0.00 C

ATOM 10 O MOL -1.163 -1.942 -1.230 1.00 0.00 O1+

ATOM 11 H MOL -2.254 0.249 -0.590 1.00 0.00 H

ATOM 12 H MOL 0.863 -2.517 -0.238 1.00 0.00 H

ATOM 13 H MOL 0.422 1.325 0.487 1.00 0.00 H

ATOM 14 H MOL 2.186 -1.625 1.551 1.00 0.00 H

ATOM 15 H MOL 0.509 -1.415 2.097 1.00 0.00 H

ATOM 16 H MOL 1.446 -0.027 1.479 1.00 0.00 H

ATOM 17 H MOL -1.272 2.967 1.413 1.00 0.00 H

ATOM 18 H MOL -2.386 2.581 0.061 1.00 0.00 H

ATOM 19 H MOL -0.820 3.405 -0.220 1.00 0.00 H

ATOM 20 H MOL -1.999 -1.581 -1.594 1.00 0.00 H

XYZ coordinates for TS_{4b}

ATOM 1 C MOL -1.216 0.207 -0.249 1.00 0.00 C

ATOM 2 C MOL -0.541 -1.055 -0.464 1.00 0.00 C

ATOM 3 C MOL 0.692 -1.495 0.031 1.00 0.00 C

ATOM 4 C MOL 1.948 -0.722 -1.360 1.00 0.00 C

ATOM 5 C MOL -0.640 1.341 0.206 1.00 0.00 C

ATOM 6 O MOL 2.377 0.332 -0.931 1.00 0.00 O

ATOM 7 O MOL 2.010 -1.522 -2.270 1.00 0.00 O

ATOM 8 C MOL 1.235 -1.113 1.388 1.00 0.00 C

ATOM 9 C MOL -1.346 2.633 0.376 1.00 0.00 C

ATOM 10 O MOL -1.167 -1.935 -1.276 1.00 0.00 O

ATOM 11 H MOL -2.275 0.226 -0.522 1.00 0.00 H

ATOM 12 H MOL 0.865 -2.540 -0.227 1.00 0.00 H

ATOM 13 H MOL 0.426 1.339 0.431 1.00 0.00 H

ATOM 14 H MOL 2.224 -1.561 1.534 1.00 0.00 H

ATOM 15 H MOL 0.568 -1.523 2.159 1.00 0.00 H

ATOM 16 H MOL 1.328 -0.037 1.553 1.00 0.00 H

ATOM 17 H MOL -1.259 2.977 1.418 1.00 0.00 H

ATOM 18 H MOL -2.405 2.571 0.104 1.00 0.00 H

ATOM 19 H MOL -0.860 3.407 -0.237 1.00 0.00 H

ATOM 20 H MOL -1.965 -1.529 -1.665 1.00 0.00 H

XYZ coordinates for 4c

ATOM 1 C MOL -1.278 0.128 -0.111 1.00 0.00 C

ATOM 2 C MOL -0.633 -1.166 -0.351 1.00 0.00 C

ATOM 3 C MOL 0.380 -1.736 0.337 1.00 0.00 C

ATOM 4 C MOL 2.489 -0.328 -1.984 1.00 0.00 C

ATOM 5 C MOL -0.655 1.278 0.204 1.00 0.00 C

ATOM 6 O MOL 2.640 0.615 -1.299 1.00 0.00 O

ATOM 7 O MOL 2.356 -1.262 -2.683 1.00 0.00 O

ATOM 8 C MOL 1.046 -1.205 1.567 1.00 0.00 C

ATOM 9 C MOL -1.341 2.584 0.431 1.00 0.00 C

ATOM 10 O MOL -1.199 -1.910 -1.387 1.00 0.00 O

ATOM 11 H MOL -2.366 0.139 -0.247 1.00 0.00 H

ATOM 12 H MOL 0.716 -2.710 -0.025 1.00 0.00 H

ATOM 13 H MOL 0.434 1.282 0.286 1.00 0.00 H

ATOM 14 H MOL 2.052 -0.807 1.358 1.00 0.00 H

ATOM 15 H MOL 1.178 -2.006 2.308 1.00 0.00 H

ATOM 16 H MOL 0.468 -0.396 2.032 1.00 0.00 H

