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Supporting Information for

Computational and Spectroscopic Studies of Organic Mixed-Valence Compounds: Where is the Charge?

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Contents

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Calculated key parameters for 1-17

Table S1: Calculated key parameters for **1**. Total dipole moment, enthalpy as difference between calculated structures of C_i and C_1 symmetry, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen atom and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the ^{14}N-HFC constants at the both nitrogen atoms. All structures were optimized in the given solvent and with a = 0.35.

1	μ_a /D	ΔH^* (C_i-C_1) /kJ mol^{-1}	$\langle S^2 \rangle$	C_{Ar}-N /Å	E_{ab}/cm^{-1}		μ_{ab} /D		a_N /MHz	
					C_1	C_i	C_1	C_i	C_1	C_i
35 % HF in gas										
	0.03	-0.02	0.78	1.426	5705	5738	21.05	21.00	11.20	11.17
				1.426					11.20	11.17
35 % HF in hexane										
	0.02	0.03	0.78	1.426	4189	4234	26.17	26.07	11.35	11.31
				1.426					11.32	11.31
35 % HF in dichloromethane										
	26.82	3.20	0.79	1.408	6800	4230	14.39	26.30	23.32	11.39
				1.428					1.67	11.39
35 % HF in acetonitrile										
	29.89	7.21	0.79	1.406	7930	4512	12.13	25.30	24.19	11.40
				1.428					1.01	11.40

Table S2: Calculated key parameters for **2**. Total dipole moment, enthalpy as difference between calculated structures of C_i and C_1 symmetry, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen atom and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the ^{14}N-HFC constants at the both nitrogen atoms. All structures were optimized in the given solvent and with a = 0.35.

2	μ_a /D	ΔH^* (C_i-C_1) /kJ mol^{-1}	$\langle S^2 \rangle$	C_{Ar}-N /Å	E_{ab}/cm^{-1}		μ_{ab} /D		a_N /MHz	
					C_1	C_i	C_1	C_i	C_1	C_i
35 % HF in gas										
	0.03	0.01	0.77	1.426	6481	6512	18.29	18.25	11.97	11.93
				1.425					11.91	11.93
35 % HF in hexane										
	1.25	-0.15	0.77	1.428	5276	5199	21.61	21.79	11.38	11.96
				1.425					12.45	11.96
35 % HF in dichloromethane										
	10.07	0.11	0.78	1.421	5745	5356	19.86	21.61	16.95	11.88
				1.428					7.21	11.88
35 % HF in acetonitrile										
	20.09	1.54	0.78	1.412	7204	5580	14.98	21.02	22.40	11.85
				1.428					2.90	11.85

Table S3: Calculated key parameters for **3**. Total dipole moment, enthalpy as difference between calculated structures of C_i and C_1 symmetry, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen atom and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the ^{14}N-HFC constants at the both nitrogen atoms. All structures were optimized in the given solvent and with a = 0.35.

3	μ_a /D	ΔH^* (C_i-C_1) /kJ mol^{-1}	$\langle S^2 \rangle$	C_{Ar}-N /Å	E_{ab}/cm^{-1}		μ_{ab} /D		a_N /MHz	
					C_1	C_i	C_1	C_i	C_1	C_i
35 % HF in gas										
	0.05	-0.01	0.77	1.426	7544	7206	15.24	15.58	12.89	13.16
				1.426					12.84	13.16
35 % HF in hexane										
	0.03	0.08	0.77	1.426	6277	6289	17.88	17.85	13.05	13.03
				1.426					13.01	13.03
35 % HF in dichloromethane										
	0.05	0.29	0.77	1.426	6653	6561	17.48	17.55	12.89	12.87
				1.426					12.84	12.87
35 % HF in acetonitrile										
	6.34	0.39	0.77	1.421	6527	6848	17.05	17.03	16.48	12.79
				1.427					9.34	12.79

Table S4: Calculated key parameters for **4**. Total dipole moment, enthalpy as difference between calculated structures of C_i and C_1 symmetry, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen atom and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the ^{14}N-HFC constants at the both nitrogen atoms. All structures were optimized in the given solvent and with a = 0.35.

4	μ_a /D	ΔH^* (C_i-C_1) /kJ mol^{-1}	$\langle S^2 \rangle$	C_{Ar}-N /Å	E_{ab}/cm^{-1}		μ_{ab} /D		a_N /MHz	
					C_1	C_i	C_1	C_i	C_1	C_i
35 % HF in gas										
	0.03	0.02	0.77	1.425	10417	10385	10.54	10.56	16.36	16.30
				1.425					16.29	16.30
35 % HF in hexane										
	0.03	0.03	0.77	1.425	9718	9559	11.76	11.84	16.38	16.24
				1.425					16.32	16.24
35 % HF in dichloromethane										
	0.03	0.24	0.77	1.425	10145	10078	11.55	11.54	16.33	16.26
				1.425					16.33	16.26
35 % HF in acetonitrile										
	0.01	0.41	0.77	1.426	10473	10437	11.27	11.22	16.36	16.27
				1.426					16.34	16.27

Table S5: Calculated key parameters for **5**. Total dipole moment μ_a (dipole moment μ_b in the IVCT excited state in brackets), enthalpy as difference between calculated structures of C_i and C_1 symmetry, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen atom and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the ^{14}N-HFC constants at the both nitrogen atoms. All structures were optimized in the given solvent and with a = 0.35.

5	μ_a /D	ΔH^* (C_i-C_1) /kJ mol^{-1}	$\langle S^2 \rangle$	C_{Ar}-N /Å	E_{ab}/cm^{-1}		μ_{ab} /D		a_N /MHz	
					C_1	C_i	C_1	C_i	C_1	C_i
35 % HF in gas										
	0.31	0.04	0.77	1.423	4145	4156	25.56	25.56	10.42	10.42
				1.423					10.51	10.42
35 % HF in hexane										
	0.10	0.07	0.77	1.423	2473	2504	34.64	34.54	10.60	10.53
				1.423					10.54	10.53
35 % HF in dichloromethane										
	40.15	10.02	0.79	1.406	6969	2421	10.62	35.46	24.40	10.58
	[-34.56]			1.426					0.30	10.58
35 % HF in acetonitrile										
	42.09	15.64	0.79	1.405	8351	2654	9.15	33.49	24.60	10.72
	[-32.13]			1.426					0.20	10.72

Table S6: Calculated key parameters for **6**. Total dipole moment μ_a (dipole moment μ_b in the IVCT excited state in brackets), enthalpy as difference between calculated structures of C_i and C_1 symmetry, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen atom and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the ^{14}N-HFC constants at the both nitrogen atoms. All structures were optimized in the given solvent and with a = 0.35.

6	μ_a /D	ΔH^* (C_i-C_1) /kJ mol^{-1}	$\langle S^2 \rangle$	C_{Ar}-N /Å	E_{ab}/cm^{-1}		μ_{ab} /D		a_N /MHz	
					C_1	C_i	C_1	C_i	C_1	C_i
35 % HF in gas										
	0.06	-0.01	0.77	1.424	4422	4390	25.27	25.30	9.86	9.90
				1.424					9.84	9.90
35 % HF in hexane										
	0.38	0.02	0.77	1.424	2796	2693	33.38	33.61	9.93	10.04
				1.424					9.92	10.04
35 % HF in dichloromethane										
	38.93	4.77	0.79	1.407	6828	2537	11.60	34.74	24.04	10.14
	[-33.49]			1.426					0.36	10.14
35 % HF in acetonitrile										
	41.24	10.27	0.79	1.405	8150	2847	9.81	32.78	24.60	10.19
	[-31.42]			1.426					0.24	10.19

Table S7: Calculated key parameters for **7**. Total dipole moment μ_a (dipole moment μ_b in the IVCT excited state in brackets), enthalpy as difference between calculated structures of C_i and C_1 symmetry, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen atom and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the ^{14}N-HFC constants at the both nitrogen atoms. All structures were optimized in the given solvent and with a = 0.35.

7	μ_a /D	ΔH^* (C_i-C_1) /kJ mol^{-1}	$\langle S^2 \rangle$	C_{Ar}-N /Å	E_{ab}/cm^{-1}		μ_{ab} /D		a_N /MHz	
					C_1	C_i	C_1	C_i	C_1	C_i
35 % HF in gas										
	0.13	0.11	0.77	1.427	5123	5153	23.83	23.78	8.44	8.48
				1.426					8.59	8.48
35 % HF in hexane										
	0.19	0.12	0.77	1.427	3841	3942	29.19	28.85	8.34	8.19
				1.427					8.46	8.19
35 % HF in dichloromethane										
	35.21	3.09	0.79	1.412	6000	3969	15.66	28.82	22.38	7.88
	[-30.51]			1.425					0.81	7.88
35 % HF in acetonitrile										
	40.02	8.35	0.79	1.408	7436	4184	12.04	27.86	24.20	7.81
	[-29.60]			1.425					0.30	7.81

Table S8: Calculated key parameters for **8**. Total dipole moment μ_a (dipole moment μ_b in the IVCT excited state in brackets), enthalpy as difference between calculated structures of C_i and C_1 symmetry, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen atom and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the ^{14}N-HFC constants at the both nitrogen atoms. All structures were optimized in the given solvent and with a = 0.35.

8	μ_a /D	ΔH^* (C_i-C_1) /kJ mol^{-1}	$\langle S^2 \rangle$	C_{Ar}-N /Å	E_{ab}/cm^{-1}		μ_{ab} /D		a_N /MHz	
					C_1	C_i	C_1	C_i	C_1	C_i
35 % HF in gas										
	0.03	-0.02	0.78	1.430	6260	6294	19.48	19.39	6.56	6.54
				1.429					6.57	6.54
35 % HF in hexane										
	0.03	0.10	0.78	1.430	5624	5644	22.85	22.78	6.27	6.27
				1.430					6.31	6.27
35 % HF in dichloromethane										
	0.04	0.32	0.78	1.430	5881	5844	22.27	22.36	5.86	5.89
	[0.19]			1.429					5.87	5.89
35 % HF in acetonitrile										
	0.05	0.46	0.78	1.430	6127	6054	21.40	21.57	5.69	5.73
	[0.73]			1.430					5.69	5.73

Table S9: Calculated key parameters for **9**. Total dipole moment μ_a (dipole moment μ_b in the IVCT excited state in brackets), enthalpy as difference between calculated structures of C_i and C_1 symmetry, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen atom and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the ^{14}N-HFC constants at the both nitrogen atoms. All structures were optimized in the given solvent and with a = 0.35.

9	μ_a /D	ΔH^* (C_i-C_1) /kJ mol^{-1}	$\langle S^2 \rangle$	C_{Ar}-N /Å	E_{ab}/cm^{-1}		μ_{ab} /D		a_N /MHz	
					C_1	C_i	C_1	C_i	C_1	C_i
35 % HF in gas										
	0.29	0.02	0.77	1.426	8296	8240	12.80	12.83	14.52	14.34
				1.424					14.04	14.34
35 % HF in hexane										
	0.45	-0.06	0.77	1.426	7523	7461	14.49	14.56	14.65	14.33
				1.424					13.93	14.33
35 % HF in dichloromethane										
	0.80	-0.04	0.77	1.426	7891	7874	14.19	14.23	14.60	14.15
	[-1.61]			1.425					13.58	14.15
35 % HF in acetonitrile										
	0.71	0.05	0.77	1.426	8065	8166	13.90	13.82	14.51	14.08
	[-1.44]			1.425					13.65	14.08

Table S10: Calculated key parameters for **10**. Total dipole moment μ_a (dipole moment μ_b in the IVCT excited state in brackets), enthalpy as difference between calculated structures of C_i and C_1 symmetry, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen atom and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the ^{14}N-HFC constants at the both nitrogen atoms. All structures were optimized in the given solvent and with a = 0.35.

10	μ_a /D	ΔH^* (C_i-C_1) /kJ mol^{-1}	$\langle S^2 \rangle$	C_{Ar}-N /Å	E_{ab}/cm^{-1}		μ_{ab} /D		a_N /MHz	
					C_1	C_i	C_1	C_i	C_1	C_i
35 % HF in gas										
	0.12	0.16	0.78	1.429	7574	7432	16.33	16.51	11.20	11.25
				1.428					11.04	11.25
35 % HF in hexane										
	0.15	0.06	0.78	1.429	6751	6689	18.75	18.83	11.05	11.00
				1.428					10.88	11.00
35 % HF in dichloromethane										
	0.06	0.27	0.77	1.429	7211	6959	18.18	18.50	10.45	10.58
	[0.05]			1.429					10.51	10.58
35 % HF in acetonitrile										
	0.08	0.29	0.77	1.429	7661	7390	17.40	17.72	10.19	10.34
	[-0.10]			1.429					10.27	10.34

Table S11: Calculated key parameters for **11**. Total dipole moment, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen/carbon atom (large one is the C-C distance) and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the $^{14}N/^{13}C$-HFC constants at the nitrogen and carbon atoms of the PTCM. All structures were optimized in the given solvent and with a = 0.35. The values in braces are calculations with a = 0.30 in TDDFT.

11	μ_a /D	$\langle S^2 \rangle$	C_{Ar}-N/C /Å	E_{ab} /cm^{-1}	μ_{ab} /D	a_N /MHz
35 % HF in gas						
	6.65	0.79	1.423	14774	3.56	0.20
			1.481	(13567)	(4.50)	97.22
35 % HF in hexane						
	6.99	0.79	1.424	14539	4.18	0.22
			1.481	(13189)	(5.07)	97.15
35 % HF in dichloromethane						
	7.49	0.79	1.425	14392	4.42	0.24
			1.481	(12956)	(5.24)	96.90
35 % HF in acetonitrile						
	7.64	0.79	1.426	14394	4.39	0.25
			1.481	(12940)	(5.19)	96.89

Table S12: Calculated key parameters for **12**. Total dipole moment, spin expectation value (theoretical value would be 0.75), key distance between the nitrogen/carbon atom (large one is the C-C distance) and the carbon atom of the outer phenyl ring, first excitation energy and transition dipole moments as well as the $^{14}N/^{13}C$-HFC constants at the nitrogen and carbon atoms of the PTCM. All structures were optimized in the given solvent and with a = 0.35. The values in braces are calculations with a = 0.30 in TDDFT.

12	μ_a /D	$\langle S^2 \rangle$	C_{Ar}-N/C /Å	E_{ab} /cm^{-1}	μ_{ab} /D	a_N /MHz
35 % HF in gas						
	7.66	0.80	1.425	15232	4.43	0.33
			1.481	(14087)	(5.26)	96.45
35 % HF in hexane						
	8.05	0.80	1.426	14904	5.18	0.36
			1.481	(13626)	(5.99)	96.36
35 % HF in dichloromethane						
	8.66	0.79	1.427	14782	5.33	0.43
			1.481	(13435)	(6.12)	96.45
35 % HF in acetonitrile						
	8.86	0.80	1.428	14745	5.34	0.45
			1.481	(13390)	(6.12)	96.24

Table S13: Calculated key parameters for **13**. Total dipole moment, spin expectation value (theoretical value would be 0.75), torsion angle of the biphenylaxis, key distance between the nitrogen/carbon atom (large one is the C-C distance) and the carbon atom of the outer phenyl ring as well as first excitation energy and transition dipole moments .All structures were optimized in the given solvent and with a = 0.35. The values in braces are calculations with a = 0.30 in TDDFT.

13	μ_a /D	$\langle S^2 \rangle$	torsion /°	C_{Ar}-N/C /Å	E_{ab} /cm^{-1}	μ_{ab} /D
35 % HF in gas						
	3.13	0.79	69.9	1.422	16000	2.01
				1.481	(13899)	(2.09)
35 % HF in hexane						
	3.16	0.79	69.8	1.423	15743	2.19
				1.481	(13628)	(2.29)
35 % HF in dichloromethane						
	3.05	0.79	71.4	1.423	15705	2.06
				1.480	(13562)	(2.15)
35 % HF in acetonitrile						
	2.83	0.79	70.4	1.423	15596	2.13
				1.481	(13454)	(2.23)

Table S14: Calculated key parameters for **13**. Total dipole moment, spin expectation value (theoretical value would be 0.75), torsion angle of the biphenylaxis, key distance between the nitrogen/carbon atom (large one is the C-C distance) and the carbon atom of the outer phenyl ring as well as first excitation energy and transition dipole moments .All structures were optimized in the given solvent and with a = 0.35. The values in braces are calculations with a = 0.30 in TDDFT. The influence of the rotational angle of the biphenylaxis was investigated by single point calculations on the bases on the optimized structure, therefore no C-N/C-C distances are given. The different diasteremere was also studied by the same procedure for dichloromethane.

molecule 14	μ_a /D	$\langle S^2 \rangle$	**torsion /°**	C_{Ar}-N/C /Å	E_{ab} /cm^{-1}	μ_{ab} /D
35 % HF in gas						
	3.71	0.79	69.1	1.420	17120	2.08
				1.480	(15087)	(2.12)
35 % HF in hexane						
	3.79	0.79	70.0	1.420	16735	2.15
				1.481	(14674)	2.21)
35 % HF in dichloromethane						
	3.94	0.79	69.4	1.421	16534	2.25
				1.480	(14463)	(2.32)
	3.73	0.79	90.0		16709	0.07
	4.28	0.79	50.0		14498	3.91
	4.44	0.79	30.0		15429	4.51
	4.02	0.79	10.0		15121	4.87
35 % HF in dichloromethane (diastereomere)						
	3.87	0.79	72.7	1.421	16624	2.07
				1.481		
35 % HF in acetonitrile						
	4.01	0.79	70.8	1.412	16545	2.10
				1.480	(14457)	(2.16)

Table S15: Calculated key parameters for **15**. Total dipole moment, spin expectation value (theoretical value would be 0.75), torsion angle of the biphenylaxis, key distance between the nitrogen/carbon atom (large one is the C-C distance, values in brackets define the distance to the tosyl-ring) and the carbon atom of the outer phenyl ring as well as first excitation energy and transition dipole moments .All structures were optimized in the given solvent and with $a = 0.35$. The values in braces are calculations with $a = 0.30$ in TDDFT.

molecule 15	μ_a /D	$\langle S^2 \rangle$	**torsion /°**	C_{Ar}-N/C /Å	E_{ab} /cm^{-1}	μ_{ab} /D
35 % HF in gas						
	2.96	0.79	70.4	1.415[1.422]	18158	1.91
				1.481	(16094)	(1.92)
35 % HF in hexane						
	3.10	0.79	71.9	1.414[1.422]	17743	1.93
				1.480	(15646)	(1.95)
35 % HF in dichloromethane						
	3.33	0.79	72.6	1.414[1.423]	17471	1.88
				1.481	(15351)	(1.91)
35 % HF in acetonitrile						
	3.40	0.79	72.0	1.413[1.423]	17407	1.92
				1.480	(15288)	(1.95)

Table S16: Calculated key parameters for **16**. Total dipole moment, spin expectation value (theoretical value would be 0.75), torsion angle of the biphenylaxis, key distance between the nitrogen/carbon atom (large one is the C-C distance) and the carbon atom of the outer phenyl ring as well as first excitation energy and transition dipole moments .All structures were optimized in the given solvent and with $a = 0.35$. The values in braces are calculations with $a = 0.30$ in TDDFT.

molecule 16	μ_a /D	$\langle S^2 \rangle$	**torsion /°**	C_{Ar}-N/C /Å	E_{ab} /cm^{-1}	μ_{ab} /D
35 % HF in gas						
	0.48	0.79	72.8	1.417	19162	1.69
				1.480	(17064)	(1.67)
35 % HF in hexane						
	0.45	0.79	72.1	1.417	18674	1.89
				1.480	(16568)	(1.88)
35 % HF in dichloromethane						
	0.35	0.79	73.6	1.417	18304	1.78
				1.480	(16167)	(1.78)
35 % HF in acetonitrile						
	0.30	0.79	74.5	1.417	18244	1.66
				1.480	(16092)	(1.66)

Table S17: Calculated key parameters for **17**. Total dipole moment (negative sign means that it points in the opposite direction compared to **11-16**), spin expectation value (theoretical value would be 0.75), torsion angle of the biphenylaxis, key distance between the nitrogen/carbon atom (large one is the C-C distance, values in brackets define the distance to the benzonitrile-ring) and the carbon atom of the outer phenyl ring as well as first excitation energy and transition dipole moments .All structures were optimized in the given solvent and with a = 0.35. The values in braces are calculations with a = 0.30 in TDDFT. The different diastereomere was also studied by the same procedure for dichloromethane.

molecule 17	μ_a /D	$\langle S^2 \rangle$	**torsion** /°	C_{Ar}-N/C /Å	E_{ab}/cm^{-1}	μ_{ab} /D
35 % HF in gas						
	-4.10	0.79	71.6	1.421[1.405]	20799	1.74
				1.480	(18906)	(1.74)
35 % HF in hexane						
	-4.43	0.79	69.6	1.422[1.404]	20274	2.07
				1.480	(18348)	(2.06)
35 % HF in dichloromethane						
	-5.18	0.79	73.6	1.423[1.400]	20095	1.77
				1.480	(18031)	(1.70)
35 % HF in dichloromethane (diastereomere)						
	-5.29	0.79	81.2	1.423[1.400]	20314	1.07
				1.480		
35 % HF in acetonitrile						
	-5.54	0.79	79.5	1.422[1.398]	20281	1.21
				1.480	(18118)	(1.13)

Electro-optical absorption spectroscopy

Dipole moments of the ground state μ_a and the dipole moment differences $\Delta\mu_{ab} = \mu_b - \mu_a$ (μ_b: Franck Condon excited state dipole moment) of mixed-valence compounds **13**-**17** have been determined by means of the electro-optical absorption (EOA) spectroscopy in anhydrous cyclohexane at 298 K (Figure S1). The difference of absorption of a solution with ($\varepsilon^E(\varphi,\tilde{\nu})$) and without ($\varepsilon(\tilde{\nu})$) an externally applied electric field **E** is measured with light parallelly ($\varphi = 0°$) and perpendicularly ($\varphi = 90°$) polarized to the direction of **E**. For uniaxial phases, induced in a solution by both an alternating and a constant electric field of about $3 \cdot 10^6$ V m^{-1}, the dichroism $\varepsilon^E(\varphi,\tilde{\nu}) - \varepsilon(\tilde{\nu})$ depends on the orientational order of the molecules due to their ground state dipole moment μ_a, the shift of the absorption band proportional to the dipole moments difference $\Delta\mu_{ab}$, and on the electric field dependence of the electric transition dipole moment μ_{ab}(**E**). UV/VIS spectra, required for the multi linear regression of the EOA spectra (Table S18), were recorded with a Perkin-Elmer Lambda 950 spectrophotometer.

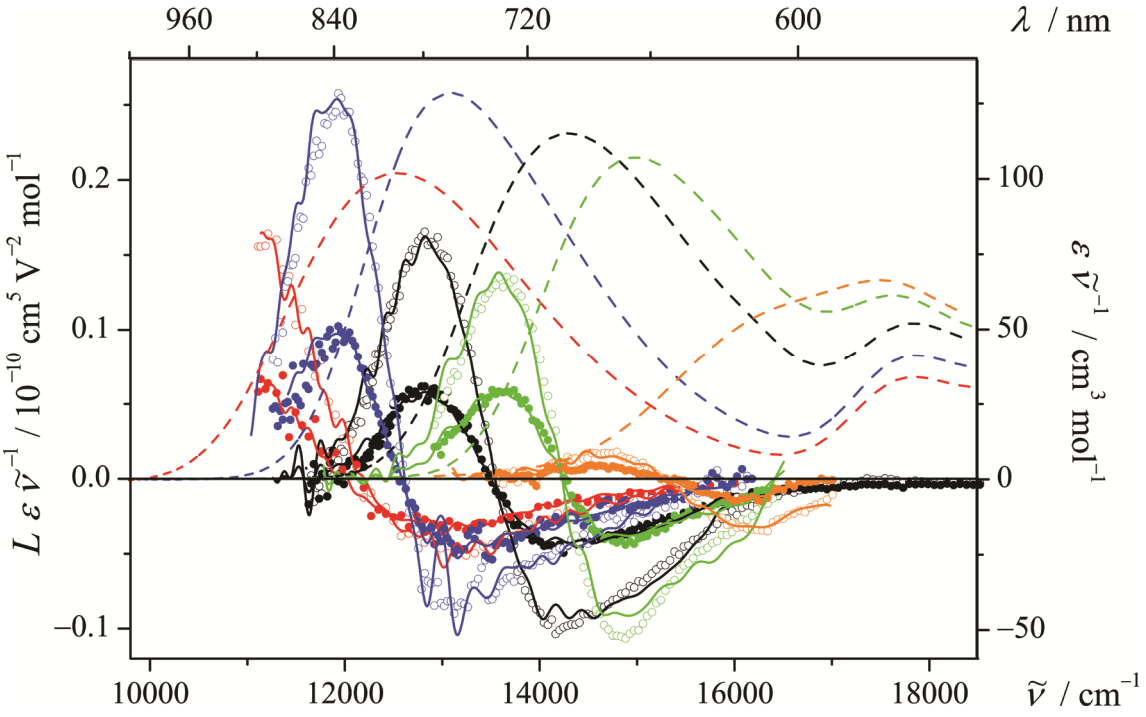
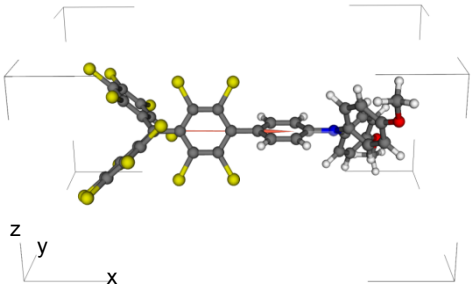


Figure S1. UV/VIS- (----) and EOA-spectrum ($\varphi = 0°$: ○; 90°: ●) as well as the multi linear regressions (—) of mixed-valence compounds **13** (----,○,●,—), **14** (----,○,●,—), **15** (----,○,●,—), **16** (----,○,●,—), and **17** (----,○ ,● ,—) measured in cyclohexane at 298 K.

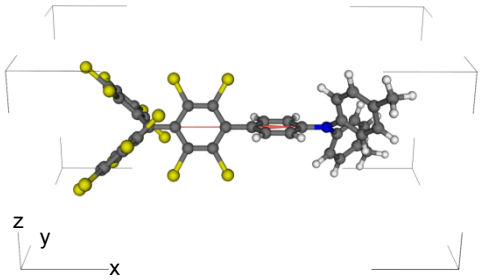
Table S18. Optical parameters (λ_{ab}: absorption wavelength; ε_{max}: molar decadic extinction coefficient), electro-optical coefficients (*D* - *I*), calculated ground-state dipole moment μ_a, dipole moment difference $\Delta\mu_{ab}$ and angle θ between μ_{ab} and $\Delta\mu_{ab}$ from analysis of the electro-optical absorption spectra of **13-17** in cyclohexane at 298 K. Cavity field corrections (Onsager´s model, spherical cavity) for cyclohexane were performed with $f = 1.2018$ ($\varepsilon_r = 2.015$).

		13 *(OMe/OMe)*	**14** *(Me/Me)*	**15** *(Me/Cl)*	**16** *(Cl/Cl)*	**17** *(CN/Cl)*
λ_{ab}	/ nm	790.4	759.5	693.4	662.2	568.4
ε_{max}	/ m^2 mol^{-1}	130	170	165	161	117
D	/ 10^{-20} V^{-2} m^2	473 ± 238	330 ± 85	–342 ± 74	–152 ± 95	–354 ± 113
E	/ 10^{-20} V^{-2} m^2	4349 ± 1429	3598 ± 507	–611 ± 445	–924 ± 572	–3685 ± 679
F	/ 10^{-40} C V^{-1} m^2	5886 ± 713	5480 ± 191	3742 ± 201	3089 ± 246	–80 ± 387
G	/ 10^{-40} C V^{-1} m^2	5054 ± 713	4726 ± 191	3479 ± 201	2555 ± 246	622 ± 387
H	/ 10^{-60} C^2 m^2	15180 ± 3395	12924 ± 744	13029 ± 620	13325 ± 772	11273 ± 1160
I	/ 10^{-60} C^2 m^2	12705 ± 3395	11963 ± 744	12284 ± 620	11278 ± 772	7700 ± 1160
μ_a	/ D	4.6 ± 0.6	4.6 ± 0.2	3.2 ± 0.2	2.5 ± 0.2	0.3 ± 0.4
$\Delta\mu_{ab}$	/ D	30.7 ± 6.9	28.4 ± 1.6	28.5 ± 1.4	28.8 ± 1.7	26.5 ± 2.7
θ	/ °	23.8 ± 5.3	15.8 ± 0.9	13.8 ± 0.2	23.1 ± 1.3	34.3 ± 3.5

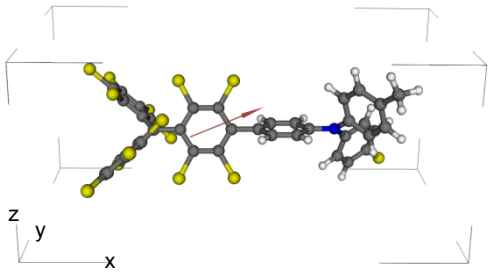
Computed dipole moments



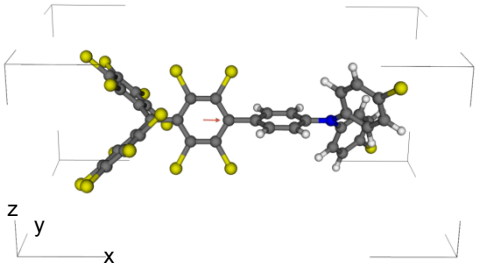
13, *X = 2.8 D; Y = 0.0 D; Z = 0.0 D;* Total = 2.8 D



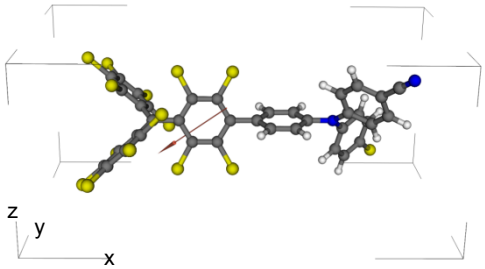
14, *X = 3.8 D; Y = 0.0 D; Z = 0.0 D;* Total = 3.8 D



15, *X = 2.0 D; Y = (-)1.9D; Z = 1.5 D;* Total = 3.2 D



16, *X = 0.5 D; Y = 0.0D; Z = 0.0 D;* Total = 0.5 D



17, *X = (-)2.1 D; Y = 3.1 D; Z = (-)2.5 D;* Total = (-)4.5 D

Figure S2. Computed dipole moments of **13-17**, obtained by Gaussian 03[84] calculations and plotted with the Molekel program (version 5.4)[96].

Cartesian coordinates of optimized structures

Table S19. Cartesian coordinates of optimized structures for **5-17**.

5 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -2336.475874521 Hartree

	X	Y	Z
C	0.0820932	0.0703383	4.0443469
C	0.0624702	0.0392609	5.4536318
C	0.0927244	0.0912618	2.8244796
C	0.0973737	0.1082619	1.4130731
C	1.1866475	-0.4266738	0.686692
C	1.1862588	-0.4171113	-0.6924863
C	0.0965608	0.1279864	-1.4106918
C	-0.992276	0.6640006	-0.6842754
C	-0.9918264	0.6543658	0.6947761
H	2.0293024	-0.8486	1.2294059
H	2.0287789	-0.8310021	-1.2415457
C	0.0917227	0.1310489	-2.8221384
H	-1.834911	1.0858913	-1.2270303
H	-1.833933	1.0690359	1.2438841
C	-1.0263743	0.5760609	6.1795993
C	-1.0558427	0.5357741	7.5565058
C	0.0101992	-0.0419759	8.2874096
C	1.1053064	-0.5738783	7.564486
C	1.1264823	-0.5354409	6.1873812
H	-1.8475864	1.0390797	5.637236
H	-1.896823	0.9693828	8.0894566
N	-0.0190168	-0.0885141	9.6711534
H	1.9261236	-1.0386081	8.1027103
H	1.9672383	-0.9682615	5.6500429
C	0.0825143	0.1286447	-4.0422311
C	0.0669566	0.120242	-5.4517962
C	1.1336746	-0.4418672	-6.1911868
C	1.1185654	-0.4557623	-7.5688653
C	0.027575	0.090572	-8.2874521
C	-1.0421688	0.6543969	-7.5504555
C	-1.0187173	0.6697982	-6.1731309
H	1.9724329	-0.8838582	-5.6581914
H	1.9422591	-0.9105716	-8.11099
N	0.0076633	0.0739015	-9.6714439
H	-1.8800737	1.098848	-8.0791456
H	-1.8420069	1.1237438	-5.6262388
C	1.2161418	0.0478351	-10.4226326
C	-1.2219046	0.0792783	-10.388138

5 with a = 0.35 in gas phase (C_i symmetry)

Energy = -2336.475889283 Hartree

	X	Y	Z
C	-0.0009058	-0.025852	4.0433852
C	-0.0027801	-0.0368044	5.4529787
C	-0.0001898	-0.0175101	2.823284
C	0.00002	-0.0086112	1.4119134
C	1.0961011	-0.5307526	0.6863333
C	1.0960889	-0.5223379	-0.6927946
C	-0.00002	0.0086112	-1.4119134
C	-1.0961011	0.5307526	-0.6863333
C	-1.0960889	0.5223379	0.6927946
H	1.9439282	-0.9411949	1.2297682
H	1.9438682	-0.9261569	-1.2412411
C	0.0001898	0.0175101	-2.823284
H	-1.9439282	0.9411949	-1.2297682
H	-1.9438682	0.9261569	1.2412411
C	-1.0832269	0.5074145	6.18597
C	-1.0903043	0.49409	7.5636378
C	-0.0092813	-0.0632575	8.2887241
C	1.0760372	-0.605461	7.5583085
C	1.0750551	-0.5933991	6.1807129
H	-1.9154991	0.9558068	5.6481336
H	-1.9246653	0.9345066	8.1013291
N	-0.0138228	-0.0789227	9.6729611
H	1.9075732	-1.0561619	8.091849
H	1.9094253	-1.0323266	5.6383366
C	0.0009058	0.025852	-4.0433852
C	0.0027801	0.0368044	-5.4529787
C	1.0832269	-0.5074145	-6.18597
C	1.0903043	-0.49409	-7.5636378
C	0.0092813	0.0632575	-8.2887241
C	-1.0760372	0.605461	-7.5583085
C	-1.0750551	0.5933991	-6.1807129
H	1.9154991	-0.9558068	-5.6481336
H	1.9246653	-0.9345066	-8.1013291
N	0.0138228	0.0789227	-9.6729611
H	-1.9075732	1.0561619	-8.091849
H	-1.9094253	1.0323266	-5.6383366
C	1.2352003	0.0802569	-10.4031547
C	-1.2038794	0.0931736	-10.4098066

C	-1.2535138	-0.1133924	10.3775117	C	-1.2352003	-0.0802569	10.4031547
C	1.1853398	-0.1113267	10.4285904	C	1.2038794	-0.0931736	10.4098066
C	2.1960449	0.823741	10.1931806	C	2.2154486	0.8310688	10.1381127
C	3.3715281	0.8096703	10.9386945	C	3.4044305	0.8238279	10.8621888
C	3.5467638	-0.1444931	11.9495081	C	3.5923082	-0.1113637	11.8883155
C	2.5258532	-1.0788258	12.1940078	C	2.5702545	-1.0339396	12.1699029
C	1.3640886	-1.0630378	11.4456862	C	1.3951942	-1.0254431	11.4422593
H	2.061156	1.5791943	9.4220856	H	2.0714219	1.5719651	9.3546786
H	4.1346582	1.5540715	10.7334533	H	4.1685911	1.5587394	10.6284479
O	4.6358396	-0.2407034	12.7261966	O	4.6952313	-0.199725	12.6462802
H	2.6795993	-1.8152364	12.9792007	H	2.7336253	-1.7556445	12.9666343
H	0.5832575	-1.7951573	11.6385705	H	0.6133601	-1.7482742	11.6638825
C	-2.2699435	-1.012617	10.0138337	C	-2.2596616	-0.9878113	10.086399
C	-3.4640353	-1.0401376	10.709505	C	-3.4395172	-0.9932446	10.8067595
C	-3.6761352	-0.1790923	11.7995924	C	-3.6281399	-0.1008566	11.8757608
C	-2.6602803	0.7100368	12.174847	C	-2.604043	0.7972884	12.2039006
C	-1.4635607	0.7377582	11.4651722	C	-1.4219528	0.8023824	11.4695462
H	-2.1121283	-1.6975777	9.1838077	H	-2.1195727	-1.6965675	9.2732847
H	-4.2557506	-1.7356207	10.4412364	H	-4.2370232	-1.6951588	10.5750415
O	-4.8643454	-0.2821041	12.4127796	O	-4.8033566	-0.1843277	12.5165583
H	-2.7928225	1.3889549	13.0113654	H	-2.719019	1.5003008	13.0229838
H	-0.6828438	1.4358725	11.7582291	H	-0.6347441	1.5073819	11.7266081
C	2.2470549	0.9632879	-10.1540706	C	2.2596616	0.9878113	-10.086399
C	3.412833	0.9445101	-10.8967361	C	3.4395172	0.9932446	-10.8067595
C	3.5802417	0.018353	-11.94019	C	3.6281399	0.1008566	-11.8757608
C	2.5499799	-0.8893082	-12.2192237	C	2.604043	-0.7972884	-12.2039006
C	1.3820112	-0.8692132	-11.462928	C	1.4219528	-0.8023824	-11.4695462
H	2.1224603	1.6978722	-9.3615458	H	2.1195727	1.6965675	-9.2732847
H	4.2149389	1.6527985	-10.7029861	H	4.2370232	1.6951588	-10.5750415
O	4.7423956	0.0809247	-12.6068399	O	4.8033566	0.1843277	-12.5165583
H	2.6489339	-1.6184158	-13.0172961	H	2.719019	-1.5003008	-13.0229838
H	0.5892703	-1.5808073	-11.6821674	H	0.6347441	-1.5073819	-11.7266081
C	-2.2374893	-0.8270273	-10.0739477	C	-2.2154486	-0.8310688	-10.1381127
C	-3.4378581	-0.8292398	-10.7788938	C	-3.4044305	-0.8238279	-10.8621888
C	-3.6335697	0.0775462	-11.8288229	C	-3.5923082	0.1113637	-11.8883155
C	-2.6077239	0.981576	-12.1533062	C	-2.5702545	1.0339396	-12.1699029
C	-1.4213585	0.9830685	-11.444255	C	-1.3951942	1.0254431	-11.4422593
H	-2.0873477	-1.5463507	-9.2718567	H	-2.0714219	-1.5719651	-9.3546786
H	-4.2047822	-1.5496966	-10.511861	H	-4.1685911	-1.5587394	-10.6284479
O	-4.7476661	0.1543333	-12.5717047	O	-4.6952313	0.199725	-12.6462802
H	-2.7770885	1.6812064	-12.9683295	H	-2.7336253	1.7556445	-12.9666343
H	-0.6365062	1.69133	-11.6994125	H	-0.6133601	1.7482742	-11.6638825
C	-5.1594409	0.5349735	13.5211005	C	-5.0733894	0.6638887	13.6079243
C	5.7059227	0.6581499	12.5551251	C	5.7690133	0.6862713	12.4351963
C	-5.8254523	-0.7152479	-12.3184276	C	-5.7690133	-0.6862713	-12.4351963

C	4.9912373	-0.8024441	-13.6749041
H	-6.1689264	0.2669344	13.8438065
H	-4.4597081	0.3587555	14.3508785
H	-5.1405355	1.6014292	13.2535465
H	6.4651484	0.3801426	13.2908372
H	6.1399773	0.583297	11.5472937
H	5.3944622	1.6969277	12.7378295
H	-6.6056526	-0.4609632	-13.0406964
H	-5.5377469	-1.767421	-12.4585066
H	-6.222311	-0.5820094	-11.3013097
H	5.9861937	-0.5565614	-14.0553082
H	4.9841729	-1.8507124	-13.3426701
H	4.2573382	-0.675393	-14.4839883

C	5.0733894	-0.6638887	-13.6079243
H	-6.0756458	0.4061859	13.9601907
H	-4.355493	0.5100343	14.4266068
H	-5.0597289	1.7224445	13.3102853
H	6.5400648	0.4177616	13.1620838
H	6.1826436	0.5859491	11.4209721
H	5.469521	1.7313784	12.6010765
H	-6.5400648	-0.4177616	-13.1620838
H	-5.469521	-1.7313784	-12.6010765
H	-6.1826436	-0.5859491	-11.4209721
H	6.0756458	-0.4061859	-13.9601907
H	5.0597289	-1.7224445	-13.3102853
H	4.355493	-0.5100343	-14.4266068

5 with *a* = 0.35 in hexane
(C_1 symmetry)

Energy = -2336.495338578 Hartree

	X	Y	Z
C	-0.0068858	0.004056	4.0431983
C	-0.0082823	-0.0150231	5.453223
C	-0.0054132	0.0178526	2.8230785
C	-0.0034869	0.0303538	1.4113072
C	1.0887018	-0.5015158	0.6869576
C	1.090029	-0.4921892	-0.6924025
C	-0.0009153	0.0493864	-1.4115695
C	-1.0929291	0.5818644	-0.6871747
C	-1.0941129	0.5726008	0.6922953
H	1.9324045	-0.9205481	1.2301611
H	1.9348469	-0.9036699	-1.2397183
C	-0.0000464	0.0563747	-2.8235837
H	-1.9366789	1.0008771	-1.2304104
H	-1.9387522	0.9843526	1.2395994
C	-1.0876749	0.526526	6.1900259
C	-1.09328	0.5045416	7.567679
C	-0.0128457	-0.0597739	8.2879179
C	1.070698	-0.6000538	7.5536901
C	1.0693565	-0.5787125	6.1761601
H	-1.919821	0.9801597	5.6564398
H	-1.9263938	0.9438408	8.1079255
N	-0.0154569	-0.0834411	9.6719914
H	1.9015835	-1.0567307	8.0827982
H	1.9028794	-1.0158444	5.6310734
C	0.0013842	0.0605562	-4.04379
C	0.003831	0.0646554	-5.45372
C	1.0854001	-0.483123	-6.1826592

5 with *a* = 0.35 in hexane
(C_i symmetry)

Energy = -2336.495310492 Hartree

	X	Y	Z
C	-0.0090367	-0.0247849	4.0437755
C	-0.0102074	-0.0345805	5.4535275
C	-0.0074944	-0.017193	2.8235367
C	-0.0044396	-0.008662	1.4115458
C	1.1063843	-0.5051197	0.6900255
C	1.1108943	-0.4965488	-0.6893324
C	0.0044396	0.008662	-1.4115458
C	-1.1063843	0.5051197	-0.6900255
C	-1.1108943	0.4965488	0.6893324
H	1.9619384	-0.8959298	1.2357623
H	1.9703464	-0.8797749	-1.2343125
C	0.0074944	0.017193	-2.8235367
H	-1.9619384	0.8959298	-1.2357623
H	-1.9703464	0.8797749	1.2343125
C	-1.0957353	0.4997133	6.1867438
C	-1.1001174	0.4890391	7.5644917
C	-0.0127235	-0.0577061	8.2886929
C	1.0767188	-0.5913476	7.5575726
C	1.07444	-0.5800156	6.1799922
H	-1.9335588	0.9390429	5.6501772
H	-1.9380581	0.9225645	8.1019876
N	-0.0152181	-0.0713174	9.6724573
H	1.9134377	-1.0339816	8.0894695
H	1.9129293	-1.0110263	5.6377325
C	0.0090367	0.0247849	-4.0437755
C	0.0102074	0.0345805	-5.4535275
C	1.0957353	-0.4997133	-6.1867438

C	1.0920535	-0.4787168	-7.5604947	C	1.1001174	-0.4890391	-7.5644917
C	0.0100138	0.0732171	-8.2885147	C	0.0127235	0.0577061	-8.2886929
C	-1.0755862	0.6201986	-7.5617753	C	-1.0767188	0.5913476	-7.5575726
C	-1.0748379	0.6165634	-6.1840368	C	-1.07444	0.5800156	-6.1799922
H	1.9181777	-0.9278388	-5.642699	H	1.9335588	-0.9390429	-5.6501772
H	1.9268278	-0.9227236	-8.0946632	H	1.9380581	-0.9225645	-8.1019876
N	0.0139492	0.0800115	-9.6726686	N	0.0152181	0.0713174	-9.6724573
H	-1.9078854	1.0671932	-8.0973097	H	-1.9134377	1.0339816	-8.0894695
H	-1.9098295	1.0582075	-5.6449745	H	-1.9129293	1.0110263	-5.6377325
C	1.2345949	0.0778414	-10.4031389	C	1.2349787	0.0756372	-10.405313
C	-1.2041615	0.0854395	-10.4083223	C	-1.2034891	0.0866674	-10.4076137
C	-1.2350526	-0.087253	10.4043975	C	-1.2349787	-0.0756372	10.405313
C	1.2036003	-0.1035898	10.406117	C	1.2034891	-0.0866674	10.4076137
C	2.2150648	0.8219514	10.1381484	C	2.2129161	0.8409389	10.1390793
C	3.406709	0.8077378	10.8576267	C	3.4047497	0.82957	10.8585108
C	3.5970289	-0.1361449	11.8752755	C	3.5977252	-0.1144305	11.8756109
C	2.5749444	-1.0594405	12.1539477	C	2.5764752	-1.037887	12.1568911
C	1.3969182	-1.0440238	11.4303702	C	1.3983441	-1.0252833	11.4333474
H	2.0687491	1.5694062	9.361585	H	2.0656257	1.5873998	9.3616253
H	4.170797	1.5434343	10.62637	H	4.1669835	1.5672283	10.6273241
O	4.7046105	-0.2315924	12.6275964	O	4.7071481	-0.2097317	12.6252625
H	2.738702	-1.7883144	12.9442151	H	2.7414739	-1.7656479	12.9479286
H	0.6163339	-1.7687494	11.6496558	H	0.619012	-1.7511888	11.6534068
C	-2.261848	-0.990359	10.0834566	C	-2.2543879	-0.9911318	10.0959876
C	-3.4401452	-0.9983432	10.8069984	C	-3.4323692	-0.9998659	10.8202211
C	-3.6245531	-0.1121096	11.8817759	C	-3.6231476	-0.1023461	11.8844271
C	-2.5980587	0.781755	12.2140339	C	-2.6047076	0.8053731	12.2038813
C	-1.4178656	0.7894567	11.4765717	C	-1.4246129	0.8133273	11.4661204
H	-2.1254648	-1.6944874	9.2659107	H	-2.1120689	-1.7043991	9.2873088
H	-4.2387912	-1.6976537	10.5708082	H	-4.2254593	-1.708407	10.5929363
O	-4.7990302	-0.1967237	12.5261862	O	-4.7955771	-0.1904224	12.5321656
H	-2.7097381	1.4802188	13.0373927	H	-2.7225034	1.51392	13.0177279
H	-0.6293132	1.4918149	11.7362421	H	-0.6418887	1.5257804	11.7163647
C	2.2593555	0.9862128	-10.0901903	C	2.2543879	0.9911318	-10.0959876
C	3.4393143	0.9876131	-10.8110546	C	3.4323692	0.9998659	-10.8202211
C	3.6273801	0.0894532	-11.8751994	C	3.6231476	0.1023461	-11.8844271
C	2.6028779	-0.8095523	-12.1998157	C	2.6047076	-0.8053731	-12.2038813
C	1.4209636	-0.8107718	-11.4650308	C	1.4246129	-0.8133273	-11.4661204
H	2.1200466	1.6994146	-9.2808635	H	2.1120689	1.7043991	-9.2873088
H	4.236304	1.6906975	-10.5807216	H	4.2254593	1.708407	-10.5929363
O	4.8034046	0.1680511	-12.5174952	O	4.7955771	0.1904224	-12.5321656
H	2.7172762	-1.5169362	-13.0151192	H	2.7225034	-1.51392	-13.0177279
H	0.6339332	-1.5173392	-11.7185496	H	0.6418887	-1.5257804	-11.7163647
C	-2.2124479	-0.8402897	-10.128459	C	-2.2129161	-0.8409389	-10.1390793
C	-3.402181	-0.8423372	-10.8511853	C	-3.4047497	-0.82957	-10.8585108

