Supporting Information For

**Exploring the cyclization reaction channel for the gas-phase elementary reaction between the silicon nitride radical (SiN, $X^2\Sigma^+$) and isoprene ($C_5H_8$, $X^1A'$) to prepare methylazasilacyclohexadienylidenes (SiNC$_5$H$_7$, $X^1A'$)**

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**Table S1.** Peak velocities ($v_p$) and speed ratios (S) of the Silicon Nitride radical (SiN) and isoprene ($C_5H_8$) beams, along with the corresponding collision energies (EC) and center-of-mass angles ($\Theta_{CM}$)

| Beam | $v_p$ (m s$^{-1}$) | S | $E_c$ (kJ mol$^{-1}$) | $\Theta_{CM}$ (degree) |
|---|---|---|---|---|
| Silicon nitride Radical (SiN) | 1204 ± 18 | 4.3 ± 0.4 | | |
| Isoprene ($C_5H_8$) | 730 ± 10 | 8.5 ± 0.2 | 25± 1 | 44.3 ± 0.5 |

**Optimized Cartesian coordinates (Å) and absolute energies for all reactants, intermediates, and product isomers involved in the reactions between silicon nitride radical (SiN) and isoprene (C₅H₈) calculated at the CBS-QB3 composite method.**

**SiN**

N  -6.442795    1.807667   0.000000
Si  -4.876575    1.756463   -0.000000

CBS-QB3 (0 K)=         -343.624031
CBS-QB3 Energy=          -343.621651
CBS-QB3 Enthalpy=        -343.620707
CBS-QB3 Free Energy=       -343.645296

**Isoprene**

C  -6.007295    2.148255   0.104357
C  -4.877481    2.867562   0.035474
H  -6.979169    2.619737   0.194562
H  -5.988505    1.064253   0.072031
C  -4.897999    4.374518   0.079906
H  -5.917905    4.750416   0.171204
H  -4.456123    4.801811   -0.826047
H  -4.317500    4.751965   0.927930
C  -3.585502    2.182670   -0.086197
C  -2.386416    2.768488   -0.164331
H  -1.481106    2.179842   -0.252598
H  -2.263801    3.845319   -0.143358
H  -3.638028    1.096537   -0.112914

CBS-QB3 (0 K)=         -194.897950
CBS-QB3 Energy=          -194.892041
CBS-QB3 Enthalpy=        -194.891097
CBS-QB3 Free Energy=       -194.926491

**P1**

C -2.749403 -0.141422 0.000000
C -1.241671 -0.006519 0.000000
C -0.420102 -1.115228 0.000000
Si 1.419232 -1.130161 0.000000
N 1.586243 0.648328 0.000000
C 0.617528 1.603993 0.000000

C -0.718680 1.321391 0.000000
H -3.057079 -1.187521 0.000000
H -3.183052 0.344816 -0.880078
H -3.183052 0.344816 0.880078
H -0.926078 -2.080797 0.000000
H 2.526912 1.022854 0.000000
H 0.951093 2.637840 0.000000
H -1.408542 2.157430 0.000000

CBS-QB3 (0 K)=         -538.081719
CBS-QB3 Energy=          -538.074795
CBS-QB3 Enthalpy=        -538.073851
CBS-QB3 Free Energy=       -538.112977

**P2**

C -2.778780 0.560967 0.000000
C -1.298278 0.262226 0.000000
C -0.387700 1.286407 0.000000
N 0.963399 1.102980 0.000000
Si 1.927802 -0.396783 0.000000
C 0.454315 -1.505678 0.000000
C -0.856186 -1.092992 0.000000
H -2.970388 1.636231 0.000000
H -3.271171 0.136494 0.880946
H -3.271171 0.136494 -0.880946
H -0.735463 2.315959 0.000000
H 1.483147 1.972182 0.000000
H 0.616783 -2.582551 0.000000
H -1.646516 -1.845347 0.000000

CBS-QB3 (0 K)=         -538.079462
CBS-QB3 Energy=          -538.072584
CBS-QB3 Enthalpy=        -538.071639
CBS-QB3 Free Energy=       -538.110432

