

Supplementary Information

Electronic structure and magnetic properties of the triangular nanographenes with radical substituents: a DFT study

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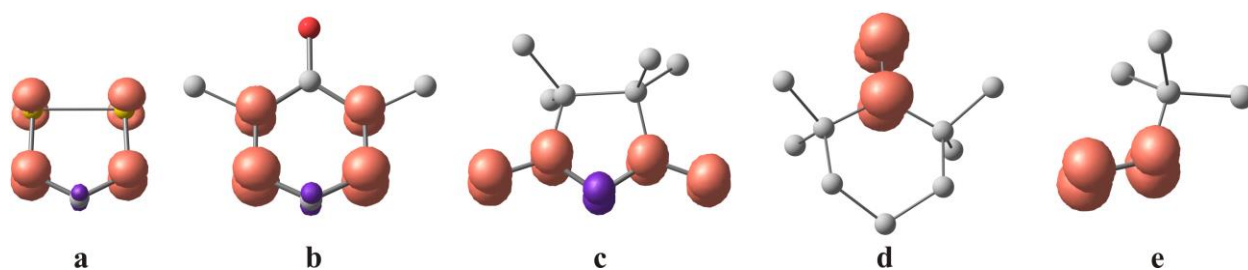


Figure S1. Spin density distribution (positive spin density is indicated in orange, negative spin density is indicated in purple) in **a–e** calculated by DFT UB3LYP/6-311++G(d,p) method.

Table S1. Spin state (S), total energies (E) and expectation values of the spin-squared operator (S^2) of **1** ($n = 3–5$) calculated by the DFT UB3LYP/6-311++G(d,p) method.

Compound	S	E , a. u.	S^2
1 ($n = 3$)	2/2	-845.8009033	2.104
BS	0	-845.7901663	1.033
1 ($n = 4$)	3/2	-1266.922765	3.913
BS1	1/2	-1266.908736	1.817
BS2	1/2	-1266.910109	1.817
1 ($n = 5$)	4/2	-1764.294394	6.227
BS1	2/2	-1764.280199	3.128
BS2	2/2	-1764.269671	2.047

Table S2. Spin state (S), total energies (E), expectation values of the spin-squared operator (S^2) and exchange spin coupling parameters corresponding to interactions between triangulene and dithiadiazolyl moieties (J) of **1'a** ($n = 2-8$) with orthogonal orientation of radical groups relative to the triangulene plane calculated by the DFT UB3LYP/6-311++G(d,p) method.

Compound	Electromer	S	E , a.u.	S^2	J , cm ⁻¹
1'a ($n = 2$)	$\alpha\alpha\alpha\alpha^*$	4/2	-3331.219226	6.090	-162
	$\beta\alpha\alpha\alpha$	2/2	-3331.220001	3.085	
	$\alpha\beta\alpha\alpha$	2/2	-3331.221501	3.028	
	$\beta\beta\alpha\alpha$	0	-3331.220759	2.047	
1'a ($n = 3$)	$\alpha\alpha\alpha\alpha$	5/2	-3676.090451	8.899	-111
	$\beta\alpha\alpha\alpha$	3/2	-3676.091288	4.876	
	$\alpha\beta\alpha\alpha$	1/2	-3676.092944	2.832	
	$\beta\beta\alpha\alpha$	1/2	-3676.092903	2.846	
1'a ($n = 4$)	$\alpha\alpha\alpha\alpha$	6/2	-4097.212513	12.207	-59
	$\beta\alpha\alpha\alpha$	4/2	-4097.213328	7.186	
	$\alpha\beta\alpha\alpha$	0	-4097.214953	3.144	
	$\beta\beta\alpha\alpha$	2/2	-4097.214141	4.165	
1'a ($n = 5$)	$\alpha\alpha\alpha\alpha$	7/2	-4594.584114	16.021	-44
	$\beta\alpha\alpha\alpha$	5/2	-4594.584923	9.999	
	$\alpha\beta\alpha\alpha$	1/2	-4594.586539	3.957	
	$\beta\beta\alpha\alpha$	3/2	-4594.585731	5.978	
1'a ($n = 6$)	$\alpha\alpha\alpha\alpha$	8/2	-5168.205330	20.338	-35
	$\beta\alpha\alpha\alpha$	6/2	-5168.206141	13.316	
	$\alpha\beta\alpha\alpha$	2/2	-5168.207760	5.273	
	$\beta\beta\alpha\alpha$	4/2	-5168.206951	8.295	
1'a ($n = 7$)	$\alpha\alpha\alpha\alpha$	9/2	-5818.076102	25.158	-30
	$\beta\alpha\alpha\alpha$	7/2	-5818.076916	17.136	
	$\alpha\beta\alpha\alpha$	3/2	-5818.078541	7.092	
	$\beta\beta\alpha\alpha$	5/2	-5818.077729	11.114	
1'a ($n = 8$)	$\alpha\alpha\alpha\alpha$	10/2	-6544.195965	30.479	-25
	$\beta\alpha\alpha\alpha$	8/2	-6544.196778	21.457	
	$\alpha\beta\alpha\alpha$	4/2	-6544.198405	9.412	
	$\beta\beta\alpha\alpha$	6/2	-6544.197592	14.434	

* α corresponds to spin-up, β corresponds to spin-down;

the ordering of the paramagnetic centers: (1) R, (2) triangulene moiety, (3) R, (4) R

Table S3. Spin state (S), total energies (E) and expectation values of the spin-squared operator (S^2) of **1a** and **1b** ($n = 2-5$) calculated by the DFT UB3LYP/6-311++G(d,p) method.

Compound	Electromer	S	E , a.u.	S^2
1a ($n = 2$)	$\alpha\alpha\alpha\alpha^*$	4/2	-3331.241863	6.070
	$\beta\alpha\alpha\alpha$	2/2	-3331.243599	3.060
	$\alpha\beta\alpha\alpha$	2/2	-3331.246961	3.061
	$\beta\beta\alpha\alpha$	0	-3331.245359	2.058
1a ($n = 3$)	$\alpha\alpha\alpha\alpha$	5/2	-3676.113126	8.874
	$\beta\alpha\alpha\alpha$	3/2	-3676.115030	4.869
	$\alpha\beta\alpha\alpha$	1/2	-3676.118981	2.865
	$\beta\beta\alpha\alpha$	1/2	-3676.117048	2.866
1a ($n = 4$)	$\alpha\alpha\alpha\alpha$	6/2	-4097.235462	12.181
	$\beta\alpha\alpha\alpha$	4/2	-4097.237156	7.180
	$\alpha\beta\alpha\alpha$	0	-4097.240946	3.178
	$\beta\beta\alpha\alpha$	2/2	-4097.239353	4.179
1a ($n = 5$)	$\alpha\alpha\alpha\alpha$	7/2	-4594.607027	15.995
	$\beta\alpha\alpha\alpha$	5/2	-4594.609087	9.994
	$\alpha\beta\alpha\alpha$	1/2	-4594.612995	3.991
	$\beta\beta\alpha\alpha$	3/2	-4594.610806	5.993
1b ($n = 2$)	$\alpha\alpha\alpha\alpha$	4/2	-1850.150671	6.083
	$\beta\alpha\alpha\alpha$	2/2	-1850.152792	3.066
	$\alpha\beta\alpha\alpha$	2/2	-1850.156920	3.056
	$\beta\beta\alpha\alpha$	0	-1850.154858	2.058
1b ($n = 3$)	$\alpha\alpha\alpha\alpha$	5/2	-2195.021435	8.887
	$\beta\alpha\alpha\alpha$	3/2	-2195.023895	4.876
	$\alpha\beta\alpha\alpha$	1/2	-2195.028895	2.860
	$\beta\beta\alpha\alpha$	1/2	-2195.026211	2.865
1b ($n = 4$)	$\alpha\alpha\alpha\alpha$	6/2	-2616.143325	12.194
	$\beta\alpha\alpha\alpha$	4/2	-2616.145681	7.187
	$\alpha\beta\alpha\alpha$	0	-2616.150409	3.173
	$\beta\beta\alpha\alpha$	2/2	-2616.148118	4.180
1b ($n = 5$)	$\alpha\alpha\alpha\alpha$	7/2	-3113.515259	16.007
	$\beta\alpha\alpha\alpha$	5/2	-3113.517554	10.001
	$\alpha\beta\alpha\alpha$	1/2	-3113.522083	3.989
	$\beta\beta\alpha\alpha$	3/2	-3113.519861	5.995

* α corresponds to spin-up, β corresponds to spin-down;

the ordering of the paramagnetic centers: (1) R, (2) triangulene moiety, (3) R, (4) R

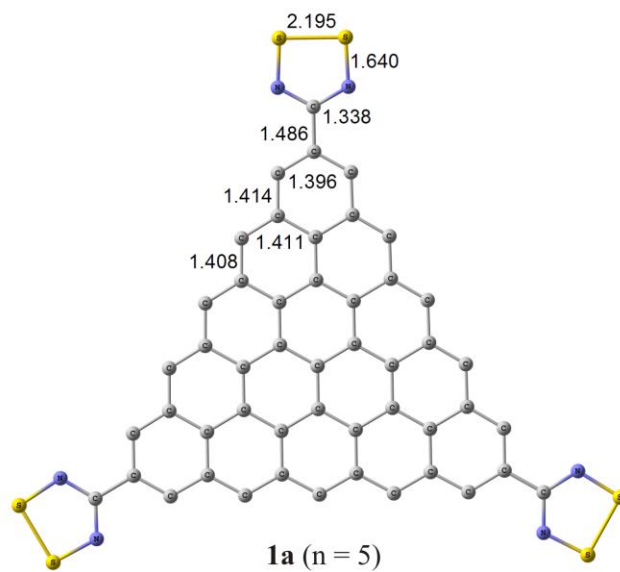
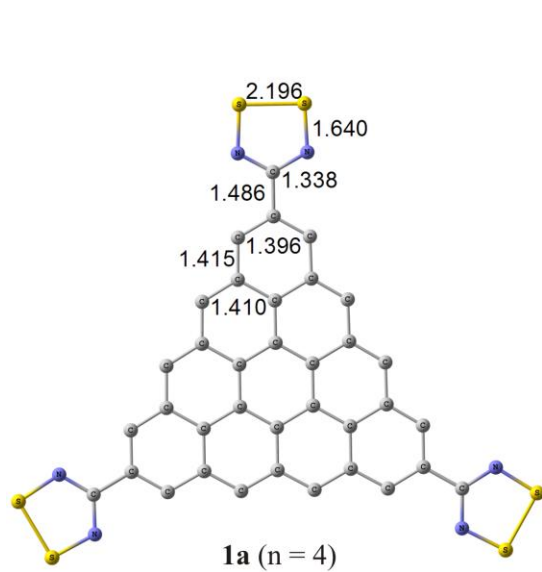
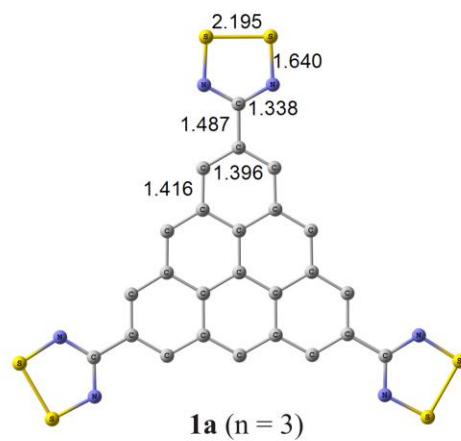
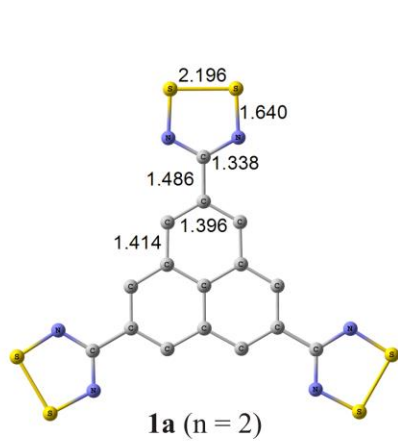


Figure S2. Optimized geometries of **1a** ($n = 2-5$) calculated by DFT UB3LYP/6-311++G(d,p) method.

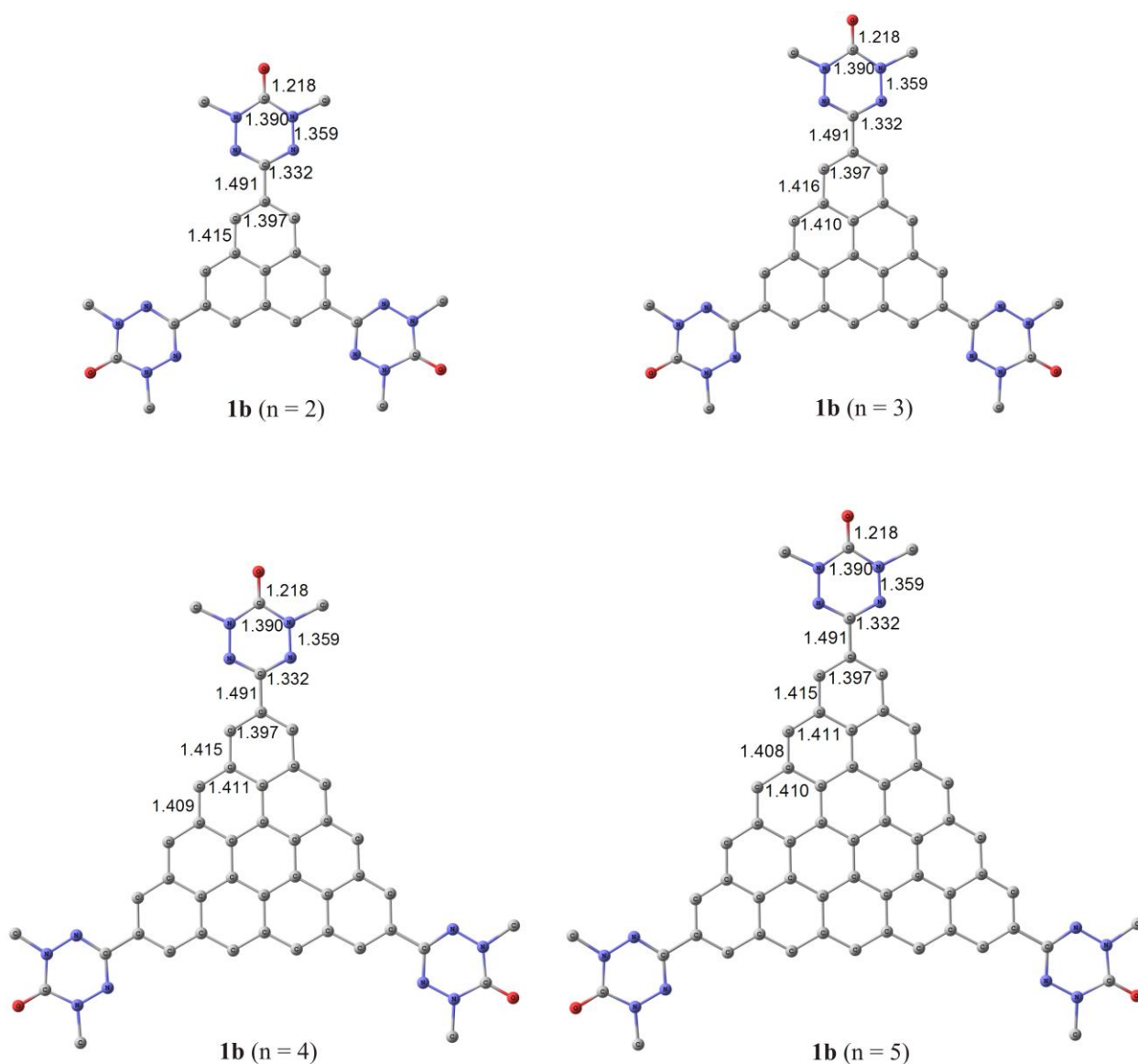


Figure S3. Optimized geometries of **1b** ($n = 2-5$) calculated by DFT UB3LYP/6-311++G(d,p) method.

Table S4. Spin state (S), total energies (E) and expectation values of the spin-squared operator (S^2) of **1c** and **1d** ($n = 2-5$) calculated by the DFT UB3LYP/6-311++G(d,p) method.

Compound	Electromer	S	E , a.u.	S^2
1c ($n = 2$)	$\alpha\alpha\alpha\alpha^*$	4/2	-2100.997983	6.155
	$\beta\alpha\alpha\alpha$	2/2	-2100.999674	3.195
	$\alpha\beta\alpha\alpha$	2/2	-2101.003264	3.291
	$\beta\beta\alpha\alpha$	0	-2101.001430	2.241
1c ($n = 3$)	$\alpha\alpha\alpha\alpha$	5/2	-2445.869660	8.949
	$\beta\alpha\alpha\alpha$	3/2	-2445.871260	4.997
	$\alpha\beta\alpha\alpha$	1/2	-2445.875258	3.097
	$\beta\beta\alpha\alpha$	1/2	-2445.873267	3.047
1c ($n = 4$)	$\alpha\alpha\alpha\alpha$	6/2	-2866.992132	12.255
	$\beta\alpha\alpha\alpha$	4/2	-2866.994298	7.306
	$\alpha\beta\alpha\alpha$	0	-2866.998229	3.407
	$\beta\beta\alpha\alpha$	2/2	-2866.996126	4.366
1c ($n = 5$)	$\alpha\alpha\alpha\alpha$	7/2	-3364.364253	16.067
	$\beta\alpha\alpha\alpha$	5/2	-3364.366260	10.119
	$\alpha\beta\alpha\alpha$	1/2	-3364.370328	4.222
	$\beta\beta\alpha\alpha$	3/2	-3364.368302	6.171
1d ($n = 2$)	$\alpha\alpha\alpha\alpha$	4/2	-1948.879463	6.060
	$\beta\alpha\alpha\alpha$	2/2	-1948.879484	3.060
	$\alpha\beta\alpha\alpha$	2/2	-1948.879485	3.060
	$\beta\beta\alpha\alpha$	0	-1948.879484	2.060
1d ($n = 3$)	$\alpha\alpha\alpha\alpha$	5/2	-2293.750622	8.867
	$\beta\alpha\alpha\alpha$	3/2	-2293.750614	4.867
	$\alpha\beta\alpha\alpha$	1/2	-2293.750623	2.867
	$\beta\beta\alpha\alpha$	1/2	-2293.750614	2.867
1d ($n = 4$)	$\alpha\alpha\alpha\alpha$	6/2	-2714.872428	12.176
	$\beta\alpha\alpha\alpha$	4/2	-2714.872310	7.176
	$\alpha\beta\alpha\alpha$	0	-2714.872818	3.176
	$\beta\beta\alpha\alpha$	2/2	-2714.872882	4.176
1d ($n = 5$)	$\alpha\alpha\alpha\alpha$	7/2	-3212.244710	15.990
	$\beta\alpha\alpha\alpha$	5/2	-3212.244754	9.990
	$\alpha\beta\alpha\alpha$	1/2	-3212.244755	3.990
	$\beta\beta\alpha\alpha$	3/2	-3212.244754	5.990

* α corresponds to spin-up, β corresponds to spin-down;

the ordering of the paramagnetic centers: (1) R, (2) triangulene moiety, (3) R, (4) R

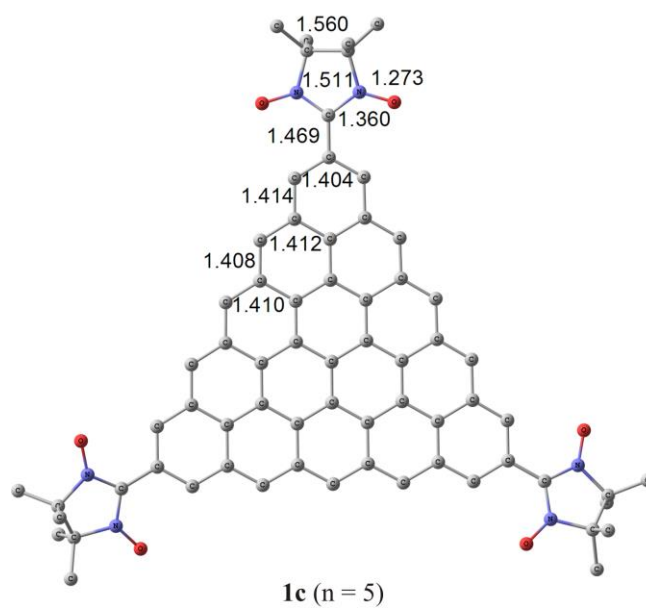
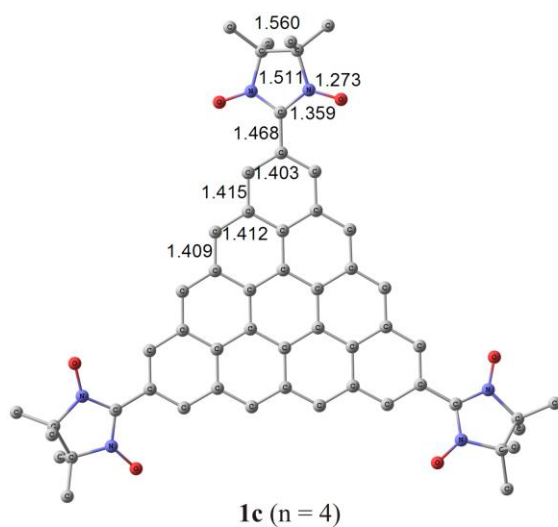
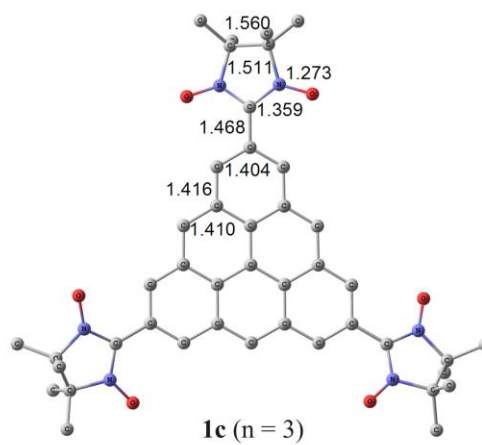
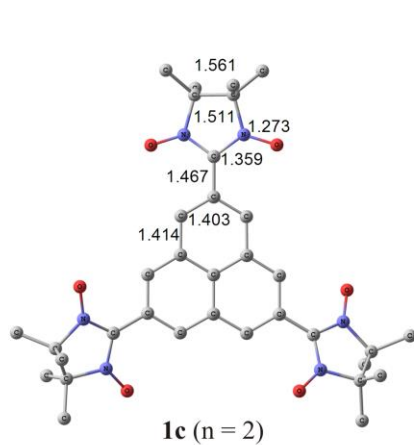


Figure S4. Optimized geometries of **1c** ($n = 2-5$) calculated by DFT UB3LYP/6-311++G(d,p) method.

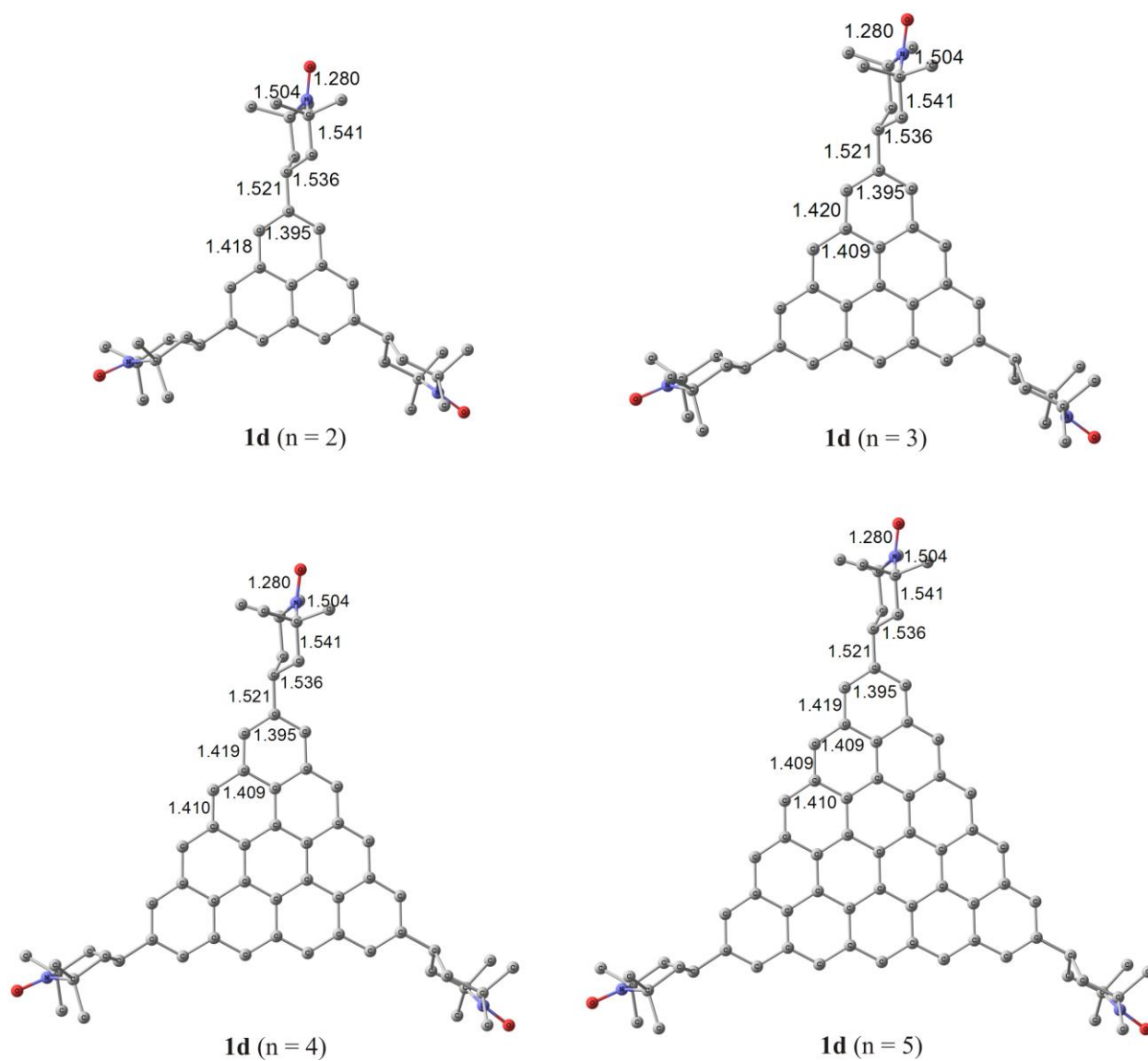


Figure S5. Optimized geometries of **1d** (n = 2–5) calculated by DFT UB3LYP/6-311++G(d,p) method.

