Supporting Information for:

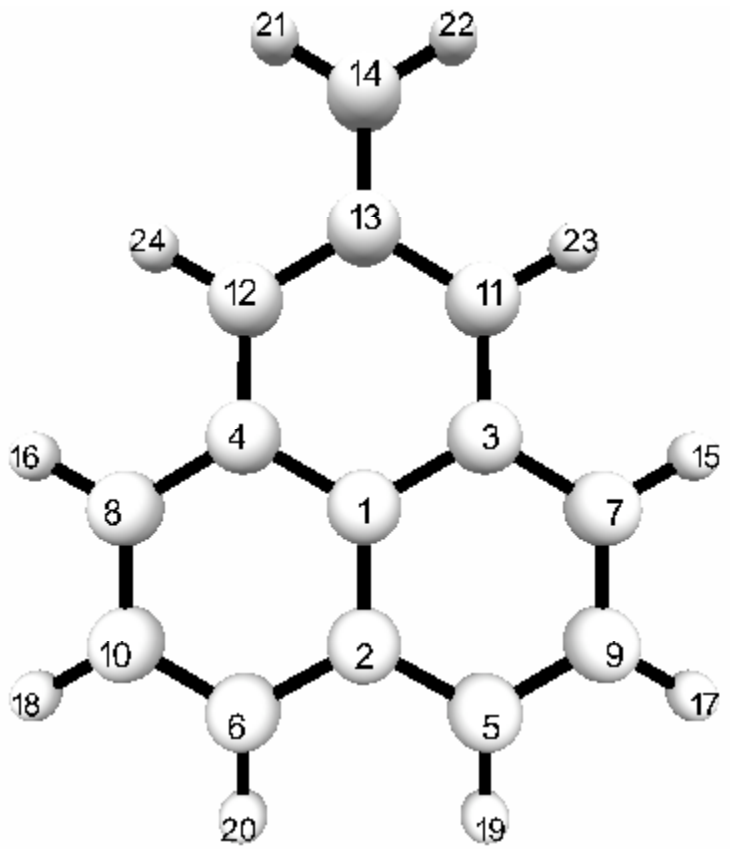
Calculations of the Relative Energies of the Low-Lying Electronic States of 2-Methylenedihydrophenalene-1,3-diyl: Effects of a 1,8-Naphtho Bridging Group on Trimethylenemethane and of a Vinylidene Bridging Group on 1,8-Naphthoquinodimethane

Hao Dong,[†] David A. Hrovat,[†] Helmut Quast,[‡] and Weston Thatcher Borden[†]*

Optimized geometries, energies, thermal corrections, and vibrational frequencies for **2, 3** and **4** discussed in the text (14 pages).

2, ($^3B_2$), CASSCF/6-31G(d), C_{2v} Geometry

Nuclear repulsion energy	780.599139 Hartrees
(14/14)CASSCF/6-31G(d) energy	-536.118398 Hartrees
Zero-point energy correction	0.198865 Hartrees
Thermal correction to Enthalpy	0.209350 Hartrees
Thermal correction to Gibbs Free Energy	0.165035 Hartrees
(14/14)CASPT2/6-31G(d) energy	-537.692591 Hartrees



	X	Y	Z
C1	0.000000	0.000000	-0.339124
C2	0.000000	0.000000	-1.760778
C3	0.000000	1.238415	0.380765
C4	0.000000	-1.238415	0.380765
C5	0.000000	1.242601	-2.449592
C6	0.000000	-1.242601	-2.449592
C7	0.000000	2.451796	-0.352338
C8	0.000000	-2.451796	-0.352338
C9	0.000000	2.443528	-1.746983
C10	0.000000	-2.443528	-1.746983
C11	0.000000	1.218372	1.791523
C12	0.000000	-1.218372	1.791523
C13	0.000000	0.000000	2.526665
C14	0.000000	0.000000	3.931169
H15	0.000000	3.385700	0.180876
H16	0.000000	-3.385700	0.180876
H17	0.000000	3.375138	-2.284031
H18	0.000000	-3.375138	-2.284031
H19	0.000000	1.245508	-3.524962
H20	0.000000	-1.245508	-3.524962
H21	0.000000	-0.918091	4.487488
H22	0.000000	0.918091	4.487488
H23	0.000000	2.151192	2.327090
H24	0.000000	-2.151192	2.327090

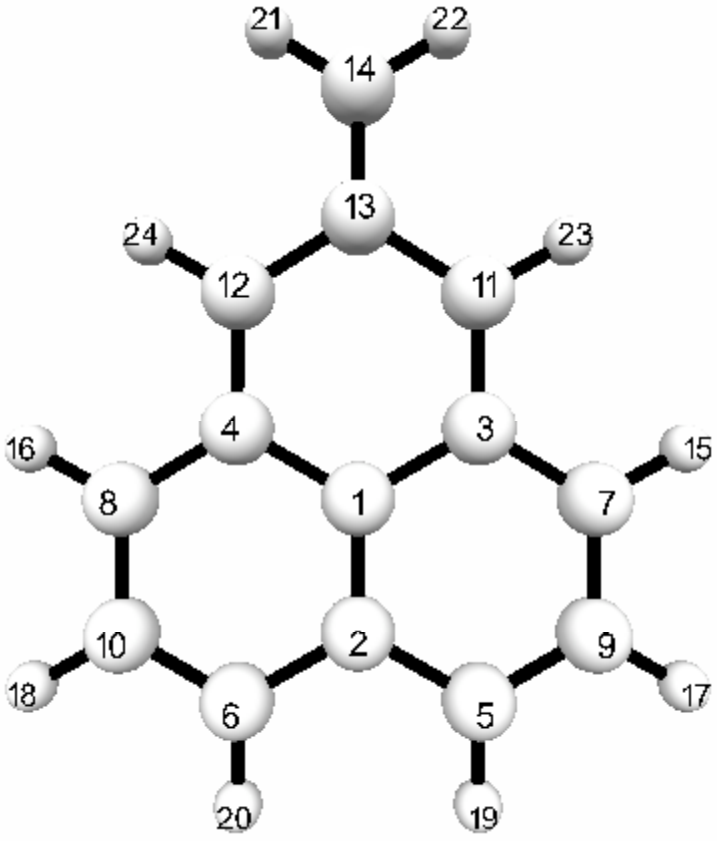
(1-2)	1.422	(1-3)	1.432	(1-4)	1.432	(2-6)	1.421	(3-7)	1.418
(3-11)	1.411	(4-8)	1.418	(4-12)	1.411	(5-9)	1.391	(5-19)	1.075
(6-10)	1.391	(6-20)	1.075	(7-9)	1.395	(7-15)	1.075	(8-10)	1.395
(8-16)	1.075	(9-17)	1.075	(10-18)	1.075	(11-13)	1.423	(11-23)	1.076
(12-13)	1.423	(12-24)	1.076	(13-14)	1.405	(14-21)	1.073	(14-22)	1.073
(2-1-3)	120.2	(2-1-4)	120.2	(3-1-4)	119.7	(1-2-5)	119.0		
(1-2-6)	119.0	(5-2-6)	122.0	(1-3-7)	118.7	(1-3-11)	119.4		
(7-3-11)	122.0	(1-4-8)	118.7	(1-4-12)	119.4	(8-4-12)	122.0		
(2-5-9)	120.7	(2-5-19)	119.2	(9-5-19)	120.2	(2-6-10)	120.7		
(2-6-20)	119.2	(10-6-20)	120.2	(3-7-9)	120.8	(3-7-15)	119.1		
(9-7-15)	120.1	(4-8-10)	120.8	(4-8-16)	119.1	(10-8-16)	120.1		
(5-9-7)	120.7	(5-9-17)	119.7	(6-10-8)	120.7	(6-10-18)	119.7		
(8-10-18)	119.6	(3-11-13)	121.9	(3-11-23)	119.0	(13-11-23)	119.0		
(4-12-13)	121.9	(4-12-24)	119.0	(13-12-24)	119.0	(11-13-12)	117.8		
(11-13-14)	121.1	(12-13-14)	121.1	(13-14-21)	121.2	(13-14-22)	121.2		
(21-14-22)	117.6								
(3-1-2-5)	0.0	(3-1-2-6)	180.0	(4-1-2-5)	180.0				
(4-1-2-6)	0.0	(2-1-3-11)	180.0	(4-1-3-11)	0.0				
(2-1-4-8)	0.0	(2-1-4-12)	180.0	(3-1-4-8)	180.0				
(3-1-4-12)	0.0	(1-2-5-9)	0.0	(1-2-5-19)	180.0				
(6-2-5-9)	180.0	(6-2-5-19)	0.0	(1-2-6-10)	0.0				
(1-2-6-20)	180.0	(5-2-6-10)	180.0	(5-2-6-20)	0.0				

