Electronic Supplementary Material (ESI) for RSC Advances.

Stability of neutral molecular polynitrogens: Energy content and decomposition mechanisms

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Supplementary Information

Part I

Structures and frequencies obtained at the M06-2X/def2-TZVPP level

(Coordinates in Angstrons and frequencies in cm^{-1})

1) $N_6(C_{2v})$-A

-Minimum:

N	0.6192257564	0.1824846652	-1.1978723201
N	0.7371349587	-0.5496772179	0.0430882858
N	0.6193902991	0.3669625547	1.1546456989
N	-0.6191787032	0.3671202215	1.1547062384
N	-0.7372544996	-0.5495071284	0.0431622453
N	-0.6193159802	0.1826297712	-1.1977843233

-Frequencies:

1	473.407
2	486.089
3	538.821
4	711.997
5	877.411
6	915.256
7	971.666
8	1015.449
9	1094.108
10	1154.737
11	1592.304
12	1661.544

-Transition state:

N	0.5820350948	0.2218634841	-1.3108199601
N	0.7622805930	-0.5596513756	0.1604955159
N	0.6509650893	0.3375580002	1.1502319525
N	-0.6508192188	0.3376794778	1.1502996950
N	-0.7624079268	-0.5594755566	0.1605545722
N	-0.5820536315	0.2220259701	-1.3107617753

-Frequencies:

1	722.895i
2	307.069
3	439.604
4	441.589
5	674.873
6	895.626
7	901.159
8	1095.164
9	1137.126
10	1192.354
11	1415.994
12	1917.137

2) $N_6(C_{2v})$-B

-Minimum:

N	0.9210258624	-0.5370954185	0.5221013569
N	-0.2691902118	0.1085146802	1.0288028283
N	-0.5481697355	1.2143983779	0.0509519804
N	-0.1563219980	0.8480166519	-1.0170568182
N	0.4130170755	-0.5297880583	-0.8314157353
N	-0.3603624714	-1.1040463816	0.2466178320

-Frequencies:

1	504.045
2	547.775
3	581.542
4	714.229
5	774.720
6	779.073
7	846.579
8	975.343
9	999.850
10	1076.422
11	1317.183
12	1781.812

-Transition state:

N	0.9468964762	-0.5205410899	0.5259384426
N	-0.2345303047	0.0105761664	1.0695375127
N	-0.5726882412	1.3000035554	-0.0109484117
N	-0.1947124179	0.9463059364	-1.0414835025
N	0.4443646590	-0.6247470429	-0.7817449837
N	-0.3893311359	-1.1115974016	0.2387030801

-Frequencies:

1	504.452i
2	449.498
3	497.792
4	503.781
5	697.018
6	731.182
7	845.371
8	895.287
9	1087.678
10	1103.105
11	1323.418
12	1969.664

3) $N_6(D_{3h})$

-Minimum:

N	1.1085321557	0.0002409814	0.1896141100
N	-0.0600737518	-0.0000406491	1.1229513141
N	-0.8465651394	0.7279772393	0.1386382099
N	0.3219809556	0.7282415330	-0.7948472221
N	0.3223309105	-0.7280920128	-0.7948810682
N	-0.8462176448	-0.7283355141	0.1385880799

-Frequencies:

1	640.156
2	712.611
3	714.459
4	883.800
5	886.448
6	978.418
7	979.317
8	999.515
9	1000.086
10	1083.645
11	1160.254
12	1312.742

-Transition states:

A) Direct decomposition:

N	1.2523283172	0.0002549827	0.5601658278
N	-0.0359794529	-0.0000314737	1.0582657416
N	-0.8057556368	0.7656842072	0.1654737806
N	0.1972577459	0.6313689549	-0.9746609993
N	0.1975596417	-0.6312335437	-0.9746691528
N	-0.8054106151	-0.7660431271	0.1654248020

-Frequencies:

1	780.881i
2	489.305
3	616.084
4	664.897
5	815.413
6	837.617
7	884.345
8	887.920
9	993.634
10	1006.922
11	1222.717
12	1492.163

B) Isomerization to $N_6(C_{2v})$-B:

N	1.1207760103	-0.2090398704	0.3514084569
N	-0.1916017325	0.0435488091	1.0482368170
N	-0.7336346976	0.9380633537	0.1165614929
N	0.1348455927	0.7672469939	-0.9083277052
N	0.3888318998	-0.6051234407	-0.7874694583
N	-0.7192180372	-0.9346957216	0.1795925343

-Frequencies:

1	1066.342i
2	390.417
3	543.110
4	773.008
5	870.286
6	882.545
7	991.409
8	993.588
9	1067.614
10	1122.247
11	1140.206
12	1232.054

4) $N_6(C_{2h})$

-Minimum:

N	0.2352432394	0.0031688392	-0.0790305392
N	0.1604788614	-0.2878235511	0.9973864529
N	0.4003787044	0.4225688071	-1.2312196424
N	-0.3692565647	-0.3969545835	-2.1219387315
N	-0.2105563305	0.0278665840	-3.2730617234
N	-0.1408560999	0.3232036018	-4.3485765236

-Frequencies:

1	54.885
2	173.273
3	301.332
4	551.445
5	585.176
6	649.115
7	694.277
8	956.300
9	1279.682
10	1353.851
11	2264.929
12	2336.102

-Transition state:

N	-0.0403373054	0.0173860719	-0.0605684947
N	-0.1901074018	0.1629109981	1.0156107669
N	0.8973383445	-0.0930723741	-1.3472945802
N	0.2591519798	-0.7289796043	-2.3357876987
N	-0.2178569765	0.0983747379	-3.2281733955
N	-0.6327556407	0.6354121706	-4.1002295978

-Frequencies:

1	760.844i
2	65.787
3	179.857
4	206.243
5	302.191
6	496.965
7	628.328
8	723.540
9	772.681
10	1109.477
11	2307.894
12	2360.965

5) $N_8(C_{2v})$-A

-Minimum:

N	-0.0001477161	-1.0738824625	-0.7086165522
N	-0.0000963501	-1.0730453312	0.7098995448
N	-0.7208599766	0.9476367490	-0.0004975643
N	0.7210468924	0.9475119867	-0.0005986980
N	0.7502132945	0.0621977708	-1.1773285743
N	0.7503915531	0.0635379795	1.1771493255
N	-0.7501288125	0.0637345306	1.1773262368
N	-0.7503136696	0.0623357228	-1.1772514669

-Frequencies:

1	511.016
2	568.232
3	694.862
4	740.838
5	801.223
6	824.685
7	838.394
8	851.243
9	878.248
10	909.939
11	921.175
12	932.646
13	987.721
14	1012.693
15	1068.099
16	1101.596
17	1172.951

```
    18    1180.826
```

-Transition state:

```
 N             -0.0001521186  -1.0400203369  -0.6653141848
 N              0.0000726067  -1.4580673956   0.4988357956
 N             -0.7198473179   0.9579812010   0.0263995106
 N              0.7200623444   0.9575697793   0.0262297231
 N              0.7714117435   0.0298906016  -1.1778906239
 N              0.6676926304   0.2610741039   1.2347172385
 N             -0.6677732484   0.2618690969   1.2348778577
 N             -0.7714666400   0.0297029498  -1.1778553169
```

-Frequencies:

```
     1     414.635i
     2     252.815
     3     420.857
     4     612.593
     5     625.706
     6     719.905
     7     752.723
     8     766.918
     9     806.564
    10     870.549
    11     895.045
    12     969.771
    13    1007.140
    14    1062.157
    15    1151.897
    16    1153.139
    17    1281.103
    18    1438.222
```

6) $N_8(C_{2v})$-B

-Minimum:

```
 N              0.8859078680   0.0679720650   1.2886385953
 N              0.0537323401  -0.8674072214   1.3015083613
 N             -0.9945215978  -0.0866367040   0.7535652285
 N             -0.9667383199  -0.1328500922  -0.7825787856
 N              0.0090664865   0.9632175002  -0.7980262397
 N             -0.0190230824   1.0097635461   0.7382226247
 N              0.9320970107  -0.0093548678  -1.2571982978
 N              0.0996176631  -0.9444501667  -1.2440418108
```

-Frequencies:

```
     1     207.158
     2     338.087
     3     425.280
     4     471.722
     5     505.498
```

6	813.295
7	873.314
8	885.919
9	893.746
10	940.151
11	982.365
12	990.847
13	1047.689
14	1132.467
15	1148.438
16	1161.166
17	1569.392
18	1601.995

-Transition states:

A) Isomerization to open chain $N_8(C_1)$:

N	1.0346339187	-0.0556438955	1.2368656004
N	0.1094002202	-0.6669924267	1.8298173038
N	-0.9507899877	-0.0362400612	1.1789831105
N	-0.9917035318	-0.0816013563	-1.3693588216
N	-0.1110731767	0.9443389391	-0.7853354793
N	-0.0928224113	0.7424972625	0.5772088929
N	0.9678297469	-0.0333108192	-1.0763646381
N	0.0345116709	-0.8130471860	-1.5918244332

-Frequencies:

1	360.190i
2	171.365
3	258.259
4	274.609
5	455.010
6	520.095
7	625.922
8	659.730
9	793.409
10	836.978
11	997.245
12	1022.006
13	1062.037
14	1125.076
15	1223.606
16	1342.522
17	1427.839
18	1499.624

B) Isomerization to $N_8(D_{2d})$:

N	0.8984762389	0.0748841580	1.3956504144
N	0.0262325327	-0.8064893301	1.3089238571
N	-0.9095938914	-0.0034964979	0.6398283297
N	-1.1181108104	-0.5099494338	-0.7977015731
N	0.1068900261	0.9767902226	-0.6872516051

```
N              0.1140761637   1.1140271498   0.7273529167
N              0.8846472698   0.0006111929  -1.1185695648
N             -0.0026310803  -0.8463770047  -1.4682412392
```

-Frequencies:

```
     1     590.976i
     2     255.107
     3     330.755
     4     349.109
     5     443.630
     6     664.661
     7     701.187
     8     756.068
     9     836.748
    10     866.674
    11     907.839
    12     981.515
    13    1049.347
    14    1085.856
    15    1118.050
    16    1160.261
    17    1385.262
    18    1605.617
```

7) $N_8(C_s)$

-Minimum:

```
N              0.6109842748   0.1668956949  -1.4967966175
N              1.0937206916  -0.2961774270  -0.1931065918
N              0.7310918654   0.7770436486   0.7662763975
N             -0.0030856976  -0.2109499852   1.5414597249
N             -0.7283570781   0.7818242645   0.7639804178
N             -0.6051347925   0.1708966827  -1.4987192574
N             -0.0041337717  -1.1005788693   0.3134290492
N             -1.0950489701  -0.2889462116  -0.1965001048
```

-Frequencies:

```
     1     409.749
     2     428.900
     3     539.557
     4     545.388
     5     769.995
     6     802.129
     7     825.818
     8     851.304
     9     896.889
    10     915.750
    11     938.188
    12     953.020
    13     995.219
    14    1008.671
    15    1080.068
```

```
16    1091.204
17    1197.853
18    1671.101
```

-Transition state:

```
N             0.5883575179   0.2021625391  -1.5981063885
N             1.1085381525  -0.3001177086  -0.1190126431
N             0.8321095043   0.7198530746   0.7735816150
N            -0.0028701857  -0.1522856741   1.5497080334
N            -0.8297575665   0.7253481006   0.7710413832
N            -0.5818723423   0.2060793429  -1.6000387227
N            -0.0042951003  -1.1083019641   0.3452037495
N            -1.1102099798  -0.2927377105  -0.1223770267
```

-Frequencies:

```
 1     625.031i
 2     329.381
 3     355.386
 4     406.434
 5     484.192
 6     754.310
 7     778.523
 8     837.536
 9     858.329
10     890.736
11     941.423
12     949.078
13    1001.770
14    1019.777
15    1100.234
16    1138.755
17    1185.491
18    1852.139
```

