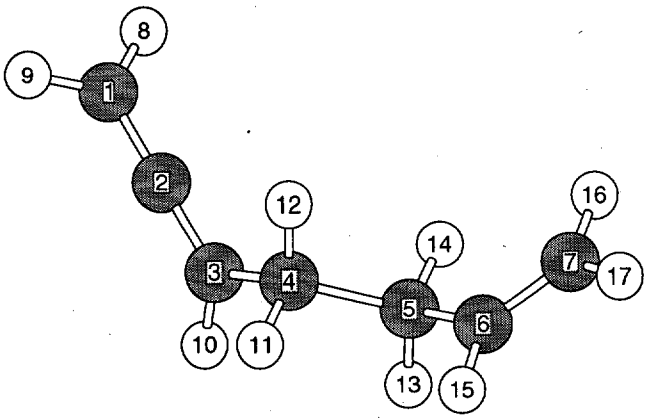
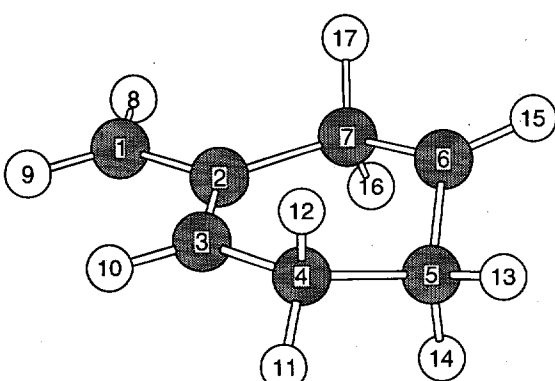
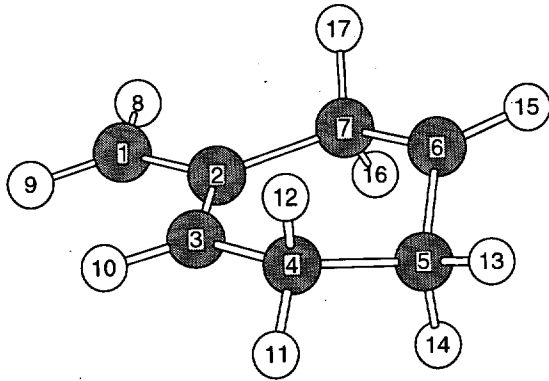
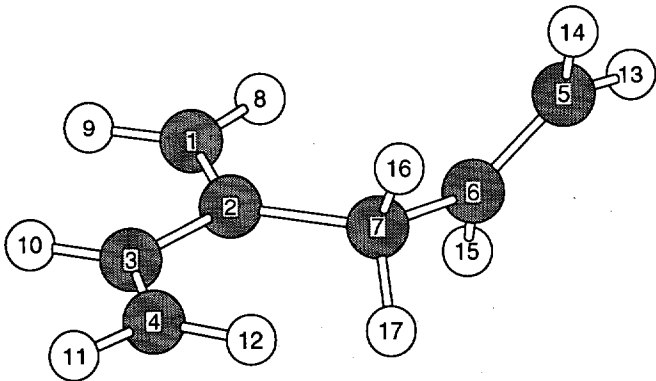
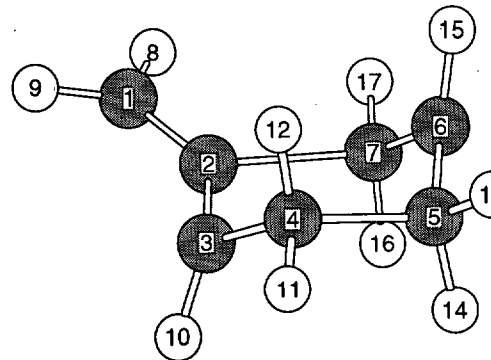


1,2,6-Heptatriene ¹ A (8/8)CASSCF/6-31G* C ₁ Geometry (1)									
Nuclear Repulsion		254.382328		CASSCF/6-31G*		-270.908615			
ZPE(kcal/mol)		96.14		CASPT2N/6-31G*		-271.738770			
C _v @ 298 (eu)		29.15							
S @ 298 (eu)		91.33							
					X	Y	Z		
				C1	3.456522	-0.821955	0.067086		
				C2	2.415895	-0.024978	-0.054737		
				C3	1.371970	0.769362	-0.168239		
				C4	0.040299	0.534257	0.502243		
				C5	-1.118611	0.349534	-0.533676		
				C6	-2.458645	0.190118	0.132103		
				C7	-3.238581	-0.894311	0.037461		
				H8	3.612725	-1.644036	-0.608846		
				H9	4.185029	-0.674892	0.844740		
				H10	1.461217	1.645708	-0.791449		
				H11	-0.195876	1.381558	1.142423		
				H12	0.092967	-0.342461	1.138064		
				H13	-1.137327	1.217298	-1.190469		
				H14	-0.902484	-0.514156	-1.154811		
				H15	-2.791615	1.020991	0.735457		
				H16	-2.950971	-1.749539	-0.549969		
				H17	-4.186763	-0.952638	0.541417		
(1-2)	1.316	(1-8)	1.076	(1-9)	1.076				
(2-3)	1.317	(3-4)	1.509	(3-10)	1.079				
(4-5)	1.565	(4-11)	1.088	(4-12)	1.084				
(5-6)	1.505	(5-13)	1.088	(5-14)	1.086				
(6-7)	1.339	(6-15)	1.079	(7-16)	1.077				
(7-17)	1.075	(2-1-8)	121.3	(2-1-9)	121.3				
(8-1-9)	117.4	(1-2-3)	179.6	(2-3-4)	124.6				
(2-3-10)	118.3	(4-3-10)	117.1	(3-4-5)	112.2				
(3-4-11)	109.4	(3-4-12)	110.1	(5-4-11)	108.7				
(5-4-12)	109.2	(11-4-12)	107.2	(4-5-6)	112.3				
(4-5-13)	108.5	(4-5-14)	109.0	(6-5-13)	109.6				
(6-5-14)	110.3	(13-5-14)	107.0	(5-6-7)	125.0				
(5-6-15)	116.1	(7-6-15)	118.9	(6-7-16)	121.8				
(6-7-17)	121.6	(16-7-17)	116.6	(8-1-2-3)	116.6				
(9-1-2-3)	-63.6	(1-2-3-4)	-27.0	(1-2-3-10)	153.8				
(2-3-4-5)	-118.1	(2-3-4-11)	121.3	(2-3-4-12)	3.8				
(10-3-4-5)	61.2	(10-3-4-11)	-59.5	(10-3-4-12)	-177.0				
(3-4-5-6)	-176.9	(3-4-5-13)	-55.5	(3-4-5-14)	60.7				
(11-4-5-6)	-55.8	(11-4-5-13)	65.6	(11-4-5-14)	-178.2				
(12-4-5-6)	60.8	(12-4-5-13)	-177.8	(12-4-5-14)	-61.6				
(4-5-6-7)	-118.0	(4-5-6-15)	61.3	(13-5-6-7)	121.2				
(13-5-6-15)	-59.5	(14-5-6-7)	3.7	(14-5-6-15)	-177.0				
(5-6-7-16)	-.6	(5-6-7-17)	179.7	(15-6-7-16)	-179.9				
(15-6-7-17)	0.4								
Frequencies(cm ⁻¹):		49.9	79.3	99.1	155.5	206.6	241.5	346.9	443.6
		500.6	575.0	644.6	808.4	821.2	873.1	898.7	967.3
		1047.4	1081.0	1101.6	1197.1	1223.9	1319.9	1381.4	1401.9
		1517.5	1584.4	1621.0	1628.4	1640.2	1792.1	2099.9	3190.2
		3262.3	3311.6	3317.6	3321.9	3325.8	3401.0	3402.8	

