Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

ELECTRONIC SUPPLEMENTARY INFORMATION

Accurate Excitation Spectra of Retinal by Multiconfiguration Pair-Density Functional Theory

Sijia S. Dong, Laura Gagliardi,* and Donald G. Truhlar*

Department of Chemistry, Chemical Theory Center, and Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN 55455, USA

**E-mail: truhlar@umn.edu, gagliard@umn.edu*

Table of Contents

Table S1 Dipole moments of **11c-dimethyl** in debye. For CASSCF calculations, the active spaces used are specified in the first column. We label the solution chosen in this article as (10,10)/TZVP #1, and the solution of the CASSCF(10,10)/TZVP calculation starting from the CASSCF(12,12) orbitals as (10,10)/TZVP #2.

	S_0	S_1	S_2
(8,8)/def2-SVP	20.62	7.84	18.68
(8,8)/def2-SVPD	17.07	3.94	5.67
(8,8)/ma-SVP	15.84	6.40	3.12
(8,8)/TZVP	20.39	7.67	18.29
(8,8)/def2-TZVP	19.71	6.79	17.83
(8,8)/ma-TZVP	15.59	6.86	3.27
(10,10)/def2-SVP	22.25	5.97	21.61
(10,10)/def2-SVPD	16.38	10.95	9.56
(10,10)/ma-SVP	16.46	10.76	9.60
(10,10)/TZVP #1	16.45	10.75	9.60
(10,10)/TZVP #2	18.35	2.79	4.05
(10,10)/def2-TZVP	21.83	5.96	21.00
(10,10)/ma-TZVP	21.81	5.94	20.97
(12,12)/def2-SVP	24.24	6.91	23.35
(12,12)/def2-SVPD	24.05	6.89	23.07
(12,12)/ma-SVP	23.98	6.74	23.00
(12,12)/TZVP	24.12	6.73	23.22
(12,12)/def2-TZVP	23.86	7.01	22.83
(12,12)/ma-TZVP	23.84	6.99	22.79
M06-2X/def2-SVP	17.04	10.31	8.35
M06-2X/ma-SVP	16.83	10.11	8.19
M06-2X/TZVP	16.89	10.16	8.17
M06-2X/def2-TZVP	16.89	10.16	8.10
M06-2X/ma-TZVP	16.87	10.14	8.07
M06-HF/def2-SVP	19.11	10.58	8.54
M06-HF/ma-SVP	18.86	10.39	8.54
M06-HF/TZVP	18.70	10.42	8.57
M06-HF/def2-TZVP	18.61	10.62	8.68
M06-HF/ma-TZVP	18.60	10.60	8.74

Table S2 Vertical excitation energies and oscillator strengths (Osc. Str.) of **11c-dimethyl**. We label the solution chosen in this article as (10,10)/TZVP #1, and the solution of the CASSCF(10,10)/TZVP calculation starting from the CASSCF(12,12) orbitals as (10,10)/TZVP #2.

	Excitation Energy (eV)				Osc. Str.	
$S_0 \rightarrow S_1$	CASSCF or TDDFT	CASPT2	MS-CASPT2	tPBE	CASPT2	tPBE
(8,8)/def2-SVP	3.35	2.40	2.45	1.77	1.22	0.90
(8,8)/def2-SVPD	2.57	2.29	2.29	1.90	1.44	1.19
(8,8)/ma-SVP	2.19	2.30	2.42	2.01	1.80	1.58
(8,8)/TZVP	3.32	2.34	2.40	1.76	1.20	0.90
(8,8)/def2-TZVP	3.67	2.41	2.28	1.87	0.86	0.67
(8,8)/ma-TZVP	2.21	2.30	2.44	2.02	1.80	1.58
(10,10)/def2-SVP	3.21	2.37	2.48	1.75	1.04	0.77
(10,10)/def2-SVPD	2.63	2.39	2.51	2.01	1.52	1.28
(10,10)/ma-SVP	2.62	2.38	2.50	2.00	1.52	1.28
(10,10)/TZVP #1	2.61	2.37	2.50	2.01	1.51	1.28
(10,10)/TZVP #2	2.24	2.30	2.27	1.91	1.43	1.19
(10,10)/def2-TZVP	3.20	2.29	2.43	1.75	1.03	0.79
(10,10)/ma-TZVP	3.19	2.28	2.43	1.75	1.03	0.79
(12,12)/def2-SVP	3.08	2.29	2.50	1.66	1.10	0.80
(12,12)/def2-SVPD	3.08	2.23	2.48	1.66	1.08	0.80
(12,12)/ma-SVP	3.04	2.25	2.47	1.66	1.11	0.82
(12,12)/TZVP	3.06	2.22	2.47	1.65	1.08	0.80
(12,12)/def2-TZVP	3.09	2.19	2.47	1.66	1.07	0.81
(12,12)/ma-TZVP	3.08	2.20	2.48	1.66	1.07	0.81
M06-2X/def2-SVP	2.46				1.45	
M06-2X/ma-SVP	2.44				1.45	
M06-2X/TZVP	2.44				1.45	
M06-2X/def2-TZVP	2.45				1.46	
M06-2X/ma-TZVP	2.44				1.45	
M06-HF/def2-SVP	2.62				1.66	
M06-HF/ma-SVP	2.59				1.65	
M06-HF/TZVP	2.59				1.66	
M06-HF/def2-TZVP	2.59				1.66	
M06-HF/ma-TZVP	2.59				1.65	
CAM-B3LYP/TZVP	2.49				1.51	
PBE0/TZVP	2.28				1.11	
Exp. (*in vacuo*)[1]	2.03					
Exp. (rhodopsin)[2]	2.49					

1. I. B. Nielsen, L. Lammich and L. H. Andersen, *Phys. Rev. Lett.*, 2006, **96**, 018304.
2. W. J. DeGrip, P. H. Bovee-Geurts, I. van der Hoef and J. Lugtenburg, *J. Am.Chem. Soc.*., 2007, **129**, 13265-13269.

	Excitation Energy (eV)				Osc. Str.	
$S_0 \rightarrow S_2$	CASSCF or TDDFT	CASPT2	MS-CASPT2	tPBE	CASPT2	tPBE
(8,8)/def2-SVP	4.04	3.46	3.52	3.18	0.10	0.09
(8,8)/def2-SVPD	3.79	3.29	3.35	2.77	0.38	0.32
(8,8)/ma-SVP	3.71	3.59	3.66	3.36	0.17	0.16
(8,8)/TZVP	4.03	3.42	3.47	3.16	0.10	0.09
(8,8)/def2-TZVP	4.09	3.47	3.81	3.29	0.26	0.25
(8,8)/ma-TZVP	3.70	3.54	3.62	3.37	0.17	0.17
(10,10)/def2-SVP	3.80	3.48	3.65	3.27	0.13	0.12
(10,10)/def2-SVPD	3.71	3.43	3.51	3.21	0.15	0.14
(10,10)/ma-SVP	3.71	3.43	3.51	3.20	0.15	0.14
(10,10)/TZVP #1	3.71	3.42	3.50	3.21	0.14	0.14
(10,10)/TZVP #2	3.56	3.36	3.39	2.79	0.32	0.27
(10,10)/def2-TZVP	3.81	3.42	3.62	3.25	0.13	0.12
(10,10)/ma-TZVP	3.81	3.42	3.62	3.25	0.13	0.12
(12,12)/def2-SVP	3.70	3.45	3.63	3.17	0.11	0.10
(12,12)/def2-SVPD	3.71	3.43	3.63	3.17	0.10	0.09
(12,12)/ma-SVP	3.70	3.43	3.61	3.16	0.10	0.09
(12,12)/TZVP	3.69	3.42	3.61	3.17	0.10	0.09
(12,12)/def2-TZVP	3.71	3.40	3.63	3.16	0.11	0.10
(12,12)/ma-TZVP	3.70	3.40	3.63	3.16	0.11	0.10
M06-2X/def2-SVP	3.58				0.41	
M06-2X/ma-SVP	3.55				0.41	
M06-2X/TZVP	3.56				0.40	
M06-2X/def2-TZVP	3.56				0.39	
M06-2X/ma-TZVP	3.55				0.39	
M06-HF/def2-SVP	4.15				0.23	
M06-HF/ma-SVP	4.10				0.23	
M06-HF/TZVP	4.10				0.23	
M06-HF/def2-TZVP	4.09				0.23	
M06-HF/ma-TZVP	4.08				0.23	
CAM-B3LYP/TZVP	3.64				0.38	
PBE0/TZVP	3.18				0.72	
Exp. (*in vacuo*)[1]	3.18					

1. I. B. Nielsen, L. Lammich and L. H. Andersen, *Physical Review Letters*, 2006, **96**, 018304.

Table S3 Vertical excitation energies (in eV) of **11c-dimethyl** and **11t-butyl** from MC-PDFT calculations with various on-top density functionals.

	tPBE	tBLYP	ftPBE	ftBLYP	trevPBE	ftrevPBE	tLSDA	ftLSDA
11c S_1	2.01	2.00	1.95	1.95	2.02	1.95	2.01	2.03
11c S_2	3.21	3.19	3.20	3.20	3.22	3.21	3.21	3.24
11t S_1	1.97	1.96	1.92	1.92	1.98	1.92	1.97	2.00
11t S_2	3.21	3.19	3.20	3.20	3.22	3.21	3.21	3.24

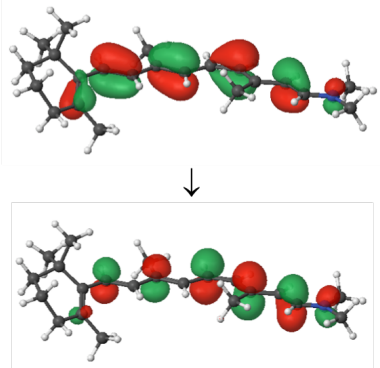
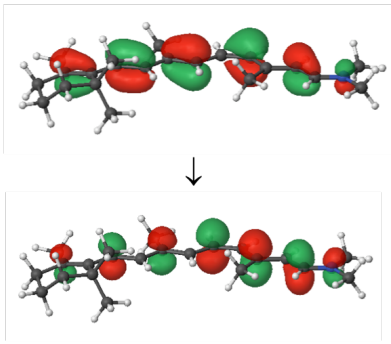
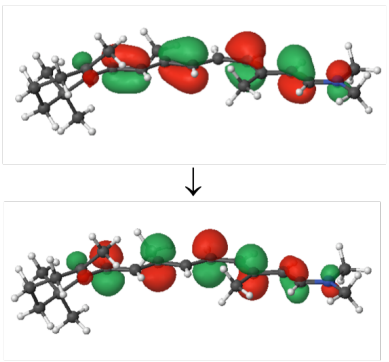
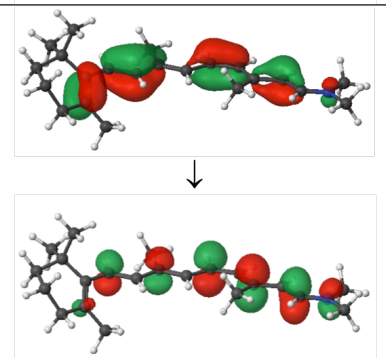
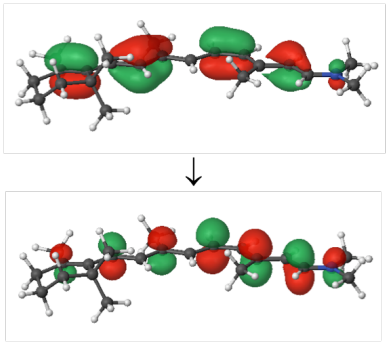
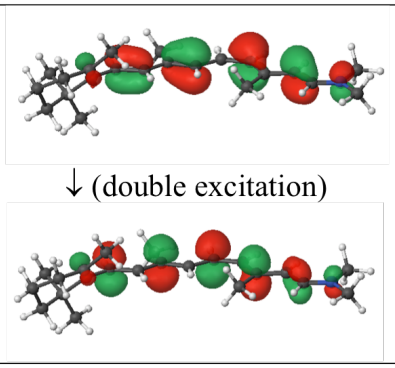
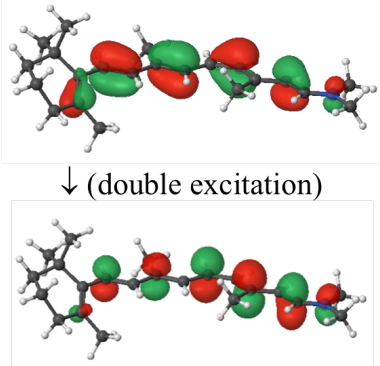
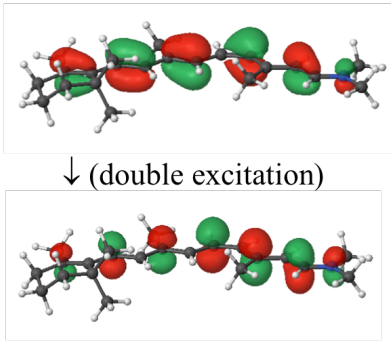
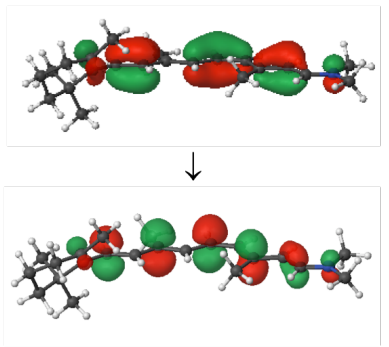
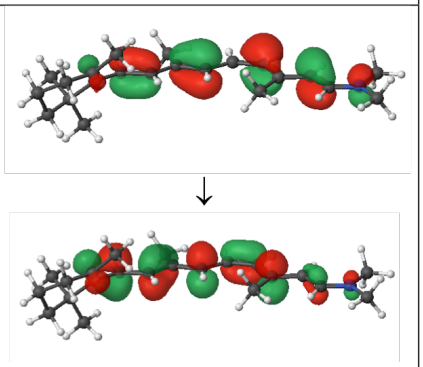
Table S4 Similar to Table 5 of the main text for **11c-dimethyl**, but this table shows the percentages of each conformation calculated from Gibbs free energy at three temperatures. Relative energies (Rel. *E*) are in kcal/mol. Torsional angles θ (in degrees) are defined in Table 1.

Rank	Label	Rel. *E*	% at 298.15 K	% at 500 K	% at 700 K	θ_6	θ_8	θ_{10}	θ_{12}	θ_{14}
1	s0048	0.00	36.5%	23.1%	17.1%	-40	178	179	179	180
2	s0096	0.37	22.0%	21.9%	19.7%	-170	-180	180	180	180
3	s0144	0.38	30.2%	25.1%	20.9%	44	-178	-179	-179	-180
4	s0003	1.69	3.6%	6.1%	6.8%	-41	177	176	-22	177
5	s0110	1.98	1.7%	4.3%	5.7%	-170	179	177	-20	177
6	s0134	2.25	1.8%	4.5%	6.0%	45	-180	177	-22	178
7	s0042	2.50	2.7%	8.8%	13.1%	-38	-25	-179	180	180
8	s0126	2.89	1.5%	6.4%	10.6%	42	26	180	-179	-180

Table S5 Similar to Table 6 of the main text for **11t-butyl**, but this table shows the percentages of each conformation calculated from Gibbs free energy at three temperatures. Relative energies (Rel. *E*) are in kcal/mol. Torsional angles θ (in degrees) are defined in Table 1.

Rank	Label	Rel. *E*	% at 298.15 K	% at 500 K	% at 700 K	θ_6	θ_8	θ_{10}	θ_{12}	θ_{14}
1	s0048	0.00	53.8%	45.3%	41.5%	-40	178	180	180	180
2	s0144	0.36	25.9%	28.1%	28.9%	44	-178	-180	-180	180
3	s0096	0.40	20.2%	26.6%	29.6%	-170	-180	180	180	179

Table S6 Molecular orbital changes for the first two excitations of the most stable three conformations of **11c-dimethyl** calculated with CASSCF(10,10)/TZVP (Solution #1).

	s0048	s0096	s0144
$S_0 \rightarrow S_1$			
$S_0 \rightarrow S_2$			
			
	↓ (double excitation)	↓ (double excitation)	
			

↓ (double excitation)

Table S7 Vertical excitation energies and oscillator strengths (Osc. Str.) of the lowest 3 kcal/mol conformations of **11c-dimethyl**.

