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Supporting Information

Rotation-Inversion Isomerization of Tertiary Carbamates: Potential Energy Surface Analysis of Multi-Paths Isomerization Using Boltzmann Statistics

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Supporting Information

Table of Content

Stationary structures of *N*-ethyl-*N*-(2,2,2-trifluoroethyl) methyl carbamate at MP2/6-311++G(d,p) With SMD Solvent Model System

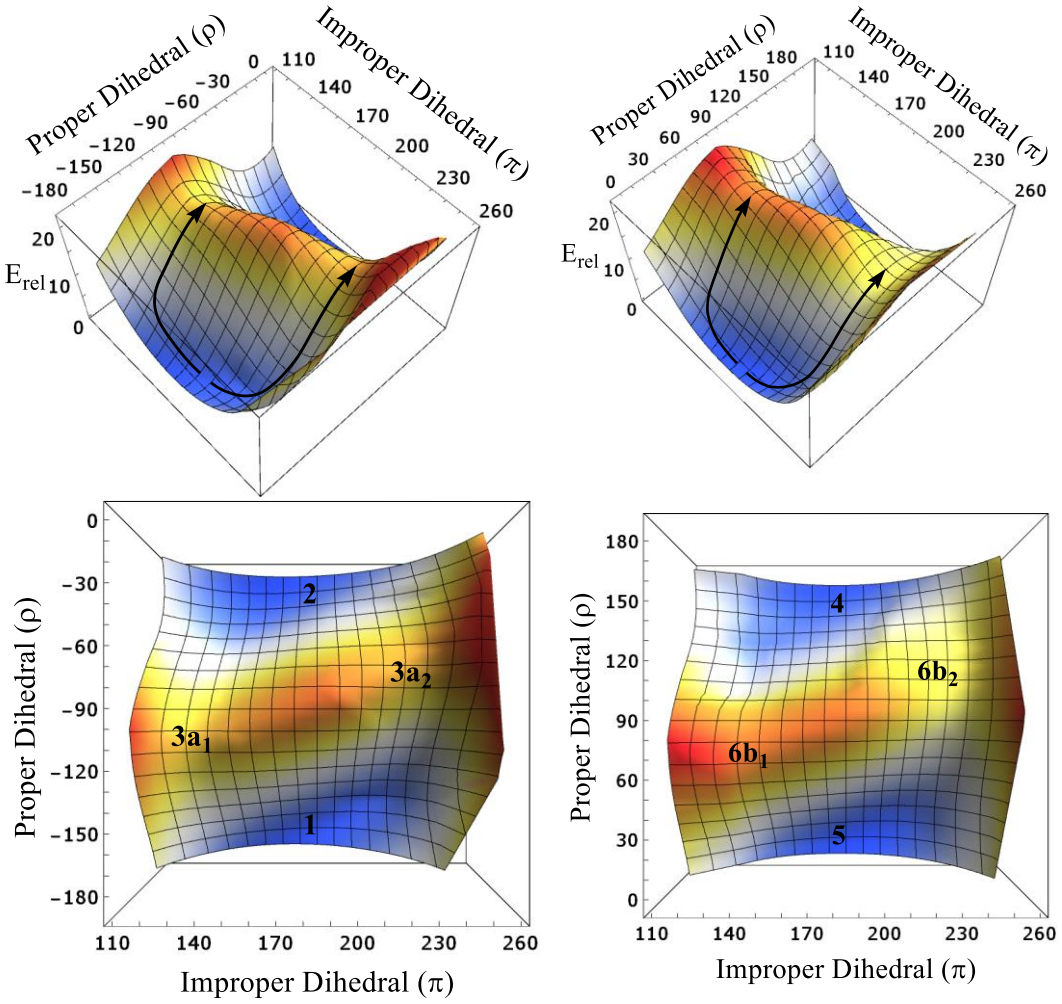

Figure S1. Rotation-inversion surfaces $E(\rho,\pi)$ for *E*/*Z*-isomerizations *E*-**1** ⇌ *Z*-**2** (left) via TS structures **3a** and *E*-**4** ⇌ *Z*-**5** (right) TS structures **6b**.

Table S1. Total Energies and Thermochemical Parameters Without SMD Solvent Model System

Species	Total E	VZPE	TE	S	ν	U_{298}	G_{298}
A	-362.161094	85.70	90.38	85.12	**i**171.4	-362.017061	-362.056561
B	-362.163499	86.26	91.63	89.37	104.2	-362.017479	-362.058997
C	-362.161695	85.94	91.02	87.90	**i**139.6	-362.016652	-362.057473
D	-362.142464	85.99	90.65	83.33	**i**97.1	-361.998006	-362.036655
E	-362.141143	85.86	90.55	83.70	**i**92.6	-361.996838	-362.035662
F	-362.129884	85.09	89.76	84.74	**i**238.1	-361.986836	-362.026156
1	-737.822943	107.92	116.00	114.70	44.8	-737.638085	-737.691641
2	-737.823206	108.01	116.03	113.72	45.9	-737.638304	-737.691916
4	-737.822545	107.97	116.02	114.15	39.1	-737.637652	-737.690943
5	-737.822763	107.97	116.01	113.86	42.3	-737.637885	-737.691037
1a	-737.821089	107.97	115.49	109.92	**i**52.1	-737.637046	-737.688326
1b	-737.821278	108.18	116.15	113.42	41.9	-737.636187	-737.689132
2a	-737.820843	107.99	115.51	110.38	**i**53.8	-737.636761	-737.688262
2b	-737.821053	108.19	116.16	113.54	39.2	-737.635937	-737.688940
TS(**1**,**4'**)	-737.816594	107.97	115.49	109.30	**i**93.8	-737.632554	-737.683541
TS(**2**,**5'**)	-737.816808	108.06	115.54	108.79	**i**87.0	-737.632688	-737.683434
TS(**1**,**4**)	-737.814094	107.87	115.42	108.37	**i**75.1	-737.630167	-737.680710
TS(**2**,**5**)	-737.814560	107.88	115.42	108.19	**i**69.9	-737.630631	-737.681090
3a$_1$	-737.794816	107.41	114.90	108.79	**i**70.0	-737.611719	-737.662463
3a$_2$	-737.794237	107.63	115.08	108.76	**i**81.7	-737.610846	-737.661577
3b$_1$	-737.796258	107.59	115.06	109.57	**i**88.9	-737.612902	-737.664017
3b$_2$	-737.793954	107.54	115.03	108.61	**i**83.1	-737.610647	-737.661308
6a$_1$	-737.790899	107.33	114.89	109.33	**i**97.0	-737.607817	-737.658816
6a$_2$	-737.800622	107.54	115.02	109.18	**i**69.8	-737.617320	-737.668252
6b$_1$	-737.791716	107.32	114.91	109.66	**i**92.2	-737.608602	-737.659757
6b$_2$	-737.799371	107.42	114.93	109.41	**i**57.6	-737.616215	-737.667257

[a]All data computed at MP2/6-311++G(d,p).

[b]Total energies (Total E) in Hartree, vibrational zero-point energies (VZPE) and thermal energies (TE) in kcal/mol, and entropy (*S*) in cal/mol^{-1} K^{-1}. Lowest vibrational wavenumber in cm^{-1}.

Table S2. Relative Energies and Isomer Populations Computed at MP2 and Higher-Order MPx Levels Without SMD Solvent Model System

Relative Energies[a,b]	MP2		MP3	MP4		
	ΔG_{rel}	ΔE_{rel}		(DQ)	(SDQ)	(SDTQ)
E_{rel}, **A** *vs.* **B**	1.53	1.51	1.38	1.35	1.41	1.56
E_{rel}, **C** *vs.* **B**	0.96	1.13	1.02	1.03	1.08	1.20
A_{cr}(**D**)	14.02	13.20	13.08	12.85	12.69	12.47
A_{cr}(**E**)	14.64	14.03	13.83	13.52	13.42	13.32
A_{cr}(**F**)	20.61	21.09	20.69	20.36	20.32	20.56
E_{rel}, **1** *vs.* **2**	0.17	0.17	0.09	0.10	0.12	0.18
E_{rel}, **4** *vs.* **2**	0.60	0.42	0.38	0.40	0.39	0.37
E_{rel}, **5** *vs.* **2**	0.54	0.28	0.30	0.29	0.26	0.23
E_{rel}, **1b** *vs.* **1**	1.57	1.04	1.20	1.20	1.12	0.95
E_{rel}, **2b** *vs.* **2**	1.86	1.35	1.44	1.47	1.42	1.30
A_{ar}(**1**,**4'**)	5.08	3.90	3.91	3.90	3.82	3.98
A_{ar}(**2**,**5'**)	5.32	3.93	3.96	3.94	3.84	4.02
A_{ar}(**1**,**1a**)	2.08	1.16	1.25	1.26	1.20	1.10
A_{ar}(**1b**,**1a**)	0.51	0.12	0.04	0.06	0.07	0.15
A_{ar}(**2**,**2a**)	2.29	1.48	1.48	1.53	1.51	1.48
A_{ar}(**2b**,**2a**)	0.43	0.13	0.04	0.06	0.09	0.18
A_{ar}(**1**,**4**)	6.86	5.58	5.60	5.55	5.41	5.55
A_{ar}(**2**,**5**)	6.79	5.31	5.34	5.36	5.33	5.43
1 to **2**						
E_{rel}, **3a$_1$** *vs.* **3b$_1$**	0.98	0.90	1.09	0.97	0.96	0.89
E_{rel}, **3a$_2$** *vs.* **3b$_1$**	1.53	1.27	1.44	1.38	1.31	1.19
E_{rel}, **3b$_2$** *vs.* **3b$_1$**	1.70	1.45	1.54	1.45	1.40	1.36
A_{cr}(**1**,**3b$_1$**)	17.33	16.75	16.61	16.42	16.22	15.89
A_{cr}(**2**,**3b$_1$**)	17.50	16.91	16.70	16.53	16.34	16.07
4 to **5**						
E_{rel}, **6a$_1$** *vs.* **6a$_2$**	5.92	6.10	5.97	5.97	5.91	5.91
E_{rel}, **6b$_1$** *vs.* **6a$_2$**	5.33	5.59	5.48	5.51	5.45	5.44
E_{rel}, **6b$_2$** *vs.* **6a$_2$**	0.62	0.79	0.76	0.69	0.74	0.81
A_{cr}(**4**,**6a$_2$**)	14.24	13.76	13.79	13.49	13.31	13.03
A_{cr}(**5**,**6a$_2$**)	14.30	13.89	13.88	13.60	13.44	13.17

Isomer Populations[c]						
p(**1**)	0.26	0.26	0.29	0.28	0.27	0.25
p(**2**)	0.35	0.35	0.33	0.34	0.34	0.34
p(**4**)	0.17	0.17	0.18	0.17	0.17	0.18
p(**5**)	0.22	0.22	0.20	0.21	0.22	0.23
p(**1**,**4**)	0.43	0.43	0.47	0.45	0.44	0.43
p(**2**,**5**)	0.57	0.57	0.53	0.55	0.56	0.57

[a] All data computed with the 6-311++G(d,p) basis set and based on the MP2(fc)/6-311++G(d,p) structures. All MPx computations employed the frozen-core approximation.