**P3**

C 2.412265 -1.286328 0.000000

C 1.098120 -0.533308 0.000000
C 1.128011 0.873275 0.000000
C -0.002983 1.703426 0.000000
N -1.280565 1.322247 0.000000
Si -1.571618 -0.312832 0.000000
H -2.949346 -0.815906 0.000000
C -0.098976 -1.273566 0.000000
H 3.267928 -0.609449 0.000000
H 2.486436 -1.931267 -0.880621
H 2.486436 -1.931267 0.880621
H 2.097068 1.361045 0.000000
H 0.181656 2.781362 0.000000
H -0.039769 -2.357407 0.000000

CBS-QB3 (0 K)=        -538.071675
CBS-QB3 Energy=          -538.064582
CBS-QB3 Enthalpy=       -538.063638
CBS-QB3 Free Energy=       -538.104295

C 1.581960 -0.957274 0.000000
C 0.458432 -0.201575 0.000000
Si -1.290257 -0.976761 0.000000
N -1.889403 0.672769 0.000000
C -0.917153 1.682856 0.000000
C 0.363014 1.253004 0.000000
H 3.083812 0.604770 0.000000
H 3.534727 -0.868648 0.876973
H 3.534727 -0.868648 -0.876973
H 1.462644 -2.040951 0.000000
H -2.857321 0.958485 0.000000
H -1.234200 2.719538 0.000000
H 1.202737 1.936203 0.000000

CBS-QB3 (0 K)=        -538.062186
CBS-QB3 Energy=          -538.054909
CBS-QB3 Enthalpy=       -538.053965
CBS-QB3 Free Energy=       -538.093855

**P4**
C 2.761893 -0.106370 0.000000
C 1.249668 -0.062959 0.000000
C 0.531438 -1.274404 0.000000
C -0.859315 -1.420904 0.000000
Si -1.738367 0.107321 0.000000
H -3.191537 0.301486 0.000000
N -0.716443 1.411819 0.000000
C 0.597168 1.184288 0.000000
H 3.150564 -0.626604 0.881485
H 3.183733 0.900822 0.000000
H 3.150564 -0.626604 -0.881485
H 1.129616 -2.185360 0.000000
H -1.279420 -2.420283 0.000000
H 1.239559 2.070203 0.000000

CBS-QB3 (0 K)=        -538.069253
CBS-QB3 Energy=          -538.062233
CBS-QB3 Enthalpy=       -538.061289
CBS-QB3 Free Energy=       -538.100590

**P6**
C -2.825921 -0.642732 0.000000
C -1.840955 0.483758 0.000000
C -0.491937 0.384578 0.000000
Si 0.543984 -1.238444 0.000000
N 1.948063 -0.193383 0.000000
C 1.706284 1.190187 0.000000
C 0.404162 1.537405 0.000000
H -3.481383 -0.581200 0.876893
H -2.342156 -1.620839 0.000000
H -3.481383 -0.581200 -0.876893
H -2.289754 1.480850 0.000000
H 2.910039 -0.498619 0.000000
H 2.546844 1.873999 0.000000
H 0.064730 2.566616 0.000000

CBS-QB3 (0 K)=        -538.061273
CBS-QB3 Energy=          -538.054076
CBS-QB3 Enthalpy=       -538.053132
CBS-QB3 Free Energy=       -538.092585

**P5**
C 3.001849 -0.482385 0.000000

**P7**
C -2.805173 -1.020708 0.000000

C -1.951173 0.198205 0.000000
C -0.591192 0.188506 0.000000
N 0.166304 -0.982708 0.000000
Si 1.721758 -0.455603 0.000000
H 2.925742 -1.297488 0.000000
C 1.514806 1.355345 0.000000
C 0.158086 1.466376 0.000000
H -3.463190 -1.034426 0.877569
H -3.463190 -1.034426 -0.877569
H -2.188279 -1.918280 0.000000
H -2.447184 1.165660 0.000000
H 2.194539 2.195520 0.000000
H -0.375333 2.412816 0.000000

CBS-QB3 (0 K)=          -538.037818
CBS-QB3 Energy=          -538.030652
CBS-QB3 Enthalpy=        -538.029708
CBS-QB3 Free Energy=        -538.069053

**P8**
C 3.052881 -0.305724 0.000000
C 1.701333 -0.938814 0.000000
C 0.484113 -0.333334 0.000000
N -0.688490 -1.098339 0.000000
Si -1.902201 0.004844 0.000000
H -3.343717 -0.277106 0.000000
C -0.979065 1.579015 0.000000
C 0.308598 1.139455 0.000000
H 3.626523 -0.631218 0.876235
H 3.026187 0.783783 0.000000
H 3.626523 -0.631218 -0.876235
H 1.674496 -2.025270 0.000000
H -1.260021 2.622906 0.000000
H 1.161814 1.808864 0.000000

