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Supporting Information available for

Kinetically persistent isomer found for pentazole: Global potential energy surface survey

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Table of Contents

1. Theoretical methods

GRRM:[1-2] The stationary points of the parent N_5H potential energy surfaces were confirmed by using the ADDF algorithm[2], implemented in the GRRM program. ADDF can follow reaction pathways starting from local minima on the PES toward TSs structures and dissociation channels. Geometric structures with weakly interacting fragments were reoptimized using the ultrafine grid and tight convergence criterion.

GPESS:[3] The GPESS platform includes isomeric search[3a] and transition state search[3k]. The isomer search was based on the grid search program.[3a] The transition state search was divided into two types, one is the isomer's conversion and the other is the isomer's decomposition. For the interconversion TS search, the "QST2" algorithm was applied, which yet has a difficulty in placing atoms in the same atomic order between reactant and product (especially for molecules with many homo-atomic elements). This was treated in GPESS by automatic enumeration of all possible combinations. Besides, the decomposition TS search was considered directing to some relatively stable molecular fragments like N_2, CO_2 and NO.

The kinetic stability of molecular N_5H(**I**) reaction pathways were determined through a systematic and automated exploration of pre-reaction complexes, TSs and product structures, using GRRM and GPESS methods at the B3LYP[4]/6-31G(d) level. The connections of all TSs were checked by the intrinsic reaction coordinate (IRC) calculations (although GRRM can automatically determine similar connection). Then, for structural and energetic refinement, the composite CBS-QB3[5] method was applied, which uses the B3LYP/6-311G(2d,d,p) geometries and frequencies followed by a series of higher level single-point energy calculations. Note that for the kinetic stability of A1 and C1, the more cost composite methods G4[6] and W1BD[7] were applied. To obtain detailed Wiberg bond indices[8] information, we performed the natural bond orbital (NBO) analysis. In the current work, all electronic state calculations were carried out within the Gaussian 03[9] and 09[10] program packages.

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D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian 03, Revision D.02; Gaussian, Inc.: Wallingford, CT, 2004.

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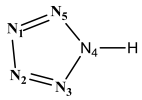
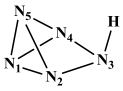
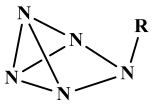
2. Table S1 The Wiberg bond index of the N_5H(A1,C1) at the B3LYP/6-311G(2d,d,p) level.

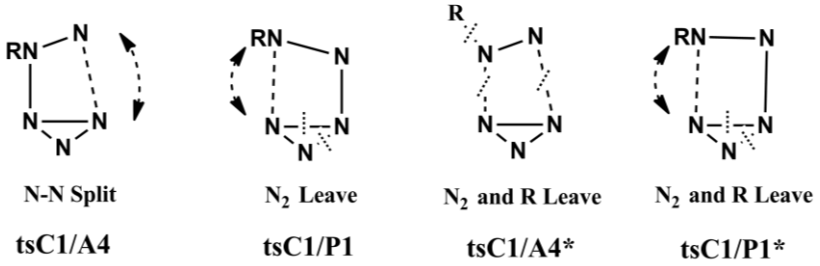
N_5H	Bond index	N_1-N_2	N_2-N_3	N_3-N_4	N_1-N_4	N_1-N_5	N_2-N_5	N_4-N_5
	Wiberg	1.347	1.573	1.286	0.000	1.573	0.000	1.286
	Wiberg	0.985	1.019	1.019	0.985	0.983	0.967	0.967

3. Table S2 The Substitution effect of C1.[a-- rate-determining barrier] The rate-determining barrier of substituted N_5R (C1) at the CBS-QB3 level with inclusion of ZPVE correction and EA (Electron Affinities) from references 1.

 3D-NNNNN-R	**tsC1/A4**	**tsC1/P1**	NPA (N_5)	Mulliken (N_5)	Hirshfield (N_5)	EA (R)
($R=NO_2$)	20.18[a]	20.71	0.341	0.265	0.162	52.41(52.42)[1]
(R=CN)		19.34 18.55[a]	0.216	0.140	0.191	90.05(89.06)[1]
（R=NCO）	21.95	17.86[a]	0.342	0.172	-0.116	83.27(83.22)[1]
($R=CF_3$)	17.66[a]	20.64	0.138	0.050	0.082	40.57(46.35)[1]
(R=F)	22.51	17.74[a]	0.232	0.072	0.224	77.93(78.43)[1]
(R=OH)	22.64	17.23[a]	0.408	0.220	0.107	40.74(42.15)[1]
($R=C_2H$)		16.85 16.63[a]	0.181	-0.024	-0.118	68.06(68.47)[1]
(R=H)	16.48[a]	18.89	0.000	0.000	0.000	12.42(17.39)[1]
(R=COOH)	17.84	15.52[a]	0.163	0.091	0.112	31.45
(R=NO)		15.46	0.343	0.236	0.156	0.24(0.60)[1]
($R=PH_2$)	12.69[a]	15.45	-0.115	-0.031	0.163	29.17(29.31)[1]
(R=SH)	17.58	12.61[a]	0.026	0.087	0.034	54.68(53.43)[1]
($R=C_6H_5$)	12.25[a]	15.83	0.154	0.004	0.058	- (25.27)[1]
(R=Cl)	21.14	15.49[a]	0.240	0.247	0.154	85.72(83.31)[1]
(R=Br)	19.68	14.50[a]	0.191	0.156	0.129	82.28(77.56)[1]
($R=CH_3$)	13.26[a]	18.60	0.121	0.011	0.023	0.24(1.84)[1]
($R=C_2H_3$)	12.37[a]	18.18	0.102	0.014	0.024	15.41(15.38)[1]
($R=NH_2$)	19.52	10.34[a]	0.232	0.072	0.020	16.32(17.78)[1]
($R=SiH_3$)		7.21[a]	-0.213	-0.147	-0.045	31.61(32.42)[1]

Note that for $R=NO_2$, the N-N cleavage (**tsC1/A4**) turns out to be the three-body fragmenation process, i.e., forming N_2, N_3 and R, and is re-named as **tsC1/A4***. For R=CN and $R=C_2H$, the N-N cleavage

(**tsC1/A4**) becomes the N_2-extrusion and is thus re-named as **tsC1/P1***.



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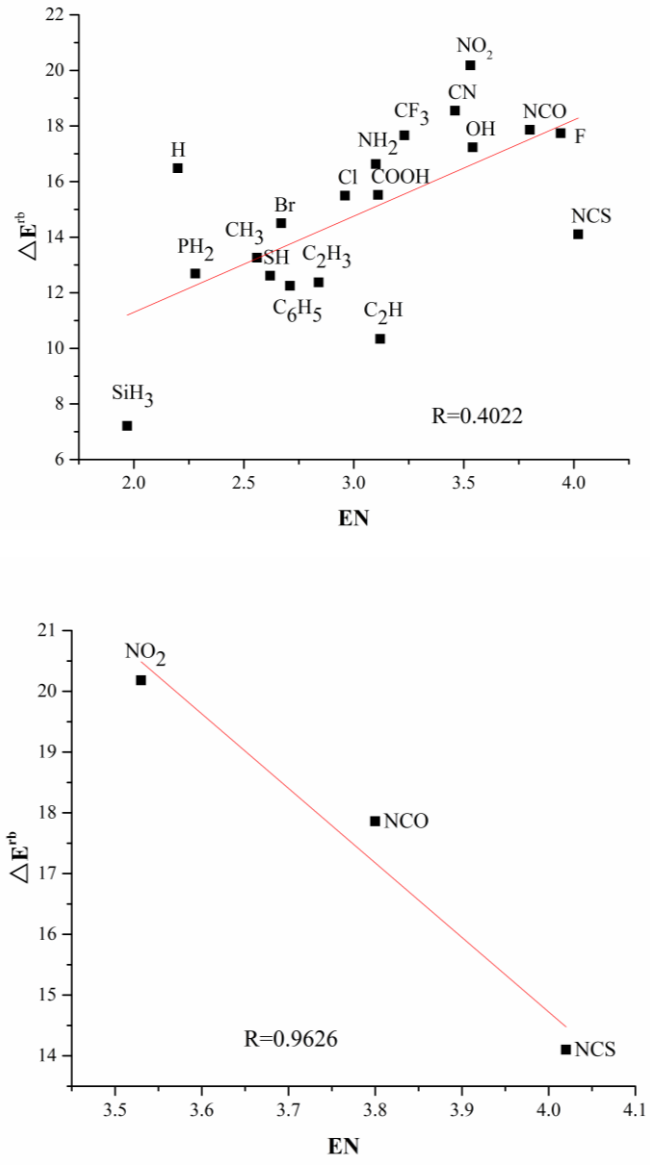
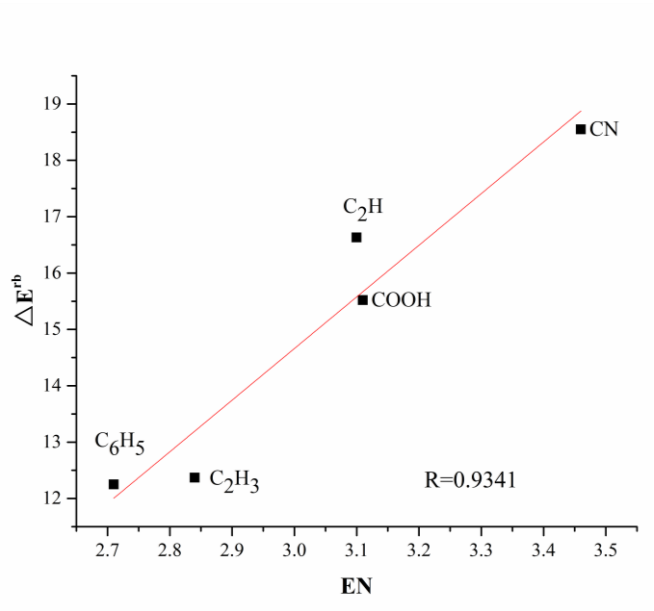
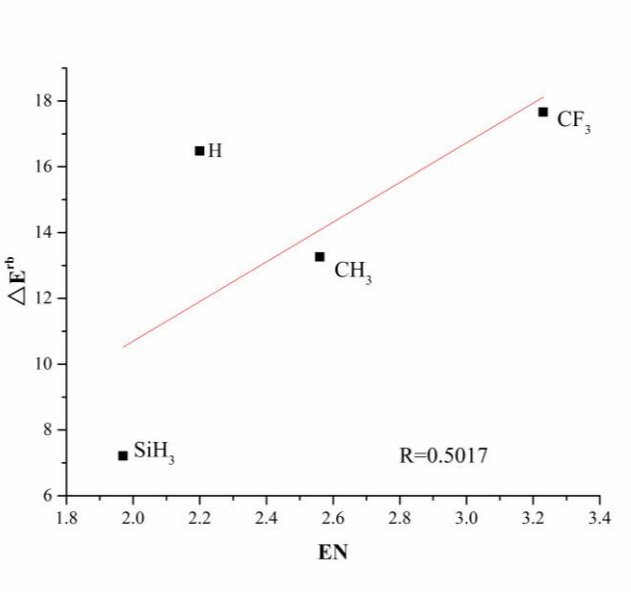
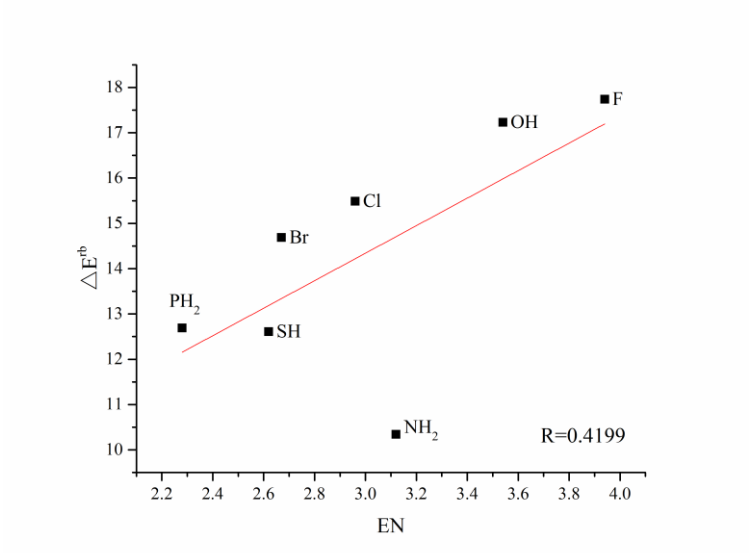
4. Fig. S1 The linear correlation coefficient R (ΔE^{rb} (the rate-determining barrier) vs EN (electronegativity))