8) $N_8(O_h)$

-Minimum:

```
N             0.0168077999  -0.0167749404   0.0167853062
N             0.0167588231  -0.0167952642   1.5121622724
N             1.5122071675  -0.0168224684   0.0168162330
N             1.5121408642  -0.0168285340   1.5122180792
N             1.5121804147  -1.5122240999   0.0168056472
N             0.0167854036  -1.5121603823   0.0168168851
N             1.5122495059  -1.5122102432   1.5121792558
N             0.0168700211  -1.5121840677   1.5122163208
```

-Frequencies:

```
 1     563.671
 2     564.017
 3     836.693
```

4	836.771
5	836.797
6	916.976
7	917.111
8	917.177
9	918.261
10	918.265
11	918.368
12	1024.672
13	1024.700
14	1024.804
15	1028.818
16	1124.622
17	1124.718
18	1180.784

-Transition state:

N	0.0033585304	-0.0262278587	0.0297961224
N	-0.1191962750	-0.0695519426	1.4635233172
N	1.6480000066	-0.0695899843	0.0655242296
N	1.5257197309	-0.0263350601	1.4991916798
N	1.5188174510	-1.5027781025	0.0227286307
N	-0.1251619698	-1.4593647860	0.0736855991
N	1.6543324063	-1.4594365723	1.4553259630
N	0.0101301198	-1.5027156931	1.5062244583

-Frequencies:

1	1938.824i
2	181.734
3	183.584
4	485.325
5	548.117
6	675.672
7	676.006
8	754.753
9	863.119
10	863.489
11	955.473
12	1009.001
13	1009.360
14	1021.424
15	1026.324
16	1050.975
17	1133.952
18	1214.827

9) $N_{10}(C_s)$

-Minimum:

N	0.0620829799	0.6339300221	-3.1801386666
N	0.9858565725	-1.0636669190	0.3897321094

N	-0.5103455483	0.6203699754	1.0074025808
N	0.1561224186	-1.9253978504	0.7848419114
N	-0.0283842466	1.7062041272	1.3826415741
N	0.3131194831	2.6803901369	1.7985837892
N	-0.2066920900	0.2432248246	-2.1732822435
N	0.3192367284	0.1143597523	-0.0632989962
N	-0.6145116402	-0.2510605926	-1.1048554985
N	-0.4764564258	-2.7583430534	1.1583642338

-Frequencies:

1	23.971
2	27.605
3	68.181
4	125.152
5	200.197
6	247.274
7	439.143
8	443.338
9	471.238
10	587.992
11	602.568
12	610.812
13	627.314
14	749.502
15	813.955
16	944.505
17	952.532
18	975.394
19	1110.839
20	1223.630
21	1274.643
22	2304.811
23	2305.008
24	2330.382

-Transition state:

N	0.1247756976	0.3628348110	-3.0662977635
N	0.9510092155	-1.1480182968	0.1268308458
N	0.0319091229	0.5553788123	1.3522143322
N	-0.1007422222	-2.0916209794	0.6555485919
N	-0.0238220399	1.7972375230	1.3266645479
N	-0.1168528995	2.9051721692	1.3959917080
N	-0.2011370332	0.3282012705	-2.0009903780
N	0.4832780679	0.0704657607	0.0746982541
N	-0.6544698880	0.2816815602	-0.8457200622
N	-0.4939480211	-3.0613326309	0.9810599240

-Frequencies:

1	749.995i
2	37.451
3	52.490
4	72.598
5	141.475
6	202.399
7	210.593

8	351.254
9	368.985
10	450.116
11	543.332
12	588.536
13	605.619
14	622.539
15	712.602
16	794.859
17	850.897
18	980.384
19	1188.248
20	1237.425
21	1271.788
22	2299.158
23	2310.955
24	2369.283

10) $N_{10}(D_{5h})$

-Minimum:

N	-0.7580393354	-0.9075663077	-0.8571471459
N	0.7364748673	-0.9330904487	-0.8484907031
N	0.7249508251	-1.1079292467	0.6163149986
N	-0.7501747916	0.2562448165	1.2265243338
N	0.7675950268	1.2330960047	0.1531059779
N	-0.7315551286	0.5390568682	-1.1431849447
N	0.7441769625	0.2307984985	1.2353614660
N	-0.7693070330	-1.0825779396	0.6075609731
N	0.7628185519	0.5135321496	-1.1344789614
N	-0.7269163084	1.2584420698	0.1444188723

-Frequencies:

1	525.137
2	526.282
3	672.139
4	733.927
5	735.378
6	759.773
7	760.729
8	798.189
9	850.507
10	850.845
11	866.541
12	867.294
13	909.449
14	950.715
15	952.505
16	953.077
17	954.795
18	1051.170
19	1051.738
20	1051.923
21	1052.624

```
   22    1086.005
   23    1086.818
   24    1105.428
```

-Transition state:

```
 N             -0.7334931553  -0.9232605824  -0.8904521922
 N              0.7892965688  -1.1111150477  -0.7610074339
 N              0.6187372170  -1.0666768137   0.5935190909
 N             -0.7254055998   0.2761991573   1.2571880727
 N              0.7510986865   1.3757410684  -0.0254383040
 N             -0.7225497265   0.4817579716  -1.1449320829
 N              0.7972296655   0.0630277921   1.3403126840
 N             -0.8037594611  -1.0659964257   0.5985597453
 N              0.7469733770   0.7404339845  -1.1619778915
 N             -0.7181275719   1.2298888957   0.1942283116
```

-Frequencies:

```
    1     670.777i
    2     405.065
    3     506.828
    4     519.627
    5     580.591
    6     601.636
    7     656.048
    8     724.290
    9     746.223
   10     805.928
   11     817.657
   12     830.812
   13     870.313
   14     903.996
   15     904.839
   16     939.696
   17     991.582
   18    1024.542
   19    1047.480
   20    1055.006
   21    1067.071
   22    1131.243
   23    1209.804
   24    1287.024
```

11) $N_{10}(C_1)$

-Minimum:

```
 N             -0.4438193965   1.1405811063  -0.3788198953
 N              1.6125289134  -0.0489313753   0.1064506090
 N             -1.5195237938  -0.6312368088  -0.5836505138
 N              0.6070294056  -1.1185932021   0.1477230919
 N              0.9058861194   1.2174155052   0.0491849608
 N             -1.1531958634   0.2617901495   0.5692945318
 N             -0.1197770313  -0.4333006499   1.2330129608
```

```
 N              1.0046633754   0.5614403317   1.3128152254
 N             -0.6498324076   0.1787400629  -1.4695744718
 N             -0.2439593212  -1.1279051196  -0.9864364990
```

-Frequencies:

```
     1     355.860
     2     438.615
     3     560.469
     4     664.985
     5     674.261
     6     725.607
     7     750.654
     8     774.794
     9     778.375
    10     795.720
    11     862.242
    12     871.789
    13     880.890
    14     890.687
    15     927.272
    16     956.412
    17     976.209
    18    1019.374
    19    1027.824
    20    1044.775
    21    1068.348
    22    1110.353
    23    1181.059
    24    1187.521
```

-Transition state:

```
 N             -0.4123925054   1.1995828797  -0.3337482600
 N              1.6510375214  -0.1490464777   0.1932520023
 N             -1.5564696702  -0.6026951583  -0.5582206116
 N              0.6848769960  -1.1157845328   0.1858104069
 N              0.8176421586   1.3490237231   0.0998738282
 N             -1.1263479728   0.2713664898   0.5516532112
 N             -0.0862509706  -0.4404072915   1.2213132441
 N              1.0199541367   0.5553641000   1.2816304355
 N             -0.6661363413   0.0638149119  -1.5666315632
 N             -0.3259133522  -1.1312186441  -1.0749326935
```

-Frequencies:

```
     1     770.943i
     2     291.827
     3     372.734
     4     458.126
     5     532.357
     6     628.684
     7     669.830
     8     714.203
     9     745.216
    10     753.066
    11     795.221
```

12	842.379
13	851.676
14	882.186
15	904.500
16	941.548
17	950.207
18	974.553
19	1014.841
20	1052.937
21	1109.182
22	1121.712
23	1218.639
24	1301.096

12) $N_{10}(C_{3v})$

-Minimum:

N	-0.5747335660	0.6834369531	-1.2904672300
N	-0.9118803041	0.9676527897	0.0494023244
N	-1.1920177407	-0.3109532639	0.7285673536
N	-0.0176770127	-0.0709051515	1.6225213333
N	-0.2336468236	-0.7648887726	-1.3501231626
N	0.8253480866	-0.9182099575	0.7239297489
N	0.8514787363	0.2537112236	-1.2935954045
N	0.3423187079	1.1304251530	0.8083016805
N	1.2945136904	0.3032358067	0.0444074620
N	-0.3836534740	-1.2734513865	-0.0429885717

-Frequencies:

1	528.584
2	529.042
3	532.773
4	680.758
5	681.539
6	737.711
7	738.912
8	799.183
9	838.518
10	866.905
11	870.296
12	916.849
13	918.132
14	933.131
15	964.275
16	966.249
17	977.601
18	1008.977
19	1020.623
20	1021.619
21	1050.889
22	1060.742
23	1060.929
24	1155.335

-Transition state:

N	-0.4844931893	0.7646582662	-1.2790240710
N	-0.8834534275	1.0041645787	0.0346709045
N	-1.2002361535	-0.3159815961	0.7163029946
N	-0.0242521072	-0.0926702094	1.6160483929
N	-0.3136930938	-1.0318244570	-1.3166408300
N	0.8291969847	-0.9268458429	0.7116279105
N	0.8206025926	0.3710376257	-1.2820722406
N	0.3379887258	1.1161805230	0.8389262041
N	1.2911711478	0.3490732834	0.0298254893
N	-0.3728314795	-1.2377921718	-0.0696647545

-Frequencies:

1	492.837i
2	309.432
3	469.315
4	612.623
5	632.146
6	665.433
7	720.315
8	766.546
9	812.945
10	814.903
11	825.008
12	869.950
13	909.506
14	916.687
15	952.401
16	974.964
17	976.476
18	998.116
19	1002.641
20	1033.530
21	1059.149
22	1083.992
23	1127.187
24	1353.911

Part II

Structures and frequencies obtained at the SOGGA11-X/def2-TZVPP level

(Coordinates in Angstrons and frequencies in cm^{-1})

1) $N_6(C_{2v})$-A

-Minimum:

N	0.6208281424	0.1817915114	-1.1973336192
N	0.7340267695	-0.5465214840	0.0425095786
N	0.6209081981	0.3644970797	1.1547461446
N	-0.6207409282	0.3646311131	1.1548002557
N	-0.7341540985	-0.5463476552	0.0425578492
N	-0.6208698852	0.1819429152	-1.1972909127

-Frequencies:

1	479.709
2	488.913
3	541.043
4	749.213
5	883.340
6	931.250
7	984.374
8	1031.697
9	1107.825
10	1169.879
11	1588.756
12	1659.600

-Transition state:

N	0.5807681130	0.2237257311	-1.3262933262
N	0.7610279337	-0.5572664621	0.1704195209
N	0.6557757002	0.3333063350	1.1558138900
N	-0.6556236371	0.3334648314	1.1558490674
N	-0.7611406139	-0.5570870384	0.1704630827
N	-0.5808074961	0.2238566029	-1.3262522348

-Frequencies:

1	707.293i
2	284.946
3	432.503
4	433.486
5	660.945
6	893.494
7	898.895
8	1119.116
9	1163.720
10	1213.982
11	1403.317
12	1941.618

2) $N_6(C_{2v})$-B

-Minimum:

N	0.9194949638	-0.5377533760	0.5216812044
N	-0.2719348620	0.1162329082	1.0254957224
N	-0.5462888874	1.2075064954	0.0568594117
N	-0.1532657518	0.8399343112	-1.0157334607
N	0.4107331508	-0.5229464131	-0.8349480358
N	-0.3587400920	-1.1029740742	0.2466466021