(1-3-7-15)	180.0	(11-3-7-9)	180.0	(11-3-7-15)	0.0
(1-3-11-13)	0.0	(1-3-11-23)	180.0	(7-3-11-13)	180.0
(7-3-11-23)	0.0	(1-4-8-10)	0.0	(1-4-8-16)	180.0
(12-4-8-10)	180.0	(12-4-8-16)	0.0	(1-4-12-13)	0.0
(8-4-12-13)	180.0	(2-5-9-17)	180.0	(19-5-9-7)	180.0
(19-5-9-17)	0.0	(2-6-10-8)	0.0	(2-6-10-18)	180.0
(20-6-10-8)	180.0	(20-6-10-18)	0.0	(15-7-9-5)	180.0
(15-7-9-17)	0.0	(4-8-10-6)	0.0	(4-8-10-18)	180.0
(16-8-10-6)	180.0	(16-8-10-18)	0.0	(3-11-13-12)	0.0
(3-11-13-14)	180.0	(23-11-13-12)	180.0	(23-11-13-14)	0.0
(4-12-13-11)	0.0	(4-12-13-14)	180.0	(24-12-13-11)	180.0
(24-12-13-14)	0.0	(11-13-14-21)	180.0	(11-13-14-22)	0.0
(12-13-14-21)	0.0	(12-13-14-22)	180.0		

Frequencies(cm^{-1}): 118.1 168.3 191.2 294.1 294.4 298.1 437.6 464.7
479.1 495.6 497.8 530.8 549.8 580.6 604.2 634.1 636.7 651.7
659.4 763.4 767.3 778.3 813.6 826.8 843.7 856.6 874.7 888.9
902.1 986.6 991.4 1024.3 1073.7 1098.6 1135.5 1170.6 1184.0 1231.2
1233.8 1282.7 1283.0 1307.7 1323.0 1401.6 1417.7 1454.3 1496.8 1514.1
1563.3 1585.4 1618.6 1635.9 1646.5 1667.2 1676.8 1704.2 3341.0 3349.9
3351.7 3356.4 3359.3 3362.2 3365.1 3377.8 3380.2 3435.6

2, ($^1A_1$), CASSCF/6-31G(d), C_{2v} Geometry

Nuclear repulsion energy	778.980450 Hartrees
(14/14)CASSCF/6-31G(d) energy	-536.086790 Hartrees
Zero-point energy correction	0.195773 Hartrees
Thermal correction to Enthalpy	0.206410 Hartrees
Thermal correction to Gibbs Free Energy	0.161622 Hartrees
(14/14)CASPT2/6-31G(d) energy	-537.662433 Hartrees



	X	Y	Z
C1	0.000000	0.000000	-0.344479
C2	0.000000	0.000000	-1.737236
C3	0.000000	1.252436	0.387031
C4	0.000000	-1.252436	0.387031
C5	0.000000	1.251659	-2.446705
C6	0.000000	-1.251659	-2.446705
C7	0.000000	2.452587	-0.347884
C8	0.000000	-2.452587	-0.347884
C9	0.000000	2.442667	-1.757268
C10	0.000000	-2.442667	-1.757268
C11	0.000000	1.242782	1.793679
C12	0.000000	-1.242782	1.793679
C13	0.000000	0.000000	2.570089
C14	0.000000	0.000000	3.921780
H15	0.000000	3.390123	0.178887
H16	0.000000	-3.390123	0.178887
H17	0.000000	3.375591	-2.291914
H18	0.000000	-3.375591	-2.291914
H19	0.000000	1.241879	-3.521859
H20	0.000000	-1.241879	-3.521859
H21	0.000000	-0.916315	4.483716
H22	0.000000	0.916315	4.483716
H23	0.000000	2.176514	2.326190
H24	0.000000	-2.176514	2.326190

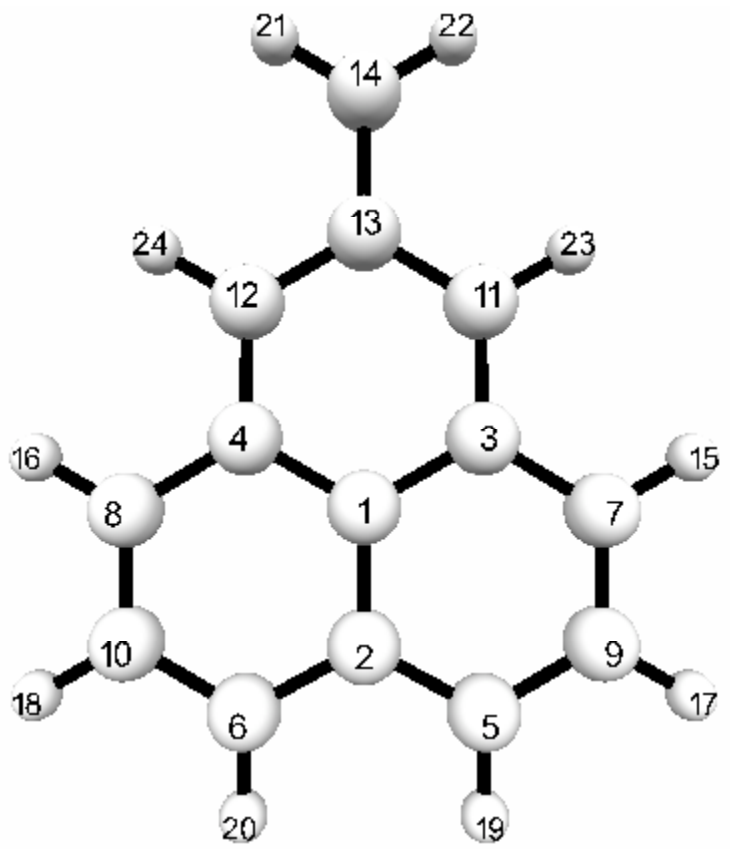
(1-2)	1.393	(1-3)	1.450	(1-4)	1.450	(2-5)	1.439	(2-6)	1.439
(3-7)	1.407	(3-11)	1.407	(4-8)	1.407	(4-12)	1.407	(5-9)	1.376

