Electronic Supplementary Information

Excited-State Aromaticity Reversals in Norcorrole

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1. Gaussian Cube Files with Isotropic Shielding Values

A zip archive of Gaussian cube files with isotropic shielding values for the T_1 electronic states of NiNc and H_2Nc is available as a separate download.

These files can be examined with various programs, including GaussView (see https://gaussian.com/gaussview6/) and Visual Molecular Dynamics (VMD, see https://www.ks.uiuc.edu/Research/vmd/). Both URLs were checked on 9 September 2024.

2. Additional Computational Details

All B3LYP, UB3LYP, TDA-B3LYP, TDA-PBE0 and TDA-ωB97X calculations reported in this paper were carried out using the GAUSSIAN "SuperFine" integration grid. All geometry optimizations included Grimme's D3 empirical dispersion corrections with Becke–Johnson damping, were carried out under the GAUSSIAN "VeryTight" convergence criteria, and were combined with analytical harmonic frequency calculations. All natural population analysis (NPA) calculations were carried out with the GAUSSIAN "Density(Current)" option.

Points making up the grids of isotropic magnetic shielding values and/or corresponding to NICS positions were specified in the GAUSSIAN input files as ghost atoms without basis functions (symbol "Bq"). To improve accuracy, the GAUSSIAN "CPHF(Separate)" option was used in all NMR calculations. Collecting all data for a grid requires running a number of separate GAUSSIAN calculations. To prepare the set of input files, use was made of a purpose-written program which is modified to include the GAUSSIAN route section, geometry and grid specification and for each molecule.

3. Comparison between the Vertical Excitation Energies Calculated with the TDA-B3LYP, TDA-PBE0 and TDA-ωB97X Methods

Table S1 Vertical $T_1 \leftarrow S_0$ and $S_1 \leftarrow S_0$ excitation energies of NiNc and H_2Nc calculated using TDA-B3LYP, TDA-PBE0 and TDA- ωB97X in the def2-TZVP basis set, at the S_0 B3LYP-D3(BJ)/def2-TZVP geometries (in eV).

State/VEE	TDA-B3LYP	TDA-PBE0	TDA- ωB97X
NiNc T_1 ($1\ ^3A_2$)	0.458	0.453	0.614
NiNc S_1 ($1\ ^1A_2$)	0.841	0.872	1.138
H_2Nc T_1 ($1\ ^3A$)	0.607	0.605	0.852
H_2Nc S_1 ($2\ ^1A$)	0.999	1.039	1.448