CBS-QB3 (0 K)=          -538.033536
CBS-QB3 Energy=          -538.026358
CBS-QB3 Enthalpy=        -538.025413
CBS-QB3 Free Energy=        -538.064718

**P9**
H -2.703769 -0.979770 0.000000
C -1.786481 -1.565496 0.000000
C -0.552652 -0.792815 0.000000

C -0.650001 0.564678 0.000000
N 0.380224 1.447402 0.000000
Si 1.512002 2.533982 0.000000
C -1.886789 -2.902274 0.000000
H -1.645909 1.007831 0.000000
H -2.854564 -3.388927 0.000000
H -1.017914 -3.550101 0.000000
C 0.769348 -1.505909 0.000000
H 0.865449 -2.150144 0.880443
H 0.865449 -2.150144 -0.880443
H 1.597484 -0.798807 0.000000

CBS-QB3 (0 K)=          -538.049363
CBS-QB3 Energy=          -538.041328
CBS-QB3 Enthalpy=        -538.040383
CBS-QB3 Free Energy=        -538.082204

**P10**
C -2.238702 -1.508881 0.000000
C -1.835516 -0.072195 0.000000
C -0.568171 0.410166 0.000000
N 0.531681 -0.410558 0.000000
Si 1.830758 -1.281422 0.000000
C -0.347962 1.868594 0.000000
C 0.832802 2.488643 0.000000
H -2.852457 -1.743749 0.878080
H -1.373485 -2.171657 0.000000
H -2.852457 -1.743749 -0.878080
H -2.636264 0.661440 0.000000
H -1.259772 2.459717 0.000000
H 1.765517 1.937073 0.000000
H 0.895905 3.570017 0.000000

CBS-QB3 (0 K)=          -538.048779
CBS-QB3 Energy=          -538.040608
CBS-QB3 Enthalpy=        -538.039663
CBS-QB3 Free Energy=        -538.082059

**P11**
H 0.052728 -1.603570 0.000000
C 1.056837 -1.191720 0.000000
C 1.138625 0.260213 0.000000
C 0.017191 1.032280 0.000000
N -1.268361 0.593289 0.000000

Si -2.779611 0.173573 0.000000
C 2.097704 -2.036816 0.000000
H 0.138080 2.115378 0.000000
H 1.944493 -3.109464 0.000000
H 3.126584 -1.695476 0.000000
C 2.490423 0.923985 0.000000
H 3.075096 0.635206 0.880181
H 3.075096 0.635206 -0.880181
H 2.396442 2.011428 0.000000

CBS-QB3 (0 K)=          -538.048303
CBS-QB3 Energy=          -538.040359
CBS-QB3 Enthalpy=          -538.039414
CBS-QB3 Free Energy=          -538.080984

**P12**
C -2.490665 1.415994 0.000000
C -2.114607 -0.046955 0.000000
C -0.707080 -0.419155 0.000000
C 0.332838 0.445882 0.000000
N 1.642352 0.079411 0.000000
Si 3.163610 -0.298151 0.000000
C -3.061076 -1.002231 0.000000
H -2.090773 1.928382 -0.880889
H -2.090773 1.928382 0.880889
H -3.574439 1.538750 0.000000
H -0.481193 -1.481699 0.000000
H 0.148084 1.518848 0.000000
H -4.116625 -0.756974 0.000000
H -2.801044 -2.055026 0.000000

CBS-QB3 (0 K)=          -538.047919
CBS-QB3 Energy=          -538.039973
CBS-QB3 Enthalpy=          -538.039029
CBS-QB3 Free Energy=          -538.080666

**P13**
C -2.890528 -0.941026 0.000000
C -1.398023 -1.051165 0.000000
C -0.478024 -0.054055 0.000000
N 0.863470 -0.364522 0.000000
Si 2.396854 -0.668925 0.000000
C -0.842753 1.374013 0.000000
C 0.013349 2.397794 0.000000

H -3.313338 -1.445145 0.877371
H -3.313338 -1.445145 -0.877371
H -3.256879 0.085044 0.000000
H -1.002117 -2.062644 0.000000
H -1.905277 1.588041 0.000000
H 1.085775 2.245127 0.000000
H -0.342479 3.421088 0.000000