2-Methylenecyclohexane-1,4-diyl ¹ A (8/8)CASSCF/6-31G* Geometry (2)									
Nuclear Repulsion		284.402612		CASSCF/6-31G*		-270.869900			
ZPE(kcal/mol)		97.49		CASPT2N/6-31G*		-271.717459			
C _v @ 298 (eu)		26.03							
S @ 298 (eu)		79.69							
				X		Y		Z	
				C1	2.474699	-0.131994	0.069987		
				C2	1.079889	-0.078901	-0.000474		
				C3	0.304853	-1.229805	-0.054347		
				C4	-1.195987	-1.255389	-0.145784		
				C5	-1.836575	0.097529	0.302085		
				C6	-1.066314	1.251646	-0.264538		
				C7	0.407005	1.319093	-0.002504		
				H8	3.067649	0.762341	0.122476		
				H9	2.998062	-1.070305	0.069577		
				H10	0.810998	-2.180665	-0.055396		
				H11	-1.589803	-2.066820	0.460932		
				H12	-1.499244	-1.464065	-1.170120		
				H13	-2.875289	0.132684	-0.009582		
				H14	-1.832436	0.140365	1.392417		
				H15	-1.581961	2.178476	-0.449363		
				H16	0.603755	1.793496	0.961415		
				H17	0.892852	1.941418	-0.748899		
				(1-2)	1.398	(1-8)	1.074	(1-9)	1.074
(2-3)	1.389	(2-7)	1.552	(3-4)	1.504				
(3-10)	1.077	(4-5)	1.562	(4-11)	1.087				
(4-12)	1.088	(5-6)	1.499	(5-13)	1.085				
(5-14)	1.091	(6-7)	1.498	(6-15)	1.077				
(7-16)	1.092	(7-17)	1.086	(2-1-8)	121.4				
(2-1-9)	121.3	(8-1-9)	117.3	(1-2-3)	121.8				
(1-2-7)	117.8	(3-2-7)	120.3	(2-3-4)	125.0				
(2-3-10)	118.0	(4-3-10)	117.0	(3-4-5)	112.1				
(3-4-11)	109.9	(3-4-12)	109.8	(5-4-11)	109.7				
(5-4-12)	108.8	(11-4-12)	106.3	(4-5-6)	110.3				
(4-5-13)	109.8	(4-5-14)	108.6	(6-5-13)	111.0				
(6-5-14)	110.2	(13-5-14)	106.8	(5-6-7)	118.3				
(5-6-15)	118.8	(7-6-15)	117.5	(2-7-6)	112.7				
(2-7-16)	108.2	(2-7-17)	108.8	(6-7-16)	110.6				
(6-7-17)	110.2	(16-7-17)	106.1	(8-1-2-3)	-179.3				
(8-1-2-7)	0.1	(9-1-2-3)	1.0	(9-1-2-7)	-179.7				
(1-2-3-4)	-179.3	(1-2-3-10)	-0.9	(7-2-3-4)	1.3				
(7-2-3-10)	179.7	(1-2-7-6)	172.3	(1-2-7-16)	-65.1				
(1-2-7-17)	49.7	(3-2-7-6)	-8.3	(3-2-7-16)	114.3				
(3-2-7-17)	-130.9	(2-3-4-5)	-19.3	(2-3-4-11)	-141.6				
(2-3-4-12)	101.7	(10-3-4-5)	162.3	(10-3-4-11)	39.9				
(10-3-4-12)	-76.7	(3-4-5-6)	43.1	(3-4-5-13)	165.7				
(3-4-5-14)	-77.8	(11-4-5-6)	165.5	(11-4-5-13)	-71.8				
(11-4-5-14)	44.6	(12-4-5-6)	-78.5	(12-4-5-13)	44.1				
(12-4-5-14)	160.6	(4-5-6-7)	-54.5	(4-5-6-15)	151.9				
(13-5-6-7)	-176.5	(13-5-6-15)	30.0	(14-5-6-7)	65.4				
(14-5-6-15)	-88.1	(5-6-7-2)	36.3	(5-6-7-16)	-84.9				
(5-6-7-17)	158.1	(15-6-7-2)	-169.8	(15-6-7-16)	68.9				
(15-6-7-17)	-48.0								
(bond)-(plane) angle		(10-3)-(2-3-4)	1.4						
(bond)-(plane) angle		(15-6)-(5-6-7)	23.0						
Frequencies(cm ⁻¹):									
125.0	195.8	277.2	375.0	445.2	457.8	503.4	576.2		
601.2	689.9	712.5	762.7	821.8	889.3	953.4	975.9	1019.7	1049.5
1113.7	1170.1	1191.3	1245.5	1267.7	1311.8	1346.1	1435.3	1450.9	1493.8
1499.1	1523.2	1571.3	1620.4	1629.9	1640.1	1644.0	3145.2	3157.9	3185.7
3220.0	3221.9	3243.7	3330.4	3339.9	3343.4	3423.7			

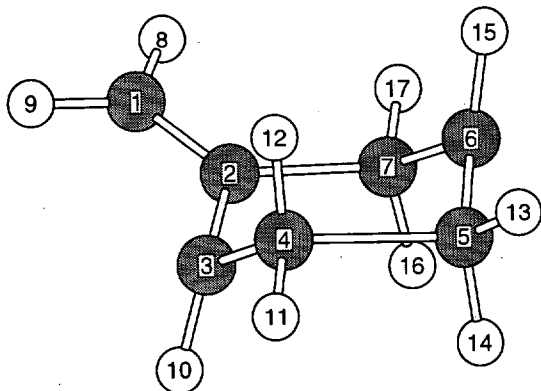
2-Methylenecyclohexane-1,4-diyl ³ A (8/8)CASSCF/6-31G* Geometry (2)									
Nuclear Repulsion		284.323252		CASSCF/6-31G*		-270.868536			
ZPE(kcal/mol)		97.44		CASPT2N/6-31G*		-271.715088			
C _v @ 298 (eu)		26.04							
S @ 298 (eu)		81.91							
				X		Y		Z	
				C1	2.475500	-0.119985	0.086545		
				C2	1.080376	-0.074377	-0.002449		
				C3	0.314385	-1.231664	-0.049387		
				C4	-1.185186	-1.255041	-0.168741		
				C5	-1.829138	0.078888	0.321704		
				C6	-1.089338	1.252791	-0.246718		
				C7	0.395866	1.320440	-0.036199		
				H8	3.065396	0.777133	0.125119		
				H9	3.000552	-1.056564	0.122090		
				H10	0.824850	-2.179962	-0.051847		
				H11	-1.590177	-2.087345	0.400288		
				H12	-1.469387	-1.424314	-1.206716		
				H13	-2.877300	0.106642	0.042285		
				H14	-1.790443	0.102925	1.412684		
				H15	-1.611927	2.187601	-0.359208		
				H16	0.615975	1.829294	0.903866		
				H17	0.857666	1.918275	-0.817086		
(1-2)	1.399	(1-8)	1.074	(1-9)	1.074				
(2-3)	1.389	(2-7)	1.554	(3-4)	1.504				
(3-10)	1.077	(4-5)	1.560	(4-11)	1.087				
(4-12)	1.089	(5-6)	1.499	(5-13)	1.085				
(5-14)	1.092	(6-7)	1.502	(6-15)	1.077				
(7-16)	1.091	(7-17)	1.086	(2-1-8)	121.5				
(2-1-9)	121.2	(8-1-9)	117.3	(1-2-3)	121.7				
(1-2-7)	118.0	(3-2-7)	120.3	(2-3-4)	124.4				
(2-3-10)	118.2	(4-3-10)	117.3	(3-4-5)	111.9				
(3-4-11)	110.0	(3-4-12)	109.8	(5-4-11)	109.7				
(5-4-12)	108.9	(11-4-12)	106.4	(4-5-6)	110.3				
(4-5-13)	109.9	(4-5-14)	108.6	(6-5-13)	111.0				
(6-5-14)	110.1	(13-5-14)	106.9	(5-6-7)	118.0				
(5-6-15)	118.7	(7-6-15)	117.1	(2-7-6)	113.5				
(2-7-16)	108.1	(2-7-17)	108.8	(6-7-16)	110.0				
(6-7-17)	110.1	(16-7-17)	106.1	(8-1-2-3)	-179.8				
(8-1-2-7)	-0.4	(9-1-2-3)	0.0	(9-1-2-7)	179.5				
(1-2-3-4)	-178.9	(1-2-3-10)	-2.2	(7-2-3-4)	1.6				
(7-2-3-10)	178.3	(1-2-7-6)	175.2	(1-2-7-16)	-62.5				
(1-2-7-17)	52.2	(3-2-7-6)	-5.3	(3-2-7-16)	117.0				
(3-2-7-17)	-128.3	(2-3-4-5)	-22.6	(2-3-4-11)	-144.8				
(2-3-4-12)	98.5	(10-3-4-5)	160.7	(10-3-4-11)	38.5				
(10-3-4-12)	-78.2	(3-4-5-6)	46.1	(3-4-5-13)	168.8				
(3-4-5-14)	-74.6	(11-4-5-6)	168.5	(11-4-5-13)	-68.8				
(11-4-5-14)	47.7	(12-4-5-6)	-75.4	(12-4-5-13)	47.3				
(12-4-5-14)	163.9	(4-5-6-7)	-53.8	(4-5-6-15)	154.6				
(13-5-6-7)	-175.8	(13-5-6-15)	32.6	(14-5-6-7)	65.9				
(14-5-6-15)	-85.6	(5-6-7-2)	32.8	(5-6-7-16)	-88.5				
(5-6-7-17)	155.0	(15-6-7-2)	-175.2	(15-6-7-16)	63.6				
(15-6-7-17)	-53.0								
(bond)-(plane) angle	(10-3)-(2-3-4)	2.9							
(bond)-(plane) angle	(15-6)-(5-6-7)	24.7							
Frequencies(cm ⁻¹):									
117.8	196.0	287.7	376.4	453.3	457.7	509.9	575.9		
603.3	684.6	706.4	756.6	814.8	889.2	951.5	973.5	1016.0	1049.4
1111.5	1167.3	1188.2	1237.4	1267.5	1312.0	1344.6	1440.0	1453.0	1494.4
1499.1	1521.4	1565.6	1618.9	1627.0	1637.0	1642.4	3150.5	3156.1	3178.5
3223.0	3224.7	3242.7	3330.6	3339.5	3342.5	3424.1			

