**Supporting Information**

for

**Negative ion formation and fragmentation upon dissociative electron attachment to the nicotinamide molecule**

Patrick Ch. Ziegler¹, Andrzej Pelc²*, Eugene Arthur-Baidoo¹, Joao Ameixa¹,³, Milan Ončák¹, Stephan Denifl¹*

¹Institute for Ion Physics and Applied Physics, University of Innsbruck, Technikerstrasse 25, 6020 Innsbruck, Austria
²Maria Curie-Skłodowska University, Department of Biophysics, Mass Spectrometry Laboratory, Pl. M. C.-Skłodowskiej 1, 20-031 Lublin, Poland
³Centre of Physics and Technological Research, Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal
*e-mail: Andrzej.Pelc@poczta.umcs.lublin.pl, Stephan.Denifl@uibk.ac.at

Table S1 – Electron affinities (in eV) for four selected molecules as optimized at the B3LYP/aug-cc-pVDZ level and single-point recalculated using various methods. The zero-point energy correction was included as calculated at the B3LYP/aug-cc-pVDZ level. Mean absolute error with respect to experimental values is also given (“Error”).

| molecule | B3LYP/aug-cc-pVDZ | B3LYP/aug-cc-pVTZ | CCSD(T)/aug-cc-pVDZ | CCSD(T)/aug-cc-pVTZ |
|----------|-------------------|-------------------|---------------------|---------------------|
| CN       | 4.04              | 4.05              | 3.74                | 3.87                |
| NCO      | 3.48              | 3.48              | 3.37                | 3.51                |
| NH2      | 0.75              | 0.76              | 0.55                | 0.68                |
| O        | 1.68              | 1.68              | 1.19                | 1.33                |
| Error    | 0.14              | 0.14              | 0.21                | 0.08                |

Cartesian coordinates (in Å) and electronic energies (in Hartree, including zero-point correction) of structures optimized at the B3LYP/aug-cc-pVDZ level

NAD

E = -416.933556
C  -0.542624  1.211717  0.101817
H  0.036724 -2.124239 -0.249663
C  -2.558069  2.020120  0.201507
H  -0.020510  2.165098  0.170555
C  -2.526925 -0.135228  0.008057
[NAD-H]-, iso2  
E = -416.331076
C -0.550357 1.223574 0.019718
C 0.195834 0.041866 0.004739
C -0.397262 -1.266603 -0.016809
N -1.776957 -1.311850 -0.018297
C -2.489502 -0.173407 -0.005486
C -1.942732 1.115903 0.013535
C 1.696051 0.131684 -0.000044

[NAD-H]-, iso3  
E = -416.314376
C -0.614152 1.222513 0.030991
C 0.172869 0.053363 -0.019374
C -0.539775 -1.161501 -0.071286
N -1.870966 -1.283951 -0.049076
C -2.697636 -0.163344 0.032270
C -1.996254 1.093855 -0.051607
C 1.647594 -1.35848 -0.014449
N 2.364464 -1.094568 -0.046250
O 2.338464 1.194209 -0.037301
H -5.590357 1.996210 0.024107
H -0.047437 2.194009 0.035261
H 1.607550 -1.873740 0.005264
H 3.284400 -1.174492 -0.046273
H -3.582998 -0.288835 -0.009541

[NAD-H]-, iso4  
E = -416.324893
C 0.395048 -1.297197 -0.014384
C -0.193365 0.001134 -0.002348
C 0.563249 1.183897 0.015931
N 1.906149 1.205452 0.014057
C 2.580196 -0.003566 -0.002210
C 1.809760 -1.219358 -0.015126
C -1.694178 0.121231 -0.000826
N -2.307282 -1.094941 0.040057
O -2.323453 1.190643 -0.031926
H 0.058566 1.254387 0.028979
H 2.417207 -2.135591 -0.026983
H -1.660277 -1.891608 0.003551
H -3.309790 -1.153908 -0.038121
H 3.600187 0.011097 -0.005217

[NAD-CNOH]  
E = -248.225812
C 1.200027 0.673556 0.000057
C 0.000299 1.387814 0.000016
C -1.199771 0.673792 -0.000125
C -1.144870 -0.723691 0.000175
N -0.000140 -1.421262 -0.000068
C 1.144440 -0.724223 -0.000035
H -2.162889 1.185183 0.000077
H -2.066324 -1.311113 -0.000124
H 2.163226 1.184320 -0.000033
H 0.000299 2.478666 -0.000027
H 2.065913 -1.311716 0.000054