ATOM 17 H MOL -1.114 2.977 1.433 1.00 0.00 H

ATOM 18 H MOL -2.430 2.497 0.331 1.00 0.00 H

ATOM 19 H MOL -0.984 3.341 -0.283 1.00 0.00 H

ATOM 20 H MOL -1.759 -1.315 -1.917 1.00 0.00 H

XYZ coordinates for 4c*

ATOM 1 C MOL -1.330 0.071 -0.181 1.00 0.00 C

ATOM 2 C MOL -0.627 -1.087 -0.535 1.00 0.00 C

ATOM 3 C MOL 0.797 -1.282 -0.347 1.00 0.00 C

ATOM 4 C MOL 1.649 0.011 -1.037 1.00 0.00 C

ATOM 5 C MOL -0.706 1.101 0.491 1.00 0.00 C

ATOM 6 O MOL 1.237 1.162 -0.733 1.00 0.00 O1-

ATOM 7 O MOL 2.605 -0.400 -1.695 1.00 0.00 O

ATOM 8 C MOL 1.358 -1.448 1.073 1.00 0.00 C

ATOM 9 C MOL -1.204 2.494 0.504 1.00 0.00 C

ATOM 10 O MOL -1.208 -2.003 -1.343 1.00 0.00 O1+

ATOM 11 H MOL -2.284 0.267 -0.679 1.00 0.00 H

ATOM 12 H MOL 1.104 -2.141 -0.949 1.00 0.00 H

ATOM 13 H MOL 0.102 0.885 1.178 1.00 0.00 H

ATOM 14 H MOL 2.443 -1.578 1.004 1.00 0.00 H

ATOM 15 H MOL 0.931 -2.343 1.544 1.00 0.00 H

ATOM 16 H MOL 1.166 -0.594 1.729 1.00 0.00 H

ATOM 17 H MOL -1.459 2.810 1.527 1.00 0.00 H

ATOM 18 H MOL -2.070 2.642 -0.150 1.00 0.00 H

ATOM 19 H MOL -0.389 3.150 0.168 1.00 0.00 H

ATOM 20 H MOL -2.114 -1.716 -1.566 1.00 0.00 H

XYZ coordinates for 4c[**]**

ATOM 1 C MOL -1.319 0.066 -0.228 1.00 0.00 C

ATOM 2 C MOL -0.623 -1.146 -0.379 1.00 0.00 C

ATOM 3 C MOL 0.800 -1.321 -0.167 1.00 0.00 C

ATOM 4 C MOL 1.631 -0.195 -1.131 1.00 0.00 C

ATOM 5 C MOL -0.715 1.163 0.331 1.00 0.00 C

ATOM 6 O MOL 1.320 1.007 -0.951 1.00 0.00 O1-

ATOM 7 O MOL 2.474 -0.754 -1.840 1.00 0.00 O

ATOM 8 C MOL 1.384 -1.230 1.252 1.00 0.00 C

ATOM 9 C MOL -1.208 2.551 0.219 1.00 0.00 C

ATOM 10 O MOL -1.214 -2.187 -0.992 1.00 0.00 O1+

ATOM 11 H MOL -2.269 0.185 -0.755 1.00 0.00 H

ATOM 12 H MOL 1.082 -2.289 -0.591 1.00 0.00 H

ATOM 13 H MOL 0.117 1.021 1.006 1.00 0.00 H

ATOM 14 H MOL 2.459 -1.439 1.201 1.00 0.00 H

ATOM 15 H MOL 0.917 -1.991 1.891 1.00 0.00 H

ATOM 16 H MOL 1.257 -0.256 1.731 1.00 0.00 H

ATOM 17 H MOL -1.708 2.844 1.157 1.00 0.00 H

ATOM 18 H MOL -1.903 2.695 -0.614 1.00 0.00 H

ATOM 19 H MOL -0.354 3.231 0.101 1.00 0.00 H

ATOM 20 H MOL -2.128 -1.954 -1.240 1.00 0.00 H

XYZ coordinates for 5a

ATOM 1 C MOL -1.976 0.097 -0.089 1.00 0.00 C

ATOM 2 C MOL -1.173 -1.161 -0.188 1.00 0.00 C

ATOM 3 C MOL 0.135 -1.162 0.078 1.00 0.00 C