3-Methylenehexa-1,5-diene 1A (8/8)CASSCF/6-31G* Geometry									
Nuclear Repulsion		267.273951		CASSCF/6-31G*		-270.933533			
ZPE(kcal/mol)		96.86		CASPT2N/6-31G*		-271.761542			
C _v @ 298 (eu)		28.36							
S @ 298 (eu)		86.67							
					X	Y	Z		
				C1	0.197972	1.804771	-0.074232		
				C2	0.578468	0.516236	0.008414		
				C3	2.011463	0.173084	-0.061184		
				C4	2.543728	-1.061418	-0.050462		
				C5	-2.898020	-0.437769	-0.362518		
				C6	-1.850949	-0.222870	0.443829		
				C7	-0.438479	-0.645451	0.146708		
				H8	-0.832449	2.103514	-0.049493		
				H9	0.924603	2.590838	-0.180678		
				H10	2.681256	1.013881	-0.139520		
				H11	3.607494	-1.201173	-0.114302		
				H12	1.949590	-1.954017	0.017318		
				H13	-3.891371	-0.129050	-0.089822		
				H14	-2.789954	-0.931143	-1.313262		
				H15	-2.009257	0.278460	1.385409		
				H16	-0.412288	-1.235301	-0.765230		
				H17	-0.092719	-1.295505	0.946257		
(1-2)	1.346	(1-8)	1.073	(1-9)	1.076				
(2-3)	1.475	(2-7)	1.550	(3-4)	1.344				
(3-10)	1.078	(4-11)	1.075	(4-12)	1.074				
(5-6)	1.339	(5-13)	1.075	(5-14)	1.077				
(6-7)	1.504	(6-15)	1.078	(7-16)	1.086				
(7-17)	1.087	(2-1-8)	122.4	(2-1-9)	121.0				
(8-1-9)	116.6	(1-2-3)	119.6	(1-2-7)	122.5				
(3-2-7)	117.9	(2-3-4)	126.7	(2-3-10)	115.2				
(4-3-10)	118.1	(3-4-11)	120.7	(3-4-12)	123.0				
(11-4-12)	116.3	(6-5-13)	121.6	(6-5-14)	121.8				
(13-5-14)	116.6	(5-6-7)	124.8	(5-6-15)	119.1				
(7-6-15)	116.2	(2-7-6)	115.0	(2-7-16)	108.4				
(2-7-17)	107.8	(6-7-16)	109.9	(6-7-17)	108.8				
(16-7-17)	106.6	(8-1-2-3)	178.7	(8-1-2-7)	0.0				
(9-1-2-3)	-0.6	(9-1-2-7)	-179.3	(1-2-3-4)	-177.0				
(1-2-3-10)	2.3	(7-2-3-4)	1.8	(7-2-3-10)	-179.0				
(1-2-7-6)	-11.1	(1-2-7-16)	112.4	(1-2-7-17)	-132.6				
(3-2-7-6)	170.2	(3-2-7-16)	-66.3	(3-2-7-17)	48.7				
(2-3-4-11)	179.5	(2-3-4-12)	-0.3	(10-3-4-11)	0.2				
(10-3-4-12)	-179.5	(13-5-6-7)	178.8	(13-5-6-15)	-0.5				
(14-5-6-7)	-0.9	(14-5-6-15)	179.8	(5-6-7-2)	117.0				
(5-6-7-16)	-5.7	(5-6-7-17)	-122.0	(15-6-7-2)	-63.7				
(15-6-7-16)	173.6	(15-6-7-17)	57.3						
Frequencies (cm ⁻¹):		69.1	93.1	141.5	222.0	308.7	390.8	436.5	469.2
		564.6	627.0	648.9	789.4	852.3	864.4	877.4	882.4
		984.5	993.2	1033.5	1051.6	1052.7	1145.0	1212.4	1357.9
		1364.0	1416.5	1423.8	1470.3	1527.9	1583.5	1598.0	1633.2
		1743.3	1788.6	1792.9	3200.5	3235.8	3319.2	3326.6	3331.3
		3338.7	3344.6	3403.9	3418.4	3424.0			

Hepta-1,2,6-triene Cope T.S. ¹ A (8/8)CASSCF/6-31G* Geometry (TS ₁ →2)													
Nuclear Repulsion		282.612112		CASSCF/6-31G*		-270.844255							
ZPE(kcal/mol)		96.91		CASPT2N/6-31G*		-271.697480							
C _v @ 298 (eu)		25.25											
S @ 298 (eu)		78.93											
					X	Y	Z						
				C1	2.428440	-0.085290	-0.293243						
				C2	1.157297	-0.228258	0.091545						
				C3	0.270451	-1.281946	0.363547						
				C4	-1.059182	-1.265521	-0.279165						
				C5	-1.849802	0.143325	0.067757						
				C6	-0.982262	1.265952	-0.323071						
				C7	0.227791	1.423771	0.389610						
				H8	2.915731	0.872309	-0.311088						
				H9	3.008693	-0.931234	-0.616030						
				H10	0.355460	-1.763941	1.324978						
				H11	-1.682340	-2.088754	0.050850						
				H12	-0.989762	-1.301767	-1.359551						
				H13	-2.790941	0.122179	-0.468636						
				H14	-2.059148	0.132929	1.131116						
				H15	-0.997071	1.561669	-1.359944						
				H16	0.167600	1.386541	1.465374						
				H17	0.915385	2.177872	0.041051						
(1-2)	1.336	(1-8)	1.075	(1-9)	1.075								
(2-3)	1.404	(2-7)	1.919	(3-4)	1.477								
(3-10)	1.079	(4-5)	1.652	(4-11)	1.084								
(4-12)	1.083	(5-6)	1.472	(5-13)	1.083								
(5-14)	1.084	(6-7)	1.413	(6-15)	1.078								
(7-16)	1.078	(7-17)	1.078	(2-1-8)	122.1								
(2-1-9)	121.0	(8-1-9)	116.8	(1-2-3)	137.5								
(1-2-7)	114.4	(3-2-7)	108.1	(2-3-4)	118.4								
(2-3-10)	117.3	(4-3-10)	117.6	(3-4-5)	110.4								
(3-4-11)	112.1	(3-4-12)	112.1	(5-4-11)	108.0								
(5-4-12)	105.6	(11-4-12)	108.4	(4-5-6)	108.2								
(4-5-13)	107.2	(4-5-14)	106.9	(6-5-13)	113.3								
(6-5-14)	112.4	(13-5-14)	108.5	(5-6-7)	117.1								
(5-6-15)	117.2	(7-6-15)	117.8	(2-7-6)	103.9								
(2-7-16)	98.8	(2-7-17)	104.1	(6-7-16)	116.8								
(6-7-17)	117.5	(16-7-17)	112.5	(8-1-2-3)	-172.0								
(8-1-2-7)	7.3	(9-1-2-3)	9.0	(9-1-2-7)	-171.7								
(1-2-3-4)	-129.7	(1-2-3-10)	79.6	(7-2-3-4)	51.0								
(7-2-3-10)	-99.7	(1-2-7-6)	131.2	(1-2-7-16)	-108.2								
(1-2-7-17)	7.7	(3-2-7-6)	-49.3	(3-2-7-16)	71.3								
(3-2-7-17)	-172.8	(2-3-4-5)	-55.8	(2-3-4-11)	-176.3								
(2-3-4-12)	61.6	(10-3-4-5)	94.8	(10-3-4-11)	-25.6								
(10-3-4-12)	-147.8	(3-4-5-6)	54.6	(3-4-5-13)	177.1								
(3-4-5-14)	-66.7	(11-4-5-6)	177.5	(11-4-5-13)	-60.0								
(11-4-5-14)	56.2	(12-4-5-6)	-66.8	(12-4-5-13)	55.7								
(12-4-5-14)	171.9	(4-5-6-7)	-65.5	(4-5-6-15)	82.9								
(13-5-6-7)	175.9	(13-5-6-15)	-35.8	(14-5-6-7)	52.4								
(14-5-6-15)	-159.3	(5-6-7-2)	59.4	(5-6-7-16)	-48.1								
(5-6-7-17)	173.7	(15-6-7-2)	-88.8	(15-6-7-16)	163.7								
(15-6-7-17)	25.5												
(bond)-(plane) angle		(10-3)-(2-3-4)	25.8										
(bond)-(plane) angle		(15-6)-(5-6-7)	27.8										
Frequencies(cm ⁻¹):													
723.6i	122.2	241.9	309.6	372.8	424.4	451.9	506.9						
611.5	651.8	715.3	789.3	824.4	880.7	885.0	952.4	1013.6	1039.4				
1063.5	1102.3	1147.4	1213.6	1239.9	1259.8	1310.7	1346.8	1377.4	1430.3				
1482.5	1549.3	1609.7	1647.0	1651.9	1665.8	1827.6	3232.8	3237.7	3276.3				
3284.2	3294.7	3317.8	3324.4	3329.6	3366.6	3408.5							

3-Methylenehexa-1,5-diene Cope T.S. ¹A (8/8)CASSCF/6-31G* Geometry (TS₂→3)

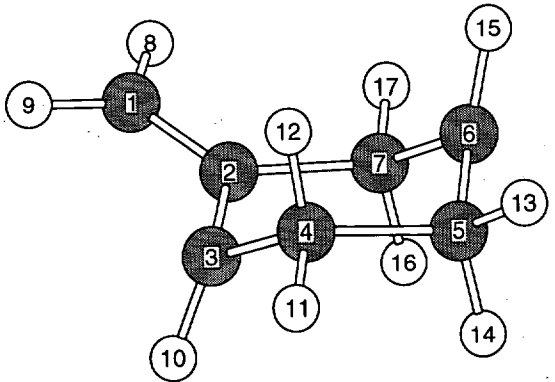
Nuclear Repulsion	284.364175	CASSCF/6-31G*	-270.850654
ZPE(kcal/mol)	96.98	CASPT2N/6-31G*	-271.702709
C _v @ 298 (eu)	24.91		
S @ 298 (eu)	78.58		

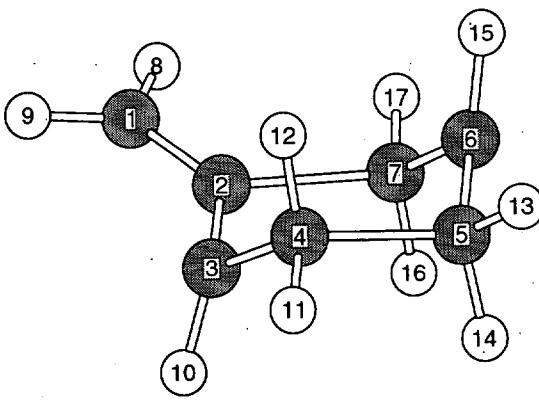


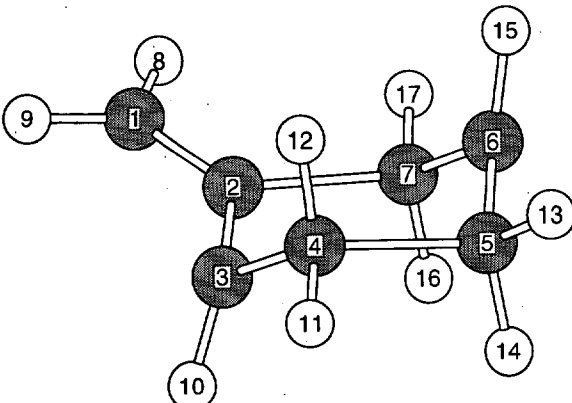
	X	Y	Z
C1	-2.369975	0.105316	-0.311209
C2	-1.096222	0.101705	0.105373
C3	-0.256934	1.272540	0.375071
C4	1.008770	1.338345	-0.296861
C5	1.884976	-0.240213	0.073995
C6	0.973171	-1.275176	-0.308454
C7	-0.336207	-1.291741	0.384750
H8	-2.921931	-0.807707	-0.449688
H9	-2.890850	1.021987	-0.521142
H10	-0.329133	1.707721	1.359835
H11	1.667263	2.134901	0.021549
H12	0.963115	1.279571	-1.373293
H13	2.808229	-0.185978	-0.485295
H14	2.066121	-0.147886	1.134588
H15	0.983404	-1.595474	-1.338071
H16	-0.215757	-1.371058	1.460681
H17	-0.975941	-2.100729	0.054847