-Frequencies:

1	504.472
2	554.855
3	643.278
4	748.968
5	779.447
6	788.306
7	841.415
8	973.708
9	1015.708
10	1085.976
11	1332.281
12	1771.841

-Transition state:

N	0.9516141410	-0.5180927661	0.5269538668
N	-0.2283809442	-0.0068342538	1.0776237834
N	-0.5777769312	1.3163376389	-0.0208640356
N	-0.2009260326	0.9633289270	-1.0476844357
N	0.4497457590	-0.6411090914	-0.7733793908
N	-0.3942769565	-1.1136303308	0.2373523496

-Frequencies:

1	517.932i
2	437.053
3	476.365
4	494.771
5	681.763
6	724.980
7	818.711
8	903.030
9	1095.913
10	1127.485
11	1341.358
12	2002.847

3) $N_6(D_{3h})$

-Minimum:

N	1.1077162652	0.0003062956	0.1905623566
N	-0.0598180766	0.0000680274	1.1225666783
N	-0.8457748265	0.7275406190	0.1376887761
N	0.3214397789	0.7273145408	-0.7943616443
N	0.3218229884	-0.7272618903	-0.7942500733
N	-0.8453870939	-0.7279674685	0.1377960442

-Frequencies:

1	648.594
2	709.764
3	711.151
4	883.515
5	889.625
6	983.415
7	983.673
8	1009.589
9	1011.922
10	1093.407
11	1172.944
12	1325.995

-Transition state:

A) Direct decomposition:

N	1.2516052888	0.0002643318	0.5558297965
N	-0.0367199921	-0.0000345478	1.0574964355
N	-0.8048631092	0.7647069610	0.1636454895
N	0.1971101576	0.6331063190	-0.9702743109
N	0.1973913573	-0.6329724901	-0.9703025714
N	-0.8045237026	-0.7650705739	0.1636051609

-Frequencies:

1	753.011i
2	491.699
3	624.196
4	678.868
5	822.817
6	857.116
7	891.115
8	892.071
9	1011.035
10	1018.149
11	1238.469
12	1496.540

B) Isomerization to $N_6(C_{2v})$-B

N	1.1229313658	-0.2031281728	0.3523245503
N	-0.1904111984	0.0411415090	1.0453845096
N	-0.7314452533	0.9374581234	0.1210657417
N	0.1342414099	0.7625503378	-0.9103566714
N	0.3885345221	-0.6050443975	-0.7840386098
N	-0.7238518104	-0.9329772759	0.1756226172

-Frequencies:

1	1052.502i
2	380.132
3	550.807
4	780.160
5	884.901
6	887.965
7	1004.023
8	1004.889
9	1082.699
10	1126.732
11	1157.087
12	1246.641

4) $N_6(C_{2h})$

-Minimum:

N	0.2321009526	-0.0009451551	-0.0783424325
N	0.1626579207	-0.2860915036	1.0031404188
N	0.3995920799	0.4209464105	-1.2281779279
N	-0.3670243564	-0.3937131530	-2.1243441750
N	-0.2071507022	0.0323739779	-3.2736450250
N	-0.1447440845	0.3194591208	-4.3550715656

-Frequencies:

1	55.420
2	173.327
3	303.180
4	542.798
5	579.869
6	643.458
7	690.559
8	962.500
9	1289.160
10	1358.359
11	2268.523
12	2335.975

-Transition state:

N	-0.0493801018	0.0148998718	-0.0366030570
N	-0.1410246347	0.1307313048	1.0539004565
N	0.8629291081	-0.0781877229	-1.3336502732
N	0.2290984180	-0.6947287080	-2.3227284754
N	-0.2214564400	0.1229874917	-3.2456002085
N	-0.6047333497	0.5963297627	-4.1717614425

-Frequencies:

1	801.817i
2	61.767
3	176.449
4	182.892
5	303.899
6	484.963
7	594.956
8	718.939
9	772.410
10	1140.168
11	2291.449
12	2331.844

5) $N_8(C_{2v})$-A

-Minimum:

N	-0.0002629192	-1.0729419744	-0.7055796995
N	-0.0001134468	-1.0720915881	0.7068478619
N	-0.7182609674	0.9455367629	-0.0005150524
N	0.7186259132	0.9452408218	-0.0006087715
N	0.7497432305	0.0627198577	-1.1752400001
N	0.7498514282	0.0641501808	1.1751088463
N	-0.7497496401	0.0643675202	1.1751369944
N	-0.7498577637	0.0630188045	-1.1751508090

-Frequencies:

1	519.621
2	576.418
3	697.697
4	745.938
5	807.752
6	840.504
7	850.809
8	863.341
9	889.453
10	922.524
11	936.854
12	943.884
13	1002.465
14	1032.715
15	1086.930
16	1122.855
17	1186.685

```
    18    1199.397
```

-Transition state:

```
 N             -0.0001476298  -1.0401779752  -0.6684931837
 N             -0.0001558473  -1.4542630191   0.5019061738
 N             -0.7171897660   0.9550855019   0.0242410427
 N              0.7174177055   0.9549125556   0.0241892942
 N              0.7709063736   0.0317146571  -1.1745933657
 N              0.6689655251   0.2603356122   1.2336220109
 N             -0.6688171905   0.2604989700   1.2336706707
 N             -0.7709791706   0.0318936973  -1.1745426429
```

-Frequencies:

```
     1     423.928i
     2     258.749
     3     437.256
     4     625.446
     5     631.727
     6     738.419
     7     758.675
     8     780.548
     9     822.214
    10     879.720
    11     909.487
    12     984.985
    13    1029.918
    14    1077.138
    15    1169.711
    16    1170.382
    17    1289.362
    18    1443.019
```

6) $N_8(C_{2v})$-B

-Minimum:

```
 N              0.8868350521   0.0705963594   1.2868157122
 N              0.0520346922  -0.8667445370   1.3027573569
 N             -0.9910834004  -0.0857950048   0.7546980386
 N             -0.9640891250  -0.1333733874  -0.7814006878
 N              0.0072664449   0.9598045096  -0.7979837636
 N             -0.0186060976   1.0063833144   0.7375054665
 N              0.9306856443  -0.0062784690  -1.2582787372
 N              0.0969432384  -0.9445923284  -1.2441218502
```

-Frequencies:

```
     1     214.977
     2     332.213
     3     411.883
     4     478.231
     5     510.867
```

6	810.587
7	879.316
8	901.168
9	910.163
10	958.754
11	999.965
12	1008.537
13	1070.447
14	1152.735
15	1165.855
16	1179.800
17	1566.697
18	1600.296

-Transition states:

A) Isomerization to open chain $N_8(C_1)$:

N	1.0253008284	-0.0464825153	1.2471352134
N	0.1026056447	-0.6560533873	1.8515827924
N	-0.9573400124	-0.0330482214	1.1972764534
N	-0.9905903612	-0.0809375520	-1.3586999292
N	-0.1068060894	0.9139456143	-0.7726374864
N	-0.0920780026	0.7450454842	0.5902082248
N	0.9747044739	-0.0419283500	-1.1136060125
N	0.0441899678	-0.8005406157	-1.6412677207

-Frequencies:

1	346.578i
2	163.106
3	235.692
4	263.724
5	462.842
6	511.401
7	634.062
8	649.194
9	791.839
10	864.470
11	1027.109
12	1044.543
13	1076.922
14	1142.784
15	1235.370
16	1347.839
17	1415.312
18	1504.155

B) Isomerization to $N_8(D_{2d})$:

N	0.8971281998	0.0758509973	1.3933718252
N	0.0210112952	-0.8072742705	1.3130777727
N	-0.9061373737	-0.0066367720	0.6386056917
N	-1.1187360082	-0.5064999870	-0.7900457998
N	0.1092285718	0.9811443600	-0.6893987729

```
 N              0.1117952272   1.1068478357   0.7237373295
 N              0.8852372963   0.0025291935  -1.1240739287
 N              0.0004592405  -0.8459609002  -1.4652825821
```

-Frequencies:

```
     1     626.328i
     2     252.767
     3     321.052
     4     338.214
     5     442.037
     6     668.400
     7     709.763
     8     755.610
     9     851.368
    10     877.934
    11     916.478
    12     994.303
    13    1051.274
    14    1092.423
    15    1132.261
    16    1176.572
    17    1407.200
    18    1601.175
```

7) $N_8(C_s)$

-Minimum:

```
 N              0.6127914564   0.1636574608  -1.4918265384
 N              1.0905042542  -0.2943523666  -0.1960177663
 N              0.7300174524   0.7775233520   0.7667130597
 N             -0.0030891188  -0.2139590823   1.5386410446
 N             -0.7272536149   0.7823218277   0.7644836205
 N             -0.6069777566   0.1677175137  -1.4937552566
 N             -0.0041430695  -1.0958427727   0.3112114346
 N             -1.0918493347  -0.2870651442  -0.1994496546
```

-Frequencies:

```
     1     407.333
     2     430.902
     3     556.421
     4     556.969
     5     780.672
     6     807.499
     7     828.876
     8     859.486
     9     918.808
    10     928.167
    11     949.133
    12     967.802
    13    1014.951
    14    1023.515
    15    1095.609
```

```
   16    1108.012
   17    1209.211
   18    1665.618
```

-Transition state:

```
 N             0.5891098961   0.2012437575  -1.5990617516
 N             1.1060748262  -0.2978972850  -0.1192296274
 N             0.8475473531   0.7133255996   0.7764368124
 N            -0.0028822125  -0.1472317307   1.5443383283
 N            -0.8452119125   0.7189826858   0.7738008621
 N            -0.5826976073   0.2051063030  -1.6009826370
 N            -0.0042517082  -1.1030073981   0.3473339561
 N            -1.1076886350  -0.2905219321  -0.1226359428
```

-Frequencies:

```
    1     627.298i
    2     330.040
    3     355.971
    4     407.526
    5     474.269
    6     758.977
    7     789.423
    8     849.151
    9     878.514
   10     900.705
   11     951.610
   12     963.350
   13    1018.617
   14    1038.198
   15    1125.880
   16    1160.346
   17    1196.412
   18    1858.160
```

8) $N_8(O_h)$

-Minimum:

```
 N             0.0184922916  -0.0184935141   0.0184914222
 N             0.0185054523  -0.0185039014   1.5104888401
 N             1.5104937494  -0.0185007607   0.0185061639
 N             1.5104929633  -0.0185151964   1.5104946978
 N             1.5104975772  -1.5104938281   0.0185067734
 N             0.0185080211  -1.5104930211   0.0185113765
 N             1.5105012057  -1.5105057583   1.5105007256
 N             0.0185087394  -1.5104940199   1.5105000005
```

-Frequencies:

```
    1     591.781
    2     591.785
    3     864.807
    4     864.809
    5     864.811
```

6	943.768
7	943.776
8	943.780
9	945.813
10	945.815
11	945.817
12	1042.451
13	1048.860
14	1048.864
15	1048.875
16	1145.628
17	1145.629
18	1209.213

-Transition state:

N	0.0054220552	-0.0275647656	0.0309688628
N	-0.1166384123	-0.0706077585	1.4624405678
N	1.6457142021	-0.0706003273	0.0665602515
N	1.5235643752	-0.0275551398	1.4980457725
N	1.5171531448	-1.5014468134	0.0241642323
N	-0.1236148188	-1.4583744932	0.0746642745
N	1.6525416267	-1.4583803972	1.4543214999
N	0.0118578272	-1.5014703049	1.5048345387

-Frequencies:

1	1853.417i
2	155.563
3	155.641
4	497.967
5	544.678
6	683.275
7	683.335
8	763.519
9	893.057
10	893.063
11	972.656
12	1026.990
13	1027.002
14	1035.157
15	1037.908
16	1070.694
17	1153.856
18	1232.308

