Supporting information

Rotational and vibrational spectroscopy of 1-cyanoadamantane and 1-isocyanoadamantane

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Table S1: Optimized equilibrium structure for AdaCN

27
AdaCN - MP2/cc-pVTZ

C	0.449098	0.000000	1.449593
H	0.831417	0.881570	1.969707
H	0.831417	-0.881571	1.969707
C	0.966513	0.000000	0.000000
C	-1.080354	0.000000	1.444101
H	-1.437748	-0.000001	2.475862
C	-1.588106	1.250027	0.721704
H	-1.243003	2.148366	1.240361
H	-2.680894	1.267054	0.731534
C	0.449098	1.255385	-0.724796
H	0.831417	1.265031	-1.748316
H	0.831417	2.146602	-0.221390
C	-1.080354	1.250628	-0.722050
H	-1.437748	2.144160	-1.237930
C	-1.588106	0.000000	-1.443407
H	-2.680894	0.000000	-1.463068
H	-1.243003	0.000001	-2.480720
C	0.449098	-1.255384	-0.724797
H	0.831417	-2.146601	-0.221392
H	0.831417	-1.265030	-1.748316
C	-1.588106	-1.250027	0.721703
H	-1.243003	-2.148367	1.240359
H	-2.680894	-1.267054	0.731534
C	-1.080354	-1.250628	-0.722051
H	-1.437748	-2.144159	-1.237932
C	2.425124	0.000000	0.000000
N	3.597827	0.000000	0.000000

Table S2: Optimized equilibrium structure for AdaNC

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27
AdaNC - MP2/cc-pVTZ
 C                     0.975874    0.000000    0.000000
 C                    -1.058573    0.000000    1.444282
 C                    -1.058573    1.250785   -0.722141
 C                    -1.058573   -1.250785   -0.722141
 C                     0.471517    0.000000    1.446219
 C                     0.471517    1.252463   -0.723110
 C                     0.471517   -1.252463   -0.723110
 C                    -1.566548    1.250165    0.721783
 C                    -1.566548   -1.250165    0.721783
 C                    -1.566548    0.000000   -1.443566
 H                    -1.414656    0.000000    2.476221
 H                    -1.414656    2.144470   -1.238110
 H                    -1.414656   -2.144470   -1.238110
 H                     0.860323   -0.882558    1.959148
 H                     0.860323    0.882558    1.959148
 H                     0.860323    2.137951   -0.215256
 H                     0.860323    1.255393   -1.743892
 H                     0.860323   -1.255393   -1.743892
 H                     0.860323   -2.137951   -0.215256
 H                    -1.221800    2.148475    1.240423
 H                    -2.659184    1.266602    0.731273
 H                    -1.221800   -2.148475    1.240423
 H                    -2.659184   -1.266602    0.731273
 H                    -1.221800    0.000000   -2.480845
 H                    -2.659184    0.000000   -1.462546
 N                     2.400837    0.000000    0.000000
 C                     3.584089    0.000000    0.000000
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