ATOM 4 C MOL 0.864 0.081 0.475 1.00 0.00 C

ATOM 5 C MOL -1.164 1.371 -0.173 1.00 0.00 C

ATOM 6 O MOL 0.174 1.311 0.057 1.00 0.00 O

ATOM 7 O MOL -1.658 2.447 -0.451 1.00 0.00 O

ATOM 8 C MOL 2.265 0.172 -0.105 1.00 0.00 C

ATOM 9 H MOL -2.525 0.131 0.867 1.00 0.00 H

ATOM 10 H MOL -2.748 0.158 -0.866 1.00 0.00 H

ATOM 11 H MOL -1.689 -2.078 -0.471 1.00 0.00 H

ATOM 12 H MOL 0.725 -2.077 0.034 1.00 0.00 H

ATOM 13 H MOL 0.925 0.139 1.574 1.00 0.00 H

ATOM 14 H MOL 2.231 0.129 -1.200 1.00 0.00 H

ATOM 15 H MOL 2.872 -0.666 0.261 1.00 0.00 H

ATOM 16 H MOL 2.743 1.108 0.200 1.00 0.00 H

XYZ coordinates for TS_{5a}

TOM 1 C MOL -1.875 0.170 0.290 1.00 0.00 C

ATOM 2 C MOL -1.182 -1.052 -0.030 1.00 0.00 C

ATOM 3 C MOL 0.200 -1.177 -0.016 1.00 0.00 C

ATOM 4 C MOL 1.011 -0.139 0.415 1.00 0.00 C

ATOM 5 C MOL -1.456 1.407 -0.736 1.00 0.00 C

ATOM 6 C MOL 2.456 -0.072 0.150 1.00 0.00 C

ATOM 7 O MOL -2.440 2.041 -1.160 1.00 0.00 O1-

ATOM 8 O MOL -0.224 1.570 -0.902 1.00 0.00 O

ATOM 9 H MOL -1.562 0.617 1.244 1.00 0.00 H

ATOM 10 H MOL -2.959 0.074 0.248 1.00 0.00 H

ATOM 11 H MOL -1.760 -1.867 -0.465 1.00 0.00 H

ATOM 12 H MOL 0.661 -2.046 -0.488 1.00 0.00 H

ATOM 13 H MOL 0.604 0.609 1.094 1.00 0.00 H

ATOM 14 H MOL 2.774 -0.754 -0.644 1.00 0.00 H

ATOM 15 H MOL 2.990 -0.336 1.080 1.00 0.00 H

ATOM 16 H MOL 2.763 0.957 -0.080 1.00 0.00 H

XYZ coordinates for 5c

ATOM 1 C MOL -1.942 -0.149 0.176 1.00 0.00 C

ATOM 2 C MOL -1.239 -1.117 -0.440 1.00 0.00 C

ATOM 3 C MOL 0.199 -1.371 -0.359 1.00 0.00 C

ATOM 4 C MOL 1.112 -0.685 0.355 1.00 0.00 C

ATOM 5 C MOL -1.550 3.634 -0.398 1.00 0.00 C

ATOM 6 O MOL -0.521 3.103 -0.200 1.00 0.00 O

ATOM 7 O MOL -2.578 4.168 -0.593 1.00 0.00 O

ATOM 8 C MOL 2.569 -1.002 0.399 1.00 0.00 C

ATOM 9 H MOL -1.472 0.583 0.833 1.00 0.00 H

ATOM 10 H MOL -3.019 -0.069 0.040 1.00 0.00 H

ATOM 11 H MOL -1.790 -1.812 -1.078 1.00 0.00 H

ATOM 12 H MOL 0.556 -2.218 -0.953 1.00 0.00 H

ATOM 13 H MOL 0.788 0.170 0.955 1.00 0.00 H

ATOM 14 H MOL 2.813 -1.881 -0.211 1.00 0.00 H

ATOM 15 H MOL 2.900 -1.198 1.431 1.00 0.00 H

ATOM 16 H MOL 3.175 -0.155 0.041 1.00 0.00 H

XYZ coordinates for TS_{5a}^{*}

ATOM 1 C MOL -0.611 -1.907 -0.371 1.00 0.00 C

ATOM 2 C MOL 0.942 -1.619 0.268 1.00 0.00 C