Table S5. Spin state (S), total energies (E) and expectation values of the spin-squared operator (S^2) of **2a–2d** calculated by the DFT UB3LYP/6-311++G(d,p) method.

Compound	Electromer	S	E , a.u.	S^2
2a	$\alpha\alpha\alpha\alpha^*$	4/2	-3363.318306	6.068
	$\beta\alpha\alpha\alpha$	2/2	-3363.319532	3.064
	$\alpha\beta\alpha\alpha$	2/2	-3363.322634	3.067
	$\alpha\alpha\alpha\beta=\alpha\alpha\beta\alpha$	2/2	-3363.319854	3.065
	$\beta\beta\alpha\alpha$	0	-3363.321376	2.065
	$\alpha\beta\beta\alpha = \alpha\beta\alpha\beta$	0	-3363.321094	2.064
2b	$\alpha\alpha\alpha\alpha$	4/2	-1882.230224	6.083
	$\beta\alpha\alpha\alpha$	2/2	-1882.230653	3.093
	$\alpha\beta\alpha\alpha$	2/2	-1882.234548	3.079
	$\alpha\alpha\alpha\beta=\alpha\alpha\beta\alpha$	2/2	-1882.232151	3.072
	$\beta\beta\alpha\alpha$	0	-1882.234046	2.068
	$\alpha\beta\beta\alpha = \alpha\beta\alpha\beta$	0	-1882.232628	2.081
2c	$\alpha\alpha\alpha\alpha$	4/2	-2133.075717	6.161
	$\beta\alpha\alpha\alpha$	2/2	-2133.075827	3.163
	$\alpha\beta\alpha\alpha$	2/2	-2133.079006	3.252
	$\alpha\alpha\alpha\beta=\alpha\alpha\beta\alpha$	2/2	-2133.077330	3.204
	$\beta\beta\alpha\alpha$	0	-2133.078924	2.250
	$\alpha\beta\beta\alpha = \alpha\beta\alpha\beta$	0	-2133.077462	2.206
2d	$\alpha\alpha\alpha\alpha$	4/2	-1980.972650	6.055
	$\beta\alpha\alpha\alpha$	2/2	-1980.972651	3.055
	$\alpha\beta\alpha\alpha$	2/2	-1980.972651	3.055
	$\alpha\alpha\alpha\beta=\alpha\alpha\beta\alpha$	2/2	-1980.972650	3.055
	$\beta\beta\alpha\alpha$	0	-1980.972651	2.055
	$\alpha\beta\beta\alpha = \alpha\beta\alpha\beta$	0	-1980.972651	2.055

* α corresponds to spin-up, β corresponds to spin-down; the ordering of the paramagnetic centers: (1) unequivalent R, (2) triangulene moiety, (3) equivalent R, (4) equivalent R

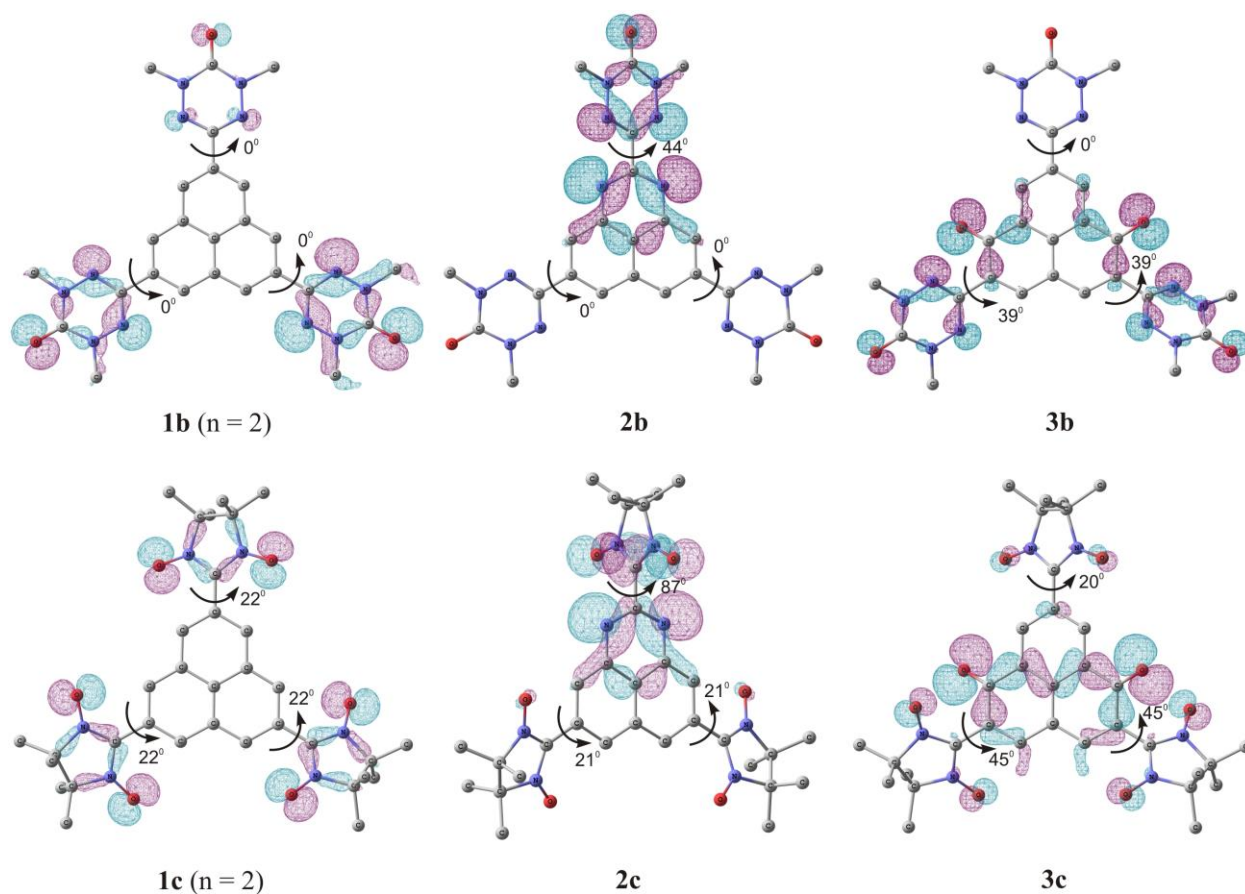


Figure S6. The shapes of orbitals and rotation angles of radicals in **1b** ($n = 2$), **1c** ($n = 2$), **2b**, **2c** and **3b**, **3c** calculated by DFT UB3LYP/6-311++G(d,p) method.

Table S6. Spin state (S), total energies (E) and expectation values of the spin-squared operator (S^2) of **3a–3d** calculated by the DFT UB3LYP/6-311++G(d,p).

Compound	Electromer	S	E , a.u.	S^2
3a	$\alpha\alpha\alpha\alpha^*$	4/2	-3480.502380	6.116
	$\beta\alpha\alpha\alpha$	2/2	-3480.502720	3.100
	$\alpha\beta\alpha\alpha$	2/2	-3480.498090	3.057
	$\alpha\alpha\alpha\beta=\alpha\alpha\beta\alpha$	2/2	-3480.501449	3.094
	$\beta\beta\alpha\alpha$	0	-3480.499080	2.073
	$\alpha\beta\beta\alpha = \alpha\beta\alpha\beta$	0	-3480.500553	2.081
3b	$\alpha\alpha\alpha\alpha$	4/2	-1999.416917	6.123
	$\beta\alpha\alpha\alpha$	2/2	-1999.415962	3.109
	$\alpha\beta\alpha\alpha$	2/2	-1999.410759	3.057
	$\alpha\alpha\alpha\beta=\alpha\alpha\beta\alpha$	2/2	-1999.414850	3.103
	$\beta\beta\alpha\alpha$	0	-1999.412663	2.078
	$\alpha\beta\beta\alpha = \alpha\beta\alpha\beta$	0	-1999.412663	2.078
3c	$\alpha\alpha\alpha\alpha$	4/2	-2250.268817	6.221
	$\beta\alpha\alpha\alpha$	2/2	-2250.267396	3.198
	$\alpha\beta\alpha\alpha$	2/2	-2250.259702	2.918
	$\alpha\alpha\alpha\beta=\alpha\alpha\beta\alpha$	2/2	-2250.265564	3.194
	$\beta\beta\alpha\alpha$	0	-2250.261416	2.058
	$\alpha\beta\beta\alpha = \alpha\beta\alpha\beta$	0	-2250.264047	2.165
3d	$\alpha\alpha\alpha\alpha$	4/2	-2098.155603	6.056
	$\beta\alpha\alpha\alpha$	2/2	-2098.155602	3.056
	$\alpha\beta\alpha\alpha$	2/2	-2098.155589	3.056
	$\alpha\alpha\alpha\beta=\alpha\alpha\beta\alpha$	2/2	-2098.155597	3.056
	$\beta\beta\alpha\alpha$	0	-2098.155590	2.056
	$\alpha\beta\beta\alpha = \alpha\beta\alpha\beta$	0	-2098.155596	2.056

* α corresponds to spin-up, β corresponds to spin-down; the ordering of the paramagnetic centers: (1) unequivalent R, (2) triangulene moiety, (3) equivalent R, (4) equivalent R

Table S7. Spin state (S), total energies (E) and expectation values of the spin-squared operator (S^2) of **4a–4d** calculated by the DFT UB3LYP/6-311++G(d,p).

Compound	Electromer	S	E , a.u.	S^2
4a	$\alpha\alpha\alpha\alpha^*$	4/2	-3900.061638	6.106
	$\beta\alpha\alpha\alpha$	2/2	-3900.060251	3.092
	$\alpha\beta\alpha\alpha$	2/2	-3900.057345	3.064
	$\beta\beta\alpha\alpha$	0	-3900.058822	2.078
4b	$\alpha\alpha\alpha\alpha$	4/2	-2418.975522	6.120
	$\beta\alpha\alpha\alpha$	2/2	-2418.974023	3.105
	$\alpha\beta\alpha\alpha$	2/2	-2418.971009	3.076
	$\beta\beta\alpha\alpha$	0	-2418.972440	2.091
4c	$\alpha\alpha\alpha\alpha$	4/2	-2669.819694	6.231
	$\beta\alpha\alpha\alpha$	2/2	-2669.817323	3.207
	$\alpha\beta\alpha\alpha$	2/2	-2669.811609	3.159
	$\beta\beta\alpha\alpha$	0	-2669.814552	2.182
4d	$\alpha\alpha\alpha\alpha$	4/2	-2517.701475	6.048
	$\beta\alpha\alpha\alpha$	2/2	-2517.701714	3.048
	$\alpha\beta\alpha\alpha$	2/2	-2517.701674	3.048
	$\beta\beta\alpha\alpha$	0	-2517.701676	2.048

* α corresponds to spin-up, β corresponds to spin-down;

the ordering of the paramagnetic centers: (1) R, (2) triangulene moiety, (3) R, (4) R

Table S8. Spin state (*S*), total energies (*E*) and expectation values of the spin-squared operator (*S*²) of **1e–4e** calculated by the DFT UB3LYP/6-311++G(d,p).

Compound	Electromer	<i>S</i>	<i>E</i> , a.u.	<i>S</i> ²
1e (<i>n</i> = 2)	αααα*	4/2	-1362.637392	6.106
	βααα	2/2	-1362.631555	3.069
	αβαα	2/2	-1362.622216	3.016
	ββαα	0	-1362.626603	2.038
1e (<i>n</i> = 3)	αααα	5/2	-1707.508942	8.914
	βααα	3/2	-1707.502936	4.874
	αβαα	1/2	-1707.490967	2.805
	ββαα	1/2	-1707.496826	2.838
1e (<i>n</i> = 4)	αααα	6/2	-2128.630686	12.225
	βααα	4/2	-2128.624660	7.184
	αβαα	0	-2128.612539	3.107
	ββαα	2/2	-2128.618561	4.145
1e (<i>n</i> = 5)	αααα	7/2	-2626.002254	16.040
	βααα	5/2	-2625.996292	9.999
	αβαα	1/2	-2625.984373	3.919
	ββαα	3/2	-2625.990336	5.959
2e	αααα	4/2	-1394.730017	6.092
	βααα	2/2	-1394.725166	3.062
	αβαα	2/2	-1394.717853	2.987
	αααβ=ααβα	2/2	-1394.724367	3.049
	ββαα	0	-1394.720851	2.017
	αββα = αβαβ	0	-1394.720819	2.021
3e	αααα	4/2	-1511.895977	6.044
	βααα	2/2	-1511.902907	2.814
	αβαα	2/2	-1511.914041	2.587
	αααβ=ααβα	2/2	-1511.903442	2.746
	ββαα	0	-1511.910209	1.591
	αββα = αβαβ	0	-1511.908533	1.672
4e	αααα	4/2	-1931.443768	6.025
	βααα	2/2	-1931.453269	2.708
	αβαα	2/2	-1931.470617	2.500
	ββαα	0	-1931.464761	1.482

*α corresponds to spin-up, β corresponds to spin-down;

the ordering of paramagnetic centers in **1e**, **4e**: (1) R, (2) triangulene moiety, (3) R, (4) R;
in **2e**, **3e**: (1) unequivalent R, (2) triangulene moiety, (3) equivalent R, (4) equivalent R

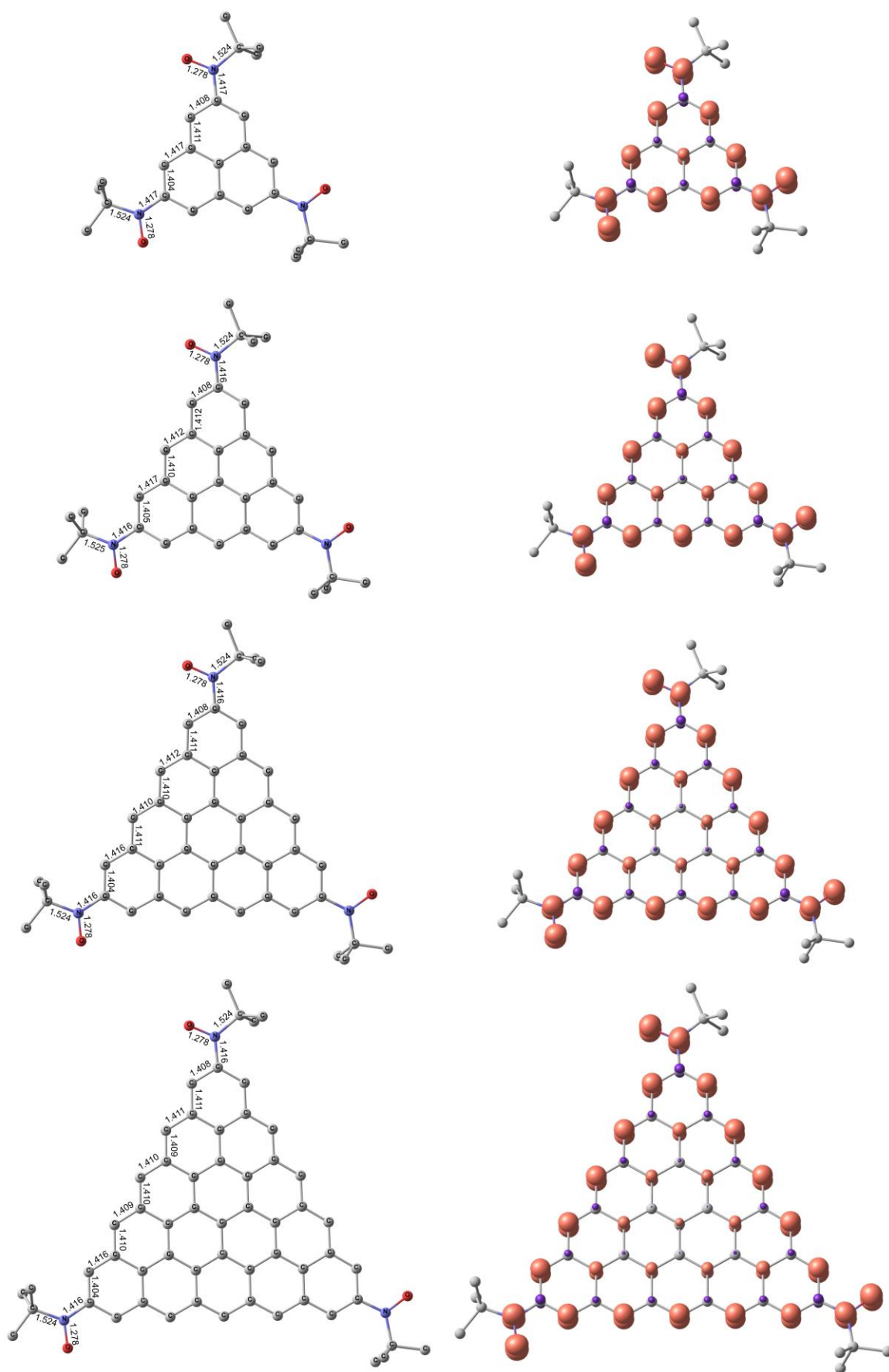


Figure S7. Optimized geometries (left column) and spin density distribution (right column: positive spin density is indicated in orange, negative spin density is indicated in purple) in **1e** (n = 2–5) calculated by DFT UB3LYP/6-311++G(d,p) method.

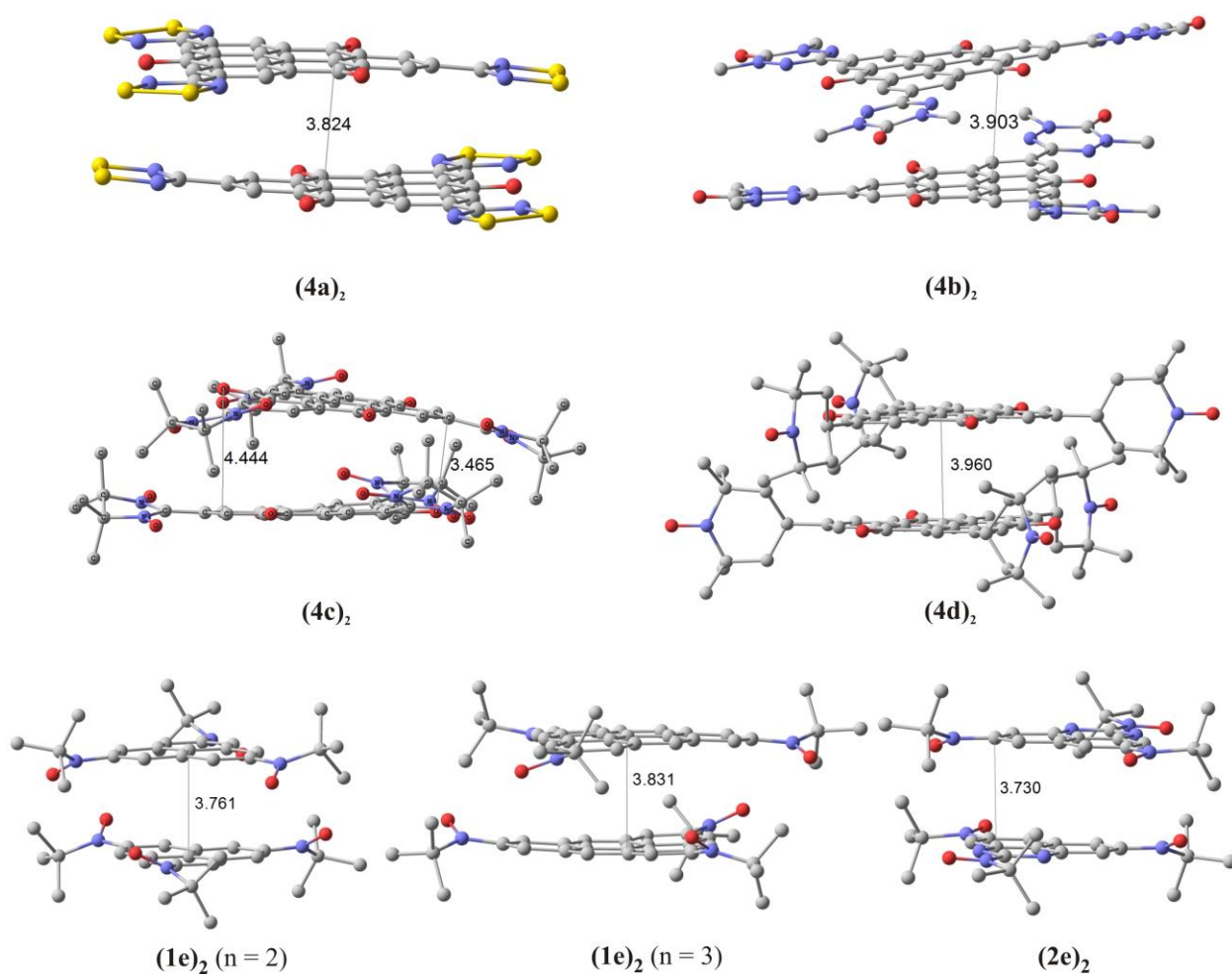


Figure S8. Optimized geometries of (4a)₂–(4d)₂, (1e)₂ (n = 2, 3) and (2e)₂ calculated by DFT CAM-UB3LYP/6-311++G(d,p) method.

Table S9. Spin state (S), total energies (E), expectation values of the spin-squared operator (S^2) and exchange spin coupling parameters (J) corresponding to the intermolecular exchange interactions of **(4a)₂**–**(4d)₂**, **(1e)₂** ($n = 2, 3$) and **(2e)₂** calculated by the DFT CAM-UB3LYP/6-311++G(d,p) method.

Compound	S	E , a.u.	S^2	J , cm ⁻¹
(4a)₂	8/2	-7798.596819	20.444	0
(4a)₂ BS	0	-7798.596844	4.445	
(4b)₂	8/2	-4835.715460	20.499	1
(4b)₂ BS	0	-4835.715397	4.496	
(4c)₂	8/2	-5337.093445	21.003	–5
(4c)₂ BS	0	-5337.093816	4.990	
(4d)₂	8/2	-5032.817819	20.206	–10
(4d)₂ BS	0	-5032.818582	4.175	
(1e)₂ ($n = 2$)	8/2	-2723.862846	20.392	–54
(1e)₂ ($n = 2$) BS	0	-2723.866827	4.276	
(1e)₂ ($n = 3$)	10/2	-3413.223507	30.660	–14
(1e)₂ ($n = 3$) BS	0	-3413.225120	5.628	
(2e)₂	8/2	-2788.058249	20.341	–6
(2e)₂ BS	0	-2788.058679	4.333	

Table S10. Spin state (S), total energies (E), expectation values of the spin-squared operator (S^2) and exchange spin coupling parameters corresponding to interactions between triangulene and dithiadiazolyl moieties (J) of structures **1a** ($n = 2$) characterized by rotation of the dithiadiazolyl substituents at 20, 40, 60 and 90°, according to the DFT UB3LYP/6-311++G(d,p) calculations.

