2,6-Diaziadamantane: A Single Crystal X-ray Diffraction Study and Theoretical Calculations

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Titration of 2-aziadamantane (5.0 mM) with sulfuric acid in methanol solution (volume corrected)

Titration of 2-aziadamantane (5.0 mM) with trifluoromethanesulfonic acid in DMSO solution (volume corrected)

Titration of 2-aziadamantane (5.0 mM) with trifluoromethanesulfonic acid in 1,1,2-trichloro-1,2,2-trifluoroethane solution

S 4

Protonated diaziadamantane, B3LYP/6-311+G* opt

1 1

N	-0.185621	-0.686412	-3.009982
C	-0.179039	-0.656659	-1.499168
C	1.136907	-0.683922	-0.773801
C	0.918330	-1.422067	0.573744
C	1.527399	0.800498	-0.513789
H	1.903250	-1.181337	-1.374938
H	2.472238	0.811721	0.034830
H	1.858639	-1.412810	1.130032
N	-0.480573	-1.756720	-2.495851
C	-1.325214	-0.006634	-0.776426
C	-0.902046	1.468800	-0.516392
C	-1.517598	-0.751973	0.571156
H	-2.236957	-0.042439	-1.379347
H	-2.321963	-0.262761	1.125586
H	-1.709302	1.962006	0.030339
N	0.940776	1.119525	2.803908
C	0.199638	0.731894	1.590135
C	0.410878	1.494792	0.295396
H	0.694983	2.528418	0.506611
H	1.701709	1.323768	-1.459031
H	-0.782309	2.007072	-1.461699
N	-0.241367	1.444721	2.802645
C	-0.198710	-0.717040	1.375296
H	-0.337520	-1.217933	2.336283
H	-1.836367	-1.785756	0.399218
H	0.663831	-2.473529	0.401861
H	-0.725996	-2.650353	-2.951700

Protonated Diazacyclopropene, B3LYP/6-311+G* opt

1 1

N	-0.179028	0.000000	0.835253
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N	0.704150	0.000000	0.000000
C	-0.589361	0.000000	-0.638506
H	-0.937974	0.947399	-1.029176
H	-0.937974	-0.947399	-1.029176
H	1.736255	0.000000	0.042616

Protonated Diazacyclobutene, B3LYP/6-311+G* opt

1 1			
N	-0.004110	0.000048	-0.940714
C	1.034019	-0.000032	0.113206
C	-0.228579	0.000036	1.017802
N	-1.031815	-0.000065	-0.235413
H	1.650905	0.899455	0.096491
H	1.650783	-0.899606	0.096477
H	-0.431679	0.894461	1.610808
H	-0.431681	-0.894287	1.610955
H	-0.019499	0.000070	-1.967886

Protonated Diazacyclopentene B3LYP/6-311+G* opt

1 1			
N	-1.263991	-0.018052	-0.041739
N	-0.594388	-0.017379	0.991520
C	0.893748	0.034073	0.877418
C	1.077857	-0.039821	-0.648299
C	-0.368369	0.030243	-1.192879
H	1.224798	0.965178	1.343707
H	1.305798	-0.803882	1.442200
H	1.685355	0.784457	-1.016609
H	1.560941	-0.970972	-0.939956
H	-0.626892	0.953179	-1.726163
H	-0.667477	-0.788586	-1.854448
H	-1.093287	-0.038325	1.885367

Protonated Diazacyclohexene B3LYP/6-311+G*

1 1

N	-1.445791	-0.074677	0.226921
N	-1.001950	0.039900	-0.919312
C	0.416754	0.136327	-1.379419
C	1.367278	-0.314879	-0.281321
C	-0.925622	0.288872	1.055417
C	-0.521502	-0.087825	1.349520
H	0.469380	-0.470497	-2.286029
H	1.378580	-1.407581	-0.227348
H	2.379019	-0.000840	-0.541911
H	1.558132	-0.064244	1.871312
H	1.026343	1.378361	1.031444
H	-0.639646	-1.105976	1.751952
H	-1.004701	0.548014	2.099748
H	0.561524	1.182101	-1.671317
H	-1.723358	0.049127	-1.646290

protonated azomethane, B3LYP/6-311+G* opt

1 1			
N	0.706909	0.000040	0.670149
N	0.637849	-0.000108	-0.562192
C	-0.550558	0.000023	-1.451471
H	-0.185721	0.000063	-2.475260
H	-1.144229	-0.895871	-1.266750
H	-1.144055	0.896059	-1.266745
C	-0.489917	0.000027	1.466553
H	-0.407131	0.869865	2.128956
H	-1.434945	-0.000417	0.926041
H	-0.406917	-0.869642	2.129217
H	1.552546	0.000120	-1.021646