4. Natural Population Analysis Charges

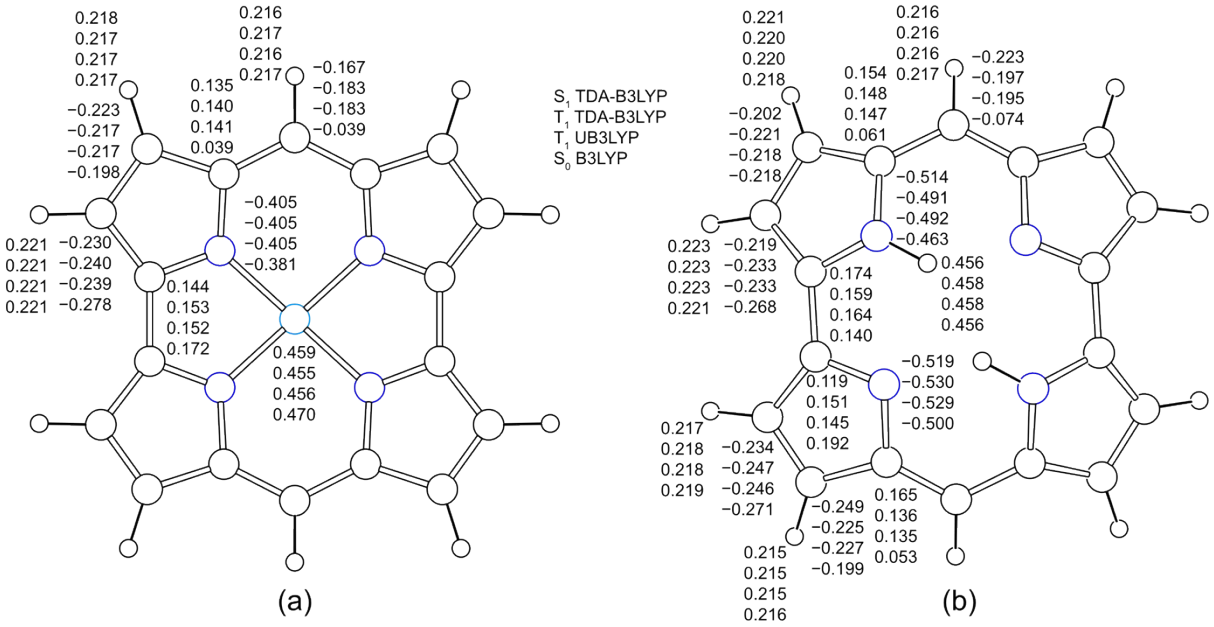

Fig. S1 Symmetry unique natural population analysis (NPA) charges (in units of *e*) at S_0, T_1 and S_1 local minimum geometries of (a) NiNc and (b) H_2Nc, arranged in columns of four numbers each including, from bottom to top, S_0 B3LYP, T_1 UB3LYP, T_1 TDA-B3LYP and S_1 TDA-B3LYP results. (a) and (b) show the S_0 B3LYP-D3(BJ) NiNc (C_{2v}) and H_2Nc (C_2) local minimum geometries, looking at the top of each bowl.

5. Cartesian Coordinates and Other Computational Data

The geometries at which NICS were calculated include the coordinates of the respective ghost atoms. All coordinates are given in Å.

UB3LYP-D3(BJ)/def2-TZVP total energy *E*, $\langle S^2 \rangle$ expectation value, lowest vibrational frequency *v* and optimized geometry of the T_1 state of NiNc, bowl-shaped local minimum of C_{2v} symmetry.

E = –2419.767717 Ha; $\langle S^2 \rangle$ = 2.0071; *v* = 60.4 cm^{-1} (A_1).

```
N    -1.219094   1.327310   0.416560
N    -1.219094  -1.327310   0.416560
N     1.219094  -1.327310   0.416560
N     1.219094   1.327310   0.416560
C    -0.716720   2.571812   0.163128
C    -1.826151   3.397186  -0.227981
C    -2.944929   2.593613  -0.244976
C    -2.534163   1.248024   0.121896
C    -3.195626   0.000000   0.027753
C    -2.534163  -1.248024   0.121896
C    -2.944929  -2.593613  -0.244976
C    -1.826151  -3.397186  -0.227981
C    -0.716720  -2.571812   0.163128
C     0.716720  -2.571812   0.163128
```

```
C    1.826151  -3.397186  -0.227981
C    2.944929  -2.593613  -0.244976
C    2.534163  -1.248024   0.121896
C    3.195626   0.000000   0.027753
C    2.534163   1.248024   0.121896
C    2.944929   2.593613  -0.244976
C    1.826151   3.397186  -0.227981
C    0.716720   2.571812   0.163128
H   -1.783103   4.443885  -0.481062
H   -3.945658   2.891856  -0.514122
H   -3.945658  -2.891856  -0.514122
H   -1.783103  -4.443885  -0.481062
H    1.783103  -4.443885  -0.481062
H    3.945658  -2.891856  -0.514122
H    3.945658   2.891856  -0.514122
H    1.783103   4.443885  -0.481062
Ni   0.000000   0.000000   0.569127
H    4.241224   0.000000  -0.248345
H   -4.241224   0.000000  -0.248345
Bq  -1.783690   0.000000   0.278965
Bq  -1.604568   0.000000  -0.704861
Bq  -1.962813   0.000000   1.262792
Bq  -1.848211   2.227589   0.045725
Bq  -1.661347   1.997198  -0.909262
Bq  -2.035076   2.457980   1.000713
Bq   0.000000   1.559649   0.345700
Bq   0.000000   1.398163  -0.641175
Bq   0.000000   1.721134   1.332576
```

UB3LYP-D3(BJ)/def2-TZVP total energy E, $\langle S^2 \rangle$ expectation value, imaginary vibrational frequency v and optimized geometry of the T_1 state of NiNc, planar TS of D_{2h} symmetry.