CBS-QB3 (0 K)=          -538.045045
CBS-QB3 Energy=          -538.036871
CBS-QB3 Enthalpy=          -538.035927
CBS-QB3 Free Energy=          -538.078235

**P14**
H 2.913046 -0.206056 0.623370
C 2.159799 -0.770626 0.074498
C 0.834542 -0.142812 0.011547
C -0.288404 -0.904326 -0.011916
N -1.564092 -0.443348 -0.105390
Si -3.062074 0.007381 -0.215959
C 2.528805 -1.924182 -0.493220
H -0.183474 -1.984923 0.068468
H 3.530936 -2.316312 -0.364864
H 1.850695 -2.504502 -1.109547
C 0.794375 1.361152 0.000520
H 1.434770 1.769255 0.790119
H 1.172465 1.757452 -0.949218
H -0.217878 1.736988 0.146082

CBS-QB3 (0 K)=          -538.044386
CBS-QB3 Energy=          -538.036153
CBS-QB3 Enthalpy=          -538.035208
CBS-QB3 Free Energy=          -538.077803

**P15**
C -2.484018 -0.126486 -0.006367
C -1.312839 0.787462 -0.162520
C -0.009390 0.432784 -0.095632
N 0.403750 -0.866342 0.088365
Si 0.961672 -2.312885 0.302580
C 1.085100 1.424038 -0.243760
C 1.079939 2.667045 0.236847
H -3.115881 0.187653 0.833481
H -2.172523 -1.156258 0.168921

H -3.121425 -0.105531 -0.898323
H -1.525717 1.832471 -0.362237
H 1.961861 1.056722 -0.771889
H 0.249106 3.053771 0.817007
H 1.915920 3.336171 0.068556

CBS-QB3 (0 K)=        -538.044021
CBS-QB3 Energy=         -538.035756
CBS-QB3 Enthalpy=       -538.034812
CBS-QB3 Free Energy=       -538.077505

**P16**
C -2.876537 -1.350472 0.048484
C -2.015899 -0.107612 0.080792
C -0.576710 -0.343274 0.244400
C 0.402141 0.439871 -0.256846
N 1.734775 0.225303 -0.086868
Si 3.279879 0.021845 0.078728
C -2.554852 1.116921 -0.014806
H -3.934541 -1.103176 -0.052249
H -2.748311 -1.932709 0.967860
H -2.592178 -2.003695 -0.783099
H -0.280289 -1.241781 0.780468
H 0.136046 1.307949 -0.859370
H -3.619876 1.251892 -0.165965
H -1.954553 2.015210 0.069832

CBS-QB3 (0 K)=        -538.043612
CBS-QB3 Energy=         -538.035500
CBS-QB3 Enthalpy=       -538.034556
CBS-QB3 Free Energy=       -538.076760

**P17**
H -2.069376 1.343461 0.245243
C -1.060182 1.027994 -0.016904
C -0.890540 -0.424605 -0.036362
C 0.285157 -1.108483 -0.065109
N 1.546183 -0.609620 -0.086238
Si 3.051235 -0.165629 -0.084065
C -0.177802 1.999332 -0.290925
H 0.227317 -2.197139 -0.051632
H -0.479828 3.039084 -0.234916
H 0.839039 1.796101 -0.589667
C -2.177038 -1.217726 0.014414

H -2.756258 -0.970100 0.911478
H -2.815189 -0.990622 -0.847012
H -1.991066 -2.293144 0.020324

CBS-QB3 (0 K)=        -538.042080
CBS-QB3 Energy=         -538.033907
CBS-QB3 Enthalpy=       -538.032963
CBS-QB3 Free Energy=       -538.075582

**P18**
C -2.685825 0.607339 -0.066662
C -1.217023 0.890898 -0.127846
C -0.196278 0.025341 0.066672
N 1.111364 0.462654 0.044414
Si 2.618792 0.881567 0.022679
C -0.343009 -1.422680 0.355631
C -1.141258 -2.277459 -0.283463
H -3.137783 0.602038 -1.066942
H -3.198990 1.392710 0.498518
H -2.904008 -0.354262 0.399351
H -0.933060 1.921126 -0.323988
H 0.315911 -1.792735 1.138122
H -1.773125 -1.969457 -1.108421
H -1.170220 -3.326026 -0.009105