C	-3.5940901	0.0851079	-11.8835906
C	-2.5757472	1.0091212	-12.1734765
C	-1.3993702	1.0098669	-11.4470098
H	-2.0650171	-1.5750736	-9.3399793
H	-4.1632014	-1.5783356	-10.611092
O	-4.6998289	0.1633313	-12.6403919
H	-2.7406999	1.7255215	-12.9747463
H	-0.6213528	1.7347294	-11.6754963
C	-5.0625172	0.6504917	13.6222791
C	5.7782221	0.6572866	12.4149471
C	-5.7685288	-0.7293981	-12.4189013
C	5.0702346	-0.6901631	-13.6042884
H	-6.0638975	0.3944631	13.9780944
H	-4.3410461	0.4921381	14.4364515
H	-5.0468231	1.709086	13.3262925
H	6.5541569	0.3837987	13.134661
H	6.1837869	0.5634549	11.3972952
H	5.4785456	1.7004251	12.5900201
H	-6.5434122	-0.4717229	-13.1454822
H	-5.4614584	-1.7730107	-12.5773714
H	-6.1788236	-0.6235749	-11.4043451
H	6.0734287	-0.4389877	-13.9583242
H	5.0517689	-1.7458679	-13.2984176
H	4.3525261	-0.5389174	-14.4231073

C	-3.5977252	0.1144305	-11.8756109
C	-2.5764752	1.037887	-12.1568911
C	-1.3983441	1.0252833	-11.4333474
H	-2.0656257	-1.5873998	-9.3616253
H	-4.1669835	-1.5672283	-10.6273241
O	-4.7071481	0.2097317	-12.6252625
H	-2.7414739	1.7656479	-12.9479286
H	-0.619012	1.7511888	-11.6534068
C	-5.0616167	0.6604263	13.6248882
C	5.7846934	0.6720122	12.4027868
C	-5.7846934	-0.6720122	-12.4027868
C	5.0616167	-0.6604263	-13.6248882
H	-6.0588094	0.3970467	13.9871953
H	-4.3346977	0.5131576	14.4362984
H	-5.057254	1.7176061	13.3235891
H	6.5645933	0.3950291	13.116946
H	6.1816884	0.5735837	11.3822075
H	5.4933757	1.7174864	12.577863
H	-6.5645933	-0.3950291	-13.116946
H	-5.4933757	-1.7174864	-12.577863
H	-6.1816884	-0.5735837	-11.3822075
H	6.0588094	-0.3970467	-13.9871953
H	5.057254	-1.7176061	-13.3235891
H	4.3346977	-0.5131576	-14.4362984

5 with a = 0.35 in DCM

(C_1 symmetry)

Energy = -2336.524359868 Hartree

	X	Y	Z
C	-0.0165245	-0.0080893	4.0130766
C	-0.0159356	-0.0273661	5.4367848
C	-0.0158147	0.0062232	2.7970598
C	-0.0137938	0.0205204	1.3732637
C	1.0283389	-0.5943468	0.6492717
C	1.0303599	-0.5827157	-0.735082
C	-0.0097708	0.0455765	-1.4489902
C	-1.051616	0.6616305	-0.7270523
C	-1.0535446	0.6486816	0.6573748
H	1.8369255	-1.0823892	1.1884392
H	1.8405457	-1.0616746	-1.2802796
C	-0.0077484	0.0564977	-2.8716152
H	-1.8603314	1.1501101	-1.2659484
H	-1.8637484	1.1270345	1.2027813
C	-1.0768992	0.5324011	6.1747281
C	-1.0778011	0.5145301	7.5590697

5 with a = 0.35 in DCM

(C_i symmetry)

Energy = -2336.520739831 Hartree

	X	Y	Z
C	-0.0357163	-0.0542906	4.0436128
C	-0.0359376	-0.0672772	5.4529354
C	-0.0298494	-0.0402928	2.8229775
C	-0.0170067	-0.0212272	1.4108953
C	1.1212762	-0.464126	0.6961602
C	1.1383213	-0.4429684	-0.6830355
C	0.0170067	0.0212272	-1.4108953
C	-1.1212762	0.464126	-0.6961602
C	-1.1383213	0.4429684	0.6830355
H	1.9879205	-0.823502	1.2459366
H	2.0189537	-0.7840928	-1.2220642
C	0.0298494	0.0402928	-2.8229775
H	-1.9879205	0.823502	-1.2459366
H	-2.0189537	0.7840928	1.2220642
C	-1.1385296	0.4289226	6.1886154
C	-1.1375173	0.4216214	7.5661265

C	-0.0147721	-0.0703115	8.2790079	C	-0.0272007	-0.0832169	8.2880799
C	1.0484011	-0.6320774	7.540845	C	1.0769282	-0.5834948	7.5533016
C	1.046173	-0.6084159	6.1568988	C	1.0696126	-0.5752282	6.1762257
H	-1.9075526	0.9973045	5.647385	H	-1.9941363	0.8366763	5.655293
H	-1.9074671	0.9654157	8.0958551	H	-1.9885196	0.8278529	8.1039585
N	-0.0146568	-0.0933816	9.6714887	N	-0.0197016	-0.0872696	9.6696908
H	1.8788182	-1.0980043	8.0634423	H	1.9308261	-0.9963196	8.0812727
H	1.8764195	-1.0570399	5.6150171	H	1.9216424	-0.9773084	5.6329539
C	-0.0049471	0.0639707	-4.0879892	C	0.0357163	0.0542906	-4.0436128
C	-0.0003598	0.0697637	-5.5065803	C	0.0359376	0.0672772	-5.4529354
C	1.0134483	-0.6002587	-6.2264055	C	1.1385296	-0.4289226	-6.1886154
C	1.0214121	-0.5956603	-7.6073467	C	1.1375173	-0.4216214	-7.5661265
C	0.0084922	0.0767425	-8.3188891	C	0.0272007	0.0832169	-8.2880799
C	-1.008201	0.7466943	-7.610285	C	-1.0769282	0.5834948	-7.5533016
C	-1.0090104	0.7442818	-6.2291809	C	-1.0696126	0.5752282	-6.1762257
H	1.78763	-1.1378087	-5.6848862	H	1.9941363	-0.8366763	-5.655293
H	1.7940433	-1.1369135	-8.1462495	H	1.9885196	-0.8278529	-8.1039585
N	0.0127927	0.079114	-9.7224538	N	0.0197016	0.0872696	-9.6696908
H	-1.7768464	1.291374	-8.15141	H	-1.9308261	0.9963196	-8.0812727
H	-1.7863679	1.2794507	-5.6898305	H	-1.9216424	0.9773084	-5.6329539
C	1.2282332	0.1639446	-10.4245345	C	1.2327541	0.0845645	-10.4155239
C	-1.1975745	-0.0065211	-10.4327919	C	-1.2047439	0.0918365	-10.3973541
C	-1.2306819	-0.010436	10.4108408	C	-1.2327541	-0.0845645	10.4155239
C	1.2034587	-0.1929401	10.4061606	C	1.2047439	-0.0918365	10.3973541
C	2.229151	0.7354806	10.2254816	C	2.1981899	0.8533812	10.1314201
C	3.4192343	0.6460222	10.9473919	C	3.3971462	0.8485973	10.8390995
C	3.5889092	-0.3762949	11.8871098	C	3.6131124	-0.1083478	11.8392551
C	2.5552071	-1.3038237	12.0821232	C	2.6063298	-1.0470707	12.1209034
C	1.3832571	-1.2165697	11.3466968	C	1.4195306	-1.0394137	11.4098387
H	2.1016178	1.5423703	9.5064945	H	2.0340984	1.6064665	9.3641714
H	4.1957562	1.3856414	10.776541	H	4.1467773	1.5996465	10.610226
O	4.6967351	-0.5447608	12.6415158	O	4.7370092	-0.2021064	12.5709502
H	2.6982764	-2.0959164	12.8142457	H	2.7862669	-1.7842981	12.9001722
H	0.5923487	-1.9476688	11.5013441	H	0.6523734	-1.7787452	11.6277989
C	-2.2753234	-0.9176876	10.1805283	C	-2.242753	-1.0218836	10.1469038
C	-3.4503926	-0.8440423	10.9115578	C	-3.4129583	-1.0214588	10.8855461
C	-3.6079976	0.1279975	11.9108018	C	-3.6026736	-0.0913495	11.9211832
C	-2.5659762	1.0275538	12.1564231	C	-2.5943031	0.8413947	12.1971165
C	-1.394123	0.9566291	11.4024969	C	-1.4212922	0.8370841	11.4479938
H	-2.1612854	-1.6862498	9.4187785	H	-2.1004545	-1.7586345	9.3598292
H	-4.2630922	-1.5456971	10.7349063	H	-4.1980422	-1.7481046	10.688368
O	-4.7827811	0.1175394	12.5780261	O	-4.7658118	-0.1726397	12.5906721
H	-2.6546019	1.7920852	12.9223107	H	-2.7130988	1.5775877	12.9858162
H	-0.592263	1.6661723	11.5959623	H	-0.6462134	1.5683835	11.6654683
C	2.2581222	1.0167774	-9.973629	C	2.242753	1.0218836	-10.1469038

C	3.4438993	1.0985492	-10.6692342
C	3.6464443	0.3304465	-11.8345862
C	2.6233041	-0.5214884	-12.2867755
C	1.429869	-0.597984	-11.58809
H	2.1058293	1.6325386	-9.0912313
H	4.2382421	1.7655839	-10.3437375
O	4.8256539	0.4742976	-12.4363165
H	2.7574946	-1.1369172	-13.1702915
H	0.6534876	-1.2773403	-11.9298436
C	-2.2244572	-0.8591633	-9.9919858
C	-3.4165611	-0.9515112	-10.6908498
C	-3.6088835	-0.184125	-11.8535053
C	-2.5799808	0.6728059	-12.2959385
C	-1.3935824	0.7589663	-11.6019524
H	-2.0745657	-1.4757076	-9.1096674
H	-4.1841737	-1.6319614	-10.337017
O	-4.7172514	-0.2026657	-12.5913504
H	-2.7516615	1.2726289	-13.1862428
H	-0.6171969	1.440257	-11.9395013
C	-5.0076691	1.0625079	13.600327
C	5.77335	0.3554578	12.5028982
C	-5.8123262	-1.0238576	-12.2194774
C	5.1168527	-0.2456793	-13.6231234
H	-6.0084477	0.864243	13.9939133
H	-4.2762203	0.9596718	14.4147191
H	-4.9721034	2.0917039	13.2155577
H	6.5475297	0.0259059	13.2012413
H	6.1830545	0.3426184	11.4826739
H	5.476912	1.3832483	12.7567615
H	-6.5884574	-0.856029	-12.9694282
H	-5.5294246	-2.0843844	-12.2207285
H	-6.1965581	-0.7457331	-11.2297191
H	6.1257815	0.0493887	-13.9196215
H	5.0927762	-1.3283806	-13.4445158
H	4.412243	0.0117345	-14.424327

C	3.4129583	1.0214588	-10.8855461
C	3.6026736	0.0913495	-11.9211832
C	2.5943031	-0.8413947	-12.1971165
C	1.4212922	-0.8370841	-11.4479938
H	2.1004545	1.7586345	-9.3598292
H	4.1980422	1.7481046	-10.688368
O	4.7658118	0.1726397	-12.5906721
H	2.7130988	-1.5775877	-12.9858162
H	0.6462134	-1.5683835	-11.6654683
C	-2.1981899	-0.8533812	-10.1314201
C	-3.3971462	-0.8485973	-10.8390995
C	-3.6131124	0.1083478	-11.8392551
C	-2.6063298	1.0470707	-12.1209034
C	-1.4195306	1.0394137	-11.4098387
H	-2.0340984	-1.6064665	-9.3641714
H	-4.1467773	-1.5996465	-10.610226
O	-4.7370092	0.2021064	-12.5709502
H	-2.7862669	1.7842981	-12.9001722
H	-0.6523734	1.7787452	-11.6277989
C	-5.0186161	0.710561	13.6643203
C	5.8070695	0.6878106	12.3276835
C	-5.8070695	-0.6878106	-12.3276835
C	5.0186161	-0.710561	-13.6643203
H	-6.0040432	0.4468338	14.0572531
H	-4.2714212	0.596563	14.4618335
H	-5.033357	1.7569881	13.329904
H	6.6065496	0.4076242	13.0185519
H	6.1757079	0.5988338	11.2963437
H	5.5156361	1.7297283	12.5188691
H	-6.6065496	-0.4076242	-13.0185519
H	-5.5156361	-1.7297283	-12.5188691
H	-6.1757079	-0.5988338	-11.2963437
H	6.0040432	-0.4468338	-14.0572531
H	5.033357	-1.7569881	-13.329904
H	4.2714212	-0.596563	-14.4618335

5 with a = 0.35 in MeCN
(C_1 symmetry)

Energy = -2336.533155063 Hartree

	X	Y	Z
C	-0.0665484	-0.0644556	4.0120532
C	-0.0566061	-0.0757396	5.4367482
C	-0.0706226	-0.0540916	2.7961394
C	-0.0703852	-0.0413033	1.3710119
C	0.9783522	-0.6443159	0.647351

5 with a = 0.35 in MeCN
(C_i symmetry)

Energy = -2336.527451887 Hartree

	X	Y	Z
C	-0.0460916	-0.0504987	4.0438855
C	-0.0460041	-0.0637594	5.4537961
C	-0.0381122	-0.0394778	2.82335
C	-0.0215783	-0.0212067	1.4106738
C	1.111643	-0.4819834	0.6995061

C	0.9812256	-0.6307739	-0.7375653	C	1.1332121	-0.4607806	-0.6799364
C	-0.0645831	-0.0127719	-1.4512886	C	0.0215783	0.0212067	-1.4106738
C	-1.1137877	0.589923	-0.729617	C	-1.111643	0.4819834	-0.6995061
C	-1.1165896	0.5754541	0.655451	C	-1.1332121	0.4607806	0.6799364
H	1.7924177	-1.1242499	1.1856957	H	1.9709955	-0.8554495	1.2513788
H	1.7974568	-1.0998711	-1.2823409	H	2.0101896	-0.8158041	-1.2159946
C	-0.0590752	0.002958	-2.8753275	C	0.0381122	0.0394778	-2.82335
H	-1.9276904	1.0702077	-1.2680949	H	-1.9709955	0.8554495	-1.2513788
H	-1.9328454	1.0445738	1.2000014	H	-2.0101896	0.8158041	1.2159946
C	-1.103492	0.5037684	6.1792468	C	-1.1415429	0.4459434	6.1906958
C	-1.0915639	0.4991471	7.5640562	C	-1.138402	0.4382892	7.5684475
C	-0.0294081	-0.092113	8.2800585	C	-0.0330243	-0.079517	8.2880136
C	1.0180826	-0.6766002	7.5370581	C	1.0636779	-0.5935858	7.5522023
C	1.0035154	-0.6652768	6.1527431	C	1.0543712	-0.5856505	6.1750419
H	-1.933303	0.9747239	5.6558485	H	-1.9929983	0.8644057	5.6590426
H	-1.9105122	0.966365	8.1033295	H	-1.9835689	0.8547119	8.1076975
N	-0.0147312	-0.0991826	9.6724685	N	-0.0223003	-0.0823685	9.6702921
H	1.847428	-1.1489735	8.055501	H	1.9134242	-1.0165066	8.0788183
H	1.8232192	-1.1297421	5.6080581	H	1.9006519	-0.9983846	5.6307951
C	-0.0506832	0.0160605	-4.0910146	C	0.0460916	0.0504987	-4.0438855
C	-0.0361606	0.0314058	-5.5116854	C	0.0460041	0.0637594	-5.4537961
C	0.9930102	-0.6180236	-6.2267592	C	1.1415429	-0.4459434	-6.1906958
C	1.0130495	-0.6009822	-7.6083324	C	1.138402	-0.4382892	-7.5684475
C	-0.0023567	0.0639258	-8.3208806	C	0.0330243	0.079517	-8.2880136
C	-1.0348989	0.7122628	-7.6176291	C	-1.0636779	0.5935858	-7.5522023
C	-1.0483155	0.6969471	-6.2357808	C	-1.0543712	0.5856505	-6.1750419
H	1.7708552	-1.1485471	-5.6835868	H	1.9929983	-0.8644057	-5.6590426
H	1.7983711	-1.1255565	-8.1453744	H	1.9835689	-0.8547119	-8.1076975
N	0.0163754	0.0813745	-9.7268483	N	0.0223003	0.0823685	-9.6702921
H	-1.8065869	1.2503607	-8.1609703	H	-1.9134242	1.0165066	-8.0788183
H	-1.8389844	1.2152982	-5.6993829	H	-1.9006519	0.9983846	-5.6307951
C	1.2359852	0.2121337	-10.4119825	C	1.2327832	0.079133	-10.4191037
C	-1.1824332	-0.0318	-10.4491863	C	-1.2042713	0.08822	-10.3934624
C	-1.2189302	0.0334393	10.4245615	C	-1.2327832	-0.079133	10.4191037
C	1.207582	-0.2236676	10.3967688	C	1.2042713	-0.08822	10.3934624
C	2.2525342	0.6807896	10.2044923	C	2.2017733	0.8498369	10.1164165
C	3.4462775	0.5668954	10.9168567	C	3.403848	0.8435812	10.8184732
C	3.600627	-0.4562311	11.858523	C	3.6196093	-0.1081183	11.82368
C	2.5478921	-1.3595818	12.065374	C	2.6089101	-1.0391231	12.1171125
C	1.3719563	-1.2480915	11.339093	C	1.4186623	-1.0299798	11.4114625
H	2.1377287	1.4881173	9.4838231	H	2.0379616	1.5993667	9.3456927
H	4.2379432	1.288071	10.736927	H	4.1560571	1.5893273	10.5810969
O	4.711258	-0.6473702	12.6036551	O	4.7477031	-0.2030675	12.5496266
H	2.6784711	-2.1527461	12.7988023	H	2.7879648	-1.7725434	12.900279
H	0.5661918	-1.9608902	11.5026184	H	0.6489215	-1.7639965	11.6378559

C	-2.2832947	-0.8611643	10.2412321	C	-2.2477869	-1.0102257	10.1470824
C	-3.4462772	-0.7388232	10.9854028	C	-3.4140922	-1.0122966	10.8921253
C	-3.5712808	0.2718555	11.9504625	C	-3.5943114	-0.0918446	11.9380801
C	-2.5095213	1.160057	12.1487126	C	-2.5818404	0.8358354	12.2162796
C	-1.3501216	1.0389903	11.3820823	C	-1.4135955	0.8352254	11.4598376
H	-2.1949364	-1.6586423	9.5060481	H	-2.1125298	-1.7415223	9.3536347
H	-4.2741194	-1.4310913	10.8450447	H	-4.2023425	-1.7347858	10.691932
O	-4.7360751	0.308594	12.6341286	O	-4.7532596	-0.1764202	12.6154703
H	-2.5729683	1.9539199	12.8868496	H	-2.6939974	1.5657734	13.0116979
H	-0.532671	1.7401183	11.538014	H	-0.6362203	1.5639101	11.6782046
C	2.2357291	1.0863256	-9.9340871	C	2.2477869	1.0102257	-10.1470824
C	3.4259255	1.2141379	-10.6144786	C	3.4140922	1.0122966	-10.8921253
C	3.6636575	0.4714168	-11.7897254	C	3.5943114	0.0918446	-11.9380801
C	2.6717255	-0.4032675	-12.2675086	C	2.5818404	-0.8358354	-12.2162796
C	1.4732936	-0.525568	-11.5849137	C	1.4135955	-0.8352254	-11.4598376
H	2.0556215	1.6828884	-9.0438356	H	2.1125298	1.7415223	-9.3536347
H	4.1961797	1.8989504	-10.2685754	H	4.2023425	1.7347858	-10.691932
O	4.8446173	0.6593921	-12.3759379	O	4.7532596	0.1764202	-12.6154703
H	2.8342868	-1.0010764	-13.1583024	H	2.6939974	-1.5657734	-13.0116979
H	0.7219699	-1.2230665	-11.9454893	H	0.6362203	-1.5639101	-11.6782046
C	-2.1946972	-0.9083115	-10.0190706	C	-2.2017733	-0.8498369	-10.1164165
C	-3.3767706	-1.0266287	-10.7297759	C	-3.403848	-0.8435812	-10.8184732
C	-3.5748543	-0.2613324	-11.8932087	C	-3.6196093	0.1081183	-11.82368
C	-2.5615432	0.6197025	-12.3246863	C	-2.6089101	1.0391231	-12.1171125
C	-1.384352	0.73148	-11.6194727	C	-1.4186623	1.0299798	-11.4114625
H	-2.039535	-1.5232237	-9.1366735	H	-2.0379616	-1.5993667	-9.3456927
H	-4.1319673	-1.7251726	-10.3847751	H	-4.1560571	-1.5893273	-10.5810969
O	-4.6758808	-0.3034412	-12.6409821	O	-4.7477031	0.2030675	-12.5496266
H	-2.7379703	1.2180741	-13.2150218	H	-2.7879648	1.7725434	-12.900279
H	-0.6214721	1.4322484	-11.9474093	H	-0.6489215	1.7639965	-11.6378559
C	-4.9296456	1.2985497	13.6212429	C	-4.9904894	0.6921435	13.7054626
C	5.8051365	0.232161	12.4557143	C	5.8223135	0.6780332	12.2899135
C	-5.7561829	-1.1493817	-12.2785016	C	-5.8223135	-0.6780332	-12.2899135
C	5.1688882	-0.0341359	-13.5708031	C	4.9904894	-0.6921435	-13.7054626
H	-5.9285143	1.1352503	14.03502	H	-5.9729726	0.4271491	14.1049382
H	-4.1892276	1.2139004	14.4293725	H	-4.2350925	0.5622566	14.4925843
H	-4.879873	2.3102507	13.1945148	H	-5.00342	1.74339	13.3869393
H	6.5776934	-0.1116964	13.1488465	H	6.6254371	0.3985288	12.9768472
H	6.2065342	0.2096542	11.4325914	H	6.1815086	0.5772881	11.2564775
H	5.5300905	1.2655257	12.7101599	H	5.5389893	1.723318	12.4739647
H	-6.5298444	-0.9972763	-13.0343026	H	-6.6254371	-0.3985288	-12.9768472
H	-5.4496169	-2.2030844	-12.2788617	H	-5.5389893	-1.723318	-12.4739647
H	-6.1534864	-0.8810035	-11.2914046	H	-6.1815086	-0.5772881	-11.2564775
H	6.1715032	0.295053	-13.8523524	H	5.9729726	-0.4271491	-14.1049382
H	5.1748084	-1.1194142	-13.408048	H	5.00342	-1.74339	-13.3869393

H	4.4646802	0.2144387	-14.3749081	H	4.2350925	-0.5622566	-14.4925843

6 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -2415.001145798 Hartree

	X	Y	Z
C	0.0429287	-0.0149427	4.032428
C	0.0277707	-0.0283485	5.4405937
C	0.0513533	-0.0044034	2.8110983
C	0.05017	0.0092158	1.4017181
C	1.1588134	-0.499248	0.6668302
C	1.0905667	-0.4579639	-0.7132953
C	-0.0277024	0.0652031	-1.4022507
C	-1.1358182	0.5747801	-0.6673611
C	-1.0677912	0.5330293	0.7127718
H	1.9229083	-0.8399889	-1.300589
C	-0.0306424	0.074178	-2.8117024
H	-1.900234	0.9148395	1.3000603
C	-1.0752091	0.4837262	6.1642568
C	-1.096641	0.4667696	7.5412295
C	-0.0084126	-0.0618957	8.2775952
C	1.0992265	-0.5721402	7.5568581
C	1.1126959	-0.556633	6.1799094
H	-1.9140446	0.9101835	5.618781
H	-1.9490556	0.8817323	8.0705306
N	-0.0273516	-0.0813186	9.6601239
H	1.9373621	-1.0005297	8.0981471
H	1.9650547	-0.9711557	5.6462814
C	-0.0243764	0.0764113	-4.0330882
C	-0.0127269	0.0761481	-5.441315
C	1.0870914	-0.4464337	-6.1624102
C	1.1034759	-0.4470345	-7.5396236
C	0.012699	0.0738929	-8.278568
C	-1.0910327	0.5965003	-7.5599461
C	-1.0991631	0.5982191	-6.1828707
H	1.9270299	-0.8676829	-5.6146231
H	1.9532217	-0.8703748	-8.066918
N	0.0254033	0.0742027	-9.6612902
H	-1.9304208	1.0199916	-8.1034623
H	-1.9485136	1.0212223	-5.6511204
C	1.2512808	0.0842181	-10.3856791
C	-1.1880758	0.0623104	-10.4066977
C	-1.2564546	-0.1028403	10.3788172
C	1.1828709	-0.0800139	10.4112482
C	2.1759417	0.8702597	10.164884

6 with a = 0.35 in gas phase (C_i symmetry)

Energy = -2415.001142038 Hartree

	X	Y	Z
C	0.0318095	-0.0474947	4.0329373
C	0.018528	-0.0536312	5.4411625
C	0.0394484	-0.0413444	2.8116851
C	0.0380216	-0.0294146	1.4019774
C	1.1370551	-0.558302	0.6672775
C	1.0700374	-0.5149691	-0.7130049
C	-0.0380216	0.0294146	-1.4019774
C	-1.1370551	0.558302	-0.6672775
C	-1.0700374	0.5149691	0.7130049
H	1.8954263	-0.9117497	-1.3003715
C	-0.0394484	0.0413444	-2.8116851
H	-1.8954263	0.9117497	1.3003715
C	-1.0779263	0.4739288	6.1633595
C	-1.0967805	0.4662009	7.5406331
C	-0.0117281	-0.0676183	8.278036
C	1.0890958	-0.5942478	7.5585537
C	1.0994429	-0.5885126	6.1813276
H	-1.9134132	0.9052003	5.6165907
H	-1.9439951	0.8931004	8.0690737
N	-0.0269136	-0.0767274	9.6611647
H	1.9242798	-1.0271022	8.1011377
H	1.9461584	-1.0154679	5.6485804
C	-0.0318095	0.0474947	-4.0329373
C	-0.018528	0.0536312	-5.4411625
C	1.0779263	-0.4739288	-6.1633595
C	1.0967805	-0.4662009	-7.5406331
C	0.0117281	0.0676183	-8.278036
C	-1.0890958	0.5942478	-7.5585537
C	-1.0994429	0.5885126	-6.1813276
H	1.9134132	-0.9052003	-5.6165907
H	1.9439951	-0.8931004	-8.0690737
N	0.0269136	0.0767274	-9.6611647
H	-1.9242798	1.0271022	-8.1011377
H	-1.9461584	1.0154679	-5.6485804
C	1.2539162	0.0922914	-10.3829852
C	-1.1858861	0.0696908	-10.4076553
C	-1.2539162	-0.0922914	10.3829852
C	1.1858861	-0.0696908	10.4076553
C	2.1805014	0.8752325	10.1463548

C	3.3566966	0.8794684	10.9027925	C	3.3639795	0.8902643	10.879808
C	3.5533769	-0.0652588	11.9181105	C	3.5622458	-0.0428746	11.9055464
C	2.5491878	-1.0140935	12.1746183	C	2.5568534	-0.9863371	12.1768428
C	1.3828294	-1.0219711	11.4325388	C	1.3876941	-1.0002155	11.4392532
H	2.0238284	1.6181551	9.3896164	H	2.0274066	1.6145765	9.3631028
H	4.106857	1.6343358	10.68791	H	4.1150614	1.6408062	10.6534719
O	4.649161	-0.1391789	12.6887828	O	4.6607956	-0.1102268	12.672883
H	2.7191481	-1.7424855	12.9639137	H	2.7278385	-1.705895	12.973917
H	0.615004	-1.7648738	11.6359459	H	0.619042	-1.738986	11.6545241
C	-2.2583694	-1.0332434	10.0580766	C	-2.2602658	-1.0196352	10.0663221
C	-3.4448487	-1.059217	10.7673853	C	-3.444644	-1.0408295	10.779354
C	-3.6623874	-0.1645482	11.8286217	C	-3.6555873	-0.1447018	11.8407631
C	-2.6601716	0.7558945	12.1615142	C	-2.6493728	0.7730369	12.1691555
C	-1.4716409	0.781815	11.4374889	C	-1.4631273	0.7945374	11.4412531
H	-2.0957851	-1.7436148	9.2505504	H	-2.1026304	-1.7316471	9.2592163
H	-4.2253651	-1.7789531	10.5323187	H	-4.22848	-1.7578421	10.5472173
O	-4.842459	-0.2687016	12.4584517	O	-4.8333731	-0.245039	12.4754133
H	-2.7969921	1.460516	12.975853	H	-2.7813905	1.4790302	12.9830977
H	-0.7007998	1.5032463	11.6984313	H	-0.6894076	1.5141515	11.6989378
C	2.2548221	1.01943	-10.0842208	C	2.2602658	1.0196352	-10.0663221
C	3.438011	1.0338295	-10.7994901	C	3.444644	1.0408295	-10.779354
C	3.6503535	0.1223731	-11.847383	C	3.6555873	0.1447018	-11.8407631
C	2.646682	-0.8032987	-12.160758	C	2.6493728	-0.7730369	-12.1691555
C	1.46153	-0.8174451	-11.4309503	C	1.4631273	-0.7945374	-11.4412531
H	2.0959775	1.7425355	-9.2872226	H	2.1026304	1.7316471	-9.2592163
H	4.2197915	1.7568132	-10.5793425	H	4.22848	1.7578421	-10.5472173
O	4.8271	0.216577	-12.4848553	O	4.8333731	0.245039	-12.4754133
H	2.7798106	-1.5211247	-12.9640557	H	2.7813905	-1.4790302	-12.9830977
H	0.6894232	-1.5430584	-11.6767039	H	0.6894076	-1.5141515	-11.6989378
C	-2.1822239	-0.8814933	-10.1397248	C	-2.1805014	-0.8752325	-10.1463548
C	-3.3662349	-0.9004183	-10.8721912	C	-3.3639795	-0.8902643	-10.879808
C	-3.5655735	0.0276428	-11.9022623	C	-3.5622458	0.0428746	-11.9055464
C	-2.5604228	0.9694752	-12.179693	C	-2.5568534	0.9863371	-12.1768428
C	-1.3906715	0.9871693	-11.4432219	C	-1.3876941	1.0002155	-11.4392532
H	-2.0284733	-1.6164927	-9.3525129	H	-2.0274066	-1.6145765	-9.3631028
H	-4.1167756	-1.6502579	-10.641814	H	-4.1150614	-1.6408062	-10.6534719
O	-4.6650261	0.0914895	-12.6684622	O	-4.6607956	0.1102268	-12.672883
H	-2.7318395	1.6846011	-12.9805984	H	-2.7278385	1.705895	-12.973917
H	-0.6219606	1.7246198	-11.6629388	H	-0.619042	1.738986	-11.6545241
C	-5.1395413	0.5789611	13.5428135	C	-5.1233515	0.6035506	13.5610191
C	5.7031312	0.7755874	12.5043928	C	5.7158056	0.8004725	12.4744122
C	-5.7203253	-0.8174225	-12.4636287	C	-5.7158056	-0.8004725	-12.4744122
C	5.1184167	-0.64792	-13.5575172	C	5.1233515	-0.6035506	-13.5610191
H	-6.1402851	0.303899	13.8863671	H	-6.1229064	0.3306872	13.9096785
H	-4.4272213	0.442676	14.3695588	H	-4.4072583	0.4660981	14.3842795

H	-5.1430929	1.6363757	13.2406002
H	6.4713045	0.5158143	13.2375721
H	6.1324555	0.7001684	11.4944494
H	5.3759905	1.8106923	12.6808797
H	-6.4916836	-0.5677156	-13.1969129
H	-5.3967151	-1.856087	-12.6248229
H	-6.1441744	-0.7244866	-11.4528668
H	6.1170919	-0.3780694	-13.9109548
H	5.1240161	-1.7004613	-13.2389111
H	4.4014874	-0.5247969	-14.3823181
C	-2.3363069	1.1371999	-1.3739366
C	2.3594296	-1.0614319	1.3733392
H	2.8196412	-0.3103911	2.0290988
H	2.0811779	-1.9118789	2.0099824
H	3.1153697	-1.4012066	0.658108
H	-2.7977145	0.3856323	-2.0282836
H	-3.0914697	1.4787683	-0.6587353
H	-2.05762	1.9864158	-2.0120408

6 with a = 0.35 in hexane
(C_1 symmetry)

Energy = -2415.020306375 Hartree

	X	Y	Z
C	0.0372701	-0.0383588	4.0339512
C	0.021905	-0.0489081	5.4421994
C	0.0474287	-0.0287957	2.8125727
C	0.0496106	-0.0131985	1.4028984
C	1.1614321	-0.5184626	0.6703882
C	1.0971071	-0.4740992	-0.7101651
C	-0.020628	0.0487432	-1.4005133
C	-1.1322333	0.5544723	-0.6679477
C	-1.0675696	0.5108395	0.7125657
H	1.932123	-0.8531306	-1.2956116
C	-0.0203057	0.0614043	-2.8102519
H	-1.902892	0.8892248	1.2979988
C	-1.0800121	0.4684691	6.1641731
C	-1.1000773	0.4566287	7.5413387
C	-0.011521	-0.0714202	8.2783035
C	1.0944396	-0.5878628	7.5587993
C	1.1068894	-0.5774289	6.1817306
H	-1.9184531	0.8951241	5.6183398
H	-1.9510374	0.8764648	8.0692058
N	-0.0283529	-0.0839407	9.660856
H	1.9323487	-1.0166281	8.1001784
H	1.9579465	-0.9960534	5.6493195

6 with a = 0.35 in hexane
(C_i symmetry)

Energy = -2415.017167939 Hartree

	X	Y	Z
C	0.0663295	-0.0506187	4.0356739
C	0.0451892	-0.0534936	5.4445987
C	0.0838697	-0.0525522	2.8147556
C	0.0705342	-0.0387825	1.4025139
C	1.1696607	-0.5261651	0.6402575
C	1.0674279	-0.4730748	-0.7384858
C	-0.0705342	0.0387825	-1.4025139
C	-1.1696607	0.5261651	-0.6402575
C	-1.0674279	0.4730748	0.7384858
H	1.8933004	-0.8383187	-1.3460057
C	-0.0838697	0.0525522	-2.8147556
H	-1.8933004	0.8383187	1.3460057
C	-1.0636454	0.4588479	6.1590431
C	-1.090206	0.4531168	7.5363665
C	-0.0017658	-0.064238	8.2809477
C	1.1118242	-0.5740974	7.5687997
C	1.1305957	-0.5695931	6.1915745
H	-1.9029719	0.8762273	5.6074546
H	-1.947102	0.8682045	8.0583018
N	-0.0257244	-0.0719615	9.6636367
H	1.9508303	-0.9936796	8.1155502
H	1.9879171	-0.9836292	5.6657226

C	-0.0132473	0.0673882	-4.0316613	C	-0.0663295	0.0506187	-4.0356739
C	-0.0035874	0.0711638	-5.4400556	C	-0.0451892	0.0534936	-5.4445987
C	1.0974672	-0.444643	-6.1643293	C	1.0636454	-0.4588479	-6.1590431
C	1.1106517	-0.4413938	-7.5416643	C	1.090206	-0.4531168	-7.5363665
C	0.0157149	0.0762603	-8.2767469	C	0.0017658	0.064238	-8.2809477
C	-1.0889002	0.5922131	-7.5546971	C	-1.1118242	0.5740974	-7.5687997
C	-1.0943991	0.590269	-6.1775339	C	-1.1305957	0.5695931	-6.1915745
H	1.9409206	-0.8634477	-5.6201487	H	1.9029719	-0.8762273	-5.6074546
H	1.961302	-0.8600562	-8.0709564	H	1.947102	-0.8682045	-8.0583018
N	0.0250788	0.0787422	-9.6590994	N	0.0257244	0.0719615	-9.6636367
H	-1.9317093	1.0135234	-8.0942974	H	-1.9508303	0.9936796	-8.1155502
H	-1.9449347	1.0079871	-5.6435843	H	-1.9879171	0.9836292	-5.6657226
C	1.2492546	0.0892023	-10.3866474	C	1.2572751	0.0910868	-10.3780034
C	-1.1897626	0.0702915	-10.4024221	C	-1.181459	0.0645506	-10.4190322
C	-1.2565254	-0.1026092	10.3807059	C	-1.2572751	-0.0910868	10.3780034
C	1.1827453	-0.0752637	10.409766	C	1.181459	-0.0645506	10.4190322
C	2.1769708	0.870609	10.1497573	C	2.1761215	0.8834305	10.1687081
C	3.3594858	0.8862908	10.8846214	C	3.356319	0.8945686	10.9075634
C	3.5567449	-0.0470573	11.9103734	C	3.5512136	-0.046667	11.9265538
C	2.5516297	-0.9908517	12.1810207	C	2.544336	-0.9908056	12.1895004
C	1.3831689	-1.0055899	11.4415723	C	1.3776901	-0.9998804	11.4471606
H	2.0249614	1.610193	9.3666831	H	2.0272222	1.6276221	9.389415
H	4.1103026	1.6371732	10.6587956	H	4.1073385	1.6476388	10.6897355
O	4.6560719	-0.1131488	12.6784963	O	4.6504918	-0.1213585	12.6940935
H	2.7202841	-1.711134	12.9780809	H	2.7101685	-1.7156893	12.9830192
H	0.6154294	-1.7456091	11.6554656	H	0.6084737	-1.7404556	11.653622
C	-2.2574077	-1.0359294	10.0658105	C	-2.2512842	-1.033426	10.0681372
C	-3.4438064	-1.0584543	10.7761917	C	-3.4398744	-1.0571276	10.7749923
C	-3.6612853	-0.1572947	11.8318069	C	-3.6664828	-0.1476426	11.8215248
C	-2.6601424	0.7665935	12.1586063	C	-2.6737549	0.787864	12.1408636
C	-1.4719831	0.7890726	11.4337091	C	-1.4827376	0.810267	11.4206179
H	-2.0950043	-1.7514569	9.2628995	H	-2.0811013	-1.7556833	9.2728721
H	-4.22302	-1.7806467	10.5440755	H	-4.2136799	-1.786526	10.5472042
O	-4.8413134	-0.2578026	12.4646003	O	-4.8465753	-0.252048	12.4537737
H	-2.797287	1.4767375	12.9679996	H	-2.8192902	1.5062029	12.9415421
H	-0.7027971	1.5142447	11.6892241	H	-0.7193992	1.5433699	11.6713072
C	2.2502414	1.0288064	-10.0920307	C	2.2512842	1.033426	-10.0681372
C	3.4317383	1.0435273	-10.8109989	C	3.4398744	1.0571276	-10.7749923
C	3.6436856	0.127754	-11.854997	C	3.6664828	0.1476426	-11.8215248
C	2.6424584	-0.8029101	-12.16128	C	2.6737549	-0.787864	-12.1408636
C	1.459307	-0.8171522	-11.4279105	C	1.4827376	-0.810267	-11.4206179
H	2.0918133	1.7552242	-9.2980898	H	2.0811013	1.7556833	-9.2728721
H	4.2110235	1.7705238	-10.5946647	H	4.2136799	1.786526	-10.5472042
O	4.8190571	0.2216457	-12.4978476	O	4.8465753	0.252048	-12.4537737
H	2.7754931	-1.5243602	-12.9612957	H	2.8192902	-1.5062029	-12.9415421

H	0.6895868	-1.5471576	-11.6677368
C	-2.1832562	-0.874871	-10.1376422
C	-3.3687089	-0.8908287	-10.867939
C	-3.5695747	0.041561	-11.893754
C	-2.5653312	0.9847917	-12.1690953
C	-1.3939211	0.999697	-11.434183
H	-2.0285784	-1.6136271	-9.3542607
H	-4.1188994	-1.6412328	-10.6385059
O	-4.6719538	0.107235	-12.6578412
H	-2.736691	1.704317	-12.9662519
H	-0.6264891	1.7389336	-11.6519676
C	-5.1355885	0.6007094	13.5437524
C	5.7118324	0.7985884	12.4745576
C	-5.7261594	-0.8053321	-12.4502381
C	5.1073048	-0.6521359	-13.5662215
H	-6.1353313	0.3289043	13.8924205
H	-4.4205344	0.4711342	14.3686731
H	-5.1391558	1.6547086	13.2313591
H	6.4839565	0.5478382	13.2065624
H	6.1336125	0.7077486	11.4631988
H	5.3863169	1.835828	12.6383055
H	-6.5006626	-0.5558917	-13.1801825
H	-5.400161	-1.8424038	-12.6141679
H	-6.1452412	-0.7143327	-11.4377555
H	6.1037151	-0.383279	-13.9265335
H	5.1158139	-1.7013776	-13.2382632
H	4.3857931	-0.536681	-14.3876402
C	-2.3323475	1.1154217	-1.3762076
C	2.3613729	-1.0797638	1.3786639
H	2.8202204	-0.3281084	2.0347291
H	2.082762	-1.9300645	2.0152798
H	3.1179534	-1.4189573	0.6639242
H	-2.7909951	0.3636088	-2.03222
H	-3.0889658	1.4546061	-0.6614928
H	-2.0538966	1.9656615	-2.012989

H	0.7193992	-1.5433699	-11.6713072
C	-2.1761215	-0.8834305	-10.1687081
C	-3.356319	-0.8945686	-10.9075634
C	-3.5512136	0.046667	-11.9265538
C	-2.544336	0.9908056	-12.1895004
C	-1.3776901	0.9998804	-11.4471606
H	-2.0272222	-1.6276221	-9.389415
H	-4.1073385	-1.6476388	-10.6897355
O	-4.6504918	0.1213585	-12.6940935
H	-2.7101685	1.7156893	-12.9830192
H	-0.6084737	1.7404556	-11.653622
C	-5.1467583	0.6094117	13.5288673
C	5.7116313	0.7845553	12.4923439
C	-5.7116313	-0.7845553	-12.4923439
C	5.1467583	-0.6094117	-13.5288673
H	-6.1429803	0.32968	13.8815235
H	-4.4284802	0.4910953	14.3526748
H	-5.1613317	1.6616752	13.2110941
H	6.4851019	0.5233193	13.219354
H	6.128632	0.697693	11.4786544
H	5.394177	1.8229146	12.6644706
H	-6.4851019	-0.5233193	-13.219354
H	-5.394177	-1.8229146	-12.6644706
H	-6.128632	-0.697693	-11.4786544
H	6.1429803	-0.32968	-13.8815235
H	5.1613317	-1.6616752	-13.2110941
H	4.4284802	-0.4910953	-14.3526748
C	-2.4100384	1.0861948	-1.2829192
C	2.4100384	-1.0861948	1.2829192
H	2.3607229	-1.0400001	2.3740191
H	2.5576586	-2.1350918	0.9936396
H	3.2999915	-0.5316719	0.9579159
H	-2.3607229	1.0400001	-2.3740191
H	-3.2999915	0.5316719	-0.9579159
H	-2.5576586	2.1350918	-0.9936396

6 with a = 0.35 in DCM

(C_1 symmetry)

Energy = -2415.046987592 Hartree

	X	Y	Z
C	0.1150074	-0.0766416	4.0777186
C	0.0741367	-0.0771551	5.4940907
C	0.1536647	-0.0776029	2.8609472
C	0.168852	-0.0629982	1.4386602
C	1.225729	-0.6470255	0.7006563

6 with a = 0.35 in DCM

(C_i symmetry)

Energy = -2415.042294313 Hartree

	X	Y	Z
C	0.0501174	-0.0401564	4.036374
C	0.0294987	-0.0450098	5.4453677
C	0.0716077	-0.0454852	2.815259
C	0.0640918	-0.0349109	1.4025012
C	1.1794191	-0.4965131	0.6471846