[b] Activation energies with respect to *N*-inversion (A_{inv}), *N*-alkyl rotation (A_{ar}), and carbamate rotation (A_{cr}), and relative isomers energies (E_{rel}) in terms of electronic energy (ΔE_{rel}) and Gibbs' free energy (ΔG_{rel}) in kcal/mol.

[c] Boltzmann populations *p*(**n**).

Table S3. Proper and Improper Dihedral Angles of the Conformations of *N*,*N*-Dimethyl Methyl Carbamate **VI** and *N*-Ethyl-*N*-(2,2,2-trifluoroethyl) Methyl Carbamate **VII** Without SMD Solvent Model System

Species[a-c]	Proper Dihedral ρ	Improper Dihedral π	ψ	Proper Dihedral α	Proper Dihedral β
A	180.00	180.00	0.00	180.00	180.00
B	-165.14	208.66	28.66	153.68	-161.57
C	175.26	167.93	12.07	159.64	145.44
D	-60.78	238.45	58.45	176.19	-176.19
E	117.39	234.79	54.79	170.76	-170.76
F	89.03	178.06	1.94	~	~
				Proper Dihedral γ	Proper Dihedral δ
1	174.79	177.77	2.23	81.79	100.71
2	-6.91	171.56	8.44	77.13	105.89
4	-176.32	184.34	4.34	75.41	-102.62
5	4.30	187.47	7.47	78.82	-107.50
1a	-171.64	192.56	12.56	133.35	90.52
1b	-166.52	199.81	19.81	151.53	87.45
2a	3.47	185.31	5.31	127.17	100.89
2b	9.77	195.19	15.19	147.72	94.98

TS(**1**,**4'**)	172.99	161.76	18.24	-175.21	94.08
TS(**2**,**5'**)	-5.98	159.64	20.36	-179.48	94.93
TS(**1**,**4**)	-176.68	185.36	5.36	80.49	-175.12
TS(**2**,**5**)	2.09	184.29	4.29	80.57	-173.03
3a$_1$	-99.92	133.93	46.07	83.78	68.39
3a$_2$	-64.52	222.17	42.17	170.69	72.21
3b$_1$	76.39	130.68	49.32	75.60	71.51
3b$_2$	118.07	231.57	51.57	169.20	72.92
6a$_1$	-101.85	152.27	27.73	58.20	-91.97
6a$_2$	-64.01	235.73	55.73	62.08	-138.98
6b$_1$	77.20	152.27	27.73	56.28	-87.60
6b$_2$	115.41	232.55	52.55	60.03	-136.06

[a]All data computed with the 6-311++G(d,p) basis set and based on the MP2(fc)/6-311++G(d,p) structures. All MPx computations employed the frozen-core approximation.

[b]Degree of pyramidalization $\psi = |\pi - 180^o|$.

[c]Proper dihdral angles $\alpha = \angle(MeO_2C{-}N{-}CH_2{-}H_{CO})$, $\beta = \angle(MeO_2C{-}N{-}CH_2{-}H_{COMe})$, $\gamma = \angle(MeO_2C{-}N{-}CH_2{-}CH_3)$, and $\delta = \angle(MeO_2C{-}N{-}CH_2{-}CF_3)$. For the parent system **A** - **E**, $\rho = \angle(H_3C{-}N{-}C(OMe){=}O)$, $\pi = \angle(H_3C{-}N{-}C_{carb}{\cdots}CH_3)$. For the fluorinated model systems **VII** $\rho = \angle(F_3CH_2C{-}N{-}C(OMe){=}O)$, $\pi = \angle(F_3C\ H_2C{-}N{-}C_{carb}{\cdots}CH_2\ CH_3)$.

Table S4. Electronic Energies from MP2 and Higher-Order MPx Calculations Without SMD Solvent Model System[a,b]

Molecule	MP2	MP3	MP4(DQ)	MP4(SDQ)	MP4(SDTQ)
A	-362.161094	-362.191858	-362.197908	-362.212551	-362.261630
B	-362.163499	-362.194059	-362.200059	-362.214801	-362.264121
C	-362.161695	-362.192440	-362.198425	-362.213076	-362.262212
D	-362.142464	-362.173207	-362.179577	-362.194580	-362.244248
E	-362.141143	-362.172022	-362.178511	-362.193421	-362.242894
F	-362.129884	-362.161095	-362.167619	-362.182425	-362.231363
1	-737.822943	-737.849565	-737.859002	-737.885731	-737.967123
2	-737.823206	-737.849713	-737.859167	-737.885930	-737.967409
4	-737.822545	-737.849101	-737.858533	-737.885309	-737.966814
5	-737.822763	-737.849243	-737.858711	-737.885512	-737.967039
1a	-737.821089	-737.847577	-737.856998	-737.883820	-737.965370
2a	-737.820843	-737.847356	-737.856729	-737.883522	-737.965045

1b	-737.821278	-737.847647	-737.857089	-737.883939	-737.965609
2b	-737.821053	-737.847424	-737.856822	-737.883672	-737.965330
TS(**1**,**4'**)	-737.816594	-737.843353	-737.852764	-737.879512	-737.961029
TS(**2**,**5'**)	-737.816808	-737.843448	-737.852852	-737.879657	-737.961285
TS(**1**,**4**)	-737.814094	-737.843448	-737.852852	-737.879657	-737.961285
TS(**2**,**5**)	-737.814560	-737.841256	-737.850655	-737.877385	-737.958909
3a$_1$	-737.794816	-737.821370	-737.831283	-737.858355	-737.940375
3a$_2$	-737.794237	-737.820800	-737.830634	-737.857797	-737.939896
3b$_1$	-737.796258	-737.823101	-737.832828	-737.859885	-737.941797
3b$_2$	-737.793954	-737.820643	-737.830518	-737.857652	-737.939624
6a$_1$	-737.790899	-737.817609	-737.827520	-737.854682	-737.936629
6a$_2$	-737.800622	-737.827128	-737.837031	-737.864097	-737.946048
6b$_1$	-737.791716	-737.818394	-737.828253	-737.855414	-737.937380
6b$_2$	-737.799371	-737.825912	-737.835929	-737.862916	-737.944762

[a] All data computed at MP2/6-311++G(d,p).

[b] Total energies (Total E) in Hartree, vibrational zero-point energies (VZPE) and thermal energies (TE) in kcal/mol, and entropy (*S*) in cal/mol^{-1} K^{-1}. Lowest vibrational wavenumber in cm^{-1}.

Table S5. Electronic Energies from MP2 and Higher-Order MPx Calculations With SMD Solvent Model System

Molecule	MP2	MP3	MP4(DQ)	MP4(SDQ)	MP4(SDTQ)
A	-362.065718	-362.169033	-362.199955	-362.205895	-362.220459
B	-362.066501	-362.170958	-362.201666	-362.207584	-362.222259
C	-362.065300	-362.169182	-362.200101	-362.205956	-362.220505
D	-362.045538	-362.151375	-362.182178	-362.188493	-362.203459
E	-362.044983	-362.150396	-362.181379	-362.187766	-362.202635
F	-362.137695	-362.160977	-362.167518	-362.182351	-362.231316
1	-737.701788	-737.832897	-737.859756	-737.869105	-737.895700
2	-737.702099	-737.833387	-737.860154	-737.869519	-737.896133
4	-737.701210	-737.832131	-737.858992	-737.868332	-737.894965
5	-737.701325	-737.832460	-737.859227	-737.868599	-737.895254
1a	-737.698436	-737.830620	-737.857350	-737.866677	-737.893367
2a	-737.698355	-737.830425	-737.857180	-737.866468	-737.893130
1b	-737.699147	-737.830893	-737.857502	-737.866851	-737.893573
2b	-737.698930	-737.830635	-737.857240	-737.866557	-737.893279
TS(**1**,**4'**)	-737.694023	-737.826753	-737.853753	-737.863067	-737.889684
TS(**2**,**5'**)	-737.694443	-737.827117	-737.853999	-737.863312	-737.889986
TS(**1**,**4**)	-737.689620	-737.822786	-737.849673	-737.858971	-737.885645
TS(**2**,**5**)	-737.690191	-737.823174	-737.850140	-737.859444	-737.886053
3a$_1$	-737.674720	-737.807051	-737.833836	-737.843623	-737.870585
3a$_2$	-737.673530	-737.805743	-737.832513	-737.842270	-737.869338
3b$_1$	-737.675348	-737.807338	-737.834365	-737.844051	-737.871002
3b$_2$	-737.672590	-737.805424	-737.832298	-737.842078	-737.869132
6a$_1$	-737.670278	-737.801881	-737.828881	-737.838664	-737.865687
6a$_2$	-737.680408	-737.812168	-737.838830	-737.848685	-737.875652
6b$_1$	-737.671167	-737.802847	-737.829739	-737.839522	-737.866588
6b$_2$	-737.679368	-737.811396	-737.838141	-737.848049	-737.874938

Table S6. Through-Space Coulombic Stabilization of TS Structures **3** and **6** Without SMD Solvent System[a]

Stability	TS Str.	E_{rel}	X_p	$X_p \cdots C{=}O$	$C{-}X_p$
2	**3a$_1$**	0.91	F	2.892	1.345
3	**3a$_2$**	1.27	F	3.197	1.342
1	**3b$_1$**	0.00	F	2.875	1.349
4	**3b$_2$**	1.45	F	3.348	1.336
4	**6a$_1$**	6.10	H	2.921	1.092
1	**6a$_2$**	0.00	H	2.596	1.095
3	**6b$_1$**	5.59	H	2.812	1.092
2	**6b$_2$**	0.79	H	2.612	1.095

[a] Relative energies (E_{rel}) based on the MP2/6-311++G(d,p) energies.

Table S7. Computed NMR Data for Model System **VII**

Parameter	1	2	4	5	TMS
B3LYP/6-311+G(2d,p)					
C-F J coupling (Hz)					
C13-F14	-352.43	-354.83	-360.39	-359.19	
C13-F15	-361.72	-360.42	-350.47	-353.00	
C13-C16	-352.68	-353.90	-354.27	-354.80	
Shielding (ppm)	47.46	47.78	47.86	48.22	183.11
B3LYP/6-311+G(2d,p) Solv.					
C-F J coupling (Hz)					
C13-F14	-354.03	-355.72	-357.99	-357.71	
C13-F15	-358.97	-358.91	-352.13	-353.96	
C13-C16	-352.66	-353.88	-353.79	-354.49	
Shielding (ppm)	46.75	47.07	47.22	47.55	184.12
B3LYP/aug-cc-pVTZ					
C-F J coupling (Hz)					
C13-F14	-351.623	-354.00	-359.473	-358.237	
C13-F15	-360.707	-359.37	-349.657	-352.186	
C13-C16	-351.642	-352.85	-353.2	-353.72	
Shielding (ppm)	47.1041	47.41	47.4945	47.821	184.40
B3LYP/aug-cc-pVTZ Solv.					
C-F J coupling (Hz)					
C13-F14	-353.144	-354.81	-357.101	-356.79	