		Excitation Energy (eV)				Osc. Str.	
Transition	Conf.	CASSCF	CASPT2	MS-CASPT2	tPBE	CASPT2	tPBE
$S_0 \rightarrow S_1$							
	s0048	2.61	2.37	2.50	2.01	1.51	1.28
	s0096	2.52	2.26	2.37	1.91	1.68	1.43
	s0144	3.21	2.33	2.46	1.77	1.04	0.79
	s0003	3.08	2.22	2.39	1.73	0.51	0.40
	s0110	2.82	2.09	2.30	1.64	0.64	0.50
	s0134	2.47	2.29	2.41	2.00	0.79	0.69
	s0042	3.17	2.29	2.49	1.75	0.92	0.70
	s0126	2.68	2.39	2.52	2.03	1.34	1.14
$S_0 \rightarrow S_2$							
	s0048	3.71	3.42	3.50	3.21	0.14	0.14
	s0096	3.44	3.24	3.31	3.04	0.15	0.14
	s0144	3.83	3.49	3.66	3.33	0.12	0.11
	s0003	3.80	3.44	3.59	3.33	0.04	0.04
	s0110	3.52	3.22	3.37	3.10	0.03	0.03
	s0134	3.77	3.47	3.55	3.28	0.08	0.08
	s0042	3.80	3.45	3.60	3.36	0.05	0.05
	s0126	3.80	3.45	3.60	3.36	0.10	0.09

Table S8 The natural occupation numbers of each root from CASSCF/TZVP calculations using different active spaces. The order of the orbitals is the same as that in Tables 3 and S9. We label the solution chosen in this article as (10,10) #1, and the solution of the CASSCF(10,10) calculation starting from the CASSCF(12,12) orbitals as (10,10) #2.

	(4,4)	(6,6)	(8,8)	(10,10) #1	(10,10) #2	(12,12)
S_0	1.963369 1.905751 0.094448 0.036432	1.984869 1.946354 1.918602 0.079081 0.021977 0.049115	1.957774 1.937971 1.918489 1.884397 0.125001 0.058183 0.039896 0.078289	1.951387 1.982823 1.931976 1.919945 1.890887 0.118715 0.057058 0.027046 0.076629 0.043532	1.995540 1.953753 1.942716 1.916000 1.876881 0.126708 0.075252 0.037675 0.025432 0.050043	1.961355 1.933788 1.947344 1.920702 1.897693 1.848466 0.167821 0.101066 0.036045 0.047157 0.061321 0.077241
S_1	1.928178 1.422221 0.570693 0.078908	1.929795 1.909903 0.714272 1.287393 0.088966 0.069671	1.934541 1.957749 1.896718 1.058975 0.941902 0.108283 0.038417 0.063415	1.921080 1.966737 1.929071 1.887162 1.231795 0.764530 0.111649 0.052160 0.077587 0.058230	1.938359 1.952079 1.912021 1.884618 1.085919 0.916755 0.123247 0.048233 0.054530 0.084240	1.971091 1.929360 1.942999 1.916643 1.886667 1.105629 0.898704 0.118784 0.035712 0.052862 0.063763 0.077786
S_2	1.724426 0.819762 1.286242 0.169570	1.907184 1.545708 0.969524 1.251242 0.259940 0.066401	1.928080 1.905645 1.599556 0.932990 1.284391 0.201242 0.056729 0.091366	1.928079 1.942822 1.910144 1.540879 1.043015 1.229341 0.209986 0.046652 0.086098 0.062983	1.925690 1.936634 1.905938 1.481470 1.298171 1.056296 0.215814 0.045279 0.056505 0.078203	1.953720 1.911039 1.922102 1.884290 1.665674 0.826085 1.308340 0.237849 0.046562 0.060913 0.076981 0.106446

Table S9 The molecular orbitals for each active space from CASSCF/TZVP calculations. The order of the orbitals is the same as that in Tables 3 and S8. We label the solution chosen in this article as (10,10) #1, and the solution of the CASSCF(10,10) calculation starting from the CASSCF(12,12) orbitals as (10,10) #2.

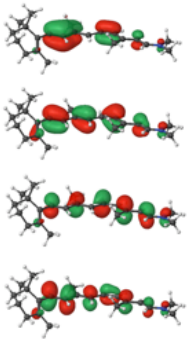
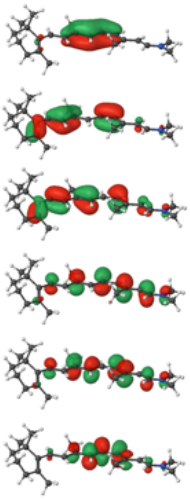
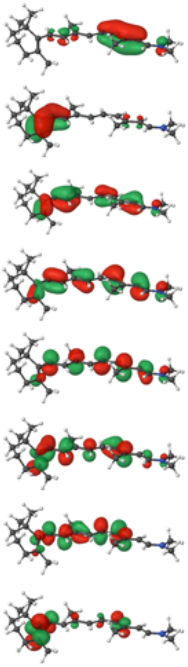
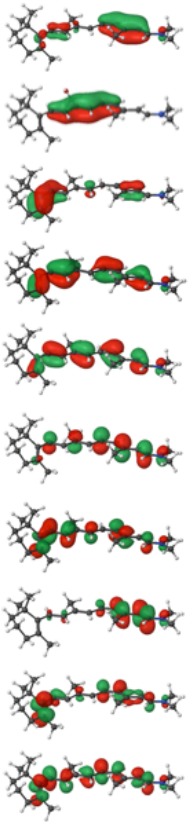
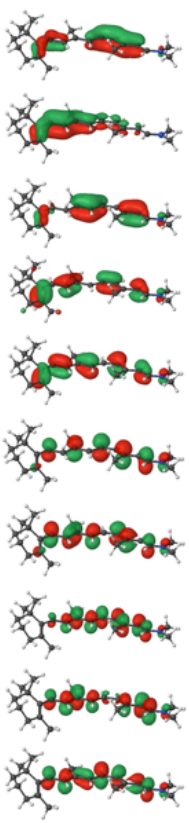
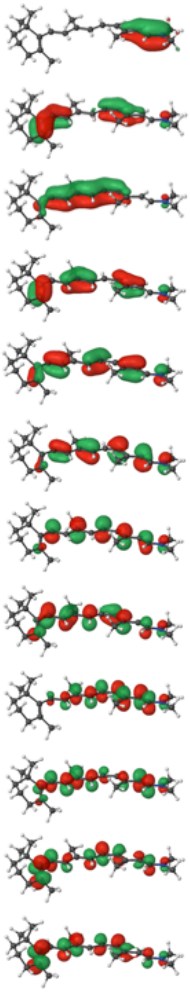
(4,4)	(6,6)	(8,8)	(10,10) #1	(10,10) #2	(12,12)
					

Table S10 Dipole moments of **11c-dimethyl** in debye calculated using CASSCF with different active spaces and calculated using KS-DFT (S_0) and TDDFT (S_1 and S_2). Calculations are carried out using the TZVP basis set. The origin of the dipole moments is the center of nuclear charges.

	S_0	S_1	S_2
(4,4)	15.89	13.18	12.64
(6,6)	14.80	5.69	1.72
(8,8)	19.92	7.24	17.82
(10,10) #1	15.99	10.32	9.20
(10,10) #2	17.91	2.42	3.66
(12,12)	23.64	6.35	22.76
M06-2X	16.43	9.64	7.64
M06-HF	18.23	9.94	8.03
CAM-B3LYP	16.09	9.63	7.48
PBE0	15.23	9.06	9.25

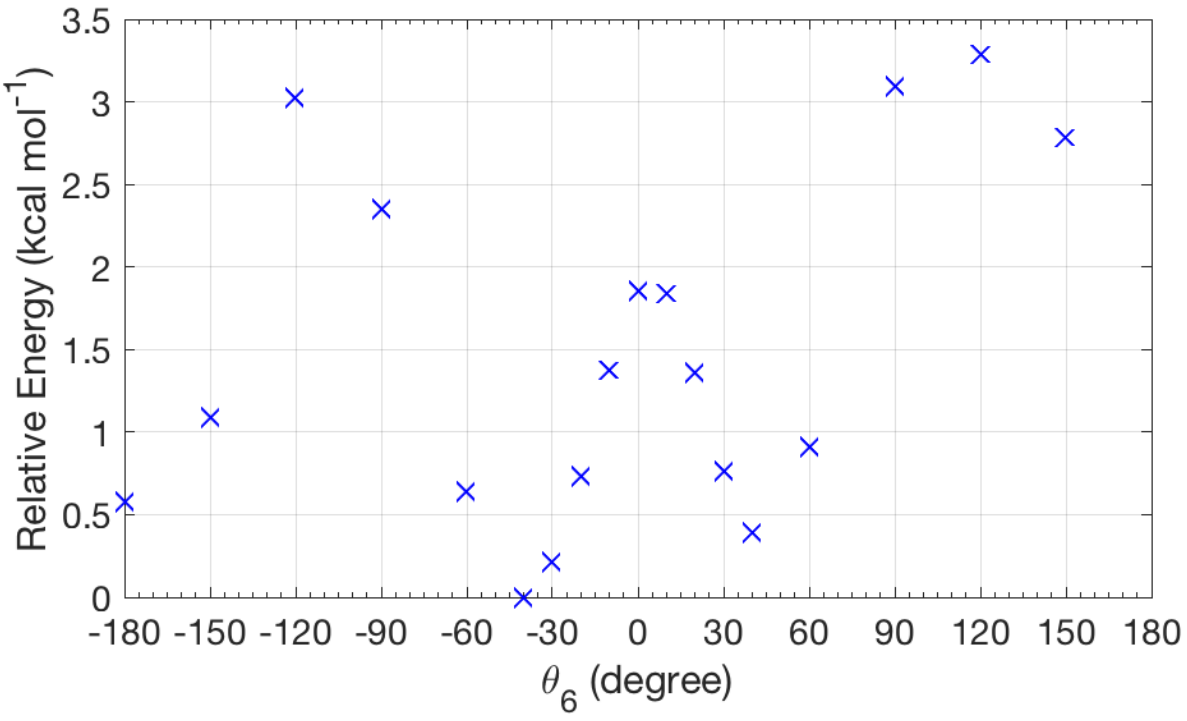


Fig. S1 Relative electronic energy of **11c-methyl** optimized with the dihedral angle θ_6 (the rotation of the β-ionone ring) fixed at various values using M06-2X/6-31+G(d,p). The initial guess of all other dihedral angles (θ_8, θ_{10}, θ_{12}, and θ_{14}) are 180°.

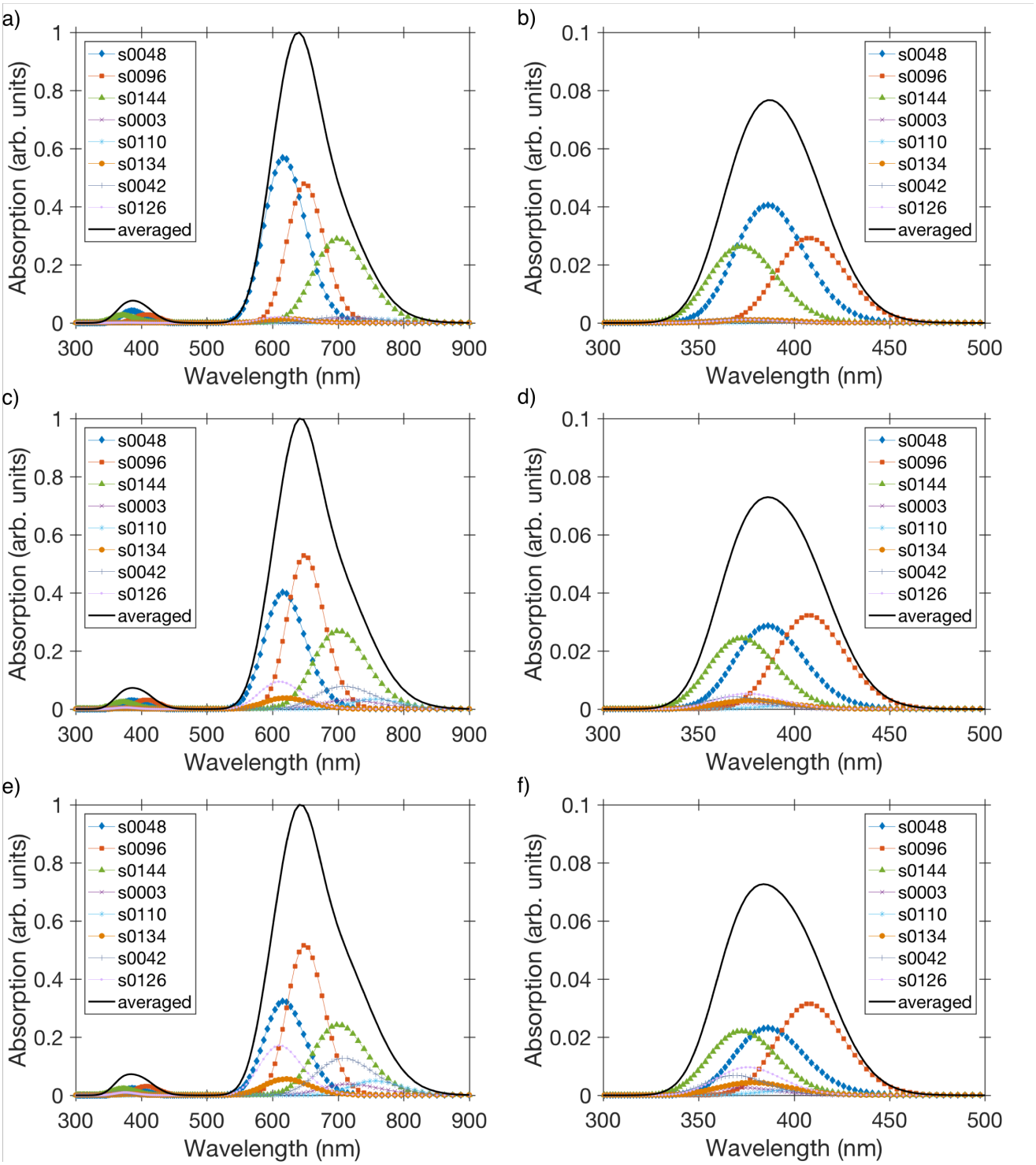


Fig. S2 Simulated spectra of **11c-methyl** with vertical excitation energies from MC-PDFT (tPBE) and thermal distributions at (a)(b) 298.15 K, (c)(d) 500 K, and (e)(f) 700K. Subplots (a), (c), and (e) are the combined spectra of the $S_0 \rightarrow S_1$ band (the longer-wavelength band) and the $S_0 \rightarrow S_2$ band (the shorter-wavelength band). The spectra are scaled such that the maximal absorption of the $S_0 \rightarrow S_1$ peak is 1.0. Subplots (b), (d), and (f) are the zoomed-in plots of the same $S_0 \rightarrow S_2$ bands in subplots (a), (c), and (e). Peak positions: 641 nm, 386 nm (298.15 K and 500 K); 641 nm, 384 nm (700 K).