CBS-QB3 (0 K)=        -538.040761
CBS-QB3 Energy=         -538.032650
CBS-QB3 Enthalpy=       -538.031706
CBS-QB3 Free Energy=       -538.073739

**P19**
C -3.096312 -0.823679 0.000000
C -2.444004 0.343612 0.000000
C -0.989845 0.541845 0.000000
C -0.118973 -0.708193 0.000000
N 1.282005 -0.489952 0.000000
Si 2.825868 -0.293990 0.000000
C -0.480580 1.778590 0.000000
H -2.589292 -1.781699 0.000000
H -4.179310 -0.854803 0.000000
H -3.027260 1.261619 0.000000
H -0.396606 -1.311329 -0.875882
H -0.396606 -1.311329 0.875882
H -1.129509 2.647185 0.000000

H 0.587217 1.951363 0.000000

CBS-QB3 (0 K)= -538.035003
CBS-QB3 Energy= -538.027198
CBS-QB3 Enthalpy= -538.026254
CBS-QB3 Free Energy= -538.067797

**P20**
C -1.161825 2.028257 0.140573
C -1.688717 0.883716 -0.304253
C -1.206264 -0.469948 -0.012099
C 0.024876 -0.652549 0.866420
N 1.242223 -0.269505 0.229158
Si 2.559998 0.117965 -0.502837
C -1.853614 -1.539344 -0.494080
H -0.273721 2.054664 0.760535
H -1.604519 2.982940 -0.118006
H -2.571206 0.928161 -0.939029
H 0.082451 -1.704403 1.167439
H -0.106092 -0.071797 1.789683
H -2.736279 -1.433222 -1.115950
H -1.521270 -2.549518 -0.283772

CBS-QB3 (0 K)= -538.034124
CBS-QB3 Energy= -538.026343
CBS-QB3 Enthalpy= -538.025399
CBS-QB3 Free Energy= -538.066962

**P21**
C -3.100306 1.344416 -0.045266
C -2.082698 0.790645 0.615847
C -0.931970 0.093108 0.008243
C 0.380914 0.318647 0.752919
N 1.519024 -0.346328 0.235851
Si 2.782860 -1.066569 -0.317693
C -1.035896 -0.677814 -1.075416
H -3.146518 1.339133 -1.128975
H -3.916306 1.827111 0.480112
H -2.064559 0.872865 1.702346
H 0.220248 0.019797 1.800063
H 0.566902 1.402403 0.783882
H -1.994965 -0.854406 -1.547193
H -0.167185 -1.161205 -1.503469

CBS-QB3 (0 K)= -538.031660
CBS-QB3 Energy= -538.023715
CBS-QB3 Enthalpy= -538.022770
CBS-QB3 Free Energy= -538.064794

**P22**
C -1.935489 1.902812 -0.533582
C -1.334191 1.081161 0.328123
C -1.119919 -0.365021 0.135921
C 0.152219 -0.936969 0.746983
N 1.339156 -0.333718 0.240353
Si 2.604464 0.352029 -0.352610
C -1.994311 -1.158686 -0.490631
H -2.297020 1.555321 -1.495517
H -2.073529 2.953662 -0.306783
H -0.935272 1.495400 1.252608
H 0.175742 -2.019244 0.577287
H 0.107837 -0.792428 1.837165
H -2.939267 -0.780944 -0.863759
H -1.794774 -2.214914 -0.634382

CBS-QB3 (0 K)= -538.031368
CBS-QB3 Energy= -538.023439
CBS-QB3 Enthalpy= -538.022494
CBS-QB3 Free Energy= -538.064710

**P23**
C -2.407979 1.822639 -0.117500
C -1.236703 1.186787 -0.054819
C -1.051704 -0.273217 0.037262
C 0.147301 -0.743317 0.855328
N 1.395684 -0.354146 0.285694
Si 2.755985 0.044832 -0.358454
C -1.858138 -1.156961 -0.557855
H -3.352306 1.289040 -0.090882
H -2.457390 2.903230 -0.186853
H -0.320893 1.772805 -0.036139
H 0.104324 -1.834060 0.950446
H 0.068545 -0.332802 1.871793
H -2.689980 -0.841152 -1.177086
H -1.700125 -2.224775 -0.453534