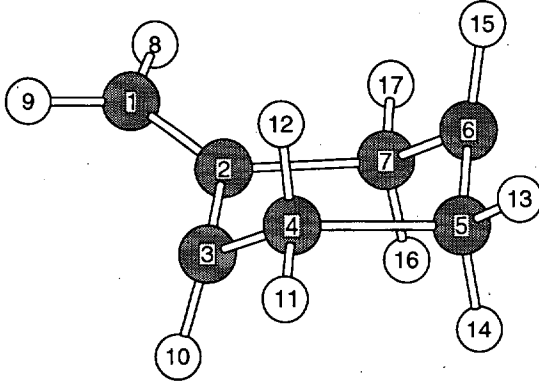
(1-2)	1.340	(1-8)	1.076	(1-9)	1.075
(2-3)	1.466	(2-7)	1.612	(3-4)	1.435
(3-10)	1.079	(4-5)	1.843	(4-11)	1.081
(4-12)	1.079	(5-6)	1.431	(5-13)	1.081
(5-14)	1.080	(6-7)	1.482	(6-15)	1.078
(7-16)	1.086	(7-17)	1.083	(2-1-8)	121.7
(2-1-9)	121.6	(8-1-9)	116.7	(1-2-3)	126.8
(1-2-7)	120.3	(3-2-7)	112.9	(2-3-4)	117.1
(2-3-10)	116.9	(4-3-10)	117.9	(3-4-5)	106.6
(3-4-11)	115.7	(3-4-12)	115.3	(5-4-11)	106.4
(5-4-12)	100.0	(11-4-12)	111.1	(4-5-6)	105.2
(4-5-13)	105.0	(4-5-14)	101.8	(6-5-13)	116.2
(6-5-14)	115.5	(13-5-14)	111.1	(5-6-7)	116.5
(5-6-15)	117.6	(7-6-15)	116.9	(2-7-6)	109.0
(2-7-16)	106.7	(2-7-17)	108.3	(6-7-16)	111.5
(6-7-17)	112.8	(16-7-17)	108.2	(8-1-2-3)	-177.7
(8-1-2-7)	1.3	(9-1-2-3)	2.1	(9-1-2-7)	-178.9
(1-2-3-4)	-126.1	(1-2-3-10)	85.8	(7-2-3-4)	54.8
(7-2-3-10)	-93.2	(1-2-7-6)	130.5	(1-2-7-16)	-109.0
(1-2-7-17)	7.4	(3-2-7-6)	-50.4	(3-2-7-16)	70.2
(3-2-7-17)	-173.5	(2-3-4-5)	-53.7	(2-3-4-11)	-171.7
(2-3-4-12)	56.3	(10-3-4-5)	94.0	(10-3-4-11)	-24.0
(10-3-4-12)	-155.9	(3-4-5-6)	53.9	(3-4-5-13)	177.1
(3-4-5-14)	-67.0	(11-4-5-6)	177.8	(11-4-5-13)	-59.0
(11-4-5-14)	57.0	(12-4-5-6)	-66.5	(12-4-5-13)	56.7
(12-4-5-14)	172.6	(4-5-6-7)	-59.9	(4-5-6-15)	86.3
(13-5-6-7)	-175.6	(13-5-6-15)	-29.4	(14-5-6-7)	51.5
(14-5-6-15)	-162.3	(5-6-7-2)	59.9	(5-6-7-16)	-57.6
(5-6-7-17)	-179.7	(15-6-7-2)	-86.5	(15-6-7-16)	156.0
(15-6-7-17)	33.9				
(bond)-(plane) angle		(10-3)-(2-3-4)	28.2		
(bond)-(plane) angle		(15-6)-(5-6-7)	29.6		

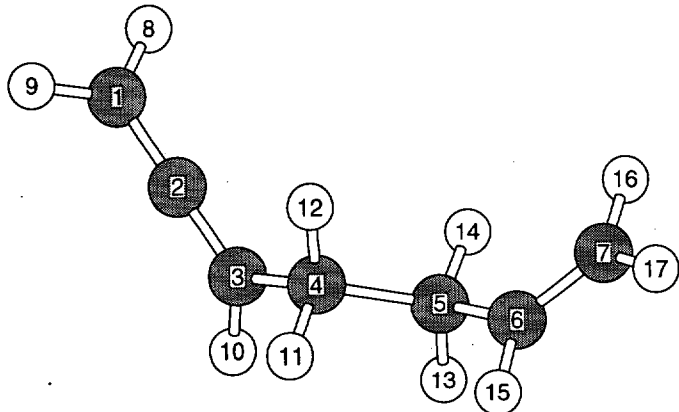
Frequencies(cm ⁻¹):	686.4i	110.9	241.6	345.8	413.6	420.5	460.9	509.5
	622.8	698.5	760.6	771.5	849.9	894.5	898.4	941.0
	998.5	1020.8	1054.8	1137.6	1176.7	1181.6	1246.8	1272.3
	1286.1	1328.5	1363.8	1388.1	1489.1	1540.7	1590.3	1638.1
	1652.6	1660.3	1787.3	3219.5	3268.9	3275.0	3279.0	3311.3
	3319.1	3328.2	3335.2	3342.4	3407.1			

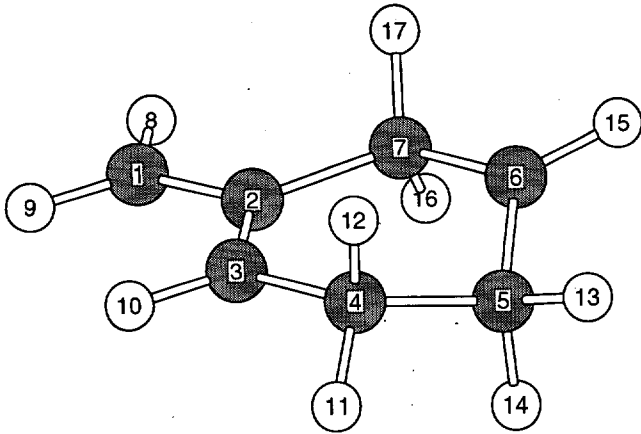
TS ₁ → ₂ to TS ₂ → ₃ Midpoint 1A (8/8)CASSCF/6-31G* Geometry (∠10-3-2-1 fixed)						
Nuclear Repulsion		285.342795	CASSCF/6-31G*		-270.854536	
			CASPT2N/6-31G*		-271.702836	
			X	Y	Z	
			C1	-0.028248	-0.006318	0.028322
			C2	-0.092975	0.029345	1.367723
			C3	1.065934	0.000092	2.273427
			C4	1.020996	-0.986060	3.387904
			C5	-0.392873	-0.886708	4.172285
			C6	-1.502447	-0.976760	3.190621
			C7	-1.493996	0.056390	2.117183
			H8	-0.914317	0.029174	-0.580893
			H9	0.912948	-0.059671	-0.488802
			H10	1.592479	0.925343	2.442565
			H11	1.831768	-0.837617	4.092994
			H12	1.091163	-2.001116	3.009866
			H13	-0.431690	-1.675441	4.915422
			H14	-0.406457	0.065451	4.694201
			H15	-1.854363	-1.960813	2.926352
			H16	-1.610410	1.050163	2.542191
			H17	-2.287114	-0.091912	1.394374
(1-2)	1.341	(1-8)	1.076	(1-9)	1.075	
(2-3)	1.471	(2-7)	1.589	(3-4)	1.489	
(3-10)	1.078	(4-5)	1.620	(4-11)	1.085	
(4-12)	1.085	(5-6)	1.484	(5-13)	1.084	
(5-14)	1.086	(6-7)	1.490	(6-15)	1.078	
(7-16)	1.087	(7-17)	1.083	(2-1-8)	121.7	
(2-1-9)	121.6	(8-1-9)	116.8	(1-2-3)	125.2	
(1-2-7)	120.9	(3-2-7)	113.9	(2-3-4)	116.8	
(2-3-10)	117.7	(4-3-10)	117.8	(3-4-5)	110.4	
(3-4-11)	111.9	(3-4-12)	110.9	(5-4-11)	109.2	
(5-4-12)	106.4	(11-4-12)	107.8	(4-5-6)	109.2	
(4-5-13)	108.6	(4-5-14)	107.3	(6-5-13)	112.5	
(6-5-14)	111.2	(13-5-14)	107.9	(5-6-7)	115.5	
(5-6-15)	117.5	(7-6-15)	117.3	(2-7-6)	109.5	
(2-7-16)	107.1	(2-7-17)	109.2	(6-7-16)	110.6	
(6-7-17)	112.4	(16-7-17)	107.9	(8-1-2-3)	-179.3	
(8-1-2-7)	2.9	(9-1-2-3)	-0.1	(9-1-2-7)	-177.8	
(1-2-3-4)	-130.3	(1-2-3-10)	81.1	(7-2-3-4)	47.6	
(7-2-3-10)	-101.0	(1-2-7-6)	130.9	(1-2-7-16)	-109.1	
(1-2-7-17)	7.5	(3-2-7-6)	-47.0	(3-2-7-16)	72.9	
(3-2-7-17)	-170.5	(2-3-4-5)	-49.2	(2-3-4-11)	-171.0	
(2-3-4-12)	68.5	(10-3-4-5)	99.4	(10-3-4-11)	-22.5	
(10-3-4-12)	-142.9	(3-4-5-6)	51.9	(3-4-5-13)	174.8	
(3-4-5-14)	-68.8	(11-4-5-6)	175.3	(11-4-5-13)	-61.7	
(11-4-5-14)	54.7	(12-4-5-6)	-68.5	(12-4-5-13)	54.4	
(12-4-5-14)	170.8	(4-5-6-7)	-57.9	(4-5-6-15)	87.2	
(13-5-6-7)	-178.5	(13-5-6-15)	-33.4	(14-5-6-7)	60.3	
(14-5-6-15)	-154.6	(5-6-7-2)	54.9	(5-6-7-16)	-62.9	
(5-6-7-17)	176.4	(15-6-7-2)	-90.3	(15-6-7-16)	151.9	
(15-6-7-17)	31.2					
(bond)-(plane) angle		(10-3)-(2-3-4)	27.5			
(bond)-(plane) angle		(15-6)-(5-6-7)	30.5			