Angle	Electromer	S	E , a.u.	S^2	J , cm ⁻¹
0°	$\alpha\alpha\alpha\alpha^*$	4/2	-3331.241863	6.070	-375
	$\beta\alpha\alpha\alpha$	2/2	-3331.243599	3.060	
	$\alpha\beta\alpha\alpha$	2/2	-3331.246961	3.061	
	$\beta\beta\alpha\alpha$	0	-3331.245359	2.058	
20°	$\alpha\alpha\alpha\alpha$	5/2	-3331.240568	6.072	-280
	$\beta\alpha\alpha\alpha$	3/2	-3331.241834	3.074	
	$\alpha\beta\alpha\alpha$	1/2	-3331.244390	3.088	
	$\beta\beta\alpha\alpha$	1/2	-3331.243105	2.080	
40°	$\alpha\alpha\alpha\alpha$	6/2	-3331.235656	6.076	-250
	$\beta\alpha\alpha\alpha$	4/2	-3331.236293	3.090	
	$\alpha\beta\alpha\alpha$	0	-3331.238504	3.118	
	$\beta\beta\alpha\alpha$	2/2	-3331.237943	2.104	
60°	$\alpha\alpha\alpha\alpha$	7/2	-3331.227521	6.083	-219
	$\beta\alpha\alpha\alpha$	5/2	-3331.227515	3.085	
	$\alpha\beta\alpha\alpha$	1/2	-3331.229508	3.091	
	$\beta\beta\alpha\alpha$	3/2	-3331.229511	2.088	
90°	$\alpha\alpha\alpha\alpha$	8/2	-3331.219989	6.089	-163
	$\beta\alpha\alpha\alpha$	6/2	-3331.220764	3.066	
	$\alpha\beta\alpha\alpha$	2/2	-3331.222262	3.026	
	$\beta\beta\alpha\alpha$	4/2	-3331.221521	2.045	

* α corresponds to spin-up, β corresponds to spin-down;

the ordering of the paramagnetic centers: (1) R, (2) triangulene moiety, (3) R, (4) R

Cartesian coordinates of the compounds
calculated by the DFT UB3LYP/6-311++G(d,p) method

1a (n = 2), $\omega_1 = 18 \text{ cm}^{-1}$

6	0.964366000	2.249281000	-0.000059000
6	-0.177618000	1.415125000	-0.000006000
6	2.249693000	1.704874000	-0.000121000
6	-0.000058000	0.000152000	-0.000009000
6	2.426073000	0.320191000	-0.000128000
6	1.314129000	-0.553591000	-0.000069000
1	0.841182000	3.324679000	-0.000050000
6	-1.490343000	1.941216000	0.000058000
6	-1.136623000	-0.861157000	0.000049000
6	1.465529000	-1.959669000	-0.000075000
6	-2.430030000	-0.289260000	0.000097000
6	-2.601272000	1.096068000	0.000105000
1	-1.636767000	3.013700000	0.000068000
6	-0.935905000	-2.261029000	0.000054000
1	-3.299750000	-0.933632000	0.000139000
6	0.351464000	-2.800615000	-0.000012000
1	-1.791540000	-2.923969000	0.000105000
1	3.428015000	-0.089365000	-0.000180000
1	2.458397000	-2.390772000	-0.000131000
16	-6.503598000	1.548245000	-0.000188000
16	-5.651465000	3.571915000	0.000660000
7	-5.022124000	0.845696000	-0.000297000
7	-4.113603000	3.003056000	0.000667000
6	-3.971091000	1.673071000	0.000172000
16	-0.267926000	-6.679888000	0.000425000
16	1.910771000	-6.406261000	-0.000542000
7	-0.544000000	-5.063749000	0.000510000
7	1.778637000	-4.771960000	-0.000577000
6	0.536635000	-4.275385000	-0.000029000
16	4.593390000	4.857743000	0.000076000
16	5.919106000	3.107508000	-0.000361000
7	3.243787000	3.926492000	0.000041000
7	4.657276000	2.060531000	-0.000363000
6	3.434416000	2.602512000	-0.000184000

1a (n = 3), $\omega_1 = 12 \text{ cm}^{-1}$

6	-3.551874000	-1.210110000	0.000000000
6	-2.136143000	-1.238185000	0.000000000
6	-1.413022000	-2.447699000	0.000000000
6	-1.420507000	0.000129000	0.000000000
6	-0.003960000	-2.469216000	0.000000000
6	0.710759000	-1.230368000	0.000000000
6	0.000306000	0.000045000	0.000000000
6	2.141024000	-1.230956000	0.000000000
6	2.824667000	-2.470929000	0.000000000
6	2.123926000	-3.678082000	0.000000000
6	0.728150000	-3.681241000	0.000000000
1	3.907071000	-2.483627000	0.000000000
6	-4.246947000	0.000252000	0.000000000
6	-3.551804000	1.210593000	0.000000000
6	-2.136125000	1.238458000	0.000000000

1	-4.103949000	2.141632000	0.000000000
6	-1.413022000	2.447948000	0.000000000
6	-0.003989000	2.469307000	0.000000000
6	0.710737000	1.230476000	0.000000000
1	-1.955341000	3.387486000	0.000000000
6	2.826979000	0.000021000	0.000000000
6	2.141000000	1.230984000	0.000000000
1	0.198065000	-4.625014000	0.000000000
1	-1.955494000	-3.387128000	0.000000000
6	0.728072000	3.681319000	0.000000000
1	0.197970000	4.625102000	0.000000000
1	3.911830000	0.000115000	0.000000000
1	-4.104272000	-2.140989000	0.000000000
6	2.824629000	2.470988000	0.000000000
6	2.123857000	3.678126000	0.000000000
1	3.907048000	2.483802000	0.000000000
16	4.960174000	6.397302000	0.000000000
16	3.058219000	7.494453000	0.000000000
7	4.204459000	4.942207000	0.000000000
7	2.176893000	6.111741000	0.000000000
6	2.866913000	4.965760000	0.000000000
16	-8.019507000	-1.097989000	0.000000000
16	-8.019698000	1.097428000	0.000000000
7	-6.381309000	-1.170340000	0.000000000
7	-6.381686000	1.170434000	0.000000000
6	-5.733649000	0.000161000	0.000000000
16	3.058219000	-7.494630000	0.000000000
16	4.959895000	-6.397443000	0.000000000
7	2.176918000	-6.111751000	0.000000000
7	4.204499000	-4.942194000	0.000000000
6	2.866994000	-4.965779000	0.000000000

1a ($n = 4$), $\omega_1 = 15 \text{ cm}^{-1}$

6	4.462866000	-2.508075000	-0.000266000
6	3.446925000	-1.523518000	-0.000062000
6	4.146924000	-3.867619000	-0.000395000
6	2.079612000	-1.940542000	-0.001155000
6	2.812768000	-4.278378000	-0.000247000
6	1.759378000	-3.333653000	-0.000078000
1	5.501614000	-2.203441000	-0.000096000
6	3.745311000	-0.145160000	-0.000011000
6	0.404971000	-3.727431000	-0.000039000
1	4.783883000	0.168650000	0.001271000
1	2.581721000	-5.335936000	-0.000076000
1	0.164330000	-4.785345000	0.001271000
6	-0.643644000	-2.786440000	-0.000107000
6	-0.320043000	-1.384716000	-0.004178000
6	1.038681000	-0.969782000	0.002847000
6	1.357776000	0.414503000	-0.004026000
6	-1.998634000	-3.172502000	-0.000078000
6	2.733587000	0.835241000	-0.000003000
6	3.024233000	2.213689000	-0.000009000
1	4.060786000	2.534107000	0.001258000
1	-2.246025000	-4.228859000	0.001297000
6	0.319210000	1.383838000	0.002864000
6	-1.039221000	0.967914000	-0.004191000
6	-1.359331000	-0.416139000	0.002697000

6	-2.091314000	1.949174000	-0.000237000
6	-3.430492000	1.511445000	-0.000267000
6	-3.766708000	0.141739000	-0.000278000
6	-2.720503000	-0.832354000	-0.001344000
6	0.639452000	2.770619000	-0.001201000
6	-1.748102000	3.315548000	-0.000218000
1	-4.226308000	2.248888000	0.001029000
6	-5.111490000	-0.298092000	-0.000403000
6	-3.043272000	-2.224857000	-0.000180000
6	-4.404056000	-2.612406000	-0.000294000
6	-5.423306000	-1.658648000	-0.000429000
1	-5.911729000	0.430904000	-0.000182000
1	-4.659571000	-3.664316000	0.000014000
6	-0.405088000	3.746513000	-0.000192000
6	2.006136000	3.189762000	-0.000077000
1	-2.539168000	4.058094000	0.001010000
6	-0.060215000	5.118635000	-0.000343000
6	2.297789000	4.574140000	-0.000262000
6	1.275413000	5.524595000	-0.000421000
1	-0.843373000	5.865996000	-0.000223000
1	3.329350000	4.902348000	-0.000079000
16	7.657152000	-5.631512000	0.000696000
16	6.163251000	-7.240153000	0.000718000
7	6.506488000	-4.463667000	0.000031000
7	4.913197000	-6.178693000	0.000038000
6	5.235014000	-4.879992000	-0.000360000
16	-8.711131000	-3.810089000	0.000687000
16	-9.351879000	-1.710355000	0.000812000
7	-7.122898000	-3.401644000	0.000086000
7	-7.806450000	-1.162827000	0.000210000
6	-6.844709000	-2.092956000	-0.000163000
16	1.054097000	9.447388000	0.000815000
16	3.193601000	8.953248000	0.000701000
7	0.615142000	7.867655000	0.000098000
7	2.895861000	7.340881000	0.000011000
6	1.609692000	6.972660000	-0.000342000

1a ($n = 5$), $\omega_1 = 13 \text{ cm}^{-1}$

6	-4.251334000	-2.465325000	-0.000436000
6	-3.570738000	-1.233180000	-0.000594000
6	-3.562753000	-3.696670000	-0.000177000
6	-2.132175000	-1.231805000	0.003338000
6	-2.133150000	-3.694671000	0.000961000
6	-1.421591000	-2.462094000	-0.002785000
1	-5.336288000	-2.469139000	-0.001734000
6	-4.253338000	0.000032000	-0.000648000
6	-0.000729000	-2.462347000	0.003375000
1	-5.338439000	-0.000026000	-0.002489000
6	0.712037000	-1.233353000	-0.004461000
6	0.000000000	0.000000000	0.006327000
6	-1.424133000	0.000034000	-0.004461000
6	-2.132091000	1.231805000	0.003375000
6	2.132862000	-1.230616000	0.003338000
6	-3.570680000	1.233214000	-0.000514000
6	-4.251198000	2.465325000	-0.000262000
1	-5.336159000	2.468933000	-0.001369000
6	-1.421440000	2.462181000	-0.002785000

6	-0.000687000	2.462420000	0.003338000
6	0.712096000	1.233318000	-0.004461000
6	0.717403000	3.708940000	-0.000594000
6	2.126697000	3.683482000	-0.000648000
6	2.853335000	2.475693000	-0.000514000
6	2.132820000	1.230542000	0.003375000
6	-2.133104000	3.694698000	0.000961000
6	-0.009367000	4.914425000	-0.000436000
1	2.669197000	4.623237000	-0.002489000
6	4.260632000	2.448983000	-0.000262000
6	2.843031000	-0.000087000	-0.002785000
6	4.266254000	-0.000026000	0.000961000
6	4.982713000	1.237058000	-0.000078000
1	4.806238000	3.386783000	-0.001369000
6	-1.420034000	4.933770000	-0.000177000
6	-3.562680000	3.696628000	-0.000078000
1	0.529806000	5.855930000	-0.001734000
6	-2.150698000	6.144917000	-0.000074000
6	-4.246127000	4.934726000	0.000088000
6	-3.546600000	6.142603000	0.000174000
1	-1.620092000	7.088466000	-0.000182000
1	-5.328632000	4.947100000	0.000100000
16	-6.381254000	-8.862309000	-0.001360000
16	-4.479390000	-9.958804000	0.001517000
7	-5.626425000	-7.406947000	-0.001443000
7	-3.598234000	-8.575933000	0.001748000
6	-4.288638000	-7.429914000	0.000154000
16	10.865612000	-1.095173000	-0.001360000
16	10.864273000	1.100136000	0.001517000
7	9.227816000	-1.169153000	-0.001443000
7	9.226093000	1.171805000	0.001748000
6	8.578813000	0.000887000	0.000154000
16	-4.484358000	9.957482000	-0.001360000
16	-6.384882000	8.858668000	0.001517000
7	-3.601392000	8.576100000	-0.001443000
7	-5.627859000	7.404129000	0.001748000
6	-4.290175000	7.429026000	0.000154000
6	4.982787000	-1.237100000	-0.000177000
6	4.260701000	-2.449101000	-0.000436000
6	2.853335000	-2.475760000	-0.000594000
6	2.126641000	-3.683515000	-0.000648000
1	4.806481000	-3.386791000	-0.001734000
1	2.669242000	-4.623211000	-0.002489000
6	0.717346000	-3.708907000	-0.000514000
6	-0.009435000	-4.914307000	-0.000262000
1	0.529921000	-5.855716000	-0.001369000
6	-4.246306000	-4.935018000	-0.000074000
6	-1.420033000	-4.933685000	-0.000078000
6	-2.150534000	-6.144617000	0.000088000
6	-3.546350000	-6.142747000	0.000174000
1	-5.328746000	-4.947274000	-0.000182000
1	-1.619998000	-7.088280000	0.000100000
6	6.397003000	-1.209900000	-0.000074000
6	6.396662000	1.209891000	0.000088000
6	7.092950000	0.000144000	0.000174000
1	6.948630000	2.141181000	0.000100000
1	6.948838000	-2.141192000	-0.000182000

1b ($n = 2$), $\omega_1 = 12 \text{ cm}^{-1}$

6	-1.237444000	2.110927000	-0.000422000
6	0.000193000	1.425357000	-0.000430000
6	-2.448110000	1.413928000	-0.000361000
6	0.000000000	0.000000000	-0.000444000
6	-2.446693000	0.016887000	-0.000367000
6	-1.234492000	-0.712511000	-0.000430000
1	-1.245769000	3.193006000	-0.000417000
6	1.237972000	2.110455000	-0.000367000
6	1.234299000	-0.712846000	-0.000430000
6	-1.209394000	-2.127122000	-0.000422000
6	2.446839000	0.016195000	-0.000422000
6	2.448552000	1.413162000	-0.000361000
1	1.247095000	3.192493000	-0.000306000
6	1.208722000	-2.127342000	-0.000367000
1	3.388109000	-0.517635000	-0.000417000
6	-0.000442000	-2.827090000	-0.000361000
1	2.141232000	-2.676262000	-0.000306000
1	-3.388327000	-0.516231000	-0.000306000
1	-2.142340000	-2.675371000	-0.000417000
7	1.159205000	-6.284106000	0.001155000
7	1.185846000	-4.925174000	0.001077000
6	0.002237000	-7.054094000	-0.000349000
6	0.000000000	-4.317923000	-0.000224000
7	-1.155960000	-6.285818000	-0.001231000
7	-1.185019000	-4.926776000	-0.001303000
8	0.003218000	-8.272015000	0.000667000
6	2.467780000	-6.929600000	0.003308000
1	3.023264000	-6.621798000	-0.884538000
1	3.019332000	-6.624370000	0.894519000
1	2.320861000	-8.005765000	0.001506000
6	-2.463278000	-6.933987000	-0.002148000
1	-3.018663000	-6.627506000	0.886228000
1	-3.016320000	-6.630063000	-0.892885000
1	-2.313874000	-8.009812000	-0.000480000
7	-6.021798000	2.138153000	0.001155000
7	-4.858249000	1.435614000	0.001077000
6	-6.110143000	3.525110000	-0.000349000
6	-3.739431000	2.158961000	-0.000224000
7	-4.865699000	4.143999000	-0.001231000
7	-3.674204000	3.489645000	-0.001303000
8	-7.165384000	4.133221000	0.000667000
6	-7.235100000	1.327640000	0.003308000
1	-7.246277000	0.692676000	-0.884538000
1	-7.246538000	0.697367000	0.894519000
1	-8.093627000	1.992958000	0.001506000
6	-4.773370000	5.600255000	-0.002148000
1	-4.230257000	5.927992000	0.886228000
1	-4.233643000	5.927241000	-0.892885000
1	-5.779764000	6.008780000	-0.000480000
7	4.862593000	4.145954000	0.001155000
7	3.672403000	3.489560000	0.001077000
6	6.107906000	3.528984000	-0.000349000
6	3.739431000	2.158961000	-0.000224000
7	6.021658000	2.141819000	-0.001231000
7	4.859223000	1.437131000	-0.001303000

8	7.162166000	4.138794000	0.000667000
6	4.767320000	5.601960000	0.003308000
1	4.223013000	5.929122000	-0.884538000
1	4.227207000	5.927003000	0.894519000
1	5.772766000	6.012808000	0.001506000
6	7.236648000	1.333732000	-0.002148000
1	7.248920000	0.699514000	0.886228000
1	7.249962000	0.702822000	-0.892885000
1	8.093638000	2.001033000	-0.000480000

1b ($n = 3$), $\omega_1 = 15 \text{ cm}^{-1}$

6	-2.638864000	2.668568000	-0.000840000
6	-2.046280000	1.382256000	-0.000471000
6	-2.818452000	0.202826000	-0.000280000
6	-0.620086000	1.278047000	-0.000360000
6	-2.223133000	-1.074933000	0.000028000
6	-0.796737000	-1.176180000	0.000176000
6	0.000117000	-0.000026000	0.000005000
6	-0.173814000	-2.463308000	0.000487000
6	-0.991700000	-3.619652000	0.000668000
6	-2.384980000	-3.520212000	0.000520000
6	-2.993873000	-2.263152000	0.000197000
1	-0.528528000	-4.597668000	0.000915000
6	-1.856159000	3.825533000	-0.001227000
6	-0.463045000	3.724288000	-0.001138000
6	0.180759000	2.462765000	-0.000624000
1	0.135434000	4.625862000	-0.001426000
6	1.585054000	2.339328000	-0.000319000
6	2.220437000	1.080957000	0.000134000
6	1.417089000	-0.102064000	0.000186000
1	2.193595000	3.237624000	-0.000436000
6	1.233691000	-2.542306000	0.000585000
6	2.042726000	-1.387862000	0.000415000
1	-4.073875000	-2.195481000	0.000079000
1	-3.900686000	0.280567000	-0.000372000
6	3.630783000	0.950865000	0.000441000
1	4.245990000	1.841105000	0.000480000
1	1.707354000	-3.518484000	0.000776000
1	-3.717449000	2.756138000	-0.000895000
6	3.457136000	-1.461188000	0.000529000
6	4.241407000	-0.305371000	0.000590000
1	3.938571000	-2.430320000	0.000636000
7	7.607372000	-1.708813000	-0.004720000
7	6.249927000	-1.638731000	-0.006168000
6	8.458025000	-0.609560000	0.001221000
6	5.728722000	-0.412690000	0.000805000
7	7.773965000	0.600389000	0.007069000
7	6.420523000	0.725835000	0.008016000
8	9.672731000	-0.697251000	0.001236000
6	8.158815000	-3.059820000	-0.013818000
1	7.802792000	-3.600092000	0.865263000
1	7.825642000	-3.580507000	-0.913667000
1	9.242609000	-2.989354000	0.000292000
6	8.513557000	1.858285000	0.016077000
1	8.239725000	2.443513000	-0.863684000
1	8.257509000	2.422016000	0.915235000
1	9.576018000	1.632973000	0.003269000

7	-2.323772000	7.442122000	-0.007128000
7	-1.705766000	6.231549000	-0.007324000
6	-3.701086000	7.629129000	-0.001389000
6	-2.507008000	5.167177000	-0.001758000
7	-4.407032000	6.431774000	0.002130000
7	-3.838955000	5.196949000	0.003383000
8	-4.232493000	8.724924000	-0.000181000
6	-1.429473000	8.595198000	-0.012468000
1	-0.795173000	8.564396000	0.875444000
1	-0.800059000	8.559602000	-0.903642000
1	-2.032660000	9.498475000	-0.013150000
6	-5.866189000	6.443329000	0.010016000
1	-6.235161000	5.910764000	-0.868420000
1	-6.227297000	5.942493000	0.910396000
1	-6.202378000	7.476045000	-0.006202000
7	-5.283697000	-5.733029000	0.000006000
7	-4.544042000	-4.592705000	-0.000002000
6	-4.757162000	-7.019363000	0.000414000
6	-3.221637000	-4.754622000	0.000703000
7	-3.367220000	-7.032273000	0.002005000
7	-2.581597000	-5.923056000	0.001585000
8	-5.440612000	-8.027363000	-0.000295000
6	-6.729374000	-5.534731000	-0.001364000
1	-7.016894000	-4.969184000	0.886961000
1	-7.015897000	-4.972533000	-0.892162000
1	-7.210384000	-6.508593000	0.000122000
6	-2.648056000	-8.301987000	0.001925000
1	-2.023389000	-8.363496000	-0.891254000
1	-2.012738000	-8.356476000	0.887884000
1	-3.374889000	-9.109083000	0.009117000

1b ($n = 4$), $\omega_1 = 13 \text{ cm}^{-1}$

6	5.035545000	0.930598000	0.000182000
6	3.755502000	0.326800000	0.000412000
6	5.180517000	2.319853000	-0.000387000
6	2.595955000	1.162317000	0.000129000
6	4.047454000	3.136590000	-0.000798000
6	2.744773000	2.583557000	-0.000522000
1	5.917920000	0.304204000	0.000256000
6	3.591015000	-1.074226000	0.001015000
6	1.590161000	3.394238000	-0.000960000
1	4.472116000	-1.707539000	0.001267000
1	4.167595000	4.212029000	-0.001277000
1	1.704904000	4.473232000	-0.001439000
6	0.293012000	2.843772000	-0.000819000
6	0.145537000	1.412698000	-0.000099000
6	1.296987000	0.580665000	0.000156000
6	1.150704000	-0.832224000	0.000850000
6	-0.864929000	3.646980000	-0.001230000
6	2.316446000	-1.675414000	0.001092000
6	2.144496000	-3.073929000	0.001497000
1	3.021757000	-3.712496000	0.001773000
1	-0.757032000	4.726699000	-0.001678000
6	-0.145759000	-1.413235000	0.000982000
6	-1.296563000	-0.580501000	0.000642000
6	-1.151366000	0.832901000	0.000116000
6	-2.609834000	-1.168149000	0.000761000

6	-3.735032000	-0.320115000	0.000430000
6	-3.609985000	1.085099000	-0.000076000
6	-2.304599000	1.666612000	-0.000335000
6	-0.291627000	-2.828855000	0.001320000
6	-2.726595000	-2.572501000	0.001197000
1	-4.726928000	-0.760071000	0.000525000
6	-4.740363000	1.936575000	-0.000485000
6	-2.160426000	3.088752000	-0.001023000
6	-3.323425000	3.895170000	-0.001418000
6	-4.599159000	3.326004000	-0.001040000
1	-5.731707000	1.502584000	-0.000442000
1	-3.222227000	4.972573000	-0.001909000
6	-1.595107000	-3.415280000	0.001492000
6	0.865109000	-3.668289000	0.001553000
1	-3.715529000	-3.019108000	0.001225000
6	-1.712611000	-4.825511000	0.001623000
6	0.692321000	-5.072967000	0.001857000
6	-0.581443000	-5.645388000	0.001702000
1	-2.696420000	-5.276291000	0.001596000
1	1.563659000	-5.714773000	0.001994000
7	-2.086086000	-8.966889000	-0.000422000
7	-1.975131000	-7.612232000	0.000542000
6	-1.012805000	-9.850340000	0.000518000
6	-0.733656000	-7.128620000	0.001836000
7	0.217157000	-9.203569000	0.001208000
7	0.383538000	-7.854201000	0.002086000
8	-1.137670000	-11.061749000	0.000631000
6	-3.453057000	-9.477857000	-0.000694000
1	-3.971367000	-9.123131000	0.892085000
1	-3.974255000	-9.112136000	-0.887315000
1	-3.414474000	-10.563331000	-0.007480000
6	1.452323000	-9.980780000	0.002396000
1	2.037630000	-9.728938000	-0.883897000
1	2.031453000	-9.737280000	0.895147000
1	1.195000000	-11.035998000	-0.003242000
7	8.809503000	2.676567000	-0.004531000
7	7.580486000	2.096083000	-0.005615000
6	9.038706000	4.047522000	0.001105000
6	6.541375000	2.929224000	-0.000768000
7	7.863200000	4.789865000	0.004782000
7	6.611643000	4.259870000	0.004564000
8	10.150131000	4.545009000	-0.000195000
6	9.934225000	1.747097000	-0.011651000
1	9.881092000	1.109762000	0.872994000
1	9.882143000	1.123627000	-0.906221000
1	10.856014000	2.321661000	-0.006612000
6	7.918806000	6.247859000	0.010031000
1	7.405916000	6.631592000	-0.873884000
1	7.420361000	6.625356000	0.904961000
1	8.961149000	6.553010000	0.003030000
7	-6.723135000	6.290002000	0.000651000
7	-5.605522000	5.516370000	0.000010000
6	-8.024992000	5.802454000	-0.001291000
6	-5.807359000	4.199579000	-0.001525000
7	-8.079763000	4.413636000	-0.002438000
7	-6.994534000	3.594939000	-0.002546000
8	-9.011746000	6.516022000	-0.002402000

6	-6.481889000	7.728987000	0.001293000
1	-5.904333000	7.997472000	0.887782000
1	-5.915164000	8.001021000	-0.891241000
1	-7.441052000	8.238619000	0.007659000
6	-9.370503000	3.733194000	-0.004733000
1	-9.448437000	3.109306000	-0.897122000
1	-9.446937000	3.101482000	0.882185000
1	-10.155393000	4.484025000	-0.000992000

1b ($n = 5$), $\omega_1 = 15 \text{ cm}^{-1}$

6	2.449853000	4.260321000	-0.001514000
6	1.219846000	3.575553000	-0.001050000
6	3.684305000	3.576589000	-0.001906000
6	1.223666000	2.137015000	-0.005414000
6	3.686481000	2.147455000	-0.002274000
6	2.456708000	1.431112000	0.001254000
1	2.449440000	5.345413000	-0.000431000
6	-0.016349000	4.253329000	-0.000357000
6	2.462400000	0.010432000	-0.004755000
1	-0.020464000	5.338530000	0.002129000
6	1.236184000	-0.707132000	0.002250000
6	0.000052000	0.000270000	-0.009488000
6	-0.005415000	1.424374000	0.001938000
6	-1.239976000	2.127590000	-0.005727000
6	1.238784000	-2.127799000	-0.005427000
6	-1.247275000	3.566113000	-0.000356000
6	-2.482557000	4.241429000	0.000913000
1	-2.490385000	5.326488000	0.003502000
6	-2.467515000	1.412262000	-0.000177000
6	-2.462307000	-0.008409000	-0.007996000
6	-1.230587000	-0.716577000	0.000071000
6	-3.706283000	-0.731016000	-0.005193000
6	-3.675170000	-2.140372000	-0.006954000
6	-2.464531000	-2.862796000	-0.006633000
6	-1.222285000	-2.137216000	-0.008708000
6	-3.702804000	2.119161000	-0.002748000
6	-4.914334000	-0.008168000	-0.004478000
1	-4.612899000	-2.686599000	-0.006364000
6	-2.431743000	-4.270137000	-0.007989000
6	0.010989000	-2.842708000	-0.000818000
6	0.016459000	-4.265826000	-0.004339000
6	-1.216841000	-4.988050000	-0.006319000
1	-3.367489000	-4.819517000	-0.008747000
6	-4.939413000	1.402661000	-0.002407000
6	-3.711710000	3.548260000	0.000622000
1	-5.853818000	-0.551127000	-0.004047000
6	-6.153450000	2.128975000	-0.000515000
6	-4.953133000	4.226825000	0.002780000
6	-6.161152000	3.525647000	0.002375000
1	-7.093080000	1.592160000	-0.000741000
1	-4.966706000	5.308890000	0.005135000
6	1.255305000	-4.978590000	0.000331000
6	2.464618000	-4.251412000	0.002032000
6	2.486583000	-2.843866000	0.000794000
6	3.691615000	-2.112216000	0.001584000
1	3.404624000	-4.793402000	0.005514000
1	4.633567000	-2.651062000	0.004839000

6	3.711917000	-0.702650000	0.000576000
6	4.914356000	0.029430000	0.000704000
1	5.858049000	-0.506119000	0.002779000
6	4.920382000	4.264713000	-0.002842000
6	4.928614000	1.440438000	-0.000425000
6	6.136976000	2.176110000	-0.001001000
6	6.133727000	3.572840000	-0.002588000
1	4.925819000	5.346873000	-0.003606000
1	7.080914000	1.646914000	-0.000245000
6	1.233281000	-6.393072000	0.001801000
6	-1.183803000	-6.402331000	-0.006435000
6	0.027442000	-7.097915000	-0.001817000
1	-2.114005000	-6.955325000	-0.009158000
1	2.167927000	-6.938529000	0.005718000
7	1.197012000	-10.550790000	0.068090000
7	1.219232000	-9.191755000	0.068478000
6	0.044111000	-11.324687000	0.004786000
6	0.033220000	-8.588716000	0.000198000
7	-1.114978000	-10.560155000	-0.059832000
7	-1.148021000	-9.201353000	-0.066010000
8	0.048999000	-12.542476000	0.006530000
6	2.505233000	-11.192787000	0.144063000
1	3.106589000	-10.890586000	-0.715444000
1	3.007961000	-10.879453000	1.060927000
1	2.360874000	-12.269306000	0.142432000
6	-2.417914000	-11.212849000	-0.135463000
1	-3.026733000	-10.902034000	0.715550000
1	-2.917167000	-10.917156000	-1.060176000
1	-2.265782000	-12.288145000	-0.117243000
7	9.704217000	4.312405000	0.007129000
7	8.543765000	3.604740000	0.009964000
6	9.786513000	5.699841000	-0.007115000
6	7.421960000	4.323281000	-0.004004000
7	8.539242000	6.313308000	-0.020523000
7	7.350812000	5.653559000	-0.019645000
8	10.839003000	6.312496000	-0.007984000
6	10.921749000	3.508231000	0.023990000
1	10.937461000	2.894480000	0.926683000
1	10.935929000	2.857366000	-0.852142000
1	11.776628000	4.178089000	0.009773000
6	8.440786000	7.769127000	-0.037546000
1	7.901588000	8.083905000	-0.932979000
1	7.894564000	8.104458000	0.846116000
1	9.445377000	8.182122000	-0.038239000
7	-8.588538000	6.246694000	0.022664000
7	-7.394921000	5.596534000	0.019964000
6	-9.830938000	5.623322000	0.013904000
6	-7.455418000	4.265733000	0.005748000
7	-9.737549000	4.236607000	-0.001255000
7	-8.571491000	3.538284000	-0.005490000
8	-10.888186000	6.227651000	0.018745000
6	-8.501692000	7.703278000	0.040661000
1	-7.974555000	8.023055000	0.941591000
1	-7.948580000	8.042035000	-0.837257000
1	-9.509429000	8.108359000	0.030790000
6	-10.948223000	3.421985000	-0.012756000
1	-10.953525000	2.796485000	-0.907359000