E = –2419.765545 Ha; $\langle S^2 \rangle$ = 2.0082; v = 44.5i cm^{-1} (B_{3u}).

```
N   0.000000   1.318402   1.204796
N   0.000000  -1.318402   1.204796
N   0.000000  -1.318402  -1.204796
N   0.000000   1.318402  -1.204796
C   0.000000   2.592686   0.722096
C   0.000000   3.452301   1.877441
C   0.000000   2.642450   2.995264
C   0.000000   1.255114   2.548359
C   0.000000   0.000000   3.216379
C   0.000000  -1.255114   2.548359
C   0.000000  -2.642450   2.995264
C   0.000000  -3.452301   1.877441
C   0.000000  -2.592686   0.722096
C   0.000000  -2.592686  -0.722096
C   0.000000  -3.452301  -1.877441
C   0.000000  -2.642450  -2.995264
C   0.000000  -1.255114  -2.548359
C   0.000000   0.000000  -3.216379
C   0.000000   1.255114  -2.548359
C   0.000000   2.642450  -2.995264
C   0.000000   3.452301  -1.877441
C   0.000000   2.592686  -0.722096
H   0.000000   4.530028   1.871529
H   0.000000   2.973337   4.021618
```

```
H   0.000000  -2.973337   4.021618
H   0.000000  -4.530028   1.871529
H   0.000000  -4.530028  -1.871529
H   0.000000  -2.973337  -4.021618
H   0.000000   2.973337  -4.021618
H   0.000000   4.530028  -1.871529
Ni  0.000000   0.000000   0.000000
H   0.000000  -0.000000  -4.297776
H   0.000000  -0.000000   4.297776
```

TDA-B3LYP-D3(BJ)/def2-TZVP total energy *E*, lowest vibrational frequency *v* and optimized geometry of the T_1 state of NiNc, bowl-shaped local minimum of C_{2v} symmetry.

E = –2419.769026 Ha; *v* = 60.4 cm^{-1} (A_1).

```
N    1.327376   1.219130   0.307388
N   -1.327376   1.219130   0.307388
N   -1.327376  -1.219130   0.307388
N    1.327376  -1.219130   0.307388
C    2.571529   0.717150   0.053978
C    3.396996   1.826857  -0.336619
C    2.593254   2.945546  -0.353282
C    1.247909   2.534691   0.013223
C    0.000000   3.195618  -0.080998
C   -1.247909   2.534691   0.013223
C   -2.593254   2.945546  -0.353282
C   -3.396996   1.826857  -0.336619
C   -2.571529   0.717150   0.053978
C   -2.571529  -0.717150   0.053978
C   -3.396996  -1.826857  -0.336619
C   -2.593254  -2.945546  -0.353282
C   -1.247909  -2.534691   0.013223
C   -0.000000  -3.195618  -0.080998
C    1.247909  -2.534691   0.013223
C    2.593254  -2.945546  -0.353282
C    3.396996  -1.826857  -0.336619
C    2.571529  -0.717150   0.053978
H    4.443710   1.783986  -0.589621
H    2.891513   3.946377  -0.622036
H   -2.891513   3.946377  -0.622036
H   -4.443710   1.783986  -0.589621
H   -4.443710  -1.783986  -0.589621
H   -2.891513  -3.946377  -0.622036
H    2.891513  -3.946377  -0.622036
H    4.443710  -1.783986  -0.589621
Ni   0.000000   0.000000   0.459641
H    0.000000  -4.241213  -0.356710
H    0.000000   4.241213  -0.356710
```

TDA-B3LYP-D3(BJ)/def2-TZVP total energy *E*, imaginary vibrational frequency *v* and optimized geometry of the T_1 state of NiNc, planar TS of D_{2h} symmetry.