9) $N_{10}(C_s)$

-Minimum:

N	0.2462747968	-1.0836495140	-3.0431509787
N	0.9773647168	-0.6563541637	0.9583222091
N	-0.5765255286	1.0226470197	0.5122789564
N	0.1467451091	-1.2262148195	1.7116927377
N	-0.1743352197	2.1670601610	0.2371360210

N	0.0823807424	3.2386135842	0.0587882969
N	-0.0596196307	-0.9203866191	-1.9821416614
N	0.3377128909	0.0720960593	-0.0818300157
N	-0.5116097208	-0.8318000706	-0.8267276426
N	-0.4683851045	-1.7820102863	2.4556313303

-Frequencies:

1	32.209
2	32.500
3	62.998
4	124.611
5	203.439
6	247.228
7	436.045
8	439.517
9	470.519
10	584.507
11	600.315
12	608.614
13	622.360
14	741.160
15	814.883
16	950.622
17	958.475
18	984.521
19	1131.758
20	1239.129
21	1288.165
22	2301.334
23	2302.893
24	2328.406

-Transition state:

N	-0.0875594267	-0.6660396795	-3.1688644255
N	0.9258123813	-0.4443154403	1.0731762865
N	-0.6640465643	0.9128452211	-0.0146844630
N	-0.1005426135	-1.1653828081	1.9100973381
N	-0.1708581945	2.0426235366	0.1226964987
N	0.1767399146	3.0957334107	0.2629214372
N	-0.0469012093	-0.8446337114	-2.0668389226
N	0.4367300104	-0.0675902680	-0.0708981022
N	-0.0601759475	-1.1584265192	-0.8653687997
N	-0.4091983506	-1.7048137418	2.8177631526

-Frequencies:

1	748.911i
2	34.750
3	44.384
4	68.777
5	137.321
6	209.867
7	216.373
8	353.923
9	372.388

10	450.483
11	539.515
12	582.407
13	602.864
14	615.563
15	713.731
16	794.300
17	856.682
18	982.822
19	1211.642
20	1248.296
21	1290.181
22	2296.868
23	2310.236
24	2341.445

10) $N_{10}(D_{5h})$

-Minimum:

N	-0.7465631747	-1.2514032076	0.0017377759
N	0.7449733410	-1.2523196177	-0.0006192338
N	0.7476826550	-0.3866869740	1.1895193247
N	-0.7435162598	1.0134936618	0.7358597093
N	0.7448057963	1.0118891241	-0.7367748180
N	-0.7481932271	-0.3868100994	-1.1891651418
N	0.7471374235	1.0124815240	0.7334697422
N	-0.7443517825	-0.3857286982	1.1918310593
N	0.7438582582	-0.3877134669	-1.1915101200
N	-0.7458373314	1.0127992364	-0.7343500487

-Frequencies:

1	536.262
2	538.797
3	685.314
4	745.091
5	746.968
6	772.110
7	776.187
8	812.763
9	868.732
10	877.797
11	880.916
12	884.021
13	921.820
14	963.175
15	968.945
16	971.070
17	973.196
18	1063.817
19	1065.088
20	1069.053
21	1075.793
22	1105.793
23	1106.522

```
    24    1120.465
```

-Transition state:

```
 N             -0.7253688286  -1.3792343752  -0.1973341250
 N              0.7339269982  -1.2298979168   0.0518152170
 N              0.7218676915  -0.4106612489   1.2174112953
 N             -0.6352865609   0.9800408339   0.7120333179
 N              0.7195779661   1.0317120889  -0.7679491067
 N             -0.7259180156  -0.6143894046  -1.2485395500
 N              0.7821186239   0.9970445262   0.7217139462
 N             -0.8004343552  -0.2286106733   1.3232112769
 N              0.7328722057  -0.3314496417  -1.1858514228
 N             -0.8033557251   1.1854458115  -0.6265108490
```

-Frequencies:

```
     1     686.340i
     2     395.280
     3     492.093
     4     522.899
     5     576.722
     6     600.546
     7     656.141
     8     736.138
     9     752.794
    10     817.555
    11     827.293
    12     838.728
    13     879.071
    14     913.398
    15     923.189
    16     954.349
    17    1005.994
    18    1042.920
    19    1065.405
    20    1070.123
    21    1083.042
    22    1152.881
    23    1231.717
    24    1306.153
```

11) $N_{10}(C_1)$

-Minimum:

```
 N             -0.4419027400   1.1374388651  -0.3787828386
 N              1.6117817452  -0.0490535516   0.1087746869
 N             -1.5182347951  -0.6291536123  -0.5798682691
 N              0.6054092321  -1.1155489067   0.1469732876
 N              0.9040810360   1.2174216070   0.0487447611
 N             -1.1493108383   0.2613811912   0.5668467401
 N             -0.1182335918  -0.4333271177   1.2280499984
 N              1.0008283241   0.5596531513   1.3120641631
 N             -0.6509288372   0.1787551132  -1.4679341144
```

```
 N             -0.2434895348  -1.1275667395  -0.9848684153
```

-Frequencies:

```
     1     360.975
     2     444.239
     3     572.275
     4     664.602
     5     682.922
     6     727.043
     7     761.704
     8     784.264
     9     789.930
    10     805.356
    11     868.159
    12     887.628
    13     892.794
    14     903.260
    15     940.055
    16     973.907
    17     989.237
    18    1038.267
    19    1048.066
    20    1063.964
    21    1083.792
    22    1128.258
    23    1194.665
    24    1202.316
```

-Transition state:

```
 N             -0.4121244077   1.1989875693  -0.3321497468
 N              1.6548022737  -0.1580953261   0.2010606355
 N             -1.5548971767  -0.6018195449  -0.5546568217
 N              0.6838509541  -1.1139534696   0.1848384328
 N              0.8122810250   1.3563697476   0.1022984884
 N             -1.1221309836   0.2708496626   0.5488935603
 N             -0.0847105192  -0.4379552826   1.2164983803
 N              1.0180775393   0.5540182667   1.2758243726
 N             -0.6701431688   0.0629732258  -1.5672696461
 N             -0.3250055357  -1.1313748489  -1.0753376555
```

-Frequencies:

```
     1     746.222i
     2     287.038
     3     368.982
     4     456.721
     5     527.124
     6     630.657
     7     677.342
     8     719.742
     9     753.376
    10     758.984
    11     806.657
    12     848.600
    13     862.844
```

14	898.816
15	921.110
16	952.992
17	965.348
18	990.286
19	1036.609
20	1070.560
21	1126.339
22	1137.847
23	1237.404
24	1315.697

12) $N_{10}(C_{3v})$

-Minimum:

N	-0.5018102379	0.7330543999	-1.2901124751
N	-0.8068299488	1.0513878138	0.0462211725
N	-1.2150741297	-0.1874524677	0.7262929018
N	-0.0258932748	-0.0633632218	1.6196592756
N	-0.3082053602	-0.7414144213	-1.3455011278
N	0.7259562947	-0.9918296579	0.7255595642
N	0.8725174337	0.1630920623	-1.2908839584
N	0.4522532227	1.0898535258	0.8031671826
N	1.3153166286	0.1713280757	0.0447731983
N	-0.5082304197	-1.2246651856	-0.0391757450

-Frequencies:

1	533.545
2	535.583
3	539.148
4	686.572
5	689.135
6	745.841
7	749.922
8	814.030
9	851.714
10	878.446
11	886.145
12	934.340
13	938.963
14	959.162
15	974.541
16	982.315
17	992.217
18	1025.661
19	1034.844
20	1038.055
21	1069.602
22	1079.337
23	1079.958
24	1176.707

-Transition state

N	-0.4005545237	0.8060678466	-1.2795832621
N	-0.7748189006	1.0855543331	0.0322216291
N	-1.2228787225	-0.1906908896	0.7132527505
N	-0.0344787565	-0.0855239610	1.6129240962
N	-0.4198123282	-1.0079488781	-1.3123347054
N	0.7280371996	-1.0013024623	0.7113327349
N	0.8555999032	0.2884301489	-1.2793233754
N	0.4465443982	1.0764674267	0.8350324968
N	1.3169470337	0.2193351598	0.0307535383
N	-0.4945853033	-1.1903887241	-0.0642759031

-Frequencies:

1	520.436i
2	266.060
3	474.085
4	617.307
5	634.460
6	680.516
7	729.341
8	777.080
9	822.123
10	831.856
11	836.302
12	883.418
13	922.363
14	933.099
15	964.117
16	989.235
17	994.899
18	1014.739
19	1024.376
20	1048.716
21	1075.923
22	1101.223
23	1146.037
24	1380.006

Part III

Graphs of selected molecular parameters against AE, DE and DE/n

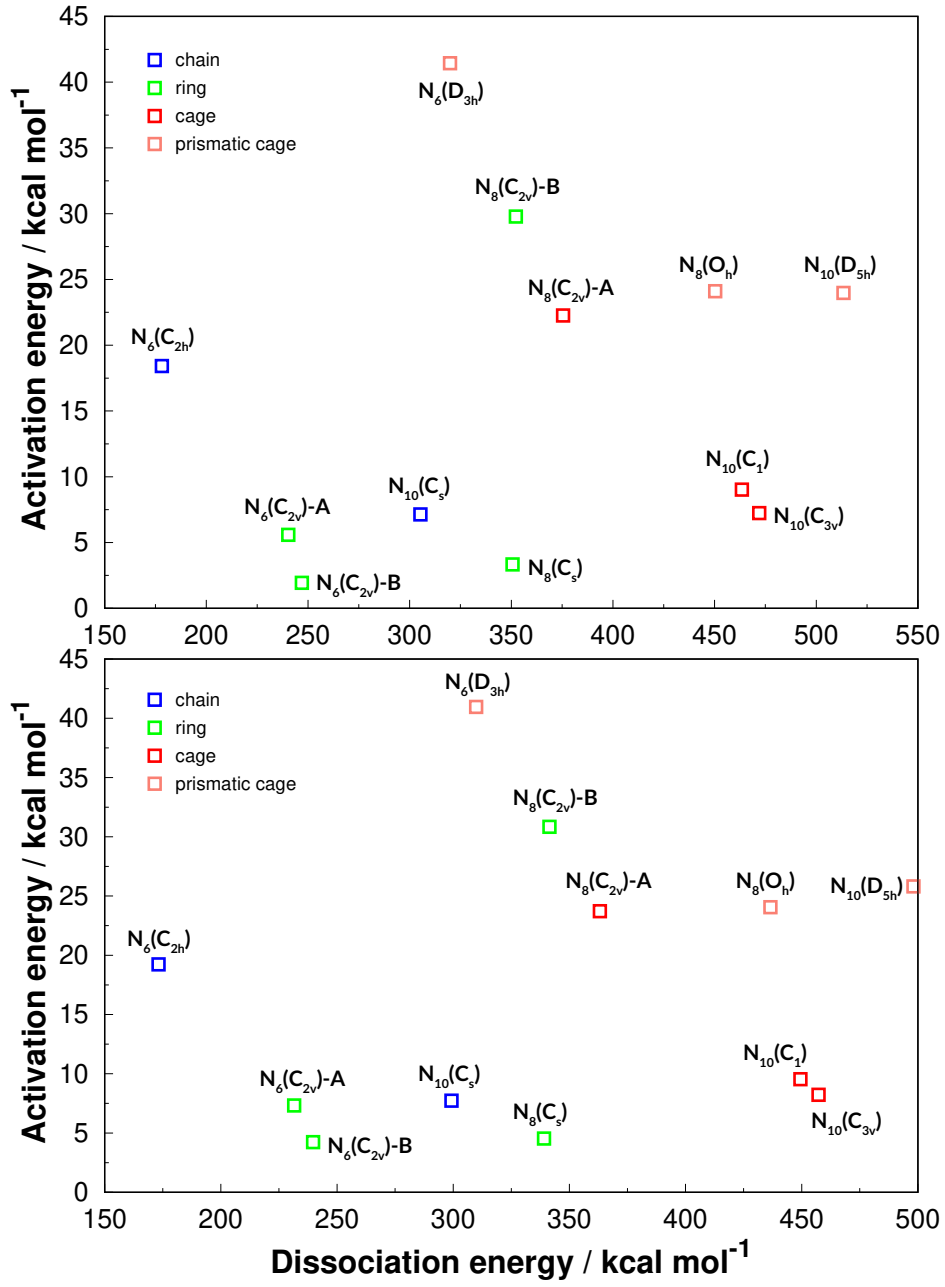

Figure S1: Calculated activation energies as a function of the dissociation energies using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