1	-10.961339000	2.782152000	0.871634000
1	-11.809151000	4.084220000	-0.011017000

1c (n = 2), $\omega_1 = 10 \text{ cm}^{-1}$

6	-0.490261000	2.398530000	-0.006385000
6	-0.949387000	1.060837000	0.000793000
6	0.882783000	2.687597000	0.000062000
6	-0.000313000	-0.000202000	0.001377000
6	1.816819000	1.640540000	0.006690000
6	1.393092000	0.291214000	0.000707000
1	-1.209574000	3.203285000	-0.029700000
6	-2.329837000	0.753049000	0.007308000
6	-0.444606000	-1.352637000	0.002477000
6	2.322045000	-0.775251000	-0.006028000
6	-1.832648000	-1.623896000	-0.004011000
6	-2.769476000	-0.579372000	0.001358000
1	-3.049795000	1.557284000	0.029692000
6	0.512109000	-2.394224000	0.009570000
1	-2.169839000	-2.649257000	-0.026530000
6	1.885859000	-2.108800000	0.001826000
1	0.175547000	-3.419774000	0.033285000
1	2.873278000	1.861838000	0.029352000
1	3.378653000	-0.554665000	-0.030136000
6	-4.205823000	-0.879760000	0.000588000
7	-4.770438000	-2.043771000	-0.414148000
8	-4.174354000	-3.069365000	-0.875041000
6	-6.277307000	-1.945687000	-0.475510000
6	-6.531586000	-0.732878000	0.473344000
7	-5.189960000	-0.039428000	0.414112000
8	-5.055009000	1.139110000	0.874984000
6	-6.624693000	-1.676323000	-1.950039000
1	-6.187071000	-0.742477000	-2.308107000
1	-7.706417000	-1.631261000	-2.090321000
1	-6.229713000	-2.493527000	-2.555609000
6	-6.895348000	-3.269518000	-0.030699000
1	-6.592882000	-4.057409000	-0.720386000
1	-7.985404000	-3.192760000	-0.046384000
1	-6.578961000	-3.560182000	0.970342000
6	-7.627563000	0.232468000	0.027035000
1	-8.595614000	-0.274485000	0.041684000
1	-7.452882000	0.625226000	-0.973893000
1	-7.666902000	1.075767000	0.716418000
6	-6.744300000	-1.119441000	1.947318000
1	-5.969264000	-1.799178000	2.306549000
1	-7.717199000	-1.595035000	2.085525000
1	-6.711721000	-0.212646000	2.553285000
6	2.864301000	-3.202288000	0.001071000
7	4.153703000	-3.109395000	-0.416606000
8	4.742094000	-2.080794000	-0.880678000
6	4.822326000	-4.463464000	-0.477580000
6	3.902334000	-5.288140000	0.475939000
7	2.630276000	-4.474023000	0.417878000
8	1.543697000	-4.946164000	0.882676000
6	4.757858000	-4.902211000	-1.950901000
1	3.729152000	-4.990220000	-2.305578000
1	5.258559000	-5.862238000	-2.090380000
1	5.266749000	-4.153294000	-2.559738000

6	6.279269000	-4.335771000	-0.037810000
1	6.807996000	-3.680989000	-0.730364000
1	6.757880000	-5.318133000	-0.053437000
1	6.376092000	-3.914766000	0.962213000
6	3.613921000	-6.721426000	0.034455000
1	4.537457000	-7.305597000	0.047825000
1	3.183311000	-6.769657000	-0.964993000
1	2.905796000	-7.175695000	0.727371000
6	4.347618000	-5.274812000	1.948648000
1	4.549541000	-4.262701000	2.304521000
1	5.246485000	-5.878960000	2.086002000
1	3.547806000	-5.698538000	2.557981000
6	1.340937000	4.081579000	0.000002000
7	2.561412000	4.513129000	0.412328000
8	3.515338000	3.806508000	0.870946000
6	2.632009000	6.021579000	0.473238000
6	1.453162000	6.409260000	-0.473102000
7	0.614693000	5.153239000	-0.412267000
8	-0.572233000	5.150489000	-0.871405000
6	2.406192000	6.397376000	1.948070000
1	1.429995000	6.067021000	2.308189000
1	2.482626000	7.477406000	2.087692000
1	3.175351000	5.913762000	2.552254000
6	4.015453000	6.488158000	0.025189000
1	4.766372000	6.099915000	0.713165000
1	4.060645000	7.579978000	0.040544000
1	4.266694000	6.141222000	-0.976397000
6	0.616740000	7.605947000	-0.025041000
1	1.228595000	8.511351000	-0.039966000
1	0.208192000	7.475704000	0.976355000
1	-0.217762000	7.739511000	-0.713285000
6	1.857913000	6.577653000	-1.947962000
1	2.447216000	5.732223000	-2.308202000
1	2.437630000	7.492113000	-2.087703000
1	0.951765000	6.645188000	-2.552015000

1c ($n = 3$), $\omega_1 = 12 \text{ cm}^{-1}$

6	2.094555000	3.115314000	0.009209000
6	1.748317000	1.742409000	0.004050000
6	2.729231000	0.729424000	0.006880000
6	0.368326000	1.372424000	-0.000817000
6	2.383431000	-0.637642000	0.003465000
6	1.002544000	-1.003734000	-0.001799000
6	-0.000447000	0.001263000	-0.002907000
6	0.633707000	-2.383887000	-0.005934000
6	1.649248000	-3.370428000	-0.001113000
6	3.006420000	-3.011617000	0.000411000
6	3.367937000	-1.655168000	0.000845000
1	1.370520000	-4.412994000	0.015305000
6	1.104825000	4.110467000	-0.001660000
6	-0.250641000	3.746369000	-0.010358000
6	-0.639544000	2.385021000	-0.004024000
1	-1.011559000	4.511465000	-0.036839000
6	-1.996331000	2.001135000	-0.005077000
6	-2.382918000	0.645129000	-0.005079000
6	-1.372343000	-0.364775000	-0.006090000
1	-2.762554000	2.768873000	-0.005897000

6	-0.734049000	-2.726960000	-0.010476000
6	-1.745075000	-1.744029000	-0.009856000
1	4.411079000	-1.378553000	-0.014709000
1	3.777233000	1.009139000	0.011024000
6	-3.745057000	0.258947000	0.000209000
1	-4.508641000	1.021435000	0.025028000
1	-1.015861000	-3.774406000	-0.013711000
1	3.136482000	3.396174000	0.035181000
6	-3.118672000	-2.087517000	-0.016145000
6	-4.111846000	-1.095779000	-0.007407000
1	-3.401603000	-3.128909000	-0.041263000
6	-5.530318000	-1.474540000	-0.004135000
7	-6.563350000	-0.676169000	0.373880000
8	-6.500542000	0.526136000	0.787026000
6	-7.863174000	-1.442042000	0.459108000
6	-7.538385000	-2.670563000	-0.446077000
7	-6.028800000	-2.683013000	-0.375984000
8	-5.376871000	-3.693581000	-0.792962000
6	-8.055580000	-1.787994000	1.945894000
1	-7.242853000	-2.408158000	2.328769000
1	-8.999345000	-2.314366000	2.100628000
1	-8.077215000	-0.859953000	2.519220000
6	-9.012304000	-0.557613000	-0.020207000
1	-9.100692000	0.305449000	0.639432000
1	-9.949709000	-1.118469000	0.013141000
1	-8.859621000	-0.190813000	-1.034454000
6	-8.086475000	-4.009616000	0.042609000
1	-9.178971000	-3.990618000	0.022120000
1	-7.759191000	-4.247582000	1.053895000
1	-7.740725000	-4.803905000	-0.618697000
6	-7.893161000	-2.471669000	-1.930066000
1	-7.509257000	-1.526531000	-2.318685000
1	-8.975023000	-2.494519000	-2.074238000
1	-7.448638000	-3.284662000	-2.506179000
6	1.486416000	5.528165000	-0.005958000
7	2.695664000	6.024627000	0.366132000
8	3.704790000	5.371113000	0.784116000
6	2.686018000	7.534292000	0.435158000
6	1.458569000	7.860770000	-0.470872000
7	0.690225000	6.562437000	-0.385177000
8	-0.511962000	6.501598000	-0.798991000
6	2.487016000	7.890437000	1.918794000
1	1.540888000	7.508690000	2.307129000
1	2.511960000	8.972344000	2.062272000
1	3.298792000	7.444667000	2.495661000
6	4.026366000	8.079559000	-0.053162000
1	4.819649000	7.732780000	0.608817000
1	4.009335000	9.172102000	-0.033369000
1	4.264294000	7.751185000	-1.064101000
6	0.576010000	9.011857000	0.007220000
1	1.138522000	9.948242000	-0.026801000
1	0.208654000	8.860698000	1.021493000
1	-0.286697000	9.101135000	-0.652764000
6	1.805669000	8.051565000	-1.957584000
1	2.424413000	7.237364000	-2.339626000
1	2.334025000	8.994170000	-2.112586000
1	0.877996000	8.074714000	-2.531450000

6	4.043650000	-4.050909000	0.001501000
7	5.346612000	-3.871899000	-0.342443000
8	5.905244000	-2.794097000	-0.724933000
6	6.090827000	-5.184439000	-0.430557000
6	5.172801000	-6.099837000	0.436738000
7	3.861785000	-5.353175000	0.346605000
8	2.782566000	-5.909319000	0.728749000
6	6.121628000	-5.555623000	-1.923425000
1	5.117703000	-5.683383000	-2.332814000
1	6.682496000	-6.478989000	-2.080213000
1	6.615346000	-4.752163000	-2.472146000
6	7.515745000	-5.001444000	0.087515000
1	8.039713000	-4.285750000	-0.545766000
1	8.047652000	-5.955314000	0.048943000
1	7.541078000	-4.626813000	1.110012000
6	4.987559000	-7.524919000	-0.080091000
1	5.940418000	-8.058532000	-0.040192000
1	4.613761000	-7.550553000	-1.102881000
1	4.270350000	-8.046924000	0.553095000
6	5.542474000	-6.129880000	1.929993000
1	5.671833000	-5.125801000	2.338498000
1	6.464566000	-6.692432000	2.088244000
1	4.737496000	-6.621439000	2.478430000

1c ($n = 4$), $\omega_1 = 12 \text{ cm}^{-1}$

6	-4.392754000	-2.631550000	-0.020957000
6	-3.035475000	-2.233253000	-0.013006000
6	-5.425140000	-1.680979000	-0.008757000
6	-2.716721000	-0.841451000	-0.004547000
6	-5.111423000	-0.313010000	0.003877000
6	-3.766732000	0.126001000	-0.001376000
1	-4.633413000	-3.683452000	-0.050234000
6	-1.987283000	-3.178594000	-0.016245000
6	-3.436859000	1.498508000	0.003111000
1	-2.232429000	-4.235351000	-0.025601000
1	-5.904677000	0.418564000	0.031850000
1	-4.236548000	2.231599000	0.006507000
6	-2.099589000	1.942378000	0.002799000
6	-1.043419000	0.964763000	0.006457000
6	-1.357496000	-0.420313000	-0.006971000
6	-0.315222000	-1.384965000	0.000225000
6	-1.760383000	3.310041000	0.004446000
6	-0.633269000	-2.788623000	-0.011368000
6	0.420001000	-3.724684000	-0.011662000
1	0.185418000	-4.783869000	-0.015961000
1	-2.552722000	4.051058000	0.000983000
6	1.041166000	-0.964491000	-0.003861000
6	1.355457000	0.420463000	0.009327000
6	0.313078000	1.384877000	0.000227000
6	2.730084000	0.846414000	0.008383000
6	3.014114000	2.226650000	0.010439000
6	1.990359000	3.198593000	0.008013000
6	0.627863000	2.772717000	0.007324000
6	2.085610000	-1.930945000	0.001721000
6	3.744806000	-0.131228000	0.010682000
1	4.048732000	2.553081000	0.013471000
6	2.282495000	4.582751000	0.011858000

6	-0.417537000	3.744816000	0.005029000
6	-0.084476000	5.119569000	-0.000853000
6	1.254993000	5.539568000	0.004057000
1	3.312623000	4.904184000	0.033003000
1	-0.875715000	5.853175000	-0.023547000
6	3.450092000	-1.511738000	0.007012000
6	1.773571000	-3.324043000	-0.005682000
1	4.782657000	0.184752000	0.011149000
6	4.474134000	-2.487482000	0.004656000
6	2.826118000	-4.269147000	-0.000348000
6	4.168591000	-3.857796000	0.002827000
1	5.505240000	-2.168917000	-0.008888000
1	2.589076000	-5.321934000	0.014160000
6	-6.826943000	-2.116315000	-0.007765000
7	-7.890361000	-1.362222000	0.376366000
8	-7.874272000	-0.161248000	0.797836000
6	-9.158476000	-2.180080000	0.457005000
6	-8.786548000	-3.385959000	-0.460371000
7	-7.277504000	-3.340801000	-0.388354000
8	-6.585989000	-4.322175000	-0.811352000
6	-9.333568000	-2.548570000	1.940402000
1	-8.495197000	-3.138322000	2.315953000
1	-10.254208000	-3.115625000	2.090539000
1	-9.393167000	-1.628509000	2.523837000
6	-10.343020000	-1.337143000	-0.010821000
1	-10.460145000	-0.482442000	0.655178000
1	-11.258245000	-1.933361000	0.024091000
1	-10.210043000	-0.958165000	-1.023365000
6	-9.283282000	-4.750218000	0.013427000
1	-10.375716000	-4.772657000	-0.007836000
1	-8.947411000	-4.986647000	1.022259000
1	-8.907429000	-5.523564000	-0.656276000
6	-9.147682000	-3.184796000	-1.942472000
1	-8.799137000	-2.221856000	-2.320600000
1	-10.227900000	-3.246191000	-2.087753000
1	-8.673032000	-3.974420000	-2.527012000
6	5.246912000	-4.854199000	0.004365000
7	5.113967000	-6.167969000	0.328579000
8	4.053213000	-6.774065000	0.685832000
6	6.453265000	-6.861234000	0.428156000
6	7.342940000	-5.899087000	-0.417017000
7	6.546555000	-4.618484000	-0.318700000
8	7.067791000	-3.513865000	-0.676977000
6	6.805316000	-6.891600000	1.925749000
1	6.888494000	-5.887333000	2.345716000
1	7.747743000	-7.417362000	2.090544000
1	6.014586000	-7.421473000	2.459044000
6	6.334336000	-8.287010000	-0.105662000
1	5.632803000	-8.845912000	0.513455000
1	7.308276000	-8.780674000	-0.059868000
1	5.973639000	-8.317385000	-1.133024000
6	8.754619000	-5.668016000	0.118074000
1	9.321633000	-6.601318000	0.077191000
1	8.755376000	-5.302189000	1.144107000
1	9.258795000	-4.927775000	-0.502907000
6	7.402363000	-6.248408000	-1.914250000
1	6.408262000	-6.412319000	-2.334552000

1	8.002838000	-7.145324000	-2.077727000
1	7.866906000	-5.417862000	-2.447916000
6	1.578998000	6.971522000	-0.001600000
7	0.730351000	7.976557000	-0.345805000
8	-0.482555000	7.872962000	-0.717818000
6	1.444418000	9.304485000	-0.448559000
6	2.710203000	9.022475000	0.417199000
7	2.779101000	7.515025000	0.334330000
8	3.828309000	6.901332000	0.712236000
6	1.737413000	9.513610000	-1.944642000
1	2.380583000	8.729045000	-2.347806000
1	2.217120000	10.479640000	-2.113234000
1	0.792472000	9.495593000	-2.489763000
6	0.533630000	10.418898000	0.062212000
1	-0.348443000	10.483756000	-0.574588000
1	1.061951000	11.374817000	0.023211000
1	0.198056000	10.245976000	1.084018000
6	4.011953000	9.625816000	-0.105579000
1	3.952487000	10.716587000	-0.073815000
1	4.232294000	9.316801000	-1.126588000
1	4.838082000	9.304798000	0.528612000
6	2.540344000	9.358986000	1.909087000
1	1.622502000	8.935411000	2.321287000
1	2.524565000	10.439902000	2.061077000
1	3.386323000	8.943350000	2.458634000

1c ($n = 5$), $\omega_1 = 11 \text{ cm}^{-1}$

6	-1.238331000	-4.756323000	0.013616000
6	-0.232374000	-3.771708000	0.010994000
6	-2.609828000	-4.420685000	0.008524000
6	-0.615258000	-2.384750000	0.000528000
6	-2.987129000	-3.044014000	-0.000602000
6	-1.990265000	-2.028601000	0.002624000
1	-0.953726000	-5.803215000	0.018168000
6	1.139156000	-4.099044000	0.012646000
6	-2.371551000	-0.660449000	-0.009660000
1	1.429614000	-5.144564000	0.018655000
6	-1.378379000	0.355154000	-0.001055000
6	0.000745000	-0.000733000	-0.008538000
6	0.381870000	-1.372995000	0.006496000
6	1.758079000	-1.725305000	0.000373000
6	-1.755884000	1.724580000	-0.011512000
6	2.145196000	-3.111086000	0.008981000
6	3.514962000	-3.435580000	0.010135000
1	3.811081000	-4.479263000	0.016598000
6	2.752230000	-0.710885000	0.005341000
6	2.373322000	0.657998000	-0.004528000
6	0.998486000	1.015603000	0.001366000
6	3.382810000	1.683303000	-0.001683000
6	2.980794000	3.034734000	-0.004423000
6	1.622173000	3.411866000	-0.005800000
6	0.615713000	2.383572000	-0.009683000
6	4.130142000	-1.066420000	0.002559000
6	4.738481000	1.304591000	-0.001594000
1	3.741038000	3.809034000	-0.003335000
6	1.218593000	4.760348000	-0.006475000
6	-0.759959000	2.737243000	-0.004473000

6	-1.140736000	4.108313000	-0.009522000
6	-0.143994000	5.130251000	-0.007347000
1	1.974428000	5.538616000	-0.002606000
6	5.133387000	-0.050902000	0.001169000
6	4.516783000	-2.440602000	0.006876000
1	5.502770000	2.074558000	-0.004495000
6	6.497192000	-0.424069000	-0.002939000
6	5.891182000	-2.773579000	0.010343000
6	6.878670000	-1.775337000	0.003185000
1	7.253745000	0.345259000	-0.022761000
1	6.181586000	-3.812814000	0.028880000
6	-2.521847000	4.469488000	-0.010074000
6	-3.498277000	3.449661000	-0.011719000
6	-3.148622000	2.086164000	-0.010086000
6	-4.117910000	1.062165000	-0.012391000
1	-4.547197000	3.726648000	-0.014650000
1	-5.168570000	1.333421000	-0.013581000
6	-3.765371000	-0.303053000	-0.010277000
6	-4.731299000	-1.326922000	-0.011838000
1	-5.783206000	-1.061506000	-0.012877000
6	-3.615024000	-5.415194000	0.006255000
6	-4.370494000	-2.691955000	-0.006633000
6	-5.346331000	-3.715227000	-0.003329000
6	-4.976182000	-5.069740000	0.001668000
1	-3.327466000	-6.455266000	-0.004380000
1	-6.391510000	-3.446754000	0.008268000
6	-2.880278000	5.837351000	-0.013786000
6	-0.542277000	6.486980000	-0.001744000
6	-1.900538000	6.843079000	-0.006498000
1	0.212850000	7.257726000	0.019073000
1	-3.924620000	6.108681000	-0.033698000
6	8.301009000	-2.141563000	0.001067000
7	9.334327000	-1.311999000	-0.304347000
8	9.270545000	-0.085151000	-0.637642000
6	10.643012000	-2.059730000	-0.413555000
6	10.314663000	-3.344042000	0.406827000
7	8.806877000	-3.367158000	0.304134000
8	8.159851000	-4.412703000	0.633619000
6	10.864682000	-2.310845000	-1.915372000
1	10.066553000	-2.915776000	-2.349815000
1	11.817692000	-2.815104000	-2.086464000
1	10.883984000	-1.349019000	-2.430184000
6	11.774380000	-1.197250000	0.141064000
1	11.867811000	-0.294549000	-0.462316000
1	12.717047000	-1.747988000	0.092015000
1	11.598247000	-0.894970000	1.172628000
6	10.887834000	-4.644754000	-0.151393000
1	11.979385000	-4.615763000	-0.107285000
1	10.583464000	-4.824925000	-1.181681000
1	10.538155000	-5.481416000	0.453164000
6	10.637465000	-3.231933000	1.907196000
1	10.235862000	-2.315324000	2.343459000
1	11.716398000	-3.253411000	2.072335000
1	10.190440000	-4.082174000	2.424736000
6	-6.005663000	-6.116975000	0.002537000
7	-5.806906000	-7.428584000	-0.297701000
8	-4.714690000	-7.990951000	-0.631111000

6	-7.110460000	-8.184666000	-0.407067000
6	-8.056473000	-7.253221000	0.411875000
7	-7.319958000	-5.938484000	0.303422000
8	-7.899123000	-4.854434000	0.634556000
6	-7.436251000	-8.251712000	-1.909336000
1	-7.559322000	-7.258412000	-2.345168000
1	-8.349780000	-8.824072000	-2.081398000
1	-6.612870000	-8.750740000	-2.422646000
6	-6.933667000	-9.596499000	0.147782000
1	-6.198758000	-10.130696000	-0.454200000
1	-7.883286000	-10.134816000	0.095779000
1	-6.586586000	-9.597606000	1.180263000
6	-9.469880000	-7.096571000	-0.145154000
1	-9.993877000	-8.054410000	-0.097671000
1	-9.474060000	-6.746205000	-1.176561000
1	-10.016653000	-6.371909000	0.457890000
6	-8.120778000	-7.580393000	1.914032000
1	-7.126325000	-7.684061000	2.352153000
1	-8.675707000	-8.504886000	2.084622000
1	-8.636873000	-6.766735000	2.425967000
6	-2.294258000	8.257950000	-0.002274000
7	-1.492115000	9.305088000	0.328528000
8	-0.271531000	9.263078000	0.687333000
6	-2.268168000	10.597515000	0.432973000
6	-3.529365000	10.250196000	-0.416045000
7	-3.523120000	8.741485000	-0.326722000
8	-4.545985000	8.076680000	-0.690281000
6	-2.554350000	10.801583000	1.930916000
1	-3.151655000	9.987737000	2.346400000
1	-3.082199000	11.742437000	2.098283000
1	-1.604271000	10.836566000	2.466221000
6	-1.417031000	11.751057000	-0.093933000
1	-0.527393000	11.854134000	0.527138000
1	-1.985660000	12.683021000	-0.044320000
1	-1.092415000	11.593352000	-1.121745000
6	-4.853087000	10.789744000	0.121342000
1	-4.849560000	11.881938000	0.084679000
1	-5.045113000	10.474676000	1.146230000
1	-5.669754000	10.424394000	-0.501028000
6	-3.395895000	10.588821000	-1.911030000
1	-2.464967000	10.207334000	-2.334794000
1	-3.433645000	11.668658000	-2.066801000
1	-4.228667000	10.131559000	-2.447640000

1d (n = 2), $\omega_1 = 8 \text{ cm}^{-1}$

6	-1.253136000	-2.098122000	-0.000276000
6	-0.005765000	-1.424415000	-0.000273000
6	-2.465177000	-1.407773000	-0.000276000
6	0.000000000	0.000000000	-0.000272000
6	-2.445356000	-0.009534000	-0.000275000
6	-1.230697000	0.717200000	-0.000273000
1	-1.256136000	-3.184005000	-0.000283000
6	1.230934000	-2.112973000	-0.000275000
6	1.236462000	0.707214000	-0.000273000
6	-1.190459000	2.134309000	-0.000276000
6	2.443595000	-0.036187000	-0.000276000
6	2.451756000	-1.431019000	-0.000276000

1	1.212130000	-3.197670000	-0.000273000
6	1.214421000	2.122507000	-0.000275000
1	3.385497000	0.504157000	-0.000283000
6	0.013421000	2.838792000	-0.000276000
1	2.163199000	2.648570000	-0.000273000
1	-3.375328000	0.549100000	-0.000273000
1	-2.129361000	2.679848000	-0.000283000
8	1.123126000	8.370405000	0.000375000
7	0.939710000	7.103684000	0.000234000
6	0.000000000	4.360057000	-0.000219000
1	-1.051571000	4.663236000	-0.000477000
6	0.682315000	4.952099000	-1.242758000
1	0.242852000	4.536454000	-2.154456000
1	1.736303000	4.654042000	-1.239925000
6	0.602616000	6.488253000	-1.330451000
6	0.601937000	6.488055000	1.330654000
6	0.681663000	4.951915000	1.242775000
1	1.735643000	4.653822000	1.240447000
1	0.241709000	4.536139000	2.154176000
6	1.642547000	6.992090000	-2.343410000
1	1.586546000	8.074638000	-2.451009000
1	1.457391000	6.528031000	-3.315886000
1	2.653673000	6.731308000	-2.021670000
6	-0.799847000	6.960277000	-1.767786000
1	-1.593078000	6.551476000	-1.139307000
1	-0.990695000	6.645903000	-2.797499000
1	-0.851761000	8.049385000	-1.722524000
6	-0.800744000	6.960024000	1.767348000
1	-0.852629000	8.049138000	1.722222000
1	-0.992116000	6.645497000	2.796917000
1	-1.593657000	6.551319000	1.138405000
6	1.641359000	6.991731000	2.344217000
1	1.585311000	8.074264000	2.451951000
1	2.652646000	6.730990000	2.022949000
1	1.455708000	6.527526000	3.316529000
8	6.687420000	-5.157858000	0.000375000
7	5.682116000	-4.365655000	0.000234000
6	3.775920000	-2.180028000	-0.000219000
1	4.564266000	-1.420931000	-0.000477000
6	3.947486000	-3.066951000	-1.242758000
1	3.807259000	-2.478543000	-2.154456000
1	3.162367000	-3.830703000	-1.239925000
6	5.317684000	-3.766007000	-1.330451000
6	5.317852000	-3.765321000	1.330654000
6	3.947653000	-3.066295000	1.242775000
1	3.162507000	-3.830022000	1.240447000
1	3.807557000	-2.477396000	2.154176000
6	5.234054000	-4.918532000	-2.343410000
1	6.199569000	-5.411308000	-2.451009000
1	4.924745000	-4.526153000	-3.315886000
1	4.502647000	-5.663803000	-2.021670000
6	6.427700000	-2.787451000	-1.767786000
1	6.470283000	-1.896092000	-1.139307000
1	6.250869000	-2.464985000	-2.797499000
1	7.396852000	-3.287046000	-1.722524000
6	6.427929000	-2.786548000	1.767348000
1	7.397073000	-3.286171000	1.722222000