(5-19) 1.075	(6-10) 1.376	(6-20) 1.075	(7-9) 1.409	(7-15) 1.075			
(8-10) 1.409	(8-16) 1.075	(9-17) 1.075	(10-18) 1.075	(11-13) 1.465			
(11-23) 1.075	(12-13) 1.465	(12-24) 1.075	(13-14) 1.352	(14-21) 1.075			
(14-22) 1.075							
(2-1-3) 120.3	(2-1-4) 120.3	(3-1-4) 119.4	(1-2-5) 119.5				
(1-2-6) 119.5	(5-2-6) 120.9	(1-3-7) 118.2	(1-3-11) 119.9				
(7-3-11) 121.9	(1-4-8) 118.2	(1-4-12) 119.9	(8-4-12) 121.9				
(2-5-9) 120.4	(2-5-19) 119.0	(9-5-19) 120.6	(2-6-10) 120.4				
(2-6-20) 119.0	(10-6-20) 120.6	(3-7-9) 121.1	(3-7-15) 119.2				
(9-7-15) 119.7	(4-8-10) 121.1	(4-8-16) 119.2	(10-8-16) 119.7				
(5-9-7) 120.5	(5-9-17) 120.1	(7-9-17) 119.4	(6-10-8) 120.5				
(6-10-18) 120.1	(8-10-18) 119.4	(3-11-13) 122.4	(3-11-23) 119.3				
(13-11-23) 118.3	(4-12-13) 122.4	(4-12-24) 119.3	(13-12-24) 118.3				
(11-13-12) 116.0	(11-13-14) 122.0	(12-13-14) 122.0	(13-14-21) 121.5				
(13-14-22) 121.5	(21-14-22) 117.0						
(3-1-2-5) 0.0	(3-1-2-6) 180.0	(4-1-2-5) 180.0					
(4-1-2-6) 0.0	(2-1-3-11) 180.0	(4-1-3-11) 0.0					
(2-1-4-8) 0.0	(2-1-4-12) 180.0	(3-1-4-8) 180.0					
(3-1-4-12) 0.0	(1-2-5-9) 0.0	(1-2-5-19) 180.0					
(6-2-5-9) 180.0	(6-2-5-19) 0.0	(1-2-6-10) 0.0					
(1-2-6-20) 180.0	(5-2-6-10) 180.0	(5-2-6-20) 0.0					
(1-3-7-15) 180.0	(11-3-7-9) 180.0	(11-3-7-15) 0.0					
(1-3-11-13) 0.0	(1-3-11-23) 180.0	(7-3-11-13) 180.0					
(7-3-11-23) 0.0	(1-4-8-10) 0.0	(1-4-8-16) 180.0					
(12-4-8-10) 180.0	(12-4-8-16) 0.0	(1-4-12-13) 0.0					
(8-4-12-13) 180.0	(2-5-9-17) 180.0	(19-5-9-7) 180.0					
(19-5-9-17) 0.0	(2-6-10-8) 0.0	(2-6-10-18) 180.0					
(20-6-10-8) 180.0	(20-6-10-18) 0.0	(15-7-9-5) 180.0					
(15-7-9-17) 0.0	(4-8-10-6) 0.0	(4-8-10-18) 180.0					
(16-8-10-6) 180.0	(16-8-10-18) 0.0	(3-11-13-12) 0.0					
(3-11-13-14) 180.0	(23-11-13-12) 180.0	(23-11-13-14) 0.0					
(4-12-13-11) 0.0	(4-12-13-14) 180.0	(24-12-13-11) 180.0					
(24-12-13-14) 0.0	(11-13-14-21) 180.0	(11-13-14-22) 0.0					
(12-13-14-21) 0.0	(12-13-14-22) 180.0						

Frequencies(cm^{-1}): -1243.8	95.8	161.2	177.5	262.3	279.4	296.0	425.4		
449.3	475.1	480.3	486.1	535.0	556.7	594.0	620.7	627.6	633.1
698.2	731.4	752.3	756.5	766.3	768.5	811.3	821.4	846.8	869.7
880.4	897.2	967.5	985.0	990.8	1046.8	1110.9	1135.2	1159.9	1208.5
1244.6	1261.7	1279.9	1306.1	1337.4	1390.8	1448.0	1449.6	1491.1	1513.9
1564.7	1570.6	1605.2	1619.3	1630.4	1699.4	1721.4	1772.9	3332.5	3350.6
3352.9	3360.9	3363.6	3366.0	3368.5	3378.4	3381.7	3414.2		

2, ($^1B_2$), CASSCF/6-31G(d), C_{2v} Geometry

Nuclear repulsion energy	780.219563 Hartrees
(14/14)CASSCF/6-31G(d) energy	-536.096425 Hartrees
Zero-point energy correction	0.196538 Hartrees
Thermal correction to Enthalpy	0.207674 Hartrees
Thermal correction to Gibbs Free Energy	0.162229 Hartrees
(14/14)CASPT2/6-31G(d) energy	-537.673722 Hartrees



	X	Y	Z
C1	0.000000	0.000000	-0.332125
C2	0.000000	0.000000	-1.773001
C3	0.000000	1.227579	0.381489
C4	0.000000	-1.227579	0.381489
C5	0.000000	1.237948	-2.451940
C6	0.000000	-1.237948	-2.451940
C7	0.000000	2.460577	-0.359810
C8	0.000000	-2.460577	-0.359810
C9	0.000000	2.451614	-1.738760
C10	0.000000	-2.451614	-1.738760
C11	0.000000	1.204821	1.786781
C12	0.000000	-1.204821	1.786781
C13	0.000000	0.000000	2.500571
C14	0.000000	0.000000	3.965705
H15	0.000000	3.391104	0.178962
H16	0.000000	-3.391104	0.178962
H17	0.000000	3.380965	-2.279817
H18	0.000000	-3.380965	-2.279817
H19	0.000000	1.248000	-3.527120
H20	0.000000	-1.248000	-3.527120
H21	0.000000	-0.920848	4.515022
H22	0.000000	0.920848	4.515022
H23	0.000000	2.137699	2.323568
H24	0.000000	-2.137699	2.323568

(1-2)	1.441	(1-3)	1.420	(1-4)	1.420	(2-5)	1.412	(2-6)	1.412
(3-7)	1.439	(3-11)	1.405	(4-8)	1.439	(4-12)	1.405	(5-9)	1.408
(5-19)	1.075	(6-10)	1.408	(6-20)	1.075	(7-9)	1.379	(7-15)	1.075
(8-10)	1.379	(8-16)	1.075	(9-17)	1.075	(10-18)	1.075	(11-13)	1.400
(11-23)	1.076	(12-13)	1.400	(12-24)	1.076	(13-14)	1.465	(14-21)	1.072
(14-22)	1.072								

(2-1-3)	120.2	(2-1-4)	120.2	(3-1-4)	119.7	(1-2-5)	118.7	
(1-2-6)	118.7	(5-2-6)	122.5	(1-3-11)	119.2	(7-3-11)	121.9	
(1-4-8)	118.8	(1-4-12)	119.2	(8-4-12)	121.9	(2-5-9)	120.8	
(2-5-19)	119.3	(9-5-19)	119.9	(2-6-10)	120.8	(2-6-20)	119.3	
(10-6-20)	119.9	(3-7-9)	120.6	(3-7-15)	118.9	(9-7-15)	120.4	
(4-8-10)	120.6	(4-8-16)	118.9	(10-8-16)	120.4	(5-9-7)	120.8	
(5-9-17)	119.4	(7-9-17)	119.8	(6-10-8)	120.8	(6-10-18)	119.4	
(8-10-18)	119.8	(3-11-13)	121.6	(3-11-23)	119.0	(13-11-23)	119.4	
(4-12-13)	121.6	(4-12-24)	119.0	(13-12-24)	119.4	(11-13-12)	118.7	
(11-13-14)	120.6	(12-13-14)	120.6	(13-14-21)	120.8	(13-14-22)	120.8	
(21-14-22)	118.4							

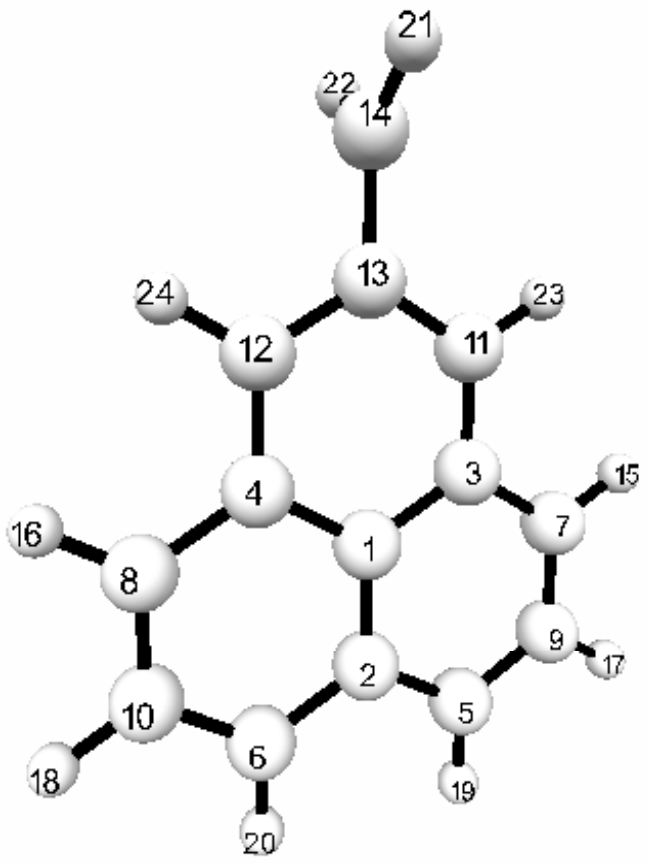
(3-1-2-5)	0.0	(3-1-2-6)	180.0	(4-1-2-5)	180.0
(4-1-2-6)	0.0	(2-1-3-11)	180.0	(4-1-3-11)	0.0
(2-1-4-8)	0.0	(2-1-4-12)	180.0	(3-1-4-8)	180.0
(3-1-4-12)	0.0	(1-2-5-9)	0.0	(1-2-5-19)	180.0
(6-2-5-9)	180.0	(6-2-5-19)	0.0	(1-2-6-10)	0.0