C	1.1547801	-0.5865525	-0.6881127	C	1.0833907	-0.4478	-0.7324411
C	0.086418	0.0241638	-1.3659572	C	-0.0640918	0.0349109	-1.4025012
C	-0.9734966	0.6104907	-0.6246027	C	-1.1794191	0.4965131	-0.6471846
C	-0.9045399	0.5522363	0.7581595	C	-1.0833907	0.4478	0.7324411
H	1.9560615	-1.029324	-1.277113	H	1.9216345	-0.7931089	-1.3345524
C	0.0752318	0.0474594	-2.7899435	C	-0.0716077	0.0454852	-2.815259
H	-1.7046888	0.9945062	1.3483323	H	-1.9216345	0.7931089	1.3345524
C	-0.9769472	0.5651549	6.1868992	C	-1.0898592	0.4422026	6.1620135
C	-1.0199814	0.5645244	7.5665354	C	-1.1132989	0.4340709	7.5393867
C	-0.005666	-0.0752372	8.3078284	C	-0.0118325	-0.0611187	8.2811043
C	1.0479071	-0.7178051	7.6258969	C	1.1105979	-0.5486847	7.5658617
C	1.0833811	-0.719699	6.2461465	C	1.1271782	-0.5409582	6.1889486
H	-1.7523995	1.0784938	5.6240771	H	-1.9397173	0.84209	5.61359
H	-1.8214728	1.0851289	8.083095	H	-1.9781311	0.8308535	8.0620685
N	-0.0444694	-0.0729107	9.7081597	N	-0.0306453	-0.0692671	9.6627473
H	1.8179862	-1.2388602	8.1876321	H	1.9596838	-0.9523012	8.1085581
H	1.8894346	-1.234479	5.7294865	H	1.992361	-0.9364056	5.661747
C	0.0676015	0.0623484	-4.0062687	C	-0.0501174	0.0401564	-4.036374
C	0.0564829	0.0766134	-5.4298888	C	-0.0294987	0.0450098	-5.4453677
C	1.1281203	-0.4540568	-6.1739776	C	1.0898592	-0.4422026	-6.1620135
C	1.1157016	-0.4472353	-7.5584736	C	1.1132989	-0.4340709	-7.5393867
C	0.0273887	0.0965902	-8.2728554	C	0.0118325	0.0611187	-8.2811043
C	-1.0452235	0.632193	-7.5286709	C	-1.1105979	0.5486847	-7.5658617
C	-1.0291784	0.6195561	-6.1447874	C	-1.1271782	0.5409582	-6.1889486
H	1.9779499	-0.8885099	-5.6512363	H	1.9397173	-0.84209	-5.61359
H	1.9543004	-0.8760408	-8.0994766	H	1.9781311	-0.8308535	-8.0620685
N	0.0110644	0.1044874	-9.6652272	N	0.0306453	0.0692671	-9.6627473
H	-1.8947217	1.0678174	-8.0466842	H	-1.9596838	0.9523012	-8.1085581
H	-1.8683262	1.0461121	-5.5987959	H	-1.992361	0.9364056	-5.661747
C	1.2200714	0.0395703	-10.4181008	C	1.2575799	0.0890623	-10.3855503
C	-1.2176069	0.1607111	-10.3869831	C	-1.1802023	0.0620417	-10.4132238
C	-1.2756228	-0.1692994	10.3835851	C	-1.2575799	-0.0890623	10.3855503
C	1.1474679	0.0254624	10.4500051	C	1.1802023	-0.0620417	10.4132238
C	2.1720263	0.895871	10.0416417	C	2.1657362	0.8975298	10.1707682
C	3.3462781	0.9980177	10.7697037	C	3.3518394	0.9048623	10.9002234
C	3.5212749	0.2231371	11.9297253	C	3.5623172	-0.0543028	11.899147
C	2.4932509	-0.6497591	12.3409805	C	2.563871	-1.0087485	12.1562941
C	1.3247711	-0.7457499	11.6177479	C	1.3905681	-1.0136528	11.4228556
H	2.034813	1.5176094	9.1608633	H	2.0045771	1.6528862	9.4050687
H	4.1128058	1.6916104	10.4398203	H	4.0953216	1.6670506	10.688719
O	4.6125747	0.2488145	12.6935288	O	4.6740844	-0.1370223	12.6511721
H	2.6509339	-1.2537963	13.2310337	H	2.7397373	-1.7481727	12.934376
H	0.5489343	-1.4388538	11.931778	H	0.6302139	-1.7651555	11.622518
C	-2.2795394	-1.0457833	9.9214619	C	-2.2489972	-1.0387058	10.091251
C	-3.4788118	-1.140778	10.5926508	C	-3.431437	-1.0630431	10.8098665

C	-3.7199582	-0.3630906	11.7436881	C	-3.6530613	-0.1457975	11.8505219
C	-2.7224349	0.5125324	12.2068001	C	-2.6641486	0.7995703	12.1518609
C	-1.5154526	0.6022797	11.5326193	C	-1.4788111	0.8206255	11.4219898
H	-2.0971555	-1.669216	9.0501351	H	-2.082096	-1.7663606	9.3005876
H	-4.2537854	-1.8260781	10.2583981	H	-4.2018748	-1.7995045	10.5927239
O	-4.9091819	-0.521922	12.3229898	O	-4.8262104	-0.2519515	12.4996538
H	-2.8860585	1.1352215	13.080239	H	-2.8071299	1.5264639	12.9451386
H	-0.7580397	1.2985233	11.8831343	H	-0.7187177	1.5613621	11.6594219
C	2.2407935	0.9811706	-10.2214458	C	2.2489972	1.0387058	-10.091251
C	3.4086564	0.9241715	-10.9654818	C	3.431437	1.0630431	-10.8098665
C	3.5822062	-0.0661316	-11.9439834	C	3.6530613	0.1457975	-11.8505219
C	2.5637067	-1.0005955	-12.1557867	C	2.6641486	-0.7995703	-12.1518609
C	1.399237	-0.9452048	-11.3893278	C	1.4788111	-0.8206255	-11.4219898
H	2.1136923	1.7634062	-9.4758119	H	2.082096	1.7663606	-9.3005876
H	4.2028522	1.6526743	-10.8153637	H	4.2018748	1.7995045	-10.5927239
O	4.7480768	-0.0379327	-12.6260248	O	4.8262104	0.2519515	-12.4996538
H	2.6653135	-1.7800396	-12.904835	H	2.8071299	-1.5264639	-12.9451386
H	0.6156766	-1.6814381	-11.5562785	H	0.7187177	-1.5613621	-11.6594219
C	-2.2149914	-0.7934312	-10.1828657	C	-2.1657362	-0.8975298	-10.1707682
C	-3.4152383	-0.7460832	-10.8918109	C	-3.3518394	-0.9048623	-10.9002234
C	-3.6239808	0.2592822	-11.8419811	C	-3.5623172	0.0543028	-11.899147
C	-2.6187515	1.2125887	-12.0605446	C	-2.563871	1.0087485	-12.1562941
C	-1.4364218	1.1669756	-11.337936	C	-1.3905681	1.0136528	-11.4228556
H	-2.0568564	-1.587047	-9.455346	H	-2.0045771	-1.6528862	-9.4050687
H	-4.1689858	-1.5045274	-10.7027158	H	-4.0953216	-1.6670506	-10.688719
O	-4.7447879	0.3873687	-12.5850728	O	-4.6740844	0.1370223	-12.6511721
H	-2.7922134	1.9911617	-12.8004975	H	-2.7397373	1.7481727	-12.934376
H	-0.6678198	1.9174534	-11.5107918	H	-0.6302139	1.7651555	-11.622518
C	-5.2361715	0.2041023	13.4963676	C	-5.1107608	0.6177287	13.5761236
C	5.7055856	1.0854096	12.3524498	C	5.7350033	0.7699311	12.4331367
C	-5.7932849	-0.5417518	-12.4238313	C	-5.7350033	-0.7699311	-12.4331367
C	4.988934	-1.0016764	-13.6270371	C	5.1107608	-0.6177287	-13.5761236
H	-6.2448137	-0.1070164	13.7772089	H	-6.0997137	0.3374144	13.9482249
H	-4.5422074	-0.0315786	14.3134718	H	-4.377086	0.5062591	14.3865312
H	-5.2292149	1.2853622	13.3074426	H	-5.1330404	1.6669997	13.2510175
H	6.4675625	0.9198605	13.117336	H	6.525529	0.4976818	13.1373926
H	6.1144072	0.8206812	11.3687698	H	6.1243628	0.6924095	11.4084072
H	5.4108449	2.1427475	12.3565768	H	5.4245219	1.8063832	12.6243717
H	-6.5841452	-0.2432896	-13.1174382	H	-6.525529	-0.4976818	-13.1373926
H	-5.4698191	-1.5635313	-12.6686541	H	-5.4245219	-1.8063832	-12.6243717
H	-6.1922496	-0.5282734	-11.3993667	H	-6.1243628	-0.6924095	-11.4084072
H	5.9787912	-0.7843213	-14.0377424	H	6.0997137	-0.3374144	-13.9482249
H	4.9881309	-2.0212783	-13.216065	H	5.1330404	-1.6669997	-13.2510175
H	4.2454421	-0.9410359	-14.4347552	H	4.377086	-0.5062591	-14.3865312
C	-2.1303962	1.2712389	-1.3202743	C	-2.4295884	1.0261518	-1.2964524

C	2.4013432	-1.3185614	1.3582806
H	2.3256273	-1.3021952	2.4489447
H	2.4795147	-2.3656965	1.0374043
H	3.3395875	-0.8237887	1.0741265
H	-2.6545248	0.5632285	-1.9761571
H	-2.850805	1.6681604	-0.5974644
H	-1.7893268	2.0980616	-1.9575992

C	2.4295884	-1.0261518	1.2964524
H	2.3808213	-0.9666448	2.3870045
H	2.5947018	-2.0759533	1.0202237
H	3.3091413	-0.4611106	0.9619097
H	-2.3808213	0.9666448	-2.3870045
H	-3.3091413	0.4611106	-0.9619097
H	-2.5947018	2.0759533	-1.0202237

6 with *a* = 0.35 in MeCN
(C_1 symmetry)

Energy = -2415.055601781 Hartree

	X	Y	Z
C	0.1098727	-0.0841924	4.0811681
C	0.0704505	-0.0828809	5.5002304
C	0.1471169	-0.0866546	2.8651844
C	0.1613297	-0.0735145	1.4408421
C	1.2129455	-0.6658001	0.7031681
C	1.1421462	-0.6054608	-0.6863308
C	0.0784812	0.0126855	-1.3639476
C	-0.9763043	0.6070443	-0.6229912
C	-0.907187	0.5489664	0.7605778
H	1.9403547	-1.0549007	-1.2745958
C	0.0677308	0.0360891	-2.789376
H	-1.7041491	0.9975008	1.350399
C	-0.9716291	0.5727377	6.1917954
C	-1.012552	0.5748156	7.5725395
C	-0.0059052	-0.0769847	8.3109308
C	1.0381815	-0.7334932	7.6308647
C	1.072491	-0.7366497	6.2500161
H	-1.7422797	1.0941839	5.6299015
H	-1.8068345	1.1056992	8.0897762
N	-0.0429705	-0.0722398	9.714556
H	1.8024432	-1.2631631	8.1924944
H	1.872577	-1.2608221	5.7335967
C	0.0609128	0.0517444	-4.0054712
C	0.0509968	0.0676237	-5.4301827
C	1.1216297	-0.4650226	-6.1739677
C	1.1107048	-0.4557537	-7.5588921
C	0.0255798	0.093279	-8.273637
C	-1.0460205	0.6306663	-7.5297384
C	-1.0320616	0.6149387	-6.1453951
H	1.9698946	-0.9030364	-5.6515489
H	1.9488734	-0.8864227	-8.0991418
N	0.0116362	0.1049942	-9.666606
H	-1.8939426	1.0698242	-8.0474166

6 with *a* = 0.35 in MeCN
(C_i symmetry)

Energy = -2415.051956648 Hartree

	X	Y	Z
C	-0.0187596	-0.0787202	4.0332101
C	-0.0303756	-0.0894316	5.4419524
C	0.004369	-0.0636997	2.8122136
C	0.0194947	-0.040613	1.4014944
C	1.1517191	-0.5145276	0.6790684
C	1.1028145	-0.461027	-0.7023748
C	-0.0194947	0.040613	-1.4014944
C	-1.1517191	0.5145276	-0.6790684
C	-1.1028145	0.461027	0.7023748
H	1.9542846	-0.8151571	-1.2798059
C	-0.004369	0.0636997	-2.8122136
H	-1.9542846	0.8151571	1.2798059
C	-1.1321534	0.4214633	6.1694439
C	-1.1388008	0.4192598	7.5470343
C	-0.0362447	-0.0904244	8.2767662
C	1.0658251	-0.6073755	7.5508886
C	1.0652525	-0.607753	6.1739511
H	-1.9802975	0.8366336	5.6298571
H	-1.9887335	0.8356254	8.0789005
N	-0.034169	-0.0834576	9.6588655
H	1.9127493	-1.0255477	8.085881
H	1.9151839	-1.0237334	5.6378211
C	0.0187596	0.0787202	-4.0332101
C	0.0303756	0.0894316	-5.4419524
C	1.1321534	-0.4214633	-6.1694439
C	1.1388008	-0.4192598	-7.5470343
C	0.0362447	0.0904244	-8.2767662
C	-1.0658251	0.6073755	-7.5508886
C	-1.0652525	0.607753	-6.1739511
H	1.9802975	-0.8366336	-5.6298571
H	1.9887335	-0.8356254	-8.0789005
N	0.034169	0.0834576	-9.6588655
H	-1.9127493	1.0255477	-8.085881

H	-1.8710941	1.04277	-5.6001414	H	-1.9151839	1.0237334	-5.6378211
C	1.2217236	0.038018	-10.4174004	C	1.2511776	0.0916095	-10.3980189
C	-1.2155546	0.16728	-10.3902913	C	-1.1877345	0.0664038	-10.3898695
C	-1.2724591	-0.1732313	10.3887811	C	-1.2511776	-0.0916095	10.3980189
C	1.1486467	0.0339313	10.4519426	C	1.1877345	-0.0664038	10.3898695
C	2.1749938	0.8966875	10.0290866	C	2.1786961	0.8753269	10.1021901
C	3.3501048	1.0062526	10.7532603	C	3.3762308	0.8934751	10.8120064
C	3.5257716	0.2459556	11.9232427	C	3.5935836	-0.0359738	11.8372027
C	2.497144	-0.6198563	12.3485298	C	2.5894697	-0.9703347	12.1414197
C	1.3270615	-0.7229014	11.6297005	C	1.4042318	-0.9864161	11.4270199
H	2.0371641	1.5075738	9.1410014	H	2.0136752	1.6087669	9.3164148
H	4.1171632	1.694045	10.4128708	H	4.1234022	1.6410876	10.5647185
O	4.6191153	0.2796774	12.6834406	O	4.7173093	-0.1052606	12.5735308
H	2.6555973	-1.2136665	13.2452741	H	2.7692118	-1.6863185	12.9404173
H	0.5517037	-1.4118673	11.9534368	H	0.6398294	-1.7229436	11.6629705
C	-2.2771718	-1.046173	9.9202007	C	-2.2476363	-1.0422274	10.1261308
C	-3.4762033	-1.1443218	10.59057	C	-3.4207658	-1.0570869	10.8605407
C	-3.71711	-0.3725601	11.7460287	C	-3.6255076	-0.1310109	11.8966407
C	-2.7196555	0.5004358	12.2147346	C	-2.6317435	0.8165166	12.1745569
C	-1.5125639	0.5928738	11.5423062	C	-1.4570562	0.8295223	11.4276217
H	-2.0948376	-1.6648439	9.0456134	H	-2.0927312	-1.7785689	9.3408986
H	-4.2511318	-1.8273844	10.2517212	H	-4.1948846	-1.7946031	10.6599315
O	-4.9066339	-0.5331276	12.3240215	O	-4.788881	-0.2300269	12.5654404
H	-2.8838692	1.1195527	13.0905214	H	-2.763168	1.5513728	12.9624609
H	-0.756064	1.2884701	11.8957311	H	-0.6941841	1.5733908	11.6460092
C	2.2449124	0.976155	-10.2172246	C	2.2476363	1.0422274	-10.1261308
C	3.4141821	0.9168883	-10.9592505	C	3.4207658	1.0570869	-10.8605407
C	3.5865627	-0.0721846	-11.9392743	C	3.6255076	0.1310109	-11.8966407
C	2.5656886	-1.0032959	-12.1546681	C	2.6317435	-0.8165166	-12.1745569
C	1.4000422	-0.9457807	-11.3899789	C	1.4570562	-0.8295223	-11.4276217
H	2.1192014	1.7575579	-9.4704744	H	2.0927312	1.7785689	-9.3408986
H	4.2100247	1.6429592	-10.8055326	H	4.1948846	1.7946031	-10.6599315
O	4.753922	-0.0466615	-12.6195028	O	4.788881	0.2300269	-12.5654404
H	2.6664241	-1.7819475	-12.9046653	H	2.763168	-1.5513728	-12.9624609
H	0.6150951	-1.6799905	-11.5594835	H	0.6941841	-1.5733908	-11.6460092
C	-2.2157689	-0.785426	-10.1926453	C	-2.1786961	-0.8753269	-10.1021901
C	-3.4146532	-0.7318848	-10.9035084	C	-3.3762308	-0.8934751	-10.8120064
C	-3.6192075	0.2785334	-11.8493256	C	-3.5935836	0.0359738	-11.8372027
C	-2.6113156	1.230512	-12.0615131	C	-2.5894697	0.9703347	-12.1414197
C	-1.4303178	1.178675	-11.3366665	C	-1.4042318	0.9864161	-11.4270199
H	-2.0612959	-1.5831228	-9.4688061	H	-2.0136752	-1.6087669	-9.3164148
H	-4.1705404	-1.4893843	-10.7192566	H	-4.1234022	-1.6410876	-10.5647185
O	-4.7386685	0.4123822	-12.5939361	O	-4.7173093	0.1052606	-12.5735308
H	-2.7809463	2.0135253	-12.7977915	H	-2.7692118	1.6863185	-12.9404173
H	-0.6599931	1.9285975	-11.5044179	H	-0.6398294	1.7229436	-11.6629705

C	-5.2333426	0.1899778	13.5003159
C	5.7129667	1.1104303	12.3273994
C	-5.7902127	-0.5158051	-12.4374082
C	4.9930777	-1.0109381	-13.6218884
H	-6.242485	-0.1208261	13.779555
H	-4.539726	-0.0493515	14.3163807
H	-5.2244603	1.2715232	13.3143098
H	6.4770259	0.9537054	13.0920075
H	6.1174019	0.831679	11.3460428
H	5.4192513	2.1677992	12.3183593
H	-6.5795109	-0.2127339	-13.1307029
H	-5.468234	-1.5369506	-12.6859139
H	-6.1897566	-0.5052033	-11.4133596
H	5.98444	-0.7968091	-14.0305006
H	4.9874777	-2.0306207	-13.2116715
H	4.2510629	-0.9462735	-14.430407
C	-2.1292713	1.2762756	-1.3174921
C	2.3839449	-1.3458118	1.3605759
H	2.3082787	-1.3289727	2.4512262
H	2.454843	-2.39343	1.0395898
H	3.3257195	-0.8577199	1.0765102
H	-2.6602341	0.5721289	-1.9720943
H	-2.8453349	1.6790329	-0.5936312
H	-1.7832326	2.1003933	-1.9556957

C	-5.0468619	0.6386272	13.6505965
C	5.7850197	0.7805088	12.3028404
C	-5.7850197	-0.7805088	-12.3028404
C	5.0468619	-0.6386272	-13.6505965
H	-6.027087	0.3589055	14.0455783
H	-4.2939958	0.5244371	14.4426401
H	-5.0755238	1.6884301	13.3282991
H	6.5857727	0.5238443	13.0013687
H	6.1530094	0.6614707	11.2744192
H	5.4903692	1.8267374	12.4623108
H	-6.5857727	-0.5238443	-13.0013687
H	-5.4903692	-1.8267374	-12.4623108
H	-6.1530094	-0.6614707	-11.2744192
H	6.027087	-0.3589055	-14.0455783
H	5.0755238	-1.6884301	-13.3282991
H	4.2939958	-0.5244371	-14.4426401
C	-2.3551872	1.0564782	-1.3963887
C	2.3551872	-1.0564782	1.3963887
H	2.7636742	-0.3179752	2.0986124
H	2.0949473	-1.9457796	1.9863647
H	3.1429988	-1.3328649	0.6885244
H	-2.7636742	0.3179752	-2.0986124
H	-3.1429988	1.3328649	-0.6885244
H	-2.0949473	1.9457796	-1.9863647

7 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -2565.241673003 Hartree

	X	Y	Z
C	0.0290172	-0.0454534	4.033594
C	0.0345327	-0.0549975	5.438278
C	0.0038345	-0.0308547	2.8123882
C	-0.0074392	-0.021545	1.4103606
C	1.1186271	-0.4583222	0.680477
C	1.1239193	-0.4560786	-0.7042772
C	-0.034334	-0.0011853	-1.4069503
C	-1.1604597	0.4348445	-0.676996
C	-1.1658922	0.4321051	0.7077491
H	1.98266	-0.7969008	1.2413669
O	2.1536623	-0.8558005	-1.459819
C	-0.0434818	0.0101066	-2.8089118
H	-2.0242916	0.7740045	-1.2378429
O	-2.1963575	0.8300128	1.4633161
C	-1.0896265	0.3967126	6.1706156
C	-1.0967626	0.3862867	7.5468504

7 with a = 0.35 in gas phase (C_i symmetry)

Energy = -2565.241715190 Hartree

	X	Y	Z
C	0.0460069	-0.044356	4.0335662
C	0.0453035	-0.0561615	5.438296
C	0.0259947	-0.0274609	2.8116456
C	0.0156043	-0.0143359	1.4100543
C	1.1412182	-0.4478865	0.6765595
C	1.1445662	-0.4413068	-0.707782
C	-0.0156043	0.0143359	-1.4100543
C	-1.1412182	0.4478865	-0.6765595
C	-1.1445662	0.4413068	0.707782
H	2.0070277	-0.7880978	1.23367
O	2.1713042	-0.8366246	-1.4694774
C	-0.0259947	0.0274609	-2.8116456
H	-2.0070277	0.7880978	-1.23367
O	-2.1713042	0.8366246	1.4694774
C	-1.0840437	0.3890911	6.167543
C	-1.0962761	0.3766662	7.5437652

C	0.0281305	-0.0743349	8.2760703	C	0.0282215	-0.0798674	8.2774668
C	1.1569815	-0.5241479	7.5454731	C	1.1623691	-0.5220389	7.5496956
C	1.1556439	-0.5162082	6.1693924	C	1.1663358	-0.5117125	6.1733359
H	-1.9557682	0.7704861	5.6292679	H	-1.9502157	0.7585731	5.6232401
H	-1.9663306	0.7538331	8.0831039	H	-1.9705454	0.7386957	8.0761207
N	0.0233971	-0.0881103	9.6555738	N	0.0188969	-0.0947611	9.6567896
H	2.0243764	-0.8978829	8.0808333	H	2.0301087	-0.8928607	8.0866687
H	2.0253063	-0.8834469	5.6290943	H	2.0403768	-0.8730621	5.6360213
C	-0.0613475	0.0266453	-4.0302791	C	-0.0460069	0.044356	-4.0335662
C	-0.0570228	0.0395901	-5.4347593	C	-0.0453035	0.0561615	-5.438296
C	1.0722018	-0.4085167	-6.1612919	C	1.0840437	-0.3890911	-6.167543
C	1.0890239	-0.3930679	-7.5372088	C	1.0962761	-0.3766662	-7.5437652
C	-0.0309512	0.07045	-8.2732669	C	-0.0282215	0.0798674	-8.2774668
C	-1.1657123	0.5152727	-7.5480222	C	-1.1623691	0.5220389	-7.5496956
C	-1.1737244	0.5014725	-6.17203	C	-1.1663358	0.5117125	-6.1733359
H	1.9347958	-0.7836987	-5.6152601	H	1.9502157	-0.7585731	-5.6232401
H	1.9625698	-0.758733	-8.0678953	H	1.9705454	-0.7386957	-8.0761207
N	-0.015626	0.0916479	-9.6518064	N	-0.0188969	0.0947611	-9.6567896
H	-2.029831	0.8909712	-8.0870413	H	-2.0301087	0.8928607	-8.0866687
H	-2.0480692	0.8648308	-5.6366699	H	-2.0403768	0.8730621	-5.6360213
C	1.2125723	0.1269186	-10.37718	C	1.2050587	0.1385433	-10.388388
C	-1.2273667	0.0807459	-10.4054004	C	-1.2341279	0.0665616	-10.40418
C	-1.198617	-0.1479678	10.3881176	C	-1.2050587	-0.1385433	10.388388
C	1.2402668	-0.0448693	10.3979277	C	1.2341279	-0.0665616	10.40418
C	2.1836113	0.9568296	10.1675569	C	2.183762	0.9325873	10.1868674
C	3.3690212	1.0051758	10.897454	C	3.366683	0.9684144	10.9220682
C	3.6198518	0.048604	11.8878142	C	3.607121	0.0007458	11.9051373
C	2.6639829	-0.9506515	12.1306893	C	2.6457458	-0.997668	12.1329408
C	1.4930955	-0.9972629	11.396184	C	1.4777996	-1.031374	11.3928738
H	1.9919087	1.7127733	9.4090543	H	1.9973376	1.6969706	9.4353068
H	4.0822306	1.7982107	10.6954114	H	4.0834216	1.760903	10.7297764
O	4.7266192	0.0097641	12.6480518	O	4.7092549	-0.0514469	12.6707384
H	2.8723563	-1.6871268	12.9022224	H	2.8484863	-1.742463	12.8988179
H	0.7616769	-1.7792879	11.587725	H	0.741776	-1.8112657	11.5748361
C	-2.1533493	-1.1387398	10.1107243	C	-2.1697199	-1.1202561	10.1132332
C	-3.3309038	-1.2008477	10.8336589	C	-3.3486494	-1.1682014	10.8354232
C	-3.5839238	-0.2842631	11.8667847	C	-3.5928627	-0.2448064	11.8650114
C	-2.6279566	0.6974959	12.155552	C	-2.6268261	0.7272772	12.1528923
C	-1.4491408	0.7592902	11.4169251	C	-1.4465479	0.7747339	11.4151678
H	-1.9624055	-1.8658249	9.3243279	H	-1.985656	-1.8518386	9.3293668
H	-4.0750202	-1.9664217	10.6304249	H	-4.1013308	-1.9268621	10.6345525
O	-4.751651	-0.4268254	12.5146823	O	-4.7628589	-0.3734454	12.5116633
H	-2.7933919	1.4202283	12.9482131	H	-2.7843403	1.4546282	12.943168
H	-0.7143285	1.5282632	11.6444326	H	-0.7025597	1.5348689	11.6425571
C	2.1815795	1.1034234	-10.0997459	C	2.1697199	1.1202561	-10.1132332

C	3.3645694	1.1416132	-10.8156702	C	3.3486494	1.1682014	-10.8354232
C	3.6084244	0.2146114	-11.8417377	C	3.5928627	0.2448064	-11.8650114
C	2.6379576	-0.7525621	-12.1308038	C	2.6268261	-0.7272772	-12.1528923
C	1.4536531	-0.7900563	-11.3991483	C	1.4465479	-0.7747339	-11.4151678
H	1.9977227	1.8378545	-9.3184772	H	1.985656	1.8518386	-9.3293668
H	4.1202678	1.8957114	-10.612103	H	4.1013308	1.9268621	-10.6345525
O	4.7825438	0.3336934	-12.483198	O	4.7628589	0.3734454	-12.5116633
H	2.7958908	-1.4821334	-12.9187508	H	2.7843403	-1.4546282	-12.943168
H	0.7068482	-1.547272	-11.627166	H	0.7025597	-1.5348689	-11.6425571
C	-2.1860123	-0.9123293	-10.2044404	C	-2.183762	-0.9325873	-10.1868674
C	-3.3651115	-0.9292064	-10.9459982	C	-3.366683	-0.9684144	-10.9220682
C	-3.5936684	0.0513231	-11.9181007	C	-3.607121	-0.0007458	-11.9051373
C	-2.6219878	1.0418452	-12.1315924	C	-2.6457458	0.997668	-12.1329408
C	-1.4573134	1.0567188	-11.3857646	C	-1.4777996	1.031374	-11.3928738
H	-2.0111211	-1.6864988	-9.4603638	H	-1.9973376	-1.6969706	-9.4353068
H	-4.0901414	-1.7171951	-10.7676003	H	-4.0834216	-1.760903	-10.7297764
O	-4.6931738	0.1218029	-12.6867263	O	-4.7092549	0.0514469	-12.6707384
H	-2.8125281	1.7961933	-12.8903739	H	-2.8484863	1.742463	-12.8988179
H	-0.7125943	1.8312484	-11.5554468	H	-0.741776	1.8112657	-11.5748361
C	-5.0762915	0.439876	13.575532	C	-5.0819722	0.5006921	13.5676376
C	5.7313814	0.9802229	12.4757894	C	5.7199022	0.9150812	12.5150216
C	-5.7123561	-0.8382288	-12.5438456	C	-5.7199022	-0.9150812	-12.5150216
C	5.0998459	-0.5462969	-13.5352131	C	5.0819722	-0.5006921	-13.5676376
H	-6.0561191	0.124786	13.9440461	H	-6.0666717	0.1985855	13.934188
H	-4.3457449	0.3686617	14.3946157	H	-4.3556173	0.4246646	14.3900734
H	-5.1395729	1.4852018	13.2394918	H	-5.1322798	1.5455151	13.2277539
H	6.5188515	0.7412246	13.195471	H	6.5020287	0.6660012	13.2371935
H	6.1535001	0.9508259	11.4603746	H	6.1488016	0.8936364	11.5022079
H	5.3550726	1.9932249	12.6805543	H	5.3477948	1.9282097	12.7268427
H	-6.4903302	-0.5731124	-13.2647101	H	-6.5020287	-0.6660012	-13.2371935
H	-5.3483958	-1.8518428	-12.7672821	H	-5.3477948	-1.9282097	-12.7268427
H	-6.1426534	-0.8247262	-11.5315382	H	-6.1488016	-0.8936364	-11.5022079
H	6.0876246	-0.2508671	-13.898792	H	6.0666717	-0.1985855	-13.934188
H	5.1425666	-1.5901117	-13.1911954	H	5.1322798	-1.5455151	-13.2277539
H	4.3766417	-0.4686486	-14.3602049	H	4.3556173	-0.4246646	-14.3900734
C	3.3356256	-1.3181481	-0.8467994	C	3.3562478	-1.3018355	-0.8657426
C	-3.3783533	1.292744	0.8504899	C	-3.3562478	1.3018355	0.8657426
H	4.0188417	-1.5831328	-1.6573277	H	4.0364545	-1.5623652	-1.6805817
H	3.7990416	-0.5376537	-0.2263452	H	3.8221546	-0.524459	-0.2432863
H	3.1472494	-2.2081135	-0.2292636	H	3.1707275	-2.1952332	-0.252334
H	-4.0628307	1.5539276	1.6611819	H	-4.0364545	1.5623652	1.6805817
H	-3.1903169	2.1849947	0.2361567	H	-3.1707275	2.1952332	0.252334
H	-3.8401771	0.5137733	0.226965	H	-3.8221546	0.524459	0.2432863

7 with *a* = 0.35 in hexane

7 with *a* = 0.35 in hexane

(C_1 symmetry)

Energy = -2565.262154920 Hartree

	X	Y	Z
C	0.0301201	-0.0633195	4.0350823
C	0.0312646	-0.0714865	5.4398255
C	0.0124983	-0.0499869	2.8128156
C	0.0085275	-0.040757	1.4110456
C	1.1423575	-0.4650407	0.6850333
C	1.1520199	-0.4600572	-0.6992839
C	-0.0097257	-0.0162119	-1.4077052
C	-1.1440251	0.40677	-0.6816883
C	-1.1535997	0.4020083	0.7026879
H	2.0091248	-0.7957444	1.2463278
O	2.1858267	-0.8457518	-1.4550931
C	-0.0129021	-0.0033361	-2.8095472
H	-2.0106894	0.7377467	-1.242987
O	-2.1875573	0.787418	1.4583701
C	-1.0982832	0.3721274	6.170163
C	-1.1061709	0.3652886	7.5464765
C	0.0223612	-0.0842876	8.278448
C	1.1556175	-0.5269613	7.5493272
C	1.1561752	-0.5215029	6.1729762
H	-1.9679804	0.7365809	5.6281812
H	-1.9803946	0.7268096	8.0791297
N	0.017998	-0.0909868	9.6575628
H	2.0260951	-0.8938507	8.0844359
H	2.0300032	-0.8822945	5.6350629
C	-0.0297285	0.0159558	-4.0317502
C	-0.0315225	0.0338	-5.4364419
C	1.1005461	-0.3960912	-6.1709032
C	1.1087227	-0.3758398	-7.5471118
C	-0.0222122	0.0741663	-8.2753154
C	-1.1588907	0.5010118	-7.5419164
C	-1.1593793	0.4825832	-6.165672
H	1.9727346	-0.759824	-5.6324122
H	1.9855136	-0.7265072	-8.0826981
N	-0.0168451	0.097398	-9.653887
H	-2.0319873	0.8669282	-8.0733147
H	-2.0359111	0.8320281	-5.6246309
C	1.2043777	0.1427722	-10.3905249
C	-1.2343394	0.0784107	-10.3984831
C	-1.2034319	-0.13253	10.3935148
C	1.2354896	-0.0564346	10.4005583
C	2.1845196	0.9406536	10.170905
C	3.3705222	0.982134	10.9008476

(C_i symmetry)

Energy = -2565.262106911 Hartree

	X	Y	Z
C	0.0215874	-0.0575011	4.0334791
C	0.0231229	-0.0699633	5.4378553
C	0.0065939	-0.0370251	2.81109
C	0.0056759	-0.0194011	1.4096275
C	1.1535475	-0.4067421	0.6847231
C	1.1670544	-0.3942741	-0.6993635
C	-0.0056759	0.0194011	-1.4096275
C	-1.1535475	0.4067421	-0.6847231
C	-1.1670544	0.3942741	0.6993635
H	2.0275614	-0.7160375	1.2469557
O	2.2134657	-0.7449049	-1.4545495
C	-0.0065939	0.0370251	-2.81109
H	-2.0275614	0.7160375	-1.2469557
O	-2.2134657	0.7449049	1.4545495
C	-1.113501	0.3513648	6.170605
C	-1.1194463	0.3428274	7.5468221
C	0.0189451	-0.0854052	8.2772691
C	1.1589987	-0.5066756	7.5452122
C	1.1569852	-0.5003424	6.169091
H	-1.9909744	0.6995588	5.6303885
H	-1.9997126	0.6870377	8.080817
N	0.0169975	-0.0928942	9.6554966
H	2.0373219	-0.8575277	8.0780018
H	2.0369346	-0.8436568	5.6296747
C	-0.0215874	0.0575011	-4.0334791
C	-0.0231229	0.0699633	-5.4378553
C	1.113501	-0.3513648	-6.170605
C	1.1194463	-0.3428274	-7.5468221
C	-0.0189451	0.0854052	-8.2772691
C	-1.1589987	0.5066756	-7.5452122
C	-1.1569852	0.5003424	-6.169091
H	1.9909744	-0.6995588	-5.6303885
H	1.9997126	-0.6870377	-8.080817
N	-0.0169975	0.0928942	-9.6554966
H	-2.0373219	0.8575277	-8.0780018
H	-2.0369346	0.8436568	-5.6296747
C	1.2035973	0.1316929	-10.3948816
C	-1.2353372	0.0658994	-10.398849
C	-1.2035973	-0.1316929	10.3948816
C	1.2353372	-0.0658994	10.398849
C	2.1838089	0.934351	10.181531
C	3.3718715	0.9650011	10.9090593

C	3.6143276	0.0226748	11.8910264	C	3.618136	-0.0093814	11.8840012
C	2.6534722	-0.9729787	12.1319872	C	2.6562422	-1.0062812	12.1149811
C	1.4822767	-1.012741	11.3964787	C	1.4828971	-1.0347045	11.3821604
H	1.9964249	1.6990002	9.4138041	H	1.9948875	1.702669	9.4347359
H	4.0867912	1.77245	10.6984412	H	4.0879634	1.7578654	10.7161176
O	4.7212984	-0.0226178	12.6520337	O	4.7293449	-0.0695998	12.6380103
H	2.8571675	-1.7121888	12.9031234	H	2.8609251	-1.7556715	12.8760539
H	0.7476415	-1.7917208	11.5875835	H	0.747832	-1.8153253	11.5647523
C	-2.1640339	-1.1214277	10.131598	C	-2.1555114	-1.1337912	10.1536435
C	-3.3410237	-1.1664007	10.8579226	C	-3.3297454	-1.1769754	10.8850301
C	-3.5860345	-0.2326988	11.8778182	C	-3.5797228	-0.2275856	11.8890847
C	-2.6237907	0.7469114	12.1525247	C	-2.6274903	0.7679593	12.1404376
C	-1.4458922	0.7913882	11.4105308	C	-1.4516794	0.808979	11.3947186
H	-1.9793025	-1.8608132	9.3553438	H	-1.9661689	-1.8849524	9.3898527
H	-4.0902259	-1.9307774	10.6654686	H	-4.0724096	-1.9517525	10.7091596
O	-4.7539837	-0.3587113	12.5310326	O	-4.7429633	-0.3544753	12.5507837
H	-2.7822516	1.4825338	12.9348464	H	-2.7912975	1.5173164	12.9085202
H	-0.7056301	1.5584137	11.6266567	H	-0.718038	1.5868863	11.5940879
C	2.1671186	1.1275452	-10.1214806	C	2.1555114	1.1337912	-10.1536435
C	3.3427192	1.1773598	-10.8498919	C	3.3297454	1.1769754	-10.8850301
C	3.58385	0.2530221	-11.8791678	C	3.5797228	0.2275856	-11.8890847
C	2.6194931	-0.7224608	-12.1607711	C	2.6274903	-0.7679593	-12.1404376
C	1.4431435	-0.7719204	-11.416503	C	1.4516794	-0.808979	-11.3947186
H	1.985377	1.8597927	-9.3377941	H	1.9661689	1.8849524	-9.3898527
H	4.0936583	1.9386582	-10.6519462	H	4.0724096	1.9517525	-10.7091596
O	4.7505952	0.3833643	-12.533952	O	4.7429633	0.3544753	-12.5507837
H	2.7747276	-1.450672	-12.9506526	H	2.7912975	-1.5173164	-12.9085202
H	0.7008973	-1.5353505	-11.6384073	H	0.718038	-1.5868863	-11.5940879
C	-2.1802544	-0.9270009	-10.1950932	C	-2.1838089	-0.934351	-10.181531
C	-3.3655466	-0.9536352	-10.927092	C	-3.3718715	-0.9650011	-10.9090593
C	-3.6114194	0.0301487	-11.8925329	C	-3.618136	0.0093814	-11.8840012
C	-2.6534457	1.0345057	-12.1071413	C	-2.6562422	1.0062812	-12.1149811
C	-1.4828684	1.0588599	-11.3698253	C	-1.4828971	1.0347045	-11.3821604
H	-1.9901168	-1.703553	-9.4571384	H	-1.9948875	-1.702669	-9.4347359
H	-4.0796596	-1.7509268	-10.7453515	H	-4.0879634	-1.7578654	-10.7161176
O	-4.7179452	0.0915202	-12.6532988	O	-4.7293449	0.0695998	-12.6380103
H	-2.8587335	1.7924464	-12.8594829	H	-2.8609251	1.7556715	-12.8760539
H	-0.7501237	1.8443241	-11.5406708	H	-0.747832	1.8153253	-11.5647523
C	-5.071503	0.530325	13.5775842	C	-5.0612437	0.5450196	13.5881619
C	5.7325814	0.9429039	12.4771894	C	5.7458781	0.891025	12.4672407
C	-5.7254029	-0.8823932	-12.5054759	C	-5.7458781	-0.891025	-12.4672407
C	5.0640297	-0.4963741	-13.5894405	C	5.0612437	-0.5450196	-13.5881619
H	-6.0538289	0.2306924	13.9521595	H	-6.0360678	0.2385644	13.9768274
H	-4.3411378	0.4670738	14.3970449	H	-4.3220004	0.5019072	14.4009828
H	-5.1253061	1.5695311	13.2226981	H	-5.131496	1.5786234	13.2199961

H	6.5201974	0.7012946	13.1957668
H	6.1521983	0.9093026	11.4612876
H	5.3617264	1.9577872	12.6805015
H	-6.5130685	-0.6250992	-13.2185593
H	-5.3501198	-1.8900444	-12.7350174
H	-6.1465752	-0.8773825	-11.4896638
H	6.0460519	-0.1950869	-13.9635392
H	5.1167327	-1.5389811	-13.2444252
H	4.3318928	-0.4241428	-14.4065984
C	3.3745344	-1.297639	-0.8430293
C	-3.3760304	1.2398945	0.8462317
H	4.0613768	-1.5515204	-1.6540603
H	3.82655	-0.5135703	-0.2195862
H	3.1938397	-2.1914306	-0.2296318
H	-4.0630204	1.4934714	1.6572344
H	-3.1949258	2.1339572	0.2333586
H	-3.8281328	0.4562905	0.2222858

7 with a = 0.35 in DCM

(C_1 symmetry)

Energy = -2565.290049708 Hartree

	X	Y	Z
C	-0.0919099	-0.0662755	4.0116406
C	-0.0648262	-0.0789458	5.433152
C	-0.1164386	-0.0509563	2.7954269
C	-0.1131044	-0.0426628	1.3764699
C	0.9822671	-0.5646615	0.6677364
C	1.011123	-0.5639179	-0.7236167
C	-0.0892698	-0.0231388	-1.4367746
C	-1.1895742	0.4994186	-0.7252438
C	-1.2167944	0.496197	0.6612044
H	1.810871	-0.970346	1.2377519
O	2.0252135	-1.0461002	-1.46023
C	-0.0795698	-0.006803	-2.8502694
H	-2.0177996	0.906316	-1.2952441
O	-2.2302884	0.9758671	1.4056805
C	-1.1358409	0.4393558	6.1879618
C	-1.1083438	0.4343974	7.5716785
C	-0.0054797	-0.0956406	8.2748911
C	1.0663206	-0.6185435	7.519994
C	1.0359126	-0.6073276	6.1368083
H	-1.9957346	0.8626162	5.6727057
H	-1.9458341	0.8540026	8.121515
N	0.0261228	-0.1025353	9.6665843
H	1.9261276	-1.0433626	8.0298249

7 with a = 0.35 in DCM

(C_i symmetry)

Energy = -2565.289021968 Hartree

	X	Y	Z
C	-0.0502825	-0.1063523	4.0320171
C	-0.0434915	-0.1253461	5.4364636
C	-0.0513536	-0.073773	2.8093464
C	-0.0241714	-0.039389	1.4082681
C	1.1469012	-0.3965034	0.7055859
C	1.1901594	-0.3635455	-0.6775391
C	0.0241714	0.039389	-1.4082681
C	-1.1469012	0.3965034	-0.7055859
C	-1.1901594	0.3635455	0.6775391
H	2.0140281	-0.6994062	1.2817555
O	2.2581371	-0.6830401	-1.413911
C	0.0513536	0.073773	-2.8093464
H	-2.0140281	0.6994062	-1.2817555
O	-2.2581371	0.6830401	1.413911
C	-1.1780426	0.2828462	6.180326
C	-1.1654944	0.2836512	7.5568651
C	-0.0110024	-0.1221807	8.2750945
C	1.1229883	-0.5403779	7.5313362
C	1.1037885	-0.5424384	6.1555417
H	-2.067762	0.617015	5.6513336
H	-2.0437812	0.6201126	8.0987747
N	0.0093741	-0.1091502	9.6526182
H	2.0127365	-0.8775889	8.0533964

H	1.8739544	-1.0241779	5.581777	H	1.9813022	-0.8784609	5.6077241
C	-0.0826089	0.0157267	-4.0687286	C	0.0502825	0.1063523	-4.0320171
C	-0.0669317	0.0360636	-5.4804749	C	0.0434915	0.1253461	-5.4364636
C	1.0216929	-0.5166179	-6.1967491	C	1.1780426	-0.2828462	-6.180326
C	1.0472207	-0.4943993	-7.5744033	C	1.1654944	-0.2836512	-7.5568651
C	-0.0229737	0.0768226	-8.2990283	C	0.0110024	0.1221807	-8.2750945
C	-1.1156329	0.6267934	-7.5915988	C	-1.1229883	0.5403779	-7.5313362
C	-1.1332866	0.6088716	-6.2134876	C	-1.1037885	0.5424384	-6.1555417
H	1.8397236	-0.9776846	-5.6490493	H	2.067762	-0.617015	-5.6513336
H	1.8792979	-0.9464697	-8.1064228	H	2.0437812	-0.6201126	-8.0987747
N	0.0000203	0.0986505	-9.6923571	N	-0.0093741	0.1091502	-9.6526182
H	-1.9302478	1.0955322	-8.1360426	H	-2.0127365	0.8775889	-8.0533964
H	-1.9684332	1.0552582	-5.6795645	H	-1.9813022	0.8784609	-5.6077241
C	1.2211114	0.2413289	-10.3859637	C	1.1985008	0.1338762	-10.4139212
C	-1.1968865	-0.0220988	-10.4304689	C	-1.2402206	0.0696536	-10.3749072
C	-1.1746597	-0.0637153	10.4336408	C	-1.1985008	-0.1338762	10.4139212
C	1.2645202	-0.1365112	10.3731199	C	1.2402206	-0.0696536	10.3749072
C	2.2435522	0.8330013	10.1530453	C	2.1825662	0.929426	10.1267537
C	3.4539009	0.806425	10.8456845	C	3.3868969	0.968168	10.8265487
C	3.6913748	-0.1930952	11.7953131	C	3.6567184	0.0019701	11.8032794
C	2.7042455	-1.1614755	12.0302361	C	2.6998558	-0.9908737	12.0689682
C	1.5116862	-1.1364962	11.3237827	C	1.5085094	-1.0261873	11.364187
H	2.0628672	1.6220572	9.4258888	H	1.9775749	1.6891897	9.3759067
H	4.1930192	1.5760374	10.6445539	H	4.0974524	1.7595115	10.6088762
O	4.8240915	-0.3016587	12.5230015	O	4.7906255	-0.0522052	12.5271923
H	2.9000823	-1.935207	12.7696415	H	2.9196269	-1.7338876	12.8324714
H	0.7574304	-1.898461	11.5088136	H	0.7790996	-1.8055616	11.572311
C	-2.1903803	-1.0090276	10.2281258	C	-2.1403107	-1.1565156	10.229021
C	-3.3496875	-0.9777455	10.9867743	C	-3.2999383	-1.1871026	10.985666
C	-3.5192881	-0.011288	11.9894947	C	-3.542855	-0.2030302	11.9572554
C	-2.5053868	0.926102	12.2103684	C	-2.6021937	0.8163976	12.1490018
C	-1.3498957	0.8975129	11.4291375	C	-1.441497	0.8437156	11.3789936
H	-2.0663045	-1.7739818	9.4643912	H	-1.955555	-1.9342674	9.4910815
H	-4.1398161	-1.709135	10.8295809	H	-4.0335733	-1.9791071	10.8518196
O	-4.6766187	-0.0643737	12.6843782	O	-4.689671	-0.3203692	12.6530697
H	-2.6038446	1.6875307	12.9780842	H	-2.7633134	1.595334	12.8876311
H	-0.5702361	1.6359979	11.6037634	H	-0.7178906	1.6415653	11.531291
C	2.1903178	1.1647135	-9.9463297	C	2.1403107	1.1565156	-10.229021
C	3.377304	1.3044316	-10.6338251	C	3.2999383	1.1871026	-10.985666
C	3.6369233	0.5276589	-11.7800679	C	3.542855	0.2030302	-11.9572554
C	2.6714638	-0.3919269	-12.2229691	C	2.6021937	-0.8163976	-12.1490018
C	1.4774306	-0.5274096	-11.5310819	C	1.441497	-0.8437156	-11.3789936
H	1.9928445	1.7873974	-9.0775265	H	1.955555	1.9342674	-9.4910815
H	4.1262246	2.0252187	-10.31493	H	4.0335733	1.9791071	-10.8518196
O	4.8127583	0.73151	-12.3770671	O	4.689671	0.3203692	-12.6530697