1	6.251227000	-2.463551000	2.796917000
1	6.470437000	-1.895512000	1.138405000
6	5.234337000	-4.917324000	2.344217000
1	6.199862000	-5.410052000	2.451951000
1	4.502885000	-5.662754000	2.022949000
1	4.925149000	-4.524443000	3.316529000
8	-7.810547000	-3.212547000	0.000375000
7	-6.621826000	-2.738029000	0.000234000
6	-3.775920000	-2.180028000	-0.000219000
1	-3.512695000	-3.242305000	-0.000477000
6	-4.629801000	-1.885148000	-1.242758000
1	-4.050110000	-2.057911000	-2.154456000
1	-4.898670000	-0.823339000	-1.239925000
6	-5.920300000	-2.722246000	-1.330451000
6	-5.919789000	-2.722734000	1.330654000
6	-4.629316000	-1.885621000	1.242775000
1	-4.898150000	-0.823800000	1.240447000
1	-4.049266000	-2.058743000	2.154176000
6	-6.876601000	-2.073558000	-2.343410000
1	-7.786115000	-2.663330000	-2.451009000
1	-6.382136000	-2.001878000	-3.315886000
1	-7.156321000	-1.067506000	-2.021670000
6	-5.627854000	-4.172826000	-1.767786000
1	-4.877205000	-4.655384000	-1.139307000
1	-5.260174000	-4.180919000	-2.797499000
1	-6.545091000	-4.762339000	-1.722524000
6	-5.627186000	-4.173476000	1.767348000
1	-6.544443000	-4.762968000	1.722222000
1	-5.259112000	-4.181946000	2.796917000
1	-4.876780000	-4.655807000	1.138405000
6	-6.875696000	-2.074407000	2.344217000
1	-7.785173000	-2.664212000	2.451951000
1	-7.155532000	-1.068236000	2.022949000
1	-6.380857000	-2.003083000	3.316529000

1d (n = 3), $\omega_1 = 9 \text{ cm}^{-1}$

8	1.115469000	9.798262000	-0.001292000
7	0.934736000	8.531094000	-0.000851000
6	0.000000000	5.785940000	0.000560000
1	-1.052026000	6.087507000	0.001363000
6	0.680036000	6.378586000	-1.242944000
1	0.240447000	5.961713000	-2.154027000
1	1.734585000	6.082472000	-1.241056000
6	0.597323000	7.914545000	-1.331082000
6	0.599429000	7.915167000	1.330200000
6	0.682062000	6.379164000	1.242649000
1	1.736634000	6.083159000	1.239193000
1	0.243996000	5.962705000	2.154655000
6	1.635334000	8.419985000	-2.345208000
1	1.577251000	9.502438000	-2.452875000
1	1.450150000	7.955402000	-3.317416000
1	2.647260000	8.161096000	-2.024384000
6	-0.806352000	8.384015000	-1.767153000
1	-1.598325000	7.974427000	-1.137562000
1	-0.997915000	8.068625000	-2.796417000
1	-0.859816000	9.473108000	-1.722616000
6	-0.803567000	8.384809000	1.768265000

1	-0.857121000	9.473880000	1.723307000
1	-0.993503000	8.069894000	2.797975000
1	-1.596527000	7.974919000	1.140116000
6	1.639022000	8.421111000	2.342452000
1	1.581078000	9.503612000	2.449703000
1	2.650450000	8.162102000	2.020157000
1	1.455380000	7.956978000	3.315168000
8	7.927809000	-5.865155000	-0.001292000
7	6.920776000	-5.075052000	-0.000851000
6	5.010771000	-2.892970000	0.000560000
1	5.797949000	-2.132672000	0.001363000
6	5.184000000	-3.778222000	-1.242944000
1	5.042772000	-3.189090000	-2.154027000
1	4.400283000	-4.543431000	-1.241056000
6	6.555535000	-4.474569000	-1.331082000
6	6.555021000	-4.476704000	1.330200000
6	5.183487000	-3.780265000	1.242649000
1	4.399853000	-4.545549000	1.239193000
1	5.041856000	-3.192659000	2.154655000
6	6.474254000	-5.626233000	-2.345208000
1	7.440727000	-6.117158000	-2.452875000
1	6.164505000	-5.233567000	-3.317416000
1	5.744086000	-6.373143000	-2.024384000
6	7.663946000	-3.493686000	-1.767153000
1	7.705219000	-2.603024000	-1.137562000
1	7.486592000	-3.170093000	-2.796417000
1	8.633860000	-3.991932000	-1.722616000
6	7.663241000	-3.496495000	1.768265000
1	8.633181000	-3.994652000	1.723307000
1	7.485485000	-3.174548000	2.797975000
1	7.704745000	-2.604827000	1.140116000
6	6.473385000	-5.629990000	2.342452000
1	7.439831000	-6.121059000	2.449703000
1	5.743363000	-6.376408000	2.020157000
1	6.163255000	-5.238885000	3.315168000
8	-9.043278000	-3.933107000	-0.001292000
7	-7.855512000	-3.456042000	-0.000851000
6	-5.010771000	-2.892970000	0.000560000
1	-4.745922000	-3.954835000	0.001363000
6	-5.864036000	-2.600365000	-1.242944000
1	-5.283219000	-2.772624000	-2.154027000
1	-6.134868000	-1.539041000	-1.241056000
6	-7.152858000	-3.439976000	-1.331082000
6	-7.154450000	-3.438463000	1.330200000
6	-5.865549000	-2.598899000	1.242649000
1	-6.136487000	-1.537610000	1.239193000
1	-5.285852000	-2.770046000	2.154655000
6	-8.109588000	-2.793752000	-2.345208000
1	-9.017978000	-3.385280000	-2.452875000
1	-7.614655000	-2.721834000	-3.317416000
1	-8.391347000	-1.787953000	-2.024384000
6	-6.857594000	-4.890329000	-1.767153000
1	-6.106894000	-5.371403000	-1.137562000
1	-6.488677000	-4.898532000	-2.796417000
1	-7.774044000	-5.481176000	-1.722616000
6	-6.859674000	-4.888314000	1.768265000
1	-7.776061000	-5.479228000	1.723307000

1	-6.491981000	-4.895346000	2.797975000
1	-6.108219000	-5.370092000	1.140116000
6	-8.112407000	-2.791121000	2.342452000
1	-9.020908000	-3.382553000	2.449703000
1	-8.393813000	-1.785694000	2.020157000
1	-7.618635000	-2.718093000	3.315168000
6	-2.488587000	-2.808444000	0.000745000
6	-1.238896000	-2.134778000	0.000734000
6	-0.010601000	-2.824283000	0.000737000
6	-1.232667000	-0.705748000	0.000733000
6	1.224489000	-2.144210000	0.000732000
6	1.227529000	-0.714647000	0.000733000
6	0.000000000	0.000000000	0.000731000
6	2.468220000	-0.005526000	0.000734000
6	3.676477000	-0.750958000	0.000745000
6	3.685666000	-2.145661000	0.000739000
6	2.466386000	-2.829266000	0.000730000
1	4.617478000	-0.209400000	0.000770000
6	-3.701030000	-2.119050000	0.000739000
6	-3.683409000	-0.721320000	0.000730000
6	-2.469185000	0.011667000	0.000732000
1	-4.613968000	-0.163966000	0.000713000
6	-2.440600000	1.421323000	0.000737000
6	-1.229324000	2.140304000	0.000734000
6	0.005138000	1.420395000	0.000733000
1	-3.378469000	1.967803000	0.000741000
6	2.451202000	1.402960000	0.000737000
6	1.244696000	2.132543000	0.000732000
1	2.448982000	-3.913831000	0.000713000
1	-0.014933000	-3.909742000	0.000741000
6	-1.187890000	3.559401000	0.000745000
1	-2.127393000	4.103553000	0.000770000
1	3.393402000	1.941939000	0.000741000
1	-2.490084000	-3.894153000	0.000770000
6	1.217023000	3.550586000	0.000730000
6	0.015364000	4.264711000	0.000739000
1	2.164986000	4.077796000	0.000713000

1d ($n = 4$), $\omega_1 = 10 \text{ cm}^{-1}$

8	3.070547000	10.851213000	0.001232000
7	2.775339000	9.605712000	0.000878000
6	2.640584000	6.708705000	-0.000311000
1	3.729967000	6.603463000	-0.001095000
6	2.224948000	7.509369000	1.243220000
1	2.481752000	6.960697000	2.154311000
1	1.135167000	7.619552000	1.241612000
6	2.863882000	8.908613000	1.331103000
6	2.862109000	8.909780000	-1.330080000
6	2.223279000	7.510466000	-1.242567000
1	1.133510000	7.620707000	-1.239396000
1	2.478831000	6.962600000	-2.154493000
6	2.082817000	9.758805000	2.345233000
1	2.533051000	10.744876000	2.453036000
1	2.085079000	9.258554000	3.317364000
1	1.046367000	9.888272000	2.024388000
6	4.341993000	8.831946000	1.767177000
1	4.928937000	8.160453000	1.137958000

1	4.404812000	8.468901000	2.796637000
1	4.790475000	9.825820000	1.722029000
6	4.339636000	8.833485000	-1.768200000
1	4.788214000	9.827298000	-1.722697000
1	4.401071000	8.471421000	-2.798088000
1	4.927387000	8.161361000	-1.140407000
6	2.079693000	9.760866000	-2.342414000
1	2.529802000	10.747021000	-2.449969000
1	1.043680000	9.890074000	-2.020057000
1	2.080631000	9.261459000	-3.314980000
8	-10.932700000	-2.766435000	0.001232000
7	-9.706460000	-2.399342000	0.000878000
6	-7.130201000	-1.067539000	-0.000311000
1	-7.583750000	-0.071486000	-0.001095000
6	-7.615778000	-1.827823000	1.243220000
1	-7.269016000	-1.331089000	2.154311000
1	-7.166309000	-2.826692000	1.241612000
6	-9.147026000	-1.974112000	1.331103000
6	-9.147151000	-1.976231000	-1.330080000
6	-7.615894000	-1.829817000	-1.242567000
1	-7.166481000	-2.828704000	-1.239396000
1	-7.269204000	-1.334569000	-2.154493000
6	-9.492781000	-3.075630000	2.345233000
1	-10.571861000	-3.178752000	2.453036000
1	-9.060682000	-2.823546000	3.317364000
1	-9.086679000	-4.037956000	2.024388000
6	-9.819686000	-0.655697000	1.767177000
1	-9.531628000	0.188358000	1.137958000
1	-9.536689000	-0.419772000	2.796637000
1	-10.904647000	-0.764237000	1.722029000
6	-9.819840000	-0.658507000	-1.768200000
1	-10.904797000	-0.766934000	-1.722697000
1	-9.537002000	-0.424271000	-2.798088000
1	-9.531639000	0.186561000	-1.140407000
6	-9.493004000	-3.079366000	-2.342414000
1	-10.572095000	-3.182638000	-2.449969000
1	-9.086895000	-4.041184000	-2.020057000
1	-9.060974000	-2.828851000	-3.314980000
8	7.862153000	-8.084779000	0.001232000
7	6.931121000	-7.206370000	0.000878000
6	4.489617000	-5.641165000	-0.000311000
1	3.853783000	-6.531977000	-0.001095000
6	5.390831000	-5.681546000	1.243220000
1	4.787265000	-5.629609000	2.154311000
1	6.031142000	-4.792859000	1.241612000
6	6.283144000	-6.934501000	1.331103000
6	6.285042000	-6.933549000	-1.330080000
6	5.392615000	-5.680649000	-1.242567000
1	6.032970000	-4.792002000	-1.239396000
1	4.790373000	-5.628031000	-2.154493000
6	7.409964000	-6.683175000	2.345233000
1	8.038810000	-7.566125000	2.453036000
1	6.975604000	-6.435008000	3.317364000
1	8.040311000	-5.850317000	2.024388000
6	5.477694000	-8.176249000	1.767177000
1	4.602691000	-8.348811000	1.137958000
1	5.131878000	-8.049130000	2.796637000

1	6.114173000	-9.061583000	1.722029000
6	5.480204000	-8.174977000	-1.768200000
1	6.116583000	-9.060364000	-1.722697000
1	5.135931000	-8.047150000	-2.798088000
1	4.604253000	-8.347922000	-1.140407000
6	7.413311000	-6.681500000	-2.342414000
1	8.042293000	-7.564384000	-2.449969000
1	8.043216000	-5.848890000	-2.020057000
1	6.980344000	-6.432608000	-3.314980000
6	2.928349000	4.201237000	-0.000535000
6	2.445848000	2.866796000	-0.000410000
6	2.068452000	5.299219000	-0.000475000
6	1.034064000	2.649015000	-0.001633000
6	0.688748000	5.075165000	-0.000441000
6	0.143245000	3.766801000	-0.000399000
1	4.002071000	4.362049000	-0.000417000
6	3.311249000	1.754611000	-0.000296000
6	-1.247589000	3.533606000	-0.000357000
1	4.383780000	1.920763000	0.001314000
1	0.000000000	5.913163000	-0.000186000
1	-1.924354000	4.382117000	0.001190000
6	-1.786008000	2.230914000	-0.000231000
6	-0.887543000	1.108362000	-0.005585000
6	0.516610000	1.323481000	0.003190000
6	1.403641000	0.214454000	-0.005585000
6	-3.175162000	1.990320000	-0.000296000
6	2.825032000	0.431271000	-0.000231000
6	3.683987000	-0.686359000	-0.000357000
1	4.757202000	-0.524519000	0.001190000
1	-3.855319000	2.836084000	0.001314000
6	0.887863000	-1.109137000	0.003190000
6	-0.516098000	-1.322816000	-0.005585000
6	-1.404473000	-0.214343000	0.003190000
6	-1.039024000	-2.662185000	-0.000231000
6	-2.436397000	-2.847247000	-0.000357000
6	-3.333768000	-1.759347000	-0.000399000
6	-2.811146000	-0.428982000	-0.001633000
6	1.777082000	-2.220033000	-0.001633000
6	-0.136087000	-3.744931000	-0.000296000
1	-2.832848000	-3.857598000	0.001190000
6	-4.739595000	-1.941109000	-0.000441000
6	-3.705643000	0.684769000	-0.000410000
6	-5.102553000	0.435406000	-0.000535000
6	-5.623484000	-0.858278000	-0.000475000
1	-5.120950000	-2.956582000	-0.000186000
1	-5.778681000	1.284871000	-0.000417000
6	1.259794000	-3.551565000	-0.000410000
6	3.190523000	-2.007454000	-0.000399000
1	-0.528461000	-4.756846000	0.001314000
6	2.174204000	-4.636643000	-0.000535000
6	4.050848000	-3.134055000	-0.000441000
6	3.555033000	-4.440941000	-0.000475000
1	1.776610000	-5.646920000	-0.000417000
1	5.120950000	-2.956582000	-0.000186000

1d ($n = 5$), $\omega_1 = 8 \text{ cm}^{-1}$

6	1.165008000	-4.774178000	-0.005311000
6	0.173747000	-3.773433000	-0.004507000
6	2.540485000	-4.462487000	-0.006105000
6	0.578257000	-2.393257000	-0.000124000
6	2.940432000	-3.090183000	-0.005473000
6	1.959179000	-2.059430000	-0.008224000
1	0.860372000	-5.815890000	-0.006270000
6	-1.202249000	-4.079721000	-0.003324000
6	2.360619000	-0.696803000	-0.001186000
1	-1.508941000	-5.120749000	-0.005241000
6	1.383221000	0.334252000	-0.007482000
6	-0.000737000	-0.000403000	0.004708000
6	-0.402990000	-1.366261000	-0.006773000
6	-1.784561000	-1.697373000	0.002582000
6	1.781873000	1.697572000	0.001403000
6	-2.192465000	-3.076392000	-0.001949000
6	-3.568161000	-3.379940000	-0.000175000
1	-3.877241000	-4.420310000	-0.001117000
6	-2.763794000	-0.668305000	-0.002800000
6	-2.362345000	0.694493000	0.004790000
6	-0.982376000	1.030972000	-0.004211000
6	-3.355165000	1.735025000	0.002378000
6	-2.932359000	3.079834000	0.003948000
6	-1.568366000	3.435903000	0.003529000
6	-0.578273000	2.392984000	0.005274000
6	-4.147039000	-1.002908000	0.002297000
6	-4.717452000	1.376766000	0.003140000
1	-3.680657000	3.865860000	0.003758000
6	-1.143328000	4.779101000	0.005924000
6	0.802462000	2.726705000	-0.002778000
6	1.204352000	4.091913000	0.002710000
6	0.221883000	5.128871000	0.005266000
1	-1.889889000	5.566842000	0.007072000
6	-5.135323000	0.029709000	0.002670000
6	-4.553529000	-2.372377000	0.001521000
1	-5.467356000	2.161364000	0.003430000
6	-6.504845000	-0.334637000	0.004075000
6	-5.940263000	-2.671201000	0.003891000
6	-6.912687000	-1.671559000	0.005025000
1	-7.242756000	0.460430000	0.005157000
1	-6.243858000	-3.713560000	0.004980000
6	2.592715000	4.431671000	-0.000283000
6	3.550304000	3.396236000	-0.003629000
6	3.179352000	2.037379000	-0.004598000
6	4.132490000	0.998775000	-0.006850000
1	4.604756000	3.653329000	-0.006274000
1	5.187383000	1.253717000	-0.010101000
6	3.758781000	-0.360486000	-0.007076000
6	4.709417000	-1.400198000	-0.008391000
1	5.764939000	-1.147652000	-0.010768000
6	3.540585000	-5.466494000	-0.006508000
6	4.329637000	-2.757382000	-0.007837000
6	5.281673000	-3.809086000	-0.008537000
6	4.902227000	-5.151058000	-0.007642000
1	3.220794000	-6.503052000	-0.005991000
1	6.336289000	-3.550971000	-0.009720000

6	2.962113000	5.799740000	0.001180000
6	0.656676000	6.479302000	0.007813000
6	2.008459000	6.821660000	0.005723000
1	-0.094154000	7.263513000	0.010778000
1	4.019810000	6.040393000	-0.001197000
8	7.935924000	-9.907857000	0.013944000
7	7.190282000	-8.867470000	0.009267000
6	5.965742000	-6.238595000	-0.006010000
1	6.933977000	-5.728457000	-0.015739000
6	5.876878000	-7.148268000	-1.240834000
1	5.900824000	-6.551567000	-2.157633000
1	4.910111000	-7.663076000	-1.228741000
6	6.997849000	-8.202060000	-1.326314000
6	7.014258000	-8.178541000	1.335083000
6	5.891172000	-7.127635000	1.244746000
1	4.924742000	-7.643186000	1.251564000
1	5.924658000	-6.515739000	2.151146000
6	6.589723000	-9.295002000	-2.326411000
1	7.379569000	-10.037604000	-2.433074000
1	6.394377000	-8.841047000	-3.301629000
1	5.682522000	-9.804800000	-1.993286000
6	8.333217000	-7.575790000	-1.779350000
1	8.628830000	-6.727393000	-1.159696000
1	8.244844000	-7.224015000	-2.810855000
1	9.124436000	-8.326121000	-1.735579000
6	8.354510000	-7.542460000	1.759143000
1	9.146684000	-8.291862000	1.716501000
1	8.279709000	-7.173987000	2.785877000
1	8.639438000	-6.703700000	1.121559000
6	6.620522000	-9.253588000	2.360062000
1	7.411958000	-9.994195000	2.468668000
1	5.708719000	-9.769132000	2.049030000
1	6.438936000	-8.782399000	3.329757000
8	4.618494000	11.823321000	-0.010989000
7	4.088308000	10.658255000	-0.008208000
6	2.419380000	8.286380000	0.006584000
1	1.494301000	8.870941000	0.022701000
6	3.221039000	8.669185000	-1.246608000
1	2.669328000	8.396818000	-2.151310000
1	4.149210000	8.087744000	-1.259796000
6	3.573454000	10.166571000	-1.333642000
6	3.613755000	10.154913000	1.327819000
6	3.258162000	8.658491000	1.238650000
1	4.186119000	8.076962000	1.219618000
1	2.733383000	8.378723000	2.157019000
6	4.698468000	10.361947000	-2.361971000
1	4.947248000	11.417123000	-2.468711000
1	4.376459000	9.972505000	-3.331467000
1	5.600110000	9.826236000	-2.055450000
6	2.353775000	11.014313000	-1.751594000
1	1.486336000	10.843100000	-1.111620000
1	2.067931000	10.768538000	-2.777976000
1	2.610287000	12.074146000	-1.707415000
6	2.407322000	10.998698000	1.789768000
1	2.662046000	12.058973000	1.746366000
1	2.152845000	10.744267000	2.822286000
1	1.520995000	10.832173000	1.174978000

6	4.769748000	10.341529000	2.322818000
1	5.020870000	11.395918000	2.431715000
1	5.661749000	9.809741000	1.983089000
1	4.478368000	9.942466000	3.298065000
8	-12.549640000	-1.906642000	-0.004250000
7	-11.275367000	-1.785906000	-0.002964000
6	-8.386500000	-2.048461000	0.007513000
1	-8.430128000	-3.141918000	0.022584000
6	-9.121176000	-1.544579000	-1.244442000
1	-8.611011000	-1.885880000	-2.150152000
1	-9.081833000	-0.450034000	-1.257224000
6	-10.594309000	-1.987748000	-1.329069000
6	-10.600405000	-1.950830000	1.331334000
6	-9.126769000	-1.510177000	1.241475000
1	-9.087162000	-0.415696000	1.224907000
1	-8.621257000	-1.826975000	2.158630000
6	-11.327572000	-1.112038000	-2.357020000
1	-12.366163000	-1.423698000	-2.461341000
1	-10.831310000	-1.197692000	-3.327436000
1	-11.313300000	-0.063011000	-2.051653000
6	-10.719627000	-3.468288000	-1.745288000
1	-10.136888000	-4.133443000	-1.105478000
1	-10.365337000	-3.593902000	-2.772052000
1	-11.765777000	-3.775654000	-1.699509000
6	-10.727340000	-3.419481000	1.787282000
1	-11.772913000	-3.729106000	1.743646000
1	-10.379109000	-3.516661000	2.819190000
1	-10.140271000	-4.101160000	1.169248000
6	-11.338390000	-1.047189000	2.331373000
1	-12.377541000	-1.355789000	2.439203000
1	-11.322421000	-0.006929000	1.997417000
1	-10.846916000	-1.106205000	3.306225000

2a, $\omega_1 = 19 \text{ cm}^{-1}$

7	1.197743000	-2.091382000	-0.000041000
6	1.209682000	-0.738988000	0.000004000
6	-0.000076000	-2.679352000	-0.000090000
6	0.000002000	-0.002938000	-0.000005000
7	-1.197860000	-2.091312000	-0.000114000
6	-1.209721000	-0.738917000	-0.000069000
6	2.439424000	-0.033046000	0.000071000
6	0.000045000	1.416854000	0.000046000
6	-2.439421000	-0.032902000	-0.000086000
6	1.245303000	2.084262000	0.000104000
6	2.446436000	1.361613000	0.000119000
1	3.363699000	-0.594501000	0.000085000
6	-1.245174000	2.084336000	0.000034000
1	1.278799000	3.166229000	0.000141000
6	-2.446349000	1.361757000	-0.000034000
1	-1.278609000	3.166305000	0.000075000
1	-3.363729000	-0.594303000	-0.000140000
16	5.187596000	4.175140000	0.000137000
16	6.267154000	2.264468000	0.000359000
7	3.724428000	3.432078000	0.000076000
7	4.878176000	1.394272000	0.000325000
6	3.741199000	2.095292000	0.000191000
16	-5.187344000	4.175446000	0.000106000

16	-6.267018000	2.264831000	-0.000247000
7	-3.724222000	3.432297000	0.000138000
7	-4.878088000	1.394560000	-0.000250000
6	-3.741070000	2.095512000	-0.000052000
16	1.104038000	-6.455620000	0.000141000
16	-1.104446000	-6.455553000	-0.000440000
7	1.171643000	-4.820107000	0.000138000
7	-1.171932000	-4.820033000	-0.000458000
6	-0.000123000	-4.182769000	-0.000195000

2b, $\omega_1 = 10 \text{ cm}^{-1}$

7	-1.207728000	2.081521000	0.055179000
6	-0.028408000	1.413965000	0.053033000
6	-2.314522000	1.336499000	0.000426000
6	0.001079000	-0.000411000	0.000606000
7	-2.406332000	0.005465000	-0.054108000
6	-1.238543000	-0.682083000	-0.051766000
6	1.197200000	2.123071000	0.109100000
6	1.230436000	-0.710165000	0.000549000
6	-1.239815000	-2.098045000	-0.107623000
6	2.431476000	0.032856000	0.055978000
6	2.411545000	1.434200000	0.109946000
1	1.171828000	3.203028000	0.149766000
6	1.187510000	-2.121807000	-0.054893000
1	3.383052000	-0.482581000	0.057355000
6	-0.036050000	-2.805243000	-0.108588000
1	2.109700000	-2.688146000	-0.056474000
1	-2.187743000	-2.616107000	-0.148166000
7	1.093511000	-6.269994000	-0.203173000
7	1.132939000	-4.912626000	-0.147616000
6	-0.071570000	-7.026064000	-0.274452000
6	-0.046929000	-4.295773000	-0.166567000
7	-1.223117000	-6.245021000	-0.282062000
7	-1.236946000	-4.888693000	-0.232548000
8	-0.082930000	-8.241686000	-0.324229000
6	2.394344000	-6.931383000	-0.182343000
1	2.984223000	-6.594401000	-1.036725000
1	2.917139000	-6.671206000	0.739939000
1	2.235429000	-8.004550000	-0.234606000
6	-2.536836000	-6.877899000	-0.357760000
1	-3.131696000	-6.571974000	0.504320000
1	-3.040406000	-6.558868000	-1.272279000
1	-2.400065000	-7.955339000	-0.360212000
7	-5.746604000	2.299181000	0.752063000
7	-4.574050000	1.607189000	0.783005000
6	-5.969790000	3.446237000	-0.000918000
6	-3.614468000	2.087005000	0.000175000
7	-4.864203000	3.826999000	-0.752725000
7	-3.678520000	3.157731000	-0.782957000
8	-7.024788000	4.054857000	-0.001785000
6	-6.794042000	1.784116000	1.627351000
1	-6.887358000	0.710572000	1.462858000
1	-6.528485000	1.964852000	2.672044000
1	-7.724580000	2.292033000	1.390098000
6	-4.942178000	4.990862000	-1.629036000
1	-4.055998000	5.605161000	-1.469444000
1	-4.972416000	4.669725000	-2.673360000