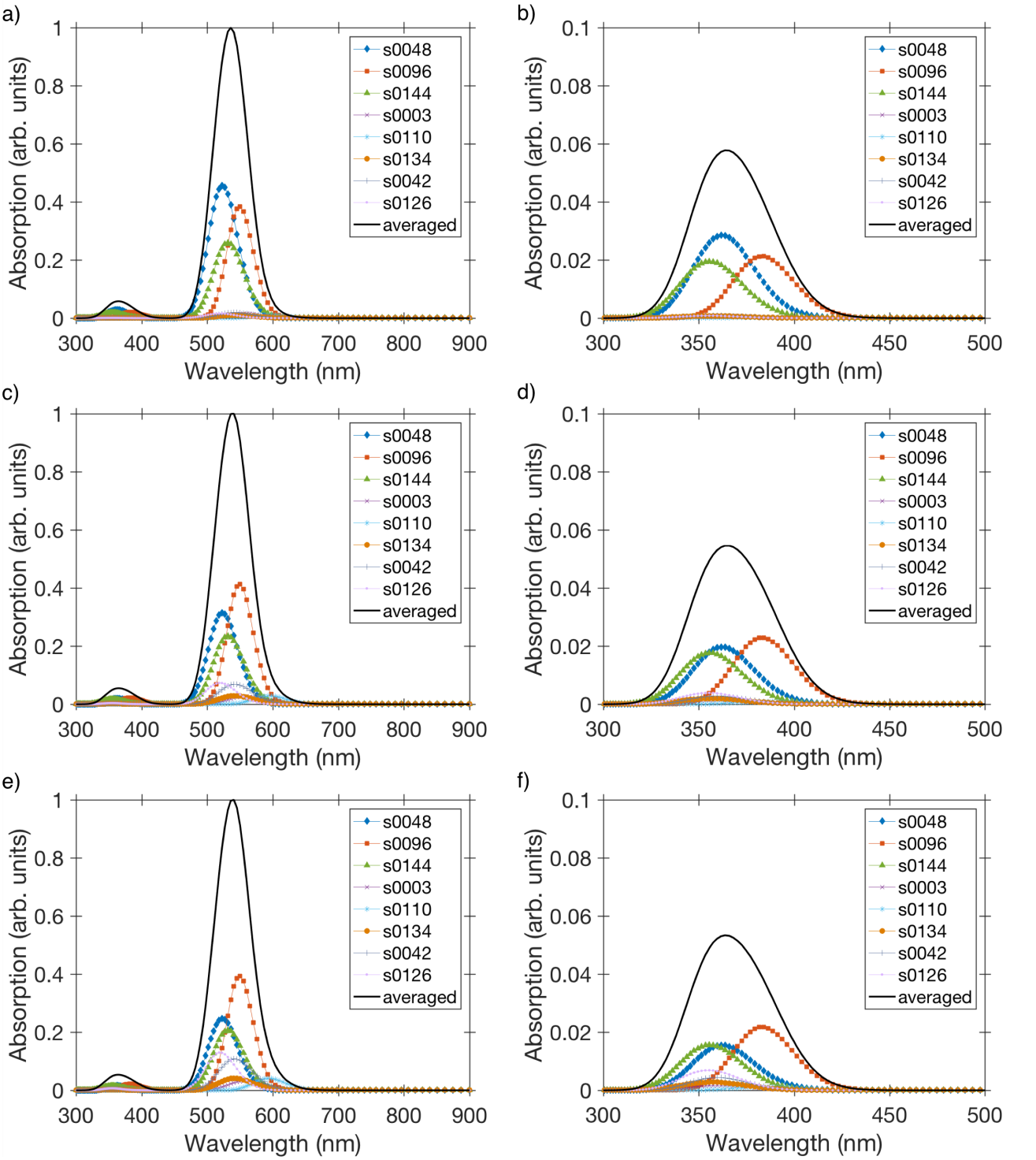


Fig. S3 Simulated spectra of **11c-methyl** with vertical excitation energies from CASPT2 and thermal distributions at (a)(b) 298.15 K, (c)(d) 500 K, and (e)(f) 700K. Subplots (a), (c), and (e) are the combined spectra of the $S_0 \rightarrow S_1$ band (the longer-wavelength band) and the $S_0 \rightarrow S_2$ band (the shorter-wavelength band). The spectra are scaled such that the maximal absorption of the $S_0 \rightarrow S_1$ peak is 1.0. Subplots (b), (d), and (f) are the zoomed-in plots of the same $S_0 \rightarrow S_2$ bands in subplots (a), (c), and (e). Peak positions: 536 nm, 364 nm (298.15 K); 541 nm, 364 nm (500 K, 700 K).

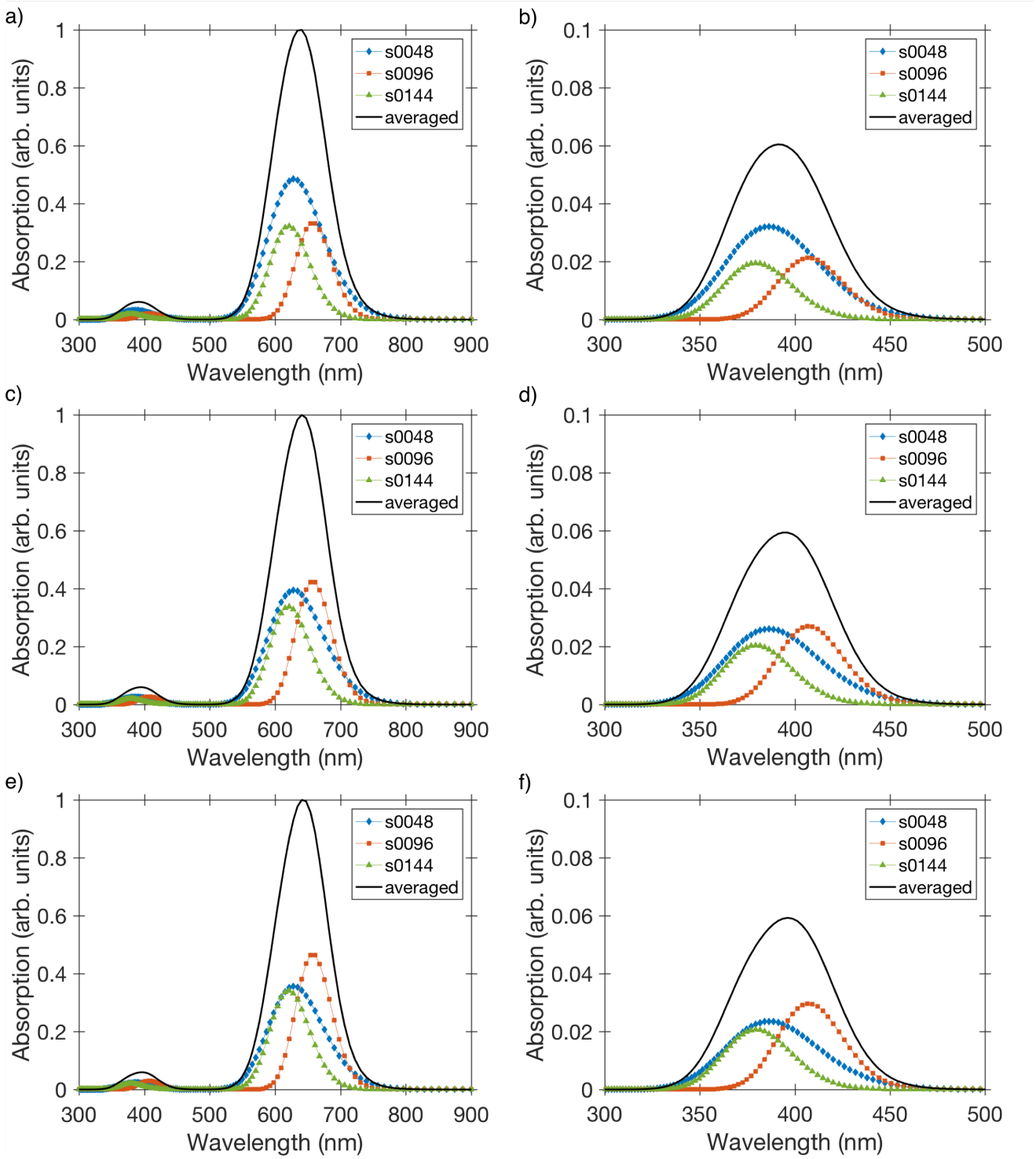


Fig. S4 Simulated spectra of **11t-butyl** with vertical excitation energies from MC-PDFT (tPBE) and thermal distributions at (a)(b) 298.15 K, (c)(d) 500 K, and (e)(f) 700K. Subplots (a), (c), and (e) are the combined spectra of the $S_0 \rightarrow S_1$ band (the longer-wavelength band) and the $S_0 \rightarrow S_2$ band (the shorter-wavelength band). The spectra are scaled such that the maximal absorption of the $S_0 \rightarrow S_1$ peak is 1.0. Subplots (b), (d), and (f) are the zoomed-in plots of the same $S_0 \rightarrow S_2$ bands in subplots (a), (c), and (e). Peak positions: 641 nm, 391 nm (298.15 K); 641 nm, 394 nm (500 K); 641 nm, 396 nm (700 K).

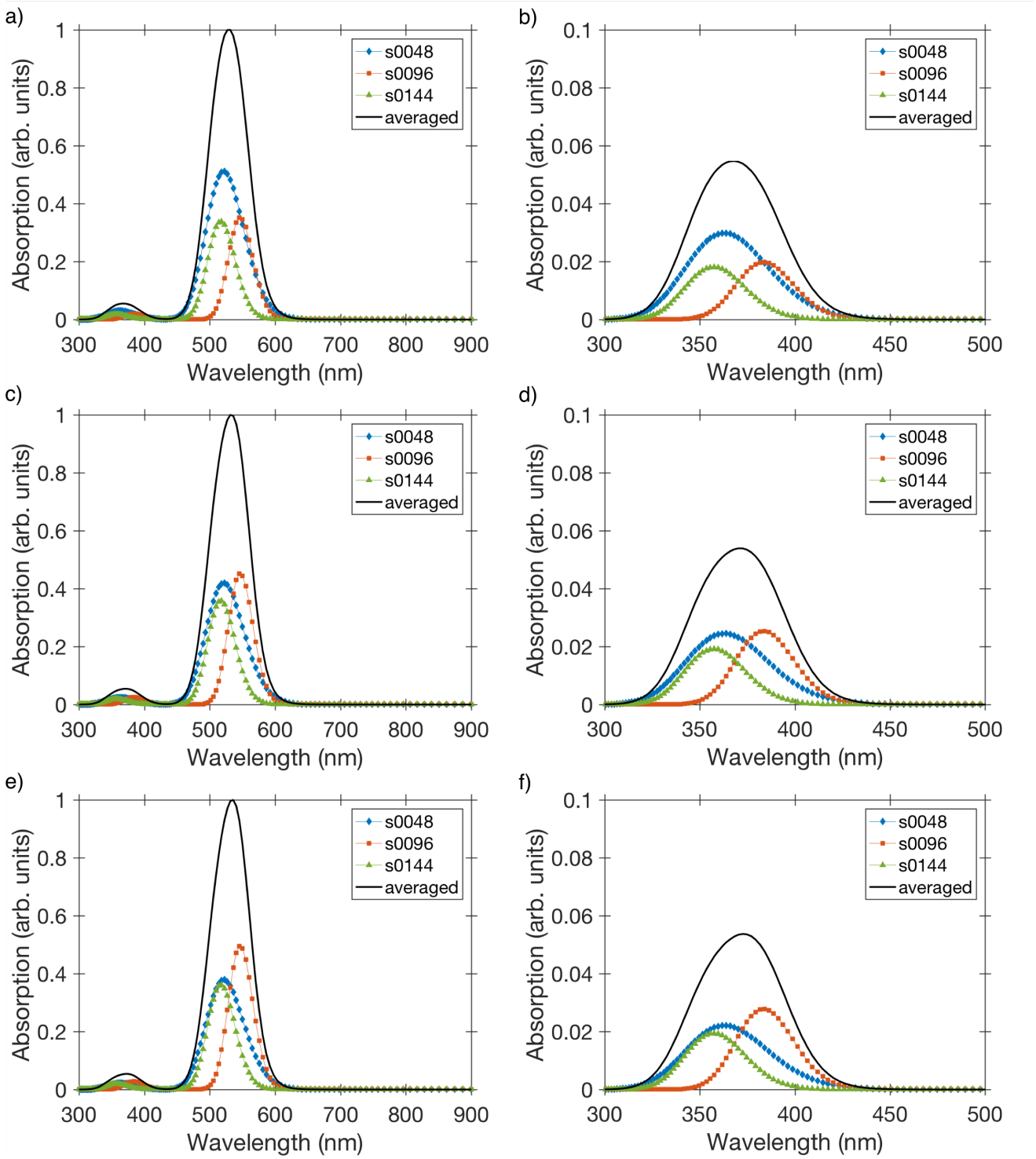


Fig. S5 Simulated spectra of **11t-butyl** with vertical excitation energies from CASPT2 and thermal distributions at (a)(b) 298.15 K, (c)(d) 500 K, and (e)(f) 700K. Subplots (a), (c), and (e) are the combined spectra of the $S_0 \rightarrow S_1$ band (the longer-wavelength band) and the $S_0 \rightarrow S_2$ band (the shorter-wavelength band). The spectra are scaled such that the maximal absorption of the $S_0 \rightarrow S_1$ peak is 1.0. Subplots (b), (d), and (f) are the zoomed-in plots of the same $S_0 \rightarrow S_2$ bands in subplots (a), (c), and (e). Peak positions: 531 nm, 370 nm (298.15 K and 500 K); 536 nm, 373 nm (700 K).

Cartesian coordinates of the molecules calculated in this study

Each structure is labeled in the format of "molecule name"-"conformation label" in the title line.

1. 11-*Z-cis*-retinal

11c-dimethyl-s0048

C	-1.147583	-5.008710	0.265151
C	-0.711879	-6.206147	1.126525
C	-0.142454	-5.782105	2.473241
C	1.115865	-4.959744	2.236253
C	0.946721	-3.888059	1.187524
C	-0.103021	-3.879166	0.326564
C	-2.501594	-4.465174	0.755295
C	2.083383	-2.897856	1.178268
C	-0.319352	-2.790710	-0.627255
C	-0.146453	-1.467983	-0.383395
C	-0.385146	-0.416325	-1.346868
C	-0.201615	0.884592	-0.922759
C	-0.822291	-0.801797	-2.732293
C	-0.373734	2.032092	-1.740709
C	-0.258995	3.382414	-1.472431
C	0.018654	4.068971	-0.257066
C	0.210173	3.315463	1.027126
C	0.093148	5.462270	-0.326963
C	0.361399	6.299615	0.760874
N	0.442420	7.614861	0.703706
C	0.249150	8.335994	-0.553623
C	-1.318691	-5.520355	-1.177505
H	0.057263	-6.773179	0.583529
H	-1.570408	-6.875796	1.251907
H	0.086908	-6.656334	3.089209
H	-0.877451	-5.186382	3.027293
H	1.944455	-5.614750	1.926939
H	1.454358	-4.478174	3.163082
H	-2.815880	-3.601760	0.158279
H	-2.453113	-4.144753	1.800180
H	-3.274395	-5.236085	0.665654
H	2.180127	-2.357305	0.236244
H	3.020770	-3.430489	1.371037
H	1.971862	-2.166801	1.989074
H	-0.713512	-3.079905	-1.599350
H	0.167154	-1.152159	0.608930
H	0.107110	1.002374	0.107766
H	-0.971782	0.047216	-3.394976
H	-0.080871	-1.462601	-3.190424
H	-1.766162	-1.353879	-2.682545
H	-0.629665	1.829011	-2.776841
H	-0.414893	4.030726	-2.330570
H	1.102458	2.685643	0.958574
H	-0.648524	2.662410	1.204616
H	0.322445	3.958680	1.897387
H	-0.062864	5.916882	-1.299488

H	0.525993	5.883417	1.749651
H	0.996336	8.022830	-1.288006
H	-0.753054	8.146945	-0.948002
H	0.361371	9.402504	-0.365610
H	-1.846519	-4.809120	-1.819987
H	-1.916204	-6.437566	-1.163513
H	-0.350927	-5.755338	-1.633054
C	0.728188	8.418707	1.890106
H	0.850103	7.767752	2.755336
H	1.647589	8.989202	1.735488
H	-0.097631	9.110968	2.073087