H	2.8483848	-1.0126274	-13.0953235
H	0.7436168	-1.2549743	-11.8683858
C	-2.174723	-0.9560649	-10.0557117
C	-3.3496765	-1.0817848	-10.7816943
C	-3.5685856	-0.2681214	-11.9058194
C	-2.5854271	0.6676178	-12.2842662
C	-1.4171233	0.7876123	-11.5622879
H	-2.0027325	-1.6072498	-9.2025304
H	-4.0806881	-1.8237889	-10.477333
O	-4.6636878	-0.3133086	-12.6670149
H	-2.7755406	1.2991022	-13.148643
H	-0.6742001	1.5258635	-11.8526668
C	-4.9101064	0.8699561	13.7145621
C	5.856204	0.642527	12.3441756
C	-5.7114564	-1.2155645	-12.3564573
C	5.1547594	0.0058385	-13.5452522
H	-5.8924771	0.6341607	14.1329812
H	-4.1547594	0.7927733	14.5097607
H	-4.9223732	1.9003889	13.3317324
H	6.6610806	0.3581343	13.0274775
H	6.2408081	0.6315977	11.3142249
H	5.5208815	1.6601017	12.5903703
H	-6.4860142	-1.0568409	-13.1102576
H	-5.3660865	-2.2564904	-12.4054069
H	-6.1273181	-1.0130452	-11.3607317
H	6.1469646	0.353189	-13.8421694
H	5.1933888	-1.0729443	-13.3451766
H	4.4430827	0.2034336	-14.357483
C	3.1576886	-1.5958019	-0.818354
C	-3.3624276	1.5245848	0.7669808
H	3.8374789	-1.9145039	-1.6125323
H	3.6633009	-0.8505833	-0.1890702
H	2.8878763	-2.4657597	-0.2040507
H	-4.0429525	1.8417468	1.5613344
H	-3.0954298	2.3962889	0.1529109
H	-3.8688695	0.7805496	0.1359729

7 with a = 0.35 in MeCN

(C_1 symmetry)

Energy = -2565.299075458 Hartree

	X	Y	Z
C	-0.0937753	-0.004523	4.0096405
C	-0.0672184	-0.0287167	5.4332319
C	-0.1158041	0.0163139	2.7940158
C	-0.1076783	0.0254466	1.3721835

H	2.7633134	-1.595334	-12.8876311
H	0.7178906	-1.6415653	-11.531291
C	-2.1825662	-0.929426	-10.1267537
C	-3.3868969	-0.968168	-10.8265487
C	-3.6567184	-0.0019701	-11.8032794
C	-2.6998558	0.9908737	-12.0689682
C	-1.5085094	1.0261873	-11.364187
H	-1.9775749	-1.6891897	-9.3759067
H	-4.0974524	-1.7595115	-10.6088762
O	-4.7906255	0.0522052	-12.5271923
H	-2.9196269	1.7338876	-12.8324714
H	-0.7790996	1.8055616	-11.572311
C	-4.9870639	0.6131308	13.670304
C	5.8113173	0.8959557	12.2968993
C	-5.8113173	-0.8959557	-12.2968993
C	4.9870639	-0.6131308	-13.670304
H	-5.9446655	0.3085914	14.1010086
H	-4.2208816	0.6067563	14.458216
H	-5.0819711	1.6314295	13.2684511
H	6.6296482	0.6428848	12.976279
H	6.1769918	0.8490169	11.2614969
H	5.4690846	1.9176847	12.512302
H	-6.6296482	-0.6428848	-12.976279
H	-5.4690846	-1.9176847	-12.512302
H	-6.1769918	-0.8490169	-11.2614969
H	5.9446655	-0.3085914	-14.1010086
H	5.0819711	-1.6314295	-13.2684511
H	4.2208816	-0.6067563	-14.458216
C	3.4596794	-1.0749021	-0.7764748
C	-3.4596794	1.0749021	0.7764748
H	4.1794643	-1.2729504	-1.5741572
H	3.8447025	-0.274571	-0.1304653
H	3.3155548	-1.987208	-0.1824353
H	-4.1794643	1.2729504	1.5741572
H	-3.3155548	1.987208	0.1824353
H	-3.8447025	0.274571	0.1304653

7 with a = 0.35 in MeCN

(C_i symmetry)

Energy = -2565.296111107 Hartree

	X	Y	Z
C	-0.0611186	-0.1226894	4.031304
C	-0.0534871	-0.1441652	5.4358076
C	-0.0598619	-0.0861292	2.8086628
C	-0.0283199	-0.0459965	1.4077333

C	0.9836021	-0.5112044	0.6682122	C	1.1475952	-0.3923701	0.7079543
C	1.0171817	-0.5137405	-0.7236036	C	1.1949782	-0.3526828	-0.6748901
C	-0.0728818	0.0376002	-1.4404137	C	0.0283199	0.0459965	-1.4077333
C	-1.167381	0.5754641	-0.7347526	C	-1.1475952	0.3923701	-0.7079543
C	-1.199698	0.5760889	0.6534093	C	-1.1949782	0.3526828	0.6748901
H	1.80569	-0.9264109	1.2410003	H	2.0149696	-0.6923485	1.2853054
O	2.0296034	-1.0104491	-1.455815	O	2.2670199	-0.6617032	-1.4092311
C	-0.0615624	0.0475369	-2.8584446	C	0.0598619	0.0861292	-2.8086628
H	-1.9890673	0.9910596	-1.3080659	H	-2.0149696	0.6923485	-1.2853054
O	-2.2122304	1.0712804	1.3916029	O	-2.2670199	0.6617032	1.4092311
C	-1.1189631	0.5193169	6.19317	C	-1.1875029	0.2623956	6.181367
C	-1.0921332	0.4987884	7.5776227	C	-1.1720193	0.2651257	7.5579833
C	-0.0105438	-0.0784944	8.2752185	C	-0.0149106	-0.1370241	8.274104
C	1.042676	-0.6291096	7.5152517	C	1.1173418	-0.5565115	7.5284447
C	1.0137945	-0.6018078	6.1314073	C	1.095738	-0.5597471	6.1526996
H	-1.9637778	0.9781952	5.6832829	H	-2.0791936	0.5944604	5.6543303
H	-1.9149745	0.9420515	8.1311695	H	-2.0498999	0.6010577	8.1008265
N	0.0198863	-0.1037835	9.6683896	N	0.0094288	-0.1182778	9.6515621
H	1.8873805	-1.0888931	8.0201616	H	2.0087159	-0.8921728	8.0485893
H	1.8378251	-1.0414718	5.5728857	H	1.9727548	-0.8952185	5.6037445
C	-0.0652886	0.0625832	-4.0752643	C	0.0611186	0.1226894	-4.031304
C	-0.053562	0.0713398	-5.4923906	C	0.0534871	0.1441652	-5.4358076
C	1.019709	-0.5099629	-6.2045959	C	1.1875029	-0.2623956	-6.181367
C	1.0390858	-0.5029004	-7.5847431	C	1.1720193	-0.2651257	-7.5579833
C	-0.0215629	0.0824376	-8.305538	C	0.0149106	0.1370241	-8.274104
C	-1.0974992	0.6634556	-7.6041373	C	-1.1173418	0.5565115	-7.5284447
C	-1.109811	0.6593348	-6.2235656	C	-1.095738	0.5597471	-6.1526996
H	1.8316865	-0.9810329	-5.6565117	H	2.0791936	-0.5944604	-5.6543303
H	1.8590332	-0.9768748	-8.1168342	H	2.0498999	-0.6010577	-8.1008265
N	-0.0047828	0.0872487	-9.706712	N	-0.0094288	0.1182778	-9.6515621
H	-1.904508	1.1428567	-8.1509344	H	-2.0087159	0.8921728	-8.0485893
H	-1.9342588	1.1268647	-5.6912414	H	-1.9727548	0.8952185	-5.6037445
C	1.209158	0.2553654	-10.3990568	C	1.1970956	0.1369196	-10.4156598
C	-1.1987773	-0.0773742	-10.4316243	C	-1.2411017	0.0740895	-10.3716064
C	-1.1786035	-0.0483154	10.4366069	C	-1.1970956	-0.1369196	10.4156598
C	1.2582048	-0.1810433	10.3715985	C	1.2411017	-0.0740895	10.3716064
C	2.2568544	0.7728965	10.1726202	C	2.1887756	0.9160583	10.1073475
C	3.4682924	0.7042373	10.8604951	C	3.3938295	0.959381	10.8054803
C	3.6874491	-0.323415	11.7841631	C	3.6591101	0.0075808	11.797454
C	2.6810584	-1.2767327	11.9980411	C	2.6969022	-0.9751929	12.0802344
C	1.4871397	-1.2094397	11.2960308	C	1.5052475	-1.016211	11.3757403
H	2.0910248	1.5834544	9.4657361	H	1.9876953	1.6650246	9.3448123
H	4.222627	1.4632064	10.6759247	H	4.1084175	1.7431979	10.5741971
O	4.8201733	-0.4733507	12.5052105	O	4.7940703	-0.0404397	12.5212977
H	2.8622836	-2.0731048	12.7170362	H	2.912343	-1.70742	12.8554601

H	0.718258	-1.9608065	11.4639948	H	0.7722479	-1.7886046	11.5966223
C	-2.2274163	-0.9500211	10.2020537	C	-2.1355949	-1.1650243	10.2464831
C	-3.3848702	-0.9029244	10.9631388	C	-3.2932814	-1.1895092	11.0068719
C	-3.5201577	0.034761	11.9978756	C	-3.5367014	-0.1934992	11.9660188
C	-2.473665	0.9277383	12.2482235	C	-2.6000097	0.8326376	12.1406036
C	-1.3205235	0.8850584	11.463948	C	-1.4415115	0.8536015	11.3670681
H	-2.1316987	-1.6937577	9.4137113	H	-1.9499918	-1.9518742	9.5184561
H	-4.20004	-1.6006564	10.7818754	H	-4.024158	-1.9860844	10.8848414
O	-4.6785337	-0.0006212	12.6933416	O	-4.6807421	-0.3056968	12.6685259
H	-2.5444501	1.6660338	13.0412353	H	-2.7624857	1.6217292	12.8680738
H	-0.5155102	1.589886	11.6611801	H	-0.720967	1.6567332	11.5057459
C	2.1662515	1.1887082	-9.949609	C	2.1355949	1.1650243	-10.2464831
C	3.3488262	1.3530174	-10.6370657	C	3.2932814	1.1895092	-11.0068719
C	3.6190202	0.5899233	-11.7911776	C	3.5367014	0.1934992	-11.9660188
C	2.6681609	-0.3422501	-12.2415028	C	2.6000097	-0.8326376	-12.1406036
C	1.4777298	-0.5018324	-11.5512369	C	1.4415115	-0.8536015	-11.3670681
H	1.9597532	1.8007349	-9.0755606	H	1.9499918	1.9518742	-9.5184561
H	4.0864696	2.0827784	-10.3124887	H	4.024158	1.9860844	-10.8848414
O	4.789794	0.8165079	-12.3869909	O	4.6807421	0.3056968	-12.6685259
H	2.8557859	-0.9551001	-13.1170711	H	2.7624857	-1.6217292	-12.8680738
H	0.7568591	-1.2410774	-11.8905874	H	0.720967	-1.6567332	-11.5057459
C	-2.1692501	-1.0014768	-10.0082106	C	-2.1887756	-0.9160583	-10.1073475
C	-3.344178	-1.1707315	-10.7220311	C	-3.3938295	-0.959381	-10.8054803
C	-3.5748368	-0.4107612	-11.882097	C	-3.6591101	-0.0075808	-11.797454
C	-2.6016628	0.516097	-12.3082665	C	-2.6969022	0.9751929	-12.0802344
C	-1.4319946	0.6790732	-11.5993005	C	-1.5052475	1.016211	-11.3757403
H	-1.9876796	-1.6124744	-9.1279747	H	-1.9876953	-1.6650246	-9.3448123
H	-4.0670433	-1.9048068	-10.3814165	H	-4.1084175	-1.7431979	-10.5741971
O	-4.6721076	-0.500329	-12.6334222	O	-4.7940703	0.0404397	-12.5212977
H	-2.8021067	1.1078471	-13.1980204	H	-2.912343	1.70742	-12.8554601
H	-0.6997543	1.4132856	-11.9242926	H	-0.7722479	1.7886046	-11.5966223
C	-4.8805518	0.9135473	13.7491569	C	-4.9724504	0.6375179	13.6795196
C	5.8704179	0.4560758	12.3471786	C	5.822109	0.8948698	12.2672591
C	-5.7132605	-1.3946779	-12.2743616	C	-5.822109	-0.8948698	-12.2672591
C	5.1411709	0.1069259	-13.5640141	C	4.9724504	-0.6375179	-13.6795196
H	-5.8718004	0.7022488	14.1596138	H	-5.9251257	0.3340999	14.1218172
H	-4.1303333	0.7870029	14.5426564	H	-4.1990588	0.6413695	14.4601582
H	-4.8542299	1.9535854	13.394422	H	-5.0741876	1.6512111	13.2682479
H	6.6713901	0.1391156	13.020605	H	6.6410004	0.6493933	12.9487605
H	6.2516735	0.4638502	11.3161791	H	6.1828409	0.8229042	11.2317308
H	5.5546261	1.4729162	12.6200398	H	5.4888259	1.9234581	12.4622279
H	-6.4927674	-1.275518	-13.0301895	H	-6.6410004	-0.6493933	-12.9487605
H	-5.3602516	-2.43381	-12.2772342	H	-5.4888259	-1.9234581	-12.4622279
H	-6.1232848	-1.1477317	-11.2867158	H	-6.1828409	-0.8229042	-11.2317308
H	6.1268852	0.4733884	-13.859142	H	5.9251257	-0.3340999	-14.1218172

H	5.1971482	-0.9724551	-13.3731967
H	4.4239556	0.3012991	-14.3717063
C	3.1527649	-1.5710946	-0.8065908
C	-3.3342565	1.6316669	0.7432666
H	3.8331325	-1.8996789	-1.5962782
H	3.6637388	-0.8300868	-0.1766421
H	2.8705387	-2.4363002	-0.1911284
H	-4.0161803	1.9594549	1.5321356
H	-3.052993	2.4979743	0.1282045
H	-3.845371	0.891873	0.1113027

H	5.0741876	-1.6512111	-13.2682479
H	4.1990588	-0.6413695	-14.4601582
C	3.4704208	-1.0465563	-0.7686097
C	-3.4704208	1.0465563	0.7686097
H	4.1942608	-1.2357559	-1.5646993
H	3.8459586	-0.2452808	-0.1185235
H	3.3309515	-1.9619074	-0.1785373
H	-4.1942608	1.2357559	1.5646993
H	-3.3309515	1.9619074	0.1785373
H	-3.8459586	0.2452808	0.1185235

8 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -2643.372774200 Hartree

	X	Y	Z
C	0.0281613	-0.0506294	4.0544929
C	0.0213874	-0.0559486	5.4565713
C	0.0289222	-0.0452374	2.828846
C	0.0259667	-0.0381043	1.4330335
C	1.2075419	-0.4142018	0.7089558
C	1.2039538	-0.4054068	-0.7184434
C	0.0185727	-0.0208406	-1.4319722
C	-1.163419	0.3543742	-0.7078412
C	-1.1597682	0.3457442	0.7195156
C	0.0156042	-0.009676	-2.827817
C	-1.135817	0.3162892	6.1849843
C	-1.1498656	0.3084488	7.5600816
C	0.0015578	-0.0695329	8.2995601
C	1.164005	-0.4384453	7.5726859
C	1.1689134	-0.4338456	6.1973743
H	-2.026662	0.6259974	5.6429542
H	-2.0479789	0.6121036	8.0886699
N	-0.0102354	-0.078872	9.6746522
H	2.0545517	-0.7469772	8.1112526
H	2.0671056	-0.7387681	5.6648005
C	0.0123443	0.0027303	-4.0534045
C	0.0086339	0.0186811	-5.4553343
C	1.1590989	-0.3474401	-6.19723
C	1.1611601	-0.3259612	-7.5723711
C	0.0038041	0.060676	-8.2980521
C	-1.1526376	0.4212555	-7.5575224
C	-1.1454024	0.4032041	-6.1824484
H	2.0544586	-0.6628069	-5.6660209
H	2.0545487	-0.6245781	-8.1118642
N	0.0034589	0.0856865	-9.6729637

8 with a = 0.35 in gas phase (C_i symmetry)

Energy = -2643.372768253 Hartree

	X	Y	Z
C	0.0098418	-0.0148012	4.0543603
C	0.0082686	-0.0239487	5.4564162
C	0.0084253	-0.0092019	2.8286472
C	0.0045685	-0.0043017	1.4327533
C	1.1870716	-0.3786071	0.7088702
C	1.1825055	-0.3743758	-0.7185997
C	-0.0045685	0.0043017	-1.4327533
C	-1.1870716	0.3786071	-0.7088702
C	-1.1825055	0.3743758	0.7185997
C	-0.0084253	0.0092019	-2.8286472
C	-1.1474305	0.3401182	6.1913964
C	-1.1562207	0.324144	7.5665208
C	-0.0003848	-0.0534582	8.2995313
C	1.1610752	-0.4126544	7.5660042
C	1.160465	-0.4004745	6.1908249
H	-2.0417852	0.6488534	5.6546183
H	-2.053709	0.620888	8.1001488
N	-0.0069782	-0.073011	9.6743527
H	2.0552292	-0.7201344	8.0991545
H	2.0578967	-0.6985412	5.6531268
C	-0.0098418	0.0148012	-4.0543603
C	-0.0082686	0.0239487	-5.4564162
C	1.1474305	-0.3401182	-6.1913964
C	1.1562207	-0.324144	-7.5665208
C	0.0003848	0.0534582	-8.2995313
C	-1.1610752	0.4126544	-7.5660042
C	-1.160465	0.4004745	-6.1908249
H	2.0417852	-0.6488534	-5.6546183
H	2.053709	-0.620888	-8.1001488
N	0.0069782	0.073011	-9.6743527

H	-2.0479025	0.7349548	-8.085147	H	-2.0552292	0.7201344	-8.0991545
H	-2.0388946	0.7027823	-5.6390836	H	-2.0578967	0.6985412	-5.6531268
C	1.2216224	0.1619768	-10.4166169	C	1.2295923	0.1478891	-10.4114629
C	-1.2165013	0.0417727	-10.4167908	C	-1.2087193	0.0282912	-10.4253565
C	-1.2357891	-0.1446678	10.407224	C	-1.2295923	-0.1478891	10.4114629
C	1.2023386	-0.0234883	10.4294933	C	1.2087193	-0.0282912	10.4253565
C	2.1077501	1.0219126	10.2500695	C	2.1122175	1.0209969	10.2594717
C	3.284219	1.0862435	10.9946402	C	3.2925497	1.0735635	10.9990242
C	3.5599773	0.100406	11.9495159	C	3.5741562	0.071314	11.9349343
C	2.6415451	-0.944775	12.13988	C	2.6579077	-0.9782841	12.111401
C	1.4808375	-1.0063386	11.3895657	C	1.4931692	-1.0276418	11.3664192
H	1.8932017	1.7997219	9.5198864	H	1.892945	1.8111239	9.5439947
H	3.9673876	1.9141043	10.8314003	H	3.9741765	1.9047996	10.8467522
O	4.6585193	0.0726373	12.7224203	O	4.6770252	0.0305512	12.7010393
H	2.8706591	-1.7021972	12.8856657	H	2.8918656	-1.7485274	12.8424653
H	0.776905	-1.821184	11.5433231	H	0.7908132	-1.8457492	11.5098284
C	-2.149836	-1.1839171	10.1792793	C	-2.1398978	-1.1900519	10.1814124
C	-3.3282907	-1.2536429	10.9013129	C	-3.3136674	-1.2709031	10.9099246
C	-3.6196952	-0.2944684	11.8844165	C	-3.604425	-0.3196456	11.9009675
C	-2.7027598	0.7357632	12.1257435	C	-2.6915551	0.7138084	12.143864
C	-1.5233826	0.8042123	11.3872082	C	-1.5167332	0.793256	11.3990166
H	-1.9279909	-1.9419035	9.4308276	H	-1.9185688	-1.9419259	9.4266552
H	-4.0433749	-2.0560306	10.7361819	H	-4.0255715	-2.0759222	10.7436958
O	-4.7847978	-0.4480177	12.5355048	O	-4.7644713	-0.484272	12.5583169
H	-2.8968989	1.4912437	12.8806983	H	-2.8854831	1.4633293	12.9048111
H	-0.8163387	1.6082959	11.5787389	H	-0.8124434	1.5993314	11.5924412
C	2.1389947	1.1969044	-10.1820787	C	2.1398978	1.1900519	-10.1814124
C	3.3084674	1.2787435	-10.9173415	C	3.3136674	1.2709031	-10.9099246
C	3.5872405	0.3367575	-11.9205152	C	3.604425	0.3196456	-11.9009675
C	2.6673295	-0.6894149	-12.1676498	C	2.6915551	-0.7138084	-12.143864
C	1.4971826	-0.7703571	-11.415831	C	1.5167332	-0.793256	-11.3990166
H	1.9266465	1.9423461	-9.4184296	H	1.9185688	1.9419259	-9.4266552
H	4.025663	2.0782635	-10.7475576	H	4.0255715	2.0759222	-10.7436958
O	4.743611	0.5020736	-12.5841783	O	4.7644713	0.484272	-12.5583169
H	2.8517981	-1.4318851	-12.9377648	H	2.8854831	-1.4633293	-12.9048111
H	0.7875219	-1.5709257	-11.6123935	H	0.8124434	-1.5993314	-11.5924412
C	-2.1184755	-1.0081007	-10.2467688	C	-2.1122175	-1.0209969	-10.2594717
C	-3.3029714	-1.0604407	-10.9794732	C	-3.2925497	-1.0735635	-10.9990242
C	-3.5905551	-0.0573543	-11.9126419	C	-3.5741562	-0.071314	-11.9349343
C	-2.6755897	0.9925016	-12.0937794	C	-2.6579077	0.9782841	-12.111401
C	-1.506672	1.0417919	-11.3553884	C	-1.4931692	1.0276418	-11.3664192
H	-1.8948498	-1.7987629	-9.5332692	H	-1.892945	-1.8111239	-9.5439947
H	-3.9832593	-1.8921722	-10.8240563	H	-3.9741765	-1.9047996	-10.8467522
O	-4.6978854	-0.0165302	-12.6723019	O	-4.6770252	-0.0305512	-12.7010393
H	-2.9140112	1.7633309	-12.8227263	H	-2.8918656	1.7485274	-12.8424653

H	-0.805452	1.8603657	-11.5017898
C	-5.148344	0.4596369	13.5476971
C	5.6251836	1.0880674	12.6059169
C	-5.6616626	-1.0356595	-12.5644027
C	5.0934619	-0.3872679	-13.6172019
H	-6.1184194	0.1286463	13.9280602
H	-4.4215564	0.4586562	14.3733038
H	-5.2478869	1.4833058	13.157835
H	6.4124654	0.8520234	13.3269091
H	6.062457	1.1181887	11.5968737
H	5.2061429	2.076342	12.8458577
H	-6.4573918	-0.7871863	-13.2718126
H	-5.2438893	-2.0184319	-12.827889
H	-6.0874748	-1.0858351	-11.5512633
H	6.0580155	-0.0489767	-14.0050916
H	5.1988611	-1.4176331	-13.2470072
H	4.3552697	-0.372155	-14.4325198
C	2.3865863	-0.7811945	-1.4047039
C	2.3934704	-0.7986068	1.3846721
C	3.5205817	-1.1487371	-0.7205055
C	3.5240419	-1.1576217	0.6903625
C	-2.349573	0.7382475	-1.383502
C	-2.3425661	0.7211316	1.405706
C	-3.4803067	1.0968274	-0.6892623
C	-3.4767809	1.0880751	0.7215849
H	2.383304	-0.7741129	-2.4908556
H	4.4174488	-1.4334465	-1.2671545
H	4.4235428	-1.4493483	1.2289289
H	2.3953976	-0.80523	2.4708448
H	-2.3516189	0.7446533	-2.469644
H	-4.3799804	1.3879447	-1.2278628
H	-4.3737757	1.3722819	1.2682802
H	-2.3393168	0.7140728	2.4918147

8 with a = 0.35 in hexane
(C_1 symmetry)

Energy = -2643.392592328 Hartree

	X	Y	Z
C	0.0083993	-0.0340935	4.0538965
C	0.0054384	-0.0457435	5.4558247
C	0.0087195	-0.0239409	2.8282241
C	0.0074923	-0.0117026	1.4326824
C	1.1935043	-0.376654	0.7096111
C	1.1918909	-0.3644875	-0.7177092
C	0.0040692	0.0125001	-1.4317041

H	-0.7908132	1.8457492	-11.5098284
C	-5.1292485	0.416988	13.5757954
C	5.6418708	1.0492815	12.5987509
C	-5.6418708	-1.0492815	-12.5987509
C	5.1292485	-0.416988	-13.5757954
H	-6.0958064	0.0787004	13.958662
H	-4.3991736	0.4167654	14.3984954
H	-5.2362931	1.4416488	13.1905983
H	6.4332341	0.8005855	13.3109673
H	6.0737278	1.099066	11.5881643
H	5.2228538	2.0322342	12.8595697
H	-6.4332341	-0.8005855	-13.3109673
H	-5.2228538	-2.0322342	-12.8595697
H	-6.0737278	-1.099066	-11.5881643
H	6.0958064	-0.0787004	-13.958662
H	5.2362931	-1.4416488	-13.1905983
H	4.3991736	-0.4167654	-14.3984954
C	2.365689	-0.7492017	-1.404455
C	2.374619	-0.7575318	1.3848906
C	3.5012006	-1.1115083	-0.7199195
C	3.5056891	-1.115775	0.6909185
C	-2.374619	0.7575318	-1.3848906
C	-2.365689	0.7492017	1.404455
C	-3.5056891	1.115775	-0.6909185
C	-3.5012006	1.1115083	0.7199195
H	2.3617723	-0.7457764	-2.490642
H	4.3984752	-1.3956594	-1.2662588
H	4.4064233	-1.4033264	1.2297394
H	2.3776018	-0.7606901	2.4710957
H	-2.3776018	0.7606901	-2.4710957
H	-4.4064233	1.4033264	-1.2297394
H	-4.3984752	1.3956594	1.2662588
H	-2.3617723	0.7457764	2.490642

8 with a = 0.35 in hexane
(C_i symmetry)

Energy = -2643.392551681 Hartree

	X	Y	Z
C	0.023425	-0.0484311	4.054138
C	0.0186977	-0.0593319	5.4561317
C	0.0207567	-0.0345965	2.8283852
C	0.0110424	-0.0181013	1.4326706
C	1.1937828	-0.3755218	0.7004645
C	1.1830677	-0.3571069	-0.7268154
C	-0.0110424	0.0181013	-1.4326706

C	-1.1820198	0.3774003	-0.7086346	C	-1.1937828	0.3755218	-0.7004645
C	-1.1803812	0.3653241	0.718699	C	-1.1830677	0.3571069	0.7268154
C	0.0025107	0.0240469	-2.8272507	C	-0.0207567	0.0345965	-2.8283852
C	-1.153571	0.3107124	6.1894977	C	-1.1410034	0.3018045	6.1866452
C	-1.1619399	0.2964661	7.5648502	C	-1.1520832	0.2917049	7.5619817
C	-0.0032297	-0.0717958	8.2980394	C	0.0047066	-0.0758745	8.298499
C	1.1601318	-0.4261752	7.5652214	C	1.1687276	-0.4352316	7.5690399
C	1.1600957	-0.4153936	6.1899045	C	1.1710436	-0.4297762	6.1935843
H	-2.0500779	0.6126859	5.6525324	H	-2.0358011	0.6043752	5.6471792
H	-2.0617511	0.5884979	8.096986	H	-2.0524284	0.5861759	8.0919227
N	-0.0084356	-0.0868594	9.6730403	N	-0.0042014	-0.0845037	9.6734961
H	2.0565207	-0.72785	8.0977872	H	2.0635538	-0.7366591	8.1043674
H	2.0596874	-0.7079892	5.652896	H	2.0708575	-0.726678	5.6593076
C	0.0015906	0.0339537	-4.0529272	C	-0.023425	0.0484311	-4.054138
C	0.0018003	0.0455032	-5.454855	C	-0.0186977	0.0593319	-5.4561317
C	1.1591467	-0.3109025	-6.1910779	C	1.1410034	-0.3018045	-6.1866452
C	1.1646548	-0.2962488	-7.5664283	C	1.1520832	-0.2917049	-7.5619817
C	0.0042976	0.0718523	-8.2972193	C	-0.0047066	0.0758745	-8.298499
C	-1.1575828	0.4259397	-7.5617674	C	-1.1687276	0.4352316	-7.5690399
C	-1.1543727	0.4153963	-6.1864583	C	-1.1710436	0.4297762	-6.1935843
H	2.0568535	-0.6128503	-5.6561142	H	2.0358011	-0.6043752	-5.6471792
H	2.06342	-0.588011	-8.1004625	H	2.0524284	-0.5861759	-8.0919227
N	0.0064636	0.0864897	-9.6721228	N	0.0042014	0.0845037	-9.6734961
H	-2.0552056	0.7275117	-8.0922655	H	-2.0635538	0.7366591	-8.1043674
H	-2.0527943	0.7079858	-5.6474863	H	-2.0708575	0.726678	-5.6593076
C	1.2262339	0.1512123	-10.4148752	C	1.2295274	0.152289	-10.4073491
C	-1.2116424	0.040015	-10.4192951	C	-1.2092132	0.0322934	-10.4272719
C	-1.2297248	-0.1572543	10.4125628	C	-1.2295274	-0.152289	10.4073491
C	1.2077305	-0.0347153	10.4227097	C	1.2092132	-0.0322934	10.4272719
C	2.1058746	1.0186647	10.2528213	C	2.1154466	1.0128825	10.249134
C	3.2859908	1.0800622	10.9920176	C	3.2962155	1.0713279	10.9875604
C	3.5724319	0.082792	11.9317287	C	3.5763303	0.0783213	11.9336935
C	2.662169	-0.9710883	12.1120163	C	2.6560555	-0.964786	12.1254602
C	1.4973849	-1.0295072	11.366549	C	1.4901726	-1.0199003	11.3814038
H	1.8828003	1.8049099	9.5344231	H	1.8987155	1.7944809	9.5238453
H	3.9631575	1.914205	10.8361378	H	3.9796496	1.8990926	10.824951
O	4.6770834	0.052159	12.6981543	O	4.683486	0.0423562	12.6963165
H	2.8984913	-1.7386333	12.8453077	H	2.886004	-1.7273804	12.8659713
H	0.8006001	-1.8519211	11.5123646	H	0.7863917	-1.8347341	11.5355018
C	-2.141201	-1.1995718	10.1897227	C	-2.1270666	-1.2098423	10.2004582
C	-3.3145962	-1.2744474	10.9204459	C	-3.3047026	-1.2830802	10.9246413
C	-3.6024347	-0.3172647	11.9063526	C	-3.6107919	-0.3078444	11.887141
C	-2.6879061	0.7161676	12.1427303	C	-2.711812	0.7432757	12.1050423
C	-1.514298	0.7900666	11.3950979	C	-1.5328272	0.8140394	11.3653308
H	-1.9221478	-1.9560542	9.4390446	H	-1.8932371	-1.9798281	9.4680456

H	-4.0270507	-2.0798129	10.7575673	H	-4.0065886	-2.1001672	10.7745089
O	-4.7628366	-0.4753697	12.567571	O	-4.772872	-0.4666117	12.5451525
H	-2.8792503	1.4703064	12.8996943	H	-2.9193248	1.5129514	12.8419237
H	-0.8097816	1.5973682	11.5823454	H	-0.8400866	1.6347608	11.538329
C	2.1401921	1.1927243	-10.1988185	C	2.1270666	1.2098423	-10.2004582
C	3.3113686	1.2628517	-10.9335768	C	3.3047026	1.2830802	-10.9246413
C	3.5944528	0.301349	-11.91664	C	3.6107919	0.3078444	-11.887141
C	2.6777339	-0.7317659	-12.1457357	C	2.711812	-0.7432757	-12.1050423
C	1.5062998	-0.8007124	-11.3941904	C	1.5328272	-0.8140394	-11.3653308
H	1.9248138	1.9522784	-9.4501708	H	1.8932371	1.9798281	-9.4680456
H	4.0257305	2.0675762	-10.7759537	H	4.0065886	2.1001672	-10.7745089
O	4.7526567	0.4553851	-12.5827243	O	4.772872	0.4666117	-12.5451525
H	2.8656982	-1.4894307	-12.9000105	H	2.9193248	-1.5129514	-12.8419237
H	0.7998829	-1.6076262	-11.5759319	H	0.8400866	-1.6347608	-11.538329
C	-2.1116759	-1.012011	-10.2513886	C	-2.1154466	-1.0128825	-10.249134
C	-3.2933775	-1.0682792	-10.9884873	C	-3.2962155	-1.0713279	-10.9875604
C	-3.5795763	-0.066905	-11.9238883	C	-3.5763303	-0.0783213	-11.9336935
C	-2.6675302	0.9857744	-12.1020288	C	-2.6560555	0.964786	-12.1254602
C	-1.5011077	1.0389709	-11.3586994	C	-1.4901726	1.0199003	-11.3814038
H	-1.8889992	-1.8011625	-9.5360435	H	-1.8987155	-1.7944809	-9.5238453
H	-3.9719294	-1.9016257	-10.8343882	H	-3.9796496	-1.8990926	-10.824951
O	-4.6857942	-0.031016	-12.6878593	O	-4.683486	-0.0423562	-12.6963165
H	-2.9036852	1.7565058	-12.8320255	H	-2.886004	1.7273804	-12.8659713
H	-0.8029212	1.8604955	-11.5028879	H	-0.7863917	1.8347341	-11.5355018
C	-5.1220871	0.437183	13.5794353	C	-5.1470038	0.4589204	13.5398409
C	5.6361325	1.0779421	12.5860851	C	5.6562291	1.0532382	12.5674947
C	-5.6466258	-1.0553458	-12.5778579	C	-5.6562291	-1.0532382	-12.5674947
C	5.1066563	-0.4611432	-13.592844	C	5.1470038	-0.4589204	-13.5398409
H	-6.0894356	0.1065938	13.9668407	H	-6.1094967	0.1205478	13.9327907
H	-4.3901091	0.4400648	14.3999622	H	-4.4156682	0.4879652	14.3604031
H	-5.224484	1.4584728	13.1852449	H	-5.2648654	1.4711358	13.1269915
H	6.4308848	0.8395909	13.29796	H	6.4538464	0.8091279	13.274322
H	6.0641371	1.1229277	11.5740812	H	6.0757806	1.0834455	11.5513843
H	5.2104446	2.0591993	12.8408274	H	5.2471748	2.0427269	12.8176188
H	-6.4424657	-0.8125199	-13.2870016	H	-6.4538464	-0.8091279	-13.274322
H	-5.2234396	-2.036383	-12.8375316	H	-5.2471748	-2.0427269	-12.8176188
H	-6.0725083	-1.1036305	-11.5651108	H	-6.0757806	-1.0834455	-11.5513843
H	6.0726193	-0.132855	-13.9856345	H	6.1094967	-0.1205478	-13.9327907
H	5.2098681	-1.4811155	-13.195461	H	5.2648654	-1.4711358	-13.1269915
H	4.3711057	-0.4662945	-14.4101582	H	4.4156682	-0.4879652	-14.3604031
C	2.377993	-0.7296936	-1.4034979	C	2.3664149	-0.7139085	-1.4214516
C	2.3810078	-0.7537353	1.3864878	C	2.38714	-0.7512846	1.3680137
C	3.5140402	-1.0906311	-0.7182003	C	3.5082401	-1.0736179	-0.7451807
C	3.515537	-1.1028694	0.6926362	C	3.5186487	-1.0931492	0.6653989
C	-2.3696136	0.7541885	-1.3855135	C	-2.38714	0.7512846	-1.3680137

C	-2.3665524	0.7303931	1.4044385
C	-3.5042274	1.1031148	-0.691702
C	-3.5026951	1.0910117	0.7191297
H	2.3773515	-0.7204771	-2.4896598
H	4.4135856	-1.3673483	-1.2643772
H	4.4162223	-1.3891337	1.2319773
H	2.3825643	-0.7634463	2.4726624
H	-2.3712156	0.7637294	-2.4716774
H	-4.4049681	1.3891519	-1.2310686
H	-4.4022953	1.3675488	1.265311
H	-2.3659319	0.72127	2.4905897

C	-2.3664149	0.7139085	1.4214516
C	-3.5186487	1.0931492	-0.6653989
C	-3.5082401	1.0736179	0.7451807
H	2.3595206	-0.6990294	-2.5072953
H	4.4052745	-1.3432305	-1.2992235
H	4.4234425	-1.3790929	1.197925
H	2.3964112	-0.7652699	2.45419
H	-2.3964112	0.7652699	-2.45419
H	-4.4234425	1.3790929	-1.197925
H	-4.4052745	1.3432305	1.2992235
H	-2.3595206	0.6990294	2.5072953

8 with *a* = 0.35 in DCM
(C_1 symmetry)

Energy = -2643.418756408 Hartree

	X	Y	Z
C	0.0023169	-0.0478135	4.052521
C	-0.0007001	-0.0603409	5.4546459
C	0.0048941	-0.0360931	2.826893
C	0.0069258	-0.0211545	1.4316609
C	1.1971875	-0.3790504	0.7113518
C	1.1995349	-0.3627823	-0.715918
C	0.0116111	0.0113767	-1.4317625
C	-1.1787633	0.3692644	-0.7114491
C	-1.1811856	0.3528077	0.7158164
C	0.0132382	0.02657	-2.8269772
C	-1.1610403	0.293032	6.1877915
C	-1.1672718	0.2800451	7.563573
C	-0.0064001	-0.0836897	8.2949409
C	1.1574678	-0.4355019	7.5622384
C	1.1567116	-0.4260286	6.1865972
H	-2.0593461	0.5912024	5.6518021
H	-2.0680904	0.569601	8.0953301
N	-0.0093163	-0.095255	9.6705449
H	2.056171	-0.7332252	8.0930324
H	2.0571747	-0.7152728	5.6493224
C	0.0132939	0.0396643	-4.0526021
C	0.0124813	0.0541962	-5.4546636
C	1.1685883	-0.3037079	-6.1922157
C	1.1701987	-0.2890085	-7.5679971
C	0.0089143	0.082144	-8.2951277
C	-1.1506819	0.4389497	-7.557855
C	-1.1455158	0.4267446	-6.1822776
H	2.0671484	-0.6073426	-5.6597394
H	2.067802	-0.5824828	-8.1030189

8 with *a* = 0.35 in DCM
(C_i symmetry)

Energy = -2643.418625317 Hartree

	X	Y	Z
C	0.0380705	-0.0816462	4.0533561
C	0.0288577	-0.0963187	5.4554308
C	0.035808	-0.0586284	2.827743
C	0.0193081	-0.0307268	1.4321773
C	1.2022469	-0.3696774	0.6912377
C	1.1831908	-0.3383455	-0.7356959
C	-0.0193081	0.0307268	-1.4321773
C	-1.2022469	0.3696774	-0.6912377
C	-1.1831908	0.3383455	0.7356959
C	-0.035808	0.0586284	-2.827743
C	-1.1334235	0.2677129	6.1805665
C	-1.1472142	0.2624518	7.5563155
C	0.0081627	-0.1018596	8.2960077
C	1.1724802	-0.469111	7.5712984
C	1.1787451	-0.4690717	6.1955308
H	-2.0266015	0.5698715	5.6383608
H	-2.0489486	0.5600771	8.081969
N	-0.0031664	-0.0991522	9.6719484
H	2.0660264	-0.7704976	8.108494
H	2.0792501	-0.7701634	5.6649347
C	-0.0380705	0.0816462	-4.0533561
C	-0.0288577	0.0963187	-5.4554308
C	1.1334235	-0.2677129	-6.1805665
C	1.1472142	-0.2624518	-7.5563155
C	-0.0081627	0.1018596	-8.2960077
C	-1.1724802	0.469111	-7.5712984
C	-1.1787451	0.4690717	-6.1955308
H	2.0266015	-0.5698715	-5.6383608
H	2.0489486	-0.5600771	-8.081969

N	0.007104	0.0960037	-9.6706795	N	0.0031664	0.0991522	-9.6719484
H	-2.0495753	0.7424598	-8.0849616	H	-2.0660264	0.7704976	-8.108494
H	-2.0426734	0.7198753	-5.6415915	H	-2.0792501	0.7701634	-5.6649347
C	1.2247273	0.1551203	-10.4171765	C	1.2300727	0.156561	-10.4039416
C	-1.2131766	0.0493137	-10.4138377	C	-1.2082016	0.037767	-10.4273052
C	-1.2293099	-0.164307	10.4122512	C	-1.2300727	-0.156561	10.4039416
C	1.2075144	-0.0350831	10.4181711	C	1.2082016	-0.037767	10.4273052
C	2.0970502	1.0258596	10.2485407	C	2.1238342	0.9952709	10.2256788
C	3.2786481	1.0949702	10.9849553	C	3.3052907	1.0604325	10.9623042
C	3.5750145	0.0976176	11.9213246	C	3.5769682	0.0870649	11.9309294
C	2.6738702	-0.9636843	12.1021528	C	2.646211	-0.9409601	12.1498606
C	1.5073397	-1.0300397	11.3582602	C	1.4795851	-1.0037206	11.4056757
H	1.8671488	1.8120611	9.5324301	H	1.9161477	1.7608516	9.48144
H	3.9490883	1.9342645	10.8280388	H	3.995696	1.8779679	10.7792055
O	4.684404	0.0758775	12.685101	O	4.6894346	0.0586337	12.6903522
H	2.9160686	-1.7329504	12.8320206	H	2.866658	-1.6895978	12.9076736
H	0.819095	-1.8598633	11.5027281	H	0.7699779	-1.8094451	11.5786565
C	-2.1289784	-1.2205867	10.210687	C	-2.1197128	-1.2245866	10.2207155
C	-3.3011481	-1.293961	10.9451353	C	-3.2992453	-1.287632	10.9445083
C	-3.5979678	-0.3205913	11.9120211	C	-3.612694	-0.2916585	11.8827568
C	-2.6961459	0.7286403	12.125875	C	-2.7235208	0.7728454	12.0739685
C	-1.5241769	0.8004272	11.3747634	C	-1.543317	0.8331313	11.3347699
H	-1.9034542	-1.9888643	9.474143	H	-1.879352	-2.0109311	9.5081947
H	-4.0035577	-2.1110606	10.7964396	H	-3.9939607	-2.1139583	10.8104897
O	-4.7567163	-0.4774245	12.5811038	O	-4.7740683	-0.4425648	12.5486384
H	-2.8957979	1.496835	12.8663619	H	-2.9392186	1.561279	12.7882661
H	-0.8305955	1.6212749	11.543177	H	-0.8595516	1.665718	11.4858911
C	2.136308	1.2011996	-10.2160342	C	2.1197128	1.2245866	-10.2207155
C	3.306136	1.2645924	-10.9551453	C	3.2992453	1.287632	-10.9445083
C	3.5886136	0.2913721	-11.9264594	C	3.612694	0.2916585	-11.8827568
C	2.6747289	-0.7473708	-12.1401246	C	2.7235208	-0.7728454	-12.0739685
C	1.505267	-0.8093192	-11.3842785	C	1.543317	-0.8331313	-11.3347699
H	1.9220558	1.9693979	-9.4760614	H	1.879352	2.0109311	-9.5081947
H	4.0177386	2.073737	-10.8066444	H	3.9939607	2.1139583	-10.8104897
O	4.7462815	0.437977	-12.5997371	O	4.7740683	0.4425648	-12.5486384
H	2.8630608	-1.5150624	-12.8840729	H	2.9392186	-1.561279	-12.7882661
H	0.8023075	-1.622179	-11.5525873	H	0.8595516	-1.665718	-11.4858911
C	-2.1115603	-1.004112	-10.2444432	C	-2.1238342	-0.9952709	-10.2256788
C	-3.2973197	-1.059158	-10.975309	C	-3.3052907	-1.0604325	-10.9623042
C	-3.5890549	-0.0550409	-11.9058689	C	-3.5769682	-0.0870649	-11.9309294
C	-2.6788795	0.9984952	-12.0868289	C	-2.646211	0.9409601	-12.1498606
C	-1.5081403	1.0508469	-11.3484567	C	-1.4795851	1.0037206	-11.4056757
H	-1.8855975	-1.7952606	-9.5325286	H	-1.9161477	-1.7608516	-9.48144
H	-3.9747791	-1.8928251	-10.8185161	H	-3.995696	-1.8779679	-10.7792055
O	-4.7021968	-0.019477	-12.6636021	O	-4.6894346	-0.0586337	-12.6903522

H	-2.9175157	1.7730999	-12.8122096
H	-0.8129056	1.8748583	-11.4928281
C	-5.1223089	0.4596018	13.5720439
C	5.6356478	1.1119758	12.5636384
C	-5.6627234	-1.046858	-12.5412165
C	5.0970597	-0.4989014	-13.5961626
H	-6.0842738	0.1289246	13.9723296
H	-4.3862569	0.49176	14.3875716
H	-5.2365724	1.4680458	13.15053
H	6.4376271	0.8817084	13.2699152
H	6.0540061	1.1580184	11.5483251
H	5.2022522	2.0889639	12.8193658
H	-6.4662795	-0.805906	-13.2421109
H	-5.2401985	-2.0268901	-12.8033434
H	-6.0759513	-1.0930996	-11.5238067
H	6.0611548	-0.177598	-13.9989595
H	5.201415	-1.5104219	-13.1794967
H	4.3573836	-0.5190183	-14.4088173
C	2.3886083	-0.7204154	-1.4000597
C	2.3840083	-0.7525213	1.3909669
C	3.5249447	-1.0782816	-0.7120678
C	3.5225929	-1.0946054	0.6986652
C	-2.365625	0.7427235	-1.3910459
C	-2.3703574	0.710408	1.3998861
C	-3.5042651	1.0846831	-0.6988153
C	-3.50668	1.0682848	0.7119041
H	2.3926126	-0.7083443	-2.4862555
H	4.4270653	-1.3491203	-1.2567272
H	4.4228678	-1.3781307	1.239903
H	2.3843462	-0.7657458	2.4771566
H	-2.3660154	0.7559886	-2.4772079
H	-4.4045319	1.3681879	-1.2400849
H	-4.4088109	1.3390617	1.2565726
H	-2.3744507	0.6983786	2.486065

8 with a = 0.35 in MeCN

(C_1 symmetry)

Energy = -2643.425652771 Hartree

	X	Y	Z
C	0.0057124	-0.0115477	4.0517979
C	0.0023969	-0.0349345	5.4538153
C	0.0080646	0.007863	2.8262848
C	0.0096164	0.0278162	1.431201
C	1.2006724	-0.3250101	0.709395
C	1.2015497	-0.3068358	-0.7178747