1	-5.844145000	5.546329000	-1.387985000
7	4.797103000	4.181847000	0.286078000
7	3.615526000	3.515763000	0.236020000
6	6.049305000	3.575226000	0.274275000
6	3.696972000	2.188828000	0.167990000
7	5.976962000	2.188260000	0.202094000
7	4.821100000	1.475486000	0.147000000
8	7.096492000	4.192869000	0.321927000
6	4.688356000	5.635991000	0.361884000
1	4.140857000	6.000974000	-0.508717000
1	4.145239000	5.910723000	1.267963000
1	5.690038000	6.055312000	0.381442000
6	7.200160000	1.392511000	0.177294000
1	7.202530000	0.708412000	1.027827000
1	7.236990000	0.814835000	-0.748245000
1	8.050071000	2.066403000	0.233787000

2c, $\omega_1 = 11 \text{ cm}^{-1}$

7	-1.201586000	-2.107912000	0.001345000
6	-1.213989000	-0.750628000	0.004343000
6	-0.000147000	-2.682101000	0.000003000
6	0.000004000	-0.022794000	-0.000002000
7	1.201357000	-2.108049000	-0.001338000
6	1.213914000	-0.750766000	-0.004342000
6	-2.442486000	-0.048440000	0.009492000
6	0.000084000	1.394706000	-0.000004000
6	2.442490000	-0.048717000	-0.009489000
6	-1.240214000	2.071326000	0.017924000
6	-2.451846000	1.354591000	0.023035000
1	-3.361469000	-0.613717000	-0.007400000
6	1.240458000	2.071185000	-0.017933000
1	-1.257526000	3.150899000	0.040094000
6	2.452009000	1.354312000	-0.023040000
1	1.257892000	3.150756000	-0.040107000
1	3.361409000	-0.614098000	0.007410000
6	-3.725991000	2.082525000	0.039089000
7	-3.899226000	3.362417000	0.458470000
8	-3.009421000	4.153498000	0.906672000
6	-5.364064000	3.730123000	0.539611000
6	-5.988910000	2.657109000	-0.407243000
7	-4.924491000	1.583454000	-0.361157000
8	-5.159856000	0.420860000	-0.815742000
6	-5.758578000	3.571720000	2.018167000
1	-5.622022000	2.547300000	2.369825000
1	-6.801102000	3.856787000	2.171077000
1	-5.127711000	4.227404000	2.620231000
6	-5.552280000	5.181419000	0.103544000
1	-5.015317000	5.836188000	0.789692000
1	-6.613228000	5.441362000	0.133938000
1	-5.175265000	5.365939000	-0.901616000
6	-7.323794000	2.073392000	0.050169000
1	-8.088829000	2.853678000	0.046214000
1	-7.268660000	1.641730000	1.048733000
1	-7.627874000	1.286421000	-0.639799000
6	-6.085262000	3.094547000	-1.879047000
1	-5.142489000	3.504739000	-2.246133000
1	-6.866069000	3.846552000	-2.007122000

1	-6.339157000	2.224135000	-2.485953000
6	3.726238000	2.082099000	-0.039089000
7	4.924673000	1.582884000	0.361172000
8	5.159892000	0.420262000	0.815762000
6	5.989224000	2.656409000	0.407256000
6	5.364517000	3.729490000	-0.539614000
7	3.899633000	3.361964000	-0.458483000
8	3.009931000	4.153146000	-0.906710000
6	6.085617000	3.093849000	1.879058000
1	5.142892000	3.504162000	2.246131000
1	6.866516000	3.845758000	2.007132000
1	6.339399000	2.223411000	2.485974000
6	7.324040000	2.072524000	-0.050139000
1	7.628019000	1.285523000	0.639838000
1	8.089170000	2.852717000	-0.046186000
1	7.268860000	1.640861000	-1.048701000
6	5.552907000	5.180767000	-0.103558000
1	6.613887000	5.440579000	-0.133945000
1	5.175905000	5.365344000	0.901595000
1	5.016032000	5.835596000	-0.789718000
6	5.759025000	3.571024000	-2.018164000
1	5.622358000	2.546615000	-2.369811000
1	6.801582000	3.855974000	-2.171070000
1	5.128236000	4.226771000	-2.620242000
6	-0.000236000	-4.168873000	0.000004000
7	0.060734000	-4.927435000	-1.107773000
8	0.130742000	-4.516206000	-2.307898000
6	-0.153811000	-6.388639000	-0.770122000
6	0.153026000	-6.388665000	0.770116000
7	-0.061312000	-4.927433000	1.107775000
8	-0.131264000	-4.516203000	2.307903000
6	-1.621016000	-6.688497000	-1.118713000
1	-2.310015000	-6.064847000	-0.546214000
1	-1.856874000	-7.737776000	-0.930229000
1	-1.776538000	-6.482013000	-2.178817000
6	0.772634000	-7.249704000	-1.625387000
1	0.526920000	-7.102271000	-2.677302000
1	0.631837000	-8.305382000	-1.379918000
1	1.822467000	-6.994052000	-1.487324000
6	-0.773542000	-7.249605000	1.625374000
1	-0.632901000	-8.305301000	1.379892000
1	-1.823338000	-6.993797000	1.487319000
1	-0.527803000	-7.102222000	2.677290000
6	1.620187000	-6.688736000	1.118704000
1	2.309277000	-6.065183000	0.546209000
1	1.855892000	-7.738049000	0.930212000
1	1.775739000	-6.482283000	2.178810000

2d, $\omega_1 = 5 \text{ cm}^{-1}$

7	-1.433541000	1.914113000	0.000038000
6	-1.261787000	0.572740000	-0.000054000
6	-0.329427000	2.675355000	0.000035000
6	0.036312000	0.010681000	-0.000134000
7	0.938213000	2.244028000	-0.000036000
6	1.134656000	0.901749000	-0.000122000
6	-2.380849000	-0.302903000	-0.000063000
6	0.228765000	-1.394903000	-0.000212000

6	2.448116000	0.365099000	-0.000184000
6	-0.917099000	-2.224037000	-0.000217000
6	-2.215653000	-1.685919000	-0.000141000
1	-3.369963000	0.141088000	-0.000001000
6	1.559404000	-1.880159000	-0.000270000
1	-0.776067000	-3.299497000	-0.000274000
6	2.662197000	-1.014780000	-0.000249000
1	1.725036000	-2.953117000	-0.000325000
1	3.271992000	1.068444000	-0.000167000
8	8.206891000	-2.040000000	0.000397000
7	6.963576000	-1.736934000	0.000256000
6	4.069764000	-1.592151000	-0.000217000
1	3.962200000	-2.681107000	-0.000529000
6	4.870515000	-1.176279000	1.243207000
1	4.321927000	-1.430016000	2.155284000
1	4.984484000	-0.087116000	1.239554000
6	6.266866000	-1.821112000	1.331129000
6	6.267319000	-1.820460000	-1.330896000
6	4.870956000	-1.175625000	-1.243131000
1	4.984978000	-0.086471000	-1.238861000
1	4.322681000	-1.428855000	-2.155537000
6	7.120235000	-1.042286000	2.344318000
1	8.103610000	-1.497915000	2.453305000
1	6.619657000	-1.040081000	3.316267000
1	7.255418000	-0.007201000	2.021757000
6	6.184228000	-3.298654000	1.768217000
1	5.511750000	-3.884245000	1.138507000
1	5.820943000	-3.360292000	2.797647000
1	7.176564000	-3.750492000	1.723819000
6	6.184773000	-3.297787000	-1.768732000
1	7.177070000	-3.749697000	-1.724198000
1	5.821863000	-3.358896000	-2.798326000
1	5.512030000	-3.883659000	-1.139562000
6	7.121057000	-1.041167000	-2.343413000
1	8.104448000	-1.496782000	-2.452305000
1	7.256181000	-0.006252000	-2.020283000
1	6.620800000	-1.038449000	-3.315527000
8	-5.986479000	-5.879609000	0.000008000
7	-5.080197000	-4.976135000	-0.000028000
6	-3.439980000	-2.588350000	-0.000118000
1	-4.311044000	-1.926848000	-0.000128000
6	-3.505963000	-3.488358000	1.243342000
1	-3.432993000	-2.887830000	2.154971000
1	-2.640441000	-4.159965000	1.239523000
6	-4.789035000	-4.337262000	1.330890000
6	-4.789067000	-4.337336000	-1.330990000
6	-3.505990000	-3.488431000	-1.243521000
1	-2.640473000	-4.160044000	-1.239682000
1	-3.433038000	-2.887959000	-2.155188000
6	-4.575619000	-5.471839000	2.345065000
1	-5.478820000	-6.071445000	2.450641000
1	-4.315721000	-5.045847000	3.317833000
1	-3.763219000	-6.129288000	2.025914000
6	-6.002650000	-3.489972000	1.766373000
1	-6.142988000	-2.607995000	1.139260000
1	-5.866392000	-3.151729000	2.797096000
1	-6.909447000	-4.094974000	1.717092000

6	-6.002692000	-3.490067000	-1.766489000
1	-6.909488000	-4.095065000	-1.717151000
1	-5.866459000	-3.151882000	-2.797234000
1	-6.143012000	-2.608056000	-1.139421000
6	-4.575680000	-5.471970000	-2.345107000
1	-5.478885000	-6.071579000	-2.450626000
1	-3.763274000	-6.129403000	-2.025939000
1	-4.315806000	-5.046033000	-3.317905000
8	-2.380460000	7.908903000	-0.000041000
7	-1.964580000	6.698129000	-0.000028000
6	-0.536734000	4.177443000	0.000175000
1	0.463157000	4.615898000	0.000510000
6	-1.315721000	4.631439000	1.242927000
1	-0.803993000	4.308725000	2.155348000
1	-2.289708000	4.133432000	1.231664000
6	-1.518036000	6.155437000	1.329512000
6	-1.517230000	6.155693000	-1.329395000
6	-1.314964000	4.631681000	-1.242972000
1	-2.288967000	4.133681000	-1.232375000
1	-0.802689000	4.309128000	-2.155141000
6	-2.631903000	6.458483000	2.343937000
1	-2.776335000	7.532767000	2.452766000
1	-2.362849000	6.035358000	3.315604000
1	-3.577347000	6.015139000	2.022668000
6	-0.225275000	6.877437000	1.763984000
1	0.628961000	6.616109000	1.136898000
1	0.019673000	6.606601000	2.794709000
1	-0.372436000	7.957776000	1.715228000
6	-0.224211000	6.877786000	-1.762950000
1	-0.371431000	7.958114000	-1.714103000
1	0.021383000	6.607125000	-2.793567000
1	0.629641000	6.616377000	-1.135376000
6	-2.630479000	6.458922000	-2.344446000
1	-2.774831000	7.533226000	-2.453184000
1	-3.576125000	6.015540000	-2.023824000
1	-2.360846000	6.035952000	-3.316019000

3a, $\omega_1 = 20 \text{ cm}^{-1}$

8	0.724197000	3.578694000	-0.001193000
6	-2.012488000	1.229155000	-0.000432000
6	-1.314106000	0.000002000	-0.000222000
6	-2.012493000	-1.229148000	-0.000111000
6	-1.387013000	2.458622000	-0.000480000
6	0.102012000	2.527707000	-0.000616000
8	0.724182000	-3.578697000	0.000727000
6	-1.387024000	-2.458617000	0.000136000
6	0.102002000	-2.527709000	0.000376000
6	0.825455000	-1.219864000	0.000216000
6	0.121370000	-0.000001000	-0.000074000
6	2.217101000	-1.210621000	0.000367000
1	2.748436000	-2.153179000	0.000612000
6	2.920184000	-0.000006000	0.000199000
6	2.217106000	1.210612000	-0.000129000
1	2.748445000	2.153168000	-0.000281000
6	0.825460000	1.219860000	-0.000236000
16	-4.477700000	-4.857313000	0.000236000
16	-2.686425000	-6.162229000	0.000033000

7	-3.561670000	-3.504027000	0.000263000
7	-1.670240000	-4.889098000	0.000042000
6	-2.219295000	-3.673868000	0.000177000
16	-2.686399000	6.162240000	0.001099000
16	-4.477677000	4.857334000	-0.001873000
7	-1.670220000	4.889103000	0.001138000
7	-3.561654000	3.504042000	-0.002026000
6	-2.219279000	3.673877000	-0.000495000
16	6.683371000	-1.100165000	0.000771000
16	6.683375000	1.100138000	0.000252000
7	5.046791000	-1.171868000	0.000674000
7	5.046796000	1.171847000	0.000125000
6	4.401385000	-0.000009000	0.000377000
1	-3.095758000	1.205108000	-0.000482000
1	-3.095763000	-1.205096000	-0.000241000

3b, $\omega_1 = 15 \text{ cm}^{-1}$

8	0.681839000	3.553984000	-0.440908000
6	-2.035499000	1.236081000	-0.040908000
6	-1.341059000	0.002329000	-0.000457000
6	-2.039999000	-1.228845000	0.040424000
6	-1.396859000	2.453223000	-0.086760000
6	0.082573000	2.511705000	-0.207473000
8	0.669033000	-3.556770000	0.438796000
6	-1.405834000	-2.448349000	0.086046000
6	0.073439000	-2.512277000	0.205852000
6	0.802880000	-1.217467000	0.089506000
6	0.095090000	-0.000308000	-0.000815000
6	2.194732000	-1.209346000	0.096382000
1	2.722329000	-2.150021000	0.177496000
6	2.904446000	-0.005464000	-0.001446000
6	2.199115000	1.201018000	-0.098964000
1	2.730101000	2.139763000	-0.180297000
6	0.807313000	1.214236000	-0.091466000
1	-3.119351000	1.218803000	-0.016537000
1	-3.123792000	-1.207586000	0.016665000
7	6.348656000	-1.165161000	0.119850000
7	4.991571000	-1.190323000	0.118875000
6	7.119436000	-0.012695000	0.001045000
6	4.388297000	-0.008150000	-0.001704000
7	6.352724000	1.141790000	-0.124204000
7	4.995755000	1.171864000	-0.122501000
8	8.335893000	-0.014278000	0.005147000
6	6.994360000	-2.467419000	0.259803000
1	6.671190000	-2.929713000	1.193995000
1	6.703285000	-3.106643000	-0.575696000
1	8.070273000	-2.319177000	0.263768000
6	7.003276000	2.442470000	-0.256222000
1	6.648661000	2.927071000	-1.167024000
1	6.749148000	3.065582000	0.603560000
1	8.077201000	2.286969000	-0.302209000
7	-2.444069000	5.867525000	0.555281000
7	-1.687041000	4.740762000	0.581761000
6	-3.702798000	5.965050000	-0.025856000
6	-2.189934000	3.697380000	-0.076366000
7	-4.112538000	4.786910000	-0.643938000
7	-3.372368000	3.647421000	-0.699204000

8	-4.376323000	6.977405000	0.005324000
6	-1.898318000	7.008111000	1.287270000
1	-2.149077000	6.935773000	2.349271000
1	-0.817079000	6.989631000	1.166633000
1	-2.320407000	7.923299000	0.879976000
6	-5.400136000	4.727998000	-1.328033000
1	-5.238760000	4.516964000	-2.386937000
1	-6.004695000	3.930804000	-0.891660000
1	-5.897420000	5.686119000	-1.207603000
7	-2.466305000	-5.858864000	-0.554508000
7	-1.704987000	-4.735006000	-0.581689000
6	-3.725153000	-5.951379000	0.027165000
6	-2.203600000	-3.689506000	0.076330000
7	-4.130116000	-4.771508000	0.645089000
7	-3.385574000	-3.634844000	0.699684000
8	-4.402571000	-6.961148000	-0.003527000
6	-1.925413000	-7.001768000	-1.286494000
1	-2.178210000	-6.929840000	-2.348042000
1	-0.843892000	-6.986210000	-1.168101000
1	-2.349244000	-7.915361000	-0.877409000
6	-5.417246000	-4.707477000	1.329610000
1	-5.254704000	-4.496559000	2.388357000
1	-6.019010000	-3.908252000	0.893084000
1	-5.918116000	-5.663801000	1.209776000

3c, $\omega_1 = 15 \text{ cm}^{-1}$

8	-3.526472000	0.563656000	-0.618300000
6	-1.225698000	-2.114006000	-0.026661000
6	0.002132000	-1.411267000	-0.000170000
6	1.232072000	-2.110313000	0.026375000
6	-2.442422000	-1.465187000	-0.050031000
6	-2.498430000	0.007032000	-0.263673000
8	3.524738000	0.574296000	0.618011000
6	2.446834000	-1.457842000	0.049753000
6	2.498421000	0.014568000	0.263263000
6	1.209227000	0.744053000	0.117904000
6	-0.000030000	0.028168000	-0.000195000
6	1.202862000	2.134420000	0.138603000
1	2.140178000	2.655877000	0.264421000
6	-0.004287000	2.847852000	-0.000215000
6	-1.209268000	2.130776000	-0.139039000
1	-2.148129000	2.649431000	-0.264933000
6	-1.211438000	0.740393000	-0.118330000
1	-1.200810000	-3.196415000	-0.003067000
1	1.210442000	-3.192790000	0.002770000
6	3.687626000	-2.192929000	-0.005418000
7	4.793683000	-1.816221000	-0.703758000
8	4.879508000	-0.843316000	-1.505491000
6	5.866716000	-2.883166000	-0.657609000
6	5.391884000	-3.739037000	0.564065000
7	3.921181000	-3.388872000	0.601566000
8	3.097549000	-4.049487000	1.309997000
6	5.789908000	-3.620502000	-2.005089000
1	4.817095000	-4.092359000	-2.157881000
1	6.563384000	-4.388042000	-2.068746000
1	5.948820000	-2.898519000	-2.807158000
6	7.233413000	-2.217927000	-0.503978000

1	7.423225000	-1.587707000	-1.373171000
1	8.014949000	-2.979984000	-0.450748000
1	7.291016000	-1.590476000	0.384369000
6	5.556776000	-5.249581000	0.413714000
1	6.618491000	-5.502481000	0.359707000
1	5.059197000	-5.636480000	-0.474760000
1	5.127026000	-5.746256000	1.283743000
6	5.970120000	-3.279025000	1.913948000
1	5.851346000	-2.204218000	2.062297000
1	7.030960000	-3.527374000	1.982223000
1	5.440989000	-3.796687000	2.715738000
6	-0.006491000	4.306266000	-0.000153000
7	-0.998345000	5.098374000	-0.492656000
8	-2.079174000	4.720730000	-1.042901000
6	-0.587368000	6.553182000	-0.524901000
6	0.567449000	6.554813000	0.525175000
7	0.982930000	5.101287000	0.492517000
8	2.064890000	4.726816000	1.042708000
6	-0.127247000	6.831822000	-1.966340000
1	0.724550000	6.210875000	-2.250498000
1	0.150685000	7.880641000	-2.086207000
1	-0.952915000	6.611881000	-2.644849000
6	-1.788758000	7.431664000	-0.183150000
1	-2.560683000	7.296621000	-0.940665000
1	-1.488099000	8.482266000	-0.176524000
1	-2.222053000	7.184836000	0.785286000
6	1.766148000	7.437086000	0.183690000
1	1.462291000	8.486770000	0.177279000
1	2.200258000	7.191810000	-0.784775000
1	2.538445000	7.304244000	0.941213000
6	0.106489000	6.831645000	1.966695000
1	-0.743517000	6.208148000	2.250628000
1	-0.174456000	7.879617000	2.086913000
1	0.932776000	6.613854000	2.645146000
6	-3.680985000	-2.204000000	0.005274000
7	-4.788152000	-1.830496000	0.703556000
8	-4.876983000	-0.857540000	1.504911000
6	-5.857913000	-2.900732000	0.657743000
6	-5.380529000	-3.755453000	-0.563748000
7	-3.910920000	-3.400804000	-0.601421000
8	-3.085317000	-4.059041000	-1.309763000
6	-5.778739000	-3.637506000	2.005397000
1	-4.804523000	-4.106469000	2.158166000
1	-6.549939000	-4.407311000	2.069351000
1	-5.939667000	-2.915805000	2.807317000
6	-7.226662000	-2.239748000	0.504051000
1	-7.418370000	-1.609913000	1.373107000
1	-8.005843000	-3.004229000	0.451061000
1	-7.286259000	-1.612687000	-0.384438000
6	-5.540781000	-5.266452000	-0.413003000
1	-6.601710000	-5.522591000	-0.358812000
1	-5.041914000	-5.651603000	0.475508000
1	-5.109612000	-5.762035000	-1.282954000
6	-5.960265000	-3.297546000	-1.913702000
1	-5.844910000	-2.222400000	-2.062275000
1	-7.020315000	-3.549271000	-1.981872000
1	-5.429539000	-3.813694000	-2.715413000

3d, $\omega_1 = 10 \text{ cm}^{-1}$

8	-3.365000000	1.654230000	0.003658000
6	-2.014791000	-1.670835000	0.002559000
6	-0.619024000	-1.411991000	0.002855000
6	0.333250000	-2.464819000	0.002315000
6	-2.973199000	-0.686082000	0.002581000
6	-2.547449000	0.731806000	0.003256000
8	3.425147000	-0.643000000	0.002849000
6	1.692717000	-2.264998000	0.002116000
6	2.215813000	-0.879741000	0.002783000
6	1.222071000	0.227447000	0.003255000
6	-0.160051000	-0.054080000	0.003285000
6	1.654779000	1.552179000	0.003400000
1	2.724245000	1.726799000	0.003227000
6	0.745524000	2.618330000	0.003613000
6	-0.621755000	2.323477000	0.003761000
1	-1.356933000	3.120679000	0.003917000
6	-1.086395000	1.007507000	0.003539000
1	-2.332178000	-2.710508000	0.002090000
1	-0.046159000	-3.483447000	0.001857000
8	-8.594014000	-1.089704000	-0.002905000
7	-7.327769000	-0.903839000	-0.001559000
6	-4.441364000	-1.051962000	0.001408000
1	-4.474268000	-2.146450000	0.001149000
6	-5.189276000	-0.542407000	-1.244611000
1	-4.670685000	-0.853213000	-2.157109000
1	-5.184684000	0.548931000	-1.226386000
6	-6.641654000	-1.050583000	-1.332014000
6	-6.644441000	-1.050966000	1.330281000
6	-5.191757000	-0.542912000	1.246117000
1	-5.186979000	0.548428000	1.228450000
1	-4.675093000	-0.854247000	2.159524000
6	-7.413173000	-0.186754000	-2.342224000
1	-8.439189000	-0.537727000	-2.446732000
1	-6.919098000	-0.237077000	-3.316279000
1	-7.436676000	0.856503000	-2.019486000
6	-6.706740000	-2.527452000	-1.774542000
1	-6.098404000	-3.180369000	-1.145414000
1	-6.348311000	-2.621411000	-2.803331000
1	-7.739186000	-2.878608000	-1.734395000
6	-6.710622000	-2.527940000	1.772304000
1	-7.743030000	-2.878951000	1.729954000
1	-6.354302000	-2.622194000	2.801797000
1	-6.101096000	-3.180792000	1.144261000
6	-7.417972000	-0.187307000	2.339099000
1	-8.444282000	-0.538106000	2.441270000
1	-7.440550000	0.856062000	2.016654000
1	-6.926014000	-0.238049000	3.314202000
8	3.580209000	7.488540000	-0.004942000
7	2.996175000	6.349872000	-0.003051000
6	1.217366000	4.061895000	0.002758000
1	0.318686000	4.685770000	0.005557000
6	2.051299000	4.399033000	-1.243691000
1	1.498019000	4.149612000	-2.154061000
1	2.951747000	3.775352000	-1.242963000

6	2.472465000	5.878477000	-1.331733000
6	2.481352000	5.878368000	1.329067000
6	2.059169000	4.399002000	1.243817000
1	2.959543000	3.775275000	1.237603000
1	1.511640000	4.149816000	2.157717000
6	3.615762000	6.016948000	-2.349127000
1	3.911531000	7.059550000	-2.458584000
1	3.287218000	5.636913000	-3.320126000
1	4.489562000	5.443930000	-2.029918000
6	1.296597000	6.778979000	-1.764418000
1	0.416645000	6.652660000	-1.131039000
1	1.008122000	6.542043000	-2.792105000
1	1.601910000	7.825836000	-1.722936000
6	1.308714000	6.779147000	1.770067000
1	1.613942000	7.825940000	1.726385000
1	1.027674000	6.542303000	2.799831000
1	0.424126000	6.653032000	1.143120000
6	3.631631000	6.016410000	2.338629000
1	3.928251000	7.058943000	2.446410000
1	4.503162000	5.443455000	2.013163000
1	3.309779000	5.636020000	3.311732000
8	5.893350000	-6.021336000	-0.003575000
7	5.008514000	-5.096754000	-0.002196000
6	2.635430000	-3.448644000	0.000783000
1	1.995006000	-4.336781000	0.000473000
6	3.541332000	-3.502044000	1.244785000
1	2.943437000	-3.430296000	2.158866000
1	4.205403000	-2.636018000	1.224228000
6	4.379711000	-4.792232000	1.330403000
6	4.378014000	-4.789934000	-1.333459000
6	3.539639000	-3.499954000	-1.244536000
1	4.203681000	-2.633911000	-1.223438000
1	2.940503000	-3.426732000	-2.157690000
6	5.522152000	-4.579508000	2.336300000
1	6.119237000	-5.484808000	2.440028000
1	5.103732000	-4.315368000	3.311283000
1	6.177867000	-3.769065000	2.010058000
6	3.530265000	-6.000781000	1.776088000
1	2.645934000	-6.142777000	1.151844000
1	3.195959000	-5.857402000	2.807264000
1	4.131746000	-6.910065000	1.729721000
6	3.528033000	-5.997731000	-1.780158000
1	4.129551000	-6.907103000	-1.736058000
1	3.192474000	-5.852604000	-2.810683000
1	2.644458000	-6.140755000	-1.155073000
6	5.519159000	-4.575392000	-2.340435000
1	6.116114000	-5.480501000	-2.446535000
1	6.175291000	-3.765533000	-2.013580000
1	5.099481000	-4.309514000	-3.314404000