11c-dimethyl-s0096

C	-0.179672	-3.733842	1.842578
C	-0.373181	-5.103501	2.524910
C	0.671761	-6.126517	2.108605
C	0.523578	-6.389979	0.618641
C	0.347073	-5.144619	-0.208689
C	0.089907	-3.918132	0.339942
C	0.991369	-3.003260	2.527910
C	0.521204	-5.405523	-1.688341
C	0.100006	-2.782138	-0.567020
C	0.065123	-1.445669	-0.302903
C	0.111081	-0.427262	-1.321540
C	0.075307	0.891559	-0.900328
C	0.189925	-0.843207	-2.764927
C	0.112741	2.015767	-1.759640
C	0.080316	3.376855	-1.506419
C	-0.017341	4.092411	-0.284222
C	-0.117299	3.368500	1.027210
C	-0.017039	5.489459	-0.370519
C	-0.103005	6.354213	0.722572
N	-0.100344	7.673139	0.650456
C	-0.003286	8.363335	-0.633981
C	-1.494026	-2.960979	2.071879
H	-1.367654	-5.492495	2.264924
H	-0.367838	-4.949858	3.610002
H	0.550887	-7.056731	2.670784
H	1.680539	-5.756214	2.322825
H	-0.346045	-7.038800	0.429386
H	1.386328	-6.940518	0.221802
H	1.215840	-2.040109	2.064989
H	1.907325	-3.599071	2.487673
H	0.748507	-2.822931	3.580677
H	-0.183203	-4.856922	-2.316132
H	0.376620	-6.469484	-1.890197
H	1.537954	-5.154336	-2.012831
H	0.185291	-3.046229	-1.615679
H	0.010647	-1.082478	0.716173
H	0.016783	1.037578	0.170283
H	0.219649	-0.005641	-3.457322

H	1.087131	-1.446372	-2.933068
H	-0.675708	-1.459547	-3.025118
H	0.183499	1.789213	-2.819740
H	0.137010	4.003156	-2.392709
H	0.773121	2.751241	1.178946
H	-0.987496	2.705927	1.019145
H	-0.212699	4.030729	1.885067
H	0.058036	5.920969	-1.363027
H	-0.178820	5.962223	1.731763
H	0.930690	8.097851	-1.137219
H	-0.850214	8.096738	-1.272486
H	-0.017446	9.437444	-0.456102
H	-1.438258	-1.905449	1.803077
H	-1.758733	-3.014589	3.133258
H	-2.310191	-3.411326	1.498010
C	-0.193719	8.507450	1.845688
H	-0.261311	7.875840	2.731046
H	0.692944	9.142089	1.923219
H	-1.083422	9.139736	1.786022

11c-dimethyl-s0144

C	1.188949	-5.044388	-0.139662
C	1.333960	-5.966835	1.081505
C	-0.010279	-6.415221	1.636387
C	-0.803701	-5.199135	2.100705
C	-0.769205	-4.032276	1.140062
C	0.145526	-3.949029	0.141447
C	0.768704	-5.861339	-1.375247
C	-1.846946	-3.010826	1.404691
C	0.192415	-2.828614	-0.799651
C	0.079357	-1.511816	-0.500385
C	0.162980	-0.439175	-1.467662
C	0.075107	0.852936	-0.990572
C	0.350352	-0.796938	-2.915317
C	0.122494	2.017310	-1.801819
C	0.075991	3.362200	-1.490317
C	0.017906	4.024281	-0.231622
C	0.029763	3.243831	1.050632
C	-0.041631	5.419618	-0.259651
C	-0.107004	6.235572	0.874666
N	-0.170583	7.552814	0.858544
C	-0.177102	8.299854	-0.398607
C	2.563374	-4.407856	-0.409884
H	1.881278	-5.428181	1.867757
H	1.950493	-6.828062	0.798613
H	0.128809	-7.111362	2.468581
H	-0.576868	-6.953208	0.868151
H	-0.412466	-4.842334	3.066383
H	-1.848406	-5.470476	2.289748
H	0.671985	-5.230320	-2.264960
H	-0.189542	-6.363847	-1.220996

H	1.526701	-6.620460	-1.596012
H	-2.050905	-2.367034	0.548862
H	-1.574844	-2.374292	2.256651
H	-2.775349	-3.519001	1.681172
H	0.408487	-3.098488	-1.833160
H	-0.051380	-1.217769	0.538475
H	-0.050177	0.950134	0.079932
H	0.395067	0.065439	-3.576049
H	1.281566	-1.358917	-3.039753
H	-0.467560	-1.439878	-3.252835
H	0.195688	1.835362	-2.870374
H	0.095398	4.028065	-2.348954
H	0.896988	2.578292	1.070698
H	-0.870160	2.624744	1.116618
H	0.070633	3.868116	1.940721
H	-0.042646	5.894304	-1.235079
H	-0.111032	5.799071	1.868398
H	0.739502	8.101864	-0.960962
H	-1.044507	8.017748	-1.001664
H	-0.232364	9.363484	-0.172759
H	2.575873	-3.824681	-1.336769
H	3.321554	-5.192151	-0.505156
H	2.857294	-3.746624	0.411976
C	-0.237744	8.333373	2.092114
H	-0.225302	7.664506	2.952175
H	0.620254	9.008246	2.147466
H	-1.158909	8.921528	2.105732

11c-dimethyl-s0003

C	-0.599462	-5.130119	-0.241898
C	-0.314871	-6.386860	0.597812
C	0.023090	-6.059827	2.045824
C	1.303210	-5.237329	2.077423
C	1.314099	-4.098659	1.086988
C	0.424432	-4.021993	0.064638
C	-2.014095	-4.600963	0.054359
C	2.440286	-3.126215	1.330308
C	0.382734	-2.876399	-0.846460
C	0.508393	-1.572845	-0.497758
C	0.470992	-0.466034	-1.429365
C	0.555799	0.808288	-0.914296
C	0.326044	-0.761882	-2.895648
C	0.651536	2.000078	-1.682755
C	0.669697	3.309852	-1.249385
C	0.352563	3.832795	0.037540
C	0.870760	5.217145	0.345281
C	-0.444452	3.142913	0.950404
C	-0.724722	3.654941	2.222880
N	-1.511163	3.089683	3.116845
C	-2.190210	1.825882	2.834653
C	-0.533467	-5.544327	-1.723906

H	0.533213	-6.926031	0.153112
H	-1.182808	-7.053107	0.533970
H	0.147034	-6.975801	2.630549
H	-0.794333	-5.494924	2.509563
H	2.171624	-5.880413	1.869154
H	1.481908	-4.821121	3.077658
H	-2.221509	-3.695126	-0.526374
H	-2.137900	-4.353206	1.112886
H	-2.764201	-5.352466	-0.214213
H	2.692917	-2.526655	0.455433
H	3.331455	-3.683407	1.638273
H	2.200548	-2.447380	2.158627
H	0.177633	-3.103613	-1.890789
H	0.635334	-1.317553	0.552303
H	0.626661	0.894458	0.166755
H	0.304368	0.133174	-3.513743
H	1.145512	-1.400365	-3.237868
H	-0.607787	-1.304471	-3.074639
H	0.828425	1.877657	-2.748421
H	0.982571	4.046340	-1.984002
H	1.323435	5.665362	-0.538900
H	1.646975	5.167626	1.116803
H	0.080158	5.884124	0.698078
H	-0.906293	2.213687	0.642857
H	-0.269572	4.589639	2.540636
H	-2.843283	1.933117	1.964321
H	-1.456422	1.037363	2.643954
H	-2.791400	1.550301	3.699549
H	-0.947538	-4.785591	-2.394799
H	-1.126761	-6.452846	-1.868776
H	0.495283	-5.761394	-2.030188
C	-1.745837	3.692450	4.427497
H	-1.186089	4.623641	4.509365
H	-2.811782	3.899908	4.551001
H	-1.420106	3.005075	5.212377

11c-dimethyl-s0110

C	0.522699	-3.812001	1.787896
C	0.490818	-5.168571	2.521341
C	1.194981	-6.274465	1.751348
C	0.452138	-6.501557	0.444486
C	0.076567	-5.233161	-0.274537
C	0.164744	-3.996823	0.303728
C	1.927758	-3.199338	1.946188
C	-0.365289	-5.486774	-1.698479
C	-0.077074	-2.851579	-0.559218
C	0.114280	-1.522294	-0.331305
C	-0.135426	-0.497544	-1.314296
C	0.087989	0.813784	-0.939461
C	-0.636904	-0.890154	-2.676588
C	0.001242	1.939714	-1.793844

C	0.158193	3.279762	-1.485405
C	0.196299	3.910161	-0.213140
C	0.768262	5.307256	-0.172602
C	-0.320089	3.315234	0.941531
C	-0.240777	3.934535	2.191508
N	-0.747273	3.459457	3.314400
C	-1.468029	2.188802	3.337266
C	-0.523521	-2.928273	2.496564
H	-0.556204	-5.463608	2.678484
H	0.933791	-5.032510	3.514575
H	1.222706	-7.198051	2.336166
H	2.235323	-5.998943	1.545686
H	-0.475407	-7.067312	0.624662
H	1.038604	-7.120981	-0.246244
H	2.037322	-2.251321	1.415570
H	2.698010	-3.872341	1.560165
H	2.135099	-3.019187	3.006705
H	-1.202265	-4.862620	-2.016249
H	-0.677973	-6.528432	-1.802762
H	0.464202	-5.331185	-2.398407
H	-0.429986	-3.104845	-1.553334
H	0.493017	-1.169662	0.620594
H	0.426244	0.974905	0.080326
H	-0.798199	-0.038943	-3.334163
H	0.071606	-1.568416	-3.161316
H	-1.590884	-1.418675	-2.587000
H	-0.115326	1.737944	-2.855664
H	0.282156	3.944637	-2.335328
H	0.982984	5.666789	-1.178655
H	1.712025	5.315534	0.383480
H	0.085512	6.015535	0.303939
H	-0.848142	2.374987	0.853024
H	0.280557	4.883084	2.292412
H	-2.336498	2.232759	2.674102
H	-0.809338	1.374967	3.019296
H	-1.806094	1.995017	4.354021
H	-0.486027	-1.879565	2.197627
H	-0.351746	-2.970135	3.577642
H	-1.535180	-3.297828	2.300741
C	-0.611492	4.171605	4.582592
H	-0.056068	5.096016	4.426991
H	-1.601558	4.409109	4.980297
H	-0.076048	3.546533	5.301988

11c-dimethyl-s0134

C	0.847585	-5.214464	-0.527938
C	1.388764	-6.184040	0.535048
C	0.364298	-6.494261	1.616757
C	-0.010296	-5.210996	2.349632
C	-0.251696	-4.027582	1.439906
C	0.154304	-4.017631	0.146584

C	-0.147696	-5.940522	-1.451569
C	-0.987827	-2.897331	2.116577
C	-0.073655	-2.881278	-0.750741
C	0.117966	-1.571833	-0.465502
C	-0.074840	-0.488478	-1.407490
C	0.165516	0.792954	-0.966087
C	-0.529956	-0.818925	-2.801022
C	0.136417	1.960283	-1.777353
C	0.302568	3.278105	-1.405622
C	0.311264	3.848171	-0.099195
C	0.947270	5.211026	0.032650
C	-0.283009	3.221153	0.994994
C	-0.236540	3.774074	2.280499
N	-0.812307	3.265086	3.351071
C	-1.585868	2.026409	3.276410
C	2.040772	-4.727751	-1.368472
H	2.275926	-5.735404	1.003554
H	1.723187	-7.100508	0.035141
H	0.761114	-7.227338	2.324969
H	-0.532723	-6.940002	1.172608
H	0.792140	-4.932103	3.050492
H	-0.900517	-5.368473	2.969263
H	-0.537382	-5.276723	-2.230361
H	-1.001921	-6.334984	-0.895435
H	0.352279	-6.774202	-1.955937
H	-0.307237	-2.330584	2.765817
H	-1.770389	-3.304247	2.764058
H	-1.450068	-2.204411	1.412577
H	-0.360560	-3.143224	-1.768915
H	0.481446	-1.295090	0.521911
H	0.470426	0.902429	0.071161
H	-0.657475	0.058531	-3.431167
H	0.190311	-1.487421	-3.283152
H	-1.490150	-1.342346	-2.767408
H	0.065228	1.803545	-2.850687
H	0.468189	3.980283	-2.217655
H	1.186534	5.621589	-0.948078
H	1.887360	5.136203	0.590333
H	0.298135	5.921874	0.549760
H	-0.843701	2.309721	0.833585
H	0.317221	4.693520	2.452892
H	-2.428854	2.146935	2.590436
H	-0.950481	1.205473	2.931602
H	-1.965129	1.789730	4.269187
H	1.725734	-4.122255	-2.224875
H	2.592268	-5.588673	-1.760270
H	2.728533	-4.128364	-0.762891
C	-0.712677	3.909094	4.659474
H	-0.114946	4.816369	4.577885
H	-1.712089	4.166325	5.019401
H	-0.238965	3.227058	5.370115

11c-dimethyl-s0042

C	1.707007	-2.109095	3.164064
C	1.588823	-3.060869	4.366820
C	1.001665	-4.412846	3.987023
C	-0.417429	-4.205141	3.478651
C	-0.540156	-3.089155	2.470588
C	0.440902	-2.166433	2.290471
C	2.926984	-2.485879	2.304906
C	-1.861877	-3.101196	1.747333
C	0.367515	-1.145978	1.246030
C	-0.119856	-1.302763	-0.010318
C	-0.141555	-0.262135	-1.022698
C	-0.147068	1.070593	-0.668756
C	-0.153662	-0.762479	-2.440739
C	-0.053975	2.133069	-1.604814
C	-0.027940	3.505542	-1.445364
C	-0.098902	4.304793	-0.270713
C	-0.232172	3.672693	1.084559
C	-0.041577	5.689724	-0.449390
C	-0.105996	6.628886	0.584499
N	-0.051831	7.937425	0.425318
C	0.087107	8.538089	-0.900531
C	1.923856	-0.691211	3.726339
H	0.940578	-2.597959	5.124355
H	2.579598	-3.172164	4.822107
H	1.000820	-5.089837	4.846024
H	1.609876	-4.887767	3.208403
H	-1.093439	-3.983887	4.318594
H	-0.811841	-5.121134	3.020035
H	3.013554	-1.823312	1.436519
H	2.855121	-3.511430	1.931499
H	3.847465	-2.395686	2.891663
H	-2.132355	-2.134518	1.321204
H	-2.647967	-3.407878	2.445324
H	-1.858587	-3.844926	0.940671
H	0.834709	-0.190413	1.480058
H	-0.439207	-2.291423	-0.330474
H	-0.232112	1.288426	0.386166
H	-0.446364	-0.015112	-3.176049
H	0.839561	-1.142726	-2.705195
H	-0.845870	-1.604990	-2.523073
H	0.022588	1.825597	-2.644627
H	0.060979	4.069217	-2.370192
H	0.623819	3.017735	1.273844
H	-1.137167	3.059632	1.120864
H	-0.284711	4.392278	1.898766
H	0.058206	6.051805	-1.467094
H	-0.209353	6.307582	1.616029
H	1.016093	8.204934	-1.371344
H	-0.762116	8.262396	-1.531844

H	0.112289	9.621209	-0.792653
H	2.252616	0.021382	2.963468
H	2.709882	-0.724241	4.487783
H	1.012299	-0.309204	4.198770
C	-0.128898	8.852823	1.561619
H	-0.230640	8.284647	2.485797
H	0.779722	9.458526	1.608831
H	-0.993793	9.511100	1.446060