E = –2419.766861 Ha; *v* = 44.5*i* cm^{-1} (B_{3u}).

```
N   0.000000   1.318491   1.204866
N   0.000000  -1.318491   1.204866
N   0.000000  -1.318491  -1.204866
```

```
N   0.000000   1.318491  -1.204866
C   0.000000   2.592344   0.722541
C   0.000000   3.452002   1.878122
C   0.000000   2.641960   2.995758
C   0.000000   1.254942   2.548843
C   0.000000   0.000000   3.216337
C   0.000000  -1.254942   2.548843
C   0.000000  -2.641960   2.995758
C   0.000000  -3.452002   1.878122
C   0.000000  -2.592344   0.722541
C   0.000000  -2.592344  -0.722541
C   0.000000  -3.452002  -1.878122
C   0.000000  -2.641960  -2.995758
C   0.000000  -1.254942  -2.548843
C   0.000000   0.000000  -3.216337
C   0.000000   1.254942  -2.548843
C   0.000000   2.641960  -2.995758
C   0.000000   3.452002  -1.878122
C   0.000000   2.592344  -0.722541
H   0.000000   4.529719   1.872328
H   0.000000   2.972776   4.022135
H   0.000000  -2.972776   4.022135
H   0.000000  -4.529719   1.872328
H   0.000000  -4.529719  -1.872328
H   0.000000  -2.972776  -4.022135
H   0.000000   2.972776  -4.022135
H   0.000000   4.529719  -1.872328
Ni  0.000000   0.000000   0.000000
H   0.000000  -0.000000  -4.297628
H   0.000000  -0.000000   4.297628
```

TDA-B3LYP-D3(BJ)/def2-TZVP total energy E, lowest vibrational frequency ν and optimized geometry of the S_1 state of NiNc, bowl-shaped local minimum of C_{2v} symmetry.

E = –2419.756198 Ha; ν = 64.0 cm^{-1} (A_1).

```
N    1.328231   1.220775   0.327247
N   -1.328231   1.220775   0.327247
N   -1.328231  -1.220775   0.327247
N    1.328231  -1.220775   0.327247
C    2.566108   0.712478   0.058457
C    3.389384   1.820789  -0.356385
C    2.587055   2.938884  -0.376055
C    1.248678   2.533888   0.013112
C    0.000000   3.193762  -0.088061
C   -1.248678   2.533888   0.013112
C   -2.587055   2.938884  -0.376055
C   -3.389384   1.820789  -0.356385
C   -2.566108   0.712478   0.058457
C   -2.566108  -0.712478   0.058457
C   -3.389384  -1.820789  -0.356385
C   -2.587055  -2.938884  -0.376055
C   -1.248678  -2.533888   0.013112
C   -0.000000  -3.193762  -0.088061
C    1.248678  -2.533888   0.013112
C    2.587055  -2.938884  -0.376055
C    3.389384  -1.820789  -0.356385
C    2.566108  -0.712478   0.058457
```

```
H    4.432304   1.773013  -0.624089
H    2.882163   3.936130  -0.661197
H   -2.882163   3.936130  -0.661197
H   -4.432304   1.773013  -0.624089
H   -4.432304  -1.773013  -0.624089
H   -2.882163  -3.936130  -0.661197
H    2.882163  -3.936130  -0.661197
H    4.432304  -1.773013  -0.624089
Ni   0.000000   0.000000   0.487769
H    0.000000  -4.234815  -0.380832
H    0.000000   4.234815  -0.380832
```

TDAB3LYP-D3(BJ)/def2-TZVP total energy *E*, imaginary vibrational frequency *v* and optimized geometry of the S_1 state of NiNc, planar TS of D_{2h} symmetry.

E = –2419.766861 Ha; *v* = 47.4*i* cm^{-1} (B_{3u}).

```
N   0.000000   1.318154   1.204446
N   0.000000  -1.318154   1.204446
N   0.000000  -1.318154  -1.204446
N   0.000000   1.318154  -1.204446
C   0.000000   2.589692   0.718236
C   0.000000   3.451156   1.878953
C   0.000000   2.642114   2.995971
C   0.000000   1.256715   2.549829
C   0.000000   0.000000   3.217392
C   0.000000  -1.256715   2.549829
C   0.000000  -2.642114   2.995971
C   0.000000  -3.451156   1.878953
C   0.000000  -2.589692   0.718236
C   0.000000  -2.589692  -0.718236
C   0.000000  -3.451156  -1.878953
C   0.000000  -2.642114  -2.995971
C   0.000000  -1.256715  -2.549829
C   0.000000   0.000000  -3.217392
C   0.000000   1.256715  -2.549829
C   0.000000   2.642114  -2.995971
C   0.000000   3.451156  -1.878953
C   0.000000   2.589692  -0.718236
H   0.000000   4.528972   1.873171
H   0.000000   2.973747   4.022102
H   0.000000  -2.973747   4.022102
H   0.000000  -4.528972   1.873171
H   0.000000  -4.528972  -1.873171
H   0.000000  -2.973747  -4.022102
H   0.000000   2.973747  -4.022102
H   0.000000   4.528972  -1.873171
Ni  0.000000   0.000000   0.000000
H   0.000000  -0.000000  -4.298777
H   0.000000  -0.000000   4.298777
```