H	-2.866658	1.6895978	-12.9076736
H	-0.7699779	1.8094451	-11.5786565
C	-5.1403212	0.5005011	13.5336558
C	5.6794398	1.049224	12.5127066
C	-5.6794398	-1.049224	-12.5127066
C	5.1403212	-0.5005011	-13.5336558
H	-6.0967953	0.1656452	13.943948
H	-4.3984379	0.5450781	14.3432898
H	-5.2658187	1.5044872	13.1048838
H	6.4841559	0.814142	13.2145169
H	6.0812084	1.0375884	11.489685
H	5.2910389	2.0527787	12.7356269
H	-6.4841559	-0.814142	-13.2145169
H	-5.2910389	-2.0527787	-12.7356269
H	-6.0812084	-1.0375884	-11.489685
H	6.0967953	-0.1656452	-13.943948
H	5.2658187	-1.5044872	-13.1048838
H	4.3984379	-0.5450781	-14.3432898
C	2.3660475	-0.6747166	-1.4404978
C	2.4032955	-0.7382421	1.3489174
C	3.5161732	-1.0281852	-0.7739743
C	3.5349051	-1.0615161	0.636119
C	-2.4032955	0.7382421	-1.3489174
C	-2.3660475	0.6747166	1.4404978
C	-3.5349051	1.0615161	-0.636119
C	-3.5161732	1.0281852	0.7739743
H	2.354972	-0.649689	-2.5257559
H	4.412325	-1.2812466	-1.3371452
H	4.445334	-1.342612	1.1611259
H	2.4212139	-0.7618039	2.4349282
H	-2.4212139	0.7618039	-2.4349282
H	-4.445334	1.342612	-1.1611259
H	-4.412325	1.2812466	1.3371452
H	-2.354972	0.649689	2.5257559

8 with a = 0.35 in MeCN

(C_i symmetry)

Energy = -2643.425465086 Hartree

	X	Y	Z
C	0.0405264	-0.1031559	4.0526772
C	0.0300946	-0.1196341	5.4549617
C	0.0389638	-0.075196	2.8271841
C	0.0210603	-0.0399815	1.4318441
C	1.2029009	-0.3759014	0.6874619
C	1.1819879	-0.3349299	-0.73913

C	0.011329	0.0642813	-1.431947	C	-0.0210603	0.0399815	-1.4318441
C	-1.1796028	0.4174822	-0.7101328	C	-1.2029009	0.3759014	-0.6874619
C	-1.1805262	0.3991478	0.7171444	C	-1.1819879	0.3349299	0.73913
C	0.0114217	0.0788046	-2.8270514	C	-0.0389638	0.075196	-2.8271841
C	-1.1611439	0.3035021	6.1888631	C	-1.1321733	0.2471984	6.1785651
C	-1.1682252	0.2776422	7.5645999	C	-1.1463307	0.2445346	7.5544293
C	-0.0053943	-0.0848109	8.2934603	C	0.0088447	-0.1184403	8.2948359
C	1.1617946	-0.4209029	7.5586747	C	1.1724831	-0.4903286	7.5714446
C	1.1622246	-0.3984925	6.182997	C	1.1790946	-0.4940463	6.1954681
H	-2.0612613	0.5999558	5.6549477	H	-2.0245434	0.5502659	5.63528
H	-2.0717874	0.5558586	8.0977075	H	-2.047898	0.5445147	8.0789095
N	-0.0094228	-0.1099338	9.6690353	N	-0.0015797	-0.1095674	9.6713012
H	2.0626227	-0.7166386	8.0869098	H	2.0656156	-0.7916766	8.1093949
H	2.0653234	-0.6758793	5.6438709	H	2.0789022	-0.7985142	5.6656144
C	0.0110391	0.0876804	-4.0527097	C	-0.0405264	0.1031559	-4.0526772
C	0.0101692	0.0940424	-5.4548412	C	-0.0300946	0.1196341	-5.4549617
C	1.1681684	-0.2647535	-6.1890071	C	1.1321733	-0.2471984	-6.1785651
C	1.1695046	-0.2622737	-7.5649824	C	1.1463307	-0.2445346	-7.5544293
C	0.0061477	0.0962819	-8.2951173	C	-0.0088447	0.1184403	-8.2948359
C	-1.1545917	0.4557141	-7.561057	C	-1.1724831	0.4903286	-7.5714446
C	-1.1493824	0.4560519	-6.1852486	C	-1.1790946	0.4940463	-6.1954681
H	2.0682103	-0.5594364	-5.6540138	H	2.0245434	-0.5502659	-5.63528
H	2.0685311	-0.5568717	-8.0968825	H	2.047898	-0.5445147	-8.0789095
N	0.0041026	0.095293	-9.6708635	N	0.0015797	0.1095674	-9.6713012
H	-2.0552047	0.750376	-8.0902283	H	-2.0656156	0.7916766	-8.1093949
H	-2.0479799	0.7496352	-5.6472034	H	-2.0789022	0.7985142	-5.6656144
C	1.2224983	0.1413116	-10.4173697	C	1.2292517	0.1620605	-10.4025712
C	-1.2153553	0.0388992	-10.4146756	C	-1.2086872	0.0402008	-10.4270976
C	-1.2296279	-0.1871834	10.4096238	C	-1.2292517	-0.1620605	10.4025712
C	1.2069568	-0.0554182	10.4181595	C	1.2086872	-0.0402008	10.4270976
C	2.0892598	1.0144769	10.2680637	C	2.1258994	0.9898039	10.2162094
C	3.2703588	1.0783066	11.0058009	C	3.3060884	1.0617973	10.9544751
C	3.5735084	0.0657776	11.923539	C	3.5746715	0.0990634	11.9345386
C	2.679889	-1.0049255	12.0847285	C	2.6421071	-0.9249893	12.1635229
C	1.5136001	-1.0656065	11.3393065	C	1.4769211	-0.9949098	11.4172012
H	1.8544281	1.8120887	9.5663327	H	1.9216049	1.747201	9.4628698
H	3.9349805	1.9248755	10.8639486	H	3.9970832	1.8771417	10.7642733
O	4.6837966	0.0380535	12.6869145	O	4.6873314	0.076592	12.6951511
H	2.9268674	-1.7864059	12.8000272	H	2.85943	-1.665511	12.9303529
H	0.8317604	-1.903269	11.4683705	H	0.7664793	-1.7983591	11.5971894
C	-2.1256313	-1.2452097	10.2017121	C	-2.1121757	-1.2382829	10.2365147
C	-3.2989678	-1.3254967	10.9340485	C	-3.29132	-1.2969948	10.9620098
C	-3.6002509	-0.3573988	11.9047463	C	-3.6105887	-0.2877436	11.8841909
C	-2.7018731	0.6933671	12.1254163	C	-2.7285987	0.7857843	12.0570547
C	-1.528927	0.7721054	11.3762979	C	-1.5488555	0.841116	11.3165814

H	-1.896941	-2.0091724	9.4616786	H	-1.8672352	-2.034246	9.5363099
H	-3.998596	-2.1439746	10.7792943	H	-3.9802438	-2.1303638	10.841484
O	-4.760474	-0.5200068	12.5712025	O	-4.7710069	-0.434514	12.5544037
H	-2.9049013	1.4577213	12.8689681	H	-2.9494943	1.5851738	12.7574464
H	-0.8383137	1.5945158	11.5493102	H	-0.8712663	1.681383	11.4528903
C	2.1286197	1.1962135	-10.2407977	C	2.1121757	1.2382829	-10.2365147
C	3.3006062	1.2455813	-10.9780282	C	3.29132	1.2969948	-10.9620098
C	3.5902506	0.2482927	-11.9223647	C	3.6105887	0.2877436	-11.8841909
C	2.6815808	-0.7996825	-12.1118822	C	2.7285987	-0.7857843	-12.0570547
C	1.5100134	-0.8469072	-11.358036	C	1.5488555	-0.841116	-11.3165814
H	1.9089411	1.9819968	-9.5211395	H	1.8672352	2.034246	-9.5363099
H	4.008095	2.0615374	-10.8475094	H	3.9802438	2.1303638	-10.841484
O	4.7502317	0.3814085	-12.5957426	O	4.7710069	0.434514	-12.5544037
H	2.8758031	-1.5861347	-12.8344486	H	2.9494943	-1.5851738	-12.7574464
H	0.8115097	-1.6674818	-11.5065258	H	0.8712663	-1.681383	-11.4528903
C	-2.1133497	-1.0131344	-10.233817	C	-2.1258994	-0.9898039	-10.2162094
C	-3.2972921	-1.0788914	-10.9667668	C	-3.3060884	-1.0617973	-10.9544751
C	-3.5875129	-0.0873028	-11.9111641	C	-3.5746715	-0.0990634	-11.9345386
C	-2.6782124	0.9648908	-12.10338	C	-2.6421071	0.9249893	-12.1635229
C	-1.5092513	1.0281703	-11.3623754	C	-1.4769211	0.9949098	-11.4172012
H	-1.8889555	-1.7951034	-9.5114068	H	-1.9216049	-1.747201	-9.4628698
H	-3.974281	-1.9110771	-10.8004597	H	-3.9970832	-1.8771417	-10.7642733
O	-4.6991778	-0.0636562	-12.6726753	O	-4.6873314	-0.076592	-12.6951511
H	-2.915116	1.7303233	-12.8391347	H	-2.85943	1.665511	-12.9303529
H	-0.8151561	1.851493	-11.5158885	H	-0.7664793	1.7983591	-11.5971894
C	-5.1309169	0.4148903	13.5634297	C	-5.1389759	0.5219347	13.5270191
C	5.627222	1.0843508	12.5831179	C	5.6850841	1.0573737	12.4999293
C	-5.6588011	-1.0914254	-12.5370903	C	-5.6850841	-1.0573737	-12.4999293
C	5.1092535	-0.5839587	-13.5627609	C	5.1389759	-0.5219347	-13.5270191
H	-6.0936999	0.0820086	13.9599122	H	-6.0923333	0.1885595	13.945601
H	-4.3974808	0.446374	14.3811671	H	-4.3943309	0.5821466	14.3328815
H	-5.2450219	1.4238191	13.1434284	H	-5.2706484	1.5185525	13.0836735
H	6.4316439	0.8480218	13.2845974	H	6.4872672	0.8298872	13.2070935
H	6.0439319	1.1515989	11.5684971	H	6.0877373	1.0235267	11.4779632
H	5.1859683	2.0528805	12.8563092	H	5.3031413	2.0673804	12.7031539
H	-6.4612834	-0.8622796	-13.2431652	H	-6.4872672	-0.8298872	-13.2070935
H	-5.2337323	-2.0742203	-12.7837178	H	-5.3031413	-2.0673804	-12.7031539
H	-6.0737399	-1.1232182	-11.5199968	H	-6.0877373	-1.0235267	-11.4779632
H	6.0739843	-0.2710902	-13.970673	H	6.0923333	-0.1885595	-13.945601
H	5.2151982	-1.5819304	-13.1153551	H	5.2706484	-1.5185525	-13.0836735
H	4.3732632	-0.6311095	-14.3774191	H	4.3943309	-0.5821466	-14.3328815
C	2.3909382	-0.6597521	-1.403702	C	2.3631879	-0.6672389	-1.4482905
C	2.3891565	-0.6954649	1.3875267	C	2.4044996	-0.7504046	1.3407404
C	3.5292357	-1.0149941	-0.7170829	C	3.5142831	-1.0264149	-0.7861626
C	3.5283307	-1.0330919	0.693533	C	3.5350418	-1.069897	0.6235765

C	-2.3680501	0.7879336	-1.3882935
C	-2.3699478	0.7520203	1.402948
C	-3.5072596	1.1254687	-0.6943066
C	-3.5082376	1.107261	0.7163061
H	2.3944007	-0.6464102	-2.4898807
H	4.4315808	-1.2822136	-1.2630885
H	4.4299632	-1.3142852	1.2336593
H	2.3911073	-0.7101354	2.4737064
H	-2.3699336	0.8027848	-2.4744686
H	-4.4088384	1.4068244	-1.2344384
H	-4.4105743	1.3745395	1.2622972
H	-2.3733439	0.7388908	2.4891378

C	-2.4044996	0.7504046	-1.3407404
C	-2.3631879	0.6672389	1.4482905
C	-3.5350418	1.069897	-0.6235765
C	-3.5142831	1.0264149	0.7861626
H	2.3508427	-0.6347084	-2.5334157
H	4.4092482	-1.2758489	-1.3530079
H	4.4458048	-1.3556366	1.1454031
H	2.4248167	-0.7816138	2.4265606
H	-2.4248167	0.7816138	-2.4265606
H	-4.4458048	1.3556366	-1.1454031
H	-4.4092482	1.2758489	1.3530079
H	-2.3508427	0.6347084	2.5334157

9 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -1876.286868530 Hartree

	X	Y	Z
C	-1.3664008	0.6883197	-2.0163995
C	-1.5636921	0.7832125	-0.6712359
C	-0.6004345	0.2909839	0.2646585
C	0.6029821	-0.2917609	-0.2590642
C	0.7960473	-0.377685	-1.6382571
C	-0.1693328	0.0990092	-2.5431515
C	1.567158	-0.7827549	0.676808
C	1.3701688	-0.6871262	2.0219943
C	0.1724099	-0.099397	2.5479206
C	-0.7939911	0.3754696	1.6439398
N	-0.0235878	-0.0154012	3.9096471
N	0.0253526	0.0151346	-3.9035394
H	-1.7010058	0.8372935	2.0235059
H	2.1110656	-1.0834425	2.7096746
H	2.4720595	-1.254541	0.2973306
H	1.7025948	-0.8407413	-2.0171522
H	-2.4689486	1.2545428	-0.2920202
H	-2.1073548	1.0848596	-2.7037111
C	1.3367267	-0.0772176	-4.4560619
C	-1.0757661	-0.0079419	-4.8085724
C	1.0766187	0.0415241	4.8119457
C	-1.3374195	0.0422626	4.4588823
C	2.3167145	0.8615253	-4.1266149
C	3.5942605	0.7805283	-4.6734386
C	3.9049066	-0.2474382	-5.5738882
C	2.9134106	-1.1842146	-5.914538
C	1.6479103	-1.099455	-5.3658327
H	2.0774387	1.6722716	-3.4415595

9 with a = 0.35 in gas phase (C_i symmetry)

Energy = -1876.286876788 Hartree

	X	Y	Z
C	-1.3613066	0.698423	-2.0197462
C	-1.5592394	0.794431	-0.6747343
C	-0.5999503	0.2953247	0.2616827
C	0.5999503	-0.2953247	-0.2616827
C	0.7940187	-0.3811967	-1.6407941
C	-0.167453	0.1024496	-2.5454731
C	1.5592394	-0.794431	0.6747343
C	1.3613066	-0.698423	2.0197462
C	0.167453	-0.1024496	2.5454731
C	-0.7940187	0.3811967	1.6407941
N	-0.0267873	-0.0182406	3.9070139
N	0.0267873	0.0182406	-3.9070139
H	-1.6979629	0.8498125	2.0193276
H	2.0988207	-1.1001902	2.7078686
H	2.461408	-1.2721372	0.2960601
H	1.6979629	-0.8498125	-2.0193276
H	-2.461408	1.2721372	-0.2960601
H	-2.0988207	1.1001902	-2.7078686
C	1.3372214	-0.0569942	-4.4617144
C	-1.0775223	-0.0230822	-4.8067725
C	1.0775223	0.0230822	4.8067725
C	-1.3372214	0.0569942	4.4617144
C	2.3164438	0.874356	-4.1080767
C	3.5935965	0.8102766	-4.657592
C	3.9057017	-0.1927349	-5.5854071
C	2.9167672	-1.1244486	-5.947181
C	1.6516452	-1.0567503	-5.3957203
H	2.0762416	1.6676619	-3.4033303

H	4.3324784	1.5296289	-4.4042444	H	4.3302689	1.5539225	-4.3697709
O	5.0992228	-0.413927	-6.1561217	O	5.0992472	-0.340192	-6.1740181
H	3.1719686	-1.9756008	-6.6139056	H	3.1768038	-1.8977591	-6.6659826
H	0.8889635	-1.8307516	-5.6342266	H	0.8951345	-1.7840734	-5.6809652
C	-2.1388159	-0.9050124	-4.6190165	C	-2.1328356	-0.9259387	-4.6010582
C	-3.1967758	-0.9337656	-5.5083851	C	-3.194733	-0.9739181	-5.4846734
C	-3.2190313	-0.0735117	-6.6197253	C	-3.2294981	-0.1270016	-6.6060639
C	-2.1520096	0.8132851	-6.8190116	C	-2.172925	0.7693315	-6.8186825
C	-1.0927698	0.8400853	-5.9176291	C	-1.1094523	0.8153307	-5.9231118
H	-2.1242465	-1.5890622	-3.773019	H	-2.1078516	-1.6006512	-3.7479429
H	-4.0227456	-1.6290743	-5.3785265	H	-4.0138107	-1.6750384	-5.3430087
H	-2.1394597	1.4894393	-7.6681855	H	-2.1716389	1.4374396	-7.6742574
H	-0.2701628	1.533788	-6.0766582	H	-0.2947769	1.5157024	-6.0931595
C	2.1363595	0.9366279	4.592916	C	2.1328356	0.9259387	4.6010582
C	3.1945483	0.9987355	5.4798562	C	3.194733	0.9739181	5.4846734
C	3.221507	0.1752351	6.6188307	C	3.2294981	0.1270016	6.6060639
C	2.1580605	-0.7090406	6.8477697	C	2.172925	-0.7693315	6.8186825
C	1.0987585	-0.770331	5.9485059	C	1.1094523	-0.8153307	5.9231118
H	2.1180081	1.5942305	3.7264999	H	2.1078516	1.6006512	3.7479429
H	4.0170941	1.6933634	5.3268894	H	4.0138107	1.6750384	5.3430087
O	4.2858028	0.3090214	7.4196697	O	4.2961429	0.2496037	7.406031
H	2.1489341	-1.3572821	7.7184468	H	2.1716389	-1.4374396	7.6742574
H	0.279944	-1.4625185	6.1311099	H	0.2947769	-1.5157024	6.0931595
C	-2.295721	-0.9135119	4.1137426	C	-2.3164438	-0.874356	4.1080767
C	-3.5768538	-0.8668404	4.6555486	C	-3.5935965	-0.8102766	4.657592
C	-3.9139401	0.1435109	5.5666063	C	-3.9057017	0.1927349	5.5854071
C	-2.9444599	1.097656	5.9228497	C	-2.9167672	1.1244486	5.947181
C	-1.6751648	1.0470166	5.3791477	C	-1.6516452	1.0567503	5.3957203
H	-2.0359964	-1.7109562	3.4206795	H	-2.0762416	-1.6676619	3.4033303
H	-4.2973355	-1.6286707	4.3743221	H	-4.3302689	-1.5539225	4.3697709
O	-5.1137821	0.2769407	6.1450872	O	-5.0992472	0.340192	6.1740181
H	-3.2233525	1.8750816	6.6300276	H	-3.1768038	1.8977591	6.6659826
H	-0.9342307	1.7924214	5.6586652	H	-0.8951345	1.7840734	5.6809652
O	-4.2836073	-0.1762177	-7.4253493	O	-4.2961429	-0.2496037	-7.406031
C	4.3935546	-0.4671563	8.5918406	C	4.4130935	-0.5518891	8.5600361
C	-6.1432561	-0.6433599	5.8629633	C	-6.1474756	-0.5566671	5.8860066
C	-4.3862607	0.637565	-8.5719821	C	-4.4130935	0.5518891	-8.5600361
C	6.1496364	0.4866659	-5.8889916	C	6.1474756	0.5566671	-5.8860066
H	5.3322609	-0.1759035	9.0701151	H	5.3507781	-0.2641509	9.0424169
H	3.5623053	-0.2694784	9.2836708	H	3.582236	-0.3765297	9.2583135
H	4.4267111	-1.5418109	8.361833	H	4.4540979	-1.6208453	8.3059754
H	-7.0093015	-0.3284284	6.450723	H	-7.0036973	-0.2340981	6.4839338
H	-6.4113074	-0.6342545	4.7965631	H	-6.4223633	-0.5275165	4.8217041
H	-5.8624105	-1.6647945	6.1571876	H	-5.8839665	-1.5872711	6.1638644
H	-5.3254173	0.3658373	-9.0608091	H	-5.3507781	0.2641509	-9.0424169

H	-4.4153977	1.7045407	-8.3079509
H	-3.5548054	0.4588862	-9.268759
H	7.0062656	0.1458104	-6.4761299
H	5.8904333	1.5106184	-6.1943053
H	6.4217715	0.4845701	-4.8235645

H	-4.4540979	1.6208453	-8.3059754
H	-3.582236	0.3765297	-9.2583135
H	7.0036973	0.2340981	-6.4839338
H	5.8839665	1.5872711	-6.1638644
H	6.4223633	0.5275165	-4.8217041

9 with a = 0.35 in hexane

(C_1 symmetry)

Energy = -1876.307513046 Hartree

	X	Y	Z
C	-1.3763356	0.6710503	-2.0165571
C	-1.574076	0.7668578	-0.6714823
C	-0.6061971	0.2835245	0.2646115
C	0.6015467	-0.2911655	-0.2583625
C	0.7958454	-0.376608	-1.6369611
C	-0.1738194	0.0916798	-2.5425332
C	1.5698154	-0.7743442	0.6777441
C	1.3718248	-0.6789047	2.0227775
C	0.169898	-0.098445	2.5479686
C	-0.8001725	0.3695447	1.6432962
N	-0.0260707	-0.0136208	3.9089468
N	0.0229956	0.0089023	-3.9018846
H	-1.7100678	0.827068	2.0208938
H	2.1159367	-1.0698253	2.7099681
H	2.478205	-1.2393298	0.2985453
H	1.7059364	-0.833818	-2.0141751
H	-2.4831164	1.2307415	-0.2924159
H	-2.121284	1.0604246	-2.7034998
C	1.3359247	-0.0791801	-4.4521511
C	-1.0755346	-0.0138285	-4.8101693
C	1.0747579	0.0426429	4.8110733
C	-1.3387714	0.0451022	4.4600131
C	2.3081054	0.8699641	-4.1301924
C	3.587051	0.7931189	-4.6746032
C	3.9063548	-0.2414401	-5.5640044
C	2.9231424	-1.1893745	-5.8961677
C	1.6557397	-1.1087313	-5.3497042
H	2.062267	1.685345	-3.4532033
H	4.3190554	1.5501775	-4.4110244
O	5.1049	-0.4036836	-6.1427507
H	3.1869976	-1.9867201	-6.5869063
H	0.9033506	-1.8492717	-5.6109191
C	-2.1317862	-0.9204718	-4.6317665
C	-3.186748	-0.949319	-5.525539
C	-3.2112301	-0.0797527	-6.6290213

9 with a = 0.35 in hexane

(C_i symmetry)

Energy = -1876.307534752 Hartree

	X	Y	Z
C	-1.3698378	0.6859938	-2.0184435
C	-1.5681234	0.7788055	-0.6732079
C	-0.6024831	0.2895227	0.2624123
C	0.6024831	-0.2895227	-0.2624123
C	0.7965074	-0.373494	-1.6412885
C	-0.1711826	0.100645	-2.5456438
C	1.5681234	-0.7788055	0.6732079
C	1.3698378	-0.6859938	2.0184435
C	0.1711826	-0.100645	2.5456438
C	-0.7965074	0.373494	1.6412885
N	-0.023497	-0.016811	3.9062447
N	0.023497	0.016811	-3.9062447
H	-1.7044788	0.8343766	2.0193718
H	2.1127305	-1.0821141	2.7040707
H	2.4747387	-1.2469027	0.2936725
H	1.7044788	-0.8343766	-2.0193718
H	-2.4747387	1.2469027	-0.2936725
H	-2.1127305	1.0821141	-2.7040707
C	1.3353541	-0.0600297	-4.4593808
C	-1.0779889	-0.0235008	-4.8096921
C	1.0779889	0.0235008	4.8096921
C	-1.3353541	0.0600297	4.4593808
C	2.3089788	0.8814077	-4.1183359
C	3.5869371	0.8162395	-4.6666414
C	3.9035494	-0.1970608	-5.5812978
C	2.920333	-1.1394336	-5.9299328
C	1.6545455	-1.0713711	-5.3785066
H	2.0651552	1.6825397	-3.4238459
H	4.3198653	1.566855	-4.3875841
O	5.0992918	-0.3437954	-6.1696224
H	3.1830366	-1.922327	-6.6374608
H	0.9020986	-1.8066613	-5.6537002
C	-2.1371903	-0.9219737	-4.6055309
C	-3.1954608	-0.9689717	-5.4943505
C	-3.2217293	-0.125954	-6.6185849

C	-2.1511439	0.8174541	-6.8167183	C	-2.1600494	0.7638374	-6.8311531
C	-1.0951805	0.8445031	-5.9110975	C	-1.1006991	0.8095891	-5.9303728
H	-2.1152026	-1.6117069	-3.791812	H	-2.1199596	-1.5932827	-3.7496381
H	-4.0072572	-1.6524686	-5.4027197	H	-4.0172253	-1.6669013	-5.3517037
H	-2.1407835	1.5016936	-7.659326	H	-2.1508491	1.427389	-7.6902377
H	-0.277887	1.5463097	-6.0611654	H	-0.2827967	1.5062723	-6.0999587
C	2.1291793	0.9446194	4.5974111	C	2.1371903	0.9219737	4.6055309
C	3.1881794	1.0046985	5.4843273	C	3.1954608	0.9689717	5.4943505
C	3.220475	0.1718204	6.6158452	C	3.2217293	0.125954	6.6185849
C	2.1628769	-0.72076	6.838571	C	2.1600494	-0.7638374	6.8311531
C	1.1025137	-0.7793512	5.9401629	C	1.1006991	-0.8095891	5.9303728
H	2.1070894	1.608763	3.7361983	H	2.1199596	1.5932827	3.7496381
H	4.0063853	1.7050866	5.3340024	H	4.0172253	1.6669013	5.3517037
O	4.2857034	0.303405	7.4186843	O	4.2860603	0.2462632	7.4249726
H	2.1585317	-1.3774213	7.7028481	H	2.1508491	-1.427389	7.6902377
H	0.2889028	-1.4790926	6.1168444	H	0.2827967	-1.5062723	6.0999587
C	-2.3012532	-0.9050867	4.1106516	C	-2.3089788	-0.8814077	4.1183359
C	-3.5818311	-0.8555506	4.6535049	C	-3.5869371	-0.8162395	4.6666414
C	-3.9138011	0.1516701	5.5696257	C	-3.9035494	0.1970608	5.5812978
C	-2.9404946	1.0997861	5.9302093	C	-2.920333	1.1394336	5.9299328
C	-1.6714878	1.0468172	5.3850196	C	-1.6545455	1.0713711	5.3785066
H	-2.0458365	-1.7006813	3.4140751	H	-2.0651552	-1.6825397	3.4238459
H	-4.3054471	-1.612743	4.3681402	H	-4.3198653	-1.566855	4.3875841
O	-5.1147725	0.2865066	6.1490979	O	-5.0992918	0.3437954	6.1696224
H	-3.2139359	1.8758602	6.6411248	H	-3.1830366	1.922327	6.6374608
H	-0.9281563	1.7887417	5.667068	H	-0.9020986	1.8066613	5.6537002
O	-4.2725474	-0.1827874	-7.4419267	O	-4.2860603	-0.2462632	-7.4249726
C	4.3948397	-0.4866836	8.5830798	C	4.3912888	-0.5574504	8.5803945
C	-6.1471066	-0.6297122	5.8564242	C	-6.1402789	-0.5668562	5.890444
C	-4.3730213	0.6449003	-8.5803704	C	-4.3912888	0.5574504	-8.5803945
C	6.1460734	0.5104447	-5.877663	C	6.1402789	0.5668562	-5.890444
H	5.3316934	-0.1975848	9.0661578	H	5.3275023	-0.2754778	9.0689952
H	3.561748	-0.3002658	9.2752404	H	3.5569322	-0.3775406	9.2728041
H	4.4319321	-1.557911	8.3398215	H	4.4269719	-1.6260599	8.3252082
H	-7.0140793	-0.3169958	6.443883	H	-6.9991598	-0.2468211	6.4858466
H	-6.4108054	-0.6111988	4.7894896	H	-6.4149612	-0.5501881	4.8262034
H	-5.8693519	-1.653622	6.1434113	H	-5.8658974	-1.5917008	6.1777361
H	-5.3070913	0.3732422	-9.0788127	H	-5.3275023	0.2754778	-9.0689952
H	-4.4103284	1.7079112	-8.3031678	H	-4.4269719	1.6260599	-8.3252082
H	-3.5356607	0.4798905	-9.2729007	H	-3.5569322	0.3775406	-9.2728041
H	7.0089264	0.1737524	-6.4579919	H	6.9991598	0.2468211	-6.4858466
H	5.8773439	1.5287755	-6.1920335	H	5.8658974	1.5917008	-6.1777361
H	6.4122832	0.5192448	-4.8111822	H	6.4149612	0.5501881	-4.8262034

9 with *a* = 0.35 in DCM

9 with *a* = 0.35 in DCM

(C_1 symmetry)

Energy = -1876.334561804 Hartree

	X	Y	Z
C	-1.3794039	0.6557974	-2.0158103
C	-1.5783395	0.7523522	-0.6711289
C	-0.6046314	0.2810908	0.2654172
C	0.6087403	-0.2831206	-0.2559832
C	0.8034824	-0.3713259	-1.6335228
C	-0.1715225	0.0864692	-2.5401759
C	1.5835821	-0.7526362	0.6811878
C	1.3844345	-0.6553762	2.0258932
C	0.1760154	-0.0865185	2.5485007
C	-0.8001628	0.3691437	1.642731
N	-0.0238984	-0.000251	3.9075709
N	0.0258356	0.0027217	-3.8980659
H	-1.7144508	0.8195076	2.0178201
H	2.1332578	-1.0363145	2.7133247
H	2.496368	-1.2088512	0.3025399
H	1.7185528	-0.8201303	-2.0080533
H	-2.4916229	1.2076426	-0.2924112
H	-2.1283133	1.0378958	-2.7022901
C	1.3386698	-0.0978048	-4.4483664
C	-1.0713273	-0.006145	-4.8095028
C	1.0724673	0.0643883	4.8147787
C	-1.3394536	0.0406188	4.453729
C	2.3148093	0.850489	-4.1378797
C	3.5939857	0.7607594	-4.6806399
C	3.9078386	-0.2858387	-5.5570768
C	2.921089	-1.2332342	-5.8780593
C	1.6532883	-1.1400331	-5.3318467
H	2.0739124	1.6748781	-3.4703469
H	4.3296337	1.5164637	-4.4237579
O	5.1094428	-0.4593324	-6.1331558
H	3.1795056	-2.0415561	-6.55828
H	0.8985716	-1.8817372	-5.5826363
C	-2.1272772	-0.9148914	-4.6474993
C	-3.1810649	-0.9289962	-5.5445898
C	-3.2029248	-0.0416392	-6.6330417
C	-2.1439209	0.8597147	-6.803165
C	-1.0897332	0.8716394	-5.8944838
H	-2.1135651	-1.6191552	-3.8185422
H	-4.0013258	-1.6342975	-5.4309851
H	-2.1316598	1.5586957	-7.6335298
H	-0.2737214	1.5777496	-6.0306217
C	2.1127006	0.9846237	4.6137134

(C_i symmetry)

Energy = -1876.334577158 Hartree

	X	Y	Z
C	-1.3805611	0.660532	-2.0205672
C	-1.5800346	0.7545888	-0.6757512
C	-0.6068274	0.2818089	0.2609876
C	0.6068274	-0.2818089	-0.2609876
C	0.8014993	-0.3689348	-1.6386871
C	-0.1738734	0.0896298	-2.5448138
C	1.5800346	-0.7545888	0.6757512
C	1.3805611	-0.660532	2.0205672
C	0.1738734	-0.0896298	2.5448138
C	-0.8014993	0.3689348	1.6386871
N	-0.0221678	-0.001144	3.9034479
N	0.0221678	0.001144	-3.9034479
H	-1.7155029	0.8187825	2.0151046
H	2.1297338	-1.0458551	2.7054389
H	2.4923308	-1.2113082	0.2969652
H	1.7155029	-0.8187825	-2.0151046
H	-2.4923308	1.2113082	-0.2969652
H	-2.1297338	1.0458551	-2.7054389
C	1.3349993	-0.0740003	-4.4557541
C	-1.0777645	-0.0376495	-4.8094936
C	1.0777645	0.0376495	4.8094936
C	-1.3349993	0.0740003	4.4557541
C	2.2973211	0.8856807	-4.1350452
C	3.5751117	0.8242387	-4.6844322
C	3.9005355	-0.202054	-5.5805239
C	2.9291882	-1.1630618	-5.9082437
C	1.6634243	-1.1001286	-5.3536603
H	2.0459005	1.6973714	-3.4560435
H	4.2995191	1.5879184	-4.4196117
O	5.0992754	-0.3422117	-6.1709632
H	3.1973826	-1.9582553	-6.6000795
H	0.920671	-1.8519035	-5.6097792
C	-2.1291781	-0.9471912	-4.6189449
C	-3.1871468	-0.9881854	-5.5097679
C	-3.2189715	-0.127644	-6.6197274
C	-2.1633835	0.7711547	-6.8203308
C	-1.1049729	0.8112862	-5.9175569
H	-2.1082179	-1.6306586	-3.7729141
H	-4.0036615	-1.6940209	-5.3750451
H	-2.1575591	1.4474679	-7.6692556
H	-0.2928656	1.5171101	-6.0759047
C	2.1291781	0.9471912	4.6189449

C	3.1664788	1.0544613	5.5073008
C	3.2055297	0.2132452	6.6317927
C	2.1626524	-0.6992683	6.8408815
C	1.1080361	-0.7676143	5.9359758
H	2.0856273	1.6547271	3.7574561
H	3.9733315	1.7694642	5.363417
O	4.2644483	0.3553856	7.4456343
H	2.1642342	-1.3640563	7.6988175
H	0.3066542	-1.4838196	6.1020588
C	-2.284189	-0.9264024	4.102746
C	-3.56852	-0.8955259	4.6379815
C	-3.9214181	0.1098677	5.5477001
C	-2.9665663	1.0756171	5.9097118
C	-1.6930668	1.0413507	5.3712638
H	-2.0130361	-1.7205716	3.4107855
H	-4.277884	-1.6648574	4.3498067
O	-5.1311649	0.2252899	6.1190488
H	-3.2548887	1.8517157	6.6148841
H	-0.9646231	1.7978981	5.6531943
O	-4.2640571	-0.1300354	-7.4529888
C	4.3765135	-0.4527531	8.600275
C	-6.1445493	-0.7113321	5.8122232
C	-4.3590186	0.7271407	-8.5727812
C	6.1535981	0.4547759	-5.8663269
H	5.3038324	-0.155773	9.0966455
H	3.5336082	-0.2913813	9.2860166
H	4.4331883	-1.5184821	8.3396007
H	-7.0248685	-0.4142869	6.3877118
H	-6.3924615	-0.6974942	4.7420491
H	-5.850739	-1.7290847	6.1030085
H	-5.2914047	0.4693806	-9.0815555
H	-4.3951568	1.7822873	-8.268637
H	-3.518781	0.578183	-9.2647229
H	7.0191948	0.1115616	-6.4385918
H	5.8892035	1.4712751	-6.1884908
H	6.4110357	0.4693511	-4.7983473

C	3.1871468	0.9881854	5.5097679
C	3.2189715	0.127644	6.6197274
C	2.1633835	-0.7711547	6.8203308
C	1.1049729	-0.8112862	5.9175569
H	2.1082179	1.6306586	3.7729141
H	4.0036615	1.6940209	5.3750451
O	4.2852627	0.2396927	7.4294913
H	2.1575591	-1.4474679	7.6692556
H	0.2928656	-1.5171101	6.0759047
C	-2.2973211	-0.8856807	4.1350452
C	-3.5751117	-0.8242387	4.6844322
C	-3.9005355	0.202054	5.5805239
C	-2.9291882	1.1630618	5.9082437
C	-1.6634243	1.1001286	5.3536603
H	-2.0459005	-1.6973714	3.4560435
H	-4.2995191	-1.5879184	4.4196117
O	-5.0992754	0.3422117	6.1709632
H	-3.1973826	1.9582553	6.6000795
H	-0.920671	1.8519035	5.6097792
O	-4.2852627	-0.2396927	-7.4294913
C	4.393914	-0.5937103	8.5659504
C	-6.122343	-0.5969439	5.9105297
C	-4.393914	0.5937103	-8.5659504
C	6.122343	0.5969439	-5.9105297
H	5.3295675	-0.3216554	9.0611647
H	3.5595678	-0.4336989	9.262463
H	4.4313964	-1.6548687	8.2835176
H	-6.9884867	-0.2821399	6.4980869
H	-6.3950461	-0.6090885	4.8463696
H	-5.8261876	-1.6087262	6.2196112
H	-5.3295675	0.3216554	-9.0611647
H	-4.4313964	1.6548687	-8.2835176
H	-3.5595678	0.4336989	-9.262463
H	6.9884867	0.2821399	-6.4980869
H	5.8261876	1.6087262	-6.2196112
H	6.3950461	0.6090885	-4.8463696

9 with a = 0.35 in MeCN

(C_1 symmetry)

Energy = -1876.341693728 Hartree

	X	Y	Z
C	-1.3818748	0.6523532	-2.0176144
C	-1.5826188	0.7465344	-0.6728331
C	-0.6089544	0.27456	0.2635739
C	0.6037074	-0.2915264	-0.2572426

9 with a = 0.35 in MeCN

(C_i symmetry)

Energy = -1876.341674155 Hartree

	X	Y	Z
C	-1.3854283	0.6492993	-2.0212991
C	-1.5860648	0.7420723	-0.67657
C	-0.6089155	0.2775648	0.26052
C	0.6089155	-0.2775648	-0.26052

C	0.7998439	-0.377865	-1.6346621	C	0.8043577	-0.3645467	-1.6379829
C	-0.1746807	0.0810246	-2.5412078	C	-0.1748296	0.0854685	-2.544769
C	1.5783735	-0.7623547	0.6793341	C	1.5860648	-0.7420723	0.67657
C	1.380121	-0.6635451	2.0240612	C	1.3854283	-0.6492993	2.0212991
C	0.1724423	-0.0931789	2.5466099	C	0.1748296	-0.0854685	2.544769
C	-0.8040724	0.3626629	1.6410336	C	-0.8043577	0.3645467	1.6379829
N	-0.0259076	-0.0050359	3.9059397	N	-0.0219561	0.0025742	3.9028446
N	0.0244957	-0.0016088	-3.8995648	N	0.0219561	-0.0025742	-3.9028446
H	-1.7178942	0.81407	2.0157576	H	-1.7218001	0.8086954	2.0125654
H	2.1286882	-1.0451762	2.7113283	H	2.1375903	-1.0288724	2.7059863
H	2.4906097	-1.2192735	0.3002736	H	2.5019685	-1.1913124	0.2979762
H	1.7145871	-0.8279075	-2.0083859	H	1.7218001	-0.8086954	-2.0125654
H	-2.4955131	1.2024022	-0.2940117	H	-2.5019685	1.1913124	-0.2979762
H	-2.1298593	1.036157	-2.7040687	H	-2.1375903	1.0288724	-2.7059863
C	1.3380202	-0.092061	-4.4490768	C	1.3346601	-0.0766113	-4.4556829
C	-1.0722089	-0.0158075	-4.8112699	C	-1.0777203	-0.0401101	-4.8098421
C	1.0726574	0.0552967	4.8110685	C	1.0777203	0.0401101	4.8098421
C	-1.3402533	0.0456398	4.4548935	C	-1.3346601	0.0766113	4.4556829
C	2.3120454	0.8537431	-4.1238973	C	2.2966102	0.8835404	-4.135636
C	3.5925982	0.7733427	-4.6649352	C	3.5738663	0.8233062	-4.68677
C	3.9095426	-0.2604644	-5.5550986	C	3.8986476	-0.2022081	-5.5838341
C	2.9248877	-1.2042323	-5.8924077	C	2.928055	-1.1644106	-5.9101794
C	1.6557913	-1.1209933	-5.3471181	C	1.6627328	-1.1025537	-5.3537746
H	2.0691825	1.6683845	-3.4453029	H	2.045979	1.6946326	-3.4555497
H	4.3264574	1.5263646	-4.3954277	H	4.2982501	1.5869076	-4.421581
O	5.1136018	-0.4239704	-6.1308694	O	5.0972523	-0.3402158	-6.1769767
H	3.1842666	-2.003155	-6.5834045	H	3.1954636	-1.9599581	-6.6019989
H	0.9030549	-1.8607986	-5.6091636	H	0.920198	-1.8548695	-5.6091444
C	-2.1279191	-0.9238855	-4.6444527	C	-2.1233487	-0.9569603	-4.6261319
C	-3.1822432	-0.9419828	-5.5412226	C	-3.1813518	-0.9974454	-5.5176245
C	-3.2039665	-0.0598965	-6.6338284	C	-3.2177144	-0.1289752	-6.6208123
C	-2.1444576	0.8394917	-6.8100333	C	-2.1666594	0.7766952	-6.8155556
C	-1.0900828	0.8557447	-5.9014457	C	-1.1087304	0.8162286	-5.9121726
H	-2.1147506	-1.6234766	-3.8116061	H	-2.0995956	-1.6453967	-3.7842762
H	-4.0026328	-1.6464206	-5.4228386	H	-3.9931973	-1.7095231	-5.3872355
H	-2.1322559	1.534378	-7.6438464	H	-2.1650771	1.459682	-7.6592245
H	-0.2747802	1.5620225	-6.0408089	H	-0.3014616	1.5289458	-6.0646341
C	2.118146	0.9680535	4.6046247	C	2.1233487	0.9569603	4.6261319
C	3.1748452	1.0329138	5.4957262	C	3.1813518	0.9974454	5.5176245
C	3.2102008	0.1948456	6.622455	C	3.2177144	0.1289752	6.6208123
C	2.1616145	-0.7093358	6.8376055	C	2.1666594	-0.7766952	6.8155556
C	1.1045978	-0.7733602	5.9347738	C	1.1087304	-0.8162286	5.9121726
H	2.0935629	1.6357769	3.7464913	H	2.0995956	1.6453967	3.7842762
H	3.9862454	1.741857	5.3470441	H	3.9931973	1.7095231	5.3872355
O	4.2732866	0.3310039	7.4337935	O	4.2841153	0.2396384	7.4320144

H	2.1604264	-1.371242	7.6977988	H	2.1650771	-1.459682	7.6592245
H	0.2987956	-1.4836521	6.1047377	H	0.3014616	-1.5289458	6.0646341
C	-2.292284	-0.9158658	4.1085783	C	-2.2966102	-0.8835404	4.135636
C	-3.5748979	-0.8753271	4.6478528	C	-3.5738663	-0.8233062	4.68677
C	-3.917308	0.1335671	5.5573541	C	-3.8986476	0.2022081	5.5838341
C	-2.9550953	1.0931848	5.9153333	C	-2.928055	1.1644106	5.9101794
C	-1.6835128	1.049887	5.3722367	C	-1.6627328	1.1025537	5.3537746
H	-2.0292368	-1.7123947	3.4162751	H	-2.045979	-1.6946326	3.4555497
H	-4.290484	-1.6399315	4.3624957	H	-4.2982501	-1.5869076	4.421581
O	-5.1251309	0.2576376	6.1334019	O	-5.0972523	0.3402158	6.1769767
H	-3.2343719	1.8726898	6.6205218	H	-3.1954636	1.9599581	6.6019989
H	-0.9491835	1.8022912	5.6499188	H	-0.920198	1.8548695	5.6091444
O	-4.2663415	-0.1511686	-7.4534175	O	-4.2841153	-0.2396384	-7.4320144
C	4.3792677	-0.4740403	8.5917034	C	4.3984	-0.6064961	8.5593094
C	-6.1466289	-0.6707766	5.8259258	C	-6.120232	-0.5999987	5.9154298
C	-4.3609199	0.7037197	-8.5756955	C	-4.3984	0.6064961	-8.5593094
C	6.1553995	0.4885348	-5.8461889	C	6.120232	0.5999987	-5.9154298
H	5.3107195	-0.1851387	9.0852312	H	5.3320741	-0.3335634	9.0578041
H	3.539458	-0.301215	9.278405	H	3.5626851	-0.4604382	9.2570701
H	4.4237917	-1.5413271	8.3353234	H	4.4430389	-1.6638242	8.2641783
H	-7.023737	-0.3685424	6.4037187	H	-6.9853292	-0.2881592	6.5061187
H	-6.3960936	-0.6524878	4.756257	H	-6.395008	-0.6087695	4.851901
H	-5.8601222	-1.6915096	6.1133148	H	-5.8214911	-1.612252	6.2201533
H	-5.2943676	0.4466484	-9.0829731	H	-5.3320741	0.3335634	-9.0578041
H	-4.3943925	1.7595991	-8.2740938	H	-4.4430389	1.6638242	-8.2641783
H	-3.5216625	0.5515633	-9.2680575	H	-3.5626851	0.4604382	-9.2570701
H	7.0247159	0.1542323	-6.4181598	H	6.9853292	0.2881592	-6.5061187
H	5.8909495	1.5086942	-6.1562276	H	5.8214911	1.612252	-6.2201533
H	6.4067406	0.4895254	-4.7767577	H	6.395008	0.6087695	-4.851901

10 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -2030.902584837 Hartree

	X	Y	Z
C	1.5258253	-1.1287869	7.6804042
C	1.2524047	-0.1043791	6.762729
C	2.2188012	0.8740766	6.5293227
C	3.4510276	0.829626	7.1777402
C	3.7249164	-0.2005615	8.0859855
C	2.7448208	-1.1774059	8.3310714
N	-0.0158905	-0.0501306	6.1060172
C	-1.1811716	-0.0567702	6.933178
C	-2.1879594	-1.014543	6.741477
C	-3.305602	-1.0280047	7.556285
C	-3.4433799	-0.0905089	8.5936436

10 with a = 0.35 in gas phase (C_i symmetry)

Energy = -2030.902644425 Hartree

	X	Y	Z
C	1.5253148	-1.1062507	7.6966258
C	1.2529986	-0.0951674	6.7633056
C	2.2246951	0.8732326	6.5086726
C	3.4594033	0.832624	7.1522492
C	3.7310626	-0.183103	8.07761
C	2.7465849	-1.150248	8.3430352
N	-0.0155803	-0.046084	6.109256
C	-1.1813459	-0.0605352	6.9338969
C	-2.1979778	-1.0031715	6.7173885
C	-3.3175239	-1.0246655	7.5290461
C	-3.4481981	-0.1113604	8.588716