11c-dimethyl-s0126

C	-0.581547	-1.962000	3.648925
C	-0.478933	-3.241468	4.494928
C	0.960679	-3.685918	4.707345
C	1.601546	-4.001254	3.360844
C	1.308369	-2.986483	2.279633
C	0.311817	-2.072235	2.401250
C	-0.163320	-0.739544	4.486606
C	2.223782	-3.103958	1.087261
C	0.025649	-1.073763	1.370844
C	0.002592	-1.259179	0.028445
C	-0.329252	-0.229565	-0.941638
C	-0.144835	1.104679	-0.649084
C	-0.871728	-0.748081	-2.244308
C	-0.551982	2.162303	-1.504058
C	-0.463168	3.535558	-1.381448
C	0.095652	4.341396	-0.350452
C	0.740546	3.715705	0.852317
C	0.014390	5.725679	-0.522518
C	0.513121	6.670568	0.379769
N	0.436552	7.978637	0.227673
C	-0.204179	8.572774	-0.944761
C	-2.053188	-1.797221	3.231265
H	-1.026992	-4.045819	3.984933
H	-0.984805	-3.070936	5.452490
H	1.001043	-4.565647	5.356071
H	1.531105	-2.897605	5.211602
H	1.250169	-4.979384	2.996884
H	2.687844	-4.101003	3.464714
H	-0.239452	0.189433	3.910815
H	0.867066	-0.826394	4.841203
H	-0.821945	-0.638616	5.355946
H	1.884332	-3.904934	0.418176
H	3.229213	-3.379684	1.417243
H	2.291999	-2.184718	0.504446
H	-0.290278	-0.098415	1.743647
H	0.146954	-2.262316	-0.365283
H	0.341470	1.328647	0.289552
H	-0.903931	-0.009840	-3.043252
H	-0.255746	-1.585526	-2.584638
H	-1.882507	-1.142206	-2.090419
H	-1.037829	1.849697	-2.424714

H	-0.889074	4.094693	-2.210234
H	1.550139	3.052042	0.536140
H	0.005822	3.113009	1.395117
H	1.156780	4.438804	1.550462
H	-0.472425	6.082769	-1.423786
H	1.010326	6.354441	1.291265
H	0.316564	8.267057	-1.856434
H	-1.251510	8.263619	-1.000638
H	-0.158347	9.656966	-0.856305
H	-2.237779	-0.845528	2.722317
H	-2.694462	-1.826330	4.118479
H	-2.362007	-2.605885	2.560937
C	0.987759	8.900391	1.218539
H	1.435138	8.336921	2.036828
H	1.751997	9.527688	0.752579
H	0.191294	9.537172	1.612048

2. 11-*Z-trans*-retinal

11t-*n*-butyl-s0048

C	-0.994813	-4.928497	0.302556
C	-0.626993	-6.058996	1.278560
C	-0.371393	-5.552380	2.691097
C	0.828947	-4.617453	2.666209
C	0.770201	-3.590352	1.562230
C	-0.089809	-3.701370	0.517298
C	-2.462332	-4.509679	0.502326
C	1.791501	-2.494675	1.731078
C	-0.217881	-2.659543	-0.501869
C	-0.208931	-1.320616	-0.285778
C	-0.358085	-0.324156	-1.321772
C	-0.362450	0.999380	-0.940817
C	-0.505048	-0.777681	-2.747520
C	-0.495575	2.117883	-1.799706
C	-0.495596	3.416881	-1.347005
C	-0.625711	4.559381	-2.179677
C	-0.773241	4.375499	-3.667076
C	-0.611685	5.813904	-1.572292
C	-0.729446	7.030920	-2.245970
N	-0.722490	8.208986	-1.655168
C	-0.809201	9.501156	-2.337710
C	-0.834647	-5.486010	-1.124282
H	0.281768	-6.559768	0.916026
H	-1.428455	-6.806515	1.263872
H	-0.187791	-6.386428	3.374461
H	-1.250877	-5.018342	3.069599
H	1.757976	-5.195635	2.548032
H	0.935593	-4.084717	3.620257
H	-2.732396	-3.694319	-0.178074
H	-2.647465	-4.162778	1.523130

H	-3.128971	-5.354335	0.297924
H	2.023033	-1.971108	0.803032
H	2.716613	-2.928310	2.125618
H	1.456082	-1.757481	2.471380
H	-0.398286	-3.006450	-1.517398
H	-0.112906	-0.948447	0.731308
H	-0.253640	1.213586	0.120926
H	-0.608813	0.045824	-3.451251
H	0.363801	-1.370749	-3.047327
H	-1.388087	-1.416605	-2.847748
H	-0.601893	1.940597	-2.866450
H	-0.390495	3.589051	-0.277898
H	-1.666607	3.783315	-3.884111
H	0.090366	3.835959	-4.065456
H	-0.857839	5.311092	-4.215515
H	-0.503063	5.850183	-0.490453
H	-0.839391	7.069837	-3.326301
H	-1.022067	9.299238	-3.391587
H	-1.664253	10.048134	-1.926276
H	-1.290341	-4.844079	-1.884287
H	-1.336977	-6.456696	-1.187875
H	0.220635	-5.635257	-1.376193
H	-0.612723	8.234270	-0.645815
C	0.472730	10.316022	-2.187851
H	0.689298	10.462810	-1.121365
H	1.311624	9.748502	-2.609023
C	0.359698	11.676770	-2.876446
H	-0.487882	12.228878	-2.452433
H	0.135728	11.527714	-3.939969
C	1.637212	12.500317	-2.729565
H	1.540411	13.467650	-3.227154
H	1.864098	12.686849	-1.675503
H	2.492404	11.979882	-3.171264

11t-*n*-butyl-s0096

C	-0.005867	-3.532877	1.910421
C	-0.020372	-4.886431	2.649870
C	0.959144	-5.891998	2.065817
C	0.536815	-6.204684	0.639262
C	0.167481	-4.989330	-0.169101
C	-0.018966	-3.754362	0.388711
C	1.248222	-2.748887	2.343426
C	0.065588	-5.289223	-1.648142
C	-0.215486	-2.644959	-0.530147
C	-0.245526	-1.303250	-0.293897
C	-0.425354	-0.315609	-1.326664
C	-0.430094	1.012556	-0.947228
C	-0.602235	-0.761471	-2.752478
C	-0.596758	2.127663	-1.798081
C	-0.593428	3.429124	-1.343022
C	-0.761793	4.568936	-2.166463

C	-0.957391	4.387885	-3.649184
C	-0.740618	5.825501	-1.557603
C	-0.898114	7.040346	-2.222250
N	-0.885997	8.219617	-1.629436
C	-1.020042	9.509741	-2.306558
C	-1.278759	-2.791649	2.366281
H	-1.032763	-5.310669	2.594717
H	0.186752	-4.700041	3.709734
H	0.979624	-6.807548	2.663593
H	1.977105	-5.486582	2.072290
H	-0.332526	-6.880964	0.637304
H	1.324357	-6.744839	0.097921
H	1.348776	-1.793638	1.824331
H	2.159664	-3.319396	2.144571
H	1.202298	-2.544177	3.418428
H	-0.760390	-4.775760	-2.143533
H	-0.084284	-6.361804	-1.792802
H	0.994893	-5.024123	-2.166224
H	-0.317783	-2.935670	-1.570442
H	-0.122252	-0.910684	0.707975
H	-0.294480	1.227327	0.111358
H	-0.727117	0.067352	-3.446164
H	0.267006	-1.340825	-3.077894
H	-1.481246	-1.406912	-2.840488
H	-0.735876	1.952938	-2.861491
H	-0.454729	3.599392	-0.277423
H	-1.853373	3.790348	-3.839051
H	-0.103596	3.856235	-4.078095
H	-1.066204	5.324739	-4.191250
H	-0.594847	5.860310	-0.480048
H	-1.048193	7.080177	-3.297683
H	-1.263485	9.304511	-3.353229
H	-1.871649	10.040744	-1.867610
H	-1.311037	-1.743431	2.067342
H	-1.336001	-2.820955	3.459550
H	-2.172777	-3.282760	1.968886
H	-0.739546	8.245487	-0.625071
C	0.249239	10.350672	-2.199184
H	0.498290	10.501496	-1.140356
H	1.085002	9.800351	-2.648443
C	0.085622	11.708926	-2.882216
H	-0.759920	12.242506	-2.431192
H	-0.168646	11.555524	-3.938297
C	1.348784	12.560263	-2.774954
H	1.216118	13.524618	-3.270145
H	1.603457	12.753149	-1.728393
H	2.201363	12.057809	-3.241859

11t-*n*-butyl-s0144

C	0.946657	-4.837880	0.049900
C	1.377172	-5.678289	1.262863

C	0.202286	-6.071855	2.146083
C	-0.464304	-4.817518	2.699495
C	-0.658981	-3.716970	1.681206
C	-0.004567	-3.712105	0.492564
C	0.250147	-5.729954	-0.993928
C	-1.644571	-2.664131	2.122453
C	-0.181837	-2.657798	-0.507164
C	-0.234667	-1.322280	-0.282631
C	-0.375580	-0.324299	-1.319300
C	-0.372919	0.999021	-0.939065
C	-0.507540	-0.777765	-2.746457
C	-0.492327	2.117848	-1.799986
C	-0.478696	3.417421	-1.349864
C	-0.593699	4.559696	-2.185436
C	-0.743624	4.374085	-3.672370
C	-0.560616	5.815253	-1.581412
C	-0.657993	7.032294	-2.258604
N	-0.631617	8.211489	-1.670964
C	-0.696919	9.503476	-2.356380
C	2.217974	-4.240010	-0.577606
H	2.091424	-5.094930	1.860649
H	1.913498	-6.564043	0.902606
H	0.535202	-6.712300	2.968004
H	-0.526664	-6.653154	1.570401
H	0.140504	-4.402480	3.520918
H	-1.435165	-5.062276	3.144826
H	-0.054819	-5.158268	-1.876766
H	-0.643708	-6.208027	-0.585217
H	0.937015	-6.512330	-1.334220
H	-2.053691	-2.083064	1.295608
H	-1.176313	-1.969005	2.831179
H	-2.475260	-3.137084	2.654148
H	-0.203637	-2.999160	-1.542002
H	-0.130856	-0.951520	0.734173
H	-0.267908	1.213193	0.123049
H	-0.615625	0.045089	-3.450262
H	0.375677	-1.354708	-3.038759
H	-1.377310	-1.431905	-2.856422
H	-0.599779	1.939865	-2.866516
H	-0.370903	3.590749	-0.281214
H	-1.638431	3.783539	-3.887458
H	0.118461	3.832189	-4.071030
H	-0.827506	5.309072	-4.221963
H	-0.451439	5.852777	-0.499684
H	-0.766322	7.070117	-3.339129
H	-0.902074	9.302261	-3.411920
H	-1.549199	10.061316	-1.953810
H	2.011635	-3.721603	-1.519962
H	2.934916	-5.039312	-0.792605
H	2.694105	-3.528251	0.104779
H	-0.522220	8.237572	-0.661564

C	0.593166	10.303071	-2.195201
H	0.801011	10.448766	-1.126806
H	1.429249	9.725088	-2.607557
C	0.503164	11.664269	-2.886369
H	-0.342399	12.226596	-2.471879
H	0.288880	11.516597	-3.952070
C	1.788471	12.473161	-2.726663
H	1.708226	13.440770	-3.226658
H	2.006012	12.658671	-1.670452
H	2.642342	11.942279	-3.158369

11t-dimethyl-s0048

C	-1.166113	-4.850731	0.531299
C	-0.732453	-5.985829	1.474172
C	-0.213225	-5.471201	2.809435
C	1.034656	-4.636473	2.561260
C	0.876883	-3.633006	1.445218
C	-0.146093	-3.697572	0.554757
C	-2.544384	-4.308480	0.950126
C	1.992567	-2.619968	1.410937
C	-0.356075	-2.672407	-0.467994
C	-0.213139	-1.333984	-0.302435
C	-0.451214	-0.352003	-1.335831
C	-0.298725	0.975923	-1.004381
C	-0.854897	-0.824531	-2.704709
C	-0.486541	2.082210	-1.869200
C	-0.321531	3.387090	-1.466641
C	-0.502106	4.518602	-2.305387
C	-0.898379	4.310679	-3.743355
C	-0.301430	5.781317	-1.746288
C	-0.442279	6.986379	-2.442656
N	-0.257009	8.186749	-1.928762
C	0.126997	8.364375	-0.529138
C	-1.285004	-5.450641	-0.882313
H	0.064353	-6.566366	0.988248
H	-1.580527	-6.666019	1.613722
H	0.014943	-6.302555	3.482599
H	-0.976661	-4.860404	3.305439
H	1.886022	-5.289918	2.317299
H	1.333700	-4.092848	3.467052
H	-2.857904	-3.488788	0.293993
H	-2.532714	-3.925301	1.974705
H	-3.298904	-5.099794	0.885459
H	2.109536	-2.136257	0.440716
H	2.933762	-3.118391	1.666495
H	1.839026	-1.842816	2.170198
H	-0.720195	-3.027012	-1.430215
H	0.070867	-0.948264	0.673716
H	-0.007119	1.204483	0.019241
H	-1.007136	-0.011507	-3.411809
H	-0.090518	-1.490489	-3.115525

H	-1.787472	-1.394330	-2.644207
H	-0.774437	1.889636	-2.899110
H	-0.034513	3.573762	-0.433872
H	-1.852781	3.779356	-3.795371
H	-0.148277	3.700233	-4.253677
H	-1.006353	5.235443	-4.305564
H	-0.017817	5.818838	-0.699646
H	-0.725086	6.985428	-3.490528
H	-0.638537	7.944503	0.129194
H	1.085200	7.874752	-0.334762
H	0.224865	9.429507	-0.325861
H	-1.808195	-4.790383	-1.580616
H	-1.864079	-6.378273	-0.829972
H	-0.299804	-5.690958	-1.295846
C	-0.425498	9.398524	-2.727957
H	-0.711225	9.131886	-3.745047
H	-1.205046	10.024830	-2.286725
H	0.513677	9.957164	-2.751801

11t-dimethyl-s0096

C	0.110031	-3.510940	1.946108
C	0.081436	-4.839120	2.729904
C	0.900178	-5.936140	2.068045
C	0.282413	-6.250082	0.714871
C	-0.090544	-5.030284	-0.085112
C	-0.110543	-3.770186	0.446527
C	1.466032	-2.822133	2.194229
C	-0.399028	-5.359396	-1.528901
C	-0.335321	-2.672959	-0.480584
C	-0.228727	-1.327645	-0.292260
C	-0.459747	-0.356252	-1.330496
C	-0.304854	0.976960	-1.004563
C	-0.856823	-0.823691	-2.704144
C	-0.485557	2.079102	-1.869659
C	-0.311093	3.386784	-1.469485
C	-0.483176	4.515251	-2.308100
C	-0.883876	4.309733	-3.745712
C	-0.269466	5.780409	-1.752830
C	-0.398796	6.983233	-2.450894
N	-0.201416	8.185080	-1.940122
C	0.184421	8.361427	-0.541757
C	-1.033538	-2.655527	2.527323
H	-0.960005	-5.180489	2.812616
H	0.431602	-4.643008	3.749654
H	0.922480	-6.834613	2.691154
H	1.939809	-5.615465	1.937623
H	-0.629508	-6.854526	0.841805
H	0.953585	-6.865110	0.101437
H	1.574068	-1.889618	1.636683
H	2.297790	-3.468867	1.901705
H	1.572648	-2.590928	3.259511

H	-1.239805	-4.795430	-1.936826
H	-0.645886	-6.420176	-1.616035
H	0.475154	-5.181638	-2.166441
H	-0.592681	-2.981704	-1.488343
H	0.053106	-0.920031	0.670815
H	-0.015296	1.207664	0.019218
H	-1.006641	-0.006132	-3.406223
H	-0.085971	-1.481281	-3.117137
H	-1.787543	-1.396605	-2.654110
H	-0.775792	1.888415	-2.899210
H	-0.020693	3.572164	-0.437434
H	-1.837935	3.777828	-3.796687
H	-0.134568	3.701881	-4.260422
H	-0.995097	5.236053	-4.304767
H	0.016163	5.817319	-0.706675
H	-0.681757	6.982972	-3.498685
H	-0.582507	7.946149	0.118073
H	1.140098	7.866619	-0.347000
H	0.288336	9.426117	-0.338809
H	-1.021359	-1.616933	2.195121
H	-0.954659	-2.649835	3.619632
H	-2.006042	-3.082452	2.262091
C	-0.357467	9.395364	-2.742835
H	-0.643374	9.127967	-3.759755
H	-1.132542	10.030702	-2.306347
H	0.586377	9.946231	-2.767548