CBS-QB3 (0 K)= -538.030894
CBS-QB3 Energy= -538.022963

CBS-QB3 Enthalpy=    -538.022019
CBS-QB3 Free Energy=    -538.064221


**P24**
H 2.231981 -1.773659 0.000000
C 2.247175 -0.687209 0.000000
C 0.934078 -0.036650 0.000000
C -0.176129 -0.816738 0.000000
Si -1.898152 -0.187688 0.000000
N -3.377122 0.319401 0.000000
C 3.426728 -0.056554 0.000000
H -0.068888 -1.898380 0.000000
H 4.355110 -0.614705 0.000000
H 3.511359 1.023704 0.000000
C 0.873720 1.467092 0.000000
H 1.377069 1.874108 0.881618
H 1.377069 1.874108 -0.881618
H -0.154849 1.835722 0.000000

CBS-QB3 (0 K)=    -537.956139
CBS-QB3 Energy=    -537.947477
CBS-QB3 Enthalpy=    -537.946533
CBS-QB3 Free Energy=    -537.989958


**P25**
H 0.663691 1.465925 0.000000
C -0.424181 1.524212 0.000000
C -1.137220 0.246228 0.000000
C -0.471622 -0.936176 0.000000
Si 1.354872 -1.131185 0.000000
N 2.903025 -1.347766 0.000000
C -0.993768 2.733512 0.000000
H -1.033166 -1.866030 0.000000
H -0.388732 3.631833 0.000000
H -2.068540 2.872430 0.000000
C -2.644957 0.261370 0.000000
H -3.025446 0.786874 0.880995
H -3.025446 0.786874 -0.880995
H -3.051920 -0.749337 0.000000

CBS-QB3 (0 K)=    -537.955707
CBS-QB3 Energy=    -537.947044

CBS-QB3 Enthalpy=    -537.946100
CBS-QB3 Free Energy=    -537.989607


**P26**
C -2.397797 1.566391 0.000000
C -2.092054 0.090892 0.000000
C -0.698893 -0.351224 0.000000
C 0.383780 0.456867 0.000000
Si 2.102175 -0.185810 0.000000
N 3.583333 -0.686033 0.000000
C -3.059214 -0.841097 0.000000
H -1.974216 2.057668 -0.881556
H -1.974216 2.057668 0.881556
H -3.474040 1.740635 0.000000
H -0.558941 -1.429612 0.000000
H 0.271528 1.537005 0.000000
H -4.108922 -0.571772 0.000000
H -2.824585 -1.899763 0.000000

CBS-QB3 (0 K)=    -537.954804
CBS-QB3 Energy=    -537.946183
CBS-QB3 Enthalpy=    -537.945239
CBS-QB3 Free Energy=    -537.988651


**P27**
C 2.229532 1.437133 0.000000
C 0.749537 1.634873 0.000000
C -0.212300 0.688457 0.000000
Si 0.293375 -1.110538 0.000000
N 0.708793 -2.616237 0.000000
C -1.642922 1.015626 0.000000
C -2.652170 0.141757 0.000000
H 2.679482 1.911855 -0.878714
H 2.517424 0.381327 0.000000
H 2.679482 1.911855 0.878714
H 0.415657 2.673303 0.000000
H -1.864971 2.081374 0.000000
H -2.491635 -0.933496 0.000000
H -3.682214 0.475203 0.000000

CBS-QB3 (0 K)=    -537.954032
CBS-QB3 Energy=    -537.945146
CBS-QB3 Enthalpy=    -537.944202
CBS-QB3 Free Energy=    -537.988215

**P28**

H -1.743679 1.362248 0.796291
C -0.988981 1.012872 0.094387
C -0.842273 -0.449450 -0.012145
C 0.361397 -1.061604 -0.059706
Si 1.981327 -0.209637 0.120888
N 3.466486 0.268231 0.225988
C -0.303635 1.906500 -0.623430
H 0.410970 -2.141776 -0.169795
H -0.443379 2.970840 -0.477337
H 0.395569 1.612407 -1.399422
C -2.127402 -1.237960 -0.031660
H -2.712259 -1.026362 0.870145
H -2.745100 -0.942571 -0.885717
H -1.946228 -2.311640 -0.082384

CBS-QB3 (0 K)=        -537.953421
CBS-QB3 Energy=        -537.944645
CBS-QB3 Enthalpy=       -537.943701
CBS-QB3 Free Energy=       -537.987366