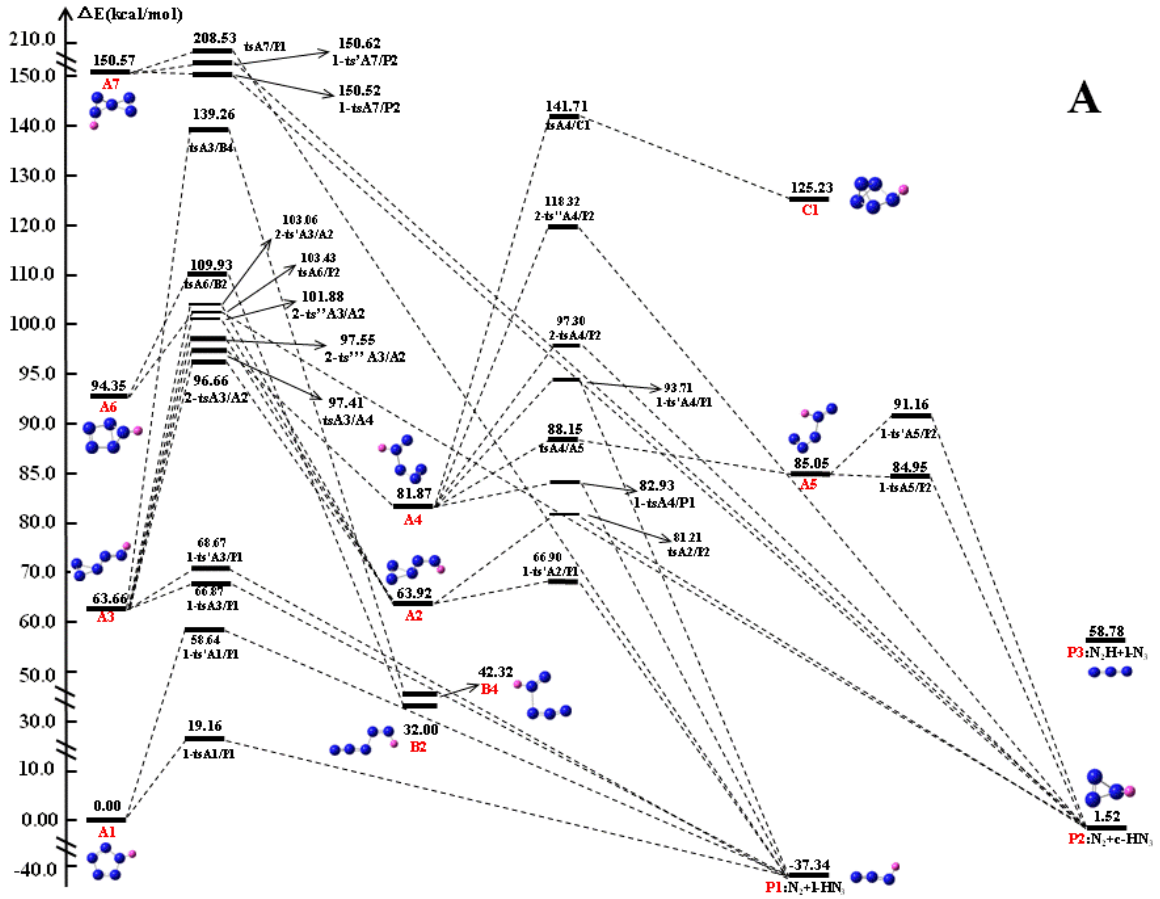


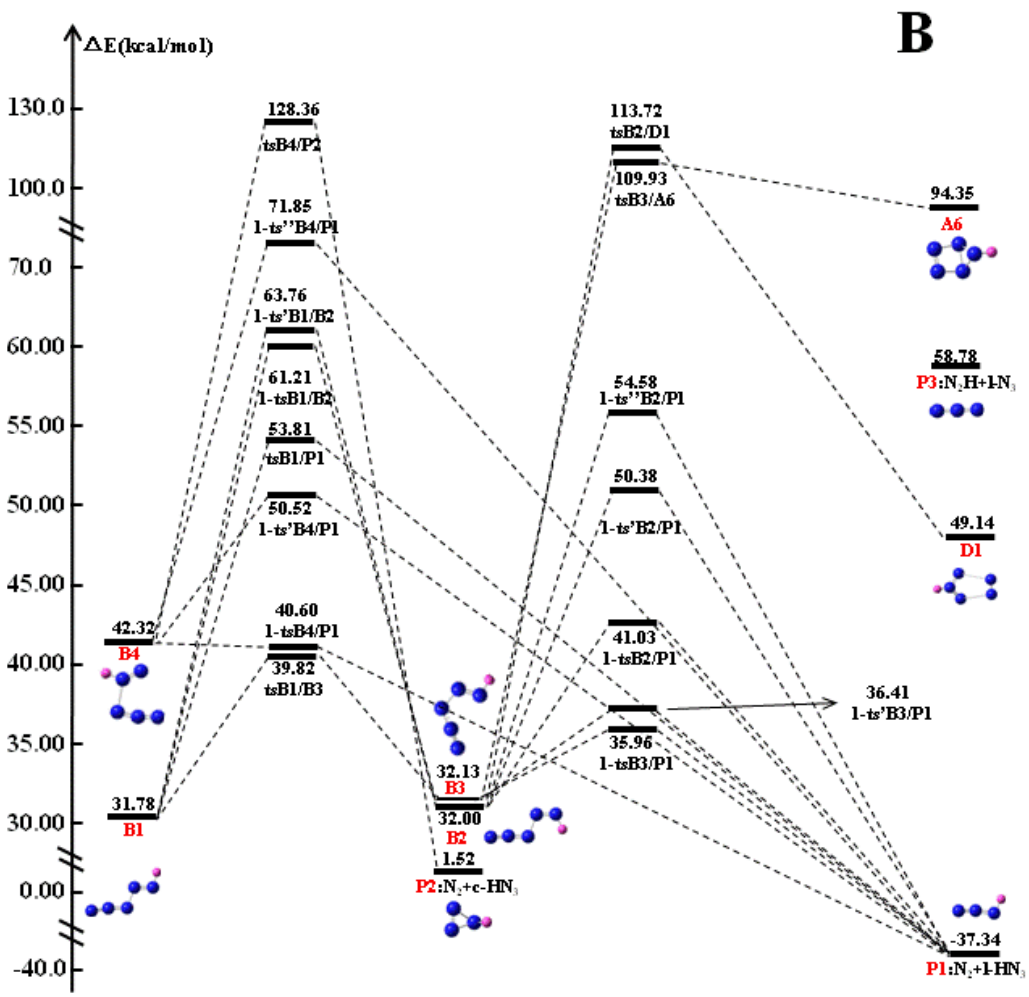

CN
C2H
COOH
C6H5
C2H3
R=0.9341
ΔErb
EN

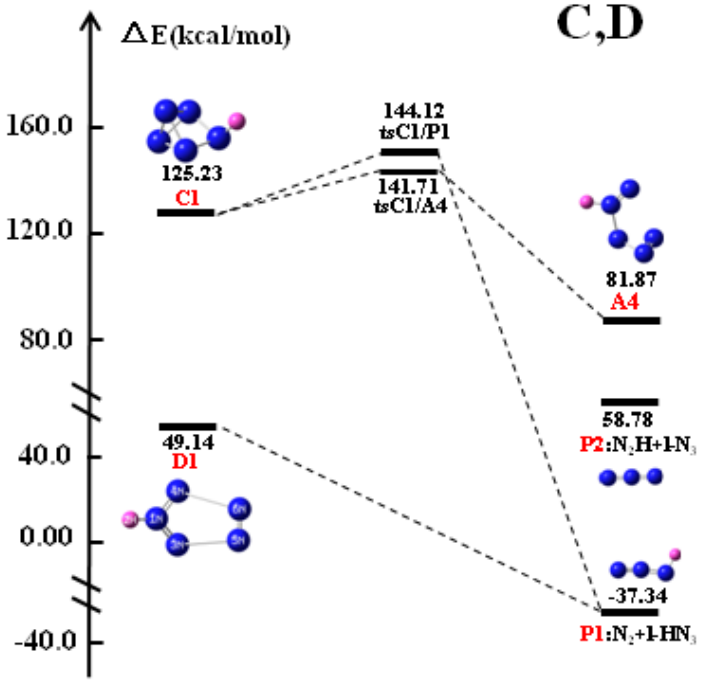

CF3
H
CH3
SiH3
R=0.5017
ΔErb
EN


F
OH
Cl
Br
PH2
SH
NH2
R=0.4199
ΔErb
EN

5. **Fig. S2 Isomerization and decomposition pathways of N_5H (A,B,C,D) in singlet state. Relative energies (kcal/mol) were obtained at CBS-QB3. The transition states for self-isomerization or interconversion between mirror isomers are not shown.**

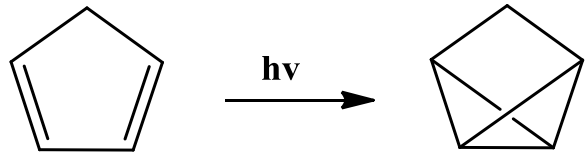



B
ΔE(kcal/mol)
130.0
100.0
70.0
60.00
55.00
50.00
45.00
40.00
35.00
30.00
0.00
-40.0
128.36
tsB4/P2
71.85
1-ts''B4/P1
63.76
1-ts'B1/B2
61.21
1-tsB1/B2
53.81
tsB1/P1
50.52
1-ts'B4/P1
40.60
1-tsB4/P1
39.82
tsB1/B3
42.32
B4
31.78
B1
32.13
B3
32.00
B2
1.52
P2:N2+c-HN3
113.72
tsB2/D1
109.93
tsB3/A6
54.58
1-ts''B2/P1
50.38
1-ts'B2/P1
41.03
1-tsB2/P1
36.41
1-ts'B3/P1
35.96
1-tsB3/P1
94.35
A6
58.78
P3:N2H+1-N3
49.14
D1
-37.34
P1:N2+1-HN3


C,D
ΔE(kcal/mol)
160.0
120.0
80.0
40.0
0.00
-40.0
125.23
C1
144.12
tsC1/P1
141.71
tsC1/A4
81.87
A4
49.14
D1
58.78
P2:N2H+1-N3
-37.34
P1:N2+1-HN3

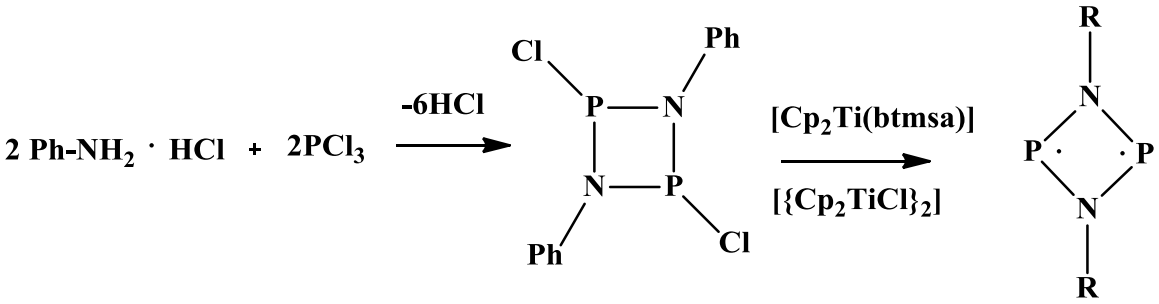
6. Fig. S3 Reference reactions for proposed synthetic routes of C1.