11t-dimethyl-s0144

C	0.721744	-4.920793	-0.029212
C	1.277926	-5.763664	1.129624
C	0.233852	-6.043616	2.200821
C	-0.242476	-4.728517	2.807218
C	-0.517697	-3.641176	1.793519
C	-0.062850	-3.715055	0.517338
C	-0.194858	-5.780487	-0.918804
C	-1.342072	-2.505651	2.346410
C	-0.320066	-2.673636	-0.478683
C	-0.238324	-1.333390	-0.295237
C	-0.468860	-0.350801	-1.330707
C	-0.310303	0.976446	-1.000977
C	-0.857301	-0.824442	-2.703509
C	-0.482940	2.081998	-1.870317
C	-0.304328	3.386126	-1.471760
C	-0.465245	4.516631	-2.316150
C	-0.859678	4.308361	-3.754562
C	-0.244173	5.778283	-1.762775
C	-0.357455	6.981874	-2.466934
N	-0.151982	8.181330	-1.958925
C	0.225396	8.360072	-0.557587
C	1.916610	-4.437032	-0.869311
H	2.119544	-5.224296	1.586283

H	1.683145	-6.696792	0.720964
H	0.646369	-6.688390	2.982255
H	-0.618353	-6.579777	1.768438
H	0.514834	-4.341942	3.507116
H	-1.144408	-4.886730	3.409108
H	-0.595379	-5.207255	-1.761578
H	-1.043756	-6.179699	-0.357897
H	0.370871	-6.620424	-1.336092
H	-1.834543	-1.914530	1.573948
H	-0.718193	-1.832065	2.947964
H	-2.109528	-2.900908	3.018153
H	-0.531670	-3.035939	-1.484569
H	0.053024	-0.949047	0.679212
H	-0.023728	1.205610	0.023912
H	-1.013945	-0.011503	-3.409718
H	-0.076151	-1.475091	-3.109476
H	-1.779394	-1.410832	-2.654409
H	-0.769372	1.889155	-2.900558
H	-0.017175	3.573035	-0.439089
H	-1.810810	3.771624	-3.808003
H	-0.105569	3.702921	-4.265261
H	-0.973875	5.233281	-4.315292
H	0.036003	5.816243	-0.715232
H	-0.632718	6.980253	-3.516805
H	-0.550323	7.954180	0.097487
H	1.175343	7.857973	-0.354591
H	0.336828	9.424675	-0.358604
H	1.600524	-3.925829	-1.784827
H	2.530373	-5.293758	-1.166681
H	2.545757	-3.748670	-0.295455
C	-0.289504	9.391205	-2.766937
H	-0.569522	9.123776	-3.785414
H	-1.061613	10.034738	-2.337569
H	0.660282	9.931796	-2.784191

11t-methyl-s0048

C	-1.182732	-4.849629	0.526983
C	-0.750144	-5.982826	1.472811
C	-0.228625	-5.465678	2.806172
C	1.020842	-4.634794	2.553618
C	0.863276	-3.632566	1.436952
C	-0.163086	-3.695733	0.549073
C	-2.561902	-4.307413	0.942486
C	1.982060	-2.623440	1.397802
C	-0.375685	-2.671575	-0.471969
C	-0.213271	-1.332962	-0.316749
C	-0.456860	-0.356798	-1.351989
C	-0.283432	0.973102	-1.031259
C	-0.888406	-0.831671	-2.711433
C	-0.471177	2.073754	-1.899434
C	-0.283450	3.381163	-1.508041

C	-0.462663	4.505439	-2.351859
C	-0.884112	4.297567	-3.782683
C	-0.238190	5.772061	-1.808151
C	-0.370949	6.973494	-2.500578
N	-0.155733	8.163232	-1.969366
C	-0.287199	9.433068	-2.673245
C	-1.298578	-5.452883	-0.885595
H	0.045139	-6.566292	0.987974
H	-1.599376	-6.660918	1.614991
H	-0.001157	-6.295656	3.481196
H	-0.989852	-4.851768	3.301764
H	1.869808	-5.290813	2.308063
H	1.324385	-4.090380	3.457437
H	-2.874889	-3.488867	0.284602
H	-2.552439	-3.922746	1.966481
H	-3.315885	-5.099133	0.877409
H	2.102875	-2.147488	0.424203
H	2.920893	-3.123077	1.659160
H	1.829351	-1.840386	2.151157
H	-0.762059	-3.025082	-1.425853
H	0.090277	-0.943819	0.651875
H	0.027042	1.204280	-0.013858
H	-1.041645	-0.020660	-3.420514
H	-0.139483	-1.509660	-3.130773
H	-1.827240	-1.388753	-2.632502
H	-0.777405	1.878822	-2.923607
H	0.021688	3.571162	-0.481209
H	-1.848068	3.782391	-3.818019
H	-0.151873	3.673687	-4.302457
H	-0.985382	5.222701	-4.345832
H	0.062790	5.826149	-0.764137
H	-0.667606	6.993629	-3.545500
H	0.668682	9.960624	-2.677370
H	-0.591243	9.238065	-3.701718
H	-1.043336	10.054148	-2.188984
H	-1.822312	-4.795844	-1.586541
H	-1.875888	-6.381516	-0.831795
H	-0.312432	-5.692377	-1.297260
H	0.123603	8.204259	-0.995015

11t-methyl-s0096

C	0.116718	-3.498542	1.940908
C	0.085714	-4.822263	2.732127
C	0.890654	-5.928631	2.068888
C	0.258380	-6.245532	0.723145
C	-0.114284	-5.028253	-0.080227
C	-0.120410	-3.764504	0.444980
C	1.480266	-2.818732	2.171853
C	-0.439086	-5.364038	-1.518652
C	-0.346008	-2.672423	-0.486010
C	-0.227924	-1.325814	-0.306561

C	-0.463361	-0.360705	-1.347326
C	-0.295236	0.974962	-1.030476
C	-0.879192	-0.831964	-2.714023
C	-0.479147	2.071300	-1.898601
C	-0.290036	3.381960	-1.507864
C	-0.466987	4.503362	-2.350224
C	-0.890680	4.297419	-3.781179
C	-0.237554	5.772783	-1.808524
C	-0.368618	6.972509	-2.499893
N	-0.147570	8.164117	-1.970310
C	-0.278811	9.432367	-2.675765
C	-1.014727	-2.631245	2.528227
H	-0.957343	-5.155645	2.826270
H	0.446593	-4.623177	3.747502
H	0.912063	-6.823932	2.696503
H	1.931343	-5.616316	1.927427
H	-0.656683	-6.842725	0.861551
H	0.919128	-6.868649	0.106547
H	1.589726	-1.889784	1.608624
H	2.304368	-3.473026	1.874547
H	1.599049	-2.582875	3.234783
H	-1.276782	-4.793838	-1.924043
H	-0.698144	-6.422655	-1.595813
H	0.432028	-5.200914	-2.164261
H	-0.615355	-2.984945	-1.489458
H	0.066796	-0.914990	0.651195
H	0.008242	1.208896	-0.011540
H	-1.029981	-0.016907	-3.418701
H	-0.118053	-1.497614	-3.132001
H	-1.813883	-1.397000	-2.650915
H	-0.784555	1.877643	-2.923228
H	0.016013	3.571069	-0.481132
H	-1.853133	3.779625	-3.817003
H	-0.157181	3.677809	-4.304380
H	-0.995735	5.224079	-4.341164
H	0.066187	5.826214	-0.765221
H	-0.669140	6.993397	-3.543665
H	0.678164	9.958027	-2.687104
H	-0.588766	9.236053	-3.702297
H	-1.030924	10.057453	-2.190175
H	-0.997624	-1.594451	2.190624
H	-0.925368	-2.620359	3.619643
H	-1.993053	-3.051907	2.274677
H	0.136376	8.205341	-0.997628

11t-methyl-s0144

C	0.717147	-4.926423	-0.045411
C	1.280891	-5.768838	1.110116
C	0.247013	-6.038497	2.193667
C	-0.213994	-4.718382	2.800959
C	-0.492504	-3.631848	1.787649

C	-0.052498	-3.713118	0.506019
C	-0.215711	-5.782848	-0.921077
C	-1.302540	-2.489006	2.346364
C	-0.314961	-2.674407	-0.489650
C	-0.232751	-1.332527	-0.310964
C	-0.471451	-0.355500	-1.347669
C	-0.307311	0.974402	-1.024181
C	-0.874166	-0.832555	-2.715032
C	-0.488620	2.074870	-1.894551
C	-0.302793	3.382133	-1.502709
C	-0.474472	4.506188	-2.348840
C	-0.890244	4.298008	-3.781260
C	-0.244054	5.772210	-1.806703
C	-0.365849	6.973233	-2.502223
N	-0.141910	8.162164	-1.973227
C	-0.262542	9.431656	-2.679747
C	1.905702	-4.453910	-0.900802
H	2.131086	-5.233482	1.555429
H	1.675437	-6.705880	0.700077
H	0.663979	-6.683173	2.972749
H	-0.613416	-6.570597	1.772717
H	0.553434	-4.334394	3.491246
H	-1.110263	-4.868336	3.413237
H	-0.622007	-5.210092	-1.761439
H	-1.060779	-6.174107	-0.348918
H	0.339270	-6.628228	-1.341684
H	-1.806150	-1.901358	1.578416
H	-0.665448	-1.813763	2.931986
H	-2.059618	-2.876069	3.034289
H	-0.532032	-3.039108	-1.493482
H	0.066409	-0.944500	0.659469
H	-0.009171	1.206451	-0.003322
H	-1.035552	-0.021597	-3.422357
H	-0.098239	-1.486023	-3.126379
H	-1.796988	-1.416719	-2.655229
H	-0.788651	1.879428	-2.920459
H	-0.001365	3.572387	-0.474841
H	-1.845193	3.767006	-3.821241
H	-0.146340	3.688818	-4.302223
H	-1.006469	5.223930	-4.340197
H	0.054371	5.826454	-0.761972
H	-0.660097	6.993406	-3.547844
H	0.697343	9.951854	-2.683233
H	-0.566443	9.237066	-3.708331
H	-1.014711	10.059298	-2.197793
H	1.583054	-3.944230	-1.814906
H	2.510167	-5.315906	-1.201835
H	2.546113	-3.767903	-0.336692
H	0.136956	8.202867	-0.998696

Vibrational frequencies ω_j (in cm^{-1}) of the mode j of **11c-dimethyl** (s0048, s0096, and s0144) ground state, the corresponding $\Delta_j^{(n)}$ (dimensionless normal coordinate displacements of the equilibrium geometry of the n^{th} excited state relative to the ground-state equilibrium geometry) for the first two excited states S_1 and S_2, and the absolute value of their product $d_j^{(n)} = |\Delta_j^{(n)}\omega_j|$.

11c-dimethyl-s0048

j	ω_j	$\Delta_j^{(1)}$	$\lvert\Delta_j^{(1)}\omega_j\rvert$	$\Delta_j^{(2)}$	$\lvert\Delta_j^{(2)}\omega_j\rvert$
1	3264.53	1.49E-02	48.49	1.97E-02	64.20
2	3241.75	-1.14E-02	36.82	-1.36E-02	44.10
3	3232.47	-6.35E-03	20.54	-3.50E-03	11.32
4	3227.54	1.50E-02	48.51	1.63E-02	52.68
5	3208.96	1.49E-02	47.67	1.94E-02	62.12
6	3205.19	-4.17E-03	13.36	-1.57E-02	50.17
7	3204.32	-1.66E-03	5.30	-3.99E-03	12.79
8	3201.45	-2.26E-03	7.24	9.63E-03	30.82
9	3201.19	-6.64E-03	21.25	6.17E-04	1.98
10	3196.72	-3.33E-03	10.65	-5.46E-03	17.44
11	3194.87	-1.46E-02	46.49	-1.16E-02	36.92
12	3177.01	1.11E-02	35.17	8.41E-03	26.71
13	3159.81	5.49E-04	1.73	-4.19E-03	13.23
14	3156.63	-2.36E-03	7.46	-1.55E-03	4.88
15	3152.23	1.36E-03	4.30	2.08E-03	6.55
16	3146.98	2.45E-03	7.72	-8.32E-03	26.18
17	3146.38	4.59E-03	14.45	9.77E-03	30.74
18	3144.19	1.07E-03	3.35	-9.44E-03	29.67
19	3139.59	-8.28E-04	2.60	-8.87E-03	27.84
20	3131.10	-2.20E-03	6.89	-7.56E-03	23.66
21	3127.74	2.26E-04	0.71	-9.30E-04	2.91
22	3114.76	-5.06E-03	15.75	-1.39E-02	43.30
23	3105.74	4.42E-03	13.71	1.17E-02	36.33
24	3085.00	-1.58E-03	4.88	-1.49E-02	45.91
25	3084.76	-2.20E-02	67.95	-3.94E-02	121.69
26	3083.27	1.65E-02	50.96	1.41E-02	43.46
27	3083.20	1.82E-02	55.99	2.87E-02	88.61
28	3079.98	9.97E-03	30.71	1.27E-02	39.13
29	3071.26	2.51E-03	7.70	-4.24E-03	13.02
30	3063.99	7.87E-03	24.10	1.25E-02	38.42
31	3058.01	-3.97E-03	12.13	-1.18E-02	36.22
32	3055.92	1.25E-02	38.27	2.86E-02	87.25
33	3049.16	-1.96E-03	5.96	4.06E-03	12.39
34	3034.08	1.62E-02	49.21	2.13E-02	64.54
35	1711.36	-9.70E-02	166.04	4.33E-02	74.15
36	1706.65	1.83E-01	311.48	5.53E-01	943.57
37	1672.36	-3.59E-01	599.73	9.10E-02	152.13

38	1636.77	1.70E-01	278.58	-2.46E-02	40.33
39	1586.64	-4.49E-02	71.30	-7.22E-02	114.52
40	1567.42	-2.20E-01	344.10	-2.45E-01	384.27
41	1522.43	4.79E-02	72.88	6.62E-02	100.81
42	1520.78	4.52E-02	68.67	2.78E-02	42.21
43	1515.32	-1.96E-02	29.75	-2.04E-02	30.84
44	1514.39	-2.47E-03	3.73	-2.02E-02	30.57
45	1509.77	4.80E-02	72.50	1.14E-01	171.66
46	1505.62	4.11E-02	61.85	7.52E-02	113.27
47	1504.55	1.80E-02	27.04	7.00E-02	105.38
48	1502.06	-2.74E-03	4.11	-1.45E-03	2.18
49	1501.67	2.88E-02	43.27	5.60E-02	84.15
50	1490.97	-8.42E-02	125.52	-1.40E-02	20.90
51	1489.42	8.22E-03	12.24	1.96E-02	29.25
52	1489.31	-1.89E-02	28.21	-1.28E-02	19.13
53	1487.52	2.51E-02	37.27	2.85E-02	42.41
54	1486.04	5.92E-02	87.97	7.58E-02	112.68
55	1485.06	-3.31E-02	49.14	-6.58E-03	9.77
56	1484.95	1.33E-02	19.70	9.98E-03	14.82
57	1482.36	-2.24E-02	33.14	-6.07E-02	90.04
58	1467.08	3.86E-02	56.61	6.67E-03	9.78
59	1462.56	-1.32E-01	193.12	-1.60E-01	234.69
60	1458.53	-1.22E-01	177.62	-1.93E-01	281.64
61	1453.96	1.76E-02	25.63	5.01E-02	72.80
62	1443.10	-8.72E-02	125.90	-9.16E-02	132.26
63	1435.10	-2.25E-02	32.29	-1.45E-01	208.52
64	1425.73	-5.89E-02	83.92	-7.89E-02	112.44
65	1417.88	-3.11E-03	4.41	4.23E-02	60.02
66	1404.46	6.00E-03	8.43	3.04E-03	4.27
67	1402.34	6.85E-03	9.61	2.68E-02	37.53
68	1393.92	-1.20E-02	16.74	1.86E-02	25.91
69	1392.83	-6.43E-02	89.57	-1.30E-01	181.28
70	1391.16	-3.64E-02	50.58	6.66E-02	92.61
71	1373.61	2.97E-02	40.79	3.56E-02	48.91
72	1360.41	-5.70E-03	7.76	-2.38E-02	32.36
73	1355.31	8.71E-02	118.04	-5.47E-02	74.12
74	1321.81	-7.41E-02	97.96	-1.00E-02	13.26
75	1315.15	1.11E-02	14.65	4.19E-02	55.09
76	1297.73	-3.55E-02	46.01	1.09E-01	141.28
77	1287.80	-7.52E-02	96.84	-2.02E-01	259.80
78	1281.44	-5.32E-02	68.18	-1.47E-01	187.94
79	1256.63	9.83E-02	123.56	7.40E-02	92.99
80	1251.04	6.42E-03	8.03	-3.83E-02	47.94
81	1245.44	-1.39E-01	173.70	-2.12E-01	264.24