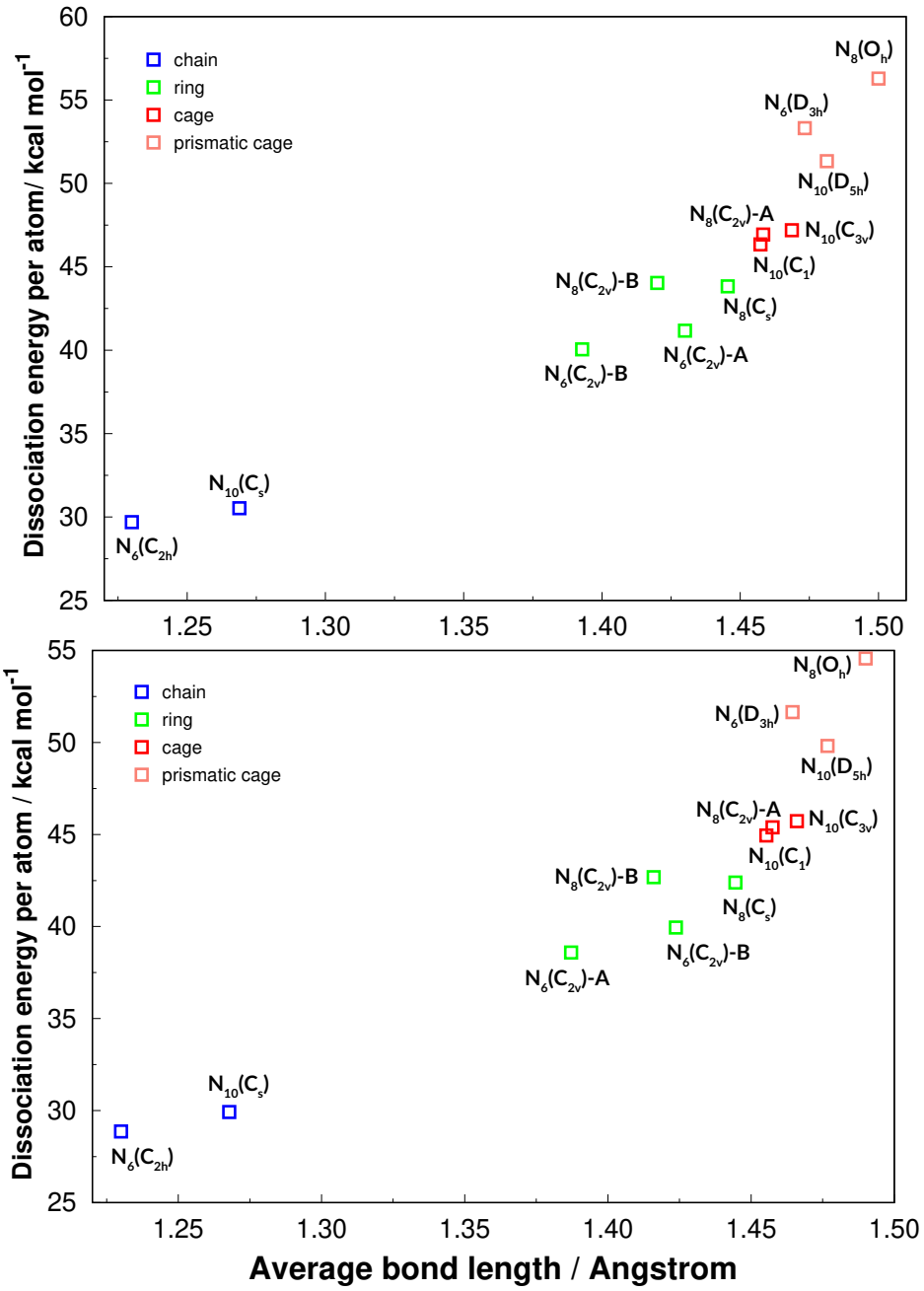

Figure S2: Calculated dissociation energies per nitrogen atom as a function of the average bond lengths using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

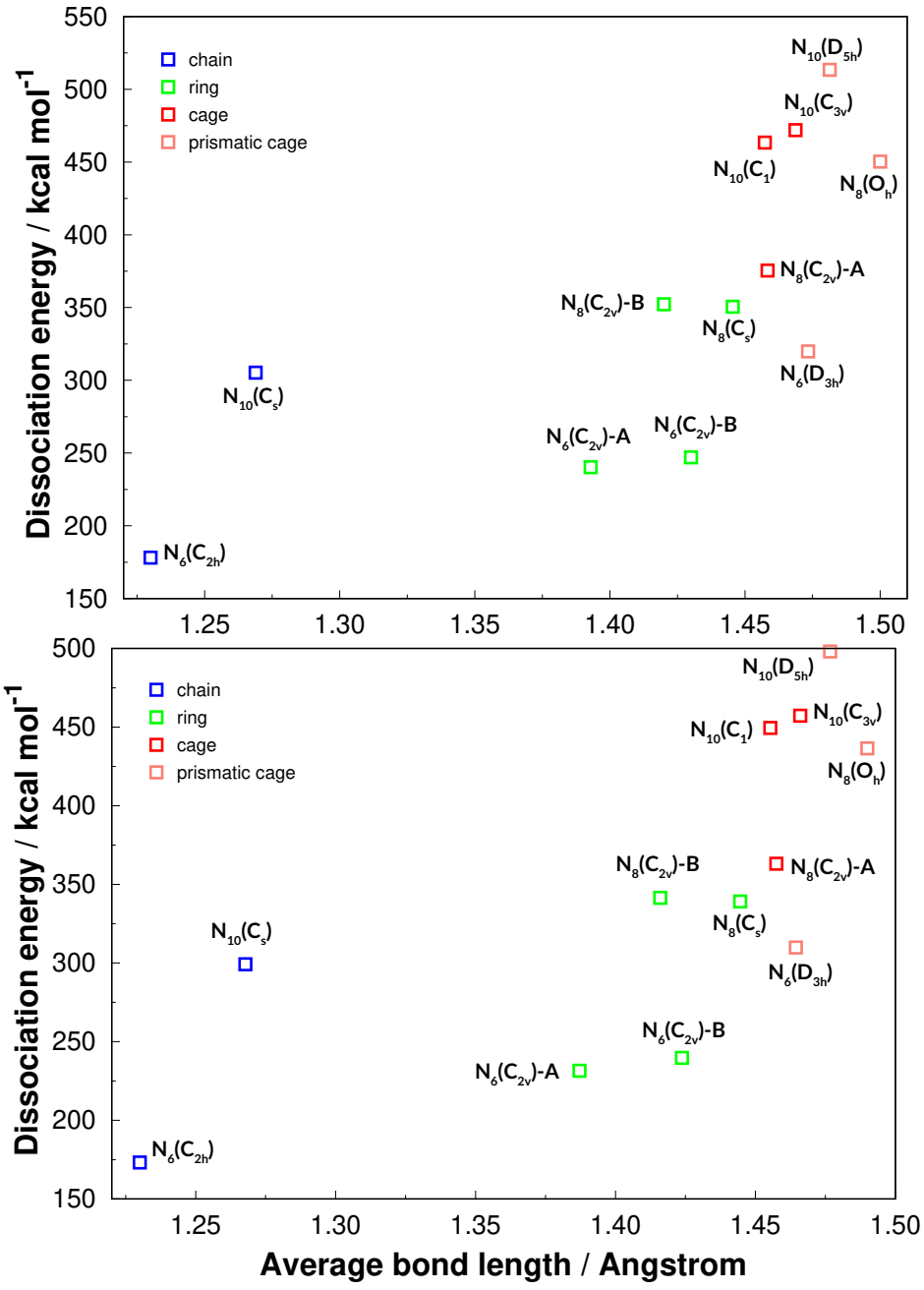

Figure S3: Calculated dissociation energies as a function of the average bond lengths using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

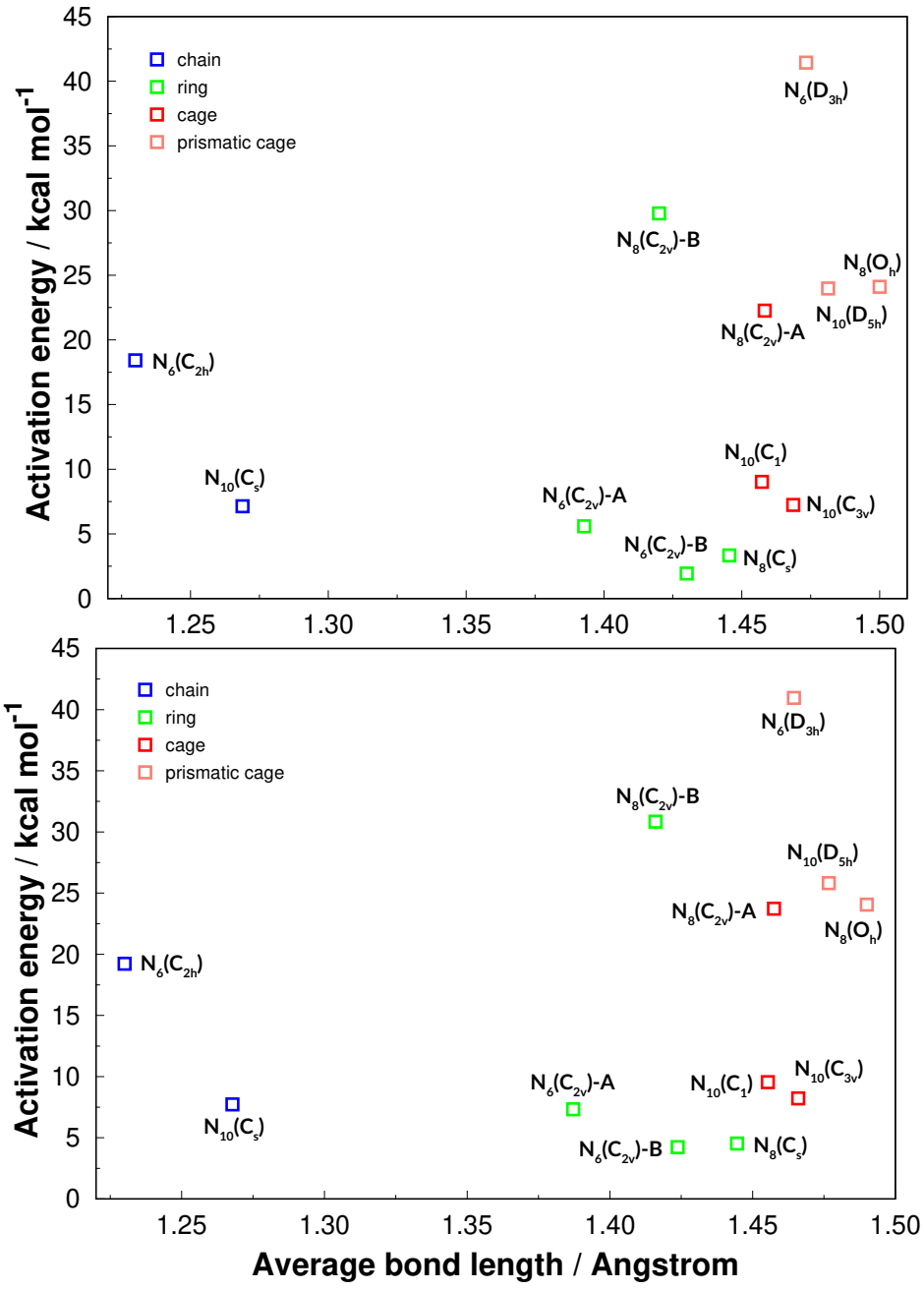

Figure S4: Calculated activation energies as a function of the average bond lengths using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