Route I :



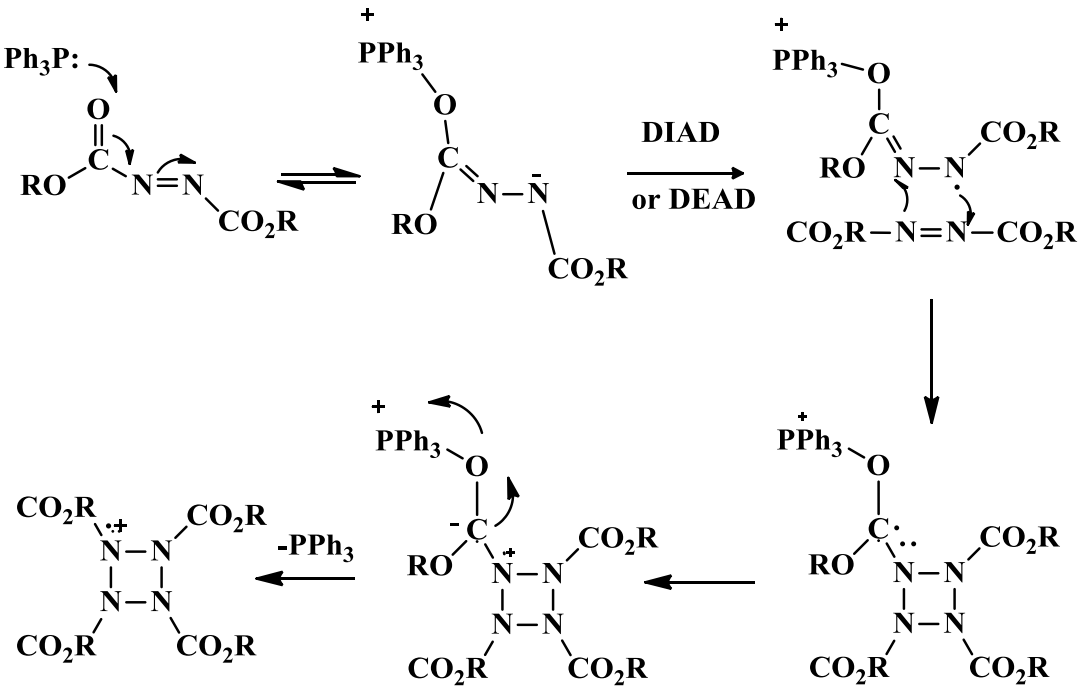
For details, see: G. D. Andrews, J. E. Baldwin, *J. Am. Chem. Soc.*, 1977, **99**, 4851.

Route II Path 1:



For details, see: A. Michaelis, G. Schroeter, *Ber. Dtsch. Chem. Ges*. 1894, **27**, 490.

Route II Path 2:



For details, see: D. Camp, M. Campitelli, G. R. Hanson and I. D. Jenkins, *J. Am. Chem. Soc.*, 2012, **134**,

16188.

7. Table S3 The half-life of C1 at different temperatures.

Isomers	$t_{1/2}^{298.15K}$(s)	$t_{1/2}^{250K}$(s)	$t_{1/2}^{200K}$(h)	$t_{1/2}^{150K}$(h)	$t_{1/2}^{100K}$(h)
C1	0.10	26.82	38.33	$5.24*10^{7}$	$7.81*10^{19}$
C1-R	24.34	21977.54	$2.19*10^{5}$	$7.39*10^{12}$	$6.24*10^{27}$

We computed the rate coefficient of **C1** and C1-NO_2 at the CBS-QB3 level at four temperatures (100, 150, 200., 250 and 298.15 K). To get the half-life values of **C1** and **C1**-NO_2 at different temperatures, we applied the conventional transition state theory (CTST), which was described below. QTS, QR are the partition functions of the transition state and the reactant, respectively. The other parameters are k_B for Boltzmann constant, h for Planck constant, T for temperature and R for universal gas constant.

$$k_{TST} = \frac{k_B T}{h}\frac{Q_{TS}}{Q_R}\exp\left[\frac{-(E_{TS}-E_R)}{RT}\right]$$

8. Fig. S4 Born-Oppenheimer molecular dynamics simulation performed at different temperatures.

We carried out the Born-Oppenheimer molecular dynamics (BOMD) simulations at 500, 1000 and 2000 K for the parent N_5H-**C1**. The structural evolution during the simulations was evaluated by the potential energy (PE, in hartree) of **C1** with respect to that for B3LYP/6-31G(d) optimized structures. The PE curves of **C1** at three temperatures are shown in Fig. S4. For 500 and 1000 K，the PE values have no sharp decrease during the 10 ps simulations, suggesting that the structure of **C1** is well maintained at these two temperatures. At 2000 K, the **C1** structure can be kept up to 4.5 ps. Afterwards, it undergoes an abrupt structural change to the weakly bound intermediate **A4** and then to the very stable fragments N_2+N_3H. Such an evolution trend is in good agreement with our PES study using GRRM and GPESS.

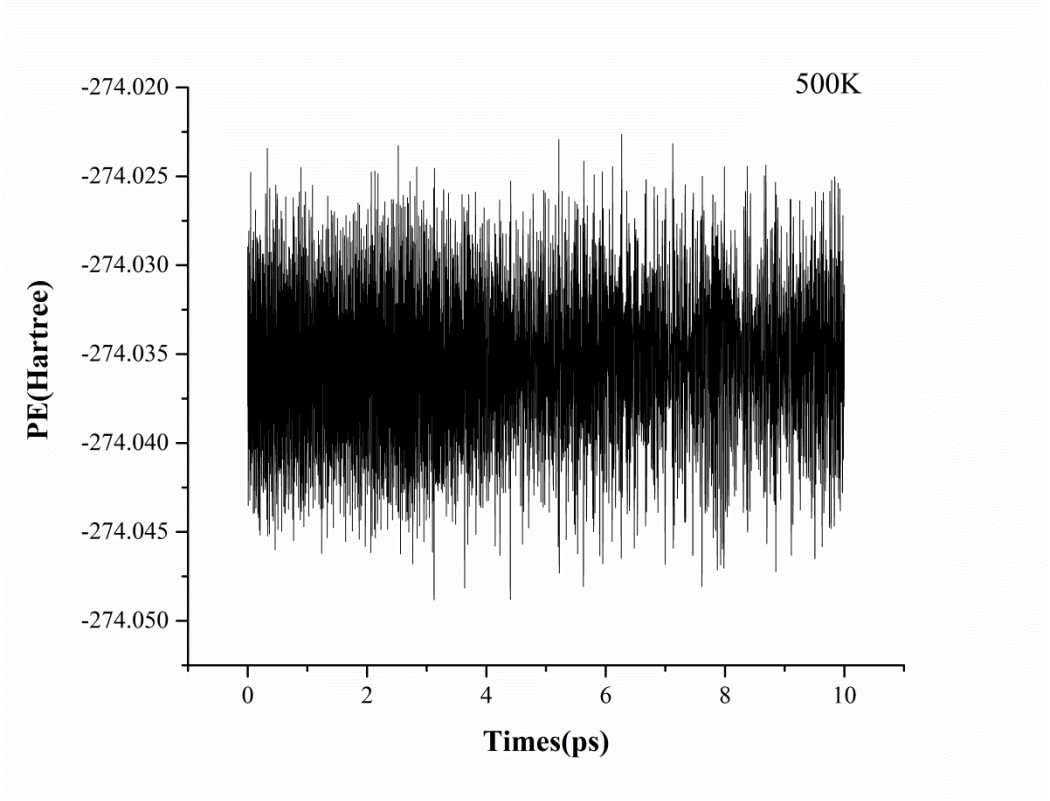


Fig. S4 a). Born-Oppenheimer molecular dynamics simulation at 500 K..

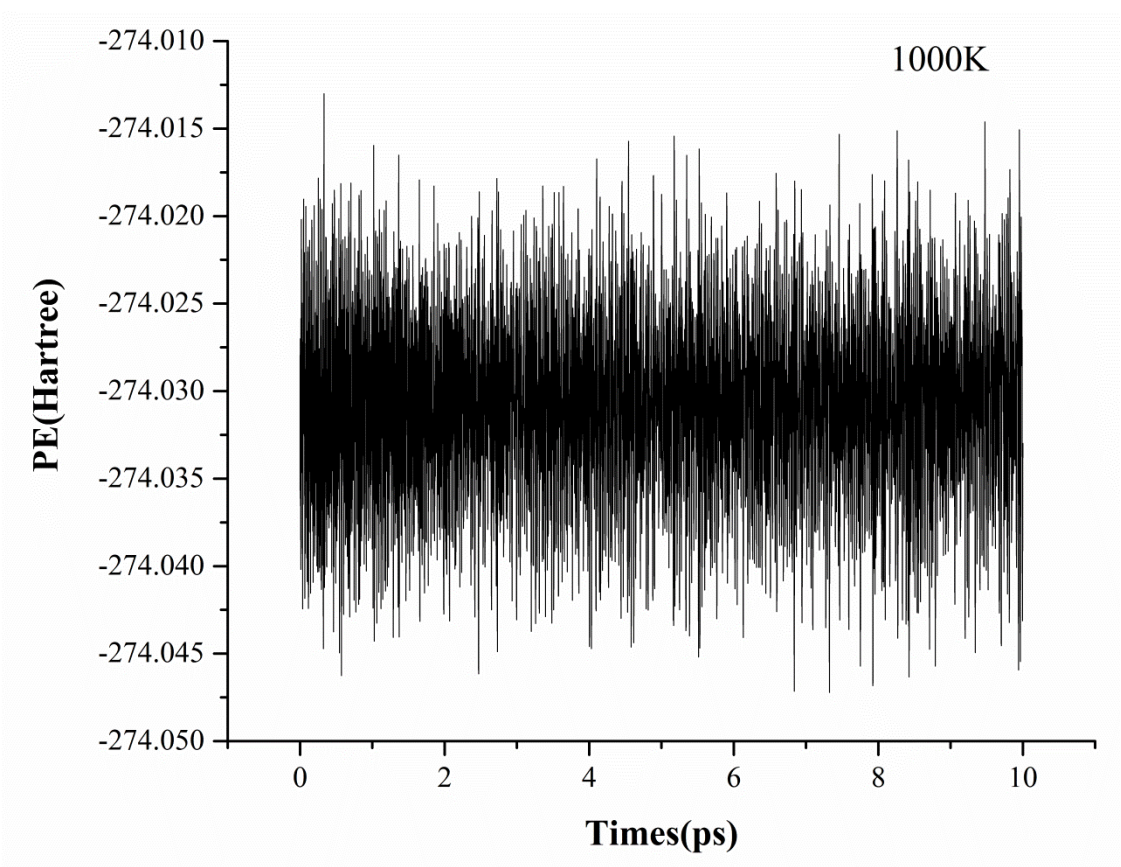


Fig. S4 b) Born-Oppenheimer molecular dynamics simulation at 1000 K.