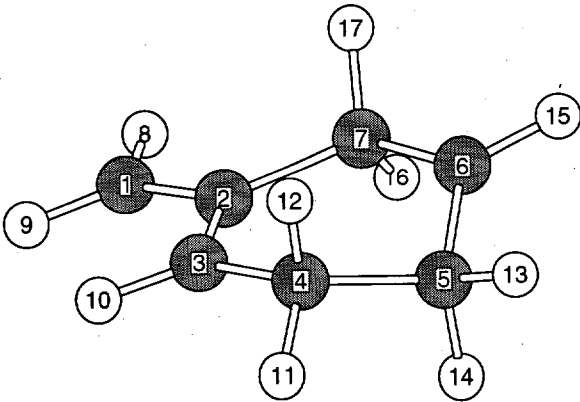
TS ₁ → ₂ to TS ₂ → ₃ (LST Point #1) ¹ A (8/8)CASSCF/6-31G* Geometry						
Nuclear Repulsion		282.336590	CASSCF/6-31G*		-270.845757	
			CASPT2N/6-31G*		-271.697588	
			X	Y	Z	
			C1	0.010264	0.009025	-0.004926
			C2	-0.007850	-0.003390	1.332222
			C3	1.026570	-0.008349	2.320822
			C4	0.948968	-1.017795	3.381206
			C5	-0.567558	-0.913088	4.162203
			C6	-1.604643	-1.027219	3.138378
			C7	-1.644915	0.013610	2.140019
			H8	-0.891439	0.090776	-0.584378
			H9	0.932694	-0.069986	-0.552087
			H10	1.480578	0.939684	2.563643
			H11	1.713223	-0.897527	4.139346
			H12	0.982982	-2.030451	3.001112
			H13	-0.587991	-1.705625	4.899550
			H14	-0.570432	0.044627	4.667573
			H15	-1.885373	-2.021444	2.829558
			H16	-1.693582	1.018572	2.534397
			H17	-2.362445	-0.125037	1.344956
(1-2)	1.337	(1-8)	1.075	(1-9)	1.075	
(2-3)	1.431	(2-7)	1.826	(3-4)	1.466	
(3-10)	1.079	(4-5)	1.709	(4-11)	1.083	
(4-12)	1.082	(5-6)	1.462	(5-13)	1.083	
(5-14)	1.083	(6-7)	1.443	(6-15)	1.078	
(7-16)	1.081	(7-17)	1.080	(2-1-8)	121.9	
(2-1-9)	121.3	(8-1-9)	116.8	(1-2-3)	132.9	
(1-2-7)	117.0	(3-2-7)	110.0	(2-3-4)	117.6	
(2-3-10)	117.2	(4-3-10)	117.7	(3-4-5)	109.6	
(3-4-11)	113.1	(3-4-12)	112.9	(5-4-11)	107.4	
(5-4-12)	104.2	(11-4-12)	109.1	(4-5-6)	107.7	
(4-5-13)	106.4	(4-5-14)	105.7	(6-5-13)	114.0	
(6-5-14)	113.2	(13-5-14)	109.2	(5-6-7)	116.6	
(5-6-15)	117.2	(7-6-15)	117.4	(2-7-6)	105.9	
(2-7-16)	102.2	(2-7-17)	105.6	(6-7-16)	114.8	
(6-7-17)	115.8	(16-7-17)	111.0	(8-1-2-3)	-175.0	
(8-1-2-7)	3.9	(9-1-2-3)	5.5	(9-1-2-7)	-175.6	
(1-2-3-4)	-129.7	(1-2-3-10)	81.2	(7-2-3-4)	51.3	
(7-2-3-10)	-97.8	(1-2-7-6)	132.0	(1-2-7-16)	-107.5	
(1-2-7-17)	8.7	(3-2-7-6)	-48.8	(3-2-7-16)	71.7	
(3-2-7-17)	-172.2	(2-3-4-5)	-54.8	(2-3-4-11)	-174.6	
(2-3-4-12)	60.9	(10-3-4-5)	94.2	(10-3-4-11)	-25.6	
(10-3-4-12)	-150.1	(3-4-5-6)	54.8	(3-4-5-13)	177.4	
(3-4-5-14)	-66.5	(11-4-5-6)	178.0	(11-4-5-13)	-59.3	
(11-4-5-14)	56.7	(12-4-5-6)	-66.3	(12-4-5-13)	56.4	
(12-4-5-14)	172.5	(4-5-6-7)	-63.2	(4-5-6-15)	83.5	
(13-5-6-7)	178.9	(13-5-6-15)	-34.4	(14-5-6-7)	53.2	
(14-5-6-15)	-160.0	(5-6-7-2)	58.5	(5-6-7-16)	-53.4	
(5-6-7-17)	175.2	(15-6-7-2)	-88.1	(15-6-7-16)	160.0	
(15-6-7-17)	28.5					
(bond)-(plane) angle		(10-3)-(2-3-4)	27.2			
(bond)-(plane) angle		(15-6)-(5-6-7)	29.2			

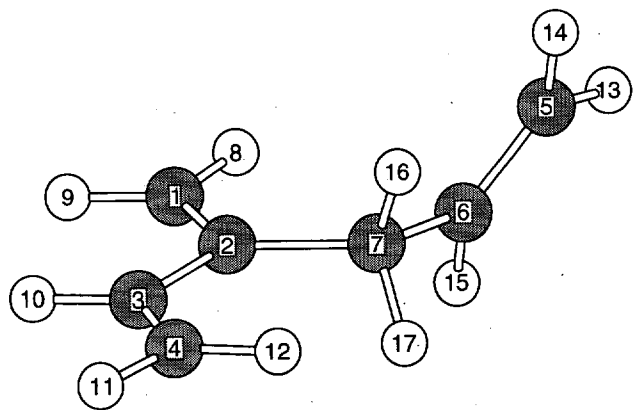
TS ₁ → ₂ to TS ₂ → ₃ (LST Point #2) 1A (8/8)CASSCF/6-31G* Geometry						
Nuclear Repulsion		282.514400	CASSCF/6-31G*		-270.847617	
			CASPT2N/6-31G*		-271.698786	
			X	Y	Z	
			C1	0.010226	0.018646	-0.005651
			C2	-0.008128	-0.005640	1.332290
			C3	1.073406	-0.014175	2.288170
			C4	1.036406	-1.026880	3.337612
			C5	-0.497073	-0.924659	4.168413
			C6	-1.539803	-1.036010	3.159824
			C7	-1.574697	0.007243	2.143128
			H8	-0.893694	0.087333	-0.583790
			H9	0.933409	-0.035036	-0.554502
			H10	1.532449	0.934032	2.520206
			H11	1.812690	-0.910657	4.083334
			H12	1.045409	-2.039801	2.958965
			H13	-0.494184	-1.720761	4.901403
			H14	-0.476117	0.033987	4.670032
			H15	-1.831218	-2.029066	2.857309
			H16	-1.645283	1.007929	2.549029
			H17	-2.319058	-0.134707	1.372507
(1-2)	1.338	(1-8)	1.075	(1-9)	1.075	
(2-3)	1.443	(2-7)	1.764	(3-4)	1.459	
(3-10)	1.079	(4-5)	1.747	(4-11)	1.083	
(4-12)	1.081	(5-6)	1.455	(5-13)	1.082	
(5-14)	1.082	(6-7)	1.457	(6-15)	1.078	
(7-16)	1.082	(7-17)	1.081	(2-1-8)	121.8	
(2-1-9)	121.4	(8-1-9)	116.8	(1-2-3)	130.7	
(1-2-7)	118.1	(3-2-7)	111.2	(2-3-4)	117.5	
(2-3-10)	117.1	(4-3-10)	117.8	(3-4-5)	108.9	
(3-4-11)	113.8	(3-4-12)	113.5	(5-4-11)	107.2	
(5-4-12)	103.2	(11-4-12)	109.6	(4-5-6)	107.2	
(4-5-13)	106.1	(4-5-14)	104.8	(6-5-13)	114.5	
(6-5-14)	113.8	(13-5-14)	109.7	(5-6-7)	116.5	
(5-6-15)	117.3	(7-6-15)	117.2	(2-7-6)	107.1	
(2-7-16)	103.7	(2-7-17)	106.4	(6-7-16)	113.7	
(6-7-17)	114.8	(16-7-17)	110.1	(8-1-2-3)	-175.9	
(8-1-2-7)	2.6	(9-1-2-3)	4.4	(9-1-2-7)	-177.0	
(1-2-3-4)	-129.9	(1-2-3-10)	81.1	(7-2-3-4)	51.5	
(7-2-3-10)	-97.5	(1-2-7-6)	132.7	(1-2-7-16)	-106.8	
(1-2-7-17)	9.4	(3-2-7-6)	-48.5	(3-2-7-16)	72.0	
(3-2-7-17)	-171.8	(2-3-4-5)	-54.1	(2-3-4-11)	-173.5	
(2-3-4-12)	60.3	(10-3-4-5)	94.7	(10-3-4-11)	-24.7	
(10-3-4-12)	-151.0	(3-4-5-6)	54.7	(3-4-5-13)	177.4	
(3-4-5-14)	-66.5	(11-4-5-6)	178.1	(11-4-5-13)	-59.1	
(11-4-5-14)	57.0	(12-4-5-6)	-66.2	(12-4-5-13)	56.6	
(12-4-5-14)	172.7	(4-5-6-7)	-62.1	(4-5-6-15)	84.2	
(13-5-6-7)	-179.4	(13-5-6-15)	-33.1	(14-5-6-7)	53.2	
(14-5-6-15)	-160.4	(5-6-7-2)	58.4	(5-6-7-16)	-55.6	
(5-6-7-17)	176.3	(15-6-7-2)	-88.0	(15-6-7-16)	158.1	
(15-6-7-17)	30.0					
(bond)-(plane) angle		(10-3)-(2-3-4)	27.3			
(bond)-(plane) angle		(15-6)-(5-6-7)	29.5			