UB3LYP-D3(BJ)/def2-TZVP total energy *E*, $\langle S^2 \rangle$ expectation value, lowest vibrational frequency *v* and optimized geometry of the T_1 state of H_2Nc, bowl-shaped local minimum of C_2 symmetry.

E = –912.467305 Ha; $\langle S^2 \rangle$ = 2.0053; *v* = 80.9 cm^{-1} (A).

```
N    1.213975   1.263100   0.579918
N   -1.335866   1.316304   0.621991
N   -1.213975  -1.263100   0.579918
N    1.335866  -1.316304   0.621991
C    2.419105   0.741377   0.258109
C    3.265849   1.783777  -0.281660
C    2.501653   2.917790  -0.321734
C    1.179294   2.554943   0.178639
C   -0.047179   3.252014   0.052003
C   -1.290748   2.599235   0.180095
C   -2.607051   2.868297  -0.336520
C   -3.328331   1.688949  -0.294357
C   -2.483420   0.678984   0.263046
C   -2.419105  -0.741377   0.258109
C   -3.265849  -1.783777  -0.281660
C   -2.501653  -2.917790  -0.321734
C   -1.179294  -2.554943   0.178639
C    0.047179  -3.252014   0.052003
C    1.290748  -2.599235   0.180095
C    2.607051  -2.868297  -0.336520
C    3.328331  -1.688949  -0.294357
C    2.483420  -0.678984   0.263046
H    4.284026   1.671685  -0.618411
H    2.793785   3.885783  -0.698172
H   -2.938706   3.810673  -0.740808
H   -4.330869   1.536120  -0.657928
H   -4.284026  -1.671685  -0.618411
H   -2.793785  -3.885783  -0.698172
H    2.938706  -3.810673  -0.740808
H    4.330869  -1.536120  -0.657928
H    0.033983  -4.262774  -0.331164
H   -0.033983   4.262774  -0.331164
H    0.445534  -0.857975   0.835538
H   -0.445534   0.857975   0.835538
Bq   2.115975   1.852197   0.082654
Bq   1.806861   1.603621  -0.835310
Bq   2.425089   2.100773   1.000619
Bq   1.242061   0.001531   0.565690
Bq   1.022487  -0.045432  -0.408775
Bq   1.461635   0.048495   1.540155
Bq   2.209083  -1.830354   0.086851
Bq   1.861888  -1.578476  -0.816483
Bq   2.556279  -2.082232   0.990185
Bq   0.121010  -1.973928   0.408031
Bq   0.138869  -1.667275  -0.543623
Bq   0.103150  -2.280582   1.359684
```

UB3LYP-D3(BJ)/def2-TZVP total energy E, $\langle S^2 \rangle$ expectation value, imaginary vibrational frequency ν and optimized geometry of the T_1 state of H_2Nc, TS of C_i symmetry.