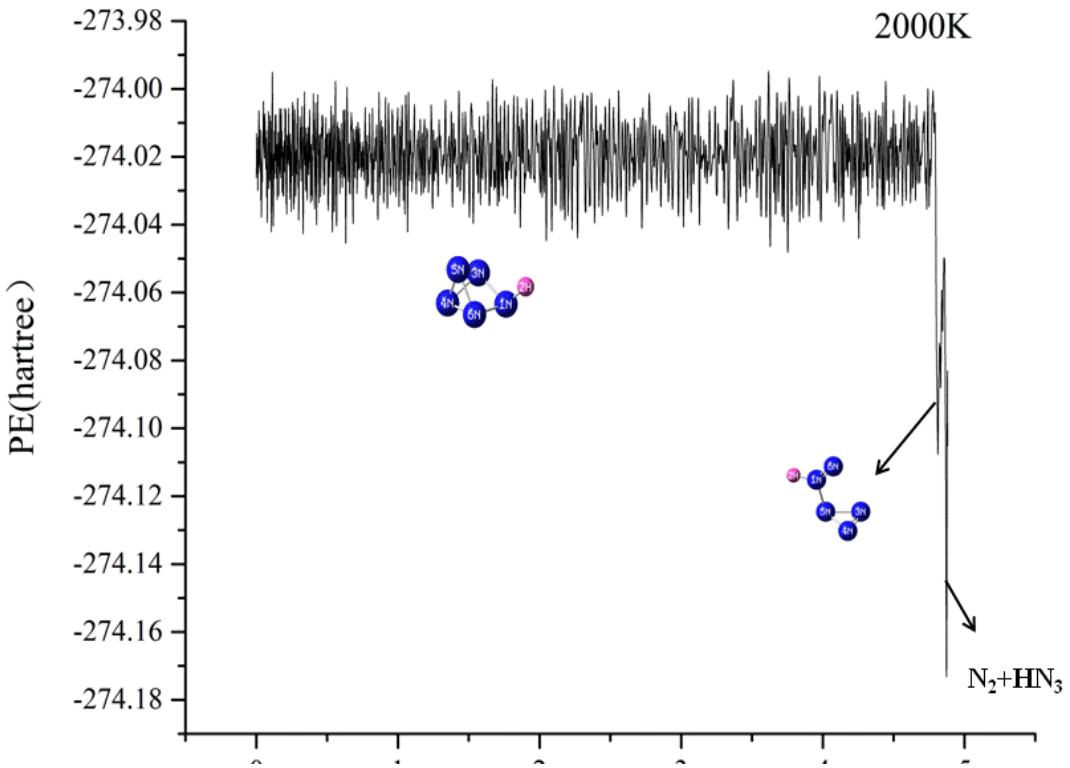


Fig. 4S c) Born-Oppenheimer molecular dynamics simulation performed at 1000 K.

9. Table S4 Cartesian coordinates of the optimized isomeric structures and Transitional structure.

"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm-1)"
"te_zpe"----"total energy with zero-point energy (a.u.)"
"te_gfe"----"total energy with Gibbs free energy (a.u.)"
"bh_zpe"----"barrier height with zero-point energy correction (kcal/mol)"
"bh_gfe"----"barrier height with Gibbs free energy correction (kcal/mol)"

##
A1 charge=0 spin=1 mol=H1N5 A1 CBS-QB3
lf=630.2 te_zpe=-274.294289 te_gfe=-274.320295 te_ms_zpe=-273.907132 te_ms_gfe=0.008477

7 1.018048 -0.000125 -0.000056
1 2.028893 -0.000255 0.000019

7 0.283513 -1.102422 -0.000161
7 -0.937690 -0.677457 0.000429
7 -0.937508 0.677685 -0.000821
7 0.283794 1.102356 0.000607

1-tsA1/P1 charge=0 spin=1 mol=H1N5 1-tsA1/P1 CBS-QB3
lf=-601.9 te_zpe=-274.269257 te_gfe=-274.295914 te_ms_zpe=-273.876595 te_ms_gfe=0.003345

7 -0.390956 1.043447 -0.102126
1 -0.676604 1.874432 0.412085
7 -1.130202 -0.027445 0.014507
7 -0.643487 -1.120368 0.009289
7 1.111936 -0.667302 0.002377
7 1.149367 0.503892 0.017083

1-ts'A1/P1 charge=0 spin=1 mol=H1N5 1-ts'A1/P1 CBS-QB3
lf=-676.9 te_zpe=-274.194141 te_gfe=-274.221303 te_ms_zpe=-273.813682 te_ms_gfe=-0.000933

7 -1.017358 0.060678 0.000063
1 -1.954512 0.602142 0.000108
7 -0.429805 1.211665 -0.000006
7 1.333077 0.448948 -0.000097
7 1.301871 -0.674034 -0.000064
7 -0.908568 -1.133278 0.000089

##
A2 charge=0 spin=1 mol=H1N5 A2 CBS-QB3
lf=140.1 te_zpe=-274.192494 te_gfe=-274.219843 te_ms_zpe=-273.805689 te_ms_gfe=0.001868

7 1.913092 -0.000017 0.158875
1 2.616140 0.000058 -0.590451
7 -0.196831 -0.000072 0.598917
7 -1.455504 -0.590113 -0.129103
7 -1.455502 0.590143 -0.128975
7 0.821010 0.000050 -0.415364

1-tsA2/A3 charge=0 spin=1 mol=H1N5 1-tsA2/A3 CBS-QB3
lf=-455.5 te_zpe=-274.135547 te_gfe=-274.163086 te_ms_zpe=-273.753090 te_ms_gfe=-0.001958

7 2.014749 -0.107765 -0.118537
1 2.537676 0.772857 -0.311159
7 -0.874455 -0.747043 -0.376550
7 -0.891702 0.794274 -0.300518
7 -1.594840 -0.015901 0.415738
7 0.983723 -0.033973 0.424318

1-ts'A2/A3 charge=0 spin=1 mol=H1N5 1-ts'A2/A3 CBS-QB3
lf=-360.6 te_zpe=-274.131675 te_gfe=-274.159519 te_ms_zpe=-273.751673 te_ms_gfe=-0.002328

1 2.518400 -0.807661 0.412351
7 1.021296 0.053895 -0.378253
7 2.014448 0.090601 0.236732
7 -1.275053 -0.081871 0.706724
7 -1.057224 0.784735 -0.232385
7 -1.063239 -0.731980 -0.391726

1-ts"A2/A3 charge=0 spin=1 mol=H1N5 1-ts"A2/A3 CBS-QB3
lf=-1327.2 te_zpe=-274.134467 te_gfe=-274.162453 te_ms_zpe=-273.744774 te_ms_gfe=-0.002666

7 1.950690 -0.000091 0.049350
1 2.862486 -0.000731 0.449128
7 -1.493948 0.594328 -0.115872
7 -0.277699 -0.000933 0.623154
7 -1.493907 -0.594003 -0.117680
7 0.905937 0.000803 -0.503112

1-ts"'A2/A3 charge=0 spin=1 mol=H1N5 1-ts"'A2/A3 CBS-QB3
lf=-330.0 te_zpe=-274.115098 te_gfe=-274.143453 te_ms_zpe=-273.742897 te_ms_gfe=-0.004257

1 -2.838891 -0.553036 0.701941
7 0.529443 -0.397244 0.008249
7 1.415847 0.639044 0.039793
7 -1.340925 0.442884 -0.004635
7 -2.291077 -0.214987 -0.118261
7 2.092268 -0.390693 -0.025423

1-tsA2/P1 charge=0 spin=1 mol=H1N5 1-tsA2/P1 CBS-QB3
lf=-463.6 te_zpe=-274.191902 te_gfe=-274.219122 te_ms_zpe=-273.800572 te_ms_gfe=0.000611

7 -1.966828 0.105773 -0.000002
1 -2.589350 -0.708196 0.000015
7 0.092320 0.640031 -0.000014
7 1.527823 -0.135957 -0.574620
7 1.527823 -0.135932 0.574626
7 -0.811231 -0.372745 0.000007

1-ts'A2/P1 charge=0 spin=1 mol=H1N5 1-ts'A2/P1 CBS-QB3
lf=-154.8 te_zpe=-274.184166 te_gfe=-274.210843 te_ms_zpe=-273.797698 te_ms_gfe=0.002589

7 1.651737 0.434425 -0.001493

1 2.530681 0.199885 -0.484778
7 -0.323082 -0.375226 0.594520
7 -1.445343 -0.322353 -0.386344
7 -1.157892 0.768326 0.030477
7 0.913054 -0.533726 -0.167905

tsA2/B4 charge=0 spin=1 mol=H1N5 tsA2/B4 CBS-QB3
lf=-1391.6 te_zpe=-274.075755 te_gfe=-274.103289 te_ms_zpe=-273.685214 te_ms_gfe=-0.000231

7 1.742272 0.441304 0.000019
1 2.687209 0.039767 0.000041
7 -0.348058 -0.097725 -0.000014
7 -1.380636 0.918531 -0.000011
7 -1.374415 -0.718125 -0.000014
7 0.976950 -0.549666 0.000014

##
A3 charge=0 spin=1 mol=H1N5 A3 CBS-QB3
lf=140.0 te_zpe=-274.193788 te_gfe=-274.221173 te_ms_zpe=-273.805269 te_ms_gfe=0.001334

7 1.964573 -0.016535 0.000003
1 1.921839 1.026402 -0.002883
7 -1.456111 -0.091852 -0.591070
7 -0.165015 0.551319 -0.001795
7 -1.455950 -0.088034 0.591704
7 0.837953 -0.501527 0.001571

1-tsA3/P1 charge=0 spin=1 mol=H1N5 1-tsA3/P1 CBS-QB3
lf=141.7 te_zpe=-274.193804 te_gfe=-274.221184 te_ms_zpe=-273.805294 te_ms_gfe=0.001325

7 -1.964594 -0.017349 0.000749
1 -1.922626 1.025365 -0.024378
7 1.456409 -0.074913 0.593482
7 0.163082 0.551857 -0.014087
7 1.456874 -0.104928 -0.588500
7 -0.837110 -0.501149 0.011838
1-ts'A3/P1 charge=0 spin=1 mol=H1N5 1-ts'A3/P1 CBS-QB3
lf=-457.9 te_zpe=-274.193205 te_gfe=-274.220507 te_ms_zpe=-273.800455 te_ms_gfe=-0.000102

7 -2.000752 -0.069368 0.000011
1 -2.037609 0.974186 -0.000074
7 1.532836 -0.088154 0.574573
7 0.046796 0.579522 -0.000057
7 1.532843 -0.088263 -0.574550
7 -0.820636 -0.472906 0.000034

tsA3/P2 charge=0 spin=1 mol=H1N5 tsA3/P2 CBS-QB3
lf=-399.8 te_zpe=-274.166503 te_gfe=-274.194892 te_ms_zpe=-273.777716 te_ms_gfe=-0.004025