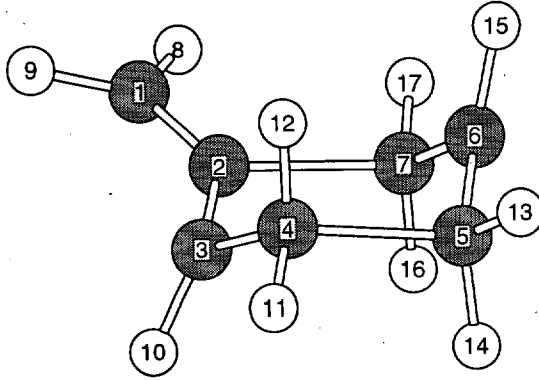
TS ₁ → ₂ to TS ₂ → ₃ (LST Point #3) ¹ A (8/8)CASSCF/6-31G* Geometry						
Nuclear Repulsion		283.046431	CASSCF/6-31G*		-270.849367	
			CASPT2N/6-31G*		-271.700475	
			X	Y	Z	
			C1	0.007199	0.015142	-0.004319
			C2	-0.005447	-0.004466	1.334474
			C3	1.116085	-0.011126	2.258926
			C4	1.122061	-1.031129	3.290114
			C5	-0.428773	-0.938152	4.169656
			C6	-1.472295	-1.040380	3.172532
			C7	-1.501769	0.010177	2.147221
			H8	-0.900583	0.070316	-0.578291
			H9	0.928200	-0.025066	-0.557757
			H10	1.567173	0.941318	2.489517
			H11	1.908165	-0.920382	4.025581
			H12	1.106921	-2.042721	2.910527
			H13	-0.403432	-1.742253	4.892605
			H14	-0.382782	0.018474	4.671781
			H15	-1.774588	-2.030092	2.869659
			H16	-1.582570	1.005027	2.568927
			H17	-2.272533	-0.125806	1.400695
(1-2)	1.339	(1-8)	1.075	(1-9)	1.075	
(2-3)	1.453	(2-7)	1.703	(3-4)	1.450	
(3-10)	1.079	(4-5)	1.785	(4-11)	1.082	
(4-12)	1.081	(5-6)	1.447	(5-13)	1.082	
(5-14)	1.081	(6-7)	1.468	(6-15)	1.078	
(7-16)	1.084	(7-17)	1.082	(2-1-8)	121.8	
(2-1-9)	121.5	(8-1-9)	116.8	(1-2-3)	129.0	
(1-2-7)	119.0	(3-2-7)	112.0	(2-3-4)	117.3	
(2-3-10)	117.0	(4-3-10)	117.9	(3-4-5)	108.1	
(3-4-11)	114.5	(3-4-12)	114.1	(5-4-11)	106.9	
(5-4-12)	102.1	(11-4-12)	110.2	(4-5-6)	106.5	
(4-5-13)	105.7	(4-5-14)	103.8	(6-5-13)	115.1	
(6-5-14)	114.4	(13-5-14)	110.3	(5-6-7)	116.4	
(5-6-15)	117.4	(7-6-15)	117.1	(2-7-6)	108.0	
(2-7-16)	105.0	(2-7-17)	107.2	(6-7-16)	112.7	
(6-7-17)	114.0	(16-7-17)	109.3	(8-1-2-3)	-176.7	
(8-1-2-7)	1.9	(9-1-2-3)	3.4	(9-1-2-7)	-178.0	
(1-2-3-4)	-128.8	(1-2-3-10)	82.6	(7-2-3-4)	52.5	
(7-2-3-10)	-96.1	(1-2-7-6)	132.2	(1-2-7-16)	-107.3	
(1-2-7-17)	8.9	(3-2-7-6)	-49.0	(3-2-7-16)	71.6	
(3-2-7-17)	-172.2	(2-3-4-5)	-53.8	(2-3-4-11)	-172.7	
(2-3-4-12)	59.0	(10-3-4-5)	94.6	(10-3-4-11)	-24.4	
(10-3-4-12)	-152.6	(3-4-5-6)	54.4	(3-4-5-13)	177.3	
(3-4-5-14)	-66.7	(11-4-5-6)	178.1	(11-4-5-13)	-59.0	
(11-4-5-14)	57.0	(12-4-5-6)	-66.2	(12-4-5-13)	56.7	
(12-4-5-14)	172.7	(4-5-6-7)	-61.1	(4-5-6-15)	85.1	
(13-5-6-7)	-177.8	(13-5-6-15)	-31.7	(14-5-6-7)	52.9	
(14-5-6-15)	-160.9	(5-6-7-2)	58.7	(5-6-7-16)	-56.9	
(5-6-7-17)	177.7	(15-6-7-2)	-87.5	(15-6-7-16)	156.9	
(15-6-7-17)	31.5					
(bond)-(plane) angle		(10-3)-(2-3-4)	27.6			
(bond)-(plane) angle		(15-6)-(5-6-7)	29.6			

1,2,6-Heptatriene ¹ A (RHF)Becke3-LYP/6-31G* Geometry (1)									
Nuclear Repulsion		254.546764		(RHF)Becke3-LYP/6-31G*		-272.680319			
ZPE(kcal/mol)		92.13							
C _v @ 298 (eu)		29.16							
S @ 298 (eu)		89.72							
					X	Y	Z		
				C1	3.455252	-0.806944	0.072774		
				C2	2.415546	-0.024019	-0.055036		
				C3	1.372782	0.758378	-0.172547		
				C4	0.034792	0.524641	0.494741		
				C5	-1.108468	0.330822	-0.528583		
				C6	-2.453377	0.191619	0.130630		
				C7	-3.248293	-0.875164	0.039779		
				H8	3.625938	-1.645740	-0.600130		
				H9	4.195021	-0.651955	0.856504		
				H10	1.451478	1.642012	-0.809969		
				H11	-0.204089	1.387541	1.134132		
				H12	0.092866	-0.350237	1.150687		
				H13	-1.118966	1.197269	-1.207677		
				H14	-0.898079	-0.550569	-1.146411		
				H15	-2.775021	1.041524	0.736083		
				H16	-2.969462	-1.746652	-0.549611		
H17	-4.209091	-0.919194	0.545843						
(1-2)	1.308	(1-8)	1.089	(1-9)	1.089				
(2-3)	1.309	(3-4)	1.513	(3-10)	1.092				
(4-5)	1.547	(4-11)	1.100	(4-12)	1.095				
(5-6)	1.504	(5-13)	1.101	(5-14)	1.097				
(6-7)	1.333	(6-15)	1.092	(7-16)	1.088				
(7-17)	1.087	(2-1-8)	121.7	(2-1-9)	121.7				
(8-1-9)	116.6	(1-2-3)	179.5	(2-3-4)	124.9				
(2-3-10)	118.6	(4-3-10)	116.5	(3-4-5)	112.4				
(3-4-11)	109.1	(3-4-12)	109.9	(5-4-11)	108.8				
(5-4-12)	109.6	(11-4-12)	106.9	(4-5-6)	112.5				
(4-5-13)	108.5	(4-5-14)	109.4	(6-5-13)	109.6				
(6-5-14)	110.1	(13-5-14)	106.7	(5-6-7)	125.3				
(5-6-15)	115.7	(7-6-15)	119.0	(6-7-16)	121.7				
(6-7-17)	121.8	(16-7-17)	116.5	(8-1-2-3)	130.0				
(9-1-2-3)	-50.1	(1-2-3-4)	-40.7	(1-2-3-10)	140.4				
(2-3-4-5)	-117.9	(2-3-4-11)	121.3	(2-3-4-12)	4.4				
(10-3-4-5)	61.0	(10-3-4-11)	-59.8	(10-3-4-12)	-176.7				
(3-4-5-6)	-176.1	(3-4-5-13)	-54.8	(3-4-5-14)	61.2				
(11-4-5-6)	-55.2	(11-4-5-13)	66.2	(11-4-5-14)	-177.9				
(12-4-5-6)	61.3	(12-4-5-13)	-177.3	(12-4-5-14)	-61.4				
(4-5-6-7)	-118.9	(4-5-6-15)	60.3	(13-5-6-7)	120.3				
(13-5-6-15)	-60.4	(14-5-6-7)	3.3	(14-5-6-15)	-177.5				
(5-6-7-16)	-.7	(5-6-7-17)	179.6	(15-6-7-16)	-179.9				
(15-6-7-17)	0.4								
Frequencies(cm-1):									
51.4	82.7	107.8	181.6	254.6	334.3	354.2	426.2		
559.9	593.8	658.0	794.1	868.1	900.6	929.7	940.4	953.0	1024.5
1035.1	1038.2	1056.2	1140.9	1161.6	1233.8	1285.8	1322.8	1340.6	1375.3
1403.1	1474.7	1506.7	1508.8	1522.8	1732.9	2074.7	3015.6	3023.1	3077.6
3101.1	3126.9	3133.8	3139.3	3155.4	3206.6	3233.8			