C	-2.4323339	0.8578247	8.7965742	C	-2.4284512	0.8220714	8.8156104
C	-1.3125625	0.8673883	7.9696934	C	-1.3069005	0.8408985	7.9912459
O	-4.5595431	-0.1834905	9.3311105	O	-4.5664772	-0.2114005	9.3217495
C	-4.7740092	0.705112	10.4023753	C	-4.7755504	0.6552654	10.412438
O	4.8749085	-0.3336612	8.7631023	O	4.8831419	-0.3115331	8.7516923
C	5.9070894	0.6081307	8.592161	C	5.9209995	0.6205786	8.5594292
C	-0.1112171	0.0011554	4.738364	C	-0.1106024	0.0092421	4.7402541
C	-1.2876266	0.4747083	4.0988923	C	-1.2763079	0.5093211	4.1027012
C	-1.3692111	0.5209097	2.7282085	C	-1.358337	0.557133	2.7318397
C	-0.3044625	0.0976633	1.8908477	C	-0.3039505	0.1104701	1.8938277
C	0.8653098	-0.3787412	2.5418936	C	0.8554515	-0.3919171	2.5435524
C	0.9657134	-0.4232061	3.9095949	C	0.9559009	-0.4383943	3.9113417
C	-0.460494	0.1694265	0.4724101	C	-0.459215	0.1851674	0.4749421
C	0.4643712	-0.1842195	-0.478239	C	0.459215	-0.1851674	-0.4749421
C	0.3078734	-0.1104683	-1.8965975	C	0.3039505	-0.1104701	-1.8938277
C	1.3674925	-0.5442023	-2.7353063	C	1.358337	-0.557133	-2.7318397
C	1.2842807	-0.4967795	-4.1059391	C	1.2763079	-0.5093211	-4.1027012
C	0.1127997	-0.0087939	-4.7430322	C	0.1106024	-0.0092421	-4.7402541
C	-0.9586732	0.4261959	-3.9133322	C	-0.9559009	0.4383943	-3.9113417
C	-0.8575284	0.3790639	-2.5457542	C	-0.8554515	0.3919171	-2.5435524
N	0.0166328	0.0461944	-6.1111791	N	0.0155803	0.046084	-6.109256
C	1.1817094	0.0685668	-6.9372668	C	1.1813459	0.0605352	-6.9338969
C	1.3161269	-0.8392646	-7.9880588	C	1.3069005	-0.8408985	-7.9912459
C	2.4368337	-0.8146809	-8.8132189	C	2.4284512	-0.8220714	-8.8156104
C	3.4465125	0.1315594	-8.5936502	C	3.4481981	0.1113604	-8.588716
C	3.3060544	1.0521879	-7.5418516	C	3.3175239	1.0246655	-7.5290461
C	2.1871864	1.0246107	-6.7291789	C	2.1979778	1.0031715	-6.7173885
O	4.5635877	0.2374658	-9.3275723	O	4.5664772	0.2114005	-9.3217495
C	4.780135	-0.6330326	-10.4132359	C	4.7755504	-0.6552654	-10.412438
C	-1.2528317	0.0904166	-6.7650942	C	-1.2529986	0.0951674	-6.7633056
C	-1.5350433	1.1096862	-7.686033	C	-1.5253148	1.1062507	-7.6966258
C	-2.7570393	1.1498689	-8.3314366	C	-2.7465849	1.150248	-8.3430352
C	-3.7317423	0.1697209	-8.0775506	C	-3.7310626	0.183103	-8.07761
C	-3.4491574	-0.8552897	-7.1660314	C	-3.4594033	-0.832624	-7.1522492
C	-2.2138688	-0.8914607	-6.5230461	C	-2.2246951	-0.8732326	-6.5086726
O	-4.8854822	0.2951548	-8.7494965	O	-4.8831419	0.3115331	-8.7516923
C	-5.91424	-0.6483433	-8.567194	C	-5.9209995	-0.6205786	-8.5594292
H	2.2726824	-0.9412866	-2.2778329	H	2.257766	-0.9642265	-2.2719335
H	2.1121124	-0.8542718	-4.7105131	H	2.1004316	-0.8771321	-4.706054
H	-1.8581477	0.824021	-4.3730052	H	-1.8507657	0.8464402	-4.3708852
H	-1.6936209	0.7454775	-1.9550019	H	-1.6873902	0.7686695	-1.9535263
H	-2.2784043	0.9074729	2.2696398	H	-2.257766	0.9642265	2.2719335
H	-2.1203932	0.8238362	4.7014082	H	-2.1004316	0.8771321	4.706054
H	1.8693883	-0.8104527	4.3698104	H	1.8507657	-0.8464402	4.3708852
H	1.7065365	-0.7356447	1.9526106	H	1.6873902	-0.7686695	1.9535263

H	0.5376111	-1.5786667	-8.1618993
H	2.515578	-1.5378268	-9.6188491
H	4.0902094	1.791433	-7.3957178
H	2.0820253	1.7522159	-5.9272158
H	-0.7896166	1.8755245	-7.8880298
H	-2.9926998	1.9383285	-9.0421584
H	-4.1748906	-1.6357911	-6.9592769
H	-1.9963344	-1.6985543	-5.8265059
H	-2.0847158	-1.754948	5.9509802
H	-4.090777	-1.7686056	7.4229332
H	-2.508663	1.593464	9.5910701
H	-0.5322213	1.6076528	8.1314695
H	2.0081359	1.6852107	5.8353146
H	4.180891	1.6080363	6.9777541
H	2.9736879	-1.9699386	9.0394925
H	0.7759214	-1.8919755	7.8757902
H	-5.7326636	0.4276717	10.8485295
H	-3.9864165	0.6171206	11.1648654
H	-4.8288593	1.748199	10.0582505
H	6.7276099	0.2911089	9.2412264
H	6.2638612	0.6335898	7.5520264
H	5.5871178	1.6176263	8.8886705
H	-6.7385827	-0.3381417	-9.2146993
H	-5.5928932	-1.65895	-8.8582901
H	-6.2659924	-0.6675189	-7.5252191
H	5.7395029	-0.347981	-10.852978
H	4.8346558	-1.6817031	-10.0864947
H	3.9937601	-0.5323853	-11.1754081
H	1.4285949	-0.5653726	-0.1431357
H	-1.42563	0.5479107	0.1368158

H	0.5200882	-1.5697076	-8.1725436
H	2.499023	-1.5397637	-9.6269505
H	4.1095753	1.7539654	-7.3765111
H	2.1004846	1.7264259	-5.9104888
H	-0.7712643	1.8611442	-7.9076995
H	-2.974326	1.9320051	-9.0636694
H	-4.1928961	-1.6032514	-6.9360592
H	-2.0144865	-1.6743165	-5.802896
H	-2.1004846	-1.7264259	5.9104888
H	-4.1095753	-1.7539654	7.3765111
H	-2.499023	1.5397637	9.6269505
H	-0.5200882	1.5697076	8.1725436
H	2.0144865	1.6743165	5.802896
H	4.1928961	1.6032514	6.9360592
H	2.974326	-1.9320051	9.0636694
H	0.7712643	-1.8611442	7.9076995
H	-5.738468	0.3773167	10.8489194
H	-3.9910942	0.5419572	11.174696
H	-4.8182397	1.7061269	10.0912622
H	6.7419145	0.3093112	9.2107229
H	6.2728744	0.6246842	7.5173903
H	5.6081284	1.6370602	8.8388727
H	-6.7419145	-0.3093112	-9.2107229
H	-5.6081284	-1.6370602	-8.8388727
H	-6.2728744	-0.6246842	-7.5173903
H	5.738468	-0.3773167	-10.8489194
H	4.8182397	-1.7061269	-10.0912622
H	3.9910942	-0.5419572	-11.174696
H	1.4173622	-0.5810622	-0.1387775
H	-1.4173622	0.5810622	0.1387775

10 with a = 0.35 in hexane

(C_1 symmetry)

Energy = -2030.923048274 Hartree

	X	Y	Z
C	1.5335039	-1.1277274	7.6775398
C	1.253656	-0.1035316	6.7617772
C	2.2151915	0.879433	6.526672
C	3.4480236	0.8416954	7.1745535
C	3.7271437	-0.1866832	8.0832345
C	2.753142	-1.1691067	8.3286188
N	-0.0145345	-0.0564859	6.10516
C	-1.1799565	-0.0659154	6.9318936
C	-2.1809077	-1.0301137	6.7438486
C	-3.3000326	-1.0450404	7.5574114

10 with a = 0.35 in hexane

(C_i symmetry)

Energy = -2030.923027219 Hartree

	X	Y	Z
C	1.5386263	-1.1081784	7.6776147
C	1.2560768	-0.088648	6.7572422
C	2.2208525	0.8874976	6.5070587
C	3.4621907	0.8444077	7.1379981
C	3.7467822	-0.1838423	8.0451769
C	2.7673625	-1.1558144	8.3109814
N	-0.0145134	-0.0402852	6.106027
C	-1.1795311	-0.0577087	6.9324608
C	-2.1829085	-1.0166622	6.7291889
C	-3.3028026	-1.0419602	7.5412358

C	-3.4443934	-0.1023026	8.5886455	C	-3.4456556	-0.1153465	8.5871429
C	-2.4400954	0.8537993	8.7868043	C	-2.4390791	0.8350414	8.8005572
C	-1.3192754	0.8654331	7.9607697	C	-1.316276	0.8564186	7.9772837
O	-4.5617267	-0.1965573	9.3270849	O	-4.5628398	-0.2194006	9.324324
C	-4.781736	0.7059249	10.388217	C	-4.776523	0.6601157	10.405895
O	4.8799919	-0.3125305	8.7598216	O	4.9097839	-0.3195047	8.7021047
C	5.9062174	0.6379249	8.5834858	C	5.9457551	0.6149031	8.4986251
C	-0.1099213	-0.0058405	4.737302	C	-0.111564	0.0120214	4.7376236
C	-1.2866477	0.4680185	4.0985451	C	-1.2846159	0.4964496	4.1003997
C	-1.3689073	0.5133837	2.7278588	C	-1.3681198	0.5426851	2.7295979
C	-0.3028849	0.0910029	1.8910758	C	-0.3078817	0.108753	1.8915159
C	0.86767	-0.3855442	2.5414142	C	0.8586758	-0.3789957	2.5406946
C	0.9672462	-0.430543	3.9092035	C	0.9605008	-0.4227852	3.9083166
C	-0.4582954	0.164528	0.473138	C	-0.4637094	0.1800463	0.4732843
C	0.470644	-0.1860782	-0.4758076	C	0.4637094	-0.1800463	-0.4732843
C	0.3135232	-0.1102846	-1.8935337	C	0.3078817	-0.108753	-1.8915159
C	1.3754913	-0.5371257	-2.7333115	C	1.3681198	-0.5426851	-2.7295979
C	1.2906106	-0.4884224	-4.1038158	C	1.2846159	-0.4964496	-4.1003997
C	0.1157603	-0.0055332	-4.7390283	C	0.111564	-0.0120214	-4.7376236
C	-0.9570438	0.4240865	-3.908028	C	-0.9605008	0.4227852	-3.9083166
C	-0.8552616	0.3750764	-2.5406256	C	-0.8586758	0.3789957	-2.5406946
N	0.017788	0.0501948	-6.1068618	N	0.0145134	0.0402852	-6.106027
C	1.1811369	0.0673774	-6.9356346	C	1.1795311	0.0577087	-6.9324608
C	1.313439	-0.8475557	-7.9802975	C	1.316276	-0.8564186	-7.9772837
C	2.4314573	-0.8267661	-8.8098129	C	2.4390791	-0.8350414	-8.8005572
C	3.4404519	0.1217877	-8.5992561	C	3.4456556	0.1153465	-8.5871429
C	3.3034709	1.0477187	-7.5518903	C	3.3028026	1.0419602	-7.5412358
C	2.1870375	1.0240986	-6.7349788	C	2.1829085	1.0166622	-6.7291889
O	4.5552585	0.2242458	-9.3401819	O	4.5628398	0.2194006	-9.324324
C	4.7680616	-0.6613149	-10.4169805	C	4.776523	-0.6601157	-10.405895
C	-1.2522363	0.0973406	-6.7592975	C	-1.2560768	0.088648	-6.7572422
C	-1.5336718	1.1190426	-7.6775399	C	-1.5386263	1.1081784	-7.6776147
C	-2.7564689	1.1617109	-8.3224462	C	-2.7673625	1.1558144	-8.3109814
C	-3.7322367	0.1831491	-8.0685025	C	-3.7467822	0.1838423	-8.0451769
C	-3.4510305	-0.8435528	-7.1584985	C	-3.4621907	-0.8444077	-7.1379981
C	-2.2151888	-0.8825495	-6.516634	C	-2.2208525	-0.8874976	-6.5070587
O	-4.888411	0.3105556	-8.7388739	O	-4.9097839	0.3195047	-8.7021047
C	-5.9167617	-0.6359994	-8.5536901	C	-5.9457551	-0.6149031	-8.4986251
H	2.281865	-0.9296057	-2.2747018	H	2.2732814	-0.9379401	-2.2708553
H	2.1203566	-0.8415146	-4.708103	H	2.1137919	-0.8534683	-4.703145
H	-1.8589203	0.8193495	-4.3647591	H	-1.8613024	0.8189461	-4.3662582
H	-1.6927895	0.736527	-1.9491203	H	-1.6950738	0.7455334	-1.9506941
H	-2.276845	0.8990988	2.2665873	H	-2.2732814	0.9379401	2.2708553
H	-2.1198022	0.8173132	4.7002731	H	-2.1137919	0.8534683	4.703145
H	1.8711155	-0.8180786	4.368588	H	1.8613024	-0.8189461	4.3662582

H	1.7089822	-0.7419572	1.9521655
H	0.5352099	-1.5886972	-8.1482132
H	2.5073406	-1.5549864	-9.6111502
H	4.0869409	1.7885125	-7.4101443
H	2.0846723	1.7564889	-5.9370543
H	-0.7864808	1.8835561	-7.8780934
H	-2.9899364	1.9525206	-9.0314143
H	-4.1778295	-1.6228689	-6.9513382
H	-1.9982212	-1.691222	-5.8217575
H	-2.0729077	-1.7745887	5.9578789
H	-4.0800369	-1.7912606	7.4252578
H	-2.52174	1.5949262	9.5756543
H	-0.5445864	1.6124686	8.1188851
H	1.9993635	1.6896442	5.8332024
H	4.1737822	1.6235741	6.9734271
H	2.9850985	-1.9613672	9.0364626
H	0.7871303	-1.8945716	7.8722618
H	-5.740057	0.4301613	10.8359361
H	-3.994517	0.630315	11.1518712
H	-4.8389518	1.7435973	10.0298049
H	6.730809	0.3275297	9.2304488
H	6.2579905	0.6634372	7.5421179
H	5.5782356	1.6447421	8.8786928
H	-6.7446993	-0.323865	-9.1955125
H	-5.5942662	-1.6444727	-8.849268
H	-6.2613889	-0.658336	-7.5098862
H	5.7257401	-0.3816306	-10.8636238
H	4.8227437	-1.7049739	-10.0759851
H	3.9783085	-0.5700973	-11.1762704
H	1.4357228	-0.5644125	-0.1396736
H	-1.4237697	0.5410661	0.1361634

H	1.6950738	-0.7455334	1.9506941
H	0.5408854	-1.6001556	-8.1478107
H	2.5200426	-1.5635796	-9.6008941
H	4.0843746	1.7842466	-7.3965837
H	2.0761109	1.7489981	-5.9318309
H	-0.7902376	1.8694223	-7.8860917
H	-3.0030759	1.9460318	-9.0199859
H	-4.1903577	-1.6207502	-6.9238884
H	-2.0013939	-1.6951613	-5.8121616
H	-2.0761109	-1.7489981	5.9318309
H	-4.0843746	-1.7842466	7.3965837
H	-2.5200426	1.5635796	9.6008941
H	-0.5408854	1.6001556	8.1478107
H	2.0013939	1.6951613	5.8121616
H	4.1903577	1.6207502	6.9238884
H	3.0030759	-1.9460318	9.0199859
H	0.7902376	-1.8694223	7.8860917
H	-5.7334448	0.3762813	10.8517471
H	-3.9859119	0.5658542	11.1638606
H	-4.8335461	1.7054915	10.0706014
H	6.7798746	0.2952399	9.1287905
H	6.2744832	0.6298714	7.4495907
H	5.639391	1.6278749	8.7959597
H	-6.7798746	-0.2952399	-9.1287905
H	-5.639391	-1.6278749	-8.7959597
H	-6.2744832	-0.6298714	-7.4495907
H	5.7334448	-0.3762813	-10.8517471
H	4.8335461	-1.7054915	-10.0706014
H	3.9859119	-0.5658542	-11.1638606
H	1.426463	-0.5621817	-0.1348458
H	-1.426463	0.5621817	0.1348458

10 with a = 0.35 in DCM
(C_1 symmetry)

Energy = -2030.950033005 Hartree

	X	Y	Z
C	1.5481734	-1.1165674	7.6737357
C	1.2546628	-0.096956	6.7577135
C	2.2041912	0.897016	6.5193202
C	3.4391531	0.8744424	7.164038
C	3.7317255	-0.1490585	8.0735415
C	2.7702399	-1.1420898	8.323348
N	-0.0148311	-0.0643412	6.1028638
C	-1.1791315	-0.083872	6.9310234
C	-2.1670506	-1.0618979	6.7488737

10 with a = 0.35 in DCM
(C_i symmetry)

Energy = -2030.949931922 Hartree

	X	Y	Z
C	1.5428096	-1.0811147	7.6960405
C	1.2612932	-0.0855851	6.7499224
C	2.233559	0.8734412	6.4639581
C	3.4830057	0.832481	7.0784417
C	3.7660286	-0.1725583	8.0115573
C	2.7781079	-1.1225718	8.3195271
N	-0.0108066	-0.0443078	6.1032136
C	-1.1751358	-0.0594378	6.9304553
C	-2.1670933	-1.0321535	6.7399922

C	-3.2853942	-1.0872916	7.5647297	C	-3.2889739	-1.0578338	7.5507503
C	-3.4396516	-0.1422137	8.5916991	C	-3.4431845	-0.117326	8.5818949
C	-2.4485233	0.8283551	8.7839841	C	-2.4504041	0.8505344	8.7793328
C	-1.3295207	0.8513154	7.9549652	C	-1.325793	0.8722663	7.9577033
O	-4.555157	-0.2474519	9.3364235	O	-4.5597594	-0.2229725	9.3251458
C	-4.7797056	0.6631334	10.3929096	C	-4.7732272	0.6723574	10.396856
O	4.8906817	-0.2585676	8.7477208	O	4.940498	-0.3052055	8.6543879
C	5.9048315	0.7058221	8.556264	C	5.9912291	0.5987718	8.3827994
C	-0.1122761	-0.0125341	4.7350317	C	-0.1118001	0.0013964	4.7337737
C	-1.2948942	0.4502051	4.098789	C	-1.2833352	0.4928255	4.0996364
C	-1.3786528	0.4987631	2.7282806	C	-1.3702302	0.5393948	2.7288995
C	-0.3074663	0.0890378	1.8908969	C	-0.3127728	0.0992658	1.8897845
C	0.8690214	-0.3782558	2.538557	C	0.8506901	-0.401201	2.5357592
C	0.969133	-0.4250407	3.9061464	C	0.9540965	-0.4460027	3.9032423
C	-0.4637347	0.1648777	0.4742	C	-0.466348	0.1790354	0.4718113
C	0.4721512	-0.1790201	-0.4724736	C	0.466348	-0.1790354	-0.4718113
C	0.3154509	-0.1012802	-1.8890568	C	0.3127728	-0.0992658	-1.8897845
C	1.3815742	-0.5206775	-2.7281721	C	1.3702302	-0.5393948	-2.7288995
C	1.2962526	-0.4709337	-4.0986354	C	1.2833352	-0.4928255	-4.0996364
C	0.1178296	0.004894	-4.7332298	C	0.1118001	-0.0013964	-4.7337737
C	-0.9583417	0.4271916	-3.9024352	C	-0.9540965	0.4460027	-3.9032423
C	-0.8571656	0.3777389	-2.5350719	C	-0.8506901	0.401201	-2.5357592
N	0.0186781	0.0591093	-6.1006771	N	0.0108066	0.0443078	-6.1032136
C	1.1803765	0.0606423	-6.9328722	C	1.1751358	0.0594378	-6.9304553
C	1.3104298	-0.8761198	-7.9580242	C	1.325793	-0.8722663	-7.9577033
C	2.4257336	-0.871518	-8.7922304	C	2.4504041	-0.8505344	-8.7793328
C	3.4339275	0.082039	-8.6039997	C	3.4431845	0.117326	-8.5818949
C	3.3000323	1.0292036	-7.575973	C	3.2889739	1.0578338	-7.5507503
C	2.1851648	1.0220057	-6.7548807	C	2.1670933	1.0321535	-6.7399922
O	4.54818	0.168014	-9.3530852	O	4.5597594	0.2229725	-9.3251458
C	4.7524761	-0.7460754	-10.4106192	C	4.7732272	-0.6723574	-10.396856
C	-1.2515292	0.116147	-6.7531183	C	-1.2612932	0.0855851	-6.7499224
C	-1.5305853	1.1496375	-7.6577191	C	-1.5428096	1.0811147	-7.6960405
C	-2.7533737	1.2013196	-8.3043676	C	-2.7781079	1.1225718	-8.3195271
C	-3.729836	0.2209204	-8.0630814	C	-3.7660286	0.1725583	-8.0115573
C	-3.4514451	-0.8169264	-7.1654442	C	-3.4830057	-0.832481	-7.0784417
C	-2.2156871	-0.8655136	-6.5234612	C	-2.233559	-0.8734412	-6.4639581
O	-4.888565	0.3564723	-8.7330202	O	-4.940498	0.3052055	-8.6543879
C	-5.9173517	-0.5939735	-8.550301	C	-5.9912291	-0.5987718	-8.3827994
H	2.2902611	-0.9068495	-2.2691621	H	2.2722952	-0.9418232	-2.270981
H	2.1288207	-0.8187434	-4.7018671	H	2.1087934	-0.8564318	-4.7035578
H	-1.8634359	0.8164698	-4.3575578	H	-1.8522168	0.8515612	-4.3579505
H	-1.6975541	0.7319746	-1.9434295	H	-1.6813977	0.7772634	-1.9440254
H	-2.29017	0.8763094	2.267786	H	-2.2722952	0.9418232	2.270981
H	-2.1317143	0.7897991	4.7009283	H	-2.1087934	0.8564318	4.7035578

H	1.8775599	-0.8045113	4.3630646
H	1.7136865	-0.7241969	1.9481331
H	0.533672	-1.6227654	-8.1074159
H	2.4994219	-1.6167419	-9.5780076
H	4.0826211	1.773861	-7.4486065
H	2.0857757	1.7697092	-5.9710194
H	-0.7835938	1.917082	-7.8475026
H	-2.9826238	2.0025367	-9.0033097
H	-4.1793306	-1.5973773	-6.9667394
H	-2.0013343	-1.6825503	-5.8378361
H	-2.0513895	-1.8082515	5.9659341
H	-4.0551273	-1.8445326	7.433645
H	-2.5384594	1.5726549	9.5688723
H	-0.5661386	1.6110708	8.1073362
H	1.9786587	1.7035365	5.8248799
H	4.1552665	1.6638649	6.9582737
H	3.0105339	-1.9319849	9.031351
H	0.8130275	-1.8937536	7.8700896
H	-5.7330593	0.3815907	10.8475237
H	-3.9877144	0.6015474	11.1522372
H	-4.8481633	1.696479	10.0256487
H	6.7387213	0.410657	9.1983668
H	6.246113	0.7285989	7.5119425
H	5.5651122	1.7094512	8.847092
H	-6.7479015	-0.2781489	-9.1868904
H	-5.5942035	-1.599401	-8.8536038
H	-6.2566274	-0.623604	-7.5054992
H	5.7087326	-0.4811324	-10.869135
H	4.8044498	-1.7805386	-10.0437641
H	3.9585405	-0.6705034	-11.1666497
H	1.4386831	-0.5520899	-0.135201
H	-1.4310554	0.5354209	0.1365123

10 with *a* = 0.35 in MeCN

(C_1 symmetry)

Energy = -2030.957133190 Hartree

	X	Y	Z
C	1.5523529	-1.1374795	7.6548082
C	1.2536502	-0.1055519	6.7549804
C	2.1957299	0.8993941	6.5350642
C	3.4289172	0.8765645	7.1836518
C	3.7264982	-0.1588296	8.0777923
C	2.7727424	-1.1637451	8.3082308
N	-0.0159904	-0.0722661	6.0992264
C	-1.1788926	-0.0872413	6.9302933

H	1.8522168	-0.8515612	4.3579505
H	1.6813977	-0.7772634	1.9440254
H	0.5614066	-1.6298915	-8.1178924
H	2.5425156	-1.5923118	-9.5659582
H	4.0601977	1.8123166	-7.4135529
H	2.0509294	1.7753642	-5.9542409
H	-0.7904985	1.8298696	-7.9332442
H	-3.0100272	1.8961054	-9.0482736
H	-4.2167757	-1.5939644	-6.8313084
H	-2.0145064	-1.664587	-5.7506788
H	-2.0509294	-1.7753642	5.9542409
H	-4.0601977	-1.8123166	7.4135529
H	-2.5425156	1.5923118	9.5659582
H	-0.5614066	1.6298915	8.1178924
H	2.0145064	1.664587	5.7506788
H	4.2167757	1.5939644	6.8313084
H	3.0100272	-1.8961054	9.0482736
H	0.7904985	-1.8298696	7.9332442
H	-5.723271	0.3860565	10.8559152
H	-3.9747984	0.5970811	11.1481903
H	-4.8426267	1.7114063	10.046221
H	6.8376481	0.2853281	8.9997064
H	6.2863302	0.5648826	7.3247716
H	5.7151858	1.6287062	8.6479704
H	-6.8376481	-0.2853281	-8.9997064
H	-5.7151858	-1.6287062	-8.6479704
H	-6.2863302	-0.5648826	-7.3247716
H	5.723271	-0.3860565	-10.8559152
H	4.8426267	-1.7114063	-10.046221
H	3.9747984	-0.5970811	-11.1481903
H	1.4267378	-0.5659371	-0.1324583
H	-1.4267378	0.5659371	0.1324583

10 with *a* = 0.35 in MeCN

(C_i symmetry)

Energy = -2030.957016095 Hartree

	X	Y	Z
C	1.5507581	-1.0904895	7.6813425
C	1.2618214	-0.0856482	6.7479814
C	2.2273041	0.8829569	6.4721882
C	3.4782528	0.842475	7.0838943
C	3.7691383	-0.1726315	8.003642
C	2.7874781	-1.1316792	8.3027699
N	-0.0107345	-0.0474582	6.1011044
C	-1.1742601	-0.0634785	6.9302388

C	-2.1597355	-1.0751013	6.766661	C	-2.1570681	-1.0476754	6.7548508
C	-3.276106	-1.0948395	7.586083	C	-3.2786526	-1.0712222	7.566877
C	-3.4346508	-0.1336372	8.5971793	C	-3.4404353	-0.1171496	8.5840415
C	-2.4503919	0.8472224	8.7707571	C	-2.4558918	0.8619034	8.7669536
C	-1.3334374	0.8638391	7.9385802	C	-1.3326086	0.8821534	7.9434605
O	-4.5486581	-0.2329281	9.3466522	O	-4.5556886	-0.2211706	9.3312009
C	-4.7759164	0.6966865	10.386705	C	-4.7712844	0.6872201	10.3923672
O	4.8849392	-0.2692024	8.7546015	O	4.9473363	-0.3067856	8.6410631
C	5.8914403	0.707382	8.580011	C	5.9943067	0.6026116	8.3693113
C	-0.114404	-0.0210451	4.7320941	C	-0.1129309	-0.0034433	4.7323551
C	-1.3035925	0.426193	4.0962385	C	-1.2926272	0.469717	4.0985798
C	-1.3881009	0.4750289	2.7259512	C	-1.3804051	0.5155783	2.728083
C	-0.3105766	0.081789	1.8882689	C	-0.31574	0.0924116	1.8887987
C	0.8727483	-0.3697132	2.5353592	C	0.8556799	-0.3902253	2.5342343
C	0.9729457	-0.4175071	3.9027463	C	0.9597832	-0.434134	3.9015263
C	-0.4674669	0.1584145	0.4724348	C	-0.4704449	0.1701818	0.4716057
C	0.475803	-0.1688132	-0.4739664	C	0.4704449	-0.1701818	-0.4716057
C	0.3179728	-0.0914605	-1.8897288	C	0.31574	-0.0924116	-1.8887987
C	1.3917144	-0.4911622	-2.729019	C	1.3804051	-0.5155783	-2.728083
C	1.3052581	-0.4421479	-4.0992446	C	1.2926272	-0.469717	-4.0985798
C	0.1184621	0.0138006	-4.7334091	C	0.1129309	0.0034433	-4.7323551
C	-0.9646592	0.4180707	-3.9022299	C	-0.9597832	0.434134	-3.9015263
C	-0.8630406	0.3683263	-2.5350322	C	-0.8556799	0.3902253	-2.5342343
N	0.0184752	0.0667664	-6.1003587	N	0.0107345	0.0474582	-6.1011044
C	1.1798974	0.0686083	-6.9337503	C	1.1742601	0.0634785	-6.9302388
C	1.3225845	-0.8853663	-7.9410377	C	1.3326086	-0.8821534	-7.9434605
C	2.4379297	-0.881159	-8.7755733	C	2.4558918	-0.8619034	-8.7669536
C	3.432555	0.08966	-8.6052082	C	3.4404353	0.1171496	-8.5840415
C	3.2860927	1.0536405	-7.5950207	C	3.2786526	1.0712222	-7.566877
C	2.1712238	1.0464537	-6.7734242	C	2.1570681	1.0476754	-6.7548508
O	4.5461473	0.1763732	-9.3568961	O	4.5556886	0.2211706	-9.3312009
C	4.7617342	-0.7564514	-10.3965576	C	4.7712844	-0.6872201	-10.3923672
C	-1.2520011	0.1192413	-6.7536322	C	-1.2618214	0.0856482	-6.7479814
C	-1.5407929	1.1611792	-7.6450681	C	-1.5507581	1.0904895	-7.6813425
C	-2.7631008	1.2074278	-8.2938442	C	-2.7874781	1.1316792	-8.3027699
C	-3.7285272	0.21299	-8.0670303	C	-3.7691383	0.1726315	-8.003642
C	-3.4406712	-0.8327032	-7.1817971	C	-3.4782528	-0.842475	-7.0838943
C	-2.2055515	-0.8756812	-6.537948	C	-2.2273041	-0.8829569	-6.4721882
O	-4.8880202	0.3428021	-8.7386338	O	-4.9473363	0.3067856	-8.6410631
C	-5.905797	-0.622631	-8.5675409	C	-5.9943067	-0.6026116	-8.3693113
H	2.3069252	-0.8616947	-2.2702427	H	2.2887119	-0.9032111	-2.269582
H	2.1439793	-0.7748558	-4.7023899	H	2.1236281	-0.8202778	-4.7024558
H	-1.8766497	0.7917702	-4.3565299	H	-1.8647606	0.8245694	-4.3556359
H	-1.7097114	0.7064645	-1.9430217	H	-1.6926501	0.7516953	-1.9423267
H	-2.3049696	0.8395711	2.2656675	H	-2.2887119	0.9032111	2.269582

H	-2.1453638	0.7532852	4.6981817	H	-2.1236281	0.8202778	4.7024558
H	1.8869002	-0.7843099	4.3587593	H	1.8647606	-0.8245694	4.3556359
H	1.7225665	-0.7020097	1.9444855	H	1.6926501	-0.7516953	1.9423267
H	0.5563318	-1.6455947	-8.0759439	H	0.5759379	-1.6500193	-8.0913139
H	2.521945	-1.6400214	-9.5471203	H	2.5540105	-1.6144378	-9.542426
H	4.058493	1.8109402	-7.480187	H	4.0435026	1.8342439	-7.4396031
H	2.0619966	1.8064581	-6.0027457	H	2.0356593	1.8001508	-5.9788965
H	-0.8023799	1.9397153	-7.8231983	H	-0.8038198	1.8474054	-7.9096614
H	-2.9994633	2.0154762	-8.9825717	H	-3.0251023	1.913348	-9.0209724
H	-4.1604537	-1.6231479	-6.9934828	H	-4.2067413	-1.6113584	-6.8441067
H	-1.9840078	-1.6981911	-5.8611991	H	-2.0032057	-1.6800802	-5.7673259
H	-2.0412157	-1.8327119	5.9950771	H	-2.0356593	-1.8001508	5.9788965
H	-4.0405438	-1.8597769	7.4686652	H	-4.0435026	-1.8342439	7.4396031
H	-2.5438872	1.6043969	9.5428534	H	-2.5540105	1.6144378	9.542426
H	-0.5756388	1.6320338	8.0756544	H	-0.5759379	1.6500193	8.0913139
H	1.9663584	1.714335	5.8518731	H	2.0032057	1.6800802	5.7673259
H	4.1393839	1.6747018	6.9923567	H	4.2067413	1.6113584	6.8441067
H	3.0166212	-1.9636018	9.0038786	H	3.0251023	-1.913348	9.0209724
H	0.8231496	-1.9238963	7.8359358	H	0.8038198	-1.8474054	7.9096614
H	-5.7258532	0.4176351	10.8499841	H	-5.71813	0.4013587	10.8581662
H	-3.9809488	0.6551289	11.1441036	H	-3.9697931	0.6268601	11.1415678
H	-4.8523185	1.7220915	9.9997162	H	-4.8475866	1.7210277	10.0284408
H	6.7262719	0.4100774	9.2199384	H	6.8465235	0.2852215	8.9760968
H	6.2348221	0.7486084	7.5371205	H	6.2799596	0.5795432	7.3086056
H	5.5418794	1.7033727	8.8845272	H	5.7180439	1.6292406	8.6460602
H	-6.7391656	-0.3105121	-9.2023081	H	-6.8465235	-0.2852215	-8.9760968
H	-5.5695236	-1.6205985	-8.8804542	H	-5.7180439	-1.6292406	-8.6460602
H	-6.2460409	-0.667317	-7.523772	H	-6.2799596	-0.5795432	-7.3086056
H	5.7140629	-0.4882075	-10.8613259	H	5.71813	-0.4013587	-10.8581662
H	4.8274015	-1.7824077	-10.0090377	H	4.8475866	-1.7210277	-10.0284408
H	3.9662448	-0.7066742	-11.1529203	H	3.9697931	-0.6268601	-11.1415678
H	1.4479574	-0.5265046	-0.1363539	H	1.4372669	-0.5399209	-0.1318472
H	-1.4400943	0.5143923	0.1344538	H	-1.4372669	0.5399209	0.1318472

11 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -8217.948650144 Hartree

	X	Y	Z
C	-1.468843	-3.2205383	-10.1355402
C	-2.2444843	-2.7098951	-11.1859184
C	-2.2661881	-1.3302041	-11.4058552
C	-1.5326625	-0.4809541	-10.5767325
C	-0.7558864	-0.9832257	-9.5332661
C	-0.7290326	-2.3715617	-9.3296523
O	-2.9237658	-3.6164445	-11.9233696
C	-3.7199081	-3.1799113	-12.9923979
N	0.010479	-0.1110931	-8.7105646
C	-0.0933309	-0.1675362	-7.316489
C	-1.2707652	-0.6114645	-6.6900595
C	-1.3559133	-0.6714366	-5.3071909
C	-0.2903021	-0.2881976	-4.47651
C	0.8839687	0.1547857	-5.1133162
C	0.9856821	0.2122053	-6.4916718
C	-0.4527642	-0.3745651	-3.0281854
C	0.4361166	0.0166379	-2.0941694
C	0.2823546	-0.0345513	-0.6357909
C	-0.3348602	-1.0828499	0.0807426
C	-0.4278114	-1.0634204	1.4767846
C	0.1124758	-0.0130456	2.2501493
C	0.7530442	1.0232228	1.5359787
C	0.82647	1.0126363	0.1429836
Cl	-0.9676241	-2.467029	-0.7593181
Cl	-1.3102046	-2.3365324	2.260639
C	0.0173143	0.0016092	3.7238384
C	-0.4675407	1.2127732	4.424415
C	0.2485375	1.7818222	5.5000118
C	-0.2113964	2.9184469	6.1742014
C	-1.4050603	3.5319482	5.7737067
C	-2.1341176	2.9958299	4.7046386
C	-1.671026	1.8492689	4.0494711
Cl	1.5469911	2.3041143	2.3959921
Cl	1.6126816	2.338107	-0.6634354
Cl	0.6953254	3.5893107	7.4814745
Cl	-1.9738856	4.9381311	6.5922357
Cl	1.7872993	1.1342755	5.9620102
Cl	-3.6143391	3.7429276	4.2230214
Cl	-2.6694274	1.1659283	2.8103221
C	0.8548825	0.842494	-9.3438649
C	1.7666561	0.4401752	-10.3310096

11 with a = 0.35 in hexane (C_1 symmetry)

Energy = -8217.954636317 Hartree

	X	Y	Z
C	-1.5757825	-3.1586091	-10.1788021
C	-2.3695441	-2.5977967	-11.1897803
C	-2.365487	-1.2114674	-11.3679348
C	-1.5875992	-0.4054793	-10.5360604
C	-0.7936093	-0.957676	-9.5315143
C	-0.7932112	-2.3513489	-9.369528
O	-3.0917247	-3.4645065	-11.9340094
C	-3.9135153	-2.9735499	-12.9632611
N	0.0170555	-0.1273903	-8.7061507
C	-0.0807304	-0.1899332	-7.3134743
C	-1.2631968	-0.6171782	-6.683193
C	-1.3445826	-0.679464	-5.3000689
C	-0.2693275	-0.316304	-4.4720961
C	0.9110035	0.1067267	-5.1120031
C	1.0084344	0.1672057	-6.4906296
C	-0.4295006	-0.3983479	-3.0233696
C	0.4646395	-0.0116838	-2.0920415
C	0.3082419	-0.0572882	-0.6336338
C	-0.3101755	-1.1033542	0.0849635
C	-0.4113716	-1.0767084	1.4802945
C	0.122156	-0.0212039	2.2514174
C	0.7663979	1.0114531	1.5352331
C	0.8465687	0.9941965	0.1428579
Cl	-0.9337316	-2.493836	-0.7523632
Cl	-1.2947106	-2.348262	2.2665469
C	0.0171118	0.0019719	3.7240645
C	-0.4757088	1.2165592	4.4132822
C	0.2320764	1.795473	5.4890279
C	-0.2342747	2.9368458	6.1505753
C	-1.4259327	3.5451288	5.7370004
C	-2.1459452	3.0000737	4.6666436
C	-1.6767572	1.8489722	4.0240972
Cl	1.5539209	2.2981138	2.3930832
Cl	1.6341044	2.3169483	-0.6672871
Cl	0.661772	3.6194546	7.4593764
Cl	-2.0030798	4.9569625	6.5403089
Cl	1.768408	1.153528	5.9674405
Cl	-3.6230963	3.7420162	4.1673283
Cl	-2.6653074	1.1543584	2.7828626
C	0.8976562	0.7924202	-9.3414733
C	1.7883555	0.3532554	-10.3317904

C	2.5767381	1.3657254	-10.9678949
C	2.5130373	2.7233699	-10.6256178
C	1.6123733	3.1335094	-9.638644
C	0.7861376	2.1972934	-9.0170157
O	3.3482674	3.5497169	-11.2942688
C	3.3386815	4.9222785	-11.0056171
C	0.4072872	-1.1927909	4.507486
C	-0.4415994	-1.7397628	5.4941784
C	-0.074907	-2.8629373	6.2436687
C	1.1582371	-3.48485	6.0107767
C	2.0196669	-2.9699114	5.0337705
C	1.647719	-1.8359981	4.3030505
Cl	-2.0251031	-1.0826233	5.742608
Cl	-1.1430667	-3.5070954	7.4375103
Cl	1.6133799	-4.8751878	6.922239
Cl	3.5471651	-3.7272277	4.759776
Cl	2.797989	-1.1774798	3.1884876
H	-1.4527843	-4.2973196	-9.9819721
H	-4.1658663	-4.0744268	-13.4373738
H	-3.1261857	-2.6596629	-13.7596504
H	-4.5266605	-2.5106342	-12.6561745
H	-2.855379	-0.9004789	-12.2105271
H	-1.5615649	0.5926389	-10.7503716
H	-0.1211521	-2.7820453	-8.5260433
H	1.8321241	-0.6121729	-10.5990689
H	3.2846788	1.0597299	-11.7350519
H	2.3577133	5.377646	-11.2113809
H	4.0859959	5.3853821	-11.6568489
H	3.608215	5.1225842	-9.95726
H	1.5321139	4.1780359	-9.3522992
H	0.079204	2.5287026	-8.2591166
H	-2.1234126	-0.906986	-7.2950249
H	1.91433	0.5456666	-6.9469692
H	1.7486201	0.4442912	-4.5195041
H	-2.2845754	-1.0154333	-4.8525526
H	1.3576165	0.4922162	-2.4206721
H	-1.4081957	-0.7833916	-2.7072486

11 with a = 0.35 in DCM (C_1 symmetry)

Energy = -8217.962802205 Hartree

	X	Y	Z
C	-1.5587756	-3.1527673	-10.2164653
C	-2.372024	-2.5804394	-11.2059565
C	-2.3873837	-1.1901437	-11.3552148
C	-1.6080087	-0.3926589	-10.5164241

C	2.6328228	1.2455523	-10.9724708
C	2.6241358	2.6051266	-10.6310316
C	1.74332	3.0518489	-9.6414968
C	0.8827999	2.1494644	-9.0162906
O	3.488783	3.3979601	-11.3027655
C	3.5336512	4.7726294	-11.0130946
C	0.4048166	-1.1858427	4.5185754
C	-0.4493394	-1.7278459	5.5032878
C	-0.0841832	-2.8437486	6.2642696
C	1.1521994	-3.463168	6.0452437
C	2.0183175	-2.9543873	5.069318
C	1.6476584	-1.8281171	4.3264777
Cl	-2.0365244	-1.0731358	5.7355364
Cl	-1.1584326	-3.4815589	7.4564917
Cl	1.6058353	-4.8444424	6.9716693
Cl	3.5489059	-3.7097365	4.8111811
Cl	2.8033112	-1.1755773	3.2134371
H	-1.5798228	-4.2396672	-10.0570881
H	-4.3944376	-3.8425736	-13.4214811
H	-3.3317763	-2.4422011	-13.7312074
H	-4.6916632	-2.2984495	-12.5768118
H	-2.9676331	-0.7440938	-12.1412512
H	-1.5966021	0.6734561	-10.6760899
H	-0.1724857	-2.8002507	-8.5968063
H	1.8118681	-0.7009497	-10.5995733
H	3.3243243	0.9093425	-11.7421338
H	2.570422	5.2641064	-11.2163195
H	4.2966573	5.2057734	-11.6663422
H	3.8135921	4.9598523	-9.9656588
H	1.704962	4.0990646	-9.3565144
H	0.1918734	2.5104825	-8.2571247
H	-2.1237584	-0.8965364	-7.2844799
H	1.942059	0.4849117	-6.9467648
H	1.7833713	0.3787298	-4.5211189
H	-2.2774469	-1.0089863	-4.8434666
H	1.3905998	0.4545039	-2.4200192
H	-1.3886067	-0.7967029	-2.6997196

11 with a = 0.35 in MeCN (C_1 symmetry)

Energy = -8217.965031199 Hartree

	X	Y	Z
C	-1.6769683	-3.0818999	-10.2273393
C	-2.4642162	-2.4790703	-11.219816
C	-2.4299359	-1.0887416	-11.3660837
C	-1.6266428	-0.3213099	-10.5218589

C	-0.7945164	-0.9564693	-9.5338293	C	-0.838085	-0.9156967	-9.5368907
C	-0.7754517	-2.3526336	-9.3997516	C	-0.8694409	-2.311824	-9.4050923
O	-3.0933117	-3.4387309	-11.960377	O	-3.2106569	-3.3098003	-11.980725
C	-3.9378427	-2.9322376	-12.9694253	C	-4.0315497	-2.770374	-12.9939552
N	0.0193659	-0.1324156	-8.7034438	N	0.0037536	-0.1220006	-8.7041487
C	-0.079625	-0.1961076	-7.3130814	C	-0.0986828	-0.1813485	-7.314618
C	-1.2530589	-0.6512033	-6.6830578	C	-1.2855816	-0.6022505	-6.6852119
C	-1.3363688	-0.7113892	-5.2997309	C	-1.3724549	-0.6583393	-5.301883
C	-0.270542	-0.3226039	-4.4702237	C	-0.2971671	-0.2979751	-4.4713313
C	0.9010423	0.1276116	-5.1089326	C	0.8873694	0.1182509	-5.1091611
C	0.9992097	0.1890955	-6.4876075	C	0.9891976	0.1749331	-6.4877377
C	-0.4314827	-0.4056587	-3.0214421	C	-0.4605246	-0.3759844	-3.0224724
C	0.4656982	-0.0240142	-2.0902805	C	0.4409167	-0.0030591	-2.0918603
C	0.3067592	-0.065955	-0.6319156	C	0.2845207	-0.0471594	-0.6330039
C	-0.3124777	-1.1095695	0.0888303	C	-0.3339202	-1.0925554	0.0858671
C	-0.4142846	-1.0801413	1.483772	C	-0.430142	-1.0684085	1.4814175
C	0.120578	-0.0240188	2.2530212	C	0.1095071	-0.0157908	2.2525886
C	0.7657783	1.006553	1.5346816	C	0.7510832	1.0176456	1.5353635
C	0.8459557	0.986535	0.1424477	C	0.8257854	1.0024816	0.143092
Cl	-0.9369935	-2.5010299	-0.7473046	Cl	-0.9622972	-2.4805379	-0.7534485
Cl	-1.3000378	-2.3493131	2.2720634	Cl	-1.3134858	-2.340265	2.2691596
C	0.0161087	0.0020227	3.7260139	C	0.0145278	0.002808	3.7262406
C	-0.4717327	1.2195546	4.4132885	C	-0.4685827	1.2159844	4.4243459
C	0.2378862	1.7969167	5.4887375	C	0.2485562	1.7862492	5.4983753
C	-0.2246563	2.9401339	6.1490293	C	-0.2096306	2.9243575	6.170186
C	-1.4132874	3.5528773	5.7345317	C	-1.4012661	3.5390802	5.7687831
C	-2.1351944	3.0092478	4.6650534	C	-2.1300777	3.0036412	4.7000727
C	-1.6706047	1.8559537	4.023824	C	-1.6696732	1.8553363	4.0471835
Cl	1.5553924	2.294356	2.3900487	Cl	1.5434347	2.3030373	2.3919081
Cl	1.6334813	2.307661	-0.671037	Cl	1.6097828	2.3263285	-0.6702629
Cl	0.673642	3.6203109	7.4585163	Cl	0.6974624	3.5950731	7.4782157
Cl	-1.9847207	4.9683416	6.5360206	Cl	-1.968522	4.947692	6.5853982
Cl	1.7720075	1.1495877	5.9680001	Cl	1.7866842	1.1367573	5.9612677
Cl	-3.6095074	3.7574039	4.1638878	Cl	-3.6076158	3.7554016	4.2149927
Cl	-2.6621164	1.1633449	2.7830808	Cl	-2.6689351	1.1721973	2.8072807
C	0.9051131	0.7841026	-9.3391796	C	0.9324599	0.7519304	-9.3399329
C	1.8201371	0.3336116	-10.3012048	C	1.8381886	0.2548037	-10.2875925
C	2.6677358	1.2224754	-10.9442282	C	2.7280316	1.1023024	-10.9299129
C	2.6359102	2.5892522	-10.6322305	C	2.748264	2.4723678	-10.6311131
C	1.7297646	3.0471255	-9.670239	C	1.8510404	2.9765021	-9.6837458
C	0.8680163	2.1475094	-9.0428442	C	0.9470555	2.1187086	-9.0571938
O	3.504064	3.3791846	-11.3024749	O	3.6550969	3.2198865	-11.2987254
C	3.5224419	4.7647153	-11.0419114	C	3.7266012	4.6072798	-11.050491
C	0.4001957	-1.1859012	4.5219229	C	0.4033562	-1.189406	4.5136279
C	-0.4544019	-1.7225137	5.5093867	C	-0.4457887	-1.7302485	5.5033566