7 -1.960151 -0.383565 -0.000151
1 -1.116117 -1.136223 -0.000160
7 1.654510 0.042830 -0.601729
7 0.306741 -0.213912 0.000106
7 1.654640 0.042696 0.601757
7 -1.496294 0.674268 0.000040

##
A4 charge=0 spin=1 mol=H1N5 A4 CBS-QB3
lf=71.0 te_zpe=-274.167867 te_gfe=-274.196121 te_ms_zpe=-273.776660 te_ms_gfe=-0.000493

7 1.128546 0.373829 0.012775
1 1.622049 1.286891 0.021912
7 -1.147740 -0.481451 -0.539212
7 -1.243577 -0.193324 0.622382
7 -0.500458 0.832900 -0.141412
7 1.531507 -0.715796 0.042337

1-tsA4/P1 charge=0 spin=1 mol=H1N5 1-ts-A4/P1 CBS-QB3
lf=-307.7 te_zpe=-274.160925 te_gfe=-274.187842 te_ms_zpe=-273.774982 te_ms_gfe=0.000430

7 1.237913 0.472749 0.049748
1 2.013620 1.151811 0.094861
7 -0.810241 -0.744238 -0.364093
7 -1.256005 0.002781 0.582392
7 -0.779143 0.787795 -0.342680
7 1.319816 -0.683631 0.061081

1-ts'A4/P1 charge=0 spin=1 mol=H1N5 1-ts'A4/P1 CBS-QB3
lf=-677.9 te_zpe=-274.152667 te_gfe=-274.180739 te_ms_zpe=-273.757789 te_ms_gfe=-0.002804

7 1.111546 0.279675 -0.000008
1 1.632407 1.223908 -0.000018
7 -1.377513 -0.296015 -0.567309
7 -1.377507 -0.296006 0.567327
7 -0.159454 0.941281 -0.000007
7 1.569727 -0.803778 0.000000

1-tsA4/P2 charge=0 spin=1 mol=H1N5 1-tsA4/P2 CBS-QB3
lf=-315.2 te_zpe=-274.143030 te_gfe=-274.172323 te_ms_zpe=-273.752076 te_ms_gfe=-0.006398

7 1.527912 -0.000123 0.171477
1 1.020102 -0.000568 1.135457
7 -1.827237 0.601550 -0.168609
7 -1.827261 -0.601406 -0.169006
7 -0.550614 -0.000120 0.342082
7 2.531472 0.000179 -0.338152

1-ts'A4/P2 charge=0 spin=1 mol=H1N5 1-tsA4/P2 CBS-QB3
lf=-197.6 te_zpe=-274.115440 te_gfe=-274.143792 te_ms_zpe=-273.718570 te_ms_gfe=-0.003324

7 -1.196274 0.076194 0.338697
1 -1.184648 0.277902 1.348297
7 1.062179 -0.916323 0.112286
7 -1.996037 -0.201673 -0.419216
7 1.677686 0.081385 -0.173474
7 0.621682 0.920718 -0.050907

tsA4/A5 charge=0 spin=1 mol=H1N5 tsA4/A5 CBS-QB3
lf=-175.7 te_zpe=-274.158265 te_gfe=-274.185611 te_ms_zpe=-273.766659 te_ms_gfe=-0.000515

7 1.073294 -0.363363 -0.094963
1 1.056310 -1.325875 -0.495653
7 -1.234078 0.747201 -0.085087
7 -1.482588 -0.390655 -0.371506
7 -0.423901 -0.237986 0.714342
7 1.916371 0.434213 -0.091979

tsA4/C1 charge=0 spin=1 mol=H1N5 tsA4/C1 CBS-QB3
lf=-589.2 te_zpe=-274.058018 te_gfe=-274.084176 te_ms_zpe=-273.681309 te_ms_gfe=0.002339

7 -1.061656 -0.335096 -0.001242
1 -1.622920 -0.841915 0.679816
7 0.208968 -0.852583 -0.362804
7 0.630925 0.560751 -0.521517
7 1.089607 -0.145666 0.615782
7 -0.635997 0.892868 0.172665

##
A5 charge=0 spin=1 mol=H1N5 A5 CBS-QB3
lf=99.4 te_zpe=-274.163395 te_gfe=-274.191695 te_ms_zpe=-273.771595 te_ms_gfe=-0.001483

7 1.019968 0.277289 0.073515
1 0.621473 1.220744 0.331541
7 -1.389515 -0.253917 0.593894
7 -1.450458 0.508654 -0.336582

7 -0.374330 -0.597267 -0.414902
7 2.105552 -0.109150 0.036712

1-tsA5/P2 charge=0 spin=1 mol=1-tsA5/P2 CBS-QB3
lf=-175.7 te_zpe=-274.158265 te_gfe=-274.185611 te_ms_zpe=-273.766659 te_ms_gfe=-0.000515

7 1.073294 -0.363363 -0.094963
1 1.056310 -1.325875 -0.495653
7 -1.234078 0.747201 -0.085087
7 -1.482588 -0.390655 -0.371506
7 -0.423901 -0.237986 0.714342
7 1.916371 0.434213 -0.091979

1-ts'A5/P2 charge=0 spin=1 mol=H1N5 1-tsA5/P2 CBS-QB3
lf=-554.1 te_zpe=-274.154981 te_gfe=-274.182939 te_ms_zpe=-273.761866 te_ms_gfe=-0.001717

7 0.977295 0.346387 0.000006
1 0.649422 1.341872 0.000020
7 -1.545645 0.107636 0.573915
7 -1.545652 0.107721 -0.573881
7 -0.060991 -0.671273 -0.000061
7 2.082218 -0.082167 0.000018

##
A6 charge=0 spin=1 mol=H1N5 A6 CBS-QB3
lf=485.2 te_zpe=-274.136303 te_gfe=-274.162424 te_ms_zpe=-273.756780 te_ms_gfe=0.005372

7 -1.106551 0.000013 -0.532756
1 -2.047765 0.000094 -0.121888
7 -0.327843 -0.747550 0.439395
7 1.027119 -0.620230 -0.164228
7 1.027281 0.619975 -0.164156
7 -0.327469 0.747779 0.439157

tsA6/B2 charge=0 spin=1 mol=H1N5 tsA6/B2 CBS-QB3
lf=-674.7 te_zpe=-274.122837 te_gfe=-274.149409 te_ms_zpe=-273.742309 te_ms_gfe=0.001450

7 1.082847 -0.000001 0.500737
1 2.099740 -0.000024 0.544818
7 0.489123 -0.804204 -0.415850
7 -1.180534 -0.587479 0.126563
7 -1.180544 0.587483 0.126570
7 0.489145 0.804205 -0.415852

tsA6/P2 charge=0 spin=1 mol=H1N5 tsA6/P2 CBS-QB3

lf=-598.5 te_zpe=-274.116562 te_gfe=-274.142836 te_ms_zpe=-273.731951 te_ms_gfe=0.002861

7 1.284058 -0.108737 -0.433209
1 2.030030 0.437085 0.023532
7 -0.088099 1.036350 0.190134
7 -1.155473 0.334591 -0.214975
7 -0.812617 -0.872316 -0.076136
7 0.482127 -0.452328 0.530825

##
A7 charge=0 spin=1 mol=H1N5 A7 CBS-QB3
lf=342.5 te_zpe=-274.054278 te_gfe=-274.081035 te_ms_zpe=-273.667184 te_ms_gfe=0.002209

7 -1.167340 -0.706700 -0.198819
1 -1.369718 -1.125568 0.719712
7 -0.041841 0.068304 0.004988
7 1.259156 0.036298 -0.622238
7 1.227084 -0.113958 0.633753
7 -1.081384 0.876851 0.079500

1-tsA7/B3 charge=0 spin=1 mol=H1N5 1-tsA7/B3 CBS-QB3
lf=-446.3 te_zpe=-274.053567 te_gfe=-274.080256 te_ms_zpe=-273.667258 te_ms_gfe=0.001647

7 -1.187390 -0.704704 -0.233145
1 -1.265480 -1.212045 0.658806
7 -0.069048 0.096362 -0.051004
7 1.211244 0.142473 -0.604101
7 1.321461 -0.215875 0.595967
7 -1.095484 0.854893 0.198167

1-ts'A7/B3 charge=0 spin=1 mol=H1N5 1-ts'A7/B3 CBS-QB3
lf=-444.7 te_zpe=-274.053967 te_gfe=-274.080663 te_ms_zpe=-273.667108 te_ms_gfe=0.001574

7 -1.168971 -0.734084 -0.159812
1 -1.474961 -1.039377 0.774904
7 -0.071500 0.080385 0.063567
7 1.340780 -0.063162 -0.611693
7 1.197675 -0.020056 0.634813
7 -1.087276 0.885400 -0.037575

tsA7/P1 charge=0 spin=1 mol=H1N5 tsA7/P1 CBS-QB3
lf=-516.9 te_zpe=-273.948815 te_gfe=-273.975511 te_ms_zpe=-273.574817 te_ms_gfe=-0.000491

1 1.452939 -0.140919 -1.128407
7 0.693659 0.541208 0.707719
7 -0.169593 -0.326981 -0.014624
7 -0.514184 0.875316 -0.499705
7 1.241253 -0.559823 -0.208550
7 -1.458697 -0.509589 0.176361

##
B1 charge=0 spin=1 mol=H1N5 B1 CBS-QB3
lf=154.3 te_zpe=-274.254708 te_gfe=-274.281973 te_ms_zpe=-273.856494 te_ms_gfe=0.004265

 7 -2.089099 0.106470 0.000075
 1 -2.746559 -0.682154 0.000238
 7 2.251738 -0.247768 0.000167
 7 1.169659 0.070541 -0.000069
 7 0.033126 0.590198 0.000044
 7 -0.973059 -0.421991 -0.000251

1-tsB1/B2 charge=0 spin=1 mol=H1N5 1-tsB1/B2 CBS-QB3
lf=-227.6 te_zpe=-274.207019 te_gfe=-274.234988 te_ms_zpe=-273.809585 te_ms_gfe=-0.000454

 7 1.956090 -0.072668 -0.223547
 1 2.507644 0.761274 -0.509458
 7 -1.136273 1.163322 -0.022025
 7 -1.189736 -0.010643 -0.068312
 7 -1.009627 -1.178134 -0.058386
 7 1.021311 -0.010631 0.445050

1-ts'B1/B2 charge=0 spin=1 mol=H1N5 1-ts'B1/B2 CBS-QB3
lf=-1042.5 te_zpe=-274.210801 te_gfe=-274.239138 te_ms_zpe=-273.805528 te_ms_gfe=-0.000818

 7 -2.159243 -0.038462 -0.000005
 1 -3.119791 0.244171 0.000026
 7 0.213455 0.781707 0.000000
 7 1.262080 0.166833 0.000001
 7 2.249294 -0.418468 0.000000
 7 -1.119901 -0.526491 0.000001

tsB1/B3 charge=0 spin=1 mol=H1N5 tsB1/B3 CBS-QB3
lf=-182.2 te_zpe=-274.241405 te_gfe=-274.268374 te_ms_zpe=-273.843670 te_ms_gfe=0.003816