2-Methylenecyclohexane-1,4-diyl ¹ A (UHF) Becke3-LYP/6-31G* Geometry (2)									
Nuclear Repulsion		284.784462		(UHF) Becke3-LYP/6-31G*		-272.654022			
ZPE(kcal/mol)		91.73		S ² before annihilation		1.00			
C _v @ 298 (eu)		27.57		S ² after annihilation		0.25			
S @ 298 (eu)		81.81							
				X		Y		Z	
				C1	2.464382	-0.145583	0.092166		
				C2	1.078418	-0.079307	-0.002725		
				C3	0.292592	-1.224743	-0.058611		
				C4	-1.202936	-1.233316	-0.168000		
				C5	-1.834439	0.093326	0.310889		
				C6	-1.060442	1.268354	-0.185420		
				C7	0.425430	1.300291	-0.049025		
				H8	3.073970	0.751549	0.146375		
				H9	2.982500	-1.100041	0.113647		
				H10	0.797788	-2.189380	-0.033100		
				H11	-1.616159	-2.078143	0.400924		
				H12	-1.499872	-1.410543	-1.215053		
				H13	-2.882690	0.152090	-0.004823		
				H14	-1.848957	0.081899	1.416882		
				H15	-1.577264	2.186410	-0.452195		
				H16	0.724204	1.851911	0.864845		
				H17	0.868446	1.880118	-0.873139		
(1-2)	1.391	(1-8)	1.086	(1-9)	1.086				
(2-3)	1.390	(2-7)	1.527	(3-4)	1.500				
(3-10)	1.089	(4-5)	1.545	(4-11)	1.099				
(4-12)	1.103	(5-6)	1.492	(5-13)	1.096				
(5-14)	1.106	(6-7)	1.492	(6-15)	1.087				
(7-16)	1.108	(7-17)	1.101	(2-1-8)	121.6				
(2-1-9)	121.2	(8-1-9)	117.2	(1-2-3)	121.8				
(1-2-7)	118.1	(3-2-7)	120.1	(2-3-4)	124.8				
(2-3-10)	117.8	(4-3-10)	117.3	(3-4-5)	112.3				
(3-4-11)	110.0	(3-4-12)	109.8	(5-4-11)	110.2				
(5-4-12)	108.8	(11-4-12)	105.5	(4-5-6)	111.2				
(4-5-13)	110.3	(4-5-14)	107.8	(6-5-13)	111.0				
(6-5-14)	110.3	(13-5-14)	106.0	(5-6-7)	120.2				
(5-6-15)	120.0	(7-6-15)	118.5	(2-7-6)	114.2				
(2-7-16)	108.0	(2-7-17)	109.1	(6-7-16)	110.8				
(6-7-17)	110.1	(16-7-17)	104.3	(8-1-2-3)	-179.3				
(8-1-2-7)	0.8	(9-1-2-3)	0.8	(9-1-2-7)	-179.1				
(1-2-3-4)	-179.7	(1-2-3-10)	-0.4	(7-2-3-4)	0.1				
(7-2-3-10)	179.4	(1-2-7-6)	178.5	(1-2-7-16)	-57.8				
(1-2-7-17)	55.0	(3-2-7-6)	-1.3	(3-2-7-16)	122.4				
(3-2-7-17)	-124.9	(2-3-4-5)	-21.6	(2-3-4-11)	-144.7				
(2-3-4-12)	99.6	(10-3-4-5)	159.2	(10-3-4-11)	36.0				
(10-3-4-12)	-79.6	(3-4-5-6)	42.6	(3-4-5-13)	166.2				
(3-4-5-14)	-78.5	(11-4-5-6)	165.6	(11-4-5-13)	-70.8				
(11-4-5-14)	44.6	(12-4-5-6)	-79.2	(12-4-5-13)	44.4				
(12-4-5-14)	159.8	(4-5-6-7)	-47.8	(4-5-6-15)	145.2				
(13-5-6-7)	-171.0	(13-5-6-15)	22.0	(14-5-6-7)	71.8				
(14-5-6-15)	-95.2	(5-6-7-2)	26.5	(5-6-7-16)	-95.6				
(5-6-7-17)	149.6	(15-6-7-2)	-166.2	(15-6-7-16)	71.6				
(15-6-7-17)	-43.2								
(bond)-(plane) angle		(10-3)-(2-3-4)	0.7						
(bond)-(plane) angle		(15-6)-(5-6-7)	11.2						
Frequencies (cm ⁻¹):									
86.9	164.9	242.5	356.4	382.2	450.6				
547.1	669.3	725.6	767.8	798.0	876.3				
902.4	909.2	959.7	1005.8	1032.7	1109.5				
1132.7	1167.1	1205.7	1252.5	1262.8	1314.8				
1349.1	1386.3	1408.5	1422.3	1480.7	1493.8				
1506.7	1517.7	1536.2	2915.1	2942.6	2988.5				
3017.7	3039.6	3074.0	3158.2	3165.1	3187.5				
3251.0									

2-Methylenecyclohexane-1,4-diyl ³ A (UHF)Becke3-LYP/6-31G* Geometry (2)									
Nuclear Repulsion		284.758397		(UHF)Becke3-LYP/6-31G*		-272.652473			
ZPE(kcal/mol)		91.62		S ² before annihilation		2.03			
C _v @ 298 (eu)		27.67		S ² after annihilation		2.00			
S @ 298 (eu)		84.55							
				X		Y		Z	
				C1	2.462979	-0.133868	0.125111		
				C2	1.078787	-0.073232	-0.006516		
				C3	0.301977	-1.225462	-0.064360		
				C4	-1.193166	-1.229141	-0.197688		
				C5	-1.822675	0.071279	0.342870		
				C6	-1.082388	1.269047	-0.153254		
				C7	0.412979	1.299638	-0.102159		
				H8	3.070896	0.764851	0.171631		
				H9	2.980011	-1.087021	0.186380		
				H10	0.810719	-2.187907	-0.037539		
				H11	-1.614545	-2.099304	0.323449		
				H12	-1.473496	-1.352899	-1.258085		
				H13	-2.883700	0.124460	0.071612		
				H14	-1.789979	0.030353	1.448916		
				H15	-1.610993	2.200274	-0.338747		
				H16	0.753379	1.911831	0.754178		
				H17	0.806756	1.825791	-0.985809		
(1-2)		1.392	(1-8)		1.086	(1-9)		1.086	
(2-3)		1.391	(2-7)		1.529	(3-4)		1.501	
(3-10)		1.089	(4-5)		1.543	(4-11)		1.098	
(4-12)		1.104	(5-6)		1.493	(5-13)		1.096	
(5-14)		1.107	(6-7)		1.497	(6-15)		1.087	
(7-16)		1.106	(7-17)		1.101	(2-1-8)		121.6	
(2-1-9)		121.1	(8-1-9)		117.2	(1-2-3)		121.6	
(1-2-7)		118.6	(3-2-7)		119.9	(2-3-4)		124.2	
(2-3-10)		118.0	(4-3-10)		117.7	(3-4-5)		111.9	
(3-4-11)		110.0	(3-4-12)		109.8	(5-4-11)		110.2	
(5-4-12)		109.1	(11-4-12)		105.6	(4-5-6)		110.9	
(4-5-13)		110.4	(4-5-14)		107.9	(6-5-13)		111.0	
(6-5-14)		110.3	(13-5-14)		106.1	(5-6-7)		120.0	
(5-6-15)		120.2	(7-6-15)		118.3	(2-7-6)		114.8	
(2-7-16)		108.3	(2-7-17)		108.9	(6-7-16)		110.2	
(6-7-17)		109.9	(16-7-17)		104.3	(8-1-2-3)		-179.9	
(8-1-2-7)		0.7	(9-1-2-3)		0.0	(9-1-2-7)		-179.4	
(1-2-3-4)		179.6	(1-2-3-10)		-2.0	(7-2-3-4)		-1.0	
(7-2-3-10)		177.4	(1-2-7-6)		-176.3	(1-2-7-16)		-52.7	
(1-2-7-17)		60.1	(3-2-7-6)		4.3	(3-2-7-16)		127.9	
(3-2-7-17)		-119.3	(2-3-4-5)		-25.1	(2-3-4-11)		-147.9	
(2-3-4-12)		96.2	(10-3-4-5)		156.6	(10-3-4-11)		33.7	
(10-3-4-12)		-82.1	(3-4-5-6)		46.2	(3-4-5-13)		169.7	
(3-4-5-14)		-74.7	(11-4-5-6)		168.9	(11-4-5-13)		-67.5	
(11-4-5-14)		48.0	(12-4-5-6)		-75.5	(12-4-5-13)		48.0	
(12-4-5-14)		163.6	(4-5-6-7)		-46.4	(4-5-6-15)		147.6	
(13-5-6-7)		-169.6	(13-5-6-15)		24.4	(14-5-6-7)		73.1	
(14-5-6-15)		-93.0	(5-6-7-2)		20.8	(5-6-7-16)		-101.8	
(5-6-7-17)		143.8	(15-6-7-2)		-172.9	(15-6-7-16)		64.5	
(15-6-7-17)		-49.9							
(bond)-(plane) angle		(10-3)-(2-3-4)		1.5					
(bond)-(plane) angle		(15-6)-(5-6-7)		12.0					
Frequencies(cm ⁻¹): 65.0 163.1 259.3 357.3 373.8 451.0 466.2 532.3									
544.0 658.3 721.0 764.7 791.8 876.8 898.1 903.2 958.6 1006.0									
1028.9 1106.5 1127.7 1168.4 1206.6 1247.2 1258.5 1326.3 1352.2 1384.9									
1407.9 1420.5 1475.6 1489.8 1502.0 1511.8 1534.4 2930.5 2941.9 2978.6									
3013.2 3049.4 3073.7 3160.0 3166.1 3188.1 3251.0									