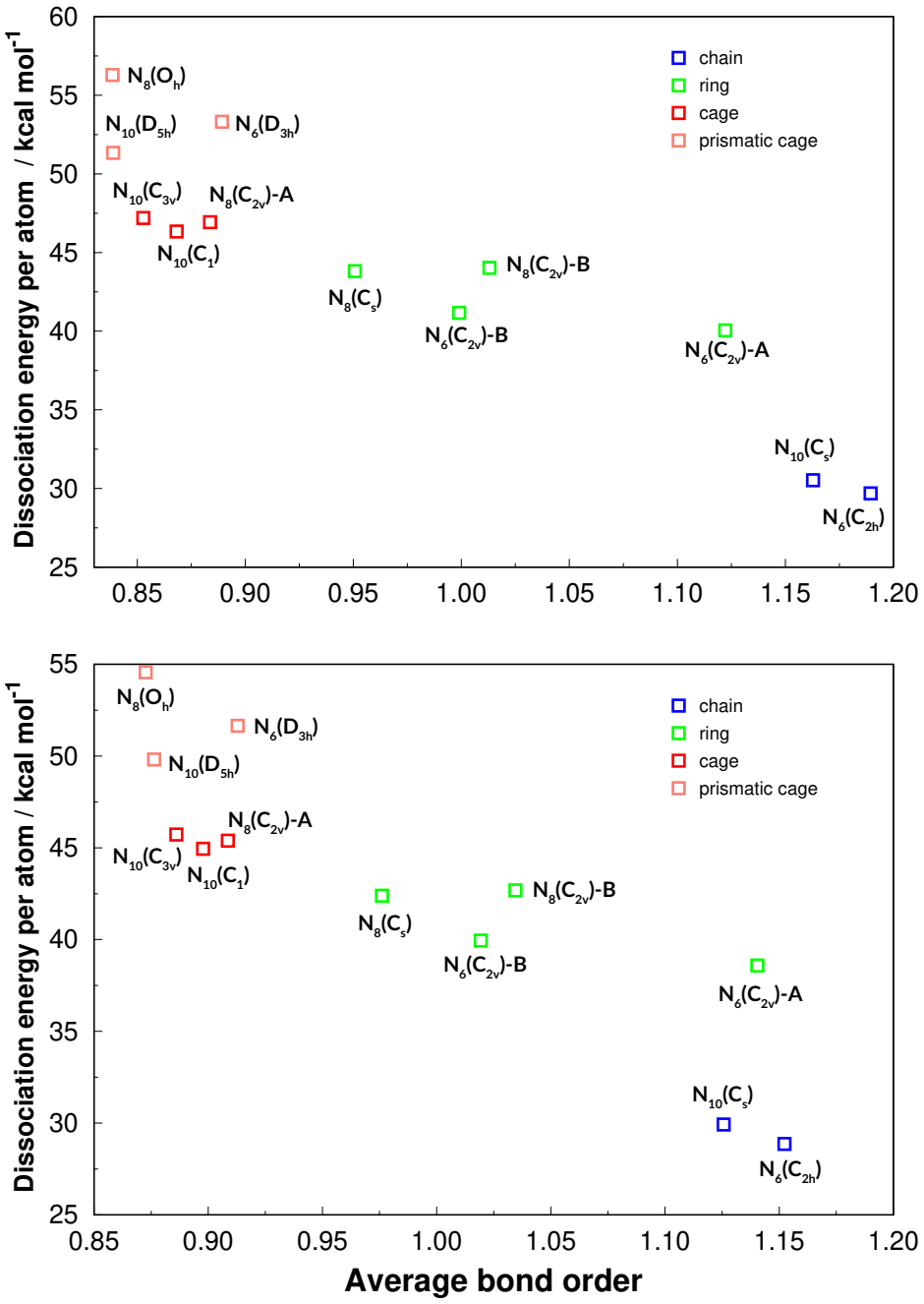

Figure S5: Calculated dissociation energies per nitrogen atom as a function of the average bond orders using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

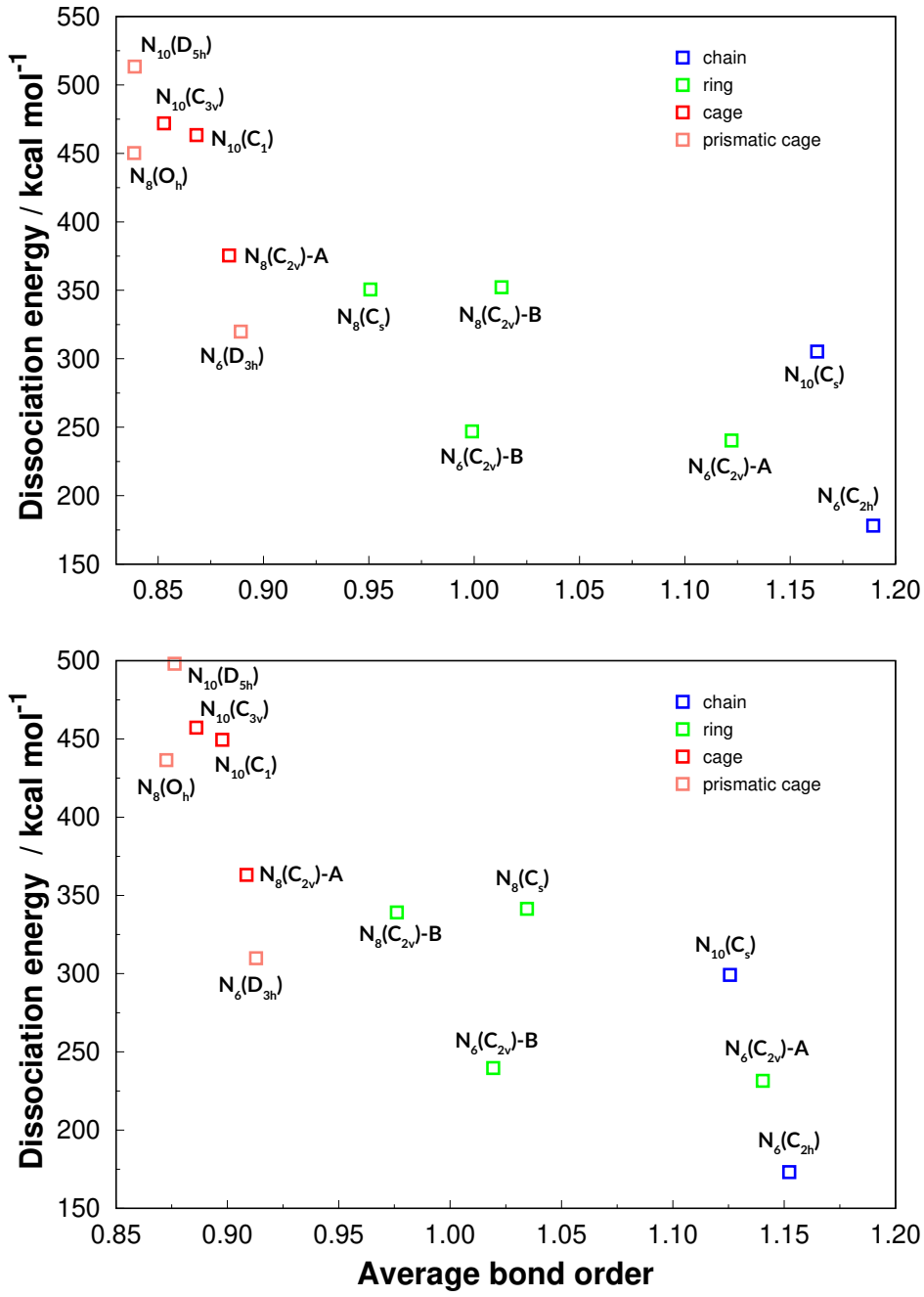

Figure S6: Calculated dissociation energies as a function of the average bond orders using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

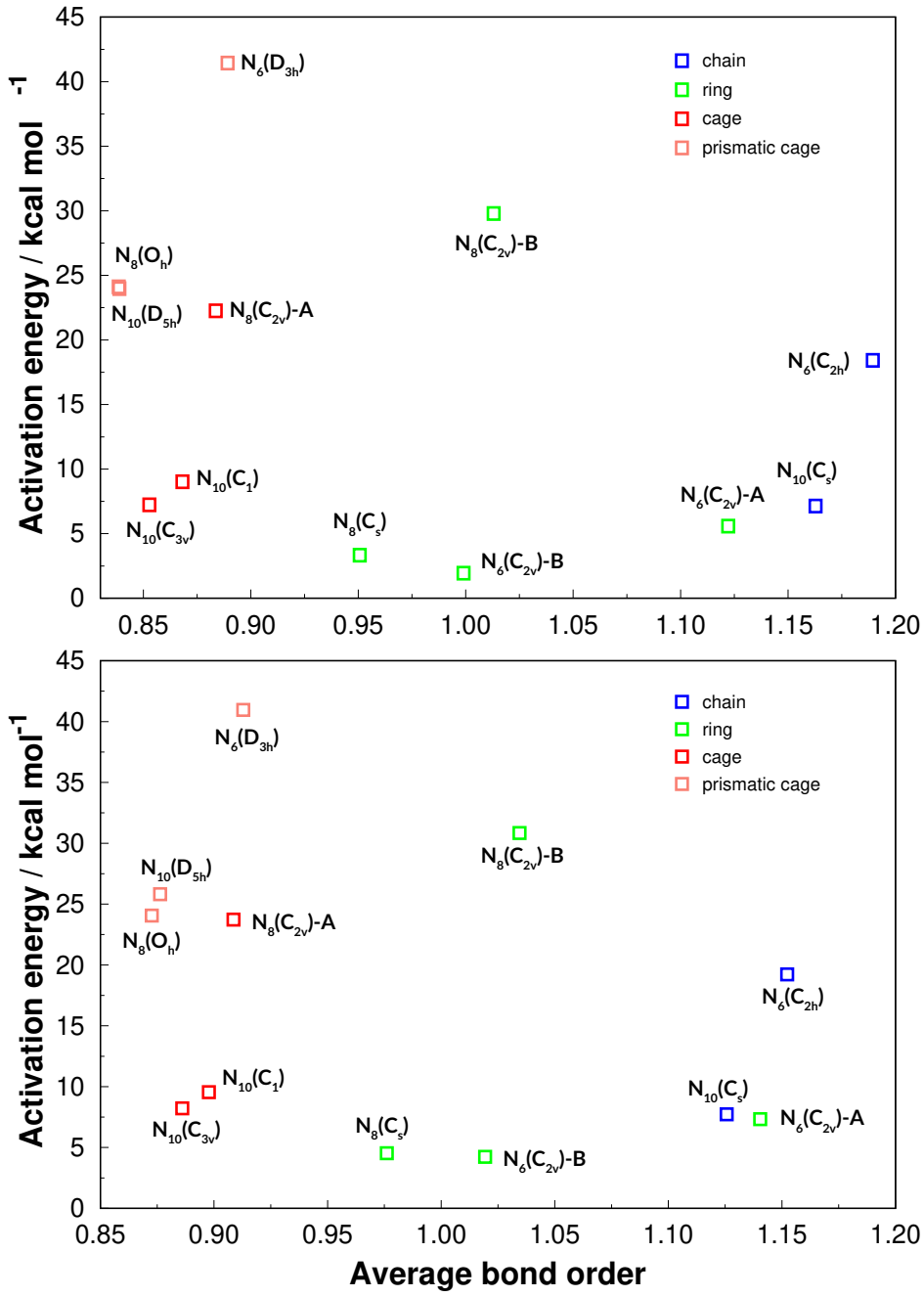

Figure S7: Calculated activation energies as a function of the average bond orders using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