Diaziadamantane, B3LYP/6-311+G* opt

0 1			
N	0.435714	3.064485	-0.433653
C	0.000030	1.723457	0.000033
C	-0.895212	0.889986	-0.897142
C	-1.788785	0.001571	-0.000512

C	0.000429	-0.001561	-1.789002
H	-1.515600	1.543871	-1.517997
H	-0.623391	-0.625740	-2.437415
H	-2.441516	-0.620744	-0.621887
N	-0.435904	3.064374	0.433856
C	0.895342	0.889961	0.897078
C	1.788834	0.001509	0.000396
C	-0.000295	-0.001563	1.788978
H	1.515702	1.543803	1.518009
H	0.623602	-0.625891	2.437183
H	2.441756	-0.620692	0.621672
N	-0.433811	-3.064443	-0.435831
C	-0.000106	-1.723516	0.000077
C	0.896991	-0.889978	-0.895239
H	1.517939	-1.543781	-1.515610
H	0.621898	0.620603	-2.441666
H	2.437290	0.625673	-0.623483
N	0.433867	-3.064476	0.435620
C	-0.897164	-0.889851	0.895404
H	-1.518269	-1.543392	1.515920
H	-0.621477	0.620749	2.441797
H	-2.437385	0.625878	0.623099

Diazacyclopropene, B3LYP/6-311+G* opt

0 1

N	0.610309	-0.539223	0.000000
N	-0.610309	-0.539223	0.000000
C	0.000000	0.806860	0.000000
H	0.000000	1.353982	-0.933839
H	0.000000	1.353982	0.933839

Diazacyclobutene, B3LYP/6-311+G* opt

0 1

N	0.840493	0.000055	0.629834
C	-0.641744	-0.000026	-0.772083
C	-0.641739	0.000026	-0.772087

N	0.840498	-0.000055	-0.629828
H	-1.016579	0.891920	1.279157
H	-1.016448	-0.892083	1.279062
H	-1.016439	0.892083	-1.279069
H	-1.016570	-0.891920	-1.279164

Diazacyclopentene B3LYP/6-311+G* opt

O 1

N	-1.112422	-0.041685	-0.616498
N	-1.112339	-0.041524	0.616681
C	0.262415	0.062577	1.191221
C	1.223724	-0.075852	-0.000104
C	0.262219	0.062640	-1.191261
H	0.317275	1.031988	1.696643
H	0.366154	-0.708013	1.957555
H	2.001166	0.688496	-0.000151
H	1.715773	-1.050348	-0.000168
H	0.316951	1.032072	-1.696666
H	0.365863	-0.707921	-1.957633

Diazacyclohexene B3LYP/6-311+G*

O 1

N	0.544921	-1.355030	0.290826
N	-0.544921	-1.355030	-0.290826
C	-1.244552	-0.093640	-0.676066
C	-0.415071	1.183092	-0.641673
C	0.415071	1.183092	0.641673
C	1.244552	-0.093640	0.676066
H	-1.655571	-0.298400	-1.667785
H	0.249555	1.220176	-1.512776
H	-1.066210	2.060206	-0.704811
H	1.066210	2.060206	0.704811
H	-0.249555	1.220176	1.512776
H	2.106418	-0.033488	0.000000
H	1.655571	-0.298400	1.667785
H	-2.106418	-0.033488	0.000000

cis-MeN=N-Me, B3LYP/6-311+G* opt

0 1

N	-0.778700	-0.001151	-0.618528
N	-0.778703	0.001149	0.618525
C	0.499408	0.001341	1.365877
H	0.259196	0.089346	2.423245
H	1.046433	-0.934078	1.204260
H	1.148829	0.832602	1.071826
C	0.499409	-0.001342	-1.365873
H	1.046355	0.934139	-1.204348
H	1.148900	-0.832521	-1.071746
H	0.259207	-0.089464	-2.423235