(1-2-6-20)	180.0	(5-2-6-10)	180.0	(5-2-6-20)	0.0
(1-3-7-15)	180.0	(11-3-7-9)	180.0	(11-3-7-15)	0.0
(1-3-11-13)	0.0	(1-3-11-23)	180.0	(7-3-11-13)	180.0
(7-3-11-23)	0.0	(1-4-8-10)	0.0	(1-4-8-16)	180.0
(12-4-8-10)	180.0	(12-4-8-16)	0.0	(1-4-12-13)	0.0
(8-4-12-13)	180.0	(2-5-9-17)	180.0	(19-5-9-7)	180.0
(19-5-9-17)	0.0	(2-6-10-8)	0.0	(2-6-10-18)	180.0
(20-6-10-8)	180.0	(20-6-10-18)	0.0	(15-7-9-5)	180.0
(15-7-9-17)	0.0	(4-8-10-6)	0.0	(4-8-10-18)	180.0
(16-8-10-6)	180.0	(16-8-10-18)	0.0	(3-11-13-12)	0.0
(3-11-13-14)	180.0	(23-11-13-12)	180.0	(23-11-13-14)	0.0
(4-12-13-11)	0.0	(4-12-13-14)	180.0	(24-12-13-11)	180.0
(24-12-13-14)	0.0	(11-13-14-21)	180.0	(11-13-14-22)	0.0
(12-13-14-21)	0.0	(12-13-14-22)	180.0		

Frequencies(cm^{-1}): 121.3 170.3 194.3 256.9 274.6 281.6 304.9 320.1
435.6 460.1 470.2 494.4 504.1 521.8 584.2 601.2 613.7 653.3
665.2 736.2 751.1 764.1 766.1 831.3 846.8 860.2 870.7 896.7
899.3 904.4 985.1 988.7 1019.8 1085.6 1117.9 1135.6 1166.6 1172.1
1192.3 1265.2 1281.8 1290.5 1376.9 1382.7 1400.5 1455.8 1516.0 1518.5
1568.3 1584.6 1614.6 1639.0 1659.3 1681.6 1687.4 1731.2 3348.5 3348.9
3351.9 3352.3 3356.0 3362.9 3366.0 3377.8 3380.7 3454.1

2, ($^1B_1$), CASSCF/6-31G(d), C_{2v} Geometry

Nuclear repulsion energy	779.70995918 Hartrees
(14/14)CASSCF/6-31G(d) energy	-536.09485023 Hartrees
Zero-point energy correction	0.196698 Hartrees
Thermal correction to Enthalpy	0.207484 Hartrees
Thermal correction to Gibbs Free Energy	0.162324 Hartrees
(14/14)CASPT2/6-31G(d) energy	-537.669692 Hartrees



	X	Y	Z
C1	0.000000	0.000000	-0.343624
C2	0.000000	0.000000	-1.771233
C3	0.000000	1.232644	0.372760
C4	0.000000	-1.232644	0.372760
C5	0.000000	1.241771	-2.455736
C6	0.000000	-1.241771	-2.455736
C7	0.000000	2.450162	-0.357544
C8	0.000000	-2.450162	-0.357544
C9	0.000000	2.443741	-1.749739
C10	0.000000	-2.443741	-1.749739
C11	0.000000	1.205401	1.789073
C12	0.000000	-1.205401	1.789073
C13	0.000000	0.000000	2.498799
C14	0.000000	0.000000	3.985970
H15	0.000000	3.382686	0.178094
H16	0.000000	-3.382686	0.178094
H17	0.000000	3.375688	-2.286294
H18	0.000000	-3.375688	-2.286294
H19	0.000000	1.247819	-3.531157
H20	0.000000	-1.247819	-3.531157
H21	0.920794	0.000000	4.537763
H22	-0.920794	0.000000	4.537763
H23	0.000000	2.136999	2.326776
H24	0.000000	-2.136999	2.326776

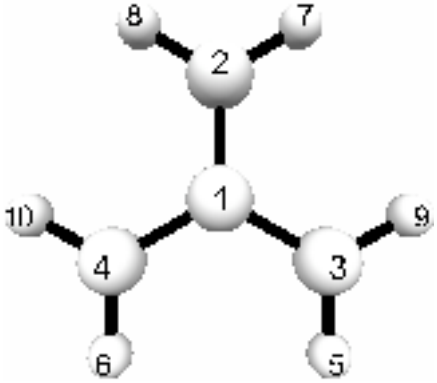
(1-2) 1.428 (1-3) 1.426 (1-4) 1.426 (2-5) 1.418 (2-6) 1.418

(3-7)	1.420	(3-11)	1.417	(4-8)	1.420	(4-12)	1.417	(5-9)	1.394
(5-19)	1.075	(6-10)	1.394	(6-20)	1.075	(7-9)	1.392	(7-15)	1.075
(8-10)	1.392	(8-16)	1.075	(9-17)	1.075	(10-18)	1.075	(11-13)	1.399
(11-23)	1.076	(12-13)	1.399	(12-24)	1.076	(13-14)	1.487	(14-21)	1.073
(14-22)	1.073								
(2-1-3)	120.2	(2-1-4)	120.2	(3-1-4)	119.7	(1-2-5)	118.9		
(1-2-6)	118.9	(5-2-6)	122.3	(1-3-11)	119.1	(7-3-11)	122.1		
(1-4-8)	118.9	(1-4-12)	119.1	(8-4-12)	122.1	(2-5-9)	120.7		
(2-5-19)	119.2	(9-5-19)	120.1	(2-6-10)	120.7	(2-6-20)	119.2		
(10-6-20)	120.1	(3-7-15)	119.2	(9-7-15)	120.1	(4-8-10)	120.7		
(4-8-16)	119.2	(10-8-16)	120.1	(5-9-7)	120.7	(5-9-17)	119.6		
(6-10-8)	120.7	(6-10-18)	119.6	(8-10-18)	119.7	(3-11-13)	121.6		
(3-11-23)	118.9	(13-11-23)	119.5	(4-12-13)	121.6	(4-12-24)	118.9		
(13-12-24)	119.5	(11-13-12)	119.0	(11-13-14)	120.5	(12-13-14)	120.5		
(13-14-21)	120.9	(13-14-22)	120.9	(21-14-22)	118.1				
(3-1-2-5)	0.0	(3-1-2-6)	180.0	(4-1-2-5)	180.0				
(4-1-2-6)	0.0	(2-1-3-11)	180.0	(4-1-3-11)	0.0				
(2-1-4-8)	0.0	(2-1-4-12)	180.0	(3-1-4-8)	180.0				
(3-1-4-12)	0.0	(1-2-5-9)	0.0	(1-2-5-19)	180.0				
(6-2-5-9)	180.0	(6-2-5-19)	0.0	(1-2-6-10)	0.0				
(1-2-6-20)	180.0	(5-2-6-10)	180.0	(5-2-6-20)	0.0				
(1-3-7-15)	180.0	(11-3-7-9)	180.0	(11-3-7-15)	0.0				
(1-3-11-13)	0.0	(1-3-11-23)	180.0	(7-3-11-13)	180.0				
(7-3-11-23)	0.0	(1-4-8-10)	0.0	(1-4-8-16)	180.0				
(12-4-8-10)	180.0	(12-4-8-16)	0.0	(1-4-12-13)	0.0				
(8-4-12-13)	180.0	(2-5-9-17)	180.0	(19-5-9-7)	180.0				
(19-5-9-17)	0.0	(2-6-10-8)	0.0	(2-6-10-18)	180.0				
(20-6-10-8)	180.0	(20-6-10-18)	0.0	(15-7-9-5)	180.0				
(15-7-9-17)	0.0	(4-8-10-6)	0.0	(4-8-10-18)	180.0				
(16-8-10-6)	180.0	(16-8-10-18)	0.0	(3-11-13-12)	0.0				
(3-11-13-14)	180.0	(23-11-13-12)	180.0	(23-11-13-14)	0.0				
(4-12-13-11)	0.0	(4-12-13-14)	180.0	(24-12-13-11)	180.0				
(24-12-13-14)	0.0	(11-13-14-21)	-90.0	(11-13-14-22)	90.0				
(12-13-14-21)	90.0	(12-13-14-22)	-90.0						