82	1238.85	-1.93E-03	2.39	4.79E-03	5.93
83	1217.93	-5.90E-02	71.87	-9.17E-02	111.72
84	1212.21	2.48E-02	30.06	-1.01E-02	12.19
85	1186.57	1.94E-02	22.99	-2.90E-01	343.72
86	1167.89	-1.48E-03	1.72	3.01E-03	3.51
87	1157.02	1.68E-01	194.94	6.16E-02	71.31
88	1154.19	8.30E-02	95.78	1.16E-01	133.76
89	1137.92	-3.77E-02	42.93	9.43E-02	107.29
90	1118.33	2.35E-03	2.63	3.57E-03	3.99
91	1088.72	1.10E-03	1.20	-3.53E-02	38.48
92	1088.51	3.59E-02	39.06	6.45E-02	70.16
93	1070.11	1.17E-01	125.57	2.99E-02	32.00
94	1055.80	-6.99E-02	73.77	-1.50E-01	158.14
95	1048.33	3.57E-02	37.37	-6.07E-02	63.67
96	1043.31	-1.11E-03	1.16	-6.07E-02	63.35
97	1035.10	1.37E-01	141.96	-5.76E-02	59.67
98	1027.43	5.35E-02	54.93	-8.48E-02	87.08
99	1017.86	4.23E-02	43.05	8.50E-02	86.56
100	1014.53	1.15E-01	116.59	3.39E-01	344.15
101	1008.00	4.96E-02	50.02	1.27E-01	127.74
102	1000.98	-1.17E-01	117.13	1.92E-01	192.58
103	989.50	-2.38E-01	235.07	1.69E-01	166.85
104	979.35	2.91E-03	2.85	-1.46E-02	14.34
105	967.37	-1.25E-02	12.14	6.74E-02	65.18
106	950.96	-7.97E-03	7.58	6.21E-03	5.90
107	934.78	3.88E-02	36.26	-2.70E-01	252.21
108	917.76	8.46E-02	77.65	-3.85E-03	3.54
109	905.61	-3.82E-02	34.62	-3.75E-02	33.93
110	897.76	-2.95E-02	26.51	2.65E-02	23.81
111	893.65	9.09E-02	81.24	6.13E-02	54.75
112	890.78	4.81E-02	42.88	1.70E-01	151.08
113	877.93	-4.19E-02	36.78	8.38E-02	73.61
114	854.51	1.00E-01	85.79	2.19E-01	186.75
115	848.97	4.70E-02	39.89	1.08E-02	9.16
116	824.15	3.49E-03	2.88	5.13E-02	42.29
117	817.25	-1.40E-01	114.71	-7.00E-02	57.21
118	761.94	-3.73E-02	28.45	-5.28E-02	40.27
119	708.72	-1.76E-02	12.46	-9.93E-02	70.41
120	666.55	4.64E-03	3.09	-1.90E-02	12.65
121	592.89	-2.04E-02	12.08	8.36E-02	49.56
122	584.33	1.29E-02	7.53	-1.25E-01	73.03
123	575.04	2.56E-02	14.74	-1.13E-01	64.98
124	557.24	6.86E-03	3.82	8.38E-02	46.67
125	549.14	-3.87E-02	21.23	9.72E-02	53.36

126	510.32	-4.72E-02	24.08	-1.94E-01	98.85
127	505.79	2.79E-01	140.89	1.06E-01	53.44
128	482.60	-1.01E-01	48.57	7.08E-02	34.15
129	473.36	-7.84E-02	37.12	-1.16E-01	54.70
130	433.82	1.50E-01	64.96	8.82E-02	38.26
131	424.84	6.18E-02	26.27	-3.20E-02	13.61
132	416.35	-4.25E-02	17.69	-1.32E-02	5.51
133	410.85	1.82E-01	74.77	-3.43E-01	141.00
134	390.06	5.60E-02	21.84	-1.53E-01	59.53
135	384.34	-3.06E-02	11.77	8.09E-02	31.09
136	377.12	8.60E-02	32.43	5.49E-02	20.69
137	348.34	-8.67E-02	30.19	-4.32E-01	150.62
138	330.94	1.92E-04	0.06	-2.62E-01	86.59
139	323.82	-2.62E-02	8.48	3.88E-01	125.66
140	303.87	1.36E-02	4.15	5.01E-01	152.20
141	290.41	-4.61E-01	133.93	8.66E-01	251.56
142	286.28	9.77E-02	27.98	2.76E-01	79.11
143	277.56	-2.73E-01	75.84	6.68E-01	185.36
144	271.01	2.96E-02	8.03	-8.62E-02	23.36
145	264.29	1.80E-01	47.60	-2.26E-02	5.98
146	258.11	1.27E-01	32.91	-1.17E+00	300.94
147	252.24	-5.19E-01	131.02	-6.14E-01	154.78
148	222.34	-3.81E-01	84.76	7.83E-01	174.00
149	218.77	2.72E-01	59.56	-6.34E-01	138.74
150	184.46	-7.58E-02	13.99	-8.91E-01	164.41
151	178.58	4.51E-01	80.59	2.86E-01	51.09
152	151.88	-4.55E-01	69.12	1.59E+00	241.81
153	144.33	1.55E-01	22.36	-4.69E-01	67.72
154	134.58	-8.37E-02	11.27	-7.36E-03	0.99
155	129.83	3.06E-01	39.74	4.54E-01	58.92
156	127.96	3.76E-01	48.05	-2.52E-01	32.21
157	100.87	-1.04E-01	10.53	-1.26E+00	126.75
158	97.91	1.28E+00	125.00	-1.71E+00	167.14
159	67.14	2.88E-01	19.36	-2.52E+00	169.03
160	57.11	-1.13E+00	64.64	2.91E+00	165.94
161	48.86	-1.24E+00	60.58	1.64E+00	79.89
162	39.82	-6.09E-01	24.26	1.50E+00	59.58
163	29.98	8.41E-01	25.21	3.04E+00	91.27
164	14.65	-2.30E+00	33.64	2.96E+00	43.32
165	14.21	1.16E-02	0.16	-5.48E+00	77.92

11c-dimethyl-s0096

j	ω_j	$\Delta_j^{(1)}$	$\lvert\Delta_j^{(1)}\omega_j\rvert$	$\Delta_j^{(2)}$	$\lvert\Delta_j^{(2)}\omega_j\rvert$
1	3269.71	1.33E-02	43.61	1.99E-02	65.01

2	3252.58	4.09E-03	13.30	1.09E-02	35.44
3	3243.46	-1.04E-02	33.76	-1.46E-02	47.31
4	3238.43	1.13E-02	36.45	9.20E-03	29.80
5	3232.48	-6.16E-03	19.90	-3.35E-03	10.82
6	3228.68	1.47E-02	47.56	1.82E-02	58.87
7	3206.57	-1.01E-03	3.24	-1.21E-02	38.93
8	3201.86	4.28E-04	1.37	2.64E-03	8.45
9	3201.60	-1.73E-03	5.54	-6.15E-03	19.70
10	3196.06	9.59E-04	3.07	3.02E-03	9.64
11	3195.81	-1.57E-02	50.27	-9.94E-03	31.75
12	3175.62	-1.05E-03	3.33	-5.05E-03	16.04
13	3166.60	-5.55E-04	1.76	-3.95E-03	12.49
14	3165.97	2.77E-03	8.77	8.47E-03	26.81
15	3157.36	-5.71E-04	1.80	7.10E-05	0.22
16	3153.36	-9.46E-04	2.98	-1.34E-03	4.21
17	3151.26	1.56E-03	4.93	1.21E-03	3.80
18	3149.81	-2.09E-04	0.66	4.90E-03	15.42
19	3146.99	-1.68E-04	0.53	-2.91E-03	9.17
20	3141.17	6.68E-03	20.98	1.35E-02	42.42
21	3140.93	8.75E-04	2.75	-1.32E-03	4.14
22	3130.42	-4.13E-04	1.29	1.22E-03	3.82
23	3107.31	-3.33E-03	10.36	-4.35E-03	13.52
24	3087.30	-7.49E-04	2.31	-4.20E-03	12.98
25	3086.06	1.71E-02	52.68	5.39E-02	166.26
26	3084.72	1.43E-02	44.18	2.08E-02	64.13
27	3081.52	2.29E-02	70.45	2.73E-02	84.26
28	3077.59	1.10E-02	33.82	1.40E-02	43.01
29	3076.80	4.43E-03	13.62	7.74E-03	23.81
30	3074.26	-1.84E-03	5.66	-8.09E-03	24.87
31	3071.45	-1.17E-03	3.60	-2.68E-03	8.22
32	3068.46	1.48E-02	45.50	3.71E-02	113.78
33	3048.54	4.61E-04	1.41	2.01E-03	6.12
34	3031.28	-1.62E-02	49.20	-2.30E-02	69.81
35	1708.92	-1.15E-01	196.84	-1.01E-01	172.40
36	1671.89	-2.13E-01	355.50	4.05E-01	677.33
37	1660.13	-1.90E-01	316.20	-4.08E-01	676.65
38	1629.59	1.98E-01	322.74	-9.43E-02	153.65
39	1580.18	-5.35E-03	8.45	-1.01E-01	160.19
40	1558.94	-1.56E-01	242.72	-2.05E-01	320.22
41	1522.98	5.35E-02	81.46	8.93E-02	135.93
42	1521.31	3.62E-02	55.03	-7.97E-03	12.13
43	1520.22	1.03E-01	156.47	4.87E-02	74.01
44	1515.32	-1.09E-02	16.47	-1.75E-02	26.59
45	1513.20	-3.69E-02	55.90	-9.61E-02	145.38

46	1509.48	-4.89E-02	73.85	-8.07E-02	121.84
47	1505.71	-3.00E-05	0.05	-1.21E-02	18.29
48	1503.23	9.23E-04	1.39	-1.00E-05	0.02
49	1502.08	-5.00E-06	0.01	-2.25E-04	0.34
50	1494.00	6.50E-05	0.10	1.64E-03	2.44
51	1489.00	1.41E-02	21.06	1.60E-02	23.84
52	1488.67	4.64E-02	69.13	1.05E-02	15.63
53	1488.05	1.47E-02	21.94	5.74E-03	8.53
54	1486.56	-7.83E-03	11.63	5.32E-03	7.90
55	1485.55	1.81E-02	26.84	1.80E-02	26.70
56	1485.15	1.55E-02	22.98	2.41E-02	35.84
57	1482.39	-1.69E-02	25.06	-6.31E-02	93.47
58	1462.93	-2.32E-02	33.90	-1.32E-02	19.24
59	1460.32	-8.24E-02	120.34	-1.24E-01	180.76
60	1458.30	-1.10E-01	160.85	-2.38E-01	347.18
61	1454.20	5.64E-03	8.20	4.04E-02	58.77
62	1443.50	-7.10E-02	102.46	-6.88E-02	99.32
63	1437.70	-2.61E-02	37.51	-2.20E-01	315.79
64	1430.91	-1.14E-02	16.27	3.77E-03	5.40
65	1416.09	-4.22E-02	59.76	1.36E-02	19.26
66	1409.01	3.07E-02	43.32	-2.63E-02	37.02
67	1407.50	-1.25E-02	17.62	4.97E-02	70.00
68	1395.24	-2.68E-03	3.73	9.10E-02	126.95
69	1394.70	-3.50E-02	48.81	1.49E-01	207.76
70	1392.45	-7.34E-02	102.25	-1.57E-02	21.80
71	1381.60	-1.35E-01	187.01	-9.74E-03	13.46
72	1373.45	-3.50E-02	48.13	-3.32E-02	45.56
73	1356.28	3.58E-02	48.52	-4.36E-02	59.12
74	1344.58	-3.98E-02	53.46	6.98E-02	93.87
75	1322.25	-5.67E-02	74.95	-1.16E-02	15.36
76	1305.57	-7.38E-03	9.63	2.81E-02	36.65
77	1289.40	-3.16E-02	40.71	-2.83E-01	365.30
78	1287.95	-1.95E-02	25.18	-5.30E-02	68.25
79	1259.29	7.05E-02	88.73	4.73E-02	59.60
80	1251.75	-4.06E-02	50.80	-1.73E-01	217.15
81	1248.62	5.04E-02	62.94	1.21E-01	150.87
82	1237.62	7.16E-02	88.60	-1.12E-03	1.38
83	1222.78	6.31E-02	77.13	-7.82E-02	95.63
84	1211.17	6.28E-02	76.12	-3.79E-02	45.85
85	1183.44	2.50E-02	29.63	1.49E-01	176.06
86	1167.04	-2.14E-03	2.50	-2.32E-03	2.71
87	1157.92	1.09E-01	125.76	6.62E-02	76.69
88	1153.43	1.54E-01	177.66	9.90E-02	114.23
89	1139.01	-4.34E-02	49.40	9.82E-02	111.87

90	1118.19	2.19E-03	2.45	2.68E-03	3.00
91	1092.02	1.74E-02	19.02	-3.19E-02	34.79
92	1089.16	3.28E-02	35.75	5.14E-02	55.98
93	1077.36	-1.57E-02	16.95	-1.16E-01	125.29
94	1067.00	-5.24E-02	55.92	-6.72E-02	71.73
95	1048.92	-1.58E-02	16.56	-1.94E-02	20.35
96	1042.91	-1.11E-02	11.53	-5.07E-03	5.28
97	1031.94	1.55E-01	159.64	-1.34E-01	138.06
98	1027.67	2.97E-02	30.55	-3.88E-02	39.90
99	1015.63	1.61E-02	16.39	2.09E-02	21.19
100	1012.64	-1.66E-01	168.59	-2.33E-01	235.63
101	1009.51	1.80E-02	18.21	-5.01E-02	50.57
102	1004.48	1.11E-02	11.15	6.58E-03	6.61
103	986.26	1.10E-01	108.40	6.40E-02	63.07
104	976.80	-3.93E-03	3.84	-1.84E-03	1.80
105	971.49	5.32E-03	5.17	-2.88E-02	28.03
106	949.62	-1.02E-03	0.97	-2.85E-03	2.71
107	928.90	-2.15E-02	19.98	-3.66E-03	3.40
108	912.50	-6.03E-03	5.50	2.51E-02	22.89
109	899.93	-4.02E-02	36.22	5.32E-02	47.92
110	894.75	5.50E-03	4.92	3.40E-03	3.04
111	891.99	6.99E-02	62.34	1.79E-01	159.87
112	882.58	-3.38E-03	2.98	-1.66E-02	14.67
113	872.80	-1.57E-02	13.71	5.21E-02	45.50
114	860.50	3.08E-02	26.51	-2.36E-02	20.33
115	849.76	6.64E-02	56.40	4.98E-02	42.32
116	828.40	1.30E-01	107.49	2.31E-01	190.97
117	823.40	4.56E-03	3.75	8.19E-03	6.74
118	750.42	-9.84E-03	7.38	-6.84E-02	51.36
119	695.50	1.99E-03	1.38	-3.67E-02	25.51
120	666.58	1.76E-03	1.18	7.72E-02	51.44
121	593.94	2.64E-02	15.67	-9.92E-02	58.93
122	588.14	5.42E-02	31.87	-1.88E-01	110.65
123	579.35	-3.83E-02	22.21	1.11E-01	64.27
124	556.52	-2.50E-02	13.90	-6.33E-02	35.20
125	535.93	-2.97E-02	15.92	-1.33E-01	71.50
126	531.66	4.80E-02	25.51	-1.56E-02	8.29
127	509.55	-1.67E-01	85.16	-1.03E-01	52.38
128	483.83	-1.55E-01	74.98	-1.35E-01	65.35
129	467.70	-6.52E-03	3.05	-1.64E-01	76.54
130	448.36	8.40E-02	37.65	3.20E-01	143.36
131	424.45	5.51E-02	23.39	1.62E-02	6.87
132	418.10	-2.40E-02	10.03	1.02E-01	42.76
133	411.48	1.07E-02	4.39	1.26E-02	5.19