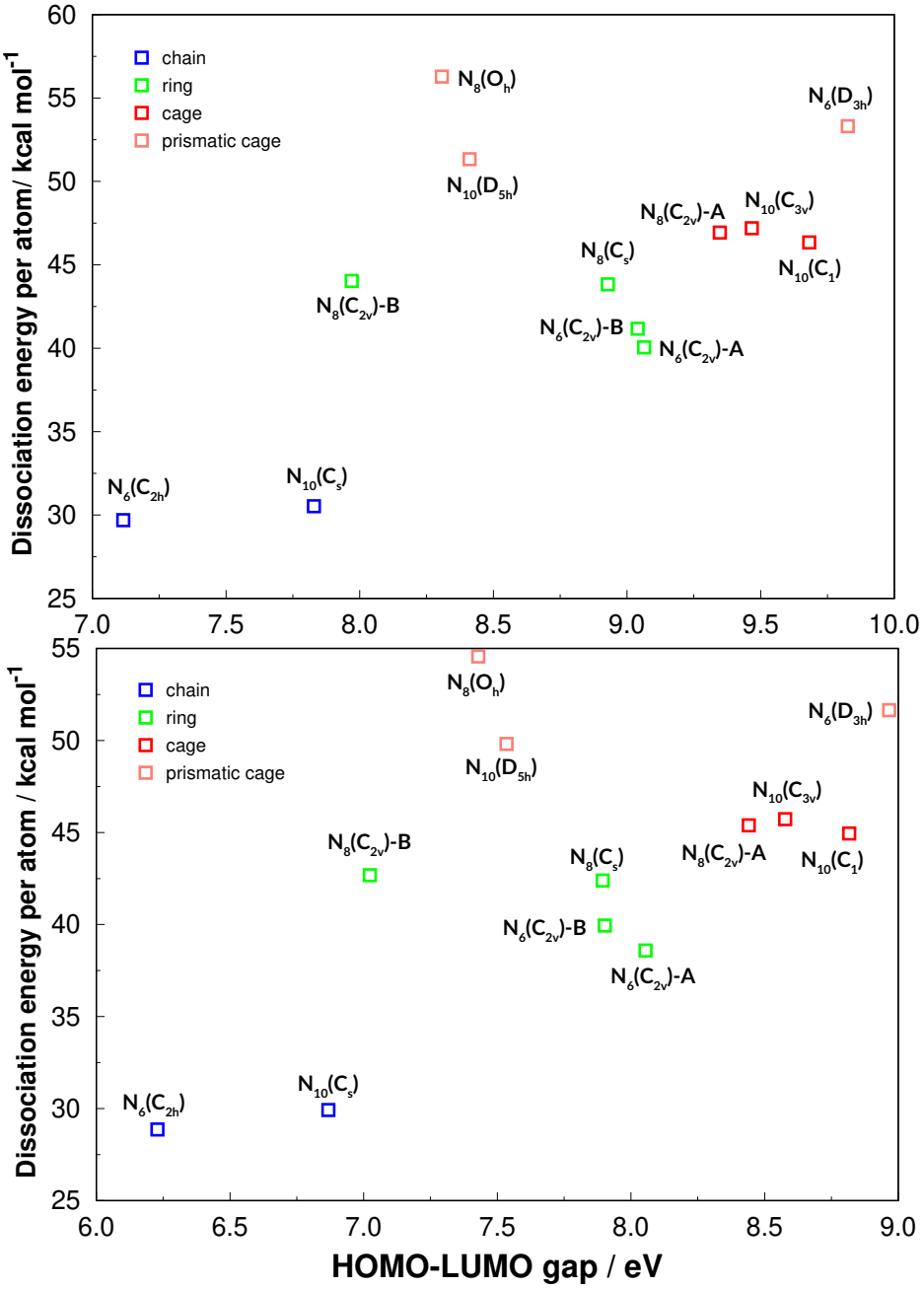

Figure S8: Calculated dissociation energies per nitrogen atom as a function of the HOMO-LUMO gaps using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

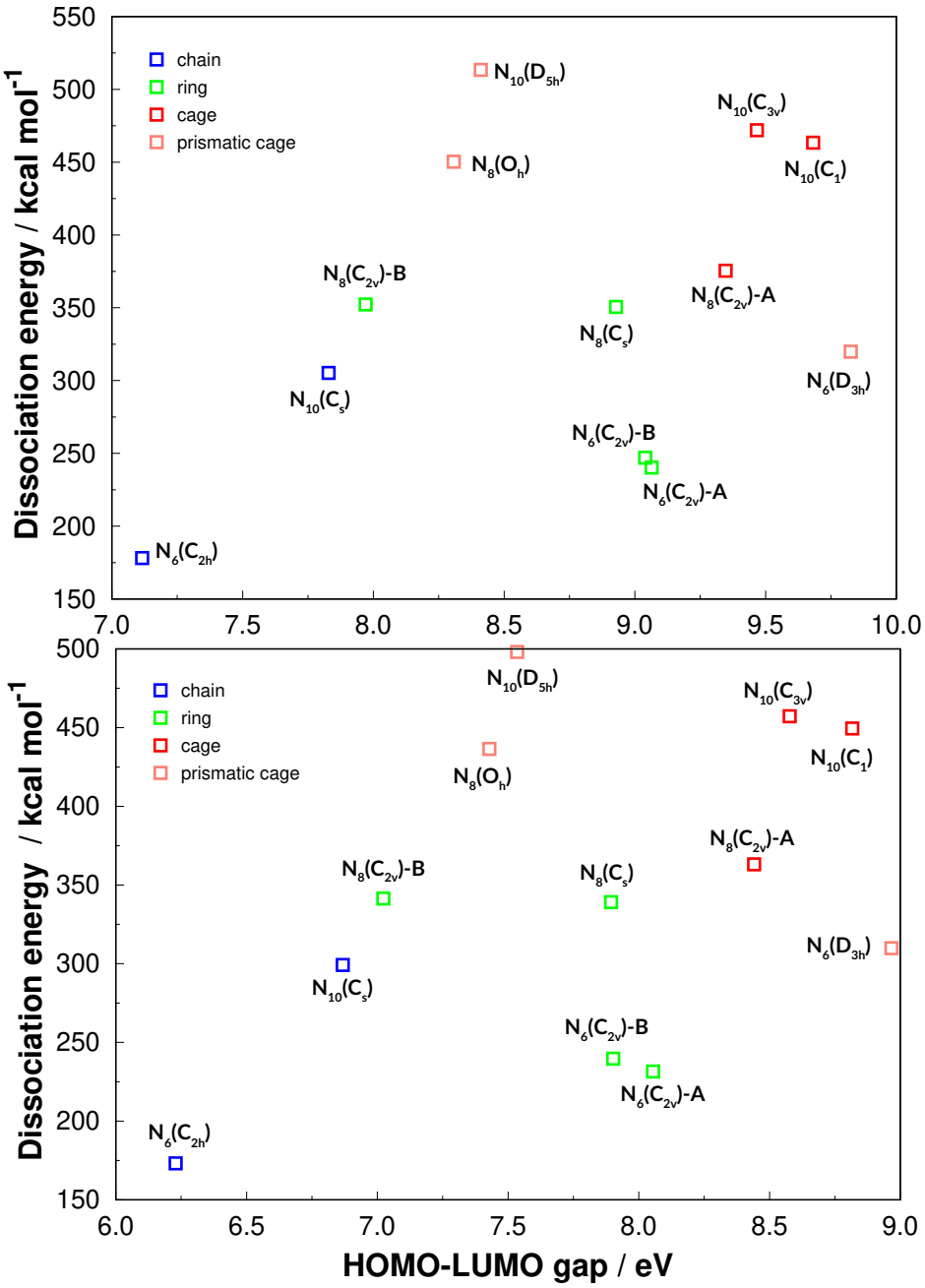

Figure S9: Calculated dissociation energies as a function of the HOMO-LUMO gaps using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

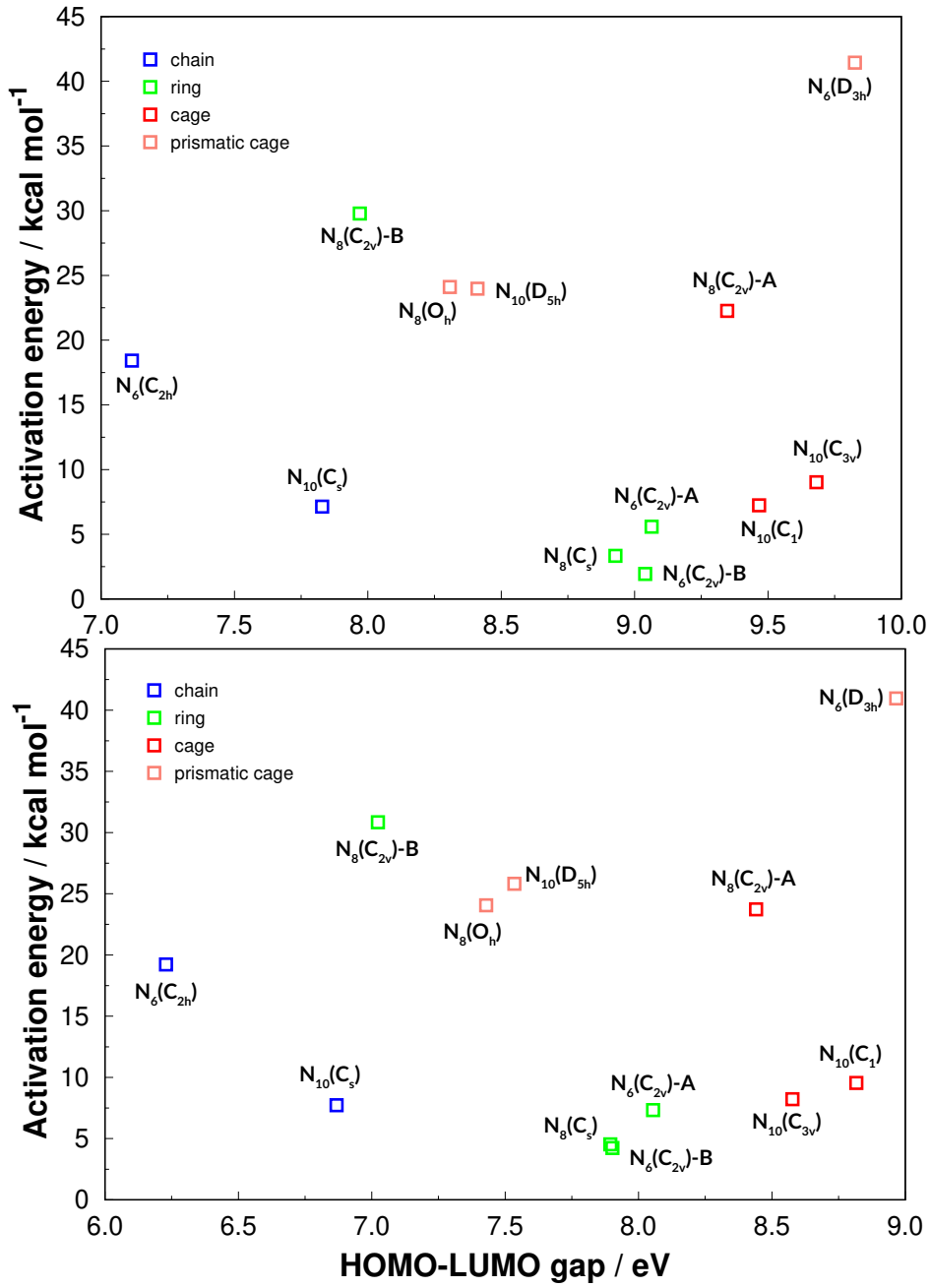

Figure S10: Calculated activation energies as a function of the HOMO-LUMO gaps using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