 7 1.696132 -0.534975 -0.277743
 1 2.549682 -0.800604 0.237673
 7 -2.026743 -0.516057 0.091214
 7 -1.070797 0.079701 -0.048265
 7 -0.092893 0.808275 -0.237738
 7 1.130061 0.277428 0.438578

tsB1/P1 charge=0 spin=1 mol=H1N5 B1-ts-B1-P1 CBS-QB3
lf=-846.5 te_zpe=-274.225594 te_gfe=-274.252943 te_ms_zpe=-273.821376 te_ms_gfe=0.001237

7 2.224168 0.106205 0.000002
1 2.780645 -0.752836 0.000028
7 -2.406957 -0.032356 -0.000008
7 -1.305578 -0.196865 0.000003
7 0.066553 0.530569 -0.000013
7 1.024578 -0.300004 0.000012

##
B2 charge=0 spin=1 mol=H1N5 B2 CBS-QB3
lf=139.5 te_zpe=-274.256386 te_gfe=-274.283841 te_ms_zpe=-273.856131 te_ms_gfe=0.003384

7 -2.132609 -0.087091 0.000051
1 -2.177899 0.948911 0.000122
7 0.015368 0.578584 -0.000054
7 1.167136 0.103919 0.000001
7 2.245462 -0.229161 0.000041
7 -0.984228 -0.501810 -0.000057

1-tsB2/P1 charge=0 spin=1 mol=H1N5 1-tsB2/P1 CBS-QB3
lf=-168.0 te_zpe=-274.240548 te_gfe=-274.267706 te_ms_zpe=-273.841742 te_ms_gfe=0.002638

7 1.676895 -0.661939 0.083117
1 1.112005 -1.089547 0.841906
7 -0.091165 0.885691 0.272465
7 -1.030170 0.116040 0.048270
7 -1.940213 -0.539825 -0.140212
7 1.225795 0.355682 -0.383912

1-ts'B2/P1 charge=0 spin=1 mol=H1N5 1-tsB2/P1 CBS-QB3
lf=-356.1 te_zpe=-274.231365 te_gfe=-274.259832 te_ms_zpe=-273.826846 te_ms_gfe=-0.001658

7 -2.181872 -0.336461 0.000391
1 -1.428474 -1.127628 0.000362
7 0.198346 -0.294216 -0.000644
7 1.386621 -0.070231 -0.000105
7 2.513781 0.158035 0.000409
7 -1.712808 0.703962 -0.000102

1-ts"B2/P1 charge=0 spin=1 mol=H1N5 1-ts"B2/P1 CBS-QB3
lf=-706.3 te_zpe=-274.223252 te_gfe=-274.250981 te_ms_zpe=-273.820147 te_ms_gfe=-0.000295

7 -2.264481 -0.086233 0.000008
1 -2.360476 0.948070 0.000073
7 -0.139117 0.506748 0.000033

7 1.338011 -0.165901 -0.000018
7 2.431916 0.004476 -0.000015
7 -1.029119 -0.394528 -0.000018

tsB2/D1 charge=0 spin=1 mol=H1N5 tsB2/D1 CBS-QB3
lf=-886.8 te_zpe=-274.097799 te_gfe=-274.125256 te_ms_zpe=-273.702576 te_ms_gfe=0.000393

7 1.186256 -0.380691 -0.504651
1 1.820367 -1.116618 -0.142653
7 1.394971 0.831558 0.109073
7 0.138108 -0.428351 0.581637
7 -0.971439 -0.080825 0.068098
7 -2.007949 0.217825 -0.233778

##

B3 charge=0 spin=1 mol=H1N5 B3 CBS-QB3
lf=162.6 te_zpe=-274.252259 te_gfe=-274.279810 te_ms_zpe=-273.855636 te_ms_gfe=0.003630

7 1.301085 -0.816661 -0.000240
1 2.299289 -1.051492 0.000115
7 1.256710 0.422599 0.000032
7 -0.044142 0.977453 0.000095
7 -0.973021 0.123134 0.000150
7 -1.869101 -0.556312 -0.000053

1-tsB3/P1 charge=0 spin=1 mol=H1N5 1-tsB3/P1 CBS-QB3
lf=-272.1 te_zpe=-274.247951 te_gfe=-274.274578 te_ms_zpe=-273.849833 te_ms_gfe=0.003525

7 -1.052636 -0.825510 0.000079
1 -1.997746 -1.216485 0.000122
7 -1.134037 0.401633 -0.000016
7 0.068922 1.144639 -0.000090
7 1.033615 0.269289 -0.000035
7 1.369528 -0.816268 0.000045

1-ts'B3/P1 charge=0 spin=1 mol=H1N5 1-ts'B3/P1 CBS-QB3
lf=-685.6 te_zpe=-274.248607 te_gfe=-274.276017 te_ms_zpe=-273.849108 te_ms_gfe=0.001964

7 -1.397036 -0.795799 0.000038
1 -2.406044 -0.964649 0.000043
7 -1.231148 0.447322 -0.000031
7 -0.036415 0.939547 -0.000054
7 0.971969 -0.060698 0.000008
7 2.036351 -0.392565 0.000033

tsB3/A6 charge=0 spin=1 mol=H1N5 tsB3/A6 CBS-QB3
lf=-598.5 te_zpe=-274.116562 te_gfe=-274.142836 te_ms_zpe=-273.731951 te_ms_gfe=0.002861

7 1.284058 -0.108737 -0.433209
1 2.030030 0.437085 0.023532
7 -0.088099 1.036350 0.190134
7 -1.155473 0.334591 -0.214975
7 -0.812617 -0.872316 -0.076136
7 0.482127 -0.452328 0.530825

##
B4 charge=0 spin=1 mol=H1N5 B4 CBS-QB3
lf=89.1 te_zpe=-274.239667 te_gfe=-274.267793 te_ms_zpe=-273.839687 te_ms_gfe=0.001873

7 -1.275004 0.228228 0.000053
1 -1.943312 1.008517 0.000075
7 0.348777 1.192451 0.000040
7 1.046816 0.203490 -0.000020
7 1.494688 -0.855563 -0.000069
7 -1.337661 -0.912680 -0.000014

1-tsB4/P1 charge=0 spin=1 mol=H1N5 1-tsB4/P1 CBS-QB3
lf=-190.7 te_zpe=-274.237619 te_gfe=-274.264674 te_ms_zpe=-273.842427 te_ms_gfe=0.002233

7 1.193368 -0.529065 0.000083
1 1.973009 -1.194813 0.000139
7 -0.944108 -1.135654 -0.000056
7 -1.060345 0.034107 -0.000071
7 -0.725158 1.175726 -0.000056
7 1.254384 0.625574 0.000080

1-ts'B4/P1 charge=0 spin=1 mol=H1N5 1-ts'B4/P1 CBS-QB3
lf=-118.4 te_zpe=-274.229278 te_gfe=-274.256908 te_ms_zpe=-273.826628 te_ms_gfe=0.001429

7 -1.269802 -0.032189 0.348687
1 -1.176176 0.010912 1.376536
7 0.266735 0.920881 -0.134688
7 1.182724 0.119801 -0.056492
7 2.066718 -0.609303 0.009828
7 -2.078349 -0.400748 -0.363983

1-ts"B4/P1 charge=0 spin=1 mol=H1N5 1-ts"B4/P1 CBS-QB3
lf=-566.0 te_zpe=-274.181141 te_gfe=-274.209110 te_ms_zpe=-273.792635 te_ms_gfe=-0.001442

7 1.211632 0.191937 0.000001
1 1.964436 0.965491 0.000002
7 0.217998 1.058441 0.000001

7 -1.015476 -0.171645 -0.000001
7 -2.120387 -0.232918 -0.000001
7 1.425598 -0.983742 -0.000001

tsB4/P2 charge=0 spin=1 mol=H1N5 tsB4/P2 CBS-QB3
lf=-886.8 te_zpe=-274.097799 te_gfe=-274.125256 te_ms_zpe=-273.702576 te_ms_gfe=0.000393

7 1.186256 -0.380691 -0.504651
1 1.820367 -1.116618 -0.142653
7 1.394971 0.831558 0.109073
7 0.138108 -0.428351 0.581637
7 -0.971439 -0.080825 0.068098
7 -2.007949 0.217825 -0.233778

##########
C1 charge=0 spin=1 mol=H1N5 C1 CBS-QB3
lf=615.6 te_zpe=-274.083530 te_gfe=-274.109479 te_ms_zpe=-273.707570 te_ms_gfe=0.005425

7 -1.183977 -0.000001 -0.135609
1 -1.694433 -0.000030 0.756122
7 -0.079983 -0.968320 -0.021207
7 0.818382 0.000029 -0.682115
7 0.767630 -0.000033 0.752071
7 -0.079990 0.968329 -0.021158

tsC1/A4 charge=0 spin=1 mol=H1N5 tsC1/A4 CBS-QB3
lf=-589.2 te_zpe=-274.058018 te_gfe=-274.084176 te_ms_zpe=-273.681309 te_ms_gfe=0.002339

7 -1.061656 -0.335096 -0.001242
1 -1.622920 -0.841915 0.679816
7 0.208968 -0.852583 -0.362804
7 0.630925 0.560751 -0.521517
7 1.089607 -0.145666 0.615782
7 -0.635997 0.892868 0.172665

tsC1/P1 charge=0 spin=1 mol=H1N5 tsC1/P1 CBS-QB3
lf=-670.7 te_zpe=-274.052164 te_gfe=-274.078249 te_ms_zpe=-273.677463 te_ms_gfe=0.002019

7 1.071954 -0.450529 -0.175545
1 1.890728 -0.448076 0.457228
7 0.577023 0.867827 -0.233279
7 -1.052499 -0.204678 -0.589685
7 -0.555094 0.650622 0.536444
7 -0.311487 -0.799231 0.396747

##########
D1 charge=0 spin=1 mol=H1N5 D1 CBS-QB3

lf=21.6 te_zpe=-274.206246 te_gfe=-274.239887 te_ms_zpe=-273.828824 te_ms_gfe=-0.007213

7	-1.465050	-0.001411	0.416740
1	-1.877391	-0.005727	1.367660
7	-1.129576	-0.937790	-0.356513
7	-1.127927	0.941979	-0.347294
7	1.992197	-0.549000	0.050764
7	1.998555	0.547040	0.040923

tsD1/A4 charge=0 spin=1 mol=H1N5 tsD1/A4 CBS-QB3
lf=-608.7 te_zpe=-274.110403 te_gfe=-274.136691 te_ms_zpe=-273.725912 te_ms_gfe=0.002269

7	-1.378523	0.033667	0.279171
1	-1.228605	-0.421710	1.198448
7	-0.494527	-0.378080	-0.587143
7	0.147401	1.049351	-0.167879
7	0.744948	-0.914618	0.055087
7	1.156216	0.269924	0.249556

tableS2. Cartesian coordinates of the optimized isomeric structures and Transitional structure of the substituted 3D-N5H(**C1**).
"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm^{-1})"
"te_zpe"----"total energy with zero-point energy (a.u.)"
"te_gfe"----"total energy with Gibbs free energy (a.u.)"
"bh_zpe"----"barrier height with zero-point energy correction (kcal mol^{-1})"
"bh_gfe"----"barrier height with Gibbs free energy correction (kcal mol^{-1})"

##########

R-Br-opt charge=0 spin=1 mol=Br1N5 R-Br-opt CBS-QB3
lf=198.6 te_zpe=-2847.606600 te_gfe=-2847.636240 te_ms_zpe=-2845.967931 te_ms_gfe=-0.009740