Parameter	1	2	4	5	TMS
C13-F15	-357.988	-357.89	-351.242	-353.069	
C13-C16	-351.566	-352.78	-352.684	-353.353	
Shielding (ppm)	46.4244	46.73	46.8783	47.1769	185.45
B3LYP/aug-cc-pVQZ					
C-F J coupling (Hz)					
C13-F14	-355.88	-358.30	-363.89	-362.63	
C13-F15	-365.11	-363.74	-353.90	-356.47	
C13-C16	-355.97	-357.20	-357.58	-358.12	
Shielding (ppm)	41.87	42.17	42.28	42.62	181.60
B3LYP/aug-cc-pVQZ Solv.					
C-F J coupling (Hz)					
C13-F14	-357.41	-359.10	-361.46	-361.14	
C13-F15	-362.33	-362.22	-355.50	-357.35	
C13-C16	-355.87	-357.10	-357.03	-357.73	
Shielding (ppm)	41.17	41.47	41.65	41.96	182.68
BHandH/6-311++G(3df,3pd)					
C-F J coupling (Hz)					
C13-F14	-292.881	-301.092	-301.553	-300.37	
C13-F15	-302.439	-293.552	-291.175	-293.55	
C13-C16	-292.677	-295.153	-294.141	-294.44	
Shielding (ppm)	56.6554	56.9808	57.0017	57.3323	189.68
BHandH/6-311++G(3df,3pd) Solv.					
C-F J coupling (Hz)					
C13-F14	-294.06	-295.60	-298.73	-298.45	
C13-F15	-299.27	-299.14	-292.44	-294.08	
C13-C16	-292.19	-293.09	-293.25	-293.73	
Shielding (ppm)	55.90	56.23	56.32	56.62	190.82
BHandH/aug-cc-pVTZ					
C-F J coupling (Hz)					
C13-F14	-294.79	-303.02	-303.48	-302.28	
C13-F15	-304.41	-295.35	-293.07	-295.47	
C13-C16	-294.49	-297.07	-295.93	-296.22	
Shielding (ppm)	57.58	57.89	57.91	58.23	190.73
BHandH/aug-cc-pVTZ Solv.					
C-F J coupling (Hz)					
C13-F14	-295.98	-301.07	-300.65	-300.37	
C13-F15	-301.22	-294.90	-294.34	-295.99	
C13-C16	-294.02	-297.52	-295.05	-295.53	
Shielding (ppm)	56.85	57.16	57.24	57.54	189.74

Parameter	1	2	4	5	TMS
BHandHLYP/6-311++G(3df,3pd)					
C-F J coupling (Hz)					
C13-F14	-296.96	-299.32	-305.83	-304.64	
C13-F15	-306.69	-305.33	-295.33	-297.83	
C13-C16	-296.93	-297.89	-298.40	-298.76	
Shielding (ppm)	57.06	56.65	57.39	57.71	188.65
BHandHLYP/6-311++G(3df,3pd) Solv.					
C-F J coupling (Hz)					
C13-F14	-297.92	-299.49	-302.72	-302.47	
C13-F15	-303.17	-303.09	-296.40	-298.10	
C13-C16	-296.09	-297.07	-297.13	-297.69	
Shielding (ppm)	56.33	56.65	56.72	57.02	188.65
BHandHLYP/aug-cc-pVTZ					
C-F J coupling (Hz)					
C13-F14	-298.90	-301.27	-307.79	-306.58	
C13-F15	-308.67	-307.27	-297.27	-299.75	
C13-C16	-298.79	-299.72	-300.23	-300.58	
Shielding (ppm)	57.95	58.24	58.26	58.57	188.69
BHandHLYP/aug-cc-pVTZ Solv.					
C-F J coupling (Hz)					
C13-F14	-299.87	-301.44	-304.67	-304.42	
C13-F15	-305.15	-305.04	-298.36	-300.05	
C13-C16	-297.97	-298.93	-298.98	-299.52	
Shielding (ppm)	57.23	57.53	57.61	57.90	189.74
BHandHLYP/aug-cc-pVQZ					
C-F J coupling (Hz)					
C13-F14	-302.20	-304.61	-311.23	-310.10	
C13-F15	-312.11	-310.69	-300.56	-303.15	
C13-C16	-302.14	-303.17	-303.66	-303.97	
Shielding (ppm)	53.63	53.92	53.97	54.29	186.32
BHandHLYP/aug-cc-pVQZ Solv.					
C-F J coupling (Hz)					
C13-F14	-303.18	-304.77	-308.07	-307.77	
C13-F15	-308.53	-308.40	-301.65	-303.33	
C13-C16	-301.30	-302.29	-302.36	-302.96	
Shielding (ppm)	52.90	53.19	53.30	53.61	187.39

47

48

Stationary structures of *N,N*-dimethyl methyl carbamate

Structure **A** SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.212606	-0.487829	0.000000
2	1	0	-2.532250	0.066354	0.887489
3	1	0	-2.532250	0.066354	-0.887489
4	7	0	-0.767648	-0.686095	0.000000
5	6	0	0.000000	0.428551	0.000000
6	6	0	-0.177627	-2.021440	0.000000
7	1	0	-0.988300	-2.750979	0.000000
8	1	0	0.439163	-2.182567	-0.888725
9	8	0	-0.429032	1.577935	0.000000
10	8	0	1.323801	0.118933	0.000000
11	6	0	2.192817	1.261570	0.000000
12	1	0	3.202595	0.852090	0.000000
13	1	0	2.033382	1.869598	-0.892466
14	1	0	2.033382	1.869598	0.892466
15	1	0	-2.695004	-1.465275	0.000000
16	1	0	0.439163	-2.182567	0.888725

Rotational constants (GHZ): 4.7038415 2.059885 1.4724947
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **A** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.209709	-0.486703	0.000000
2	1	0	-2.525574	0.072443	0.885265
3	1	0	-2.525574	0.072443	-0.885265
4	7	0	-0.766512	-0.690399	0.000000
5	6	0	0.000000	0.432115	0.000000
6	6	0	-0.173313	-2.022111	0.000000
7	1	0	-0.981805	-2.754435	0.000000
8	1	0	0.446228	-2.181363	-0.886953
9	8	0	-0.430011	1.574656	0.000000
10	8	0	1.326253	0.116852	0.000000
11	6	0	2.184417	1.264216	0.000000
12	1	0	3.197272	0.863925	0.000000
13	1	0	2.013531	1.873215	-0.889342
14	1	0	2.013531	1.873215	0.889342
15	1	0	-2.696559	-1.462451	0.000000
16	1	0	0.446228	-2.181363	0.886953

Rotational constants (GHZ): 4.6998416 2.0667976 1.4754098
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **B** SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.098655	-0.826592	0.051898
2	1	0	2.301164	-0.928447	1.126606
3	1	0	1.833238	-1.802491	-0.352322
4	7	0	1.018332	0.119499	-0.200366
5	6	0	-0.254386	-0.352310	-0.049165
6	6	0	1.329338	1.522201	0.057799
7	1	0	2.314592	1.733273	-0.364083
8	1	0	0.596047	2.167508	-0.422843
9	8	0	-0.563579	-1.534471	0.028557
10	8	0	-1.161340	0.656530	-0.031847
11	6	0	-2.526988	0.216419	0.037856
12	1	0	-3.120213	1.130251	0.044105
13	1	0	-2.781532	-0.392632	-0.831538
14	1	0	-2.703670	-0.353755	0.951605
15	1	0	3.000643	-0.465005	-0.446791
16	1	0	1.351034	1.740034	1.133820

Rotational constants (GHZ): 4.8129058 2.0340020 1.4759194
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **B** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.095880	-0.832700	0.047625
2	1	0	2.363221	-0.882965	1.112057
3	1	0	1.780499	-1.820770	-0.283215
4	7	0	1.018991	0.117943	-0.188372
5	6	0	-0.259527	-0.353974	-0.044095
6	6	0	1.339574	1.518163	0.053477
7	1	0	2.297431	1.736081	-0.425816
8	1	0	0.573069	2.157928	-0.378750
9	8	0	-0.573572	-1.529721	0.027027
10	8	0	-1.161544	0.665023	-0.026516
11	6	0	-2.522726	0.219696	0.033482
12	1	0	-3.120059	1.130104	0.050220
13	1	0	-2.768655	-0.384064	-0.841730
14	1	0	-2.696030	-0.369315	0.935442
15	1	0	2.973520	-0.519152	-0.523246
16	1	0	1.425787	1.737026	1.126627

Rotational constants (GHZ): 4.8202548 2.0341434 1.4757457
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **C**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.081013	-0.864118	0.034181
2	1	0	-2.252829	-1.377310	-0.917292
3	1	0	-1.825550	-1.613013	0.786868
4	7	0	-1.016888	0.125805	-0.079437
5	6	0	0.260075	-0.342923	-0.019826
6	6	0	-1.362484	1.536370	0.007507
7	1	0	-2.227277	1.730079	-0.633072
8	1	0	-1.611117	1.828477	1.035655
9	8	0	0.564073	-1.525116	-0.008042
10	8	0	1.171152	0.670200	0.012779
11	6	0	2.529140	0.212966	0.013368
12	1	0	3.134779	1.117914	0.034177
13	1	0	2.729074	-0.401557	0.892604
14	1	0	2.740253	-0.368663	-0.885638
15	1	0	-2.997679	-0.351952	0.333521
16	1	0	-0.527555	2.140944	-0.340041

Rotational constants (GHZ): 4.7724399 2.0333594 1.4663353
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **C** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.081013	-0.864118	-0.034181
2	1	0	2.252829	-1.377310	0.917292
3	1	0	1.825550	-1.613013	-0.786868
4	7	0	1.016888	0.125805	0.079437
5	6	0	-0.260075	-0.342923	0.019826
6	6	0	1.362484	1.536370	-0.007507
7	1	0	2.227277	1.730079	0.633072
8	1	0	1.611117	1.828477	-1.035655
9	8	0	-0.564073	-1.525116	0.008042
10	8	0	-1.171152	0.670200	-0.012779
11	6	0	-2.529140	0.212966	-0.013368
12	1	0	-3.134779	1.117914	-0.034177
13	1	0	-2.729074	-0.401557	-0.892604
14	1	0	-2.740253	-0.368663	0.885638
15	1	0	2.997679	-0.351952	-0.333521
16	1	0	0.527555	2.140944	0.340041

Rotational constants (GHZ): 4.7724386 2.0333593 1.4663352
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **D**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.742519	-1.208964	-0.101008
2	1	0	1.973125	-1.235577	0.974365
3	1	0	1.157063	-2.094312	-0.364165
4	7	0	0.999517	-0.000000	-0.484296
5	6	0	-0.271841	0.000000	0.165391
6	6	0	1.742519	1.208964	-0.101008
7	1	0	2.677480	1.228727	-0.666547
8	1	0	1.157063	2.094312	-0.364166
9	8	0	-0.454383	0.000000	1.366801
10	8	0	-1.253350	-0.000000	-0.741550
11	6	0	-2.583162	-0.000000	-0.181874
12	1	0	-3.253885	-0.000001	-1.039456
13	1	0	-2.738204	-0.893364	0.425612
14	1	0	-2.738205	0.893365	0.425611
15	1	0	2.677480	-1.228727	-0.666548
16	1	0	1.973124	1.235578	0.974364