134	397.27	3.11E-02	12.36	-1.61E-01	63.95
135	388.15	-2.31E-02	8.98	-8.15E-02	31.64
136	385.47	7.30E-02	28.15	2.36E-01	90.98
137	346.85	-1.87E-01	64.86	-3.27E-01	113.57
138	328.37	1.65E-02	5.43	-6.84E-02	22.45
139	316.99	-1.45E-01	46.04	-7.25E-02	22.97
140	303.22	-1.59E-01	48.27	-2.71E-01	82.05
141	288.34	2.52E-03	0.73	-1.60E-01	46.17
142	283.18	7.46E-02	21.12	1.79E-02	5.07
143	274.53	5.26E-02	14.44	-4.10E-02	11.26
144	263.78	-4.50E-01	118.77	-3.81E-01	100.55
145	260.19	-1.08E-01	28.01	2.06E-01	53.69
146	246.00	-1.53E-01	37.61	7.48E-02	18.39
147	220.87	1.60E-01	35.31	6.76E-02	14.92
148	197.10	2.18E-01	42.88	4.29E-01	84.58
149	186.64	-4.74E-01	88.38	-6.60E-01	123.20
150	179.34	-2.87E-01	51.41	-4.45E-01	79.79
151	164.28	-7.16E-02	11.76	-3.10E-01	50.99
152	142.28	3.12E-02	4.44	-3.62E-01	51.57
153	136.08	-3.82E-02	5.20	-3.36E-02	4.57
154	129.95	-1.56E-01	20.27	-9.92E-01	128.95
155	126.62	-2.72E-02	3.44	1.94E-02	2.45
156	118.33	-2.94E-01	34.84	-6.88E-01	81.37
157	101.42	5.96E-01	60.47	1.35E+00	137.20
158	98.55	-3.61E-01	35.61	-5.20E-01	51.23
159	81.57	-2.36E-01	19.28	1.14E-01	9.33
160	61.06	7.84E-02	4.79	2.79E-01	17.03
161	49.42	8.26E-02	4.08	-1.01E+00	49.82
162	39.93	-4.16E-02	1.66	-1.03E-02	0.41
163	30.76	9.61E-01	29.55	3.40E-01	10.45
164	15.04	2.09E-01	3.14	1.10E+00	16.53
165	12.06	-9.07E-01	10.94	-4.72E-01	5.70

11c-dimethyl-s0144

j	ω_j	$\Delta_j^{(1)}$	$\lvert\Delta_j^{(1)}\omega_j\rvert$	$\Delta_j^{(2)}$	$\lvert\Delta_j^{(2)}\omega_j\rvert$
1	3265.35	1.49E-02	48.63	1.96E-02	64.11
2	3241.90	-1.15E-02	37.19	-1.35E-02	43.86
3	3232.81	-6.68E-03	21.60	-4.70E-03	15.20
4	3228.19	1.58E-02	50.94	1.61E-02	52.12
5	3205.59	-1.30E-03	4.16	-9.21E-03	29.54
6	3204.44	-1.74E-03	5.58	-2.65E-03	8.50
7	3202.27	5.94E-03	19.02	1.85E-02	59.17
8	3201.58	1.18E-03	3.76	4.49E-03	14.37
9	3197.39	-3.34E-03	10.67	-4.07E-03	13.02

10	3195.14	-1.70E-02	54.16	-1.09E-02	34.77
11	3183.99	1.55E-02	49.31	8.52E-03	27.13
12	3178.21	8.83E-03	28.05	8.10E-03	25.75
13	3159.55	-2.59E-04	0.82	4.55E-03	14.37
14	3157.27	-5.53E-04	1.75	-3.75E-03	11.84
15	3155.90	1.94E-03	6.12	2.60E-03	8.21
16	3152.57	-1.82E-03	5.74	-4.41E-03	13.89
17	3145.32	-3.28E-03	10.33	-1.34E-02	42.01
18	3141.42	-2.39E-03	7.51	9.24E-03	29.01
19	3135.22	3.68E-03	11.53	7.88E-03	24.69
20	3133.21	-3.72E-03	11.65	2.43E-04	0.76
21	3127.92	5.70E-05	0.18	-3.58E-03	11.19
22	3123.17	5.89E-03	18.38	1.48E-02	46.12
23	3104.16	4.88E-03	15.16	2.46E-03	7.64
24	3096.77	3.20E-03	9.90	-1.06E-04	0.33
25	3085.18	-1.20E-02	36.97	-8.96E-03	27.65
26	3084.01	1.96E-02	60.40	4.18E-02	129.03
27	3082.80	2.51E-02	77.48	2.56E-02	78.82
28	3080.13	2.49E-03	7.66	3.44E-03	10.58
29	3079.42	1.04E-02	32.12	1.31E-02	40.35
30	3066.17	6.75E-03	20.68	1.59E-02	48.87
31	3058.85	5.25E-03	16.07	1.01E-02	30.96
32	3056.16	1.10E-02	33.65	2.86E-02	87.26
33	3048.63	-7.21E-04	2.20	-6.00E-03	18.30
34	3029.58	1.40E-02	42.44	2.03E-02	61.42
35	1711.44	-2.78E-02	47.63	2.13E-01	365.34
36	1709.04	-2.30E-01	392.74	-5.46E-01	932.97
37	1677.35	-3.59E-01	602.43	7.92E-02	132.83
38	1637.89	1.64E-01	267.88	-1.86E-02	30.48
39	1587.22	-4.17E-02	66.14	-7.19E-02	114.17
40	1568.52	-2.19E-01	344.04	-2.46E-01	386.43
41	1521.99	4.37E-02	66.48	6.01E-02	91.43
42	1517.94	-7.04E-03	10.68	-3.13E-02	47.56
43	1515.03	2.54E-02	38.43	6.59E-03	9.98
44	1511.47	-4.63E-02	69.92	-4.03E-02	60.92
45	1510.31	4.94E-02	74.57	1.28E-01	193.69
46	1506.67	3.20E-02	48.15	1.03E-01	155.09
47	1504.54	1.78E-02	26.81	7.40E-02	111.36
48	1501.52	-3.08E-04	0.46	-3.71E-04	0.56
49	1501.41	2.24E-02	33.66	-7.69E-03	11.55
50	1491.76	-9.05E-02	135.07	-4.10E-02	61.12
51	1489.35	2.12E-02	31.59	1.01E-02	15.08
52	1488.87	-1.37E-02	20.35	-3.13E-02	46.64
53	1487.50	-2.39E-02	35.48	-2.51E-02	37.33

54	1486.41	-6.36E-02	94.52	-7.98E-02	118.64
55	1485.54	-3.44E-02	51.16	-2.73E-02	40.49
56	1484.22	7.05E-04	1.05	2.66E-02	39.52
57	1482.51	2.60E-02	38.53	5.51E-02	81.63
58	1470.78	3.26E-02	47.96	8.06E-02	118.51
59	1462.14	-1.19E-01	173.43	-1.60E-01	234.48
60	1458.28	-1.17E-01	170.27	-1.82E-01	265.81
61	1453.25	-2.13E-02	30.95	-4.37E-02	63.48
62	1443.05	-8.17E-02	117.90	-8.73E-02	125.97
63	1435.29	-2.29E-02	32.91	-1.41E-01	202.48
64	1427.87	5.15E-02	73.54	8.29E-02	118.30
65	1416.07	-8.91E-03	12.61	2.99E-02	42.29
66	1407.17	1.01E-02	14.20	2.37E-02	33.41
67	1403.40	2.31E-03	3.24	-3.70E-02	51.88
68	1394.12	2.87E-03	4.00	8.07E-03	11.25
69	1393.74	-7.23E-02	100.73	-1.45E-01	201.60
70	1390.90	-3.43E-02	47.68	6.29E-02	87.52
71	1375.25	-2.20E-02	30.28	-3.16E-02	43.49
72	1357.94	3.05E-02	41.42	-2.91E-02	39.50
73	1354.16	-7.30E-02	98.83	5.34E-02	72.35
74	1321.61	-7.64E-02	101.01	-6.36E-03	8.41
75	1312.62	-1.78E-02	23.41	6.22E-02	81.58
76	1297.15	1.59E-02	20.60	-5.60E-02	72.63
77	1287.75	-7.07E-02	91.02	-2.07E-01	267.08
78	1280.69	-5.36E-02	68.69	-1.54E-01	196.97
79	1257.34	7.99E-02	100.47	1.18E-01	148.24
80	1251.77	-4.79E-02	59.97	5.46E-02	68.33
81	1246.09	-1.10E-01	137.28	-2.16E-01	269.49
82	1238.45	-9.54E-02	118.19	1.91E-03	2.37
83	1217.35	3.70E-02	45.08	1.14E-01	138.57
84	1211.04	-5.05E-02	61.21	9.92E-02	120.12
85	1190.61	-9.69E-03	11.53	-2.66E-01	317.24
86	1167.62	6.14E-04	0.72	-1.45E-03	1.69
87	1159.86	9.77E-02	113.34	7.93E-02	91.98
88	1153.12	1.65E-01	189.81	8.05E-02	92.82
89	1137.50	-4.25E-02	48.35	9.58E-02	108.92
90	1117.46	-3.35E-03	3.74	-7.82E-03	8.74
91	1092.62	4.23E-02	46.20	6.91E-03	7.55
92	1087.69	4.00E-02	43.49	6.78E-02	73.78
93	1070.71	-3.70E-02	39.60	4.21E-02	45.04
94	1056.93	1.06E-01	112.53	1.90E-01	200.97
95	1050.11	-3.93E-02	41.25	7.97E-02	83.74
96	1044.96	-4.38E-03	4.58	6.52E-02	68.11
97	1034.08	1.31E-01	135.77	-9.54E-02	98.61

98	1026.95	1.23E-02	12.63	8.95E-02	91.95
99	1019.11	-4.18E-02	42.62	-1.06E-01	108.19
100	1017.56	1.95E-02	19.85	2.80E-01	285.14
101	1013.22	1.48E-01	150.22	1.85E-01	187.53
102	997.60	2.70E-01	268.87	-2.68E-01	266.89
103	991.36	-7.80E-02	77.35	9.02E-03	8.94
104	981.27	-1.16E-03	1.14	9.74E-03	9.56
105	962.33	4.70E-03	4.52	-1.12E-01	107.76
106	949.53	2.56E-02	24.29	-4.35E-02	41.32
107	935.41	-7.40E-02	69.25	2.33E-01	218.02
108	918.16	6.58E-02	60.43	6.18E-02	56.78
109	907.81	-3.59E-02	32.62	-1.31E-01	118.60
110	898.36	4.33E-02	38.86	-1.84E-02	16.56
111	894.50	9.48E-02	84.77	3.37E-02	30.10
112	891.40	6.18E-02	55.12	1.52E-01	135.81
113	879.06	5.35E-02	47.01	-4.17E-03	3.67
114	855.39	-5.15E-02	44.03	-8.83E-02	75.52
115	848.91	5.85E-02	49.68	2.82E-02	23.90
116	824.91	4.26E-03	3.51	-4.74E-02	39.07
117	814.46	1.20E-01	97.53	2.93E-02	23.83
118	765.77	-2.41E-02	18.48	1.93E-02	14.80
119	715.98	-2.45E-02	17.53	-1.63E-01	116.63
120	646.71	1.61E-02	10.44	-7.16E-02	46.28
121	589.27	-1.68E-02	9.88	8.62E-02	50.80
122	586.90	-5.98E-02	35.09	2.06E-01	121.09
123	579.00	5.99E-02	34.65	-1.41E-01	81.63
124	556.65	-1.40E-02	7.82	-4.44E-02	24.74
125	546.56	3.29E-02	17.96	-8.34E-03	4.56
126	518.03	2.34E-01	121.08	1.56E-01	81.02
127	503.07	-4.20E-02	21.14	-6.94E-02	34.91
128	481.63	1.07E-01	51.76	1.24E-01	59.49
129	468.10	-1.80E-01	84.29	1.86E-02	8.70
130	439.65	-2.70E-02	11.86	1.24E-02	5.47
131	425.51	4.34E-02	18.48	-2.31E-01	98.29
132	420.95	-8.56E-03	3.60	-6.90E-01	290.37
133	416.77	-3.91E-02	16.29	-3.97E-02	16.55
134	390.54	-9.07E-02	35.42	2.03E-01	79.45
135	389.44	1.24E-01	48.23	-1.79E-01	69.53
136	362.55	9.15E-02	33.18	-6.29E-01	228.10
137	351.43	-2.93E-03	1.03	-4.43E-01	155.62
138	330.09	-1.27E-01	41.83	1.07E-01	35.30
139	327.79	2.06E-01	67.50	-7.05E-01	231.03
140	303.14	3.51E-03	1.06	-5.77E-01	174.97
141	296.30	3.63E-01	107.58	-4.15E-01	123.02

142	281.75	1.92E-01	54.18	-4.39E-01	123.56
143	277.43	-5.09E-02	14.12	3.68E-01	102.00
144	271.94	7.49E-02	20.37	-5.62E-02	15.28
145	261.89	-5.54E-01	144.96	6.47E-01	169.37
146	254.27	2.22E-02	5.65	1.49E+00	377.84
147	242.72	1.86E-01	45.13	5.99E-01	145.31
148	213.89	-1.29E-01	27.62	4.63E-01	98.93
149	204.47	3.82E-01	78.13	2.66E-01	54.47
150	179.93	-3.11E-01	55.94	2.02E-01	36.38
151	170.63	3.82E-01	65.15	5.95E-01	101.57
152	153.34	4.60E-01	70.56	-1.22E+00	187.79
153	136.16	1.37E-01	18.67	-1.83E-01	24.91
154	130.52	-5.10E-01	66.51	4.80E-01	62.62
155	127.29	-2.63E-01	33.46	6.40E-02	8.14
156	111.99	4.33E-01	48.54	-7.99E-02	8.95
157	97.62	-1.92E-01	18.72	-9.88E-01	96.49
158	95.66	-1.19E+00	113.42	2.12E+00	202.43
159	66.40	4.68E-01	31.07	-2.60E+00	172.36
160	62.38	8.88E-01	55.37	4.35E-02	2.71
161	54.82	-4.38E-01	24.04	2.34E+00	128.32
162	39.37	6.52E-01	25.68	-1.50E+00	58.95
163	29.17	5.98E-01	17.44	3.87E+00	112.90
164	14.20	2.02E+00	28.62	-3.09E+00	43.83
165	12.52	1.16E-01	1.46	6.06E+00	75.86