C	-0.092021	-2.8375016	6.2723442
C	1.1409889	-3.4630233	6.0521157
C	2.0068782	-2.9599867	5.0735849
C	1.6400799	-1.8337405	4.329372
Cl	-2.0388113	-1.0608312	5.7427778
Cl	-1.1663417	-3.4673787	7.4695589
Cl	1.5903965	-4.8445023	6.9807284
Cl	3.5340574	-3.7240635	4.8127582
Cl	2.7969863	-1.18834	3.2126386
H	-1.5466152	-4.2361059	-10.1154397
H	-4.4148673	-3.7963253	-13.4401022
H	-3.3714558	-2.3774069	-13.7310428
H	-4.7162925	-2.2760059	-12.5544311
H	-3.0051216	-0.7141954	-12.1106956
H	-1.6324941	0.6886818	-10.6343018
H	-0.1395395	-2.8109186	-8.6450188
H	1.861899	-0.725652	-10.5462534
H	3.3779019	0.8758488	-11.6922813
H	2.5562817	5.2340458	-11.276724
H	4.2926205	5.1940012	-11.6887067
H	3.7770741	4.9765465	-9.9935722
H	1.6731522	4.0996651	-9.4092782
H	0.1575026	2.5172627	-8.3062115
H	-2.1065691	-0.9522969	-7.2837892
H	1.9256475	0.5312391	-6.9404589
H	1.7654566	0.4243842	-4.5182578
H	-2.2627704	-1.060859	-4.8448138
H	1.3961488	0.4336931	-2.4178724
H	-1.3927166	-0.7998426	-2.6985248

C	-0.080336	-2.848863	6.2590098
C	1.1507916	-3.4743681	6.0287172
C	2.0110605	-2.9679872	5.0467971
C	1.6409872	-1.83796	4.3097537
Cl	-2.0271979	-1.0667989	5.7506267
Cl	-1.1481104	-3.4828068	7.4593551
Cl	1.6047666	-4.8602371	6.9487086
Cl	3.535615	-3.7330898	4.7728497
Cl	2.7914698	-1.189091	3.1881615
H	-1.7036913	-4.1652418	-10.1278453
H	-4.5362822	-3.6157368	-13.4695352
H	-3.4409842	-2.2344565	-13.750361
H	-4.7880258	-2.0880911	-12.5810637
H	-3.0269595	-0.5894412	-12.1231896
H	-1.6128049	0.7605046	-10.6374106
H	-0.2541659	-2.7944281	-8.648375
H	1.8394802	-0.8076729	-10.5221034
H	3.4306368	0.7189483	-11.6671188
H	2.7825309	5.1121947	-11.2999107
H	4.5201032	4.9985922	-11.6931276
H	3.9788136	4.8178943	-10.0015324
H	1.8343607	4.0330265	-9.4338951
H	0.2441373	2.5245649	-8.332449
H	-2.1465761	-0.8805131	-7.2862243
H	1.9262089	0.4892735	-6.9388398
H	1.7595403	0.3907455	-4.5181751
H	-2.3086578	-0.9819111	-4.8479808
H	1.3757593	0.4457672	-2.4197748
H	-1.4262715	-0.7591335	-2.6992813

12 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -8216.712915636 Hartree

	X	Y	Z
C	1.2377459	-4.2475888	-2.1505696
C	0.1703232	-4.5322604	-1.2707147
C	-0.7176091	-5.5607846	-1.6535603
C	-0.5503599	-6.2747765	-2.8453606
C	0.5124555	-5.9624292	-3.7025979
C	1.4070215	-4.9426888	-3.3533368
C	-0.0049097	-3.7856024	-0.0040066
C	-0.1886146	-4.5250074	1.2657536
C	0.68828	-5.5611005	1.6535329
C	0.5130591	-6.2679454	2.8484365
C	-0.5461761	-5.9399797	3.7042222

12 with a = 0.35 in hexane (C_1 symmetry)

Energy = -8216.718892990 Hartree

	X	Y	Z
C	1.2437019	-4.2567309	-2.1465706
C	0.1737122	-4.5364039	-1.2682796
C	-0.7161652	-5.5633735	-1.6507283
C	-0.548845	-6.2795447	-2.8409985
C	0.5164471	-5.9721609	-3.6965679
C	1.4125513	-4.9538071	-3.3480397
C	-0.0020211	-3.7865243	-0.0035874
C	-0.1914785	-4.5224712	1.267174
C	0.6792014	-5.5626022	1.6580816
C	0.4969431	-6.2678673	2.8526482
C	-0.5637961	-5.9354278	3.7044251

C	-1.4301053	-4.912803	3.3497933	C	-1.4401164	-4.9026953	3.3481479
C	-1.2529753	-4.2248316	2.1440862	C	-1.2566209	-4.2165929	2.1425693
Cl	2.0803424	-5.9296011	0.6907868	Cl	2.0729329	-5.9376447	0.6998827
Cl	1.6101855	-7.5250673	3.292358	Cl	1.5859984	-7.5312599	3.2998363
Cl	-0.7619655	-6.7968246	5.1841055	Cl	-0.7893293	-6.7921739	5.183138
Cl	-2.7464568	-4.522195	4.3964979	Cl	-2.7563593	-4.503519	4.3923091
Cl	-2.4392204	-3.0418772	1.7046252	Cl	-2.4359042	-3.0274419	1.6996174
Cl	-1.6607633	-7.5223762	-3.2831632	Cl	-1.6618426	-7.5253895	-3.278435
Cl	0.7190468	-6.828687	-5.1782539	Cl	0.7230216	-6.8416757	-5.170548
Cl	2.7267951	-4.5705919	-4.4023568	Cl	2.7347358	-4.586352	-4.3961902
Cl	2.4369396	-3.0756791	-1.7168137	Cl	2.4454854	-3.0870411	-1.7125857
C	0.0036615	-2.3111638	-0.0069625	C	0.0106075	-2.312185	-0.0099846
C	0.794629	-1.5707864	0.9045121	C	0.7996926	-1.5718296	0.9031368
C	0.7998197	-0.17662	0.9069692	C	0.8064866	-0.1778146	0.9043473
C	0.0222129	0.5564684	-0.0146994	C	0.0337122	0.5555877	-0.0209604
C	-0.7650043	-0.1713987	-0.932371	C	-0.7506442	-0.1723027	-0.9408816
C	-0.7779494	-1.5655064	-0.9222397	C	-0.7663535	-1.5662147	-0.9289391
C	0.0318997	1.9715501	-0.0188653	C	0.0440674	1.9708027	-0.02567
C	0.0404361	3.1857717	-0.0226312	C	0.0520205	3.1854128	-0.0297643
C	0.0503719	4.6063583	-0.0265675	C	0.0609724	4.6059491	-0.033777
C	0.7929524	5.3304081	0.9250648	C	0.7923953	5.3307354	0.9265862
C	0.8060686	6.7138214	0.9223623	C	0.8032147	6.7140755	0.9247431
C	0.0694913	7.4436889	-0.0332637	C	0.0763915	7.4441712	-0.0393242
C	-0.6765016	6.7193496	-0.9855339	C	-0.6578096	6.7183789	-1.0007715
C	-0.6819038	5.3356013	-0.9818083	C	-0.661824	5.334699	-0.9972855
N	0.0794216	8.8385782	-0.0374893	N	0.0839843	8.8372781	-0.0418417
C	0.3644472	9.5771402	1.1468896	C	0.374548	9.575743	1.1423442
C	-0.365579	9.3715725	2.3175649	C	-0.3637655	9.3833652	2.310165
C	-0.0909799	10.0977518	3.4762954	C	-0.0854706	10.1101834	3.4676463
C	0.9164346	11.0670809	3.469692	C	0.9349933	11.0663447	3.4620547
C	1.6432343	11.2877043	2.2916304	C	1.670577	11.2733283	2.2865791
C	1.3755264	10.5484641	1.1512462	C	1.3981628	10.5334488	1.1471501
O	1.2546157	11.8288085	4.532839	O	1.2772084	11.8270177	4.5245303
C	0.5720963	11.6636063	5.7473884	C	0.5836548	11.6741229	5.7379088
Cl	1.7868154	0.6947304	2.0284114	Cl	1.7898754	0.6938818	2.0293507
Cl	1.8712257	-2.390556	1.9897993	Cl	1.871236	-2.3923123	1.9932504
Cl	-1.8653355	-2.3771928	-2.0028052	Cl	-1.8515259	-2.3772394	-2.0126059
Cl	-1.7406357	0.7065595	-2.0585061	Cl	-1.7201444	0.7064327	-2.0723853
C	-0.2013073	9.5726327	-1.225691	C	-0.2074098	9.5748552	-1.2261809
C	-1.1856403	10.5597522	-1.2344468	C	-1.2044884	10.5493158	-1.2272492
C	-1.4483443	11.3080067	-2.3820635	C	-1.477506	11.3024587	-2.3693616
C	-0.7294839	11.0615387	-3.5549057	C	-0.7555154	11.0733932	-3.5442506
C	0.2590562	10.0670748	-3.5530723	C	0.2459589	10.0915169	-3.5499072
C	0.5249992	9.341821	-2.4036513	C	0.521628	9.3612143	-2.405481
O	-0.9105882	11.7221442	-4.7191456	O	-0.9459059	11.7408221	-4.7030361

C	-1.8872221	12.7261168	-4.7998597
H	-1.2702322	4.7972268	-1.7219179
H	1.3746337	4.7875451	1.6671634
H	1.398147	7.2446219	1.6622513
H	-1.2611084	7.2543075	-1.728364
H	-1.1593091	8.6270664	2.3290621
H	1.9514242	10.7226371	0.2447116
H	-0.6782328	9.9059232	4.3694754
H	2.4253795	12.0435656	2.3014308
H	1.3034269	8.5813672	-2.4120567
H	-1.7542017	10.7534074	-0.3272319
H	0.8175149	9.8924178	-4.4700618
H	-2.2199643	12.0714476	-2.3475976
H	-1.8554793	13.1130791	-5.8227011
H	-2.8958451	12.3330767	-4.5998922
H	-1.684276	13.5520766	-4.1010452
H	1.0144066	12.3717287	6.4544162
H	-0.5014429	11.8852235	5.6472635
H	0.6875033	10.644218	6.1466514
Cl	-2.1135073	-5.9099061	-0.6890668

C	-1.9361984	12.7362559	-4.7737716
H	-1.2417147	4.7971629	-1.7446545
H	1.3666438	4.7897522	1.6758325
H	1.3861922	7.2440657	1.672272
H	-1.2350785	7.2513922	-1.7505884
H	-1.1677534	8.6499009	2.3211286
H	1.9810214	10.6971037	0.2430376
H	-0.6793702	9.9294444	4.3586471
H	2.4628474	12.0187525	2.295593
H	1.3104372	8.6116077	-2.4201565
H	-1.775787	10.7296073	-0.3189486
H	0.8073991	9.9294501	-4.4675283
H	-2.2588237	12.055581	-2.3290943
H	-1.9102304	13.1317565	-5.7932426
H	-2.9386383	12.328573	-4.5752869
H	-1.7400478	13.5571456	-4.0679986
H	1.0306014	12.3791788	6.4447018
H	-0.4855711	11.9088371	5.6284946
H	0.6848897	10.6547998	6.1395498
Cl	-2.1150219	-5.9067597	-0.6880818

12 with a = 0.35 in DCM (C_1 symmetry)

Energy = -8216.727150541 Hartree

	X	Y	Z
C	1.3580317	-4.263631	-2.0726776
C	0.2418055	-4.5416059	-1.2535779
C	-0.6252588	-5.5699263	-1.6818926
C	-0.3894477	-6.2924231	-2.856244
C	0.721846	-5.9880186	-3.6516385
C	1.5957769	-4.9672776	-3.2581772
C	-0.0042865	-3.788263	-0.0028604
C	-0.264801	-4.5202027	1.2575577
C	0.5821821	-5.5595183	1.699201
C	0.3322999	-6.2624738	2.8824267
C	-0.7728012	-5.9264143	3.6736003
C	-1.6266897	-4.8939321	3.2670836
C	-1.3752004	-4.2100693	2.0729027
Cl	2.0266516	-5.9381068	0.8202549
Cl	1.3927577	-7.527268	3.391528
Cl	-1.0813394	-6.7800399	5.1393251
Cl	-2.9981255	-4.4902435	4.2366017
Cl	-2.5263489	-3.0193389	1.5630983
Cl	-1.4745408	-7.5425878	-3.3493511
Cl	1.0133288	-6.8657699	-5.1065286
Cl	2.9747052	-4.6027405	-4.232496

12 with a = 0.35 in MeCN (C_1 symmetry)

Energy = -8216.729384905 Hartree

	X	Y	Z
C	1.3091842	-4.2556672	-2.1052032
C	0.214022	-4.536968	-1.259224
C	-0.6618444	-5.5658169	-1.6677199
C	-0.4549702	-6.2847457	-2.8497265
C	0.6352044	-5.9764802	-3.6723546
C	1.5171265	-4.9550934	-3.2987439
C	-0.0020216	-3.7866859	-0.0012027
C	-0.2300166	-4.5226941	1.263167
C	0.6282483	-5.5631515	1.6794445
C	0.4051861	-6.2743202	2.8631401
C	-0.6833838	-5.9459463	3.6800161
C	-1.5478292	-4.9125865	3.2987053
C	-1.3235203	-4.2204027	2.1039376
Cl	2.0548208	-5.9319315	0.7676258
Cl	1.4789827	-7.5401933	3.3410462
Cl	-0.9592112	-6.8106381	5.1458153
Cl	-2.8991974	-4.5184725	4.3000163
Cl	-2.487063	-3.0277531	1.6270165
Cl	-1.5502677	-7.5355957	-3.3183376
Cl	0.8903607	-6.8496153	-5.1368607
Cl	2.8697047	-4.5852222	-4.3076295

Cl	2.5327431	-3.089891	-1.5775333	Cl	2.4939738	-3.0806166	-1.6370627
C	0.009886	-2.3135073	-0.0125887	C	0.0093471	-2.3124392	-0.0083101
C	0.7534292	-1.5712832	0.9361142	C	0.7698905	-1.5708895	0.9278115
C	0.7624136	-0.1774764	0.9328805	C	0.776469	-0.1771014	0.926759
C	0.0359834	0.554124	-0.0302871	C	0.03257	0.5546704	-0.0229988
C	-0.7032786	-0.1759648	-0.9847545	C	-0.7226965	-0.1746534	-0.9655313
C	-0.7198204	-1.5696836	-0.9707603	C	-0.7387952	-1.5683087	-0.9522747
C	0.0477295	1.9696127	-0.0380476	C	0.0435542	1.9701435	-0.0298632
C	0.0569538	3.1847921	-0.0436145	C	0.0523227	3.1855705	-0.0349601
C	0.0666294	4.6051213	-0.0485178	C	0.0620133	4.6058701	-0.0394377
C	0.8405063	5.3303522	0.878767	C	0.7933586	5.3312074	0.9221445
C	0.8513047	6.7134417	0.876808	C	0.804235	6.7142593	0.9207186
C	0.0811246	7.445806	-0.0535505	C	0.0786092	7.4469455	-0.0451752
C	-0.6955122	6.7181343	-0.9820439	C	-0.6547925	6.719002	-1.008534
C	-0.698754	5.334761	-0.9790579	C	-0.6600022	5.3356882	-1.0043254
N	0.0869287	8.8354798	-0.0545123	N	0.0863662	8.8354925	-0.0472238
C	0.4929545	9.5758944	1.096222	C	0.4469539	9.5770739	1.1183419
C	-0.1574368	9.4165185	2.3200026	C	-0.2653235	9.434462	2.3093283
C	0.23138	10.145819	3.4435654	C	0.0776704	10.1658417	3.4463362
C	1.2763542	11.0709794	3.3462524	C	1.1398536	11.0751574	3.3953448
C	1.9238745	11.2446006	2.114344	C	1.8506267	11.2310954	2.1961526
C	1.5412695	10.5016157	1.0080986	C	1.5118581	10.4867273	1.0763789
O	1.7213402	11.8308877	4.3704198	O	1.5439402	11.8352817	4.4359838
C	1.1187993	11.70609	5.6393642	C	0.8743204	11.7294004	5.6741249
Cl	1.691382	0.697039	2.1021517	Cl	1.7241234	0.697799	2.0810363
Cl	1.7660887	-2.3901729	2.0824527	Cl	1.8063223	-2.3898119	2.0528825
Cl	-1.7473089	-2.3839987	-2.1070891	Cl	-1.7883992	-2.3820444	-2.0688575
Cl	-1.6161712	0.700923	-2.1648261	Cl	-1.656092	0.7037771	-2.128687
C	-0.3217041	9.5786077	-1.2021696	C	-0.2734049	9.5787679	-1.2115769
C	-1.3426598	10.5233882	-1.1063645	C	-1.3075946	10.5126724	-1.1626283
C	-1.731155	11.2816384	-2.211239	C	-1.6487922	11.2718306	-2.2824105
C	-1.1018371	11.0873873	-3.4448774	C	-0.9566617	11.0893348	-3.4839932
C	-0.0759112	10.135868	-3.5470847	C	0.0827387	10.1483231	-3.5390657
C	0.3142128	9.4001025	-2.4392345	C	0.4247498	9.4112205	-2.4160775
O	-1.4078493	11.7627284	-4.5738095	O	-1.2132741	11.7672462	-4.6235199
C	-2.4330624	12.7307164	-4.5459198	C	-2.2474204	12.727769	-4.6412016
H	-1.3121027	4.7995821	-1.7010506	H	-1.2403636	4.8011019	-1.7536215
H	1.4480302	4.7914343	1.6028992	H	1.3670696	4.7928383	1.6738482
H	1.4680153	7.2405323	1.5984776	H	1.3864192	7.2410338	1.6707886
H	-1.3078818	7.2484953	-1.7050212	H	-1.231978	7.2491579	-1.7601156
H	-0.979617	8.7083859	2.4028803	H	-1.1012127	8.7390612	2.3556302
H	2.0560293	10.6394252	0.0594349	H	2.0752772	10.6108952	0.1537198
H	-0.2958774	9.9920119	4.3802198	H	-0.4975914	10.0261064	4.3565874
H	2.7361396	11.9656026	2.0498757	H	2.6758466	11.9397338	2.1672118
H	1.120459	8.6749127	-2.5301816	H	1.2421627	8.6947547	-2.4697142

H	-1.8421533	10.6763555	-0.15191
H	0.4135159	9.9995271	-4.5092339
H	-2.5275254	12.0107233	-2.0960564
H	-2.5042983	13.1390071	-5.5578074
H	-3.400591	12.2876083	-4.2699718
H	-2.2007655	13.5463085	-3.8463653
H	1.6388838	12.4037607	6.3015067
H	0.051998	11.9697689	5.6087384
H	1.2243289	10.6873481	6.0391089
Cl	-2.0766334	-5.9091342	-0.7982548

H	-1.855588	10.6566922	-0.2336178
H	0.6212872	10.0209802	-4.4759769
H	-2.4578773	11.9918296	-2.2044168
H	-2.2723074	13.1405485	-5.6533916
H	-3.2232076	12.2751471	-4.4149329
H	-2.0555915	13.5410973	-3.9271466
H	1.3703876	12.4244437	6.3570469
H	-0.1849924	12.0087641	5.5857053
H	0.9437814	10.7123345	6.085302
Cl	-2.0897726	-5.9094632	-0.7482369

13 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -8140.646692510 Hartree

	X	Y	Z
C	-0.1067529	8.8876399	-1.7089801
C	0.597828	7.8599718	-1.0645512
C	1.9027714	7.5905029	-1.4793697
C	2.4927975	8.3063144	-2.521091
C	1.7835717	9.331769	-3.1534163
C	0.4785215	9.6175877	-2.7308483
N	-0.0014487	7.1288843	-0.0021154
C	-0.6025515	7.8570835	1.0611724
C	-1.9041549	7.5787725	1.4809644
C	-2.4952733	8.2909027	2.5245364
C	-1.7909231	9.3213584	3.1541301
C	-0.4896613	9.6162479	2.7265125
C	0.0972021	8.8896987	1.7030313
O	-2.2749949	10.0758162	4.1666302
C	-3.5736071	9.8423645	4.6411609
O	2.2659648	10.0894359	-4.1642582
C	3.5692592	9.8674442	-4.6317395
C	-0.0000391	5.7266313	-0.0035971
C	0.0036793	4.9998899	1.1998328
C	0.0041861	3.612054	1.1922103
C	0.0026157	2.8923083	-0.0069899
C	0.0000478	3.6148286	-1.2044392
C	-0.0019346	5.0027465	-1.2086992
C	0.0030872	1.4029437	-0.0081527
C	1.1295052	0.6711582	0.4018711
C	1.133374	-0.72795	0.4002083
C	0.0023696	-1.4680471	-0.0057394
C	-1.1276334	-0.7280619	-0.4145124
C	-1.1231154	0.6710109	-0.4183288
C	0.0010486	-2.9479976	-0.0016965

13 with a = 0.35 in hexane (C_1 symmetry)

Energy = -8140.652284958 Hartree

	X	Y	Z
C	-0.1444099	8.8671934	-1.7273769
C	0.5772863	7.8559156	-1.0764167
C	1.8838972	7.5994395	-1.494463
C	2.4600535	8.3126583	-2.5457565
C	1.733993	9.322689	-3.1846283
C	0.4267215	9.5953846	-2.7591372
N	-0.0079627	7.127596	-0.0032832
C	-0.5830146	7.8625664	1.0704162
C	-1.8816171	7.6011386	1.5100773
C	-2.4486061	8.322344	2.5608493
C	-1.7221102	9.3457201	3.1774952
C	-0.4235175	9.6237537	2.7299167
C	0.1392155	8.8876592	1.6992138
O	-2.1829632	10.1083161	4.1946905
C	-3.4796643	9.8889996	4.6897589
O	2.202928	10.0764511	-4.2045232
C	3.5076537	9.8606888	-4.6799256
C	-0.0080101	5.7263516	-0.0007369
C	-0.0125608	5.0010969	1.2042016
C	-0.0114368	3.6130696	1.1993022
C	-0.0067049	2.8907848	0.0014794
C	-0.0024042	3.6111515	-1.197482
C	-0.0022047	4.9991145	-1.2044907
C	-0.006001	1.4016115	0.002411
C	1.1178216	0.6701027	0.4200874
C	1.1235735	-0.7284288	0.4170776
C	-0.0033281	-1.469745	0.0023398
C	-1.1318679	-0.7305994	-0.4119
C	-1.1287599	0.6682747	-0.4147537
C	-0.0013681	-2.9497103	0.0012302

C	0.4334681	-3.6863531	1.2066671	C	0.4241786	-3.691789	1.2096292
C	1.3913853	-4.7213885	1.1366633	C	1.3844663	-4.7248115	1.1421244
C	1.7963743	-5.4306894	2.2730035	C	1.7819509	-5.4385728	2.2780789
C	1.2591245	-5.1077115	3.5256238	C	1.2352194	-5.1221805	3.5280191
C	0.3131867	-4.0798855	3.6288125	C	0.2875859	-4.0960126	3.6289439
C	-0.0948589	-3.3889573	2.482117	C	-0.1133144	-3.4006285	2.4826354
Cl	2.1720962	-5.0862135	-0.3659378	Cl	2.1764852	-5.0819216	-0.3566802
Cl	2.9743868	-6.6865675	2.1484562	Cl	2.9625512	-6.692826	2.1563729
Cl	1.7587396	-5.9703183	4.9314218	Cl	1.7257206	-5.9907971	4.9336553
Cl	-0.3606022	-3.6935064	5.1707338	Cl	-0.3974735	-3.7170416	5.168126
Cl	-1.3494622	-2.2075783	2.6525749	Cl	-1.3706291	-2.2212686	2.6495569
Cl	2.6045467	-1.549458	0.811491	Cl	2.5931446	-1.5485721	0.8379401
Cl	2.5636298	1.5255471	0.8753483	Cl	2.5487545	1.5254893	0.9035374
Cl	-2.5567072	1.5252261	-0.8937763	Cl	-2.5613158	1.5214663	-0.8972052
Cl	-2.5991047	-1.5491418	-0.8256273	Cl	-2.5997996	-1.5538645	-0.8324263
C	-0.4328409	-3.6933449	-1.2051142	C	-0.424608	-3.6910372	-1.2084552
C	-1.3924767	-4.7263185	-1.1280637	C	-1.3810462	-4.7277288	-1.1425701
C	-1.7979545	-5.443336	-2.2593525	C	-1.7759982	-5.4410777	-2.2796666
C	-1.2594904	-5.1304712	-3.5140138	C	-1.2307408	-5.1204928	-3.529171
C	-0.3123369	-4.1044826	-3.6243023	C	-0.2868046	-4.0907852	-3.6284843
C	0.0960656	-3.405648	-2.482526	C	0.1118302	-3.3959781	-2.4810512
Cl	-2.1745065	-5.0788643	0.3767648	Cl	-2.1719028	-5.0900043	0.3556031
Cl	1.351687	-2.2265619	-2.6610132	Cl	1.364843	-2.2118054	-2.6462722
Cl	0.3626971	-3.7303273	-5.1686906	Cl	0.396419	-3.7064711	-5.167155
Cl	-1.7591922	-6.0031302	-4.9135668	Cl	-1.7181763	-5.9885919	-4.9361915
Cl	-2.977992	-6.6964032	-2.1261367	Cl	-2.9515885	-6.7002018	-2.1598632
H	-0.0121598	3.0834655	-2.1546342	H	-0.0087588	3.0787398	-2.1471924
H	0.0177276	3.078432	2.1411242	H	-0.0045412	3.0822108	2.1498719
H	0.0118917	5.5304921	2.1481259	H	-0.0100283	5.5317401	2.1524195
H	-0.0106424	5.5356502	-2.1557066	H	-0.0048498	5.5285044	-2.1534268
H	-2.4657967	6.7867677	0.9898758	H	-2.4610261	6.8161029	1.0284013
H	1.111711	9.1227037	1.3869744	H	1.151539	9.108654	1.3677095
H	-3.5082646	8.0394246	2.824995	H	-3.4600765	8.0838895	2.8764253
H	0.0481475	10.4190704	3.2258738	H	0.1328256	10.4212357	3.2177959
H	2.4678316	6.8025635	-0.9856342	H	2.4621856	6.8241526	-0.9959193
H	-1.1238259	9.1137828	-1.3961226	H	-1.1633382	9.0829015	-1.4128953
H	3.5086472	8.0618517	-2.8176526	H	3.4776642	8.0788389	-2.8446219
H	-0.0628967	10.4167141	-3.2322406	H	-0.12889	10.3821072	-3.264927
H	-3.7457745	10.558105	5.4506107	H	-3.6333507	10.6109648	5.4970619
H	-4.3312489	10.0024212	3.8586601	H	-4.2449884	10.0518721	3.9162694
H	-3.6877655	8.8223398	5.0393926	H	-3.5955971	8.8723991	5.0946064
H	3.7400115	10.5859956	-5.4389769	H	3.6659105	10.5727857	-5.495061
H	4.3209526	10.0324976	-3.8445741	H	4.2615298	10.0402045	-3.8989269
H	3.6940284	8.849031	-5.0309269	H	3.6365051	8.8395874	-5.0691777

13 with a = 0.35 in DCM (C_1 symmetry)

Energy = -8140.659949373 Hartree

	X	Y	Z
C	-0.1428494	8.8719405	-1.731591
C	0.5785763	7.8628919	-1.0771385
C	1.8924445	7.6183331	-1.4800324
C	2.477432	8.342662	-2.518836
C	1.7513149	9.350258	-3.1623171
C	0.4361055	9.6106946	-2.7524436
N	-0.0153204	7.1263024	-0.0135417
C	-0.5971603	7.8570838	1.0604735
C	-1.9107721	7.617184	1.4676527
C	-2.4848077	8.3329765	2.5183871
C	-1.7486504	9.3294	3.1681547
C	-0.4338491	9.5852023	2.7541754
C	0.1345359	8.8540658	1.7218828
O	-2.215616	10.0834905	4.1886817
C	-3.5339232	9.8869001	4.6474677
O	2.229178	10.1128584	-4.1712749
C	3.5459504	9.906994	-4.6303788
C	-0.0116047	5.725891	-0.0149524
C	-0.0515933	4.9974026	1.1879807
C	-0.0487657	3.609008	1.1801027
C	-0.0060393	2.8900979	-0.0189699
C	0.0339901	3.6121959	-1.2161887
C	0.0313608	5.0005743	-1.2198229
C	-0.0030106	1.4006917	-0.0194067
C	1.1202236	0.6709273	0.4007019
C	1.1273457	-0.7276946	0.4005956
C	0.0004954	-1.4707367	-0.0116281
C	-1.1273307	-0.7329078	-0.4301468
C	-1.1235895	0.6658772	-0.4378267
C	0.0014206	-2.9506267	-0.0024081
C	0.4279123	-3.6842295	1.2108711
C	1.3858646	-4.7196353	1.1493101
C	1.7840517	-5.4252708	2.2898181
C	1.2415608	-5.0976078	3.5383596
C	0.2969378	-4.0685744	3.6334891
C	-0.1059591	-3.382045	2.4828505
Cl	2.174298	-5.0894791	-0.34867
Cl	2.9607904	-6.6844335	2.1747577
Cl	1.7344836	-5.9564733	4.9495297
Cl	-0.3820431	-3.6745809	5.1721536
Cl	-1.3609109	-2.1986528	2.6435496
Cl	2.5975107	-1.5458079	0.8250206

13 with a = 0.35 in MeCN (C_1 symmetry)

Energy = -8140.661994123 Hartree

	X	Y	Z
C	-0.1298517	8.8826725	-1.7112043
C	0.5869498	7.8618438	-1.0697711
C	1.8920675	7.6014294	-1.492204
C	2.4714389	8.3199053	-2.5381611
C	1.7502813	9.3399582	-3.1678268
C	0.4447564	9.6168033	-2.7380829
N	-0.0010437	7.1283341	-0.0015735
C	-0.5903075	7.8580047	1.0685616
C	-1.8951526	7.5943817	1.4898307
C	-2.4759996	8.3090514	2.5375777
C	-1.7565895	9.3284114	3.1703924
C	-0.4513873	9.6085542	2.741749
C	0.1246457	8.8782523	1.712927
O	-2.2319649	10.0835532	4.1865504
C	-3.5406015	9.8575015	4.6629212
O	2.2242267	10.0986713	-4.1819619
C	3.5332258	9.8764206	-4.6589537
C	0.00052	5.7270236	-0.0031377
C	-0.0094881	4.9994026	1.2006674
C	-0.0080667	3.6110075	1.193731
C	0.0029515	2.8917863	-0.0060993
C	0.0130084	3.6134885	-1.2044144
C	0.012082	5.0019236	-1.2084425
C	0.003275	1.4024791	-0.0070514
C	1.1276681	0.6696754	0.4051146
C	1.1320432	-0.7289258	0.4035246
C	0.0023118	-1.4693829	-0.0048385
C	-1.1265152	-0.7288395	-0.4154785
C	-1.1212299	0.6697749	-0.419079
C	0.0011736	-2.9494102	-0.0014061
C	0.4297462	-3.6882346	1.2079126
C	1.3861281	-4.7248036	1.1401285
C	1.7853324	-5.435859	2.2767935
C	1.2455363	-5.1130602	3.5276397
C	0.3022864	-4.0834546	3.6288966
C	-0.1013521	-3.3910201	2.4821827
Cl	2.1709995	-5.0895767	-0.3609911
Cl	2.9602117	-6.6962284	2.1543923
Cl	1.7390184	-5.9786547	4.9345856
Cl	-0.3738361	-3.6954045	5.1704092
Cl	-1.3539421	-2.2061278	2.650437
Cl	2.6024358	-1.5508162	0.81961

Cl	2.5487623	1.5304288	0.8862029
Cl	-2.5535211	1.519535	-0.9295236
Cl	-2.5951867	-1.5565762	-0.8514743
C	-0.4258949	-3.70111	-1.2050831
C	-1.3833461	-4.7358659	-1.1284924
C	-1.7790876	-5.4600328	-2.2581845
C	-1.2351038	-5.1517514	-3.5110347
C	-0.2912264	-4.1234417	-3.6209234
C	0.1092959	-3.4181792	-2.4808982
Cl	-2.1732378	-5.0826262	0.374232
Cl	1.3616767	-2.2346505	-2.6589131
Cl	0.3899215	-3.7545912	-5.1648982
Cl	-1.7240003	-6.0339458	-4.9091312
Cl	-2.9548071	-6.7183793	-2.1248949
H	0.0585476	3.0824005	-2.1671571
H	-0.0710881	3.0764742	2.129556
H	-0.0792525	5.524211	2.1378312
H	0.0568584	5.5303654	-2.1682108
H	-2.4977715	6.8536426	0.9610836
H	1.1592981	9.0571268	1.4177165
H	-3.5079022	8.1126124	2.8082299
H	0.1317036	10.360658	3.266888
H	2.4720731	6.8462175	-0.9783069
H	-1.1678234	9.0784219	-1.4304784
H	3.5014948	8.1199989	-2.8039173
H	-0.121379	10.3953798	-3.2597428
H	-3.6911702	10.6001101	5.4613854
H	-4.2718082	10.0798308	3.855644
H	-3.6816018	8.8673985	5.0320105
H	3.7102457	10.6235735	-5.4398503
H	4.2851086	10.0884418	-3.8370196
H	3.6844913	8.8885808	-5.0208477

Cl	2.5624688	1.5248133	0.8807984
Cl	-2.5553762	1.5251039	-0.8964154
Cl	-2.5973211	-1.5503203	-0.8309692
C	-0.4288591	-3.6938567	-1.206704
C	-1.3873353	-4.7280944	-1.1333101
C	-1.7877096	-5.44471	-2.2660675
C	-1.2468456	-5.1300926	-3.5185431
C	-0.3016372	-4.1028192	-3.6253793
C	0.1029509	-3.4046199	-2.4824888
Cl	-2.1732175	-5.0827713	0.369683
Cl	1.3574899	-2.2227009	-2.656919
Cl	0.3757263	-3.7248972	-5.1688574
Cl	-1.7415869	-6.0027349	-4.9206816
Cl	-2.9653087	-6.7018515	-2.1368776
H	0.0126717	3.0834964	-2.155552
H	-0.0068756	3.0790373	2.1437642
H	-0.0125261	5.5270693	2.1506221
H	0.0142325	5.531543	-2.1573145
H	-2.4705737	6.8133894	0.9969337
H	1.1423681	9.1004595	1.3988751
H	-3.4916206	8.0693505	2.8383239
H	0.1020584	10.4016021	3.2406859
H	2.4689125	6.819982	-1.0016987
H	-1.1478772	9.1023197	-1.3962998
H	3.4873163	8.0826353	-2.8399827
H	-0.1101333	10.4103578	-3.23461
H	-3.7055482	10.5723938	5.4737189
H	-4.291812	10.0265889	3.8784585
H	-3.6576582	8.8375031	5.0558158
H	3.6969564	10.5939944	-5.4676325
H	4.2841399	10.0444973	-3.8739593
H	3.6521672	8.8577997	-5.0549167

14 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -7990.406325303 Hartree

	X	Y	Z
C	2.1064745	7.828882	-1.2012772
C	0.7728099	8.1664139	-0.9499236
C	0.2151654	9.2460151	-1.6472168
C	0.9755399	9.9637001	-2.562302
C	2.3084275	9.6275368	-2.8302601
C	2.852501	8.544469	-2.1340273
N	0.0002219	7.4435148	-0.0029274
C	-0.7722149	8.1657859	0.9447341

14 with a = 0.35 in hexane (C_1 symmetry)

Energy = -7990.410327010 Hartree

	X	Y	Z
C	2.1166757	7.8367836	-1.178947
C	0.7787254	8.1697076	-0.944125
C	0.2267338	9.2495006	-1.6459212
C	0.9964689	9.9716294	-2.550131
C	2.3338207	9.6393303	-2.8024669
C	2.8726218	8.5566574	-2.1008646
N	-0.0037219	7.4433541	-0.0076152
C	-0.7859311	8.1628047	0.9348013

C	-2.1061749	7.8288811	1.1947932	C	-2.1256576	7.8320187	1.1619512
C	-2.8519089	8.5430262	2.1289236	C	-2.8814012	8.5434184	2.0905855
C	-2.3071412	9.6241875	2.8275433	C	-2.3402002	9.6152878	2.8068185
C	-0.9740275	9.9602437	2.5602815	C	-1.001006	9.9457813	2.561933
C	-0.213963	9.2437799	1.6440134	C	-0.2316209	9.2318395	1.6508995
C	-0.0009848	6.0371982	-0.0028267	C	-0.0020901	6.0372137	-0.0101339
C	-0.1210217	5.3149411	1.1954351	C	-0.1373104	5.3126423	1.1854855
C	-0.1235554	3.9267731	1.1903457	C	-0.1372604	3.9242912	1.1781259
C	-0.0028597	3.2067995	-0.0024527	C	0.0009638	3.2068011	-0.0144158
C	0.1182789	3.9262499	-1.1955559	C	0.1371887	3.9279832	-1.2049515
C	0.1171299	5.3144756	-1.2010845	C	0.1340371	5.3164499	-1.2079873
C	-0.0022712	1.7171108	-0.0020348	C	0.0024914	1.7169944	-0.0150358
C	1.0682215	0.9860695	0.537692	C	1.0747348	0.986567	0.5214963
C	1.0724902	-0.413034	0.537223	C	1.0793826	-0.4123171	0.5224099
C	-0.0008927	-1.1536526	-0.0019202	C	0.0027036	-1.1535728	-0.0091838
C	-1.0750619	-0.414081	-0.5408066	C	-1.0734917	-0.414667	-0.5450144
C	-1.0721002	0.9850278	-0.5414929	C	-1.0689033	0.9842646	-0.550172
C	-0.000779	-2.6338889	-0.0007296	C	0.0011699	-2.6339029	-0.0021361
C	0.2863471	-3.3728701	1.2495059	C	0.28885	-3.3680202	1.2510214
C	1.2488145	-4.405052	1.2931904	C	1.2493633	-4.4019381	1.2979562
C	1.5206953	-5.1110974	2.4704415	C	1.5209838	-5.1035653	2.4777175
C	0.8389598	-4.788933	3.6509562	C	0.8422005	-4.7746805	3.6577807
C	-0.1166836	-3.7650885	3.6410299	C	-0.1116842	-3.7494774	3.644779
C	-0.3899434	-3.0774149	2.4532465	C	-0.3852595	-3.0661802	2.454711
Cl	2.1998847	-4.7701296	-0.1076839	Cl	2.1978604	-4.7751263	-0.1028347
Cl	2.7097228	-6.3625439	2.4872518	Cl	2.7074096	-6.3580072	2.4982027
Cl	1.1741969	-5.6475154	5.1070272	Cl	1.1781916	-5.6274721	5.1173967
Cl	-0.9686558	-3.3799946	5.0923731	Cl	-0.9610142	-3.3567394	5.0960004
Cl	-1.6611857	-1.9015912	2.472659	Cl	-1.6546656	-1.8879091	2.4712479
Cl	2.4860373	-1.2325661	1.118696	Cl	2.4939317	-1.232092	1.1021363
Cl	2.4368131	1.8406689	1.1762977	Cl	2.4451022	1.8428675	1.1551488
Cl	-2.4414791	1.838512	-1.1797491	Cl	-2.4393277	1.837757	-1.1874545
Cl	-2.4875338	-1.235188	-1.1226321	Cl	-2.4874899	-1.2368837	-1.1226477
C	-0.2872961	-3.3763779	-1.2489638	C	-0.2881662	-3.3811158	-1.2469885
C	0.3894675	-3.0845361	-2.4534188	C	0.3866972	-3.0944293	-2.4539227
C	0.1183326	-3.7774094	-3.6386657	C	0.1131239	-3.7921403	-3.6356263
C	-0.8360161	-4.8026135	-3.6453796	C	-0.8416203	-4.8166573	-3.6365581
C	-1.5185805	-5.1207873	-2.4642272	C	-1.5219015	-5.1298957	-2.4531064
C	-1.248694	-4.4096892	-1.2896141	C	-1.2500462	-4.4141966	-1.2819327
Cl	1.6593709	-1.9072949	-2.4764393	Cl	1.6568006	-1.9172507	-2.4841247
Cl	-2.2009831	-4.7700622	0.1116572	Cl	-2.2001326	-4.7684618	0.1226931
Cl	-2.7058554	-6.3739756	-2.4771363	Cl	-2.7099162	-6.3829762	-2.4588722
Cl	-1.1684036	-5.6678508	-5.0981346	Cl	-1.1770703	-5.687574	-5.0855637
Cl	0.9712887	-3.3973883	-5.0907501	Cl	0.9634278	-3.4179461	-5.0911884
H	0.202094	3.3926603	-2.1407524	H	0.2354785	3.3968006	-2.150021

H	-0.2078082	3.3938471	2.1358677
H	-0.2076117	5.8485014	2.1382895
H	0.2044205	5.847951	-2.1438911
H	-2.5602156	6.9998632	0.6564232
H	0.8230192	9.5174368	1.4626472
H	-3.8882421	8.2575723	2.3071889
H	-0.5145659	10.7944047	3.0905629
H	2.5599332	6.9978605	-0.6655997
H	-0.8216125	9.5200222	-1.4653615
H	3.8887157	8.2588877	-2.3127798
H	0.5162341	10.7986482	-3.0914951
C	-3.1165816	10.4080863	3.827525
C	3.1190628	10.414415	-3.8269544
H	4.1097213	9.9704156	-3.9784632
H	2.6183591	10.4596284	-4.8037585
H	3.2662741	11.4513331	-3.4930146
H	-4.1152572	9.9767274	3.9618889
H	-2.625728	10.430651	4.8102028
H	-3.2444308	11.4520716	3.5083016

H	-0.234599	3.3898682	2.1214553
H	-0.2384023	5.8436436	2.1283911
H	0.233842	5.8505554	-2.1493037
H	-2.5774528	7.0107769	0.6097791
H	0.8095362	9.5014116	1.4875081
H	-3.9224429	8.263871	2.249795
H	-0.5445432	10.7732587	3.1051214
H	2.5671668	7.0074421	-0.637974
H	-0.8129527	9.5210544	-1.476691
H	3.9122109	8.2751739	-2.2660594
H	0.541678	10.8073956	-3.0819124
C	-3.1579266	10.391444	3.8061951
C	3.1521458	10.4251269	-3.79379
H	4.1750993	10.0381396	-3.8651937
H	2.707786	10.3864359	-4.798183
H	3.212948	11.4851348	-3.5108779
H	-4.1836639	10.0101299	3.8672078
H	-2.718387	10.3345998	4.8118612
H	-3.2104187	11.4559616	3.539134

14 with a = 0.35 in DCM (C_1 symmetry)

Energy = -7990.415614688 Hartree

	X	Y	Z
C	2.0962456	7.8445321	-1.2122282
C	0.7592459	8.1678046	-0.9587262
C	0.1853658	9.2352412	-1.6619116
C	0.9328993	9.9550857	-2.5872746
C	2.2689817	9.6314191	-2.8593808
C	2.8302373	8.5613429	-2.1546598
N	-0.0008358	7.4440103	-0.0009232
C	-0.7598548	8.1684302	0.9572304
C	-2.0969847	7.8460931	1.2113994
C	-2.8299844	8.5634262	2.1541617
C	-2.2676111	9.6331716	2.8585599
C	-0.9315051	9.9559624	2.5857011
C	-0.1848891	9.2354764	1.660049
C	-0.0007934	6.0385105	-0.0006111
C	-0.1248548	5.3155022	1.1976527
C	-0.1255474	3.9268883	1.1930191
C	-0.00044	3.2075407	-0.0002058
C	0.1246281	3.9265822	-1.1936042
C	0.1236905	5.3152163	-1.1986753
C	-0.0004318	1.7179674	-0.0000391
C	1.0701572	0.9856804	0.5370509
C	1.0741126	-0.412991	0.5372657

14 with a = 0.35 in MeCN (C_1 symmetry)

Energy = -7990.417053927 Hartree

	X	Y	Z
C	2.1259311	7.8505237	-1.1577411
C	0.781078	8.1671893	-0.9399279
C	0.2189333	9.2279555	-1.6624176
C	0.9858814	9.9491319	-2.5708722
C	2.3312931	9.6339141	-2.805195
C	2.8801425	8.5687035	-2.0832407
N	-0.0000742	7.4424266	0.0002172
C	-0.7812597	8.1672574	0.9402206
C	-2.1251379	7.8481664	1.1607525
C	-2.879354	8.5663306	2.0862149
C	-2.3316748	9.6341324	2.8052928
C	-0.9872758	9.9516136	2.5684104
C	-0.2202078	9.2304004	1.6600454
C	0.0002433	6.0369478	0.0003605
C	-0.1570526	5.3135676	1.1947001
C	-0.1580917	3.9248108	1.1897468
C	0.0004906	3.2061781	0.0002829
C	0.1590881	3.9249136	-1.1891134
C	0.1576073	5.3136557	-1.1940226
C	0.0004966	1.7163371	0.0001584
C	1.0691159	0.9843092	0.5406159
C	1.0745825	-0.4142828	0.5377294