C5H4N.H2O  
E = -323.980827
C -1.635968 -1.179138 0.000000
C -0.618459 -2.147061 0.000000
C 0.671720 -1.662926 0.000000
C 0.992063 -0.319086 0.000000
N 0.000000 0.596541 -0.000000
C -1.269711 0.170327 0.000000
H 2.014304 0.059586 -0.000000
H -2.688054 -1.467055 0.000000
H -0.847800 -3.213634 0.000000
H -2.835874 0.948126 -0.000000
H 0.884260 2.336757 -0.000000
O 1.588260 3.015677 -0.000000
H 1.129276 3.862315 -0.000000

CS4N.H2O  
E = -323.980827
C -1.635968 -1.179138 0.000000
C -0.618459 -2.147061 0.000000
C 0.671720 -1.662926 0.000000
C 0.992063 -0.319086 0.000000
N 0.000000 0.596541 -0.000000
C -1.269711 0.170327 0.000000
H 2.014304 0.059586 -0.000000
H -2.688054 -1.467055 0.000000
H -0.847800 -3.213634 0.000000
H -2.835874 0.948126 -0.000000
H 0.884260 2.336757 -0.000000
O 1.588260 3.015677 -0.000000
H 1.129276 3.862315 -0.000000

CN pathway, TS1  
E = -416.893297
H 3.206475 0.146523 0.095635
o 2.388487 1.117440 -0.046323
 1.621482 0.020270 -0.017579
c 0.209417 0.022214 -0.019031
c -0.555130 0.020270 -0.019031
n -1.874585 -1.274752 -0.029382
c -2.584107 -0.195470 0.016748
c -1.946380 1.154570 0.030331
-0.565559 1.239734 0.017314
h -0.050099 2.199340 0.031932
h -2.554464 2.063576 0.065828
h -3.672597 -0.192785 -0.039757
h -0.018203 -2.150613 -0.100704
h 2.301341 -1.847606 0.528398

CN pathway, LM2
E = -416.929514
C 0.498937 -1.220196 0.000121
C -0.240797 0.022486 0.000013
C 0.572294 1.211798 0.000186
N 1.893034 1.244799 0.000047
C 2.567098 0.051860 -0.000188
C 1.882057 -1.183914 -0.000019
C -1.665637 0.085844 -0.000043
N -2.504673 1.103547 -0.000073
O -2.291287 1.150446 -0.040719
H 0.078287 2.190150 0.000322
H 2.454905 -2.116368 0.000016
H -0.036835 -2.161012 -0.00398
H -1.995188 1.985903 -0.00274
H 3.657841 -1.027578 -0.00381
H -3.230951 -0.929339 0.000156

CN pathway, TS2
E = -416.918136
c -1.862855 1.162918 0.065562
c -0.493793 1.213987 0.101189
c 0.263368 -0.025627 0.030063
C -0.544199 -1.210988 -0.046088
N -1.862057 -1.262992 -0.080938
C -2.550571 -0.067406 -0.033299
C 1.702836 -0.094467 0.011065
O 2.368346 1.127048 -0.130445

CN pathway, LM3
E = -416.923772
c 0.209417 0.022214 -0.019031
c -0.555130 -1.197339 -0.048294
n -1.874585 -1.274752 -0.029382
c -2.584107 -0.195470 0.016748
c -1.946380 1.154570 0.030331
-0.565559 1.239734 0.017314
h -0.050099 2.199340 0.031932
h -2.554464 2.063576 0.065828
h -3.672597 -0.192785 -0.039757
h -0.018203 -2.150613 -0.100704
h 2.301341 -1.847606 0.528398

CN pathway, TS3
E = -416.919222
c 1.909248 1.145478 0.035714
c 0.520213 1.218357 0.034882
-0.257804 0.002528 0.003339
c 0.526040 -1.204945 -0.034741
n 1.846398 -1.274256 -0.036295
h 2.550096 -0.100572 0.001921
h -1.687208 -0.094507 0.008863
-2.381616 1.152296 -0.044458
n -2.419254 -1.181183 -0.056969
h 0.025543 -2.146682 -0.075631
h 2.507575 2.060447 0.069065
h 0.051261 2.204096 0.086603
h -2.730888 -1.632784 0.797897
h 3.639456 -0.180127 0.00358
h -1.742453 1.866773 -0.172786

CN pathway, LM4
E = -416.921744
C 2.558492 -0.076941 0.029417
C 1.896908 1.158735 -0.029203
C 0.508755 1.215594 -0.061904
C -0.246781 -0.021807 -0.023248
C 0.549452 -1.218688 0.012211
N 1.867813 -1.271933 0.040421
C -1.676025 -0.107818 -0.009369
N -2.376624 -1.213359 -0.064952
C 0.234675 1.150446 -0.040719
C 2.494889 -1.144242 -0.022964
h -0.090042 -2.199043 0.031674
h -2.425884 2.125307 -0.038868
h 0.061755 2.152578 -0.093480
h 1.938887 -2.001241 -0.055617
h -3.648600 -0.082613 0.033722
h 2.376269 1.477303 0.868582