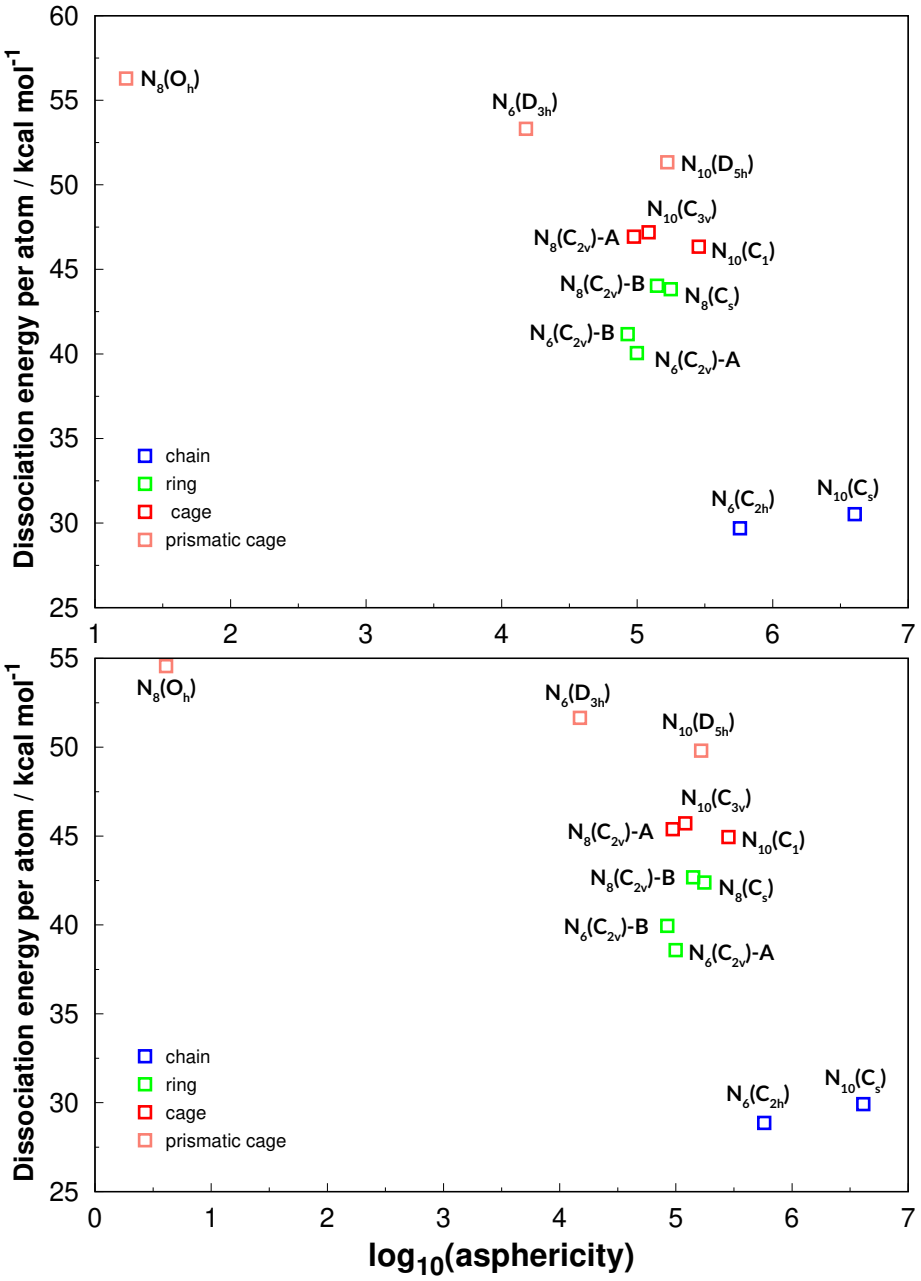

Figure S11: Calculated dissociation energies per nitrogen atom as a function of the asphericities using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

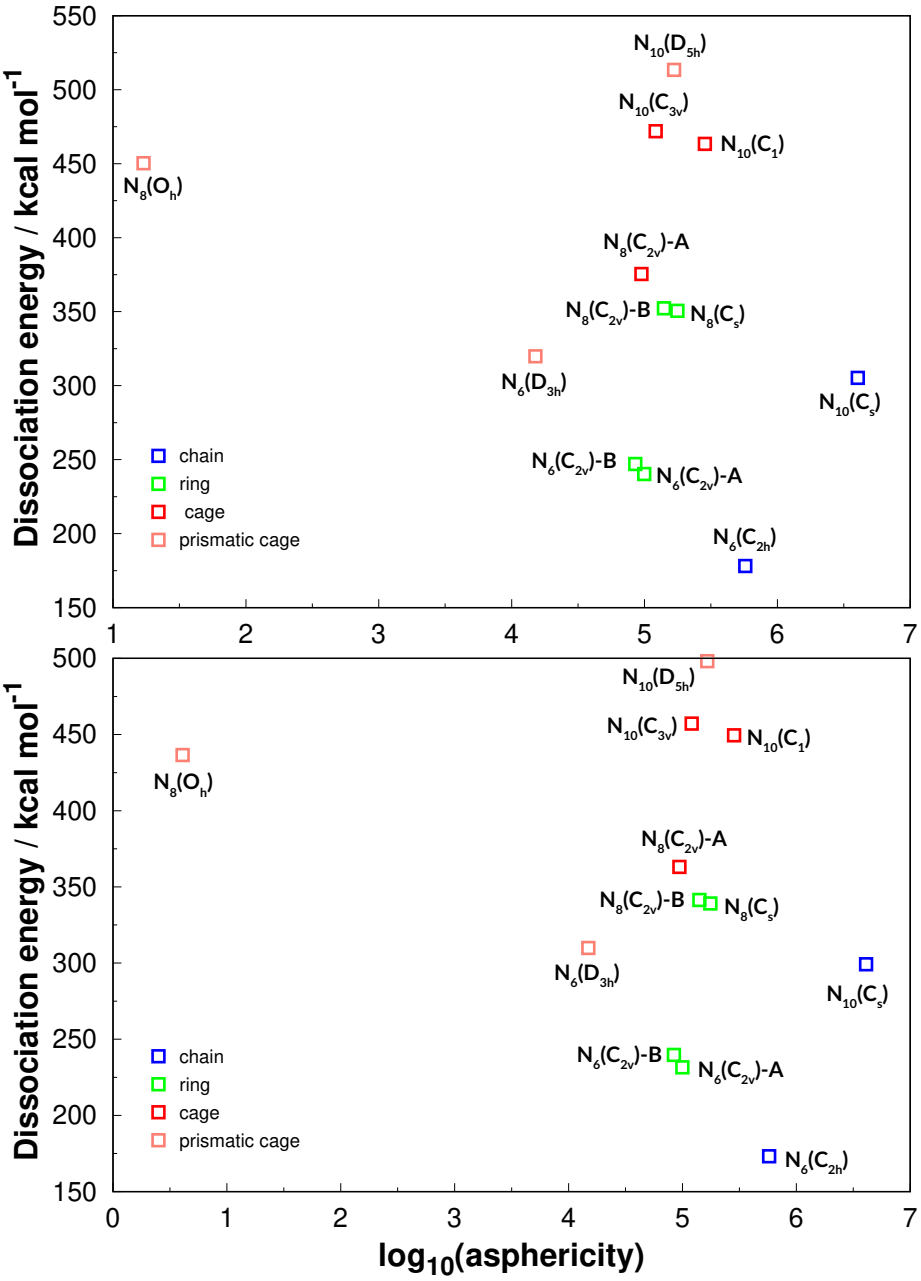

Figure S12: Calculated dissociation energies as a function of the asphericities using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.

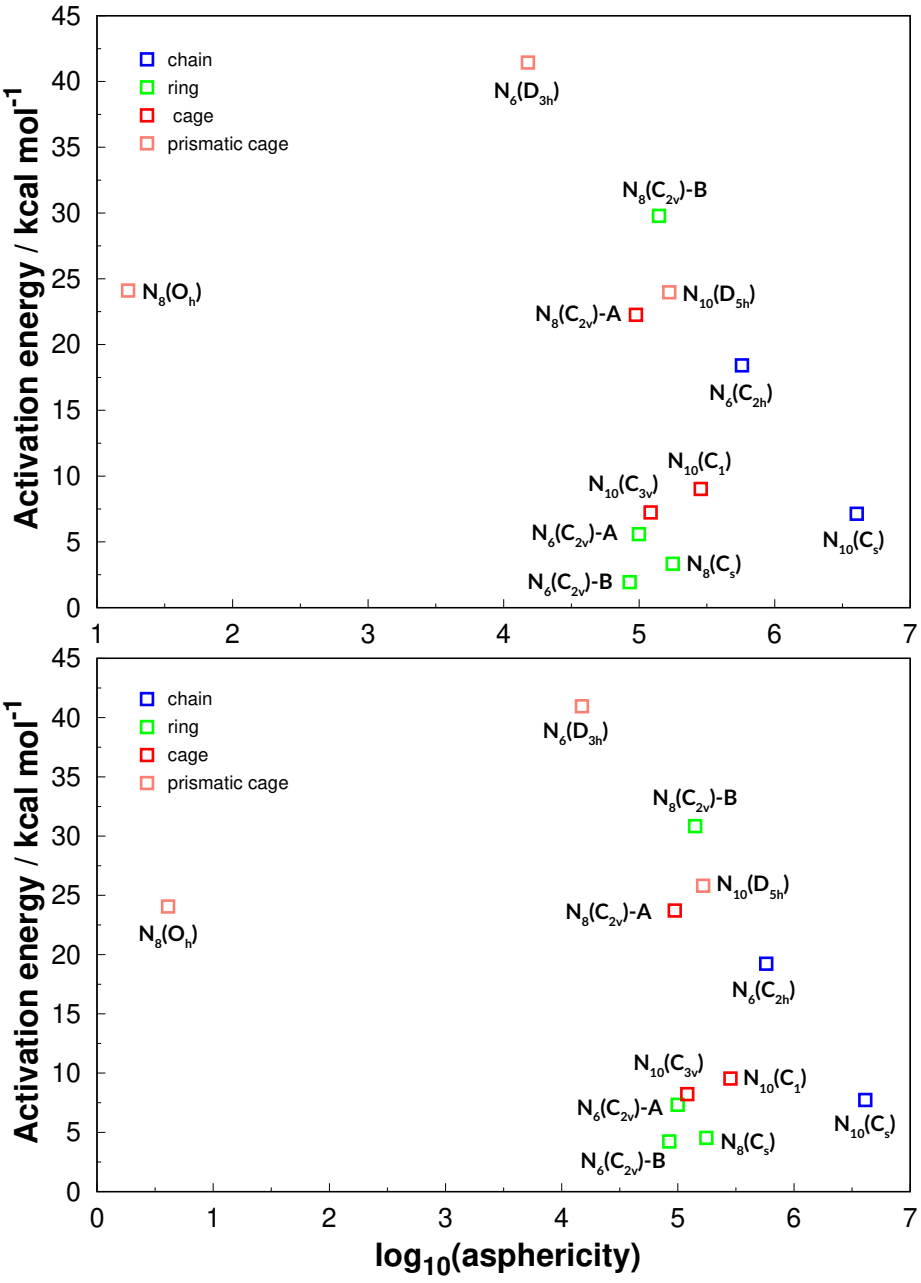

Figure S13: Calculated activation energies as a function of the asphericities using the def2-TZVPP basis set. The M06-2X functional is shown in the upper panel, while the SOGGA11-X one is on the lower panel.