**P29**

H 2.897916 -0.156103 0.484319
C 2.132670 -0.730513 -0.033207
C 0.783872 -0.133601 -0.028026
C -0.328536 -0.903298 -0.073402
Si -2.040680 -0.249091 -0.115025
N -3.511254 0.280784 -0.142921
C 2.483391 -1.858303 -0.655102
H -0.235867 -1.985368 -0.074541
H 3.502306 -2.224256 -0.616632
H 1.776266 -2.438716 -1.237664
C 0.750234 1.369469 0.052986
H 1.251533 1.708102 0.965801
H 1.290115 1.810561 -0.790691
H -0.266847 1.769021 0.057072

CBS-QB3 (0 K)=        -537.952537
CBS-QB3 Energy=        -537.943734
CBS-QB3 Enthalpy=       -537.942790
CBS-QB3 Free Energy=       -537.986704

**P30**

C -3.001084 0.138494 0.000000
C -1.633283 -0.470427 0.000000
C -0.443268 0.173808 0.000000
Si 1.071260 -0.918410 0.000000
N 2.341633 -1.827623 0.000000
C -0.254731 1.628020 0.000000
C 0.924610 2.255482 0.000000
H -3.560640 -0.203843 0.877427
H -3.560640 -0.203843 -0.877427
H -2.997444 1.227190 0.000000
H -1.629644 -1.558152 0.000000
H -1.159539 2.228608 0.000000
H 1.870395 1.718703 0.000000
H 0.985202 3.336568 0.000000

CBS-QB3 (0 K)=        -537.951526
CBS-QB3 Energy=        -537.942527
CBS-QB3 Enthalpy=       -537.941582
CBS-QB3 Free Energy=       -537.986099

**P31**

C -1.220884 2.013467 0.168223
C -1.746150 0.873333 -0.291694
C -1.287219 -0.483762 0.018840
C -0.079859 -0.658906 0.909229
Si 1.558021 -0.181456 0.063356
N 2.961368 0.100011 -0.560815
C -1.918119 -1.552272 -0.490357
H -0.381591 2.047178 0.854315
H -1.622941 2.972767 -0.132873
H -2.593552 0.925094 -0.969836
H 0.038002 -1.700426 1.215853
H -0.143851 -0.049191 1.815292
H -2.783919 -1.435168 -1.131622
H -1.593264 -2.565247 -0.284131

CBS-QB3 (0 K)=        -537.950904
CBS-QB3 Energy=        -537.942467
CBS-QB3 Enthalpy=       -537.941523
CBS-QB3 Free Energy=       -537.984859

**P32**

C -2.923179 -1.364246 0.048517
C -2.089148 -0.105468 0.064318

C -0.636941 -0.303595 0.209764
C 0.323571 0.490351 -0.303880
Si 2.115120 0.177791 -0.044742
N 3.649780 -0.057356 0.137945
C -2.628824 1.117853 -0.008130
H -3.985447 -1.134314 -0.040434
H -2.773653 -1.940781 0.967708
H -2.640657 -2.013479 -0.786259
H -0.345638 -1.194543 0.764076
H 0.058598 1.354634 -0.907242
H -3.699149 1.254119 -0.110171
H -2.025341 2.015305 0.059894

CBS-QB3 (0 K)=          -537.950175
CBS-QB3 Energy=          -537.941367
CBS-QB3 Enthalpy=        -537.940423
CBS-QB3 Free Energy=      -537.984470

**P33**
C 1.040240 -2.519092 -0.032805
C 1.289659 -1.058273 -0.220984
C 0.396656 -0.053113 -0.135561
Si -1.396447 -0.453544 0.195350
N -2.912217 -0.738466 0.447912
C 0.746700 1.375899 -0.285468
C 1.807557 1.952641 0.281540
H 1.341088 -3.078527 -0.924707
H -0.009170 -2.747826 0.177717
H 1.642233 -2.903356 0.798022
H 2.314784 -0.781209 -0.467293
H 0.070432 1.981076 -0.884510
H 2.477622 1.402394 0.933205
H 2.027598 3.000844 0.117864

CBS-QB3 (0 K)=          -537.949379
CBS-QB3 Energy=          -537.940496
CBS-QB3 Enthalpy=        -537.939551
CBS-QB3 Free Energy=      -537.983609

**P34**
C -2.855143 -1.396728 0.000000
C -2.448222 -0.124102 0.000000
C -1.058678 0.351248 0.000000
C 0.027219 -0.709943 0.000000