Rotational constants (GHZ): 5.0993024 1.7165740 1.6924928
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **D** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.741677	1.207815	-0.099458
2	1	0	-1.959003	1.244435	0.978726
3	1	0	-1.161931	2.091652	-0.378040
4	7	0	-1.000521	-0.000002	-0.480885
5	6	0	0.272883	0.000001	0.165850
6	6	0	-1.741677	-1.207816	-0.099452
7	1	0	-2.681552	-1.221518	-0.656865
8	1	0	-1.161931	-2.091654	-0.378029
9	8	0	0.460351	0.000005	1.364745
10	8	0	1.253716	-0.000002	-0.747881
11	6	0	2.575757	-0.000001	-0.181521
12	1	0	3.252355	-0.000001	-1.033789
13	1	0	2.726007	0.889648	0.432450
14	1	0	2.726008	-0.889649	0.432451
15	1	0	-2.681552	1.221514	-0.656872
16	1	0	-1.959003	-1.244430	0.978732

Rotational constants (GHZ): 5.1030926 1.7198590 1.6963344
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **E**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.612710	-0.312819	-1.211789
2	1	0	1.330170	-1.375401	-1.236201
3	1	0	1.204002	0.188039	-2.093758
4	7	0	1.140754	0.369666	-0.000011
5	6	0	-0.278046	0.495896	-0.000014
6	6	0	1.612708	-0.312754	1.211805
7	1	0	2.702707	-0.234483	1.243783
8	1	0	1.203996	0.188148	2.093747
9	8	0	-0.867421	1.554331	-0.000040
10	8	0	-0.893935	-0.700255	0.000016
11	6	0	-2.334090	-0.643474	0.000020
12	1	0	-2.663715	-1.681374	0.000041
13	1	0	-2.692078	-0.128184	0.893131
14	1	0	-2.692086	-0.128219	-0.893108
15	1	0	2.702710	-0.234552	-1.243768
16	1	0	1.330171	-1.375336	1.236272

Rotational constants (GHZ): 4.3117434 1.8958900 1.8048965
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **E** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.613822	-0.309600	-1.211117
2	1	0	1.323176	-1.370221	-1.248731
3	1	0	1.216254	0.202954	-2.090960
4	7	0	1.139408	0.365754	-0.000010
5	6	0	-0.278550	0.499901	-0.000012
6	6	0	1.613824	-0.309536	1.211132
7	1	0	2.704378	-0.236834	1.235982
8	1	0	1.216257	0.203064	2.090948
9	8	0	-0.873953	1.550206	-0.000038
10	8	0	-0.894257	-0.708188	0.000017
11	6	0	-2.329223	-0.642668	0.000016
12	1	0	-2.667324	-1.677480	0.000042
13	1	0	-2.684851	-0.119694	0.889548
14	1	0	-2.684852	-0.119737	-0.889539
15	1	0	2.704376	-0.236900	-1.235972
16	1	0	1.323178	-1.370156	1.248802

Rotational constants (GHZ): 4.3175618 1.8966438 1.8059301
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **F**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.756933	-1.249525	-0.207122
2	1	0	1.074458	-2.083715	-0.022690
3	1	0	2.150870	-1.349710	-1.228388
4	7	0	1.049769	-0.000036	-0.035311
5	6	0	-0.293475	0.000196	0.340076
6	6	0	1.757018	1.249253	-0.208208
7	1	0	2.151604	1.348138	-1.229344
8	1	0	1.074362	2.083640	-0.025364
9	8	0	-0.722147	0.000830	1.479261
10	8	0	-1.107299	-0.000352	-0.737544
11	6	0	-2.515859	-0.000247	-0.433204
12	1	0	-3.020280	-0.000666	-1.398444
13	1	0	-2.781381	-0.892663	0.136812
14	1	0	-2.781431	0.892618	0.136085
15	1	0	2.595833	-1.334850	0.498077
16	1	0	2.595445	1.335570	0.497440

Rotational constants (GHZ): 4.6382089 1.6943507 1.6875388
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **F** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.753933	-1.247075	-0.211552
2	1	0	2.655248	-1.286660	0.415304
3	1	0	1.107152	-2.078577	0.079905
4	7	0	1.052054	0.000000	-0.019497
5	6	0	-0.296186	0.000000	0.349421
6	6	0	1.753933	1.247075	-0.211552
7	1	0	2.052260	1.396541	-1.259707
8	1	0	1.107152	2.078577	0.079905
9	8	0	-0.733807	0.000000	1.480955
10	8	0	-1.100604	0.000000	-0.742357
11	6	0	-2.505882	0.000000	-0.442688
12	1	0	-3.008256	0.000000	-1.408517
13	1	0	-2.772473	-0.889147	0.131716
14	1	0	-2.772473	0.889147	0.131716
15	1	0	2.052260	-1.396541	-1.259707
16	1	0	2.655248	1.286660	0.415304

Rotational constants (GHZ): 4.6276078 1.6974074 1.6941061
Standard basis: 6-311++G(d,p) (5D, 7F)

Stationary structures of *N*-ethyl-*N*-(2,2,2-trifluoroethyl) methyl carbamate

Structure **1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.172049	2.863984	0.620256
2	1	0	-2.189499	2.511679	0.811056
3	1	0	-0.609181	2.841661	1.559374
4	1	0	-1.223601	3.902455	0.277003
5	6	0	-0.497631	1.996836	-0.437206
6	1	0	0.511508	2.356620	-0.651113
7	1	0	-1.063030	2.013499	-1.370364
8	7	0	-0.381138	0.597279	-0.012739
9	6	0	-1.475626	-0.209874	-0.169779
10	6	0	0.743027	0.219843	0.814526
11	1	0	1.118687	1.094171	1.354131
12	1	0	0.464858	-0.546323	1.538262
13	6	0	1.888128	-0.325438	-0.011948
14	9	0	2.364330	0.587943	-0.882826
15	9	0	1.535042	-1.402858	-0.731205
16	9	0	2.914322	-0.688581	0.785099
17	8	0	-2.489388	0.113963	-0.770143
18	8	0	-1.295044	-1.417211	0.412951
19	6	0	-2.392658	-2.328909	0.232805
20	1	0	-2.089434	-3.241520	0.744619
21	1	0	-3.303873	-1.928155	0.680388
22	1	0	-2.555403	-2.526252	-0.828179

Rotational constants (GHZ): 1.1453414 0.7115001 0.5056771
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **1** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.147744	-2.874482	0.603966
2	1	0	2.172210	-2.534058	0.772717
3	1	0	0.607791	-2.857308	1.556141
4	1	0	1.180003	-3.909774	0.250510
5	6	0	0.464494	-1.984136	-0.430764
6	1	0	-0.552437	-2.325912	-0.637622
7	1	0	1.019287	-1.995561	-1.370508
8	7	0	0.376397	-0.589546	0.010199
9	6	0	1.487602	0.198048	-0.160347
10	6	0	-0.746103	-0.180898	0.820243
11	1	0	-1.122840	-1.032148	1.396258
12	1	0	-0.457575	0.610619	1.511600
13	6	0	-1.897772	0.342019	-0.017404
14	9	0	-2.385092	-0.605975	-0.842164

15	9	0	-1.538787	1.384802	-0.775441
16	9	0	-2.907353	0.738228	0.782333
17	8	0	2.489428	-0.147628	-0.759299
18	8	0	1.327499	1.414276	0.419751
19	6	0	2.438014	2.299919	0.213122
20	1	0	2.160533	3.225173	0.715350
21	1	0	3.347730	1.882996	0.647976
22	1	0	2.592327	2.473297	-0.852877

Rotational constants (GHZ): 1.1512701 0.7065916 0.5035656
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **2**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.289312	2.631764	0.508673
2	1	0	-2.237365	2.203190	0.845271
3	1	0	-0.641165	2.779630	1.378589
4	1	0	-1.490190	3.611346	0.062353
5	6	0	-0.622480	1.720151	-0.516548
6	1	0	0.315473	2.157145	-0.867904
7	1	0	-1.263047	1.575650	-1.386972
8	7	0	-0.295501	0.398665	0.036237
9	6	0	-1.246028	-0.574761	0.207152
10	6	0	0.925412	0.262110	0.798514
11	1	0	1.236560	1.231102	1.198532
12	1	0	0.785381	-0.439930	1.622420
13	6	0	2.056468	-0.263800	-0.057136
14	9	0	2.355936	0.571206	-1.074343
15	9	0	1.772770	-1.457019	-0.603318
16	9	0	3.178155	-0.410577	0.677672
17	8	0	-1.083587	-1.605902	0.842832
18	8	0	-2.387813	-0.258020	-0.441171
19	6	0	-3.420148	-1.254388	-0.334164
20	1	0	-4.260094	-0.853352	-0.900053
21	1	0	-3.087947	-2.199349	-0.767533
22	1	0	-3.703109	-1.403645	0.709303

Rotational constants (GHZ): 1.4103735 0.5996162 0.4845415
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **2** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.251145	2.627591	0.510009
2	1	0	-2.217430	2.219358	0.815829
3	1	0	-0.627063	2.757385	1.399787
4	1	0	-1.415878	3.613804	0.064708
5	6	0	-0.579495	1.699797	-0.500500

6	1	0	0.373647	2.115455	-0.836154
7	1	0	-1.207528	1.569384	-1.382303
8	7	0	-0.293620	0.372392	0.054124
9	6	0	-1.272995	-0.579873	0.213611
10	6	0	0.921798	0.186960	0.811600
11	1	0	1.228031	1.122664	1.289853
12	1	0	0.766063	-0.576495	1.576096
13	6	0	2.069113	-0.275713	-0.063689
14	9	0	2.380561	0.639864	-1.005384
15	9	0	1.791635	-1.420103	-0.697080
16	9	0	3.172302	-0.470507	0.684387
17	8	0	-1.148645	-1.614841	0.842497
18	8	0	-2.402222	-0.219960	-0.444121
19	6	0	-3.451925	-1.195660	-0.355006
20	1	0	-4.280181	-0.773876	-0.922003
21	1	0	-3.130647	-2.142979	-0.790570
22	1	0	-3.739326	-1.354930	0.685415

Rotational constants (GHZ): 1.4234985 0.5934070 0.4821517
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.002960	2.678691	0.707959
2	1	0	-0.882781	2.506574	1.332022
3	1	0	0.879799	2.292304	1.222792
4	1	0	0.119247	3.759118	0.575439
5	6	0	-0.176711	2.015716	-0.654324
6	1	0	0.701044	2.193354	-1.281282
7	1	0	-1.049505	2.431827	-1.166423
8	7	0	-0.345381	0.558853	-0.574035
9	6	0	-1.565436	0.088232	-0.172366
10	6	0	0.706563	-0.322105	-1.026532
11	1	0	0.293692	-1.282822	-1.333125
12	1	0	1.229994	0.126357	-1.875696
13	6	0	1.742487	-0.598319	0.043265
14	9	0	1.195478	-1.049405	1.183472
15	9	0	2.455629	0.503110	0.357332
16	9	0	2.621375	-1.528742	-0.382599
17	8	0	-2.506830	0.804028	0.135096
18	8	0	-1.608251	-1.264593	-0.161158
19	6	0	-2.859798	-1.810677	0.290675
20	1	0	-2.730085	-2.891209	0.243641
21	1	0	-3.064456	-1.498892	1.316451
22	1	0	-3.675842	-1.497962	-0.362996