Frequencies(cm^{-1}): -260.2 117.8 139.0 176.6 191.5 284.0 290.1 303.6
436.4 468.4 486.2 503.6 505.3 533.0 548.6 602.9 634.7 656.0
658.6 759.1 772.4 781.0 831.7 858.8 860.8 865.5 891.3 893.2
907.7 988.1 992.8 1034.4 1097.3 1097.9 1123.6 1175.1 1178.4 1213.0
1238.6 1270.4 1284.5 1289.2 1331.1 1388.9 1410.1 1414.7 1488.1 1520.9
1569.5 1590.2 1596.9 1659.0 1665.4 1680.9 1697.3 1714.9 3335.5 3349.6
3351.4 3357.1 3359.2 3362.1 3364.8 3377.3 3379.8 3435.1

3 (Trimethylenemethane), ($^3B_2$), CASSCF/6-31G(d), C_{2v} Geometry

Nuclear repulsion energy	105.514818 Hartrees
(4/4)CASSCF/6-31G(d) energy	-154.904651 Hartrees
Zero-point energy correction	0.084397 Hartrees
Thermal correction to Enthalpy	0.090174 Hartrees
Thermal correction to Gibbs Free Energy	0.058701 Hartrees
(4/4)CASPT2/6-31G(d) energy	-155.353253 Hartrees



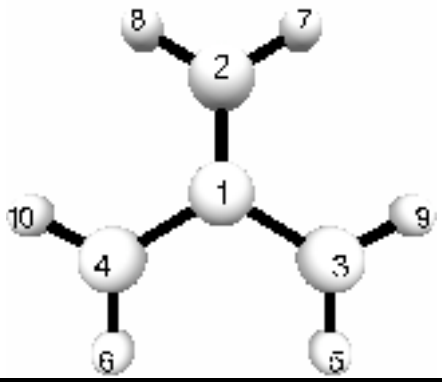
	X	Y	Z
C1	0.000000	0.000000	-0.000001
C2	0.000000	0.000000	1.415608
C3	0.000000	1.225961	-0.707806
C4	0.000000	-1.225961	-0.707806
H5	0.000000	1.248112	-1.780916
H6	0.000000	-1.248112	-1.780916
H7	0.000000	0.918267	1.971342
H8	0.000000	-0.918267	1.971342
H9	0.000000	2.166372	-0.190427
H10	0.000000	-2.166372	-0.190427

(1-2)	1.416	(1-3)	1.416	(2-7)	1.073	(3-5)	1.073	(3-9)	1.073
(4-10)	1.073								
(2-1-3)	120.0	(3-1-4)	120.0	(1-2-7)	121.2	(7-2-8)	117.6		
(1-3-5)	121.2	(1-3-9)	121.2	(5-3-9)	117.6	(1-4-10)	121.2		
(6-4-10)	117.6								
(3-1-2-7)	0.0	(3-1-2-8)	180.0	(2-1-3-5)	180.0				
(2-1-3-9)	0.0	(4-1-3-5)	0.0	(4-1-3-9)	180.0				
(2-1-4-10)	0.0	(3-1-4-10)	180.0						

Frequencies(cm^{-1}): 453.4 453.4 502.1 511.3 511.3 514.2 594.3 594.3
647.6 972.9 1034.9 1081.4 1081.4 1425.6 1425.7 1623.6 1623.6 1654.1
3339.7 3339.7 3350.0 3434.6 3439.6 3439.6

3 (Trimethylenemethane), ($^1A_1$), CASSCF/6-31G(d), C_{2v} Geometry

Nuclear repulsion energy	104.695458 Hartrees
(4/4)CASSCF/6-31G(d) energy	-154.873163 Hartrees
Zero-point energy correction	0.080668 Hartrees
Thermal correction to Enthalpy	0.087261 Hartrees
Thermal correction to Gibbs Free Energy	0.054008 Hartrees
(4/4)CASPT2/6-31G(d) energy	-155.322574 Hartrees



	X	Y	Z
C1	0.000000	0.000000	0.049202
C2	0.000000	0.000000	1.396140
C3	0.000000	1.260463	-0.716295
C4	0.000000	-1.260463	-0.716295
H5	0.000000	1.258039	-1.788342
H6	0.000000	-1.258039	-1.788342
H7	0.000000	0.915963	1.959022
H8	0.000000	-0.915963	1.959022
H9	0.000000	2.204758	-0.208394
H10	0.000000	-2.204758	-0.208394

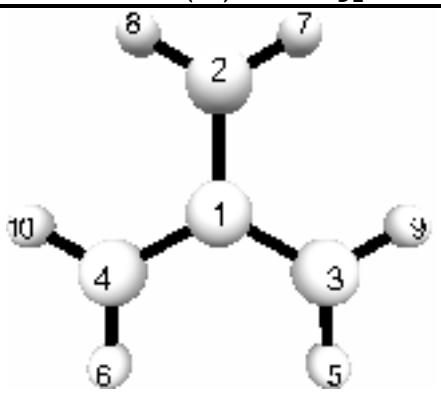
(1-2)	1.347	(1-3)	1.475	(2-7)	1.075	(3-5)	1.072	(3-9)	1.072
(4-10)	1.072								
(2-1-3)	121.3	(3-1-4)	117.5	(1-2-7)	121.6	(7-2-8)	116.9		
(1-3-5)	121.1	(1-3-9)	120.5	(5-3-9)	118.4	(1-4-10)	120.5		
(6-4-10)	118.4								

(3-1-2-7)	0.0	(3-1-2-8)	180.0	(2-1-3-5)	180.0
(2-1-3-9)	0.0	(4-1-3-5)	0.0	(4-1-3-9)	180.0
(2-1-4-10)	0.0	(3-1-4-10)	180.0		

Frequencies(cm^{-1}): -70.9 145.7 288.1 298.3 387.9 416.3 505.4 586.6
738.8 816.0 912.5 1025.0 1122.6 1255.7 1554.9 1582.1 1634.7 1777.9
3331.4 3345.1 3356.9 3411.6 3455.3 3458.0

3 (Trimethylenemethane), ($^1B_2$), CASSCF/6-31G(d), C_{2v} Geometry

Nuclear repulsion energy	104.741159 Hartrees
(4/4)CASSCF/6-31G(d) energy	-154.872519 Hartrees
Zero-point energy correction	0.079504 Hartrees
Thermal correction to Enthalpy	0.084779 Hartrees
Thermal correction to Gibbs Free Energy	0.053962 Hartrees
(4/4)CASPT2/6-31G(d) energy	-155.321566 Hartrees