7	0.390984	0.000001	-0.774183
7	1.270283	-0.974132	-0.107475
7	2.384009	0.000000	-0.254914
7	1.635677	-0.000003	0.962675
7	1.270285	0.974135	-0.107471
35	-1.390247	0.000000	0.056274

R-Br-TS charge=0 spin=1 mol=Br1N5 R-Br-TS CBS-QB3
lf=-607.2 te_zpe=-2847.583903 te_gfe=-2847.613844 te_ms_zpe=-2845.944528 te_ms_gfe=-0.012461

7	-0.394847	-0.277987	-0.620421
7	-1.040076	0.947081	-0.352218
7	-2.506987	-0.250128	-0.345371
7	-1.833846	0.534473	0.717178
7	-1.529941	-0.876423	0.347651

35 1.461139 -0.015403 0.050636

##
R-C2H3-opt charge=0 spin=1 mol=C2H3N5 R-C2H3-opt CBS-QB3
lf=71.0 te_zpe=-351.465443 te_gfe=-351.495237 te_ms_zpe=-350.951152 te_ms_gfe=0.033231

 7 -0.275498 -0.504972 0.003902
 7 0.781565 -0.099530 0.972703
 7 1.816094 -0.503562 0.003338
 7 1.393998 0.864369 -0.006398
 7 0.781055 -0.113495 -0.971207
 6 -1.389811 0.392335 -0.002237
 1 -1.181447 1.460596 -0.009013
 6 -2.617282 -0.111009 0.000479
 1 -3.486375 0.535167 -0.004127
 1 -2.770121 -1.183387 0.007325

R-C2H3-TS charge=0 spin=1 mol=C2H3N5 R-C2H3-TS CBS-QB3
lf=-476.0 te_zpe=-351.446810 te_gfe=-351.476440 te_ms_zpe=-350.931435 te_ms_gfe=0.031997

 7 -0.184027 0.420860 -0.332209
 7 0.534240 -0.810075 -0.444671
 7 1.762638 0.010369 -0.354812
 7 1.350373 -0.708686 0.811005
 7 0.893858 1.070031 0.118825
 6 -1.495916 0.522981 0.130619
 1 -1.713436 1.505044 0.533533
 6 -2.382400 -0.463736 0.023128
 1 -3.395741 -0.318301 0.369176
 1 -2.120502 -1.419708 -0.412156

##
R-C2H-opt charge=0 spin=1 mol=C2H1N5 R-C2H-opt CBS-QB3
lf=161.3 te_zpe=-350.220984 te_gfe=-350.250015 te_ms_zpe=-349.708165 te_ms_gfe=0.010071

 7 -0.261480 0.000073 -0.676495
 7 0.711141 -0.974978 -0.080576
 7 1.796616 0.000007 -0.292410
 7 1.119342 -0.000089 0.975270
 7 0.711173 0.974989 -0.080413
 6 -1.501538 0.000040 -0.140505
 6 -2.646454 -0.000014 0.225044
 1 -3.649581 -0.000167 0.575132

R-C2H-TS charge=0 spin=1 mol=C2H1N5 R-C2H-TS CBS-QB3

lf=-535.2 te_zpe=-350.195672 te_gfe=-350.224967 te_ms_zpe=-349.681658 te_ms_gfe=0.007865

 7 -0.283063 0.255254 -0.313248
 7 0.734810 -0.767443 -0.551875
 7 1.714629 0.297968 -0.268231
 7 1.441091 -0.703180 0.732695
 7 0.615756 1.063100 0.268462
 6 -1.561455 0.035890 -0.034654
 6 -2.737662 -0.150440 0.135077
 1 -3.767865 -0.332599 0.322832

##
R-C6H5-opt charge=0 spin=1 mol=C6H5N5 R-C6H5-opt CBS-QB3
lf=27.4 te_zpe=-505.109320 te_gfe=-505.143452 te_ms_zpe=-504.326522 te_ms_gfe=0.076909

 7 1.049326 -0.421318 -0.634630
 7 1.891824 -0.880371 0.503218
 7 3.026793 -0.129825 -0.063031
 7 2.203339 0.532407 0.906820
 7 1.947176 0.742920 -0.560153
 6 -0.319526 -0.163955 -0.300055
 6 -1.156371 -1.274662 -0.169041
 6 -0.827099 1.128849 -0.176185
 6 -2.503003 -1.086129 0.115445
 1 -0.744961 -2.269434 -0.291953
 6 -2.186558 1.304282 0.077250
 1 -0.173412 1.984283 -0.287167
 6 -3.023425 0.203372 0.232888
 1 -3.151365 -1.947032 0.229387
 1 -2.586109 2.308111 0.162924
 1 -4.077472 0.346833 0.439427

R-C6H5-TS charge=0 spin=1 mol=C6H5N5 R-C6H5-TS CBS-QB3
lf=-485.8 te_zpe=-505.090848 te_gfe=-505.125115 te_ms_zpe=-504.306997 te_ms_gfe=0.075294

 7 1.031343 0.094342 -0.532441
 7 1.930418 -0.936618 -0.121748
 7 2.991010 0.092690 -0.180233
 7 2.490196 -0.272967 1.107166
 7 1.905310 1.053910 -0.207001
 6 -0.349070 0.049920 -0.254929
 6 -0.989014 -1.190087 -0.227130
 6 -1.055775 1.239308 -0.065442
 6 -2.357773 -1.233530 0.016736
 1 -0.419547 -2.096639 -0.388165

6 -2.421691 1.173578 0.180887
1 -0.535885 2.188294 -0.095197
6 -3.076890 -0.057606 0.220802
1 -2.861794 -2.192209 0.046449
1 -2.976285 2.090225 0.343113
1 -4.143141 -0.098656 0.408057

##
R-CF3-opt charge=0 spin=1 mol=C1F3N5 R-CF3-opt CBS-QB3
lf=57.3 te_zpe=-611.207163 te_gfe=-611.239098 te_ms_zpe=-610.452528 te_ms_gfe=0.003455

7 0.224679 0.000000 -0.700365
7 1.195055 -0.973568 -0.171697
7 2.274060 0.000000 -0.449559
7 1.697284 -0.000002 0.858373
7 1.195054 0.973569 -0.171695
6 -1.059001 0.000000 -0.022224
9 -0.986720 -0.000009 1.318578
9 -1.714910 1.092743 -0.404952
9 -1.714918 -1.092733 -0.404966

R-CF3-TS charge=0 spin=1 mol=C1F3N5 R-CF3-TS CBS-QB3
lf=-631.1 te_zpe=-611.179115 te_gfe=-611.211508 te_ms_zpe=-610.424380 te_ms_gfe=0.000253

7 0.250176 0.305197 -0.471159
7 1.220808 -0.745287 -0.584161
7 2.244057 0.298087 -0.285296
7 1.918288 -0.601819 0.721261
7 1.057322 1.179163 0.070218
6 -1.090024 -0.015975 0.006320
9 -1.043774 -0.717510 1.133897
9 -1.735864 1.121932 0.218684
9 -1.697519 -0.732372 -0.929688

##
R-CH3-opt charge=0 spin=1 mol=C1H3N5 R-CH3-opt CBS-QB3
lf=204.8 te_zpe=-313.383126 te_gfe=-313.411034 te_ms_zpe=-312.936590 te_ms_gfe=0.030658

7 0.613816 0.000043 -0.606497
7 -0.382193 0.969866 -0.112586
7 -1.454191 0.000024 -0.401385
7 -0.899104 -0.000067 0.919412
7 -0.382180 -0.969846 -0.112704
6 1.840702 -0.000010 0.187130
1 2.410403 0.885833 -0.097226

1 1.662015 -0.000029 1.268033
1 2.410338 -0.885883 -0.097264

R-CH3-TS charge=0 spin=1 mol=C1H3N5 R-CH3-TS CBS-QB3
lf=-471.3 te_zpe=-313.362916 te_gfe=-313.391094 te_ms_zpe=-312.915455 te_ms_gfe=0.028560

7 -0.601364 0.252396 -0.367888
7 0.410237 -0.720572 -0.605897
7 1.384344 0.335336 -0.257703
7 1.124844 -0.671357 0.715505
7 0.226769 1.079575 0.243105
6 -1.877244 -0.180433 0.170097
1 -2.398311 -0.749194 -0.598833
1 -1.694245 -0.798919 1.056489
1 -2.457793 0.703066 0.431907

##
R-Cl-opt charge=0 spin=1 mol=Cl1N5 R-Cl-opt CBS-QB3
lf=239.4 te_zpe=-733.682945 te_gfe=-733.711406 te_ms_zpe=-732.837416 te_ms_gfe=-0.008088

7 -0.181869 0.000000 -0.728688
7 0.734773 -0.975007 -0.102826
7 1.834506 0.000000 -0.305082
7 1.146680 -0.000002 0.949187
7 0.734774 0.975008 -0.102823
17 -1.757767 0.000000 0.119507

R-Cl-TS charge=0 spin=1 mol=Cl1N5 R-Cl-TS CBS-QB3
lf=-628.2 te_zpe=-733.658417 te_gfe=-733.687186 te_ms_zpe=-732.812733 te_ms_gfe=-0.010918

7 0.207758 -0.287838 -0.570982
7 -0.474266 0.943813 -0.341000
7 -1.923919 -0.253237 -0.396735
7 -1.309640 0.549682 0.694352
7 -1.011182 -0.874695 0.361921
17 1.857573 -0.032004 0.103948

##
R-CN-opt charge=0 spin=1 mol=C1N6 R-CN-opt CBS-QB3
lf=163.3 te_zpe=-366.320710 te_gfe=-366.349597 te_ms_zpe=-365.800726 te_ms_gfe=-0.000322

7 0.296004 0.000192 -0.662395
7 -0.679273 0.975126 -0.084320
7 -1.760847 0.000056 -0.319017

7 -1.110160 -0.000251 0.962776
7 -0.679225 -0.975122 -0.084784
6 1.529888 0.000199 -0.102556
7 2.622169 -0.000171 0.275645

R-CN-TS charge=0 spin=1 mol=C1N6 R-CN-TS CBS-QB3
lf=-763.3 te_zpe=-366.292388 te_gfe=-366.321782 te_ms_zpe=-365.771165 te_ms_gfe=-0.003750

7 0.363778 -0.223755 -0.499650
7 -0.447562 0.961354 -0.288539
7 -1.841357 -0.251834 -0.424813
7 -1.266307 0.504278 0.721984
7 -0.951496 -0.903599 0.336030
6 1.628279 -0.066969 -0.081923
7 2.747277 -0.029042 0.225209

##
R-COOH-opt charge=0 spin=1 mol=C1H1N5O2 R-COOH-opt CBS-QB3
lf=87.1 te_zpe=-462.689982 te_gfe=-462.720716 te_ms_zpe=-462.062900 te_ms_gfe=0.014698

7 0.036826 -0.005896 -0.631281
7 0.961437 -0.989112 -0.040389
7 2.079888 -0.072538 -0.339870
7 1.462128 0.026316 0.949478
7 1.034103 0.956670 -0.150999
6 -1.263084 0.126964 -0.076495
8 -1.778998 1.184831 0.136760
8 -1.811119 -1.086561 0.061472
1 -2.721217 -0.956025 0.364546

R-COOH-TS charge=0 spin=1 mol=C1H1N5O2 R-COOH-TS CBS-QB3
lf=-486.9 te_zpe=-462.665790 te_gfe=-462.696900 te_ms_zpe=-462.038172 te_ms_gfe=0.011802