Rotational constants (GHZ): 1.215205 0.7239196 0.5254801
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **4** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.035190	2.645777	0.703938
2	1	0	-0.861150	2.495070	1.308253
3	1	0	0.899392	2.236502	1.230782
4	1	0	0.186742	3.722126	0.573061
5	6	0	-0.136850	1.983452	-0.660312
6	1	0	0.752825	2.139377	-1.277367
7	1	0	-0.995362	2.418583	-1.180853
8	7	0	-0.343338	0.532487	-0.580409
9	6	0	-1.580717	0.101002	-0.174640
10	6	0	0.690466	-0.379264	-1.005179
11	1	0	0.256651	-1.350061	-1.241687
12	1	0	1.195766	0.009604	-1.895221
13	6	0	1.755538	-0.607372	0.050714
14	9	0	1.232919	-0.995191	1.220584
15	9	0	2.476747	0.508777	0.281830
16	9	0	2.614534	-1.560438	-0.358493
17	8	0	-2.496967	0.842911	0.128690
18	8	0	-1.661273	-1.254453	-0.160168
19	6	0	-2.928548	-1.748869	0.298186
20	1	0	-2.842930	-2.833298	0.253290
21	1	0	-3.116833	-1.421101	1.321695
22	1	0	-3.734094	-1.398563	-0.348793

Rotational constants (GHZ): 1.2364924 0.7121132 0.5229814
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **5**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.523967	2.429774	0.564345
2	1	0	-1.364872	2.102568	1.179969
3	1	0	0.403125	2.282128	1.123211
4	1	0	-0.639494	3.500569	0.363902
5	6	0	-0.493750	1.668287	-0.757033
6	1	0	0.346514	2.008077	-1.368660
7	1	0	-1.411884	1.850863	-1.321923
8	7	0	-0.322858	0.217029	-0.594531
9	6	0	-1.353378	-0.605253	-0.223415
10	6	0	0.917082	-0.414324	-0.979130
11	1	0	0.741210	-1.474710	-1.166477
12	1	0	1.323493	0.051127	-1.881644
13	6	0	1.978809	-0.323617	0.095720
14	9	0	1.548032	-0.781679	1.281637
15	9	0	2.399280	0.944627	0.292768
16	9	0	3.063569	-1.046092	-0.250655
17	8	0	-1.275440	-1.819191	-0.098981

18	8	0	-2.484195	0.104310	-0.017288
19	6	0	-3.605944	-0.686131	0.414185
20	1	0	-4.419126	0.026397	0.547411
21	1	0	-3.870957	-1.425126	-0.343881
22	1	0	-3.381971	-1.186177	1.358180

Rotational constants (GHZ): 1.5171358 0.6091288 0.5015310
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **5** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.470018	2.425946	0.541396
2	1	0	-1.317553	2.124371	1.159559
3	1	0	0.454693	2.265292	1.098884
4	1	0	-0.562652	3.495374	0.325008
5	6	0	-0.461091	1.639186	-0.767066
6	1	0	0.384629	1.950678	-1.387363
7	1	0	-1.378076	1.832557	-1.330538
8	7	0	-0.324422	0.188967	-0.581561
9	6	0	-1.380688	-0.608878	-0.213299
10	6	0	0.901091	-0.480199	-0.943161
11	1	0	0.699967	-1.547384	-1.050959
12	1	0	1.297191	-0.086910	-1.885090
13	6	0	1.988018	-0.331633	0.102309
14	9	0	1.578267	-0.713675	1.317292
15	9	0	2.411501	0.947194	0.204799
16	9	0	3.057278	-1.077641	-0.231858
17	8	0	-1.342013	-1.820656	-0.097559
18	8	0	-2.489623	0.140258	0.000927
19	6	0	-3.631292	-0.629069	0.408866
20	1	0	-4.429404	0.098713	0.546094
21	1	0	-3.900318	-1.353826	-0.360923
22	1	0	-3.423964	-1.153456	1.342936

Rotational constants (GHZ): 1.5314902 0.6040401 0.4987983
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **1a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.832628	2.965519	0.563533
2	1	0	0.170439	3.151088	1.414844
3	1	0	1.788328	2.586073	0.935103
4	1	0	1.030916	3.919622	0.065125
5	6	0	0.172910	2.017864	-0.430470
6	1	0	0.850229	1.797775	-1.263038
7	1	0	-0.721263	2.481661	-0.845734
8	7	0	-0.272872	0.766162	0.197725
9	6	0	-1.532826	0.304232	-0.093529
10	6	0	0.686700	-0.068416	0.885767
11	1	0	1.374153	0.546036	1.470980
12	1	0	0.176615	-0.753590	1.560937
13	6	0	1.526822	-0.904644	-0.059502
14	9	0	2.370504	-0.151175	-0.796907
15	9	0	0.777936	-1.609822	-0.923688
16	9	0	2.283908	-1.780522	0.631802
17	8	0	-2.346229	0.884695	-0.795595
18	8	0	-1.784785	-0.873054	0.524330
19	6	0	-3.086952	-1.416949	0.246826
20	1	0	-3.124035	-2.356166	0.797424
21	1	0	-3.869122	-0.740855	0.596422
22	1	0	-3.204877	-1.599864	-0.822624

Rotational constants (GHZ): 1.1055061 0.7573189 0.5225348
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **1a** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.817071	2.959588	0.560077
2	1	0	0.145736	3.153181	1.401551
3	1	0	1.766467	2.578902	0.946288
4	1	0	1.027759	3.909118	0.059418
5	6	0	0.165993	2.002161	-0.432584
6	1	0	0.851210	1.778774	-1.257739
7	1	0	-0.729166	2.454734	-0.858894
8	7	0	-0.279353	0.756566	0.203253
9	6	0	-1.545790	0.299374	-0.089902
10	6	0	0.678542	-0.083456	0.883125
11	1	0	1.352756	0.525130	1.490551
12	1	0	0.160149	-0.782898	1.536650
13	6	0	1.541848	-0.898607	-0.063318
14	9	0	2.387618	-0.117793	-0.767855
15	9	0	0.810736	-1.590550	-0.947268
16	9	0	2.292279	-1.774225	0.631564

17	8	0	-2.358074	0.883851	-0.781231
18	8	0	-1.792653	-0.886428	0.523056
19	6	0	-3.093029	-1.421526	0.235288
20	1	0	-3.136981	-2.366020	0.775111
21	1	0	-3.872764	-0.742097	0.582706
22	1	0	-3.207386	-1.586263	-0.837090

Rotational constants (GHZ): 1.1137733 0.7518899 0.5211382
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **1b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.359736	2.707994	0.499209
2	1	0	0.956756	2.927571	1.492942
3	1	0	2.283253	2.133873	0.607773
4	1	0	1.618064	3.655656	0.016964
5	6	0	0.322622	1.997982	-0.359748
6	1	0	0.746195	1.730551	-1.335550
7	1	0	-0.520784	2.664560	-0.540200
8	7	0	-0.235302	0.804357	0.297306
9	6	0	-1.514021	0.442713	-0.056508
10	6	0	0.648934	-0.152255	0.926328
11	1	0	1.389421	0.357794	1.545081
12	1	0	0.077382	-0.826968	1.561438
13	6	0	1.404966	-1.003714	-0.074420
14	9	0	2.292541	-0.283258	-0.791927
15	9	0	0.585626	-1.601259	-0.957277
16	9	0	2.099854	-1.971665	0.555912
17	8	0	-2.237872	1.090593	-0.796064
18	8	0	-1.894985	-0.704828	0.549496
19	6	0	-3.223739	-1.138248	0.209752
20	1	0	-3.365321	-2.070871	0.754675
21	1	0	-3.961953	-0.398780	0.524914
22	1	0	-3.306205	-1.311195	-0.864679

Rotational constants (GHZ): 1.1418198 0.7602045 0.5310761
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **1b** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.336877	2.706468	0.498175
2	1	0	0.925899	2.927918	1.487738
3	1	0	2.260098	2.133756	0.614188
4	1	0	1.599153	3.652588	0.016513
5	6	0	0.308103	1.985124	-0.363660
6	1	0	0.741984	1.713272	-1.333689
7	1	0	-0.541424	2.639848	-0.558903

8	7	0	-0.245053	0.796109	0.300681
9	6	0	-1.528538	0.434696	-0.053547
10	6	0	0.641260	-0.160910	0.921867
11	1	0	1.368181	0.349252	1.557499
12	1	0	0.063838	-0.846806	1.539096
13	6	0	1.422170	-0.994561	-0.078335
14	9	0	2.318772	-0.249893	-0.758514
15	9	0	0.622680	-1.576195	-0.983743
16	9	0	2.106921	-1.964306	0.555834
17	8	0	-2.256366	1.084435	-0.779347
18	8	0	-1.898148	-0.725565	0.545276
19	6	0	-3.224388	-1.152622	0.200309
20	1	0	-3.366746	-2.093027	0.730161
21	1	0	-3.960432	-0.413986	0.521350
22	1	0	-3.307332	-1.302165	-0.877209

Rotational constants (GHZ): 1.1506887 0.7552590 0.5298439
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **2a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.042754	2.921096	0.411314
2	1	0	-0.573329	2.968054	1.314701
3	1	0	1.094719	2.867504	0.703924
4	1	0	-0.095375	3.850145	-0.150795
5	6	0	-0.380060	1.746462	-0.463732
6	1	0	0.262027	1.676753	-1.348437
7	1	0	-1.400713	1.896642	-0.808425
8	7	0	-0.354714	0.468368	0.263756
9	6	0	-1.402819	-0.417417	0.285892
10	6	0	0.869588	0.028550	0.892943
11	1	0	1.359857	0.851015	1.417700
12	1	0	0.641059	-0.761975	1.607946
13	6	0	1.866522	-0.536993	-0.096823
14	9	0	2.378716	0.414341	-0.908858
15	9	0	1.324343	-1.475280	-0.889937
16	9	0	2.907104	-1.100579	0.548815
17	8	0	-1.381415	-1.502141	0.850476
18	8	0	-2.478639	0.055527	-0.380007
19	6	0	-3.614519	-0.827424	-0.361514
20	1	0	-4.383601	-0.309125	-0.932947
21	1	0	-3.368573	-1.779629	-0.834405
22	1	0	-3.952901	-0.997031	0.662032

Rotational constants (GHZ): 1.3234113 0.6350799 0.4959767
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **2a** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.045208	2.890984	0.429433
2	1	0	-0.595701	2.935317	1.314724
3	1	0	1.087595	2.824514	0.751422
4	1	0	-0.065388	3.826804	-0.126442
5	6	0	-0.359421	1.722086	-0.464791
6	1	0	0.305991	1.657777	-1.332291
7	1	0	-1.370928	1.873303	-0.835250
8	7	0	-0.355707	0.443039	0.255322
9	6	0	-1.425494	-0.423227	0.284127
10	6	0	0.855221	-0.023218	0.888625
11	1	0	1.328749	0.770212	1.472138
12	1	0	0.602231	-0.851617	1.551124
13	6	0	1.884128	-0.535504	-0.100737
14	9	0	2.408676	0.464606	-0.843872
15	9	0	1.367267	-1.431356	-0.950280
16	9	0	2.905635	-1.119662	0.552023
17	8	0	-1.428573	-1.502288	0.849762
18	8	0	-2.492217	0.076698	-0.384772
19	6	0	-3.634450	-0.793257	-0.369665
20	1	0	-4.397011	-0.268272	-0.942680
21	1	0	-3.392644	-1.749243	-0.836188
22	1	0	-3.971993	-0.964821	0.653470