E = –912.462284 Ha; $\langle S^2 \rangle$ = 2.0058; ν = 48.0i cm^{-1} (A_u).

```
N   0.003648   1.187209   1.211260
N   0.285122  -1.294875   1.263554
N  -0.003648  -1.187209  -1.211260
N  -0.285122   1.294875  -1.263554
C  -0.051397   2.450019   0.741208
C  -0.041901   3.360216   1.867267
```

```
C   0.000529   2.582862   2.997551
C   0.034213   1.188785   2.559525
C   0.076670  -0.039756   3.274286
C   0.135417  -1.287309   2.605361
C  -0.034532  -2.677740   2.955819
C  -0.038262  -3.418580   1.783995
C   0.130409  -2.510685   0.687734
C   0.051397  -2.450019  -0.741208
C   0.041901  -3.360216  -1.867267
C  -0.000529  -2.582862  -2.997551
C  -0.034213  -1.188785  -2.559525
C  -0.076670   0.039756  -3.274286
C  -0.135417   1.287309  -2.605361
C   0.034532   2.677740  -2.955819
C   0.038262   3.418580  -1.783995
C  -0.130409   2.510685  -0.687734
H  -0.084197   4.436905   1.825075
H   0.008984   2.931589   4.018694
H  -0.169088  -3.062461   3.953589
H  -0.175934  -4.484097   1.704111
H   0.084197  -4.436905  -1.825075
H  -0.008984  -2.931589  -4.018694
H   0.169088   3.062461  -3.953589
H   0.175934   4.484097  -1.704111
H  -0.023488   0.025491  -4.353693
H   0.023488  -0.025491   4.353693
H  -0.312598   0.395511  -0.775706
H   0.312598  -0.395511   0.775706
```

TDA-B3LYP-D3(BJ)/def2-TZVP total energy E, lowest vibrational frequency v and optimized geometry of the T_1 state of H_2Nc, bowl-shaped local minimum of C_2 symmetry.

E = –912.468873 Ha; v = 81.0 cm^{-1} (A).

```
N  -1.236630   1.241170  -0.521509
N   1.312357   1.339751  -0.561370
N   1.236630  -1.241170  -0.521509
N  -1.312357  -1.339751  -0.561370
C  -2.430704   0.699240  -0.198618
C  -3.297033   1.728262   0.339849
C  -2.554054   2.875083   0.378158
C  -1.223970   2.535263  -0.120887
C  -0.012487   3.252625   0.006588
C   1.244559   2.621008  -0.119539
C   2.554054   2.913501   0.398136
C   3.297343   1.746538   0.355422
C   2.472018   0.722891  -0.203263
C   2.430704  -0.699240  -0.198618
C   3.297033  -1.728262   0.339849
C   2.554054  -2.875083   0.378158
C   1.223970  -2.535263  -0.120887
C   0.012487  -3.252625   0.006588
C  -1.244559  -2.621008  -0.119539
C  -2.554054  -2.913501   0.398136
C  -3.297343  -1.746538   0.355422
C  -2.472018  -0.722891  -0.203263
H  -4.313033   1.597984   0.676634
H  -2.863476   3.838298   0.753028
```

```
H   2.868344   3.861245   0.803665
H   4.302305   1.612065   0.719550
H   4.313033  -1.597984   0.676634
H   2.863476  -3.838298   0.753028
H  -2.868344  -3.861245   0.803665
H  -4.302305  -1.612065   0.719550
H   0.043524  -4.263271   0.388657
H  -0.043524   4.263271   0.388657
H  -0.431226  -0.865355  -0.776461
H   0.431226   0.865355  -0.776461
```

TDA-B3LYP-D3(BJ)/def2-TZVP total energy *E*, imaginary vibrational frequency *v* and optimized geometry of the T_1 state of H_2Nc, TS of C_i symmetry.

E = –912.463883 Ha; *v* = 47.7*i* cm^{-1} (A_u).

```
N   0.007408   1.187788   1.210812
N   0.284361  -1.295178   1.263524
N  -0.007408  -1.187788  -1.210812
N  -0.284361   1.295178  -1.263524
C  -0.050027   2.449297   0.741893
C  -0.043198   3.359976   1.869213
C  -0.000352   2.582983   2.998682
C   0.036119   1.188253   2.560547
C   0.078491  -0.038105   3.274214
C   0.135388  -1.287434   2.605098
C  -0.035164  -2.676492   2.956168
C  -0.039259  -3.418402   1.783886
C   0.129748  -2.511567   0.688143
C   0.050027  -2.449297  -0.741893
C   0.043198  -3.359976  -1.869213
C   0.000352  -2.582983  -2.998682
C  -0.036119  -1.188253  -2.560547
C  -0.078491   0.038105  -3.274214
C  -0.135388   1.287434  -2.605098
C   0.035164   2.676492  -2.956168
C   0.039259   3.418402  -1.783886
C  -0.129748   2.511567  -0.688143
H  -0.087547   4.436579   1.826922
H   0.006279   2.931386   4.019944
H  -0.169691  -3.060873   3.954051
H  -0.177617  -4.483879   1.704762
H   0.087547  -4.436579  -1.826922
H  -0.006279  -2.931386  -4.019944
H   0.169691   3.060873  -3.954051
H   0.177617   4.483879  -1.704762
H  -0.026954   0.023898  -4.353571
H   0.026954  -0.023898   4.353571
H  -0.313499   0.396446  -0.775129
H   0.313499  -0.396446   0.775129
```