ATOM 3 C MOL 1.514 -0.475 -0.377 1.00 0.00 C

ATOM 4 C MOL 0.904 0.772 -0.335 1.00 0.00 C

ATOM 5 C MOL -0.246 0.949 0.425 1.00 0.00 C

ATOM 6 O MOL -1.363 -0.904 -0.304 1.00 0.00 O1-

ATOM 7 O MOL -0.757 -3.069 -0.745 1.00 0.00 O

ATOM 8 C MOL -1.215 2.045 0.224 1.00 0.00 C

ATOM 9 H MOL 1.502 -2.546 0.145 1.00 0.00 H

ATOM 10 H MOL 0.654 -1.464 1.315 1.00 0.00 H

ATOM 11 H MOL 2.324 -0.632 -1.091 1.00 0.00 H

ATOM 12 H MOL 1.193 1.538 -1.056 1.00 0.00 H

ATOM 13 H MOL -0.375 0.359 1.331 1.00 0.00 H

ATOM 14 H MOL -2.218 1.610 0.108 1.00 0.00 H

ATOM 15 H MOL -0.987 2.656 -0.656 1.00 0.00 H

ATOM 16 H MOL -1.261 2.686 1.117 1.00 0.00 H

XYZ coordinates for TS_{5a}**

ATOM 1 C MOL -1.858 0.033 0.363 1.00 0.00 C

ATOM 2 C MOL -1.182 -1.134 -0.112 1.00 0.00 C

ATOM 3 C MOL 0.204 -1.218 -0.126 1.00 0.00 C

ATOM 4 C MOL 0.953 -0.180 0.417 1.00 0.00 C

ATOM 5 C MOL -1.343 1.391 -0.566 1.00 0.00 C

ATOM 6 C MOL 2.371 0.084 0.091 1.00 0.00 C

ATOM 7 O MOL -2.288 2.023 -1.018 1.00 0.00 O1-

ATOM 8 O MOL -0.094 1.522 -0.567 1.00 0.00 O

ATOM 9 H MOL -1.532 0.400 1.344 1.00 0.00 H

ATOM 10 H MOL -2.945 0.010 0.288 1.00 0.00 H

ATOM 11 H MOL -1.753 -1.868 -0.682 1.00 0.00 H

ATOM 12 H MOL 0.696 -1.962 -0.754 1.00 0.00 H

ATOM 13 H MOL 0.555 0.362 1.273 1.00 0.00 H

ATOM 14 H MOL 2.745 -0.563 -0.709 1.00 0.00 H

ATOM 15 H MOL 3.005 -0.032 0.983 1.00 0.00 H

ATOM 16 H MOL 2.467 1.132 -0.226 1.00 0.00 H

XYZ coordinates for 6a

ATOM 1 C MOL 1 -1.801 0.580 0.168 1.00 0.00 C

ATOM 2 C MOL 1 -1.136 -0.760 0.035 1.00 0.00 C

ATOM 3 C MOL 1 0.198 -0.830 -0.020 1.00 0.00 C

ATOM 4 C MOL 1 1.101 0.366 0.015 1.00 0.00 C

ATOM 5 C MOL 1 -0.919 1.698 0.659 1.00 0.00 C

ATOM 6 C MOL 1 1.532 0.783 -1.391 1.00 0.00 C

ATOM 7 C MOL 1 2.304 0.128 0.922 1.00 0.00 C

ATOM 8 C MOL 1 -2.036 -1.954 -0.039 1.00 0.00 C

ATOM 9 O MOL 1 0.420 1.555 0.615 1.00 0.00 O

ATOM 10 O MOL 1 -1.374 2.742 1.114 1.00 0.00 O

ATOM 11 H MOL 1 -2.666 0.534 0.843 1.00 0.00 H

ATOM 12 H MOL 1 -2.214 0.900 -0.804 1.00 0.00 H

ATOM 13 H MOL 1 0.702 -1.791 -0.137 1.00 0.00 H

ATOM 14 H MOL 1 0.658 1.018 -2.011 1.00 0.00 H

ATOM 15 H MOL 1 2.080 -0.040 -1.867 1.00 0.00 H

ATOM 16 H MOL 1 2.190 1.659 -1.346 1.00 0.00 H