Rotational constants (GHZ): 1.3425988 0.6262802 0.4934133
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **2b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.480201	2.857158	0.336570
2	1	0	0.131677	2.993541	1.365181
3	1	0	1.550837	2.640221	0.349073
4	1	0	0.342242	3.800724	-0.200281
5	6	0	-0.331970	1.778909	-0.369431
6	1	0	0.052726	1.609348	-1.382362
7	1	0	-1.364783	2.111187	-0.458152
8	7	0	-0.357242	0.511986	0.381644
9	6	0	-1.426422	-0.350378	0.328720
10	6	0	0.863859	-0.026468	0.937258
11	1	0	1.425480	0.741771	1.471408
12	1	0	0.614341	-0.828471	1.632190
13	6	0	1.779887	-0.615111	-0.115858
14	9	0	2.290284	0.328336	-0.937219
15	9	0	1.151313	-1.509787	-0.896653
16	9	0	2.825574	-1.240284	0.460765
17	8	0	-1.459944	-1.450195	0.861238

18	8	0	-2.456403	0.175464	-0.368114
19	6	0	-3.626289	-0.661713	-0.408399
20	1	0	-4.354873	-0.100140	-0.991832
21	1	0	-3.401415	-1.611617	-0.896161
22	1	0	-4.004911	-0.841376	0.599242

Rotational constants (GHZ): 1.3286038 0.6515852 0.5074330
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **2b** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.492279	2.831167	0.354407
2	1	0	0.109179	2.972830	1.369403
3	1	0	1.558069	2.597758	0.403656
4	1	0	0.388908	3.775794	-0.187181
5	6	0	-0.305104	1.755388	-0.375513
6	1	0	0.114274	1.581958	-1.373980
7	1	0	-1.333577	2.088661	-0.502030
8	7	0	-0.359890	0.496038	0.380306
9	6	0	-1.446588	-0.351398	0.329101
10	6	0	0.847747	-0.069597	0.935539
11	1	0	1.399150	0.671163	1.518349
12	1	0	0.570702	-0.900386	1.585101
13	6	0	1.790143	-0.616783	-0.120062
14	9	0	2.329870	0.369265	-0.870814
15	9	0	1.173571	-1.458638	-0.959459
16	9	0	2.809397	-1.275882	0.459847
17	8	0	-1.499780	-1.445718	0.860787
18	8	0	-2.468082	0.196455	-0.370741
19	6	0	-3.639405	-0.633281	-0.415846
20	1	0	-4.362026	-0.070462	-1.004426
21	1	0	-3.412884	-1.587245	-0.893980
22	1	0	-4.019631	-0.813921	0.590659

Rotational constants (GHZ): 1.3448400 0.6451365 0.5060741
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure TS(**1**,**4'**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.406073	2.673594	0.147196
2	1	0	1.784112	2.543382	1.164474
3	1	0	2.066345	2.155046	-0.550235
4	1	0	1.448783	3.743513	-0.078592
5	6	0	-0.041994	2.234563	-0.005348
6	1	0	-0.397095	2.497051	-1.004085

7	1	0	-0.670214	2.772591	0.714694
8	7	0	-0.272529	0.781833	0.163382
9	6	0	-1.572281	0.387869	-0.032867
10	6	0	0.655417	-0.073590	0.873124
11	1	0	1.361953	0.524853	1.448455
12	1	0	0.131346	-0.739131	1.560938
13	6	0	1.473725	-0.950100	-0.055506
14	9	0	2.243222	-0.234841	-0.898863
15	9	0	0.717168	-1.758076	-0.814943
16	9	0	2.301859	-1.735299	0.667324
17	8	0	-2.439921	1.110007	-0.501060
18	8	0	-1.780988	-0.890769	0.351651
19	6	0	-3.109159	-1.377126	0.091584
20	1	0	-3.105389	-2.409597	0.438943
21	1	0	-3.848346	-0.793673	0.643328
22	1	0	-3.327449	-1.338091	-0.977082

Rotational constants (GHZ): 1.1392630 0.7572743 0.5116212
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure TS(**1**,**4'**) NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.817071	2.959588	0.560077
2	1	0	0.145736	3.153181	1.401551
3	1	0	1.766467	2.578902	0.946288
4	1	0	1.027759	3.909118	0.059418
5	6	0	0.165993	2.002161	-0.432584
6	1	0	0.851210	1.778774	-1.257739
7	1	0	-0.729166	2.454734	-0.858894
8	7	0	-0.279353	0.756566	0.203253
9	6	0	-1.545790	0.299374	-0.089902
10	6	0	0.678542	-0.083456	0.883125
11	1	0	1.352756	0.525130	1.490551
12	1	0	0.160149	-0.782898	1.536650
13	6	0	1.541848	-0.898607	-0.063318
14	9	0	2.387618	-0.117793	-0.767855
15	9	0	0.810736	-1.590550	-0.947268
16	9	0	2.292279	-1.774225	0.631564
17	8	0	-2.358074	0.883851	-0.781231
18	8	0	-1.792653	-0.886428	0.523056
19	6	0	-3.093029	-1.421526	0.235288
20	1	0	-3.136981	-2.366020	0.775111
21	1	0	-3.872764	-0.742097	0.582706
22	1	0	-3.207386	-1.586263	-0.837090

Rotational constants (GHZ): 1.1137733 0.7518899 0.5211382
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure TS(**2,5'**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.570146	2.829369	0.055065
2	1	0	1.033308	2.881161	1.043304
3	1	0	1.318493	2.520073	-0.677054
4	1	0	0.240765	3.840697	-0.202361
5	6	0	-0.656481	1.929694	0.029628
6	1	0	-1.149615	2.024504	-0.939372
7	1	0	-1.367360	2.258802	0.796662
8	7	0	-0.366069	0.490419	0.232651
9	6	0	-1.408341	-0.405944	0.226923
10	6	0	0.842527	0.030516	0.884972
11	1	0	1.357737	0.852532	1.381209
12	1	0	0.607121	-0.736550	1.626241
13	6	0	1.822184	-0.589386	-0.090943
14	9	0	2.262040	0.290429	-1.013515
15	9	0	1.299313	-1.625159	-0.764611
16	9	0	2.908637	-1.043651	0.570039
17	8	0	-1.340769	-1.563055	0.613570
18	8	0	-2.527965	0.157309	-0.276527
19	6	0	-3.657711	-0.731614	-0.338367
20	1	0	-4.465988	-0.132545	-0.755998
21	1	0	-3.441490	-1.581692	-0.987748
22	1	0	-3.924471	-1.084323	0.659330

Rotational constants (GHZ): 1.3409614 0.6431912 0.4902506
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure TS(**2,5'**) NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.045208	2.890984	0.429433
2	1	0	-0.595701	2.935317	1.314724
3	1	0	1.087595	2.824514	0.751422
4	1	0	-0.065388	3.826804	-0.126442
5	6	0	-0.359421	1.722086	-0.464791
6	1	0	0.305991	1.657777	-1.332291
7	1	0	-1.370928	1.873303	-0.835250
8	7	0	-0.355707	0.443039	0.255322
9	6	0	-1.425494	-0.423227	0.284127
10	6	0	0.855221	-0.023218	0.888625
11	1	0	1.328749	0.770212	1.472138
12	1	0	0.602231	-0.851617	1.551124
13	6	0	1.884128	-0.535504	-0.100737
14	9	0	2.408676	0.464606	-0.843872
15	9	0	1.367267	-1.431356	-0.950280
16	9	0	2.905635	-1.119662	0.552023
17	8	0	-1.428573	-1.502288	0.849762

18	8	0	-2.492217	0.076698	-0.384772
19	6	0	-3.634450	-0.793257	-0.369665
20	1	0	-4.397011	-0.268272	-0.942680
21	1	0	-3.392644	-1.749243	-0.836188
22	1	0	-3.971993	-0.964821	0.653470

Rotational constants (GHZ): 1.3425988 0.6262802 0.4934133
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure TS(**1**,**4**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.023998	2.606521	-0.643403
2	1	0	0.990887	2.686067	-1.040766
3	1	0	-0.691515	2.263777	-1.437819
4	1	0	-0.347551	3.603452	-0.324626
5	6	0	-0.053895	1.654632	0.547768
6	1	0	-1.053646	1.596500	0.973581
7	1	0	0.610928	2.020513	1.334415
8	7	0	0.391970	0.296326	0.198520
9	6	0	1.742675	0.101704	0.145654
10	6	0	-0.475389	-0.867346	0.034681
11	1	0	-0.247369	-1.371133	-0.907873
12	1	0	-0.337070	-1.587559	0.848381
13	6	0	-1.955063	-0.573509	-0.009402
14	9	0	-2.287748	0.349414	-0.928474
15	9	0	-2.455140	-0.159938	1.172184
16	9	0	-2.609476	-1.707775	-0.327778
17	8	0	2.581164	0.972508	0.328675
18	8	0	2.043545	-1.189726	-0.137605
19	6	0	3.453366	-1.461966	-0.220619
20	1	0	3.523726	-2.525670	-0.444990
21	1	0	3.911408	-0.875697	-1.019147
22	1	0	3.943849	-1.242313	0.729188

Rotational constants (GHZ): 1.4015405 0.5883987 0.4645997
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure TS(**1**,**4**) NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.008614	2.604961	-0.643557
2	1	0	1.009692	2.671201	-1.032507
3	1	0	-0.677712	2.266049	-1.437418
4	1	0	-0.322637	3.605492	-0.328398
5	6	0	-0.050739	1.653389	0.548935
6	1	0	-1.052046	1.599445	0.971777
7	1	0	0.618542	2.013843	1.334436
8	7	0	0.388403	0.292818	0.201121

9	6	0	1.742940	0.099413	0.146422
10	6	0	-0.480304	-0.866225	0.033662
11	1	0	-0.248566	-1.371579	-0.907119
12	1	0	-0.341947	-1.591510	0.843393
13	6	0	-1.961458	-0.569268	-0.010465
14	9	0	-2.284781	0.353818	-0.930487
15	9	0	-2.451708	-0.152556	1.172547
16	9	0	-2.613701	-1.702677	-0.326988
17	8	0	2.580762	0.964771	0.326555
18	8	0	2.038232	-1.198775	-0.138051
19	6	0	3.447118	-1.461540	-0.219600
20	1	0	3.525681	-2.524214	-0.443279
21	1	0	3.901658	-0.866982	-1.013528
22	1	0	3.934617	-1.231100	0.728746

Rotational constants (GHZ): 1.4035963 0.5889815 0.4652261
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure TS(**2**,**5**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.463418	2.375208	-0.562280
2	1	0	1.455706	2.254083	-1.003411
3	1	0	-0.290734	2.230962	-1.339664
4	1	0	0.377514	3.399373	-0.182666
5	6	0	0.262967	1.390779	0.586006
6	1	0	-0.709225	1.539438	1.052933
7	1	0	1.013806	1.558007	1.361393
8	7	0	0.363212	-0.016485	0.164558
9	6	0	1.574763	-0.619730	-0.011574
10	6	0	-0.758431	-0.932054	-0.022277
11	1	0	-0.669090	-1.426135	-0.993300
12	1	0	-0.768061	-1.709134	0.750406
13	6	0	-2.128092	-0.302573	-0.001353
14	9	0	-2.259259	0.716336	-0.869196
15	9	0	-2.488207	0.159279	1.213628
16	9	0	-3.037809	-1.236177	-0.342285
17	8	0	1.720140	-1.793750	-0.330458
18	8	0	2.597547	0.234908	0.213966
19	6	0	3.900671	-0.346069	0.033560
20	1	0	4.601482	0.461666	0.241444
21	1	0	4.055466	-1.170022	0.732384
22	1	0	4.024847	-0.700417	-0.991300