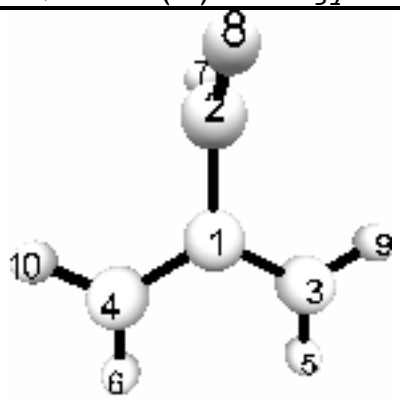
	X	Y	Z
C1	0.000000	0.000000	-0.045287
C2	0.000000	0.000000	1.471970
C3	0.000000	1.214038	-0.718476
C4	0.000000	-1.214038	-0.718476
H5	0.000000	1.250258	-1.791909
H6	0.000000	-1.250258	-1.791909
H7	0.000000	0.923076	2.016158
H8	0.000000	-0.923076	2.016158
H9	0.000000	2.150678	-0.193470
H10	0.000000	-2.150678	-0.193470

(1-2) 1.517	(1-3) 1.388	(2-7) 1.072	(3-5) 1.074	(3-9) 1.074	
(4-10) 1.074					
(2-1-3) 119.0	(3-1-4) 122.0	(1-2-7) 120.5	(7-2-8) 119.0		
(1-3-5) 120.9	(1-3-9) 121.7	(5-3-9) 117.3	(1-4-10) 121.7		
(6-4-10) 117.3					
(3-1-2-7)	0.0	(3-1-2-8)	180.0	(2-1-3-5)	180.0
(2-1-3-9)	0.0	(4-1-3-5)	0.0	(4-1-3-9)	180.0
(2-1-4-10)	0.0	(3-1-4-10)	180.0		

Frequencies(cm^{-1}): -678.2 -436.4 -282.3 386.6 453.1 499.2 582.4 596.7
699.1 726.3 908.7 1024.4 1124.9 1171.2 1485.8 1600.7 1612.7 1674.6
3326.2 3343.7 3357.7 3428.4 3431.8 3465.3

3 (Trimethylenemethane), ($^1B_1$), CASSCF/6-31G(d), C_{2v} Geometry

Nuclear repulsion energy	104.745781 Hartrees
(4/4)CASSCF/6-31G(d) energy	-154.881323 Hartrees
Zero-point energy correction	0.082405 Hartrees
Thermal correction to Enthalpy	0.088240 Hartrees
Thermal correction to Gibbs Free Energy	0.056517 Hartrees
(4/4)CASPT2/6-31G(d) energy	-155.329437 Hartrees



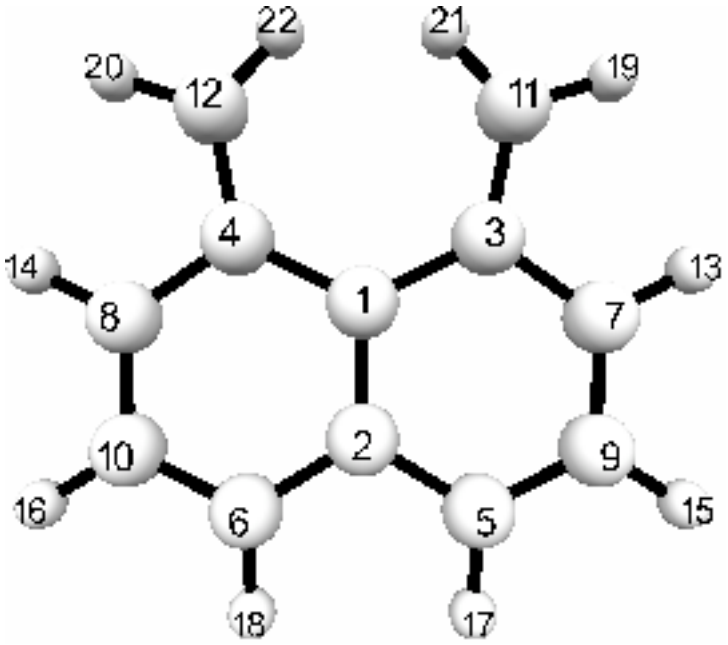
	X	Y	Z
C1	0.000000	0.000000	-0.034560
C2	0.000000	0.000000	1.459006
C3	0.000000	1.216936	-0.716502
C4	0.000000	-1.216936	-0.716502
H5	0.000000	1.248903	-1.790792
H6	0.000000	-1.248903	-1.790792
H7	-0.921239	0.000000	2.009579
H8	0.921239	0.000000	2.009579
H9	0.000000	2.153685	-0.192678
H10	0.000000	-2.153685	-0.192678

(1-2) 1.494 (1-3) 1.395 (2-7) 1.073 (3-5) 1.075 (3-9) 1.073
(4-10) 1.073
(2-1-3) 119.3 (3-1-4) 121.5 (1-2-7) 120.9 (7-2-8) 118.3
(1-3-5) 121.0 (1-3-9) 121.5 (5-3-9) 117.5 (1-4-10) 121.5
(6-4-10) 117.5
(3-1-2-7) 90.0 (2-1-3-5) 180.0 (2-1-3-9) 0.0
(4-1-3-5) 0.0 (4-1-3-9) 180.0 (2-1-4-10) 0.0
(3-1-4-10) 180.0

Frequencies(cm^{-1}): -315.4 278.5 384.0 447.4 450.8 543.8 585.3 678.6
690.4 926.4 1040.7 1087.4 1118.8 1268.2 1485.3 1600.2 1612.6 1663.7
3330.1 3336.6 3341.7 3428.7 3431.5 3439.0

4 (1,8-Naphthoquinodimethane), ($^3B_2$), CASSCF/6-31G(d), C_{2v} Geometry

Nuclear repulsion energy	618.073285 Hartrees
(12/12)CASSCF/6-31G(d) energy	-460.302499 Hartrees
Zero-point energy correction	0.184204 Hartrees
Thermal correction to Enthalpy	0.193695 Hartrees
Thermal correction to Gibbs Free Energy	0.151749 Hartrees
(12/12)CASPT2/6-31G(d) energy	-461.655368 Hartrees



	X	Y	Z
C1	0.000000	0.000000	-0.272905
C2	0.000000	0.000000	1.160144
C3	0.000000	1.310076	-0.938059
C4	0.000000	-1.310076	-0.938059
C5	0.000000	1.213331	1.905090
C6	0.000000	-1.213331	1.905090
C7	0.000000	2.486057	-0.115845
C8	0.000000	-2.486057	-0.115845
C9	0.000000	2.443805	1.267599
C10	0.000000	-2.443805	1.267599
C11	0.000000	1.576931	-2.309479
C12	0.000000	-1.576931	-2.309479
H13	0.000000	3.438237	-0.613598
H14	0.000000	-3.438237	-0.613598
H15	0.000000	3.355686	1.837106
H16	0.000000	-3.355686	1.837106
H17	0.000000	1.155047	2.978218
H18	0.000000	-1.155047	2.978218
H19	0.000000	2.602213	-2.627701
H20	0.000000	-2.602213	-2.627701
H21	0.000000	0.858356	-3.090971
H22	0.000000	-0.858356	-3.090971