CN pathway, TS4
E = -416.865924
o -2.898626 0.922065 0.889873
h -3.242550 -0.565875 -0.226931
c -1.446882 -0.419747 -0.372876
n -2.471651 -0.094492 -0.052247
n -0.930349 -0.194718 -0.238847
n 0.521538 1.075470 -0.528810
C 1.880849 1.216379 -0.314288
C 2.637003 1.041690 0.191713
n 2.074039 -1.059656 0.499681
n 0.777473 -1.211454 0.301261
n 0.347102 -2.181454 0.566005
h -2.788996 1.160020 1.820632
h 0.094438 1.899228 -0.885187
h 2.373028 2.168389 -0.527951
h 3.711181 0.237151 0.366343
CN pathway, LM5
E = -416.940759

o -5.096555 0.005210 0.114243
h -4.123886 0.007936 -0.081254
c -1.097207 0.013263 -0.172443
n -2.277299 0.008182 -0.251929
c 0.295666 0.029114 -0.079325
c 1.071961 1.260744 -0.025179
c 2.449206 1.156104 0.069397
c 3.079875 -0.102731 0.112118
n 2.359064 -1.282328 0.061407
c 1.049733 -1.196467 -0.028762
h 0.498404 -2.143152 -0.068130
h -5.116321 -0.042556 1.075891
h 0.573089 2.228995 -0.059756
h 3.061208 2.061987 0.111691
h 4.164195 -0.102731 0.112118

NCO pathway, TS
E = -416.314587

c -0.054131 -0.307719 -0.000018
h 2.028882 -1.622982 -0.000022
c 2.801086 0.024204 0.000005
n 2.964048 -1.200993 -0.000010
o 2.925558 1.194744 0.000022
c -0.567853 1.018442 -0.000020
c -1.944396 1.286591 -0.000006
c -2.838775 0.218232 0.000011
n -2.433261 -1.066310 0.000014
c -1.093961 -1.273520 0.000000
h -0.836645 -2.343766 0.000006
h 0.124139 1.864159 -0.000035
h -2.326689 2.310434 -0.000009
h -3.921733 0.384755 0.000022

O
E = -75.077162
O 0.00000 0.00000 0.00000

NH2
E = -55.872209
N 0.00000 0.00000 0.143266
H -0.00000 0.807952 -0.501432
H -0.00000 -0.807952 -0.501432

CN
E = -92.720216
N 0.00000 0.00000 0.541845
C 0.00000 0.00000 -0.632152

C5H4N
E = -247.551143
C -1.179144 -0.812271 -0.000000
C 0.075785 -1.382457 -0.000000
C 1.252458 -0.654864 0.000000
N 1.200908 -0.807952 -0.501432
C 0.00000 1.285155 0.000000
C -1.125234 0.591728 -0.000000
H 2.240668 -1.116338 0.000000
H -2.163621 1.131522 -0.000000

[NAD-H], iso6
E = -416.264538
C 1.892518 1.142718 0.042124
C 0.503493 1.219816 0.044667
C -0.232653 0.026926 0.03839
C 0.468033 -1.190441 -0.040755
N 1.803546 -1.272262 -0.041318
C 2.491825 -0.122964 0.007785
C -1.715982 0.071128 0.019338
O -2.363248 1.121149 -0.116177
N -2.402987 -1.122371 0.040429
H -0.800755 -2.131944 -0.089038
H 2.508782 2.040875 0.074123
H -0.019063 2.175355 0.077212
H -3.330797 -0.958293 0.450852
H 3.580497 -0.215850 0.002559

NCO
E = -168.019808
N 0.009369 1.271717 0.000000
C 0.000000 0.040182 0.000000
O -0.008198 -1.142889 -0.000000

[NAD-CN]-
E = -324.007113
N 1.120721 -1.167813 -0.018131
C 1.830532 0.026982 0.003315
C 1.156701 1.216695 0.002158
C -0.268878 1.262144 -0.003306
C -0.959628 0.029652 0.00039
C -0.285936 -1.174532 0.002919
O -2.331263 0.089439 0.002311
H -0.774809 -2.145274 -0.002252
H 1.733448 2.140754 0.005583
H -0.821848 2.197290 -0.001547
H 2.914128 -0.054145 0.007712
H -2.697386 -0.803480 0.001566
H 1.614302 -2.041612 0.064812