C	-0.0002427	-1.1534372	-0.000155	C	0.000282	-1.1546574	0.0000112
C	-1.0747349	-0.4130928	-0.5375116	C	-1.0738119	-0.4140802	-0.5377991
C	-1.0710156	0.9855975	-0.5370448	C	-1.0682096	0.9844966	-0.5403453
C	-0.0001488	-2.633559	-0.0001061	C	0.0001689	-2.6349051	-0.0000177
C	0.2861356	-3.3742106	1.2494045	C	0.2872316	-3.3758569	1.249157
C	1.2468578	-4.4081446	1.2915502	C	1.247906	-4.409774	1.2907718
C	1.5153017	-5.1179278	2.4668161	C	1.5172787	-5.1190697	2.4660313
C	0.8342395	-4.7970366	3.6474157	C	0.8369528	-4.7982705	3.6469437
C	-0.1184995	-3.7712636	3.6395331	C	-0.1160479	-3.7727192	3.639515
C	-0.3896518	-3.0798509	2.4538769	C	-0.3880495	-3.0816817	2.4539442
Cl	2.1989325	-4.77156	-0.109691	Cl	2.1988186	-4.7731428	-0.1114109
Cl	2.7012597	-6.3735473	2.4811734	Cl	2.7031586	-6.3750029	2.479662
Cl	1.1664435	-5.6607998	5.1018882	Cl	1.1705177	-5.6614026	5.1015344
Cl	-0.970059	-3.3872017	5.0923626	Cl	-0.9664637	-3.3883261	5.0930455
Cl	-1.658025	-1.9000193	2.4759876	Cl	-1.6566881	-1.9019645	2.4765107
Cl	2.4876885	-1.2344178	1.1182266	Cl	2.4872982	-1.2351246	1.1217657
Cl	2.4409277	1.8406856	1.1736063	Cl	2.4363488	1.8404194	1.1837745
Cl	-2.4418752	1.840566	-1.1734545	Cl	-2.4354739	1.8408743	-1.1830909
Cl	-2.4882398	-1.2346747	-1.1185231	Cl	-2.4866156	-1.2346561	-1.122024
C	-0.2863856	-3.3747676	-1.249316	C	-0.2871289	-3.3757046	-1.2492308
C	0.389483	-3.0808572	-2.4538929	C	0.3881853	-3.0815252	-2.4540167
C	0.1187524	-3.7730631	-3.6391591	C	0.1158253	-3.7723686	-3.6396211
C	-0.833742	-4.7991448	-3.6465522	C	-0.8374272	-4.7976725	-3.6471568
C	-1.514932	-5.1194596	-2.4659197	C	-1.5178162	-5.1184501	-2.4662607
C	-1.2468104	-4.4089528	-1.2910095	C	-1.2480941	-4.4093395	-1.2909632
Cl	1.6573127	-1.9004644	-2.4765246	Cl	1.657196	-1.9022429	-2.4765337
Cl	-2.1991184	-4.7717011	0.1102399	Cl	-2.1990464	-4.7725783	0.1112435
Cl	-2.7003457	-6.3755894	-2.4798132	Cl	-2.7041533	-6.3739139	-2.4799996
Cl	-1.165425	-5.6635321	-5.1007668	Cl	-1.1712975	-5.6604956	-5.1018591
Cl	0.9706098	-3.3897133	-5.0919847	Cl	0.9661929	-3.3880028	-5.0932086
H	0.2136926	3.3939386	-2.1389663	H	0.2750951	3.3929082	-2.1318257
H	-0.214278	3.3944361	2.1385115	H	-0.273985	3.3928115	2.1324795
H	-0.216369	5.8463795	2.1416148	H	-0.2747557	5.844056	2.1359676
H	0.2154378	5.8464411	-2.1424124	H	0.2753327	5.8441065	-2.135306
H	-2.5662651	7.0282043	0.6688024	H	-2.5828253	7.0310991	0.6070244
H	0.854232	9.4997204	1.4758726	H	0.8248704	9.4897758	1.5044875
H	-3.8695271	8.290762	2.3338841	H	-3.9233081	8.2952167	2.2410557
H	-0.459454	10.7822763	3.1170699	H	-0.5251076	10.7731417	3.1156899
H	2.5645522	7.0260312	-0.6697145	H	2.5844815	7.0354999	-0.6017166
H	-0.8536889	9.5001569	-1.4782895	H	-0.8268683	9.4855607	-1.5087418
H	3.8696438	8.287871	-2.3339254	H	3.9249997	8.2997644	-2.2357289
H	0.4615759	10.7813812	-3.1193226	H	0.5229367	10.768893	-3.1201463
C	-3.0583427	10.4092739	3.8795486	C	-3.1514608	10.4254301	3.7911391
C	3.0610474	10.4080127	-3.8789539	C	3.1503891	10.4242426	-3.7923938
H	4.1076363	10.0839109	-3.9041579	H	4.1434282	9.982363	-3.9333355

H	2.6456851	10.2779516	-4.8884012
H	3.0442422	11.4846473	-3.662507
H	-4.1086139	10.0966438	3.894373
H	-2.6519932	10.2647441	4.8907634
H	-3.0276797	11.4875917	3.6735952

H	2.6571836	10.4716841	-4.7726663
H	3.289959	11.4607917	-3.4540032
H	-4.1359442	9.9705342	3.9496502
H	-2.6477833	10.4943758	4.7646801
H	-3.3113248	11.4548136	3.4398352

15 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -8410.599267722 Hartree

	X	Y	Z
C	-1.3908231	-4.6280544	-1.1052929
C	-0.4041498	-3.6203385	-1.175715
C	0.1875875	-3.3916082	-2.4374021
C	-0.1864859	-4.122246	-3.5709659
C	-1.1622148	-5.1219188	-3.4671422
C	-1.7631205	-5.3765082	-2.2276641
C	-0.0054225	-2.8422639	0.0189715
C	0.3535452	-3.544749	1.2718604
C	1.2871384	-4.604009	1.2829316
C	1.622781	-5.2796739	2.4615552
C	1.0384178	-4.897479	3.6759425
C	0.1151434	-3.8444397	3.698818
C	-0.2233301	-3.1874295	2.5103626
Cl	2.123828	-5.0436462	-0.1686056
Cl	2.7727192	-6.5669054	2.436656
Cl	1.4527687	-5.7184649	5.1331653
Cl	-0.6171068	-3.3850637	5.1931055
Cl	-1.4548574	-1.9718199	2.5805891
Cl	1.4781557	-2.2485141	-2.6009284
Cl	0.5657648	-3.8206541	-5.0952873
Cl	-1.6202342	-6.0336794	-4.8557555
Cl	-2.9776575	-6.5968633	-2.1033185
Cl	-2.2463867	-4.9081738	0.3744173
C	0.0339521	-1.3634122	-0.0375963
C	1.1669168	-0.6373812	0.3873084
C	1.1987364	0.7605761	0.3402252
C	0.107589	1.5027288	-0.1386569
C	-1.0202938	0.7854887	-0.5679256
C	-1.0601755	-0.6121786	-0.5168404
C	0.1441792	2.9917273	-0.1872615
C	0.1086639	3.7494579	0.9875852
C	0.1445638	5.1369337	0.9481629
C	0.2097891	5.8168019	-0.2777314
C	0.2447549	5.0574497	-1.4571958
C	0.2153299	3.6700957	-1.4078718

15 with a = 0.35 in hexane (C_1 symmetry)

Energy = -8410.603444009 Hartree

	X	Y	Z
C	-1.3955259	-4.6237772	-1.1063682
C	-0.4105684	-3.6143039	-1.1762761
C	0.1766652	-3.3803869	-2.4394432
C	-0.2007336	-4.1071238	-3.5741453
C	-1.1749977	-5.1080184	-3.4708007
C	-1.7706909	-5.3682809	-2.2301867
C	-0.0078856	-2.8412679	0.0204359
C	0.356554	-3.5502084	1.267732
C	1.2888838	-4.6105618	1.2691893
C	1.627696	-5.2935297	2.4425193
C	1.0485783	-4.9175928	3.6612562
C	0.1274133	-3.8629933	3.6937827
C	-0.2147019	-3.1988074	2.5105364
Cl	2.1195029	-5.0423921	-0.1884084
Cl	2.7756963	-6.5830271	2.4052473
Cl	1.4664807	-5.7483976	5.1125194
Cl	-0.5946866	-3.4075376	5.1948014
Cl	-1.4422818	-1.9796983	2.5919295
Cl	1.4661879	-2.2361126	-2.6039511
Cl	0.5481617	-3.7999798	-5.0996512
Cl	-1.6365175	-6.0158501	-4.8614664
Cl	-2.9837666	-6.5907153	-2.1060176
Cl	-2.2449822	-4.911191	0.3757531
C	0.0303672	-1.3620447	-0.0295266
C	1.1638903	-0.6363735	0.3948442
C	1.1961509	0.7615863	0.3496898
C	0.1040849	1.5041102	-0.1246796
C	-1.025272	0.7885608	-0.5511596
C	-1.0652366	-0.6090209	-0.5025184
C	0.1419355	2.9925448	-0.1741749
C	0.0787034	3.7517255	0.9986441
C	0.1157811	5.1397694	0.9582611
C	0.2125636	5.8172431	-0.2667007
C	0.2747934	5.05696	-1.4442857
C	0.2425178	3.6692084	-1.3937987

N	0.2458203	7.224965	-0.3259469
C	-0.4949372	8.0011994	0.5960144
C	-1.8074561	7.6513102	0.9435112
C	-2.5333951	8.4165336	1.8491081
C	-1.96046	9.5577925	2.4059442
C	-0.6622798	9.9287162	2.0640408
C	0.0658489	9.1495736	1.1718652
Cl	-2.8725895	10.5260494	3.5332117
Cl	2.6334059	1.5979998	0.8413431
Cl	2.5983482	-1.4781435	0.8878754
Cl	-2.5332918	-1.4116035	-0.961127
Cl	-2.4109468	1.6578677	-1.1299612
C	1.0250589	7.8826898	-1.316856
C	2.3543257	7.514488	-1.5442607
C	3.1060579	8.1564394	-2.5247231
C	2.5709137	9.1942354	-3.2932428
C	1.2412681	9.5607245	-3.0496634
C	0.4751699	8.9151754	-2.0866352
C	3.3901736	9.9060588	-4.3379062
H	0.2349231	3.1056594	-2.3384468
H	0.0664905	3.2469593	1.952278
H	0.1264426	5.7012188	1.8772126
H	0.2923248	5.5614724	-2.4190535
H	-2.2640321	6.769941	0.4996537
H	1.08316	9.4349123	0.9154855
H	-3.5507529	8.1385221	2.113284
H	-0.2198824	10.8178567	2.506487
H	2.7987968	6.7168273	-0.9529217
H	-0.5597308	9.2093051	-1.9253677
H	4.1385718	7.8480209	-2.6858171
H	0.7890607	10.3603056	-3.6363443
H	4.3439714	9.3963216	-4.5164768
H	2.8548274	9.9651296	-5.2949018
H	3.6173076	10.937348	-4.0317119

15 with a = 0.35 in MeCN (C_1 symmetry)

Energy = -8410.610488292 Hartree

	X	Y	Z
C	-1.3961983	-4.6200141	-1.1110227
C	-0.4098548	-3.6117733	-1.1780097
C	0.17597	-3.3736325	-2.4406606
C	-0.203856	-4.095252	-3.5774795
C	-1.1781993	-5.0956112	-3.476843
C	-1.7726004	-5.3598509	-2.2370581
C	-0.0064562	-2.8420722	0.0206114
N	0.2537271	7.2251761	-0.3161811
C	-0.5084552	8.0052819	0.5844139
C	-1.8303919	7.6589367	0.8998401
C	-2.5775659	8.4284048	1.7846804
C	-2.0149633	9.5693257	2.3526797
C	-0.7077914	9.9376525	2.0436948
C	0.0405123	9.1544192	1.1713164
Cl	-2.9544391	10.5430282	3.4556765
Cl	2.6316018	1.5996257	0.8491637
Cl	2.5963293	-1.4782093	0.8912233
Cl	-2.5401581	-1.4067277	-0.9437603
Cl	-2.4169841	1.6640598	-1.1074695
C	1.060751	7.8786014	-1.2883311
C	2.3979958	7.5145249	-1.4710311
C	3.177477	8.1521384	-2.4329438
C	2.6620249	9.1815027	-3.2262943
C	1.3233474	9.5442811	-3.0276441
C	0.5302182	8.9030823	-2.0828957
C	3.5093049	9.8868579	-4.2530494
H	0.2855819	3.1015663	-2.3223352
H	0.0107934	3.2487613	1.9623567
H	0.0756419	5.7049973	1.8860727
H	0.3483445	5.5593438	-2.405282
H	-2.2789266	6.7779556	0.4473934
H	1.064447	9.4382958	0.9399922
H	-3.6021298	8.152754	2.0218225
H	-0.2731935	10.8261045	2.4951873
H	2.8277627	6.7244912	-0.8590632
H	-0.5100808	9.1959407	-1.9551437
H	4.2153777	7.8463838	-2.5597392
H	0.885749	10.3356501	-3.6364027
H	4.4916297	9.412009	-4.3575001
H	3.0260055	9.8847397	-5.2393252
H	3.6744377	10.9385385	-3.9786573

15 with a = 0.35 in DCM (C_1 symmetry)

Energy = -8410.609023636 Hartree

	X	Y	Z
C	-1.3956075	-4.6281781	-1.1029461
C	-0.4103161	-3.6192747	-1.1756489
C	0.1755921	-3.3878913	-2.4395072
C	-0.2022421	-4.117503	-3.5719383
C	-1.1751377	-5.1188184	-3.4655333
C	-1.7702135	-5.375918	-2.2244405
C	-0.0077327	-2.842806	0.0187179

C	0.3562575	-3.5470601	1.2691001	C	0.3567715	-3.553301	1.2671055
C	1.2893013	-4.6068375	1.275015	C	1.287204	-4.6154059	1.2668392
C	1.6285378	-5.2842323	2.4510836	C	1.6234983	-5.3016901	2.4384899
C	1.0503825	-4.9031932	3.6680736	C	1.0451427	-4.9274675	3.6573943
C	0.1287972	-3.84959	3.6962855	C	0.126948	-3.8712079	3.6919484
C	-0.2146998	-3.1910555	2.510641	C	-0.2137972	-3.2036212	2.5106411
Cl	2.1200516	-5.0450822	-0.1809625	Cl	2.1182327	-5.0457336	-0.1914638
Cl	2.776611	-6.5742503	2.4195266	Cl	2.767551	-6.5952384	2.3989757
Cl	1.4703926	-5.7267812	5.123028	Cl	1.4609357	-5.7626847	5.1070579
Cl	-0.5953416	-3.3901448	5.1955332	Cl	-0.5967813	-3.4195378	5.1939616
Cl	-1.4445652	-1.9733471	2.5880718	Cl	-1.439558	-1.9821964	2.595431
Cl	1.4636489	-2.2417281	-2.6070173	Cl	1.4660664	-2.228672	-2.601743
Cl	0.5420428	-3.811219	-5.100198	Cl	0.5395717	-3.7800145	-5.1044827
Cl	-1.6371812	-6.0301046	-4.853959	Cl	-1.6431155	-5.9968414	-4.8710078
Cl	-2.9815635	-6.600395	-2.0965301	Cl	-2.9852951	-6.5839285	-2.1160186
Cl	-2.2453384	-4.9111269	0.3802451	Cl	-2.2449009	-4.9116066	0.3711987
C	0.0311555	-1.3639237	-0.0356652	C	0.0330442	-1.3629066	-0.027343
C	1.164628	-0.6379107	0.3878018	C	1.1673234	-0.638945	0.397397
C	1.1950446	0.7597787	0.3431386	C	1.1997658	0.7587139	0.3546254
C	0.1035785	1.5025154	-0.1321219	C	0.1095807	1.5039184	-0.1197751
C	-1.0240782	0.7854653	-0.5600233	C	-1.0195937	0.7888248	-0.5470726
C	-1.0641023	-0.6119181	-0.5109843	C	-1.0617354	-0.608406	-0.4997665
C	0.1402624	2.9917833	-0.1790713	C	0.1486105	2.9930578	-0.1667382
C	0.0613626	3.7475835	0.9950167	C	0.0842281	3.7489633	1.0082712
C	0.0995278	5.1355349	0.9567496	C	0.1220317	5.1369346	0.9691614
C	0.2113207	5.8152301	-0.2661222	C	0.2187688	5.8163055	-0.2552153
C	0.2890242	5.0565828	-1.4442355	C	0.2832497	5.0574942	-1.4340061
C	0.2565514	3.6686361	-1.3971626	C	0.251109	3.6695104	-1.3863432
N	0.2546372	7.2235912	-0.3130398	N	0.2599844	7.2249444	-0.303368
C	-0.5186528	8.0046605	0.575909	C	-0.5103991	8.0058244	0.5877398
C	-1.8434436	7.656328	0.8778808	C	-1.8282441	7.6469978	0.9082024
C	-2.6030549	8.4284024	1.7500791	C	-2.5850135	8.4187261	1.7832785
C	-2.0479589	9.5732085	2.3174648	C	-2.0339037	9.5734666	2.3340123
C	-0.7382293	9.9440942	2.023229	C	-0.7317371	9.9555293	2.0212175
C	0.021416	9.1577768	1.1634198	C	0.0253644	9.1694082	1.1588395
Cl	-3.0040262	10.5532229	3.4054861	Cl	-2.9868489	10.5532748	3.4266058
Cl	2.6293634	1.5994597	0.8448696	Cl	2.6363559	1.5950983	0.8561704
Cl	2.5980959	-1.4791111	0.8843779	Cl	2.599284	-1.4832612	0.8933747
Cl	-2.5385648	-1.4113333	-0.9537275	Cl	-2.5377273	-1.4052783	-0.9423852
Cl	-2.4152961	1.6606566	-1.1192133	Cl	-2.4105855	1.6664737	-1.1036544
C	1.0780285	7.8764289	-1.2725667	C	1.0728079	7.8766719	-1.2729436
C	2.4203065	7.5175782	-1.4263592	C	2.4150516	7.5213227	-1.4364826
C	3.2165733	8.1549375	-2.3753779	C	3.2005594	8.155312	-2.3965941
C	2.7114633	9.1783714	-3.1839335	C	2.6845886	9.1724084	-3.206878
C	1.3668416	9.5353611	-3.0138435	C	1.340218	9.5255762	-3.0272815

C	0.5581071	8.8937604	-2.0825587
C	3.5756473	9.8833013	-4.1967611
H	0.3119763	3.105144	-2.3269488
H	-0.0179039	3.245978	1.9579104
H	0.0482466	5.6978173	1.8858681
H	0.3723744	5.559229	-2.4044359
H	-2.2864653	6.7728121	0.4249594
H	1.047659	9.442735	0.9454753
H	-3.6295107	8.1502319	1.9762457
H	-0.3090439	10.8355099	2.474117
H	2.8423273	6.7324001	-0.8024622
H	-0.4866624	9.1800555	-1.9804496
H	4.2588333	7.8547414	-2.4788488
H	0.9382339	10.3233153	-3.633009
H	4.5586142	9.4068526	-4.2856328
H	3.1067453	9.883874	-5.1899047
H	3.7371241	10.9343893	-3.9182005

C	0.5419851	8.8868388	-2.0845762
C	3.5398445	9.8774339	-4.2271955
H	0.2946572	3.1061981	-2.3168364
H	0.0163464	3.2475591	1.9720999
H	0.0815713	5.6991313	1.898898
H	0.3554575	5.5596278	-2.3953897
H	-2.2684266	6.7557073	0.4681192
H	1.0459576	9.4630232	0.9265541
H	-3.6058313	8.1320029	2.0238487
H	-0.305828	10.8549769	2.4591007
H	2.8453264	6.7410768	-0.8120021
H	-0.5030877	9.1696971	-1.975937
H	4.2426761	7.8574291	-2.5081108
H	0.9029418	10.3074152	-3.6480917
H	4.4911841	9.3556715	-4.3819758
H	3.0280898	9.9498597	-5.1957965
H	3.7713366	10.904147	-3.9088688

16 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -8830.791813406 Hartree

	X	Y	Z
C	2.0666889	7.3576512	-1.2746572
C	0.7557212	7.74465	-0.9660503
C	0.2098821	8.8550529	-1.6232488
C	0.9546807	9.5665657	-2.557313
C	2.2528163	9.1610399	-2.8582453
C	2.8096608	8.0542603	-2.2211402
N	-0.0021169	7.0321787	-0.0041362
C	-0.7562347	7.7477603	0.9581869
C	-2.0710131	7.371087	1.2633476
C	-2.8100416	8.0699742	2.2111559
C	-2.2464648	9.1703239	2.8535472
C	-0.9445013	9.5659415	2.5556565
C	-0.2038042	8.8520875	1.6202195
C	-0.005198	5.6199966	-0.0035095
C	0.0020243	4.9031865	1.2016321
C	-0.0040353	3.514338	1.1982215
C	-0.0080442	2.796485	-0.001417
C	-0.0112399	3.5125481	-1.2021916
C	-0.0140689	4.9014602	-1.2076477
C	-0.0069254	1.3055952	-0.0003469
C	1.1402541	0.5785954	0.3517018
C	1.1470464	-0.820496	0.3464989
C	-0.0029682	-1.5610831	-0.0010032

16 with a = 0.35 in hexane (C_1 symmetry)

Energy = -8830.796163522 Hartree

	X	Y	Z
C	2.0577766	7.3697317	-1.2860936
C	0.7463583	7.7481385	-0.9683908
C	0.187483	8.8527473	-1.6248371
C	0.9192595	9.566361	-2.5678326
C	2.217819	9.1684533	-2.8772086
C	2.7884516	8.0681105	-2.2411347
N	0.0008789	7.0332486	0.0011476
C	-0.7460932	7.7464742	0.970631
C	-2.0560814	7.3643328	1.2898618
C	-2.7882008	8.0610052	2.2449901
C	-2.2208929	9.1637325	2.8799507
C	-0.9238304	9.5653503	2.5690039
C	-0.1905161	8.8534255	1.6259637
C	0.0020736	5.6208535	0.0009236
C	0.0216029	4.9033121	1.2056398
C	0.0179276	3.5142802	1.2012567
C	0.003001	2.7977117	0.0006412
C	-0.0118106	3.5145856	-1.1997685
C	-0.0165652	4.9036	-1.203951
C	0.002687	1.3071182	0.0002776
C	1.1477096	0.5771581	0.3538602
C	1.151377	-0.8218506	0.3512663
C	0.0013748	-1.5607465	0.0002284

C	-1.1548925	-0.8235091	-0.3486145
C	-1.1521053	0.5756502	-0.3526267
C	-0.0011659	-3.0414946	-0.0000029
C	0.4929825	-3.7800076	1.1841581
C	1.4490265	-4.8123986	1.0650249
C	1.9147658	-5.5190989	2.1795721
C	1.4419667	-5.1965759	3.4580878
C	0.4987295	-4.1721064	3.6094402
C	0.0295771	-3.4839602	2.4847954
Cl	2.1520834	-5.1758574	-0.4756335
Cl	3.0888702	-6.7708463	1.9951962
Cl	2.0172041	-6.0552233	4.8367039
Cl	-0.0957356	-3.7864736	5.1835312
Cl	-1.219004	-2.3067948	2.7185306
Cl	2.6380306	-1.6380256	0.6837725
Cl	2.5908274	1.4400283	0.7563575
Cl	-2.6049623	1.4332828	-0.7572573
Cl	-2.6435017	-1.6450404	-0.6866607
C	-0.4932365	-3.7839393	-1.1824946
C	-0.0300939	-3.4901024	-2.4836925
C	-0.4959442	-4.1834233	-3.6065135
C	-1.4354852	-5.2109219	-3.4526713
C	-1.9086012	-5.5307013	-2.1735436
C	-1.446217	-4.8188203	-1.0609288
Cl	1.2147107	-2.3095126	-2.720128
Cl	-2.1494423	-5.179408	0.4803303
Cl	-3.0788625	-6.7856294	-1.986275
Cl	-2.0059261	-6.0764977	-4.8289532
Cl	0.0977693	-3.7999986	-5.1813984
H	-0.0264386	2.9766886	-2.149646
H	0.0100622	2.980167	2.1466408
H	0.0160423	5.4399077	2.1470524
H	-0.026627	5.4368305	-2.1538606
H	-2.5182951	6.5209627	0.7536846
H	0.8169001	9.1547251	1.3988327
H	-3.8296807	7.7726229	2.4432248
H	-0.5091158	10.4216449	3.0656915
H	2.5079897	6.5027544	-0.7678454
H	-0.8080722	9.1644199	-1.3986723
H	3.8265151	7.7501302	-2.456473
H	0.525727	10.4274678	-3.0639807
Cl	-3.1740387	10.0554303	4.0336904
Cl	3.1855919	10.0434225	-4.0367632

16 with a = 0.35 in DCM (C_1 symmetry)

C	-1.1477879	-0.8208234	-0.3513444
C	-1.1429573	0.5781742	-0.3533547
C	0.0008231	-3.0412867	-0.0001364
C	0.4909663	-3.7824152	1.1840176
C	1.4448434	-4.8167688	1.0651745
C	1.9040904	-5.5286166	2.1788471
C	1.4293842	-5.2075403	3.4567982
C	0.4896311	-4.18018	3.6081543
C	0.0256894	-3.4875922	2.4842741
Cl	2.1499433	-5.1794539	-0.4750391
Cl	3.0742255	-6.7846832	1.9944809
Cl	1.9975737	-6.0722997	4.8349489
Cl	-0.1071144	-3.7957825	5.1821717
Cl	-1.2195969	-2.3065046	2.7177764
Cl	2.6409791	-1.642543	0.6895377
Cl	2.6004422	1.4349908	0.7604988
Cl	-2.5949705	1.4373647	-0.7596976
Cl	-2.6382248	-1.6400722	-0.6895181
C	-0.4902006	-3.7811349	-1.1847399
C	-0.0249806	-3.4855535	-2.4848256
C	-0.4907067	-4.1758396	-3.6093796
C	-1.4320959	-5.2018145	-3.4588569
C	-1.9066554	-5.5237725	-2.1810698
C	-1.4455328	-4.8142465	-1.0666711
Cl	1.2223407	-2.3064379	-2.7173922
Cl	-2.1504449	-5.1777559	0.4734327
Cl	-3.0788289	-6.7781045	-1.9978109
Cl	-2.0026606	-6.0636043	-4.8378949
Cl	0.105562	-3.7901083	-5.1832382
H	-0.034326	2.9801991	-2.1478706
H	0.0409019	2.9798083	2.1493063
H	0.0437631	5.4385373	2.1517892
H	-0.0391428	5.4389619	-2.1500124
H	-2.5065114	6.5126619	0.7856392
H	0.8267852	9.1601146	1.3947661
H	-3.8041001	7.7589436	2.487222
H	-0.48537	10.4228779	3.0733351
H	2.5104032	6.5199322	-0.7806979
H	-0.8310395	9.1560925	-1.3946427
H	3.8055513	7.769358	-2.4823931
H	0.4786	10.4220975	-3.0732681
Cl	-3.1403478	10.0468949	4.070977
Cl	3.1353937	10.0538219	-4.0681826

16 with a = 0.35 in MeCN (C_1 symmetry)

Energy = -8830.802058766 Hartree

	X	Y	Z
C	2.0776895	7.3626123	-1.253982
C	0.7627982	7.7465082	-0.9571189
C	0.2201811	8.856698	-1.618142
C	0.970957	9.5708878	-2.5459324
C	2.2722777	9.1663586	-2.8338292
C	2.8282969	8.0610352	-2.1936627
N	-0.0027582	7.0319937	-0.0035616
C	-0.7652263	7.7461329	0.953277
C	-2.0842335	7.3708998	1.2421118
C	-2.8321728	8.0680869	2.1848699
C	-2.2686125	9.1633567	2.8356421
C	-0.9628829	9.5592515	2.5558203
C	-0.2149845	8.8460014	1.6248834
C	-0.0034923	5.6195303	-0.0035511
C	-0.0112634	4.9029695	1.2021089
C	-0.0161498	3.5136871	1.198728
C	-0.0052369	2.7976196	-0.0022014
C	0.0061572	3.512581	-1.2037784
C	0.0025827	4.9018786	-1.2085098
C	-0.0042739	1.3072499	-0.0015499
C	1.1420014	0.5786727	0.3492498
C	1.1481076	-0.8199598	0.3466755
C	-0.0017957	-1.5608599	-0.0001681
C	-1.1529086	-0.8222748	-0.3478238
C	-1.1492254	0.5764204	-0.3518144
C	-0.0003742	-3.0414075	0.0002734
C	0.4949754	-3.7811026	1.1832139
C	1.4494661	-4.8145348	1.0618955
C	1.9145516	-5.5235332	2.1746617
C	1.4445338	-5.2019368	3.4537077
C	0.5040579	-4.1761208	3.6075025
C	0.0341873	-3.4858256	2.4849886
Cl	2.1497237	-5.1774379	-0.4808039
Cl	3.0858057	-6.7788429	1.9870648
Cl	2.0200334	-6.064136	4.8309761
Cl	-0.0862236	-3.7900514	5.1841026
Cl	-1.2118048	-2.305945	2.722292
Cl	2.6396716	-1.6384961	0.6836268
Cl	2.5940789	1.4397131	0.7533108
Cl	-2.6025617	1.4346448	-0.7571954
Cl	-2.6431232	-1.6437024	-0.6838157
C	-0.494163	-3.7826853	-1.1823144
C	-0.0342921	-3.4867938	-2.4842484

Energy = -8830.803643578 Hartree

	X	Y	Z
C	2.1009573	7.3661479	-1.2129869
C	0.7791032	7.74531	-0.9419379
C	0.240107	8.8458686	-1.6215932
C	1.001252	9.5551121	-2.545053
C	2.3090244	9.1543276	-2.8076444
C	2.8625364	8.0593766	-2.1478421
N	0.0020287	7.0328258	0.0041165
C	-0.7758102	7.7477236	0.9473868
C	-2.0952251	7.3643802	1.2248181
C	-2.8574818	8.0608475	2.1566824
C	-2.3073684	9.1631585	2.8069796
C	-1.0022448	9.568174	2.5379333
C	-0.2402049	8.8557778	1.6176489
C	0.0016727	5.6200741	0.0044487
C	-0.0171035	4.9032441	1.2098091
C	-0.0220098	3.5138436	1.2061245
C	0.0012379	2.7986878	0.0048156
C	0.0246535	3.5135987	-1.1965932
C	0.0199435	4.9029634	-1.2006747
C	0.0010463	1.3080888	0.0044984
C	1.1491134	0.5785062	0.3463923
C	1.1539741	-0.8201746	0.3417887
C	0.000701	-1.5592167	0.0024883
C	-1.1525247	-0.8194304	-0.3354429
C	-1.1473448	0.5792292	-0.3378372
C	0.0007173	-3.0398459	0.0005647
C	0.5001744	-3.7822171	1.1799278
C	1.4512801	-4.8180213	1.052331
C	1.9184617	-5.531182	2.1614191
C	1.4547488	-5.2111325	3.4431349
C	0.518493	-4.1825156	3.6032232
C	0.0459002	-3.488331	2.4842964
Cl	2.1442765	-5.1790284	-0.4941988
Cl	3.0845125	-6.7904055	1.9659965
Cl	2.0328979	-6.0787779	4.8161015
Cl	-0.0635067	-3.7976665	5.1834219
Cl	-1.1958012	-2.3053796	2.7294361
Cl	2.6464473	-1.6412145	0.6695005
Cl	2.6040625	1.4392645	0.7414033
Cl	-2.6023208	1.4408279	-0.7308874
Cl	-2.6452686	-1.6395489	-0.6643217
C	-0.4989068	-3.7783429	-1.1812514
C	-0.0459871	-3.4789898	-2.4848512

C	-0.5026276	-4.1787128	-3.6064223
C	-1.4404434	-5.2068686	-3.4520356
C	-1.9095266	-5.5290846	-2.1727862
C	-1.446128	-4.8184098	-1.0604224
Cl	1.2087016	-2.303924	-2.7223101
Cl	-2.1451286	-5.1821176	0.4826406
Cl	-3.0774885	-6.7873585	-1.9844233
Cl	-2.0137901	-6.0712973	-4.8288119
Cl	0.0857725	-3.7913042	-5.1833884
H	0.0045458	2.9780569	-2.1521298
H	-0.0153668	2.97982	2.1474537
H	-0.0079729	5.4374744	2.1488687
H	-0.0002528	5.4355014	-2.1558066
H	-2.5309643	6.5254534	0.7244358
H	0.809183	9.1470062	1.4182337
H	-3.8550678	7.771221	2.4028372
H	-0.5277975	10.4109252	3.0728161
H	2.5193295	6.5093194	-0.7448953
H	-0.8006081	9.1650444	-1.4057426
H	3.8478408	7.7568809	-2.4172916
H	0.541284	10.4305005	-3.0542764
Cl	-3.2086507	10.0490146	4.0133807
Cl	3.2157365	10.0532815	-4.0077907

C	-0.52134	-4.1668725	-3.6064412
C	-1.4586279	-5.1950716	-3.4500006
C	-1.9204199	-5.5211759	-2.1691021
C	-1.4507821	-4.813946	-1.0572224
Cl	1.1976356	-2.2973127	-2.7262188
Cl	-2.1416667	-5.1822243	0.4885408
Cl	-3.0874992	-6.7801318	-1.9780934
Cl	-2.040784	-6.0544106	-4.8264855
Cl	0.0579422	-3.774185	-5.1856749
H	0.033572	2.9796166	-2.145207
H	-0.0316794	2.9801335	2.1548963
H	-0.0236596	5.4372114	2.1569418
H	0.0263886	5.4367588	-2.1479004
H	-2.5311746	6.5133785	0.7071427
H	0.7836402	9.163549	1.4195369
H	-3.8802524	7.757264	2.36585
H	-0.5779709	10.4254776	3.0546419
H	2.5393028	6.5209098	-0.6878803
H	-0.7858005	9.1500399	-1.4284998
H	3.8871918	7.7589313	-2.3522664
H	0.5743145	10.4065161	-3.0692742
Cl	-3.2655008	10.0477272	3.9725744
Cl	3.2660201	10.0347925	-3.9771483

17 with a = 0.35 in gas phase (C_1 symmetry)

Energy = -8463.470263833 Hartree

	X	Y	Z
C	1.4223595	4.7152113	-1.1086505
C	0.4763194	3.6709725	-1.2008344
C	0.0009617	3.3501676	-2.4912851
C	0.447976	4.0273101	-3.6315806
C	1.3811704	5.0645432	-3.5067783
C	1.8660882	5.4109023	-2.2389766
C	0.0042122	2.9458504	0.0004062
C	-0.4819628	3.7001411	1.1776812
C	-1.4463044	4.7240656	1.0517797
C	-1.9034473	5.447612	2.159084
C	-1.4135503	5.1507011	3.4375151
C	-0.462535	4.1343847	3.595832
C	-0.0023282	3.4292689	2.4779971
Cl	-2.1690639	5.0562076	-0.4868422
Cl	-3.0874424	6.6886096	1.9667043
Cl	-1.9776028	6.0302853	4.8072884
Cl	0.1528384	3.7803916	5.1692104

17 with a = 0.35 in hexane (C_1 symmetry)

Energy = -8463.476537470 Hartree

	X	Y	Z
C	1.4164859	4.7138615	-1.1175396
C	0.4706409	3.6689228	-1.2036467
C	-0.0116362	3.3471683	-2.4913068
C	0.4285428	4.0241262	-3.6341464
C	1.3608917	5.0624085	-3.5151515
C	1.8525404	5.4096654	-2.2505244
C	0.0050677	2.945148	0.0009182
C	-0.474215	3.7015458	1.1797647
C	-1.4382218	4.7261819	1.0576893
C	-1.8865357	5.4534166	2.1659285
C	-1.3889871	5.1591582	3.4416753
C	-0.4387345	4.1419873	3.5963927
C	0.013199	3.4331722	2.4777231
Cl	-2.1706837	5.0551391	-0.4772848
Cl	-3.0699001	6.6963164	1.9779267
Cl	-1.9421853	6.0440096	4.8129615
Cl	0.18544	3.7902731	5.1672998

Cl	1.2564915	2.2641899	2.7182009	Cl	1.2713857	2.2661342	2.7129609
Cl	-1.2369506	2.1555787	-2.69272	Cl	-1.2498342	2.1514771	-2.68544
Cl	-0.1611045	3.6117433	-5.1923785	Cl	-0.1884998	3.6068161	-5.1918187
Cl	1.9290328	5.9097211	-4.9045484	Cl	1.8996803	5.9080532	-4.9166155
Cl	3.0283707	6.6777775	-2.0875532	Cl	3.0139723	6.6788002	-2.1061559
Cl	2.1394849	5.1092237	0.4178696	Cl	2.1423414	5.1088858	0.4048945
C	0.018408	1.465125	0.0232631	C	0.0183489	1.4643815	0.0258048
C	-1.1233234	0.7208157	0.3890579	C	-1.1222172	0.7210994	0.3965757
C	-1.1064454	-0.6781491	0.4106988	C	-1.1065946	-0.6777605	0.4180519
C	0.0457383	-1.4004569	0.0654053	C	0.0437116	-1.4024253	0.0701983
C	1.1844079	-0.6666724	-0.3001745	C	1.1813492	-0.6686196	-0.2997556
C	1.1749502	0.7323806	-0.3187008	C	1.1726214	0.7302954	-0.3204082
C	0.0604583	-2.8913483	0.0854934	C	0.0575548	-2.8929971	0.0925752
C	0.0435122	-3.5916121	1.2958281	C	0.002323	-3.5916438	1.3031035
C	0.0549645	-4.9805449	1.3177096	C	0.0117995	-4.9804525	1.3277384
C	0.0971183	-5.7095437	0.1224024	C	0.090257	-5.7118598	0.1353977
C	0.1142324	-5.0114953	-1.0912616	C	0.1457368	-5.0155586	-1.0783387
C	0.091793	-3.6223913	-1.1057883	C	0.1251063	-3.6263666	-1.0960037
N	0.1046969	-7.127525	0.1349783	N	0.092972	-7.1295585	0.1502242
C	0.9210514	-7.8376947	1.0307994	C	0.8619026	-7.8446301	1.0819028
C	2.1775471	-7.3367416	1.4146441	C	2.0958028	-7.3458084	1.537084
C	2.9794562	-8.0388189	2.3002157	C	2.8489333	-8.053238	2.4601612
C	2.5586091	-9.2708947	2.8225565	C	2.3994621	-9.2890421	2.9499558
C	1.3092612	-9.7780489	2.4362365	C	1.1740955	-9.796054	2.4916764
C	0.5018904	-9.0710909	1.5594045	C	0.4160583	-9.0833818	1.5766567
Cl	-2.550075	-1.5444746	0.8305649	Cl	-2.5527384	-1.5403702	0.8395403
Cl	-2.6178678	1.5316474	0.7246597	Cl	-2.6148896	1.5344168	0.7367036
Cl	2.6542315	1.5611945	-0.6768516	Cl	2.6507052	1.5589689	-0.6859513
Cl	2.6447932	-1.5171657	-0.6938076	Cl	2.6427129	-1.5179692	-0.6948498
C	-0.730348	-7.8254484	-0.7791035	C	-0.6909973	-7.8255891	-0.8107996
C	-2.0795579	-7.4784099	-0.91425	C	-2.0375215	-7.4946439	-1.0004664
C	-2.8968218	-8.1456636	-1.8201705	C	-2.8036673	-8.157912	-1.9531767
C	-2.3713906	-9.1818115	-2.5891657	C	-2.227452	-9.1732606	-2.7136004
C	-1.0320469	-9.5448976	-2.4620491	C	-0.8904546	-9.521358	-2.5323219
C	-0.2159226	-8.8614051	-1.5676157	C	-0.1259375	-8.8414749	-1.5903492
Cl	-3.3935075	-10.0272632	-3.7171174	Cl	-3.1855998	-10.0136164	-3.9027693
H	0.1129293	-3.0988461	-2.0597497	H	0.1757191	-3.1058334	-2.0503597
H	0.0057905	-3.0443784	2.2358836	H	-0.0644575	-3.0439456	2.2411348
H	0.028925	-5.5062456	2.2693718	H	-0.0464477	-5.5028172	2.2796945
H	0.1472278	-5.5623791	-2.0282477	H	0.2074622	-5.5663402	-2.0138203
H	2.5268054	-6.3913089	1.0087591	H	2.4671077	-6.3978987	1.1579737
H	-0.4688756	-9.4724034	1.2818879	H	-0.5371279	-9.4842216	1.2437849
H	3.9510184	-7.6394517	2.5826174	H	3.8029666	-7.6546352	2.7975563
H	0.9663984	-10.7280194	2.8399788	H	0.8098723	-10.7488783	2.8688468
H	-2.4911623	-6.6763254	-0.305802	H	-2.4884791	-6.7091045	-0.3984264

H	0.833169	-9.1346648	-1.4789236
H	-3.944246	-7.8732758	-1.9231887
H	-0.6292856	-10.3492436	-3.0726087
C	3.3908405	-9.9990428	3.7351702
N	4.0602005	-10.5848699	4.4711535

H	0.9218767	-9.1019099	-1.4589248
H	-3.8490776	-7.8975964	-2.0986298
H	-0.4477401	-10.3096405	-3.1360071
C	3.1783162	-10.0213804	3.9044909
N	3.8034155	-10.6111481	4.6758664

17 with a = 0.35 in DCM (C_1 symmetry)

Energy = -8463.485720700 Hartree

	X	Y	Z
C	1.4182494	4.7165166	-1.1054127
C	0.480081	3.6651607	-1.1967028
C	0.0110922	3.336929	-2.4876213
C	0.4574332	4.0131884	-3.6281718
C	1.3815159	5.0577281	-3.5040568
C	1.8592109	5.4119075	-2.236425
C	0.0094695	2.9407971	0.0055923
C	-0.4836301	3.6959859	1.1794139
C	-1.4518701	4.7155162	1.0482353
C	-1.9130858	5.4412202	2.1518129
C	-1.4255365	5.1504839	3.4318085
C	-0.4719966	4.1383325	3.5955785
C	-0.0061394	3.4313433	2.4817842
Cl	-2.1728592	5.0395681	-0.4935576
Cl	-3.1005446	6.6793175	1.9523976
Cl	-1.9955329	6.0337175	4.7979051
Cl	0.1391589	3.789962	5.1729824
Cl	1.2557535	2.2704754	2.7289339
Cl	-1.2178724	2.1327058	-2.6892848
Cl	-0.1419835	3.5863241	-5.1907408
Cl	1.9275798	5.9029276	-4.903611
Cl	3.0103406	6.6905116	-2.0854457
Cl	2.1279162	5.1210181	0.4225489
C	0.0319925	1.4603068	0.0325408
C	-1.1064724	0.7102575	0.3963523
C	-1.0823436	-0.6881721	0.4184029
C	0.0729665	-1.4052424	0.0748906
C	1.2078756	-0.665872	-0.2886567
C	1.1923861	0.7326787	-0.3068767
C	0.0931093	-2.89634	0.0919636
C	0.1154721	-3.5967165	1.3022636
C	0.126196	-4.9862531	1.3201781
C	0.1278312	-5.7099999	0.1215086
C	0.1081212	-5.0116718	-1.0913788
C	0.0864201	-3.6219663	-1.1030741
N	0.1236614	-7.130506	0.1285585

17 with a = 0.35 in MeCN (C_1 symmetry)

Energy = -8463.488369935 Hartree

	X	Y	Z
C	1.355739	4.7123478	-1.1775302
C	0.4145695	3.660555	-1.2212658
C	-0.1201302	3.3332202	-2.4867659
C	0.267083	4.0104073	-3.6481997
C	1.1957606	5.0551071	-3.5708489
C	1.7373466	5.4087716	-2.3291857
C	0.0065841	2.9352669	0.0030215
C	-0.4236335	3.6898757	1.201729
C	-1.3963465	4.7102929	1.1215328
C	-1.7970245	5.4374327	2.2473928
C	-1.2428347	5.1467563	3.4998565
C	-0.2839786	4.1329265	3.6135491
C	0.1214035	3.4248116	2.4771333
Cl	-2.1970475	5.034312	-0.3804023
Cl	-2.9912589	6.6776794	2.1098402
Cl	-1.7381486	6.0321992	4.8935624
Cl	0.4090177	3.7843125	5.1568853
Cl	1.3923514	2.2615334	2.6579741
Cl	-1.3578529	2.1290416	-2.6260893
Cl	-0.4113159	3.5841727	-5.1784402
Cl	1.6691509	5.9016476	-4.9960237
Cl	2.8933727	6.6888119	-2.2361712
Cl	2.1430933	5.1158807	0.3121821
C	0.0288446	1.4545284	0.0270479
C	-1.0878267	0.7049954	0.4543503
C	-1.0626614	-0.6934557	0.4740184
C	0.0699822	-1.4089621	0.0632673
C	1.1833706	-0.6716961	-0.3619981
C	1.1690423	0.726775	-0.3757423
C	0.0902069	-2.9006927	0.0741874
C	0.3076824	-3.5999905	1.2650641
C	0.3240348	-4.9899007	1.2780674
C	0.1344555	-5.7096958	0.0929046
C	-0.0824366	-5.0122452	-1.1001662
C	-0.1091417	-3.6220031	-1.1063733
N	0.1440982	-7.132386	0.0983341

C	0.9912306	-7.853512	0.9552804	C	1.1796701	-7.840163	0.7145252
C	2.2549909	-7.3390648	1.3035445	C	2.4723888	-7.288097	0.8104054
C	3.1107559	-8.0558378	2.122934	C	3.4974544	-7.984065	1.4276157
C	2.7361838	-9.3164183	2.61494	C	3.2686069	-9.2620054	1.9627634
C	1.4802866	-9.8383111	2.2668094	C	1.9846424	-9.8221383	1.8649973
C	0.6216418	-9.1171461	1.4543067	C	0.9577654	-9.122061	1.2549072
Cl	-2.521904	-1.5629078	0.8373954	Cl	-2.4693323	-1.5732746	0.983379
Cl	-2.606149	1.5146303	0.7300185	Cl	-2.5671315	1.5084348	0.8710041
Cl	2.6688141	1.569441	-0.6634416	Cl	2.6255464	1.561979	-0.8099122
Cl	2.671751	-1.5115252	-0.6823566	Cl	2.6169912	-1.5230823	-0.8436903
C	-0.7901429	-7.8066851	-0.7268887	C	-0.930678	-7.8129741	-0.537624
C	-2.1443811	-7.4542013	-0.7315267	C	-2.2542656	-7.4556319	-0.2565672
C	-3.0405492	-8.0937631	-1.5818947	C	-3.3124854	-8.0978116	-0.8917974
C	-2.5826182	-9.1049605	-2.4233161	C	-3.0461178	-9.1144026	-1.8059822
C	-1.2391263	-9.4741689	-2.4280085	C	-1.735266	-9.4875352	-2.0954906
C	-0.3465901	-8.8175784	-1.5872911	C	-0.6827781	-8.8292065	-1.4681449
Cl	-3.7044613	-9.9178559	-3.4866927	Cl	-4.3712316	-9.9306672	-2.6006265
H	0.075171	-3.097525	-2.0567174	H	-0.2742612	-3.094785	-2.0441343
H	0.1092022	-3.0518063	2.2443932	H	0.454462	-3.0553359	2.195815
H	0.1284896	-5.5134553	2.2714364	H	0.482333	-5.5203191	2.2142828
H	0.1107421	-5.5602347	-2.0304069	H	-0.2291855	-5.5614144	-2.0274204
H	2.5699837	-6.3726209	0.9208691	H	2.6743145	-6.3069291	0.3908641
H	-0.3517445	-9.5315936	1.2084479	H	-0.0314138	-9.5677042	1.2044816
H	4.0853989	-7.6440458	2.3746518	H	4.4891048	-7.5410856	1.4852043
H	1.1721025	-10.8091254	2.6478943	H	1.7890215	-10.8070243	2.2828661
H	-2.5003153	-6.6719309	-0.0650379	H	-2.459713	-6.6686903	0.4653983
H	0.7054019	-9.0934119	-1.6013701	H	0.3411694	-9.1083666	-1.7053156
H	-4.0917215	-7.816542	-1.5827484	H	-4.3387691	-7.8167328	-0.6693705
H	-0.8908699	-10.258656	-3.09526	H	-1.5377005	-10.2759516	-2.8173808
C	3.6211184	-10.0595857	3.4596421	C	4.3272713	-9.9817635	2.601419
N	4.333613	-10.6605792	4.1427331	N	5.181678	-10.563454	3.1189745