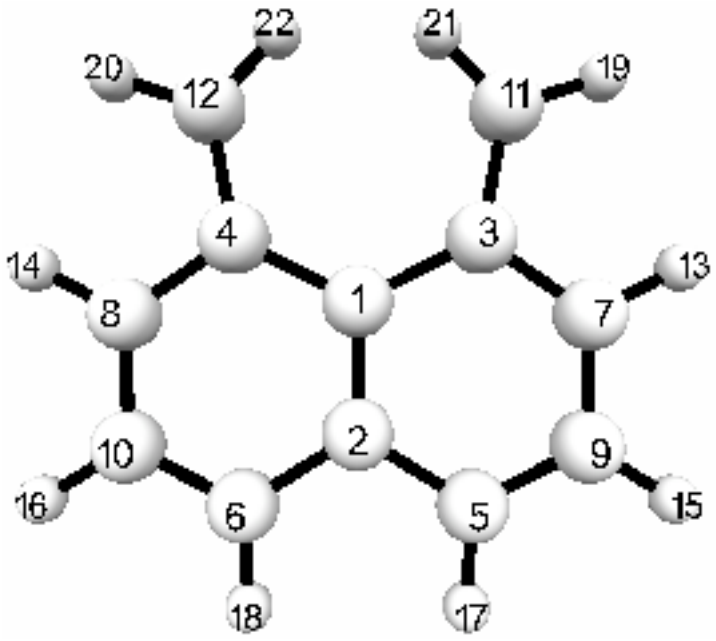
(1-2)	1.433	(1-3)	1.469	(1-4)	1.469	(2-5)	1.424	(2-6)	1.424
(3-7)	1.435	(3-11)	1.397	(4-8)	1.435	(4-12)	1.397	(5-9)	1.386
(5-17)	1.075	(6-10)	1.386	(6-18)	1.075	(7-9)	1.384	(7-13)	1.074
(8-10)	1.384	(8-14)	1.074	(9-15)	1.075	(10-16)	1.075	(11-19)	1.074
(11-21)	1.062	(12-20)	1.074	(12-22)	1.062				
(2-1-3)	116.9	(2-1-4)	116.9	(3-1-4)	126.2	(1-2-5)	121.5		
(1-2-6)	121.5	(5-2-6)	116.9	(1-3-7)	118.1	(1-3-11)	127.9		
(7-3-11)	113.9	(1-4-8)	118.1	(1-4-12)	127.9	(8-4-12)	113.9		
(2-5-9)	121.1	(2-5-17)	118.4	(9-5-17)	120.5	(2-6-10)	121.1		
(2-6-18)	118.4	(10-6-18)	120.5	(3-7-9)	123.2	(3-7-13)	117.4		
(9-7-13)	119.3	(4-8-10)	123.2	(4-8-14)	117.4	(10-8-14)	119.3		
(5-9-7)	119.1	(5-9-15)	120.6	(7-9-15)	120.2	(6-10-8)	119.1		
(6-10-16)	120.6	(8-10-16)	120.2	(3-11-19)	118.3	(3-11-21)	126.4		
(19-11-21)	115.4	(4-12-20)	118.3	(4-12-22)	126.4	(20-12-22)	115.4		
(3-1-2-5)	0.0	(3-1-2-6)	180.0	(4-1-2-5)	180.0				
(4-1-2-6)	0.0	(2-1-3-11)	180.0	(4-1-3-11)	0.0				
(2-1-4-8)	0.0	(2-1-4-12)	180.0	(3-1-4-8)	180.0				
(3-1-4-12)	0.0	(1-2-5-17)	180.0	(6-2-5-17)	0.0				
(1-2-6-10)	0.0	(1-2-6-18)	180.0	(5-2-6-10)	180.0				
(5-2-6-18)	0.0	(1-3-7-13)	180.0	(11-3-7-13)	0.0				
(1-3-11-19)	180.0	(1-3-11-21)	0.0	(7-3-11-19)	0.0				
(7-3-11-21)	180.0	(1-4-8-10)	0.0	(1-4-8-14)	180.0				
(12-4-8-10)	180.0	(12-4-8-14)	0.0	(2-5-9-15)	180.0				

(17-5-9-15)	0.0	(2-6-10-8)	0.0	(2-6-10-16)	180.0
(18-6-10-8)	180.0	(18-6-10-16)	0.0	(13-7-9-15)	0.0
(4-8-10-6)	0.0	(4-8-10-16)	180.0	(14-8-10-6)	180.0
(14-8-10-16)	0.0				

Frequencies(cm^{-1}): -194.1 123.2 195.8 257.6 361.8 369.2 378.8 445.5
482.2 494.9 503.0 560.5 580.2 582.9 609.6 633.4 672.0 697.4
707.8 760.8 761.6 814.3 836.0 854.5 873.4 879.6 979.6 984.4
1016.3 1035.9 1095.8 1102.8 1187.8 1218.7 1221.0 1276.3 1287.7 1299.3
1317.3 1408.3 1411.2 1483.5 1538.1 1553.9 1599.5 1630.6 1646.2 1672.3
1692.8 1705.9 3352.9 3355.6 3362.4 3367.7 3371.3 3376.8 3383.4 3386.7
3513.9 3581.5

4 (1,8-Naphthoquinodimethane), ($^1A_1$), CASSCF/6-31G(d), C_{2v} Geometry

Nuclear repulsion energy	618.418880 Hartrees
(12/12)CASSCF/6-31G(d) energy	-460.292838 Hartrees
Zero-point energy correction	0.183773 Hartrees
Thermal correction to Enthalpy	0.193538 Hartrees
Thermal correction to Gibbs Free Energy	0.151072 Hartrees
(12/12)CASPT2/6-31G(d) energy	-461.649552 Hartrees



	X	Y	Z
C1	0.000000	0.000000	-0.259972
C2	0.000000	0.000000	1.149928
C3	0.000000	1.311050	-0.930526
C4	0.000000	-1.311050	-0.930526
C5	0.000000	1.218920	1.909096
C6	0.000000	-1.218920	1.909096
C7	0.000000	2.468312	-0.124015
C8	0.000000	-2.468312	-0.124015
C9	0.000000	2.433324	1.278792
C10	0.000000	-2.433324	1.278792
C11	0.000000	1.574927	-2.322161
C12	0.000000	-1.574927	-2.322161
H13	0.000000	3.423304	-0.616980
H14	0.000000	-3.423304	-0.616980
H15	0.000000	3.350508	1.839519
H16	0.000000	-3.350508	1.839519
H17	0.000000	1.153629	2.981910
H18	0.000000	-1.153629	2.981910
H19	0.000000	2.600212	-2.639320
H20	0.000000	-2.600212	-2.639320
H21	0.000000	0.853921	-3.100129
H22	0.000000	-0.853921	-3.100129

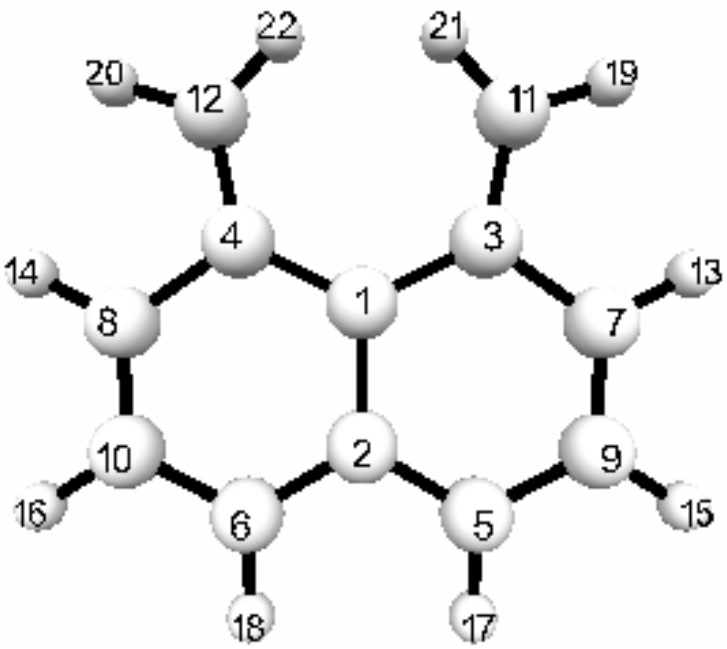
(1-2)	1.410	(1-3)	1.473	(1-4)	1.473	(2-5)	1.436	(2-6)	1.436	
(3-11)	1.416	(4-8)	1.411	(4-12)	1.416	(5-9)	1.368	(5-17)	1.075	
(6-10)	1.368	(6-18)	1.075	(7-9)	1.403	(7-13)	1.075	(8-10)	1.403	
(8-14)	1.075	(9-15)	1.075	(10-16)	1.075	(11-19)	1.073	(11-21)	1.061	
(12-20)	1.073	(12-22)	1.061							
(2-1-3)	117.1	(2-1-4)	117.1	(3-1-4)	125.8	(1-2-5)	121.9			
(1-2-6)	121.9	(5-2-6)	116.2	(1-3-7)	118.0	(1-3-11)	127.8			
(7-3-11)	114.1	(1-4-8)	118.0	(1-4-12)	127.8	(8-4-12)	114.1			
(2-5-9)	120.7	(2-5-17)	118.4	(9-5-17)	120.9	(2-6-10)	120.7			
(2-6-18)	118.4	(10-6-18)	120.9	(3-7-9)	123.4	(3-7-13)	117.8			
(9-7-13)	118.7	(4-8-10)	123.4	(4-8-14)	117.8	(10-8-14)	118.7			
(5-9-7)	118.9	(5-9-15)	121.1	(7-9-15)	120.0	(6-10-8)	118.9			
(6-10-16)	121.1	(8-10-16)	120.0	(3-11-19)	117.9	(3-11-21)	126.4			