TDA-B3LYP-D3(BJ)/def2-TZVP total energy *E*, lowest vibrational frequency *v* and optimized geometry of the S_1 state of H_2Nc, bowl-shaped local minimum of C_2 symmetry.

E = – 912.457951 Ha; *v* = 85.5 cm^{-1} (A).

```
N  -1.246011   1.256065  -0.562942
```

```
N   1.315694   1.348056  -0.625646
N   1.246011  -1.256065  -0.562942
N  -1.315694  -1.348056  -0.625646
C  -2.439514   0.684711  -0.213395
C  -3.286906   1.691528   0.386972
C  -2.542644   2.837504   0.444495
C  -1.232198   2.516978  -0.113101
C  -0.000184   3.247011   0.013429
C   1.232198   2.620431  -0.138384
C   2.547569   2.902652   0.404681
C   3.280771   1.744971   0.364044
C   2.458510   0.717264  -0.226852
C   2.439514  -0.684711  -0.213395
C   3.286906  -1.691528   0.386972
C   2.542644  -2.837504   0.444495
C   1.232198  -2.516978  -0.113101
C   0.000184  -3.247011   0.013429
C  -1.232198  -2.620431  -0.138384
C  -2.547569  -2.902652   0.404681
C  -3.280771  -1.744971   0.364044
C  -2.458510  -0.717264  -0.226852
H  -4.291042   1.547371   0.752549
H  -2.837443   3.784686   0.868468
H   2.853891   3.844933   0.829310
H   4.276660   1.599425   0.748909
H   4.291042  -1.547371   0.752549
H   2.837443  -3.784686   0.868468
H  -2.853891  -3.844933   0.829310
H  -4.276660  -1.599425   0.748909
H   0.028681  -4.243283   0.430979
H  -0.028681   4.243283   0.430979
H  -0.436326  -0.874213  -0.841434
H   0.436326   0.874213  -0.841434
```

TDAB3LYP-D3(BJ)/def2-TZVP total energy E, imaginary vibrational frequency v and optimized geometry of the S_1 state of NiNc, TS of C_i symmetry.

E = –912.450687 Ha; v = 47.1i cm^{-1} (A_u).

```
N  -0.059699   1.181339   1.217849
N   0.351303  -1.290515   1.261968
N   0.059699  -1.181339  -1.217849
N  -0.351303   1.290515  -1.261968
C  -0.087785   2.454012   0.733594
C  -0.030038   3.362087   1.855436
C   0.018380   2.584199   2.989275
C   0.009456   1.195164   2.552534
C   0.053980  -0.057022   3.274590
C   0.153450  -1.279588   2.606611
C  -0.032581  -2.679386   2.948738
C  -0.023599  -3.412227   1.785278
C   0.171919  -2.497507   0.678807
C   0.087785  -2.454012  -0.733594
C   0.030038  -3.362087  -1.855436
C  -0.018380  -2.584199  -2.989275
C  -0.009456  -1.195164  -2.552534
C  -0.053980   0.057022  -3.274590
C  -0.153450   1.279588  -2.606611
```

```
C   0.032581   2.679386  -2.948738
C   0.023599   3.412227  -1.785278
C  -0.171919   2.497507  -0.678807
H  -0.043577   4.439685   1.813971
H   0.062327   2.935440   4.008585
H  -0.192416  -3.063214   3.943384
H  -0.172071  -4.475925   1.698598
H   0.043577  -4.439685  -1.813971
H  -0.062327  -2.935440  -4.008585
H   0.192416   3.063214  -3.943384
H   0.172071   4.475925  -1.698598
H   0.036452   0.048371  -4.351459
H  -0.036452  -0.048371   4.351459
H  -0.356619   0.395340  -0.770690
H   0.356619  -0.395340   0.770690
```