ATOM 17 H MOL 1 2.900 -0.703 0.525 1.00 0.00 H

ATOM 18 H MOL 1 1.980 -0.130 1.937 1.00 0.00 H

ATOM 19 H MOL 1 2.937 1.022 0.961 1.00 0.00 H

ATOM 20 H MOL 1 -1.466 -2.882 -0.161 1.00 0.00 H

ATOM 21 H MOL 1 -2.734 -1.860 -0.885 1.00 0.00 H

ATOM 22 H MOL 1 -2.655 -2.035 0.867 1.00 0.00 H

XYZ coordinates for TS_{6a}

ATOM 1 C MOL -1.705 0.436 0.445 1.00 0.00 C

ATOM 2 C MOL -1.063 -0.725 -0.153 1.00 0.00 C

ATOM 3 C MOL 0.312 -0.807 -0.373 1.00 0.00 C

ATOM 4 C MOL 1.334 -0.020 0.151 1.00 0.00 C

ATOM 5 C MOL -1.383 1.833 -0.360 1.00 0.00 C

ATOM 6 O MOL -0.182 2.046 -0.627 1.00 0.00 O1-

ATOM 7 O MOL -2.407 2.531 -0.542 1.00 0.00 O

ATOM 8 C MOL -1.938 -1.764 -0.771 1.00 0.00 C

ATOM 9 C MOL 2.624 0.025 -0.586 1.00 0.00 C

ATOM 10 C MOL 1.349 0.607 1.498 1.00 0.00 C

ATOM 11 H MOL -1.318 0.700 1.435 1.00 0.00 H

ATOM 12 H MOL -2.791 0.330 0.500 1.00 0.00 H

ATOM 13 H MOL 0.614 -1.502 -1.160 1.00 0.00 H

ATOM 14 H MOL -1.358 -2.547 -1.269 1.00 0.00 H

ATOM 15 H MOL -2.631 -1.308 -1.493 1.00 0.00 H

ATOM 16 H MOL -2.570 -2.227 0.002 1.00 0.00 H

ATOM 17 H MOL 2.521 -0.303 -1.625 1.00 0.00 H

ATOM 18 H MOL 3.360 -0.625 -0.086 1.00 0.00 H

ATOM 19 H MOL 3.043 1.040 -0.552 1.00 0.00 H

ATOM 20 H MOL 2.112 0.078 2.093 1.00 0.00 H

ATOM 21 H MOL 0.404 0.548 2.037 1.00 0.00 H

ATOM 22 H MOL 1.676 1.652 1.437 1.00 0.00 H

XYZ coordinates for 6b

ATOM 1 C MOL -1.817 -0.201 -1.163 1.00 0.00 C

ATOM 2 C MOL -1.296 -0.921 -0.149 1.00 0.00 C

ATOM 3 C MOL 0.009 -0.646 0.471 1.00 0.00 C

ATOM 4 C MOL 1.173 -0.271 -0.109 1.00 0.00 C

ATOM 5 C MOL -0.466 3.921 1.355 1.00 0.00 C

ATOM 6 C MOL 1.375 -0.085 -1.585 1.00 0.00 C

ATOM 7 C MOL 2.391 -0.019 0.734 1.00 0.00 C

ATOM 8 C MOL -2.069 -2.056 0.476 1.00 0.00 C

ATOM 9 O MOL 0.508 3.395 0.964 1.00 0.00 O

ATOM 10 O MOL -1.442 4.446 1.746 1.00 0.00 O

ATOM 11 H MOL -2.795 -0.447 -1.580 1.00 0.00 H

ATOM 12 H MOL -1.302 0.662 -1.582 1.00 0.00 H

ATOM 13 H MOL 0.036 -0.816 1.553 1.00 0.00 H

ATOM 14 H MOL 0.580 -0.552 -2.177 1.00 0.00 H

ATOM 15 H MOL 2.345 -0.502 -1.892 1.00 0.00 H

ATOM 16 H MOL 1.398 0.985 -1.847 1.00 0.00 H

ATOM 17 H MOL 3.228 -0.661 0.421 1.00 0.00 H

ATOM 18 H MOL 2.195 -0.191 1.800 1.00 0.00 H

ATOM 19 H MOL 2.734 1.020 0.611 1.00 0.00 H

ATOM 20 H MOL -2.232 -1.866 1.548 1.00 0.00 H