4a, $\omega_1 = 18 \text{ cm}^{-1}$

8	2.565394000	-3.250248000	-0.000030000
8	1.532509000	3.846402000	-0.000109000
6	-1.576958000	-3.959318000	0.000021000
6	-0.193693000	-3.747231000	0.000017000
1	0.489992000	-4.586157000	0.000039000
6	0.331587000	-2.459983000	0.000002000

6	1.807564000	-2.290033000	-0.000005000
6	2.315879000	-0.894023000	-0.000020000
6	1.419646000	0.206472000	-0.000038000
6	0.000462000	-0.000121000	-0.000033000
6	-0.530358000	-1.332452000	-0.000016000
6	3.689935000	-0.682301000	-0.000023000
1	4.347439000	-1.541903000	-0.000008000
6	4.217683000	0.613770000	-0.000061000
6	3.342371000	1.705687000	-0.000084000
1	3.727090000	2.717212000	-0.000118000
6	1.965079000	1.516769000	-0.000065000
6	1.079948000	2.709993000	-0.000062000
8	-4.096928000	-0.596298000	-0.000053000
6	-2.435372000	-2.854109000	-0.000005000
1	-3.508603000	-2.993214000	-0.000003000
6	-1.931531000	-1.558456000	-0.000016000
6	-2.886405000	-0.420348000	-0.000038000
6	-2.295356000	0.942699000	-0.000066000
6	-0.888008000	1.125664000	-0.000061000
6	-3.147590000	2.041022000	-0.000101000
1	-4.215973000	1.868701000	-0.000103000
6	-2.639691000	3.345036000	-0.000138000
6	-1.253415000	3.536271000	-0.000127000
1	-0.837888000	4.535540000	-0.000150000
6	-0.383119000	2.452070000	-0.000088000
16	-1.950420000	-7.859631000	-0.000358000
16	-3.993698000	-7.042737000	-0.000619000
7	-1.275842000	-6.366789000	-0.000045000
7	-3.453363000	-5.496553000	-0.000257000
6	-2.125100000	-5.332524000	0.000078000
16	7.779469000	2.245324000	-0.000185000
16	8.097590000	0.068195000	0.000349000
7	6.149744000	2.080519000	-0.000315000
7	6.488743000	-0.239897000	0.000280000
6	5.680800000	0.827057000	-0.000088000
16	-5.833999000	5.613323000	-0.000001000
16	-4.107435000	6.977796000	-0.000119000
7	-4.876061000	4.284840000	-0.000083000
7	-3.036069000	5.738557000	-0.000171000
6	-3.556049000	4.505410000	-0.000186000

4b, $\omega_1 = 14 \text{ cm}^{-1}$

8	4.090213000	0.645211000	0.013588000
8	-1.486371000	-3.864845000	0.013641000
6	1.531149000	3.981393000	0.013627000
6	2.400534000	2.883357000	0.013651000
1	3.471725000	3.033392000	0.013671000
6	1.912775000	1.581286000	0.013633000
6	2.880674000	0.454426000	0.013607000
6	2.306626000	-0.915650000	0.013596000
6	0.901178000	-1.114308000	0.013625000
6	-0.000043000	0.000030000	0.013625000
6	0.514405000	1.337670000	0.013625000
6	3.171508000	-2.004374000	0.013586000
1	4.236868000	-1.817371000	0.013546000
6	2.682311000	-3.316697000	0.013629000
6	1.296690000	-3.520591000	0.013676000

1	0.890970000	-4.523262000	0.013714000
6	0.412960000	-2.447117000	0.013653000
6	-1.046873000	-2.721945000	0.013639000
8	-2.603918000	3.219663000	0.013645000
6	0.150042000	3.748887000	0.013608000
1	-0.544631000	4.577985000	0.013586000
6	-0.360360000	2.455511000	0.013615000
6	-1.833908000	2.267575000	0.013640000
6	-2.325842000	0.865926000	0.013654000
6	-1.415699000	-0.223297000	0.013633000
6	-3.697361000	0.637288000	0.013671000
1	-4.362909000	1.489939000	0.013700000
6	-4.213591000	-0.664635000	0.013629000
6	-3.321690000	-1.744463000	0.013601000
1	-3.692395000	-2.760609000	0.013569000
6	-1.946396000	-1.539783000	0.013615000
7	-7.795111000	-0.054468000	0.014418000
7	-6.459448000	0.183795000	0.014535000
6	-8.373700000	-1.320499000	0.013990000
6	-5.676542000	-0.895325000	0.013616000
7	-7.433707000	-2.347144000	0.013310000
7	-6.089499000	-2.162954000	0.012873000
8	-9.574931000	-1.509855000	0.013976000
6	-8.639366000	1.137331000	0.015474000
1	-8.424383000	1.729972000	0.906322000
1	-8.421606000	1.733211000	-0.872499000
1	-9.678843000	0.822669000	0.013368000
6	-7.870350000	-3.740868000	0.012229000
1	-7.483840000	-4.238499000	-0.878855000
1	-7.479431000	-4.240962000	0.899964000
1	-8.956216000	-3.761251000	0.014795000
7	5.749456000	-5.264141000	0.013317000
7	4.917866000	-4.192108000	0.012861000
6	5.330334000	-6.591518000	0.014052000
6	3.613575000	-4.468300000	0.013633000
7	3.944621000	-6.723474000	0.014505000
7	3.070473000	-5.685872000	0.014600000
8	6.094939000	-7.537130000	0.014059000
6	7.174788000	-4.945445000	0.012207000
1	7.412490000	-4.361915000	-0.878889000
1	7.412447000	-4.356826000	0.899920000
1	7.735369000	-5.875645000	0.014785000
6	3.334591000	-8.050501000	0.015616000
1	2.713870000	-8.160572000	0.906482000
1	2.709649000	-8.159849000	-0.872347000
1	4.126810000	-8.793409000	0.013524000
7	3.850518000	6.777822000	0.014390000
7	3.388923000	5.502014000	0.014489000
6	3.043468000	7.911956000	0.014043000
6	2.062910000	5.363650000	0.013629000
7	1.684336000	7.611313000	0.013419000
7	1.171643000	6.355152000	0.012962000
8	3.480163000	9.046901000	0.014046000
6	5.304788000	6.912928000	0.015374000
1	5.710518000	6.430347000	0.906188000
1	5.711842000	6.426372000	-0.872632000
1	5.552176000	7.970438000	0.013285000

6	0.695786000	8.686444000	0.012429000
1	0.071509000	8.600657000	-0.878624000
1	0.067272000	8.598013000	0.900198000
1	1.221193000	9.636954000	0.014996000

4c, $\omega_1 = 12 \text{ cm}^{-1}$

8	-4.131722000	-0.260791000	-0.023860000
8	2.291321000	-3.448030000	-0.030063000
6	-2.365203000	3.558206000	-0.028621000
6	-2.974334000	2.287651000	-0.047347000
1	-4.049712000	2.191762000	-0.071738000
6	-2.210405000	1.127967000	-0.033935000
6	-2.911756000	-0.183892000	-0.025444000
6	-2.051178000	-1.397275000	-0.019300000
6	-0.636872000	-1.283425000	-0.027825000
6	-0.000150000	-0.000290000	-0.028506000
6	-0.793005000	1.192685000	-0.028247000
6	-2.663274000	-2.643808000	-0.005388000
1	-3.742142000	-2.683921000	0.021582000
6	-1.899248000	-3.827545000	-0.027190000
6	-0.494472000	-3.719928000	-0.049024000
1	0.126178000	-4.603307000	-0.075614000
6	0.127946000	-2.478531000	-0.035729000
6	1.614734000	-2.429963000	-0.029554000
8	1.839954000	3.708058000	-0.031506000
6	-0.957912000	3.627840000	-0.009472000
1	-0.453138000	4.582221000	0.014895000
6	-0.184490000	2.474453000	-0.022464000
6	1.296614000	2.613075000	-0.030384000
6	2.082064000	1.349725000	-0.036805000
6	1.429403000	0.089874000	-0.029358000
6	3.468333000	1.431466000	-0.049963000
1	3.922993000	2.410679000	-0.075572000
6	4.264184000	0.268702000	-0.029267000
6	3.620796000	-0.984862000	-0.009231000
1	4.194884000	-1.899191000	0.016236000
6	2.235233000	-1.077974000	-0.022527000
6	5.715835000	0.360447000	-0.028179000
7	6.575011000	-0.628056000	0.349426000
8	6.270934000	-1.785416000	0.774231000
6	7.999980000	-0.128731000	0.431856000
6	7.921139000	1.134577000	-0.481667000
7	6.444186000	1.449573000	-0.403802000
8	5.997458000	2.559315000	-0.829636000
6	8.254595000	0.184010000	1.916642000
1	7.580221000	0.955545000	2.293318000
1	9.283252000	0.515807000	2.069186000
1	8.093643000	-0.725353000	2.497678000
6	8.953681000	-1.223720000	-0.040545000
1	8.873426000	-2.083190000	0.624884000
1	9.982195000	-0.855776000	-0.010301000
1	8.731451000	-1.560536000	-1.052314000
6	8.726917000	2.341511000	-0.006490000
1	9.793860000	2.106911000	-0.033459000
1	8.460567000	2.647155000	1.004517000
1	8.540437000	3.184022000	-0.672309000
6	8.217925000	0.856999000	-1.965632000

1	7.648313000	0.006014000	-2.344193000
1	9.280879000	0.658875000	-2.115253000
1	7.944277000	1.738607000	-2.547314000
6	-2.545683000	-5.130547000	-0.027140000
7	-3.828607000	-5.381710000	0.358210000
8	-4.675263000	-4.541287000	0.793270000
6	-4.108495000	-6.865835000	0.435133000
6	-2.981377000	-7.424949000	-0.488916000
7	-1.969318000	-6.303904000	-0.412460000
8	-0.787995000	-6.469361000	-0.847792000
6	-3.955068000	-7.250071000	1.917007000
1	-2.947035000	-7.054174000	2.287706000
1	-4.181617000	-8.307418000	2.065942000
1	-4.657776000	-6.658476000	2.505790000
6	-5.536972000	-7.141327000	-0.028955000
1	-6.236325000	-6.644428000	0.643307000
1	-5.733251000	-8.215993000	-0.002002000
1	-5.724107000	-6.775989000	-1.037929000
6	-2.335927000	-8.728643000	-0.024642000
1	-3.072597000	-9.535345000	-0.051045000
1	-1.931564000	-8.656018000	0.984174000
1	-1.517346000	-8.984750000	-0.697139000
6	-3.380244000	-7.535846000	-1.970742000
1	-3.834561000	-6.615060000	-2.341794000
1	-4.084703000	-8.356291000	-2.119496000
1	-2.483984000	-7.737253000	-2.559488000
6	-3.170343000	4.769596000	-0.028990000
7	-4.477192000	4.855753000	-0.406425000
8	-5.214467000	3.913725000	-0.832360000
6	-4.942322000	6.292403000	-0.486443000
6	-3.888809000	6.992917000	0.427904000
7	-2.744031000	6.008079000	0.348082000
8	-1.590115000	6.323457000	0.774016000
6	-4.847956000	6.686869000	-1.970611000
1	-3.825719000	6.617943000	-2.347712000
1	-5.206774000	7.706674000	-2.121514000
1	-5.474388000	6.009123000	-2.552599000
6	-6.391143000	6.387663000	-0.013629000
1	-7.026606000	5.804435000	-0.679925000
1	-6.721157000	7.429010000	-0.042150000
1	-6.524470000	6.005155000	0.997519000
6	-3.415990000	8.365693000	-0.045146000
1	-4.248387000	9.073102000	-0.016496000
1	-3.011862000	8.340568000	-1.056368000
1	-2.632108000	8.725934000	0.620952000
6	-4.289011000	7.058685000	1.912043000
1	-4.620808000	6.089378000	2.289235000
1	-5.090633000	7.784061000	2.062857000
1	-3.421699000	7.374231000	2.493988000

4d, $\omega_1 = 5 \text{ cm}^{-1}$

8	2.820516000	3.030845000	-0.020696000
8	-4.032982000	0.925185000	-0.020287000
6	4.170509000	-0.956509000	-0.019759000
6	3.733688000	0.374101000	-0.019942000
1	4.439040000	1.196822000	-0.020045000
6	2.380481000	0.701630000	-0.019985000

6	1.985468000	2.133043000	-0.020190000
6	0.529935000	2.422355000	-0.020349000
6	-0.418537000	1.369600000	-0.020108000
6	0.001635000	-0.000503000	-0.019868000
6	1.398274000	-0.321642000	-0.019830000
6	0.101201000	3.749007000	-0.020724000
1	0.862685000	4.521182000	-0.020964000
6	-1.254927000	4.087868000	-0.020758000
6	-2.188793000	3.044219000	-0.020408000
1	-3.253963000	3.243746000	-0.020344000
6	-1.795826000	1.708589000	-0.020142000
6	-2.837943000	0.650864000	-0.019897000
8	1.217350000	-3.957398000	-0.019737000
6	3.198906000	-1.961462000	-0.019632000
1	3.486845000	-3.007034000	-0.019508000
6	1.835636000	-1.669442000	-0.019651000
6	0.857315000	-2.785340000	-0.019482000
6	-0.579863000	-2.411787000	-0.019783000
6	-0.974791000	-1.049468000	-0.019854000
6	-1.540221000	-3.419914000	-0.019971000
1	-1.180609000	-4.442216000	-0.019909000
6	-2.910945000	-3.132705000	-0.020225000
6	-3.295264000	-1.788751000	-0.020189000
1	-4.344685000	-1.515197000	-0.020331000
6	-2.360713000	-0.754270000	-0.019984000
8	-3.962775000	9.027379000	-0.016107000
7	-3.407536000	7.874477000	-0.017078000
6	-1.686234000	5.542700000	-0.020657000
1	-0.771042000	6.142088000	-0.023320000
6	-2.512135000	5.901552000	1.225411000
1	-1.965447000	5.638944000	2.136059000
1	-3.427862000	5.300596000	1.224336000
6	-2.895767000	7.391302000	1.312248000
6	-2.902839000	7.390142000	-1.348682000
6	-2.518691000	5.900467000	-1.262614000
1	-3.434446000	5.299618000	-1.256281000
1	-1.976815000	5.637114000	-2.175921000
6	-4.035288000	7.558812000	2.329521000
1	-4.306276000	8.608325000	2.437060000
1	-3.715538000	7.173065000	3.301225000
1	-4.922517000	7.006110000	2.011669000
6	-1.697775000	8.262206000	1.744460000
1	-0.820183000	8.111146000	1.113297000
1	-1.417600000	8.020870000	2.773390000
1	-1.975875000	9.316441000	1.699485000
6	-1.707222000	8.260725000	-1.788076000
1	-1.985116000	9.314988000	-1.742485000
1	-1.432605000	8.018531000	-2.818301000
1	-0.826225000	8.110225000	-1.161544000
6	-4.047783000	7.556727000	-2.360004000
1	-4.319364000	8.606139000	-2.467030000
1	-4.933290000	7.004295000	-2.036925000
1	-3.733224000	7.170119000	-3.333060000
8	-5.849678000	-7.938851000	-0.018131000
7	-5.124514000	-6.884509000	-0.018560000
6	-3.956473000	-4.232318000	-0.020263000
1	-4.932163000	-3.737497000	-0.021659000

6	-3.855581000	-5.128825000	1.224705000
1	-3.898410000	-4.525117000	2.136179000
1	-2.878918000	-5.624635000	1.221776000
6	-4.957350000	-6.202360000	1.311456000
6	-4.955005000	-6.205058000	-1.349661000
6	-3.853341000	-5.131388000	-1.263155000
1	-2.876755000	-5.627304000	-1.257480000
1	-3.894504000	-4.529581000	-2.175965000
6	-4.534341000	-7.276160000	2.326155000
1	-5.309826000	-8.033528000	2.433395000
1	-4.357286000	-6.808794000	3.298517000
1	-3.614004000	-7.770253000	2.005921000
6	-6.307972000	-5.596892000	1.746956000
1	-6.614990000	-4.760066000	1.117025000
1	-6.236074000	-5.234636000	2.776047000
1	-7.084093000	-6.362692000	1.702845000
6	-6.304847000	-5.600454000	-1.788759000
1	-7.081065000	-6.366143000	-1.744404000
1	-6.231150000	-5.240340000	-2.818474000
1	-6.612941000	-4.762315000	-1.161104000
6	-4.530255000	-7.280930000	-2.361435000
1	-5.305582000	-8.038481000	-2.468510000
1	-3.610507000	-7.774413000	-2.038576000
1	-4.351460000	-6.815545000	-3.334429000
8	9.802325000	-1.089217000	-0.016916000
7	8.526462000	-0.991098000	-0.017544000
6	5.645929000	-1.311069000	-0.019462000
1	5.706365000	-2.403402000	-0.020398000
6	6.370697000	-0.773699000	1.225285000
1	5.869872000	-1.113281000	2.136843000
1	6.309547000	0.319883000	1.221933000
6	7.852257000	-1.187876000	1.312533000
6	7.853731000	-1.185602000	-1.348707000
6	6.372093000	-0.771503000	-1.262401000
1	6.311075000	0.322072000	-1.257213000
1	5.872291000	-1.109434000	-2.175136000
6	8.568545000	-0.282530000	2.326800000
1	9.612885000	-0.572920000	2.434055000
1	8.075511000	-0.363677000	3.299216000
1	8.533752000	0.761347000	2.006161000
6	8.006091000	-2.659703000	1.749007000
1	7.436979000	-3.345582000	1.118940000
1	7.655705000	-2.778732000	2.777839000
1	9.058004000	-2.946741000	1.706011000
6	8.008026000	-2.656684000	-1.787516000
1	9.059889000	-2.943805000	-1.743850000
1	7.658774000	-2.773952000	-2.816936000
1	7.438217000	-3.343634000	-1.159251000
6	8.571182000	-0.278553000	-2.360627000
1	9.615628000	-0.568803000	-2.467221000
1	8.536077000	0.764775000	-2.038243000
1	8.079223000	-0.358014000	-3.333728000

1e ($n = 2$), $\omega_1 = 7 \text{ cm}^{-1}$

6	2.276422000	0.907127000	0.202829000
6	0.875990000	1.120071000	0.204555000
6	2.808093000	-0.392427000	0.200840000

6	0.000003000	-0.000240000	0.204328000
6	1.932151000	-1.495362000	0.200701000
6	0.532261000	-1.319019000	0.202447000
1	2.907380000	1.779523000	0.203218000
6	0.328760000	2.420551000	0.206443000
6	-1.408210000	0.198272000	0.206045000
6	-0.352384000	-2.425388000	0.202353000
6	-1.924067000	1.517587000	0.207895000
6	-1.064349000	2.627780000	0.207980000
1	0.974848000	3.286327000	0.206699000
6	-2.260820000	-0.925923000	0.205955000
1	-2.995123000	1.627601000	0.209535000
6	-1.743652000	-2.235993000	0.204135000
1	-3.333655000	-0.799377000	0.207278000
1	2.358836000	-2.487806000	0.199242000
1	0.087720000	-3.407969000	0.200836000
6	-2.963161000	4.430153000	0.207187000
7	-1.508921000	3.972951000	0.209919000
8	-0.617476000	4.889260000	0.213786000
6	-3.663018000	3.948946000	-1.078538000
1	-4.674633000	4.361734000	-1.109020000
1	-3.744414000	2.866487000	-1.157130000
1	-3.123981000	4.311588000	-1.956922000
6	-2.961994000	5.965650000	0.206265000
1	-2.463983000	6.367593000	1.088084000
1	-4.001355000	6.303559000	0.203925000
1	-2.460423000	6.366456000	-0.674084000
6	-2.354880000	-4.781732000	0.203177000
7	-2.686169000	-3.293717000	0.204160000
8	-3.925482000	-2.979947000	0.205218000
6	-1.589263000	-5.148836000	-1.082752000
1	-1.440539000	-6.231307000	-1.111810000
1	-0.611323000	-4.677906000	-1.163019000
1	-2.173790000	-4.864835000	-1.960989000
6	-3.685181000	-5.548543000	0.204403000
1	-4.281644000	-5.316807000	1.086295000
1	-3.458094000	-6.617602000	0.203670000
1	-4.283733000	-5.316029000	-0.675858000
7	4.195417000	-0.679527000	0.199070000
8	4.543696000	-1.909563000	0.198655000
6	5.318086000	0.351833000	0.197495000
6	6.647532000	-0.416449000	0.194480000
1	6.747193000	-1.050345000	1.075071000
1	7.459685000	0.314904000	0.193151000
1	6.743617000	-1.049563000	-0.687079000
6	5.250091000	1.200762000	-1.086718000
1	5.293625000	0.554155000	-1.966281000
1	6.113442000	1.870394000	-1.116889000
1	4.353373000	1.812807000	-1.163291000
6	5.254998000	1.199225000	1.482983000
1	4.358662000	1.811318000	1.563609000
1	5.301676000	0.551536000	2.361585000
1	6.118553000	1.868697000	1.510782000
6	-3.667137000	3.950401000	1.491232000
1	-3.748686000	2.868004000	1.570756000
1	-3.130867000	4.314051000	2.370888000
1	-4.678884000	4.363130000	1.518076000

6	-1.586301000	-5.149942000	1.487022000
1	-1.437968000	-6.232493000	1.515016000
1	-0.607960000	-4.679506000	1.565241000
1	-2.168589000	-4.866283000	2.366855000

1e (n = 3), $\omega_1 = 8 \text{ cm}^{-1}$

6	-2.844421000	-2.450960000	0.000091000
6	-1.522316000	-1.942120000	0.000121000
6	-0.399322000	-2.795338000	0.000122000
6	-1.315912000	-0.528671000	0.000165000
6	0.919032000	-2.290160000	0.000176000
6	1.116891000	-0.874605000	0.000233000
6	0.000391000	0.000650000	0.000224000
6	2.444157000	-0.346292000	0.000316000
6	3.545621000	-1.237278000	0.000330000
6	3.354164000	-2.628623000	0.000223000
6	2.043537000	-3.143244000	0.000167000
1	4.530546000	-0.802364000	0.000481000
6	-3.954137000	-1.589848000	0.000089000
6	-3.744283000	-0.197520000	0.000126000
6	-2.443167000	0.350091000	0.000168000
1	-4.607614000	0.451705000	0.000132000
6	-2.221341000	1.744340000	0.000212000
6	-0.920841000	2.290317000	0.000264000
6	0.200265000	1.405147000	0.000282000
1	-3.077369000	2.411267000	0.000210000
6	2.621597000	1.052923000	0.000394000
6	1.524924000	1.942161000	0.000373000
1	1.913560000	-4.215530000	0.000121000
1	-0.548529000	-3.870165000	0.000086000
6	-0.700362000	3.689628000	0.000316000
1	-1.570797000	4.323500000	0.000363000
1	3.627249000	1.460541000	0.000467000
1	-2.957839000	-3.521874000	0.000102000
6	1.701221000	3.342725000	0.000423000
6	0.600102000	4.220335000	0.000372000
1	2.695133000	3.765650000	0.000496000
7	-5.299185000	-2.033144000	0.000089000
8	-6.215243000	-1.141612000	0.000384000
6	-5.757772000	-3.486914000	-0.000249000
6	-7.293248000	-3.485413000	-0.000465000
1	-7.694477000	-2.985648000	0.880629000
1	-7.630901000	-4.524921000	-0.000739000
1	-7.694223000	-2.985274000	-0.881466000
6	-5.277538000	-4.188922000	-1.285173000
1	-5.640755000	-3.651563000	-2.164321000
1	-5.689867000	-5.200806000	-1.313979000
1	-4.194996000	-4.269173000	-1.364120000
6	-5.277890000	-4.189368000	1.284566000
1	-4.195364000	-4.269613000	1.363786000
1	-5.641365000	-3.652320000	2.163796000
1	-5.690198000	-5.201273000	1.312903000
7	4.410317000	-3.572163000	0.000239000
8	4.094979000	-4.811002000	0.000776000
6	5.899301000	-3.244207000	-0.000368000
6	6.662663000	-4.576817000	-0.000757000
1	6.429394000	-5.173757000	0.880392000

1	7.732615000	-4.353526000	-0.001261000
1	6.428561000	-5.173714000	-0.881720000
6	6.268928000	-2.477943000	-1.285182000
1	5.979237000	-3.058129000	-2.164400000
1	7.352324000	-2.336458000	-1.315847000
1	5.804260000	-1.496605000	-1.361627000
6	6.269936000	-2.478091000	1.284244000
1	5.805310000	-1.496764000	1.361153000
1	5.980919000	-3.058383000	2.163612000
1	7.353354000	-2.336590000	1.314101000
7	0.888076000	5.607079000	0.000448000
8	2.117926000	5.955323000	0.001154000
6	-0.142819000	6.730378000	-0.000280000
6	0.625484000	8.059851000	-0.000444000
1	1.258658000	8.158180000	0.880805000
1	-0.106060000	8.871931000	-0.000991000
1	1.259304000	8.157578000	-0.881302000
6	-0.989965000	6.665549000	-1.285800000
1	-0.342051000	6.714704000	-2.164040000
1	-1.661942000	7.527212000	-1.313146000
1	-1.598865000	5.767300000	-1.367781000
6	-0.990842000	6.666357000	1.284706000
1	-1.599686000	5.768085000	1.366890000
1	-0.343529000	6.716196000	2.163351000
1	-1.662946000	7.527954000	1.310999000

1e (n = 4), $\omega_1 = 10 \text{ cm}^{-1}$

6	-3.471697000	-3.759727000	0.000487000
6	-2.807279000	-2.514848000	0.000507000
6	-2.757258000	-4.972806000	0.000477000
6	-1.377690000	-2.484177000	0.000529000
6	-1.353172000	-4.940688000	0.000547000
6	-0.648089000	-3.712357000	0.000562000
1	-4.551114000	-3.799442000	0.000467000
6	-3.517082000	-1.294698000	0.000480000
6	0.761846000	-3.668883000	0.000615000
1	-4.601783000	-1.318080000	0.000469000
1	-0.766195000	-5.843546000	0.000643000
1	1.319887000	-4.599837000	0.000653000
6	1.471216000	-2.450016000	0.000606000
6	0.731603000	-1.217655000	0.000547000
6	-0.688516000	-1.242831000	0.000525000
6	-1.420002000	-0.024583000	0.000478000
6	2.880096000	-2.398722000	0.000644000
6	-2.857055000	-0.048946000	0.000467000
6	-3.557948000	1.174800000	0.000434000
1	-4.643196000	1.157008000	0.000427000
1	3.442696000	-3.326410000	0.000694000
6	-0.731746000	1.217870000	0.000466000
6	0.689017000	1.242244000	0.000480000
6	1.420880000	0.024953000	0.000530000
6	1.386433000	2.498959000	0.000468000
6	2.796675000	2.494066000	0.000481000
6	3.539280000	1.294755000	0.000508000
6	2.840500000	0.048790000	0.000546000
6	-1.462201000	2.435393000	0.000424000