3-Methylenehepta-1,5-diene 1A (RHF)Becke3-LYP/6-31G* Geometry (3)									
Nuclear Repulsion		267.855322		(RHF)Becke3-LYP/6-31G*		-272.699220			
ZPE(kcal/mol)		92.63							
C _v @ 298 (eu)		28.82							
S @ 298 (eu)		86.73							
					X	Y	Z		
				C1	0.199539	1.798788	-0.078028		
				C2	0.574590	0.510838	-0.001600		
				C3	2.002853	0.168590	-0.057376		
				C4	2.533757	-1.061820	-0.035088		
				C5	-2.898909	-0.445539	-0.336512		
				C6	-1.838690	-0.214081	0.437909		
				C7	-0.428323	-0.627965	0.117512		
				H8	-0.843392	2.098001	-0.063331		
				H9	0.935490	2.593423	-0.171379		
				H10	2.675155	1.023246	-0.135484		
				H11	3.608446	-1.208473	-0.089054		
				H12	1.929903	-1.962164	0.033043		
				H13	-3.899946	-0.140455	-0.043190		
				H14	-2.807293	-0.953334	-1.294764		
				H15	-1.975979	0.302845	1.388460		
				H16	-0.415915	-1.215925	-0.811168		
				H17	-0.075367	-1.310029	0.905956		
(1-2)	1.344	(1-8)	1.085	(1-9)	1.087				
(2-3)	1.470	(2-7)	1.522	(3-4)	1.340				
(3-10)	1.090	(4-11)	1.086	(4-12)	1.086				
(5-6)	1.333	(5-13)	1.087	(5-14)	1.088				
(6-7)	1.504	(6-15)	1.091	(7-16)	1.099				
(7-17)	1.101	(2-1-8)	122.1	(2-1-9)	121.1				
(8-1-9)	116.8	(1-2-3)	119.5	(1-2-7)	122.5				
(3-2-7)	118.0	(2-3-4)	126.7	(2-3-10)	114.8				
(4-3-10)	118.5	(3-4-11)	121.0	(3-4-12)	122.8				
(11-4-12)	116.2	(6-5-13)	121.8	(6-5-14)	121.7				
(13-5-14)	116.5	(5-6-7)	125.0	(5-6-15)	119.2				
(7-6-15)	115.7	(2-7-6)	115.4	(2-7-16)	109.1				
(2-7-17)	108.0	(6-7-16)	109.7	(6-7-17)	108.6				
(16-7-17)	105.7	(8-1-2-3)	178.6	(8-1-2-7)	-0.3				
(9-1-2-3)	-0.6	(9-1-2-7)	-179.5	(1-2-3-4)	-177.8				
(1-2-3-10)	1.5	(7-2-3-4)	1.1	(7-2-3-10)	-179.6				
(1-2-7-6)	-12.5	(1-2-7-16)	111.5	(1-2-7-17)	-134.1				
(3-2-7-6)	168.6	(3-2-7-16)	-67.4	(3-2-7-17)	47.0				
(2-3-4-11)	179.5	(2-3-4-12)	-0.2	(10-3-4-11)	0.3				
(10-3-4-12)	-179.5	(13-5-6-7)	178.7	(13-5-6-15)	-0.5				
(14-5-6-7)	-1.1	(14-5-6-15)	179.7	(5-6-7-2)	119.3				
(5-6-7-16)	-4.3	(5-6-7-17)	-119.4	(15-6-7-2)	-61.4				
(15-6-7-16)	174.9	(15-6-7-17)	59.9						
Frequencies (cm ⁻¹):		67.3	96.1	158.6	213.8	296.7	403.0	413.9	455.0
		542.6	625.2	651.3	794.1	847.7	923.3	927.0	937.6
		937.6	943.3	953.8	986.3	1036.2	1042.7	1076.1	1147.9
		1147.9	1265.9	1282.0	1335.6	1344.4	1385.1	1448.5	1473.3
		1473.3	1487.6	1505.9	1681.1	1719.7	1734.3	3014.3	3050.4
		3050.4	3146.7	3149.9	3157.4	3168.9	3173.4	3234.7	3248.5
		3248.5	3251.3						

1,2,6-Heptatriene Cope T.S. ¹ A (UHF)Becke3-LYP/6-31G* Geometry (TS ₁ →2)									
Nuclear Repulsion		283.701643		(UHF)Becke3-LYP/6-31G*		-272.629512			
ZPE(kcal/mol)		91.89		S ² before annihilation		0.00			
C _v @ 298 (eu)		26.77		S ² after annihilation		0.00			
S @ 298 (eu)		80.59							
				X		Y		Z	
				C1	2.078119	0.628898	-1.110837		
				C2	0.916271	0.100302	-0.725706		
				C3	-0.303665	-0.257171	-1.296887		
				C4	-1.548242	0.138324	-0.686566		
				C5	-1.546447	-0.392382	0.984413		
				C6	-0.337484	0.134733	1.542928		
				C7	0.894010	-0.355219	1.055031		
				H8	2.958590	0.635340	-0.474375		
				H9	2.182892	1.086267	-2.091331		
				H10	-0.309986	-1.126239	-1.955768		
				H11	-2.434762	-0.300622	-1.152326		
				H12	-1.691014	1.213017	-0.562995		
				H13	-2.476559	-0.003457	1.404104		
				H14	-1.591210	-1.479860	0.902009		
				H15	-0.362319	1.141811	1.957135		
				H16	0.993151	-1.437487	0.964449		
				H17	1.798839	0.099859	1.455483		
(1-2)	1.333	(1-8)	1.086	(1-9)	1.087				
(2-3)	1.394	(2-7)	1.838	(3-4)	1.441				
(3-10)	1.091	(4-5)	1.753	(4-11)	1.093				
(4-12)	1.091	(5-6)	1.432	(5-13)	1.092				
(5-14)	1.092	(6-7)	1.412	(6-15)	1.089				
(7-16)	1.091	(7-17)	1.089	(2-1-8)	122.6				
(2-1-9)	120.8	(8-1-9)	116.6	(1-2-3)	138.3				
(1-2-7)	112.9	(3-2-7)	108.8	(2-3-4)	120.8				
(2-3-10)	117.2	(4-3-10)	118.0	(3-4-5)	108.6				
(3-4-11)	114.2	(3-4-12)	115.5	(5-4-11)	106.6				
(5-4-12)	101.0	(11-4-12)	109.7	(4-5-6)	105.1				
(4-5-13)	104.9	(4-5-14)	103.3	(6-5-13)	116.0				
(6-5-14)	115.5	(13-5-14)	110.4	(5-6-7)	118.3				
(5-6-15)	118.0	(7-6-15)	118.2	(2-7-6)	105.0				
(2-7-16)	99.5	(2-7-17)	104.0	(6-7-16)	116.9				
(6-7-17)	116.9	(16-7-17)	111.7	(8-1-2-3)	-168.1				
(8-1-2-7)	9.2	(9-1-2-3)	12.4	(9-1-2-7)	-170.3				
(1-2-3-4)	-132.2	(1-2-3-10)	70.8	(7-2-3-4)	50.4				
(7-2-3-10)	-106.6	(1-2-7-6)	134.3	(1-2-7-16)	-104.4				
(1-2-7-17)	10.9	(3-2-7-6)	-47.6	(3-2-7-16)	73.7				
(3-2-7-17)	-171.0	(2-3-4-5)	-54.1	(2-3-4-11)	-172.9				
(2-3-4-12)	58.5	(10-3-4-5)	102.7	(10-3-4-11)	-16.0				
(10-3-4-12)	-144.7	(3-4-5-6)	53.3	(3-4-5-13)	176.1				
(3-4-5-14)	-68.1	(11-4-5-6)	176.8	(11-4-5-13)	-60.4				
(11-4-5-14)	55.3	(12-4-5-6)	-68.6	(12-4-5-13)	54.2				
(12-4-5-14)	169.9	(4-5-6-7)	-65.9	(4-5-6-15)	87.3				
(13-5-6-7)	178.7	(13-5-6-15)	-28.1	(14-5-6-7)	47.2				
(14-5-6-15)	-159.6	(5-6-7-2)	62.0	(5-6-7-16)	-47.1				
(5-6-7-17)	176.7	(15-6-7-2)	-91.2	(15-6-7-16)	159.8				
(15-6-7-17)	23.5								
(bond)-(plane) angle		(10-3)-(2-3-4)	20.3						
(bond)-(plane) angle		(15-6)-(5-6-7)	23.4						
Frequencies(cm ⁻¹):									
442.8i	97.2	199.9	320.2	347.6	395.2	411.8	457.1		
522.6	621.3	684.2	766.1	806.8	871.7	892.8	920.2	979.0	989.8
1023.1	1057.7	1071.2	1138.8	1150.3	1197.6	1236.0	1247.3	1279.1	1303.2
1388.4	1462.8	1507.1	1542.4	1547.4	1564.3	1775.4	3092.9	3103.5	3117.1
3135.2	3150.3	3153.3	3156.4	3169.3	3191.7	3230.7			