(19-11-21)	115.6	(4-12-20)	117.9	(4-12-22)	126.4	(20-12-22)	115.6
(3-1-2-5)	0.0	(3-1-2-6)	180.0	(4-1-2-5)	180.0		
(4-1-2-6)	0.0	(2-1-3-11)	180.0	(4-1-3-11)	0.0		
(2-1-4-8)	0.0	(2-1-4-12)	180.0	(3-1-4-8)	180.0		
(3-1-4-12)	0.0	(1-2-5-17)	180.0	(6-2-5-17)	0.0		
(1-2-6-10)	0.0	(1-2-6-18)	180.0	(5-2-6-10)	180.0		
(5-2-6-18)	0.0	(1-3-7-13)	180.0	(11-3-7-13)	0.0		
(1-3-11-19)	180.0	(1-3-11-21)	0.0	(7-3-11-19)	0.0		
(7-3-11-21)	180.0	(1-4-8-10)	0.0	(1-4-8-14)	180.0		
(12-4-8-10)	180.0	(12-4-8-14)	0.0	(2-5-9-15)	180.0		
(17-5-9-15)	0.0	(2-6-10-8)	0.0	(2-6-10-16)	180.0		
(18-6-10-8)	180.0	(18-6-10-16)	0.0	(13-7-9-15)	0.0		
(4-8-10-6)	0.0	(4-8-10-16)	180.0	(14-8-10-6)	180.0		
(14-8-10-16)	0.0						

Frequencies(cm^{-1}): -217.9 117.4 186.3 258.5 304.2 353.2 363.3 373.8
487.2 494.9 500.9 503.1 578.9 587.6 610.0 621.5 630.4 655.3
671.1 766.0 767.8 828.6 836.0 882.5 886.7 897.7 986.4 989.7
993.7 1038.8 1043.6 1096.1 1177.1 1214.0 1225.1 1264.3 1285.4 1286.3
1334.8 1402.1 1448.9 1515.0 1558.0 1560.0 1606.3 1623.1 1634.0 1694.4
1714.0 1734.8 3352.9 3355.5 3362.3 3367.7 3373.0 3378.5 3383.5 3387.2
3524.2 3593.6

4 (1,8-Naphthoquinodimethane), ($^1B_2$), CASSCF/6-31G(d), C_{2v} Geometry

Nuclear repulsion energy	615.774124 Hartrees
(12/12)CASSCF/6-31G(d) energy	-460.259428 Hartrees
Zero-point energy correction	0.186929 Hartrees
Thermal correction to Enthalpy	0.196588 Hartrees
Thermal correction to Gibbs Free Energy	0.154241 Hartrees
(12/12)CASPT2/6-31G(d) energy	-461.612372 Hartrees



	X	Y	Z
C1	0.000000	0.000000	-0.306046
C2	0.000000	0.000000	1.201736
C3	0.000000	1.297356	-0.954197
C4	0.000000	-1.297356	-0.954197
C5	0.000000	1.202854	1.912828
C6	0.000000	-1.202854	1.912828
C7	0.000000	2.512584	-0.101597
C8	0.000000	-2.512584	-0.101597
C9	0.000000	2.466952	1.248993
C10	0.000000	-2.466952	1.248993
C11	0.000000	1.578351	-2.307073
C12	0.000000	-1.578351	-2.307073
H13	0.000000	3.458584	-0.610582
H14	0.000000	-3.458584	-0.610582
H15	0.000000	3.372548	1.828449
H16	0.000000	-3.372548	1.828449
H17	0.000000	1.166112	2.986821
H18	0.000000	-1.166112	2.986821
H19	0.000000	2.605518	-2.620114
H20	0.000000	-2.605518	-2.620114
H21	0.000000	0.865674	-3.095396
H22	0.000000	-0.865674	-3.095396

(1-2)	1.508	(1-3)	1.450	(1-4)	1.450	(2-5)	1.397
(2-6)	1.397	(3-7)	1.484	(3-11)	1.382	(4-8)	1.484
(4-12)	1.382	(5-9)	1.428	(5-17)	1.075	(6-10)	1.428
(6-18)	1.075	(7-9)	1.351	(7-13)	1.074		

(8-10)	1.351	(8-14)	1.074	(9-15)	1.075	(10-16) 1.075	(11-19) 1.074
(11-21)	1.063	(12-20)	1.074	(12-22)	1.063		
(2-1-3)	116.5	(2-1-4)	116.5	(3-1-4)	126.9	(1-2-5)	120.6
(1-2-6)	120.6	(5-2-6)	118.8	(1-3-7)	118.4	(1-3-11)	128.3
(7-3-11)	113.3	(1-4-8)	118.4	(1-4-12)	128.3	(8-4-12)	113.3
(2-5-9)	121.7	(2-5-17)	118.6	(9-5-17)	119.7	(2-6-10)	121.7
(2-6-18)	118.6	(10-6-18)	119.7	(3-7-9)	123.1	(3-7-13)	116.7
(9-7-13)	120.2	(4-8-10)	123.1	(4-8-14)	116.7	(10-8-14)	120.2
(5-9-7)	119.6	(5-9-15)	119.7	(7-9-15)	120.7	(6-10-8)	119.6
(6-10-16)	119.7	(8-10-16)	120.7	(3-11-19)	118.7	(3-11-21)	126.2
(19-11-21)	115.2	(4-12-20)	118.7	(4-12-22)	126.2	(20-12-22)	115.2
(3-1-2-5)	0.0	(3-1-2-6)	180.0	(4-1-2-5)	180.0		
(4-1-2-6)	0.0	(2-1-3-11)	180.0	(4-1-3-11)	0.0		
(2-1-4-8)	0.0	(2-1-4-12)	180.0	(3-1-4-8)	180.0		
(3-1-4-12)	0.0	(1-2-5-17)	180.0	(6-2-5-17)	0.0		
(1-2-6-10)	0.0	(1-2-6-18)	180.0	(5-2-6-10)	180.0		
(5-2-6-18)	0.0	(1-3-7-13)	180.0	(11-3-7-13)	0.0		
(1-3-11-19)	180.0	(1-3-11-21)	0.0	(7-3-11-19)	0.0		
(7-3-11-21)	180.0	(1-4-8-10)	0.0	(1-4-8-14)	180.0		
(12-4-8-10)	180.0	(12-4-8-14)	0.0	(2-5-9-15)	180.0		
(17-5-9-15)	0.0	(2-6-10-8)	0.0	(2-6-10-16)	180.0		
(18-6-10-8)	180.0	(18-6-10-16)	0.0	(13-7-9-15)	0.0		
(4-8-10-6)	0.0	(4-8-10-16)	180.0	(14-8-10-6)	180.0		
(14-8-10-16)	0.0						

Frequencies(cm^{-1}): -181.8 109.7 172.6 239.4 362.8 367.8 394.5 434.8
476.0 498.3 498.4 540.1 559.5 568.5 610.3 613.6 649.5 723.4
727.2 751.6 764.6 778.6 804.5 831.0 834.4 851.3 972.1 973.6
987.0 1005.5 1093.1 1123.7 1166.8 1192.4 1207.6 1275.1 1300.7 1398.8
1427.7 1427.7 1456.4 1523.8 1557.8 1564.1 1593.6 1650.7 1711.5 1720.5
1761.1 2741.2 3355.9 3357.1 3363.4 3367.8 3375.9 3382.4 3387.1 3389.5
3511.6 3568.1