Stereodynamics of 1-(Methylsulfonyl)-3,5-Bis(trifluoromethylsulfonyl)-1,3,5-Triazinane: Experimental and Theoretical Analysis

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Table S1. B3LYP / 6-311+G(d,p) Energies (a.u.) for the Conformers of 1-(Methylsulfonyl)-3,5-bis(trifluoromethylsulfonyl)-1,3,5-triazinane **2a-c**, 1-cyanopiperidine **3** and 1-carbonyl piperidinium Cation **4**

2a	**2b**	**2c**	**3**	**4**
-2643.5494346	-2643.5423984	-2643.5405594	-344.2338945	-364.4638690

Table S2. B3LYP / 6-311+G(d,p) Calculated Geometry (Cartesians in Å) for the Conformer **2a** of 1-(Methylsulfonyl)-3,5-bis(trifluoromethylsulfonyl)-1,3,5-triazinane

x	y	z
-1.219612	0.982027	-1.229325
-1.209185	-0.386258	-0.666307
-2.181562	-0.781282	0.625277
-2.574128	0.427810	1.330861
-1.636254	-1.951076	1.284175
0.000595	-1.159169	-0.972176
1.209250	-0.385155	-0.664755
2.182498	-0.780657	0.625811
1.637885	-1.950944	1.284393
1.219472	0.982956	-1.228050
-0.000507	1.688296	-0.898392
-0.001359	3.126802	0.010984
-1.278554	3.759506	-0.294864
1.275025	3.761095	-0.294990
2.575042	0.428254	1.331698
-0.000870	2.673745	1.752637
-3.745282	-1.364410	-0.265051
-4.662607	-1.703441	0.632683
-4.217561	-0.379842	-1.035929
-3.459931	-2.417398	-1.032207
3.745965	-1.362971	-0.265498
4.663588	-1.702919	0.631573
4.218020	-0.377694	-1.035613
3.460306	-2.415216	-1.033608
-2.082175	1.539634	-0.874911
-1.291713	0.875526	-2.317471
0.000680	-2.088983	-0.409829
0.001273	-1.369355	-2.045608
2.081261	1.541187	-0.872727
1.292813	0.876473	-2.316121
-0.001580	3.616450	2.300669
-0.905901	2.104991	1.960825
0.905115	2.106451	1.960705

Table S3. B3LYP / 6-311+G(d,p) Calculated Geometry (Cartesians in Å) for the Conformer **2b** of 1-(Methylsulfonyl)-3,5-bis(trifluoromethylsulfonyl)-1,3,5-triazinane

x	y	z
-1.211960	0.844917	-1.697690
-1.035898	-0.440452	-0.989484
-2.314574	-1.490528	-0.798631
-1.818016	-2.847602	-0.952094
-3.450854	-0.964320	-1.533113
0.332757	-0.972225	-1.058075
1.257437	0.053507	-0.581415
2.264672	-0.208613	0.713196
1.703779	-1.230077	1.572450
1.099997	1.379421	-1.194958
-0.286383	1.841076	-1.170615
-0.831909	2.667482	0.253160
-0.247798	2.077381	1.450802
-2.277351	2.774517	0.093444
2.766116	1.072655	1.169533
-0.104055	4.295225	0.008125
3.740936	-1.035540	-0.133925
4.667660	-1.339383	0.766917
4.261808	-0.204950	-1.044200
3.339367	-2.151726	-0.753854
-2.236931	1.187580	-1.594581
-0.976866	0.716360	-2.760682
0.416264	-1.868716	-0.450717
0.584301	-1.215622	-2.097956
1.756752	2.079683	-0.686213
1.394510	1.316335	-2.247844
-0.444540	4.892357	0.854170
0.981712	4.217029	0.025346
-0.472035	4.701957	-0.931051
-2.745189	-1.315209	1.038331
-3.725243	-2.172401	1.321160
-1.675745	-1.603259	1.774135
-3.148093	-0.077092	1.293342

Table S4. B3LYP / 6-311+G(d,p) Calculated Geometry (Cartesians in Å) for the Conformer **2c** of 1-(Methylsulfonyl)-3,5-bis(trifluoromethylsulfonyl)-1,3,5-triazinane

x	y	z
-1.175351	0.946064	-1.289419
-1.170892	-0.210070	-0.383539
-2.432138	-0.531025	0.646793
-3.330858	0.606417	0.634219
-1.935902	-1.180297	1.840826
0.066434	-0.987526	-0.362402
1.197175	-0.069986	-0.181877
2.490731	-0.485445	0.765816
2.031953	-1.408871	1.783144
1.241283	1.069784	-1.119781
-0.015375	1.809281	-1.087931
-0.127037	3.031014	0.141617
1.221021	3.573741	0.249433
-0.838079	2.529198	1.309639
3.271475	0.704357	1.027838
-1.171896	4.245987	-0.679718
-3.351928	-1.883093	-0.305315
-4.424324	-2.270643	0.374025
-3.729301	-1.412610	-1.500676
-2.542876	-2.932391	-0.496760
3.555944	-1.527387	-0.402941
4.651605	-1.945013	0.216280
3.898584	-0.793705	-1.470623
2.851652	-2.586275	-0.826713
-2.102086	1.494841	-1.147240
-1.130033	0.586709	-2.323367
0.045297	-1.698075	0.460597
0.166663	-1.518321	-1.317514
2.064722	1.726280	-0.850147
1.374425	0.701297	-2.143282
-1.242344	5.080046	0.018646
-0.688437	4.551247	-1.604853
-2.161314	3.825094	-0.850175

Table S5. B3LYP / 6-311+G(d,p) Calculated Geometry (Cartesians in Å) for 1-Cyanopiperidine **3**

x	y	z
-0.036335	1.248952	0.289919
1.386904	1.263267	-0.268333
2.156370	0.000105	0.141027
1.387081	-1.263163	-0.268340
-0.036168	-1.249038	0.289899
-0.717678	-0.000089	-0.106307
-2.051066	-0.000144	-0.089528
-3.211323	0.000067	-0.111406
-0.619770	2.085263	-0.096737
-0.015132	1.331966	1.387297
1.899458	2.161290	0.089156
1.337869	1.328714	-1.360435
3.152070	0.000178	-0.310882
2.304410	0.000111	1.228502
1.899751	-2.161114	0.089164
1.338072	-1.328622	-1.360443
-0.619481	-2.085429	-0.096770
-0.014952	-1.332074	1.387275

Table S6. B3LYP / 6-311+G(d,p) Calculated Geometry (Cartesians in Å) for 1-carbonyl piperidinium Cation **4**

x	y	z
0.059353	1.304505	0.486851
1.328846	1.268859	-0.353854
2.153578	0.000242	-0.094090
1.329238	-1.268600	-0.354018
0.059814	-1.304692	0.486783
-0.707520	-0.000266	0.277670
-3.000490	0.000046	-0.404136
-1.907732	-0.000208	-0.079223
-0.606905	2.125501	0.222466
0.264623	1.343054	1.558737
1.904931	2.163559	-0.101528
1.067858	1.348087	-1.413751
3.035964	0.000428	-0.735851
2.518614	0.000217	0.939214
1.905603	-2.163159	-0.101849
1.068214	-1.347754	-1.413912
-0.606188	-2.125943	0.222546
0.265267	-1.343143	1.558640