ATOM 21 H MOL -1.509 -3.001 0.409 1.00 0.00 H

ATOM 22 H MOL -3.045 -2.194 -0.002 1.00 0.00 H

XYZ coordinates for TS_{6a}^{*}

ATOM 1 C MOL -1.604 0.569 -0.492 1.00 0.00 C

ATOM 2 C MOL -1.126 -0.708 -0.007 1.00 0.00 C

ATOM 3 C MOL 0.226 -0.947 0.221 1.00 0.00 C

ATOM 4 C MOL 1.286 -0.102 -0.131 1.00 0.00 C

ATOM 5 C MOL -1.094 1.816 0.515 1.00 0.00 C

ATOM 6 C MOL 1.455 0.561 -1.459 1.00 0.00 C

ATOM 7 C MOL 2.494 -0.079 0.739 1.00 0.00 C

ATOM 8 C MOL -2.137 -1.662 0.545 1.00 0.00 C

ATOM 9 O MOL 0.143 1.825 0.719 1.00 0.00 O1-

ATOM 10 O MOL -2.022 2.560 0.848 1.00 0.00 O

ATOM 11 H MOL -2.692 0.636 -0.542 1.00 0.00 H

ATOM 12 H MOL -1.162 0.912 -1.431 1.00 0.00 H

ATOM 13 H MOL 0.459 -1.731 0.946 1.00 0.00 H

ATOM 14 H MOL 0.579 0.495 -2.106 1.00 0.00 H

ATOM 15 H MOL 2.287 0.049 -1.969 1.00 0.00 H

ATOM 16 H16 MOL 1 1.750 1.610 -1.342 1.00 0.00 H

ATOM 17 H17 MOL 1 3.417 -0.238 0.163 1.00 0.00 H

ATOM 18 H18 MOL 1 2.437 -0.799 1.561 1.00 0.00 H

ATOM 19 H19 MOL 1 2.560 0.930 1.174 1.00 0.00 H

ATOM 20 H20 MOL 1 -1.673 -2.540 1.009 1.00 0.00 H

ATOM 21 H21 MOL 1 -2.814 -1.999 -0.253 1.00 0.00 H

ATOM 22 H22 MOL 1 -2.770 -1.159 1.291 1.00 0.00 H

XYZ coordinates for TS_{6a}[**]**

ATOM 1 C MOL -1.716 0.289 -0.282 1.00 0.00 C

ATOM 2 C MOL -0.927 -0.919 -0.290 1.00 0.00 C

ATOM 3 C MOL 0.459 -0.884 -0.149 1.00 0.00 C

ATOM 4 C MOL 1.244 0.275 -0.143 1.00 0.00 C

ATOM 5 C MOL -1.402 1.180 1.137 1.00 0.00 C

ATOM 6 C MOL 1.161 1.374 -1.155 1.00 0.00 C

ATOM 7 C MOL 2.467 0.302 0.710 1.00 0.00 C

ATOM 8 C MOL -1.647 -2.221 -0.120 1.00 0.00 C

ATOM 9 O MOL -0.181 1.414 1.306 1.00 0.00 O1-

ATOM 10 O MOL -2.436 1.489 1.722 1.00 0.00 O

ATOM 11 H MOL -2.793 0.117 -0.296 1.00 0.00 H

ATOM 12 H MOL -1.438 1.051 -1.013 1.00 0.00 H

ATOM 13 H MOL 0.923 -1.785 0.259 1.00 0.00 H

ATOM 14 H MOL 0.289 1.307 -1.808 1.00 0.00 H

ATOM 15 H MOL 2.056 1.297 -1.792 1.00 0.00 H

ATOM 16 H MOL 1.187 2.358 -0.674 1.00 0.00 H

ATOM 17 H MOL 3.366 0.551 0.128 1.00 0.00 H

ATOM 18 H MOL 2.624 -0.636 1.252 1.00 0.00 H

ATOM 19 H MOL 2.328 1.105 1.449 1.00 0.00 H

ATOM 20 H MOL -0.961 -3.061 0.038 1.00 0.00 H

ATOM 21 H MOL -2.260 -2.433 -1.008 1.00 0.00 H

ATOM 22 H MOL -2.343 -2.166 0.730 1.00 0.00 H