6	0.637572000	3.693450000	0.000439000
1	3.323896000	3.442813000	0.000466000
6	4.955554000	1.298301000	0.000514000
6	3.581887000	-1.173940000	0.000614000
6	4.992213000	-1.126851000	0.000626000
6	5.685448000	0.098462000	0.000546000
1	5.444120000	2.257938000	0.000570000
1	5.566417000	-2.041732000	0.000685000
6	-0.774014000	3.688828000	0.000419000
6	-2.890621000	2.417556000	0.000405000
1	1.159678000	4.644517000	0.000434000
6	-1.519981000	4.886666000	0.000383000
6	-3.601849000	3.642300000	0.000373000
6	-2.927757000	4.874339000	0.000339000
1	-1.014782000	5.841389000	0.000387000
1	-4.677199000	3.585508000	0.000445000
7	7.100051000	0.032602000	0.000589000
8	7.637290000	-1.127250000	0.001549000
6	8.047572000	1.226799000	-0.000618000
6	9.480968000	0.676120000	-0.001184000
1	9.677219000	0.066197000	0.880068000
1	10.168748000	1.525527000	-0.002163000
1	9.676080000	0.065097000	-0.881932000
6	7.849844000	2.053566000	-1.285850000
1	7.995202000	1.420945000	-2.164593000
1	8.597854000	2.850038000	-1.315762000
1	6.868222000	2.517192000	-1.364552000
6	7.851352000	2.054902000	1.283992000
1	6.869832000	2.518645000	1.363329000
1	7.997679000	1.423170000	2.163213000
1	8.599422000	2.851380000	1.312245000
7	-3.578098000	6.132310000	0.000345000
8	-2.842291000	7.177535000	0.001100000
6	-5.086022000	6.355774000	-0.000549000
6	-5.325874000	7.872459000	-0.000726000
1	-4.895627000	8.347165000	0.880558000
1	-6.405377000	8.043361000	-0.001453000
1	-4.894451000	8.347131000	-0.881459000
6	-5.703347000	5.771443000	-1.285838000
1	-5.228117000	6.213707000	-2.164524000
1	-6.767070000	6.021183000	-1.315629000
1	-5.614230000	4.689524000	-1.364745000
6	-5.704803000	5.771487000	1.284064000
1	-5.615745000	4.689568000	1.363100000
1	-5.230564000	6.213790000	2.163265000
1	-6.768566000	6.021200000	1.312653000
7	-3.521908000	-6.164790000	0.000454000
8	-4.794959000	-6.049762000	0.001106000
6	-2.962064000	-7.582642000	-0.000522000
6	-4.156006000	-8.548254000	-0.001390000
1	-4.782558000	-8.412991000	0.879671000
1	-3.764616000	-9.568735000	-0.002197000
1	-4.782420000	-8.411552000	-0.882333000
6	-2.146921000	-7.825070000	-1.285512000
1	-2.767345000	-7.635084000	-2.164432000
1	-1.830861000	-8.871014000	-1.314997000
1	-1.254874000	-7.206436000	-1.364083000

6	-2.147266000	-7.826927000	1.284339000
1	-1.255223000	-7.208423000	1.364015000
1	-2.767922000	-7.638162000	2.163357000
1	-1.831235000	-8.872919000	1.312435000

1e (n = 5), $\omega_1 = 11 \text{ cm}^{-1}$

6	0.000077000	-0.077580000	4.914132000
6	0.000058000	0.667071000	3.717816000
6	0.000281000	-1.488845000	4.914070000
6	0.004419000	-0.033225000	2.461741000
6	0.001434000	-2.180623000	3.662521000
6	-0.001870000	-1.454516000	2.442181000
1	-0.001269000	0.447974000	5.863256000
6	-0.000133000	2.076819000	3.711090000
6	0.004403000	-2.148125000	1.201963000
1	-0.002213000	2.606295000	4.658406000
6	-0.003393000	-1.423662000	-0.019535000
6	0.007544000	0.000195000	0.000034000
6	-0.003477000	0.695175000	1.242919000
6	0.004263000	2.115245000	1.259580000
6	0.004526000	-2.114981000	-1.259752000
6	-0.000007000	2.819476000	2.512898000
6	-0.000016000	4.228918000	2.502426000
1	-0.001262000	4.760019000	3.449046000
6	-0.001977000	2.842494000	0.038774000
6	0.004380000	2.148781000	-1.201884000
6	-0.003466000	0.729064000	-1.223295000
6	0.000042000	2.886403000	-2.436416000
6	-0.000103000	2.175704000	-3.653937000
6	0.000064000	0.766718000	-3.698010000
6	0.004338000	0.033454000	-2.461447000
6	0.001304000	4.262383000	0.057434000
6	0.000045000	4.294755000	-2.389687000
1	-0.002177000	2.731370000	-4.586132000
6	0.000093000	0.052912000	-4.913393000
6	-0.001841000	-1.387404000	-2.480867000
6	0.001485000	-2.081198000	-3.719854000
6	0.000359000	-1.356920000	-4.951233000
1	-0.001166000	0.607166000	-5.846647000
6	0.000203000	5.000331000	-1.167464000
6	0.000199000	4.966593000	1.300391000
1	-0.001273000	4.853946000	-3.319390000
6	0.000201000	6.410694000	-1.125671000
6	0.000043000	6.382807000	1.299021000
6	0.000143000	7.108593000	0.096840000
1	0.000043000	6.981211000	-2.042864000
1	-0.000195000	6.874567000	2.257044000
6	0.000439000	-3.510946000	-3.746451000
6	0.000310000	-4.216638000	-2.524300000
6	0.000260000	-3.552921000	-1.281287000
6	0.000128000	-4.251978000	-0.057054000
1	-0.000959000	-5.301380000	-2.543725000
1	-0.001882000	-5.337116000	-0.072174000
6	0.000215000	-3.585644000	1.185183000
6	0.000238000	-4.281302000	2.411024000
1	-0.000948000	-5.366650000	2.397660000
6	0.000272000	-2.230262000	6.114583000

6	0.000399000	-3.609150000	3.650874000
6	0.000245000	-4.316098000	4.878012000
6	0.000272000	-3.637946000	6.107674000
1	0.000063000	-1.721229000	7.067276000
1	0.000047000	-5.391645000	4.824776000
6	0.000453000	-4.179971000	-4.988712000
6	0.000221000	-2.066234000	-6.177053000
6	0.000362000	-3.470297000	-6.204431000
1	-0.000068000	-1.482256000	-7.081878000
1	0.000325000	-5.259546000	-5.024078000
7	0.000227000	-4.283764000	7.367991000
8	0.001008000	-3.544085000	8.410452000
6	-0.000663000	-5.790813000	7.596947000
6	-0.000880000	-6.025110000	9.114505000
1	0.880359000	-5.593071000	9.587668000
1	-0.001553000	-7.103974000	9.289399000
1	-0.881637000	-5.591986000	9.587576000
6	-1.285940000	-6.410193000	7.014762000
1	-2.164631000	-5.933470000	7.455400000
1	-1.315717000	-7.473058000	7.268141000
1	-1.364861000	-6.324691000	5.932537000
6	1.283954000	-6.411716000	7.014912000
1	1.362948000	-6.326618000	5.932661000
1	2.163156000	-5.935804000	7.455404000
1	1.312606000	-7.474542000	7.268584000
7	0.000131000	8.522966000	0.025804000
8	0.001167000	9.055778000	-1.136065000
6	-0.001098000	9.474927000	1.216397000
6	-0.001341000	10.906231000	0.660301000
1	0.880016000	11.100010000	0.049739000
1	-0.002298000	11.597246000	1.507077000
1	-0.881965000	11.099187000	0.048419000
6	-1.286499000	9.280439000	2.043675000
1	-2.165113000	9.423768000	1.410416000
1	-1.316372000	10.031257000	2.837508000
1	-1.365498000	8.300421000	2.510665000
6	1.283341000	9.281585000	2.045451000
1	1.362376000	8.301792000	2.512907000
1	2.162698000	9.425285000	1.413312000
1	1.311653000	10.032698000	2.839062000
7	0.000338000	-4.239317000	-7.393627000
8	0.001243000	-5.511900000	-7.273766000
6	-0.000716000	-3.684799000	-8.813509000
6	-0.000877000	-4.882374000	-9.774622000
1	0.880446000	-5.508016000	-9.636858000
1	-0.001692000	-4.494863000	-10.796583000
1	-0.881538000	-5.508694000	-9.635708000
6	-1.286077000	-2.871183000	-9.059069000
1	-2.164706000	-3.491402000	-8.867092000
1	-1.315532000	-2.558784000	-10.106115000
1	-1.365246000	-1.977071000	-8.443476000
6	1.283775000	-2.870279000	-9.060661000
1	1.362879000	-1.975870000	-8.445493000
1	2.163075000	-3.489751000	-8.869357000
1	1.311921000	-2.558237000	-10.107850000

2e, $\omega_1 = 8 \text{ cm}^{-1}$

7	-1.364391000	1.950626000	0.536086000
6	-1.197333000	0.608090000	0.486263000
6	-0.251130000	2.694140000	0.550251000
6	0.098706000	0.045646000	0.454350000
7	1.019830000	2.267920000	0.521110000
6	1.200024000	0.933090000	0.473285000
6	-2.320278000	-0.252007000	0.465059000
6	0.290003000	-1.356819000	0.403737000
6	2.517848000	0.405824000	0.440486000
6	-0.849902000	-2.195189000	0.383956000
6	-2.149536000	-1.648506000	0.413199000
1	-3.315915000	0.163753000	0.488078000
6	1.609217000	-1.854587000	0.373544000
1	-0.685327000	-3.258267000	0.343573000
6	2.722479000	-0.979403000	0.391256000
1	1.797606000	-2.917650000	0.335848000
1	3.318283000	1.124482000	0.456464000
7	-3.329874000	-2.431657000	0.390315000
8	-4.445967000	-1.812299000	0.393033000
6	-3.389067000	-3.956409000	0.366878000
6	-4.871499000	-4.356163000	0.375596000
1	-5.381185000	-3.990326000	1.266473000
1	-4.926269000	-5.447544000	0.361982000
1	-5.398101000	-3.967378000	-0.495340000
6	-2.755571000	-4.486397000	-0.934089000
1	-3.255646000	-4.047752000	-1.800669000
1	-2.891739000	-5.569843000	-0.978934000
1	-1.689623000	-4.284156000	-1.022569000
6	-2.729321000	-4.527371000	1.636786000
1	-1.662584000	-4.324409000	1.711438000
1	-3.213675000	-4.119790000	2.527131000
1	-2.861733000	-5.612107000	1.647752000
7	4.002365000	-1.581292000	0.358487000
8	4.049513000	-2.857309000	0.330266000
6	5.336560000	-0.838793000	0.349611000
6	6.446554000	-1.898173000	0.297013000
1	6.414779000	-2.558548000	1.163198000
1	7.407481000	-1.378063000	0.286804000
1	6.372412000	-2.514494000	-0.598568000
6	5.440928000	0.035368000	-0.914432000
1	5.314081000	-0.579613000	-1.808562000
1	6.436586000	0.484153000	-0.952699000
1	4.713265000	0.843925000	-0.953648000
6	5.498027000	-0.033946000	1.653417000
1	4.786829000	0.782931000	1.760864000
1	5.391915000	-0.693074000	2.518268000
1	6.501787000	0.397363000	1.680138000
7	-0.418039000	4.100633000	0.602007000
8	0.623571000	4.825804000	0.626430000
6	-1.779314000	4.799806000	0.630123000
6	-1.506040000	6.308262000	0.673720000
1	-0.940868000	6.591252000	1.561899000
1	-2.469715000	6.823162000	0.692274000
1	-0.947572000	6.642943000	-0.200698000
6	-2.562290000	4.465216000	-0.651631000
1	-1.977893000	4.730594000	-1.536677000

1	-3.483105000	5.054714000	-0.668041000
1	-2.824303000	3.410777000	-0.701837000
6	-2.547826000	4.387977000	1.898153000
1	-2.806185000	3.331406000	1.888347000
1	-1.954321000	4.602338000	2.790918000
1	-3.469881000	4.972583000	1.959119000

3e, $\omega_1 = 13 \text{ cm}^{-1}$

8	1.082635000	3.772628000	0.371683000
6	-1.963587000	1.868827000	0.599940000
6	-1.479970000	0.544612000	0.460682000
6	-2.356694000	-0.566837000	0.506998000
6	-1.133564000	2.958648000	0.535003000
6	0.327012000	2.805385000	0.371346000
8	-0.060287000	-3.304778000	0.059318000
6	-1.911166000	-1.854542000	0.347485000
6	-0.479150000	-2.152540000	0.163044000
6	0.432168000	-0.980527000	0.110776000
6	-0.072534000	0.325716000	0.252783000
6	1.798726000	-1.194179000	-0.061428000
1	2.121463000	-2.219361000	-0.136742000
6	2.690121000	-0.115129000	-0.107025000
6	2.187516000	1.190088000	0.041479000
1	2.867981000	2.029178000	0.025328000
6	0.826893000	1.412796000	0.214944000
1	-3.020788000	2.029542000	0.779796000
1	-3.412541000	-0.399357000	0.688745000
7	4.095813000	-0.261156000	-0.268989000
8	4.812168000	0.763887000	-0.005957000
6	4.810038000	-1.518339000	-0.745692000
6	6.262733000	-1.125349000	-1.050155000
1	6.314313000	-0.349554000	-1.815053000
1	6.784208000	-2.013113000	-1.415763000
1	6.775075000	-0.757447000	-0.162612000
6	4.808814000	-2.571562000	0.379211000
1	5.261757000	-2.156999000	1.282621000
1	5.405256000	-3.431975000	0.065079000
1	3.814539000	-2.937117000	0.633977000
6	4.163644000	-2.035973000	-2.043847000
1	3.145832000	-2.400190000	-1.915794000
1	4.154266000	-1.250693000	-2.803583000
1	4.762142000	-2.866211000	-2.426036000
7	-1.679430000	4.258375000	0.777059000
8	-2.243870000	4.410254000	1.921596000
6	-1.713088000	5.408500000	-0.196469000
6	-3.182185000	5.855197000	-0.302986000
1	-3.804788000	5.062717000	-0.727910000
1	-3.249244000	6.729350000	-0.955152000
1	-3.576635000	6.118777000	0.678203000
6	-0.842935000	6.539388000	0.373880000
1	-1.202517000	6.827452000	1.363347000
1	-0.894911000	7.412375000	-0.282394000
1	0.195566000	6.217208000	0.456243000
6	-1.203909000	4.956872000	-1.569914000
1	-0.143125000	4.709266000	-1.550491000
1	-1.768547000	4.099959000	-1.948183000
1	-1.341804000	5.778101000	-2.276928000

7	-2.838847000	-2.933315000	0.499325000
8	-3.380099000	-3.030995000	1.660605000
6	-3.254386000	-3.908292000	-0.570879000
6	-2.777566000	-5.307536000	-0.150981000
1	-1.689347000	-5.335751000	-0.086174000
1	-3.111480000	-6.047103000	-0.883795000
1	-3.195486000	-5.569743000	0.822461000
6	-4.790884000	-3.858080000	-0.644668000
1	-5.229107000	-4.085083000	0.327218000
1	-5.145527000	-4.593885000	-1.370612000
1	-5.137552000	-2.870321000	-0.961252000
6	-2.650844000	-3.501450000	-1.919727000
1	-2.933255000	-2.482746000	-2.199602000
1	-1.564350000	-3.586656000	-1.921418000
1	-3.039159000	-4.172797000	-2.689059000

4e, $\omega_1 = 15 \text{ cm}^{-1}$

8	-4.126012000	0.271830000	0.113390000
8	2.305834000	3.438269000	0.151674000
6	-2.378433000	-3.536649000	0.124238000
6	-2.979726000	-2.275474000	0.129994000
1	-4.050140000	-2.145077000	0.159613000
6	-2.207090000	-1.115735000	0.124944000
6	-2.902693000	0.196241000	0.126925000
6	-2.041801000	1.405502000	0.139836000
6	-0.627603000	1.284556000	0.134580000
6	0.003860000	-0.001583000	0.131457000
6	-0.794393000	-1.191586000	0.128452000
6	-2.641594000	2.658793000	0.145407000
1	-3.720397000	2.729533000	0.158087000
6	-1.866281000	3.827531000	0.141956000
6	-0.473625000	3.719014000	0.155290000
1	0.173096000	4.581842000	0.196518000
6	0.144833000	2.470133000	0.143780000
6	1.628645000	2.416538000	0.152758000
8	1.831481000	-3.715273000	0.132062000
6	-0.978307000	-3.623182000	0.139994000
1	-0.499781000	-4.592425000	0.157963000
6	-0.192769000	-2.477119000	0.139809000
6	1.285049000	-2.618098000	0.139056000
6	2.073524000	-1.359771000	0.140430000
6	1.433179000	-0.097857000	0.139218000
6	3.464176000	-1.448601000	0.153148000
1	3.888534000	-2.439984000	0.186374000
6	4.254877000	-0.296958000	0.149704000
6	3.630544000	0.958985000	0.163426000
1	4.230826000	1.857922000	0.184792000
6	2.245370000	1.066145000	0.156052000
7	-3.117350000	-4.755380000	0.153124000
8	-2.524652000	-5.765186000	0.670614000
6	-4.525377000	-4.950558000	-0.379745000
6	-4.707281000	-6.455730000	-0.627284000
1	-3.970204000	-6.831115000	-1.339511000
1	-5.705316000	-6.617782000	-1.040862000
1	-4.609992000	-7.028743000	0.292961000
6	-5.540473000	-4.486307000	0.682407000
1	-5.369635000	-5.015331000	1.622537000

1	-6.553513000	-4.714892000	0.341321000
1	-5.492797000	-3.414464000	0.878185000
6	-4.700764000	-4.207902000	-1.715859000
1	-4.671873000	-3.123242000	-1.623362000
1	-3.932591000	-4.513031000	-2.430735000
1	-5.673884000	-4.472831000	-2.135442000
7	-2.552213000	5.076974000	0.177926000
8	-3.709991000	5.071626000	0.724638000
6	-2.033478000	6.389119000	-0.381072000
6	-3.257371000	7.278927000	-0.646484000
1	-3.947662000	6.802700000	-1.345411000
1	-2.911258000	8.218059000	-1.084367000
1	-3.801969000	7.496499000	0.270419000
6	-1.131520000	7.066488000	0.668419000
1	-1.672705000	7.183724000	1.609771000
1	-0.843424000	8.059754000	0.314340000
1	-0.215502000	6.507997000	0.865512000
6	-1.297615000	6.151959000	-1.710688000
1	-0.368126000	5.595137000	-1.602320000
1	-1.938057000	5.619518000	-2.418209000
1	-1.047775000	7.121321000	-2.148129000
7	5.679782000	-0.328854000	0.184386000
8	6.255995000	0.675720000	0.730228000
6	6.554164000	-1.435150000	-0.377579000
6	7.938927000	-0.823533000	-0.638756000
1	7.875823000	0.011298000	-1.339347000
1	8.579174000	-1.594863000	-1.073026000
1	8.396952000	-0.460636000	0.279483000
6	6.684918000	-2.559576000	0.667590000
1	7.068205000	-2.156602000	1.607610000
1	7.390317000	-3.312106000	0.305707000
1	5.739138000	-3.063744000	0.870165000
6	5.981508000	-1.946342000	-1.710753000
1	5.038164000	-2.480547000	-1.606863000
1	5.835093000	-1.120187000	-2.410863000
1	6.699980000	-2.639104000	-2.154852000

(4a)₂

8	-1.282562000	-1.829396000	-0.903240000
8	-2.941781000	5.098493000	-0.500118000
6	-5.323228000	-2.914439000	-0.795812000
6	-3.971292000	-2.580575000	-0.827991000
1	-3.216829000	-3.352438000	-0.901814000
6	-3.568583000	-1.257005000	-0.776174000
6	-2.120510000	-0.950785000	-0.831336000
6	-1.741797000	0.481983000	-0.806551000
6	-2.726114000	1.487902000	-0.702825000
6	-4.116377000	1.151388000	-0.641936000
6	-4.522464000	-0.220183000	-0.688973000
6	-0.402415000	0.817613000	-0.904392000
1	0.328343000	0.024479000	-0.990955000
6	0.000500000	2.151099000	-0.904495000
6	-0.960658000	3.151701000	-0.778431000
1	-0.668875000	4.193508000	-0.766952000
6	-2.304703000	2.834581000	-0.676795000
6	-3.290947000	3.935150000	-0.555127000
8	-8.121683000	0.186889000	-0.599371000

6	-6.273645000	-1.899915000	-0.713794000
1	-7.328653000	-2.137791000	-0.693113000
6	-5.888970000	-0.571259000	-0.659448000
6	-6.937917000	0.472129000	-0.591936000
6	-6.476980000	1.877835000	-0.526934000
6	-5.100227000	2.187735000	-0.556597000
6	-7.421751000	2.886829000	-0.453029000
1	-8.469619000	2.618696000	-0.436023000
6	-7.034378000	4.223799000	-0.405065000
6	-5.678735000	4.541908000	-0.435542000
1	-5.356019000	5.574120000	-0.408203000
6	-4.720010000	3.546134000	-0.510557000
16	-5.362787000	-6.808022000	-0.956584000
16	-7.420729000	-6.197180000	-0.936737000
7	-4.810644000	-5.274896000	-0.887378000
7	-7.045713000	-4.609945000	-0.869512000
6	-5.744589000	-4.327670000	-0.853660000
16	3.367012000	4.067035000	-1.326194000
16	3.860342000	1.983537000	-1.398138000
7	1.774837000	3.780599000	-1.106767000
7	2.313068000	1.511965000	-1.188864000
6	1.426663000	2.497191000	-1.066892000
16	-10.391585000	6.199796000	-0.255589000
16	-8.833294000	7.674371000	-0.182322000
7	-9.338198000	4.955785000	-0.338633000
7	-7.646092000	6.558059000	-0.255951000
6	-8.049981000	5.292188000	-0.329999000
8	2.324254000	2.511992000	-4.605492000
8	-4.515859000	4.523057000	-4.290591000
6	1.239473000	-1.525205000	-4.807162000
6	1.626006000	-0.188081000	-4.756778000
1	2.673682000	0.080776000	-4.774187000
6	0.680614000	0.820127000	-4.680068000
6	1.140662000	2.226032000	-4.612848000
6	0.091076000	3.268596000	-4.542897000
6	-1.275171000	2.916554000	-4.512935000
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1	1.529740000	4.836022000	-4.507417000
6	-0.476130000	5.611145000	-4.401738000
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6	-0.115955000	-1.844254000	-4.776452000
1	-0.438020000	-2.876617000	-4.805832000
6	-1.075279000	-0.849273000	-4.698728000
6	-2.504073000	-1.239320000	-4.654181000
6	-3.490940000	-0.139665000	-4.529456000
6	-3.070376000	1.207237000	-4.500994000
6	-4.834713000	-0.457867000	-4.427582000
1	-5.125839000	-1.499839000	-4.440905000
6	-5.796443000	0.541876000	-4.299105000
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6	-4.055258000	2.212299000	-4.394522000
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7	3.543708000	-2.255578000	-4.877084000
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6	2.255702000	-2.592792000	-4.885139000
16	-0.439181000	9.504463000	-4.234390000
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7	-7.569442000	-1.088974000	-4.096073000
7	-8.109666000	1.179274000	-4.016253000
6	-7.222361000	0.194690000	-4.136924000

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1	0.374603000	3.060582000	-1.597875000
6	0.355168000	0.944395000	-1.808178000
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1	6.141482000	7.071322000	2.831380000
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6	8.198221000	2.027032000	2.380004000
1	8.377447000	1.855847000	3.443595000
1	7.875938000	1.100830000	1.910870000
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7	4.082365000	-0.376262000	1.332961000
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6	4.714167000	-2.829674000	-3.234054000
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1	4.948921000	-3.799398000	-3.676274000
1	5.324735000	-2.695382000	-2.343454000
6	2.950628000	-3.874539000	-1.828899000
1	3.377286000	-3.590779000	-0.866644000
1	3.409487000	-4.815217000	-2.139417000
1	1.892242000	-4.073905000	-1.671401000
6	2.434452000	-3.063204000	-4.190027000
1	1.356121000	-3.072274000	-4.044871000
1	2.671438000	-2.303811000	-4.937867000
1	2.721916000	-4.036000000	-4.592874000
7	-4.328062000	-2.126032000	-1.303680000
8	-4.097758000	-3.374362000	-1.262312000
6	-5.773305000	-1.686133000	-1.217643000
6	-6.635105000	-2.946687000	-1.279817000
1	-6.484042000	-3.490411000	-2.211891000
1	-7.681202000	-2.641416000	-1.216863000
1	-6.416294000	-3.623084000	-0.456387000
6	-6.020925000	-0.990119000	0.124809000
1	-5.818259000	-1.680294000	0.945429000
1	-7.070660000	-0.694457000	0.182860000
1	-5.409980000	-0.106332000	0.289823000
6	-6.130508000	-0.807963000	-2.423278000
1	-5.635167000	0.159366000	-2.432298000
1	-5.886174000	-1.324744000	-3.353501000
1	-7.206489000	-0.625254000	-2.413940000
7	-1.201422000	4.331617000	-1.537244000
8	-2.332939000	4.822039000	-1.257853000
6	-0.055834000	5.288700000	-1.806574000
6	-0.627642000	6.702602000	-1.732660000
1	-1.411770000	6.858996000	-2.472622000
1	0.185835000	7.403241000	-1.929486000
1	-1.045451000	6.918903000	-0.750604000
6	1.020303000	5.123922000	-0.730312000
1	0.593121000	5.289508000	0.261776000
1	1.798971000	5.873761000	-0.884233000
1	1.480617000	4.140347000	-0.762207000
6	0.502628000	5.051452000	-3.212899000
1	0.985849000	4.082095000	-3.298283000
1	-0.294182000	5.120377000	-3.956885000
1	1.237882000	5.827636000	-3.435330000