7 0.037157 0.129396 -0.412063
7 0.922361 1.097867 -0.241336
7 1.721771 -0.369088 0.960242
7 2.018562 0.163174 -0.353957
7 1.027165 -0.913027 -0.194082
6 -1.320692 0.114245 -0.013828
8 -1.776957 -1.134136 -0.126879
1 -2.706329 -1.129973 0.143755
8 -1.905371 1.094916 0.330327

##
R-F-opt charge=0 spin=1 mol=F1N5 R-F-opt CBS-QB3

lf=297.2 te_zpe=-373.299677 te_gfe=-373.327106 te_ms_zpe=-372.820100 te_ms_gfe=-0.005595

7 -0.733910 0.526271 0.000000
7 -0.044805 -0.335608 0.978085
7 -0.154265 -1.445867 0.000000
7 1.035392 -0.658812 0.000000
7 -0.044805 -0.335608 -0.978085
9 -0.044805 1.749708 0.000000

R-F-TS charge=0 spin=1 mol=F1N5 R-F-TS CBS-QB3
lf=-622.8 te_zpe=-373.271157 te_gfe=-373.298903 te_ms_zpe=-372.791835 te_ms_gfe=-0.008459

7 0.672564 -0.315578 -0.473498
7 -0.021296 0.934080 -0.318135
7 -1.453505 -0.260698 -0.486492
7 -0.954169 0.585009 0.637351
7 -0.659536 -0.859929 0.390511
9 1.879066 -0.064465 0.194649

##
R-NCO-opt charge=0 spin=1 mol=C1N6O1 R-NCO-opt CBS-QB3
lf=44.1 te_zpe=-441.569611 te_gfe=-441.600865 te_ms_zpe=-440.951924 te_ms_gfe=0.002042

7 0.135835 0.000407 -0.543456
7 1.174146 -0.974526 -0.096985
7 2.214779 0.000383 -0.480789
7 1.748992 -0.001153 0.875478
7 1.174518 0.975185 -0.095238
7 -0.923572 -0.000700 0.381453
6 -2.105341 0.000655 0.054569
8 -3.255106 -0.000138 -0.076332

R-NCO-TS charge=0 spin=1 mol=C1N6O1 R-NCO-TS CBS-QB3
lf=-650.2 te_zpe=-441.541208 te_gfe=-441.572618 te_ms_zpe=-440.923452 te_ms_gfe=-0.001032

7 -0.302697 0.945432 0.226288
7 -0.649457 -0.316352 0.902086
7 -2.256734 -0.076826 0.122447
7 -1.180728 -1.047632 -0.154579
7 -1.458993 0.236847 -0.895610
7 1.035858 0.946735 0.023693
6 1.874010 0.042437 -0.058002
8 2.805649 -0.634006 -0.152782

##

R-NH2-opt charge=0 spin=1 mol=H2N6 R-NH2-opt CBS-QB3
lf=286.8 te_zpe=-329.421367 te_gfe=-329.448982 te_ms_zpe=-328.965398 te_ms_gfe=0.019634

7 0.667454 -0.015953 -0.582097
7 -0.376129 0.983772 -0.114533
7 -1.422156 0.004785 -0.425668
7 -0.896420 0.005081 0.904792
7 -0.369432 -0.975380 -0.097929
7 1.789485 -0.082694 0.190036
1 2.570791 0.350732 -0.280500
1 1.679593 0.211995 1.158290

R-NH2-TS charge=0 spin=1 mol=H2N6 R-NH2-TS CBS-QB3
lf=-595.6 te_zpe=-329.407108 te_gfe=-329.434977 te_ms_zpe=-328.948914 te_ms_gfe=0.017295

7 0.744103 -0.313896 -0.457667
7 -0.092325 0.882829 -0.384610
7 -1.470938 -0.169071 -0.476360
7 -0.957306 0.545194 0.677392
7 -0.742393 -0.927547 0.361097
7 1.870253 -0.008160 0.144973
1 2.653942 -0.614660 -0.047599
1 1.886301 0.549216 0.993816

##
R-NO2-opt charge=0 spin=1 mol=N6O2 R-NO2-opt CBS-QB3
lf=68.7 te_zpe=-478.606433 te_gfe=-478.637149 te_ms_zpe=-477.968873 te_ms_gfe=0.001517

7 -0.043515 -0.000001 -0.730971
7 -0.949520 0.980284 -0.106928
7 -2.047243 -0.000001 -0.279182
7 -1.342948 0.000001 0.961603
7 -0.949520 -0.980285 -0.106925
7 1.301425 0.000000 -0.046206
8 1.763700 1.094170 0.135018
8 1.763705 -1.094168 0.135015

R-NO2-TS charge=0 spin=1 mol=N6O2 R-NO2-TS CBS-QB3
lf=-738.5 te_zpe=-478.578739 te_gfe=-478.610404 te_ms_zpe=-477.936721 te_ms_gfe=-0.002642

7 0.128930 0.277645 -0.659616
7 0.992845 -0.828237 -0.478088
7 2.077029 0.155925 -0.087927
7 1.490092 -0.464095 0.935955
7 0.850917 1.165306 -0.029279

7 -1.389961 -0.038104 -0.010611
8 -1.968948 0.959895 0.269129
8 -1.662172 -1.194780 0.019242

##
R-NO-opt charge=0 spin=1 mol=N6O1 R-NO-opt CBS-QB3
lf=142.8 te_zpe=-403.398658 te_gfe=-403.427791 te_ms_zpe=-402.853099 te_ms_gfe=-0.002749

7 0.261159 0.340623 -0.554265
7 -0.873732 0.956859 0.137523
7 -1.740495 -0.119712 -0.391700
7 -1.145181 -0.308270 0.893668
7 -0.494406 -0.916898 -0.320636
7 1.497912 0.541740 0.096112
8 2.182900 -0.432549 0.121887

R-NO-TS charge=0 spin=1 mol=N6O1 R-NO-TS CBS-QB3
lf=-538.1 te_zpe=-403.375995 te_gfe=-403.405922 te_ms_zpe=-402.828461 te_ms_gfe=-0.006727

7 -0.258623 0.428017 -0.299716
7 0.570956 -0.805890 -0.487891
7 1.714575 0.118846 -0.334329
7 1.301221 -0.767063 0.733719
7 0.791553 1.109238 0.161155
7 -1.556755 0.438441 0.293361
8 -2.242561 -0.456391 -0.058012

##
R-OH-opt charge=0 spin=1 mol=H1N5O1 R-OH-opt CBS-QB3
lf=300.2 te_zpe=-349.286081 te_gfe=-349.313619 te_ms_zpe=-348.820283 te_ms_gfe=0.007133

7 0.659432 0.000117 -0.586809
7 -0.350391 0.976784 -0.097986
7 -1.409647 0.000045 -0.427726
7 -0.878837 -0.000227 0.900090
7 -0.350264 -0.976669 -0.098340
8 1.726451 -0.000085 0.306316
1 2.496338 0.000330 -0.275125

R-OH-TS charge=0 spin=1 mol=H1N5O1 R-OH-TS CBS-QB3
lf=-641.6 te_zpe=-349.259077 te_gfe=-349.286824 te_ms_zpe=-348.792820 te_ms_gfe=0.004410

7 0.715203 -0.339943 -0.463398
7 -0.041704 0.899926 -0.375766
7 -1.461778 -0.215162 -0.471445

 7 -0.946189 0.583360 0.644078
 7 -0.693995 -0.882713 0.392662
 8 1.899879 -0.110969 0.136164
 1 1.800215 0.569481 0.827763

##
R-PH2-opt charge=0 spin=1 mol=H2N5P1 R-PH2-opt CBS-QB3
lf=191.6 te_zpe=-616.051393 te_gfe=-616.080465 te_ms_zpe=-615.214913 te_ms_gfe=0.009180

 7 0.211544 0.000576 -0.630155
 7 -0.769991 0.975251 -0.100691
 7 -1.857318 0.010955 -0.372032
 7 -1.257832 -0.001858 0.931594
 7 -0.777677 -0.965283 -0.115722
15 1.819271 -0.113539 0.079267
 1 2.265859 1.079018 -0.532327
 1 1.603993 0.486582 1.352357

R-PH2-TS charge=0 spin=1 mol=H2N5P1 R-PH2-TS CBS-QB3
lf=-477.6 te_zpe=-616.030600 te_gfe=-616.060110 te_ms_zpe=-615.194687 te_ms_gfe=0.006658

 7 -0.198833 0.302338 -0.381167
 7 0.811958 -0.694456 -0.631157
 7 1.791919 0.326057 -0.212781
 7 1.468096 -0.733921 0.701025
 7 0.657028 1.068946 0.291121
15 -1.855414 -0.169027 -0.000994
 1 -2.262472 1.154407 0.284075
 1 -1.617489 -0.501754 1.361550

##
R-SH-opt charge=0 spin=1 mol=H1N5S1 R-SH-opt CBS-QB3
lf=215.9 te_zpe=-672.288661 te_gfe=-672.317424 te_ms_zpe=-671.448500 te_ms_gfe=0.000518

 7 0.226473 0.000000 -0.653469
 7 -0.757348 0.974007 -0.106991
 7 -1.836942 0.000000 -0.370717
 7 -1.231912 0.000000 0.927660
 7 -0.757347 -0.974006 -0.106992
16 1.752008 0.000000 0.194721
 1 2.467399 0.000000 -0.941982

R-SH-TS charge=0 spin=1 mol=H1N5S1 R-SH-TS CBS-QB3
lf=-653.8 te_zpe=-672.269091 te_gfe=-672.297976 te_ms_zpe=-671.428400 te_ms_gfe=-0.001702

 7 0.280624 -0.315871 -0.490284
 7 -0.499094 0.895113 -0.412657
 7 -1.913068 -0.238943 -0.418263
 7 -1.336354 0.561079 0.662366
 7 -1.046332 -0.888373 0.392217
16 1.820455 0.046521 0.155818
 1 2.472280 -0.835365 -0.626742

##
R-SIH3-opt charge=0 spin=1 mol=H3N5Si1 R-SIH3-opt CBS-QB3
lf=-147.2 te_zpe=-564.800518 te_gfe=-564.829478 te_ms_zpe=-563.967378 te_ms_gfe=0.016298

 7 -0.181411 -0.000003 -0.598160
 7 0.809642 -0.966112 -0.107852
 7 1.893365 0.000003 -0.392336
 7 1.321513 -0.000001 0.926311
 7 0.809637 0.966111 -0.107849
14 -1.841798 0.000000 0.086154
 1 -1.999500 1.223063 0.898930
 1 -2.785108 -0.000127 -1.045040
 1 -1.999446 -1.222923 0.899155

R-SIH3-TS charge=0 spin=1 mol=H3N5Si1 R-SIH3-TS CBS-QB3
lf=-487.5 te_zpe=-564.787937 te_gfe=-564.817932 te_ms_zpe=-563.955885 te_ms_gfe=0.013872

 7 -0.176596 0.276384 -0.400408
 7 0.836663 -0.738447 -0.593215
 7 1.828096 0.305612 -0.250646
 7 1.490501 -0.675719 0.745365
 7 0.708667 1.052417 0.248079
14 -1.860151 -0.078062 0.085686
 1 -2.433994 1.237911 0.408526
 1 -2.476852 -0.696228 -1.098586
 1 -1.858367 -0.990550 1.246228