Rotational constants (GHZ): 1.6964892 0.5346825 0.4534813
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure TS(**2**,**5**) NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.456753	2.381546	-0.560067
2	1	0	1.447309	2.256523	-1.002223
3	1	0	-0.301501	2.237293	-1.332386
4	1	0	0.374665	3.405567	-0.180547
5	6	0	0.260112	1.393187	0.587359
6	1	0	-0.711687	1.537291	1.056699
7	1	0	1.015401	1.559231	1.358894
8	7	0	0.361406	-0.011306	0.162173
9	6	0	1.574946	-0.619252	-0.014626
10	6	0	-0.756245	-0.930720	-0.018177
11	1	0	-0.657951	-1.436341	-0.982380
12	1	0	-0.759960	-1.705668	0.756831
13	6	0	-2.129584	-0.304971	-0.002033
14	9	0	-2.254787	0.709586	-0.874388
15	9	0	-2.482936	0.161763	1.212132
16	9	0	-3.032918	-1.242060	-0.338371
17	8	0	1.719066	-1.790060	-0.328319
18	8	0	2.599161	0.241521	0.207470
19	6	0	3.894418	-0.352946	0.035809
20	1	0	4.603271	0.446073	0.247084
21	1	0	4.031226	-1.182007	0.731783
22	1	0	4.016943	-0.715180	-0.986117

Rotational constants (GHZ): 1.6937378 0.5360285 0.4541890
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **3a**$_1$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.740625	2.449449	-0.494685
2	1	0	2.405801	1.770346	-1.030323
3	1	0	0.951788	2.782111	-1.176403
4	1	0	2.313130	3.335548	-0.199099
5	6	0	1.162022	1.806896	0.766270
6	1	0	0.546692	2.541672	1.297853
7	1	0	1.969122	1.514523	1.445515
8	7	0	0.302684	0.613517	0.597058
9	6	0	1.015291	-0.613342	0.464734
10	6	0	-0.753999	0.807419	-0.386038
11	1	0	-1.131446	1.827315	-0.271243
12	1	0	-0.433691	0.668585	-1.428305
13	6	0	-1.938505	-0.105110	-0.162692
14	9	0	-1.648766	-1.398232	-0.408232
15	9	0	-2.937604	0.236563	-1.006939
16	9	0	-2.427799	-0.034967	1.083533
17	8	0	0.812530	-1.585753	1.156814

18	8	0	1.942361	-0.565056	-0.507754
19	6	0	2.712859	-1.775590	-0.666561
20	1	0	3.412824	-1.565490	-1.473894
21	1	0	3.248637	-2.005332	0.256134
22	1	0	2.056990	-2.606023	-0.933549

Rotational constants (GHZ): 1.2487797 0.6707228 0.5348833
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **3a$_1$** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.751805	2.446572	-0.501796
2	1	0	2.390508	1.751949	-1.048469
3	1	0	0.959137	2.796029	-1.170242
4	1	0	2.346405	3.320326	-0.215587
5	6	0	1.176702	1.805723	0.764301
6	1	0	0.574601	2.544294	1.307189
7	1	0	1.987464	1.507211	1.436389
8	7	0	0.310123	0.623136	0.598695
9	6	0	1.004899	-0.614507	0.472667
10	6	0	-0.757320	0.824172	-0.365488
11	1	0	-1.142197	1.838496	-0.226327
12	1	0	-0.444954	0.713820	-1.414624
13	6	0	-1.936422	-0.104519	-0.157388
14	9	0	-1.628721	-1.381983	-0.444211
15	9	0	-2.932954	0.259968	-0.994596
16	9	0	-2.416389	-0.064417	1.087391
17	8	0	0.801786	-1.583790	1.160960
18	8	0	1.933617	-0.573191	-0.512868
19	6	0	2.675930	-1.797157	-0.668233
20	1	0	3.378118	-1.607926	-1.478317
21	1	0	3.204810	-2.038208	0.255383
22	1	0	2.001041	-2.615911	-0.922619

Rotational constants (GHZ): 1.2442493 0.6755637 0.5376365
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **3a$_2$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.697147	2.875459	0.042432
2	1	0	0.308678	3.209833	1.009239
3	1	0	1.726854	2.532504	0.172064
4	1	0	0.718618	3.732340	-0.638012
5	6	0	-0.196723	1.796851	-0.550505
6	1	0	0.210189	1.440434	-1.505602
7	1	0	-1.187530	2.219639	-0.750581
8	7	0	-0.424070	0.684680	0.397923

9	6	0	-1.444745	-0.185282	-0.085051
10	6	0	0.728092	0.019678	0.980174
11	1	0	1.316022	0.765120	1.521465
12	1	0	0.378477	-0.716700	1.710956
13	6	0	1.718963	-0.712219	0.082699
14	9	0	1.254772	-1.865786	-0.419806
15	9	0	2.819050	-1.023774	0.810522
16	9	0	2.137900	0.036678	-0.956336
17	8	0	-1.341617	-0.972784	-1.002260
18	8	0	-2.572404	0.019586	0.606888
19	6	0	-3.697037	-0.766277	0.157630
20	1	0	-4.524804	-0.473985	0.801493
21	1	0	-3.923304	-0.539087	-0.885711
22	1	0	-3.482216	-1.830578	0.268513

Rotational constants (GHZ): 1.3150499 0.6467123 0.5065919
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **3a**$_2$ NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.728771	2.858386	-0.040186
2	1	0	-0.371081	3.173403	-1.024589
3	1	0	-1.758416	2.503679	-0.128309
4	1	0	-0.739159	3.729595	0.620973
5	6	0	0.191056	1.796146	0.546303
6	1	0	-0.197050	1.438939	1.508994
7	1	0	1.178184	2.235870	0.727698
8	7	0	0.422478	0.685240	-0.398060
9	6	0	1.447296	-0.180407	0.086235
10	6	0	-0.725964	0.015262	-0.976640
11	1	0	-1.314677	0.757442	-1.521523
12	1	0	-0.372474	-0.717506	-1.708995
13	6	0	-1.716771	-0.721470	-0.078236
14	9	0	-1.246586	-1.870826	0.414719
15	9	0	-2.815344	-1.023140	-0.809067
16	9	0	-2.125495	0.034741	0.958332
17	8	0	1.351363	-0.967297	1.001631
18	8	0	2.575999	0.032968	-0.610504
19	6	0	3.694581	-0.751777	-0.157617
20	1	0	4.523788	-0.465830	-0.801644
21	1	0	3.917671	-0.525322	0.886499
22	1	0	3.475235	-1.816131	-0.256696

Rotational constants (GHZ): 1.3211096 0.6474952 0.5077808
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **3b$_1$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.032937	-2.472747	-0.365294
2	1	0	-2.514807	-1.842913	-1.114496
3	1	0	-1.213562	-3.020815	-0.840001
4	1	0	-2.757194	-3.211163	-0.006473
5	6	0	-1.541001	-1.643894	0.823751
6	1	0	-1.075675	-2.298503	1.569979
7	1	0	-2.388037	-1.155200	1.315945
8	7	0	-0.550848	-0.582585	0.546346
9	6	0	-1.145805	0.564693	-0.065068
10	6	0	0.606696	-1.078367	-0.182269
11	1	0	0.896476	-2.034904	0.261861
12	1	0	0.427157	-1.231765	-1.256775
13	6	0	1.812278	-0.169630	-0.063763
14	9	0	1.623078	1.001174	-0.705591
15	9	0	2.876214	-0.767492	-0.640578
16	9	0	2.136729	0.106062	1.201823
17	8	0	-1.851270	0.560189	-1.052749
18	8	0	-0.824376	1.658614	0.630997
19	6	0	-1.301111	2.884337	0.047562
20	1	0	-0.936472	3.672572	0.702939
21	1	0	-0.898172	3.000622	-0.960126
22	1	0	-2.391506	2.885701	0.006349

Rotational constants (GHZ): 1.0835013 0.7852302 0.5463558
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **3b$_1$** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.032937	-2.472747	-0.365294
2	1	0	-2.514807	-1.842913	-1.114496
3	1	0	-1.213562	-3.020815	-0.840001
4	1	0	-2.757194	-3.211163	-0.006473
5	6	0	-1.541001	-1.643894	0.823751
6	1	0	-1.075675	-2.298503	1.569979
7	1	0	-2.388037	-1.155200	1.315945
8	7	0	-0.550848	-0.582585	0.546346
9	6	0	-1.145805	0.564693	-0.065068
10	6	0	0.606696	-1.078367	-0.182269
11	1	0	0.896476	-2.034904	0.261861
12	1	0	0.427157	-1.231765	-1.256775
13	6	0	1.812278	-0.169630	-0.063763
14	9	0	1.623078	1.001174	-0.705591
15	9	0	2.876214	-0.767492	-0.640578
16	9	0	2.136729	0.106062	1.201823
17	8	0	-1.851270	0.560189	-1.052749

18	8	0	-0.824376	1.658614	0.630997
19	6	0	-1.301111	2.884337	0.047562
20	1	0	-0.936472	3.672572	0.702939
21	1	0	-0.898172	3.000622	-0.960126
22	1	0	-2.391506	2.885701	0.006349

Rotational constants (GHZ): 1.0835013 0.7852302 0.5463558
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **3b$_2$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.009990	2.753506	0.134354
2	1	0	-0.813719	2.772007	0.874258
3	1	0	0.950483	2.688684	0.653416
4	1	0	-0.022014	3.701766	-0.413516
5	6	0	-0.196115	1.615488	-0.867595
6	1	0	0.633546	1.604377	-1.579186
7	1	0	-1.108311	1.778996	-1.451451
8	7	0	-0.317330	0.243083	-0.312797
9	6	0	-1.639603	-0.008284	0.158431
10	6	0	0.654817	-0.144221	0.703425
11	1	0	0.885944	0.641679	1.433085
12	1	0	0.276722	-1.013534	1.250148
13	6	0	1.956347	-0.586965	0.077275
14	9	0	1.799108	-1.611819	-0.775198
15	9	0	2.817487	-0.992009	1.035778
16	9	0	2.567855	0.404354	-0.603638
17	8	0	-2.203354	0.593496	1.051059
18	8	0	-2.185184	-1.013968	-0.530866
19	6	0	-3.528728	-1.356725	-0.126865
20	1	0	-3.816756	-2.185255	-0.771514
21	1	0	-3.541213	-1.662556	0.920635
22	1	0	-4.195469	-0.505493	-0.274467

Rotational constants (GHZ): 1.3489548 0.5851918 0.4768021
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **3b$_2$** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.132226	2.807102	-0.363577
2	1	0	1.067672	3.289345	0.615939
3	1	0	2.071347	2.251678	-0.429349
4	1	0	1.159471	3.584887	-1.131957
5	6	0	-0.077972	1.913812	-0.600850
6	1	0	0.021833	1.385311	-1.557747
7	1	0	-0.978844	2.534925	-0.652047
8	7	0	-0.305789	0.981592	0.520311

9	6	0	-1.565773	0.327910	0.410487
10	6	0	0.798895	0.173804	0.995396
11	1	0	1.613981	0.847961	1.268603
12	1	0	0.490065	-0.342263	1.910194
13	6	0	1.426670	-0.890656	0.091140
14	9	0	0.763121	-2.056616	0.092229
15	9	0	2.674887	-1.158674	0.540082
16	9	0	1.540524	-0.484626	-1.184929
17	8	0	-2.553902	0.640260	1.032436
18	8	0	-1.528853	-0.657863	-0.505990
19	6	0	-2.762134	-1.380985	-0.662418
20	1	0	-2.553739	-2.146544	-1.407267
21	1	0	-3.056045	-1.833135	0.286301
22	1	0	-3.551434	-0.709168	-1.003931

Rotational constants (GHZ): 1.1312828 0.7863704 0.5624466
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **6a$_1$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.344223	2.156104	-1.099115
2	1	0	-0.385957	1.553458	-1.639943
3	1	0	1.340368	1.900000	-1.465724
4	1	0	0.159406	3.211647	-1.326428
5	6	0	0.245839	1.958607	0.416595
6	1	0	1.030129	2.548589	0.907182
7	1	0	-0.712256	2.341080	0.782605
8	7	0	0.351978	0.587700	0.932819
9	6	0	1.536566	-0.131640	0.623523
10	6	0	-0.840491	-0.194417	1.151646
11	1	0	-1.468045	0.303961	1.900617
12	1	0	-0.552509	-1.166672	1.563793
13	6	0	-1.771116	-0.481505	-0.021189
14	9	0	-1.170296	-1.081285	-1.054726
15	9	0	-2.766498	-1.291154	0.399044
16	9	0	-2.349908	0.644558	-0.487743
17	8	0	2.420146	-0.356171	1.420427
18	8	0	1.572662	-0.536927	-0.660390
19	6	0	2.758573	-1.268699	-1.019471
20	1	0	2.635284	-1.515710	-2.072280
21	1	0	2.840644	-2.173982	-0.415505
22	1	0	3.645371	-0.651251	-0.865455

Rotational constants (GHZ): 1.3185465 0.6631180 0.5958211
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **6a$_1$** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.344223	2.156104	-1.099115
2	1	0	-0.385957	1.553458	-1.639943
3	1	0	1.340368	1.900000	-1.465724
4	1	0	0.159406	3.211647	-1.326428
5	6	0	0.245839	1.958607	0.416595
6	1	0	1.030129	2.548589	0.907182
7	1	0	-0.712256	2.341080	0.782605
8	7	0	0.351978	0.587700	0.932819
9	6	0	1.536566	-0.131640	0.623523
10	6	0	-0.840491	-0.194417	1.151646
11	1	0	-1.468045	0.303961	1.900617
12	1	0	-0.552509	-1.166672	1.563793
13	6	0	-1.771116	-0.481505	-0.021189
14	9	0	-1.170296	-1.081285	-1.054726
15	9	0	-2.766498	-1.291154	0.399044
16	9	0	-2.349908	0.644558	-0.487743
17	8	0	2.420146	-0.356171	1.420427
18	8	0	1.572662	-0.536927	-0.660390
19	6	0	2.758573	-1.268699	-1.019471
20	1	0	2.635284	-1.515710	-2.072280
21	1	0	2.840644	-2.173982	-0.415505
22	1	0	3.645371	-0.651251	-0.865455

Rotational constants (GHZ): 1.3185466 0.6631181 0.5958212
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **6a$_2$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.501029	2.421563	-0.632751
2	1	0	1.271015	2.205460	-1.679849
3	1	0	2.479583	1.992340	-0.392591
4	1	0	1.575623	3.505720	-0.504454
5	6	0	0.411115	1.875154	0.276187
6	1	0	0.645382	2.080531	1.332178
7	1	0	-0.545120	2.348343	0.040511
8	7	0	0.226201	0.421781	0.066225
9	6	0	1.434361	-0.278502	0.379207
10	6	0	-0.888241	-0.117501	0.847255
11	1	0	-1.187113	0.544075	1.669871
12	1	0	-0.641153	-1.095300	1.270620
13	6	0	-2.086200	-0.328374	-0.047388
14	9	0	-1.843447	-1.229344	-1.014950
15	9	0	-3.137227	-0.784786	0.668210
16	9	0	-2.483907	0.806479	-0.654152
17	8	0	1.975815	-0.288795	1.466536

18	8	0	1.886050	-0.918285	-0.698442
19	6	0	3.110464	-1.655394	-0.486267
20	1	0	3.337315	-2.112858	-1.447547
21	1	0	2.961662	-2.419895	0.278175
22	1	0	3.910541	-0.977062	-0.184660

Rotational constants (GHZ): 1.3640785 0.5772820 0.4914988
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **6a$_2$** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.436305	2.437777	-0.610331
2	1	0	1.213805	2.223989	-1.658515
3	1	0	2.425896	2.034445	-0.373206
4	1	0	1.477989	3.521386	-0.468303
5	6	0	0.364232	1.839553	0.289303
6	1	0	0.593934	2.031965	1.349503
7	1	0	-0.606789	2.284481	0.061230
8	7	0	0.231069	0.387714	0.050359
9	6	0	1.459111	-0.274735	0.369465
10	6	0	-0.867420	-0.202707	0.811622
11	1	0	-1.134212	0.387267	1.698987
12	1	0	-0.610286	-1.211538	1.146175
13	6	0	-2.100444	-0.342217	-0.054766
14	9	0	-1.897832	-1.171956	-1.085487
15	9	0	-3.119854	-0.840610	0.676108
16	9	0	-2.506895	0.838376	-0.556243
17	8	0	1.991747	-0.276562	1.459581
18	8	0	1.941127	-0.892685	-0.712221
19	6	0	3.181467	-1.588524	-0.484007
20	1	0	3.439422	-2.033008	-1.442903
21	1	0	3.048300	-2.357921	0.278231
22	1	0	3.953192	-0.888260	-0.159708

Rotational constants (GHZ): 1.3841968 0.5693371 0.4876692
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **6b$_1$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.019265	2.478481	0.589818
2	1	0	0.869702	2.053768	1.126010
3	1	0	-0.867942	2.388460	1.221857
4	1	0	0.210798	3.545134	0.426721
5	6	0	-0.201020	1.807376	-0.766482
6	1	0	-1.081103	2.253461	-1.246703

7	1	0	0.652027	1.992028	-1.426832
8	7	0	-0.396289	0.350258	-0.758803
9	6	0	-1.432635	-0.137293	0.076690
10	6	0	0.710438	-0.541605	-1.003680
11	1	0	1.175227	-0.289417	-1.963408
12	1	0	0.334782	-1.567562	-1.071859
13	6	0	1.845795	-0.570373	0.008253
14	9	0	1.443346	-0.838417	1.258445
15	9	0	2.737396	-1.526452	-0.340604
16	9	0	2.524751	0.595831	0.049324
17	8	0	-1.412705	-0.215501	1.287618
18	8	0	-2.486344	-0.499445	-0.673788
19	6	0	-3.610047	-1.003851	0.078050
20	1	0	-4.362775	-1.255876	-0.667167
21	1	0	-3.985546	-0.236748	0.757794
22	1	0	-3.318977	-1.890559	0.644188

Rotational constants (GHZ): 1.4322979 0.6126438 0.5282693
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **6b$_1$** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.057750	2.459019	0.582682
2	1	0	0.937478	2.051443	1.081722
3	1	0	-0.800408	2.337407	1.247553
4	1	0	0.215810	3.530659	0.420304
5	6	0	-0.193993	1.784584	-0.768154
6	1	0	-1.079761	2.231247	-1.237760
7	1	0	0.648047	1.962347	-1.444855
8	7	0	-0.398111	0.331623	-0.747601
9	6	0	-1.445830	-0.139926	0.083573
10	6	0	0.699421	-0.571637	-0.978775
11	1	0	1.146478	-0.361366	-1.957555
12	1	0	0.315004	-1.596229	-1.004367
13	6	0	1.855600	-0.569898	0.013643
14	9	0	1.467054	-0.759573	1.277457
15	9	0	2.719379	-1.557031	-0.307074
16	9	0	2.547290	0.588462	-0.031031
17	8	0	-1.435994	-0.221992	1.292128
18	8	0	-2.502422	-0.485387	-0.678618
19	6	0	-3.632261	-0.964952	0.072819
20	1	0	-4.389616	-1.205736	-0.670708
21	1	0	-3.989732	-0.191043	0.754331
22	1	0	-3.356827	-1.850921	0.647561

Rotational constants (GHZ): 1.4518991 0.6076747 0.5268526
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **6b$_2$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.456592	2.517537	0.188073
2	1	0	-1.061524	2.699845	1.191446
3	1	0	-2.444643	2.054674	0.281571
4	1	0	-1.587469	3.477861	-0.319725
5	6	0	-0.499992	1.647490	-0.612163
6	1	0	-0.907990	1.440630	-1.613056
7	1	0	0.456707	2.160685	-0.734393
8	7	0	-0.211298	0.381326	0.098722
9	6	0	-1.408654	-0.335380	0.403868
10	6	0	0.744278	-0.464008	-0.616195
11	1	0	0.803071	-0.227219	-1.686260
12	1	0	0.486609	-1.522060	-0.513624
13	6	0	2.124544	-0.307272	-0.022272
14	9	0	2.172469	-0.696292	1.262332
15	9	0	3.016602	-1.060677	-0.702192
16	9	0	2.566300	0.964775	-0.067057
17	8	0	-1.799612	-0.561804	1.525682
18	8	0	-2.048261	-0.723746	-0.713165
19	6	0	-3.268648	-1.461661	-0.488565
20	1	0	-3.650337	-1.694766	-1.481273
21	1	0	-3.982813	-0.847756	0.063073
22	1	0	-3.057504	-2.377254	0.066817

Rotational constants (GHZ): 1.4250362 0.5579935 0.4852806
Standard basis: 6-311++G(d,p) (5D, 7F)

Structure **6b$_2$** NO SMD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.432883	2.511438	0.194237
2	1	0	-1.038342	2.684875	1.198318
3	1	0	-2.422050	2.051968	0.286486
4	1	0	-1.558260	3.472985	-0.311347
5	6	0	-0.480665	1.631268	-0.602791
6	1	0	-0.886095	1.430111	-1.606960
7	1	0	0.482687	2.133342	-0.717245
8	7	0	-0.213890	0.366467	0.110914
9	6	0	-1.418001	-0.339015	0.411708
10	6	0	0.741880	-0.489191	-0.584193
11	1	0	0.781389	-0.291907	-1.664247
12	1	0	0.490625	-1.544253	-0.443974
13	6	0	2.134663	-0.308199	-0.018153
14	9	0	2.204694	-0.666911	1.268175
15	9	0	3.009291	-1.073475	-0.705302
16	9	0	2.558869	0.965656	-0.110711
17	8	0	-1.816631	-0.585092	1.522476

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     18          8           0       -2.064005   -0.701416   -0.722325
     19          6           0       -3.292926   -1.417173   -0.501911
     20          1           0       -3.685082   -1.631298   -1.494400
     21          1           0       -3.991425   -0.800562    0.066456
     22          1           0       -3.099232   -2.340667    0.046456
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           1.4378669   0.5547913   0.4844436
 Standard basis: 6-311++G(d,p) (5D, 7F)
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