Si 1.802350 -0.069798 0.000000
N 3.280829 0.429479 0.000000
C -0.798530 1.665416 0.000000
H -2.167024 -2.234354 0.000000
H -3.909906 -1.642437 0.000000
H -3.196360 0.664441 0.000000
H -0.063266 -1.361036 -0.877144
H -0.063266 -1.361036 0.877144
H -1.602563 2.392160 0.000000
H 0.211136 2.065530 0.000000

CBS-QB3 (0 K)=          -537.948948
CBS-QB3 Energy=          -537.940415
CBS-QB3 Enthalpy=        -537.939471
CBS-QB3 Free Energy=      -537.983128

**P35**
C -2.744887 0.615620 -0.038800
C -1.270191 0.858065 -0.126469
C -0.284143 -0.037859 0.092327
Si 1.465714 0.600368 -0.009913
N 2.952245 1.081538 -0.059346
C -0.448271 -1.472565 0.413654
C -1.149605 -2.341915 -0.315181
H -3.201410 0.687442 -1.032866
H -3.211842 1.393635 0.573413
H -2.983706 -0.361907 0.377957
H -0.990312 1.880342 -0.373073
H 0.088095 -1.829964 1.290178
H -1.659006 -2.047338 -1.225907
H -1.217194 -3.384405 -0.027010

CBS-QB3 (0 K)=          -537.947241
CBS-QB3 Energy=          -537.938334
CBS-QB3 Enthalpy=        -537.937390
CBS-QB3 Free Energy=      -537.981592

**P36**
C -1.960050 1.910174 -0.489732
C -1.484963 1.059361 0.420604
C -1.208542 -0.372833 0.186348
C 0.037333 -0.918472 0.849499
Si 1.639827 -0.301550 0.022122
N 2.975067 0.141773 -0.655298

C -1.997262 -1.160482 -0.553146
H -2.161110 1.600563 -1.509464
H -2.147916 2.948387 -0.243458
H -1.247431 1.432822 1.415596
H 0.075853 -2.009775 0.820804
H 0.106807 -0.605510 1.896604
H -2.916094 -0.784211 -0.985426
H -1.755872 -2.201784 -0.733873

CBS-QB3 (0 K)=        -537.946358
CBS-QB3 Energy=          -537.937748
CBS-QB3 Enthalpy=        -537.936804
CBS-QB3 Free Energy=        -537.980883


**P37**
C -2.496354 1.812939 -0.073183
C -1.313537 1.200119 -0.020934
C -1.110973 -0.260469 0.052976
C 0.036923 -0.728359 0.923445
Si 1.748065 -0.409605 0.151114
N 3.149131 -0.132716 -0.480292
C -1.871075 -1.140442 -0.609268
H -3.428442 1.259321 -0.039927
H -2.565848 2.891985 -0.140583
H -0.410353 1.809695 -0.004779
H -0.010573 -1.804417 1.106717
H 0.048485 -0.219393 1.892367
H -2.664609 -0.810190 -1.267933
H -1.714217 -2.209565 -0.522318

CBS-QB3 (0 K)=        -537.945966
CBS-QB3 Energy=          -537.937340
CBS-QB3 Enthalpy=        -537.936396
CBS-QB3 Free Energy=        -537.980512


**P38**
C -3.146520 1.378728 -0.062987
C -2.168120 0.800006 0.633849
C -0.997945 0.110060 0.049280
C 0.299341 0.362500 0.802962
Si 1.839761 -0.478628 0.104554
N 3.130753 -1.152608 -0.456375
C -1.086683 -0.671434 -1.030537
H -3.137872 1.402810 -1.147207

H -3.982997 1.855266 0.434404
H -2.195024 0.850576 1.721073
H 0.212712 0.029088 1.844390
H 0.523655 1.434875 0.844311
H -2.040995 -0.861684 -1.505739
H -0.220522 -1.157754 -1.470727

CBS-QB3 (0 K)=        -537.944874
CBS-QB3 Energy=          -537.936176
CBS-QB3 Enthalpy=        -537.935232
CBS-QB3 Free Energy=        -537.979572

**i1**
C -2.079598 1.470799 -0.163831
C -1.786568 -0.007857 0.014352
C -2.764875 -0.930797 -0.313338
Si 3.236596 -0.651257 0.115972
N 1.861767 -0.063252 0.548150
C 0.587088 0.455931 0.928094
C -0.550257 -0.431662 0.504246
H -3.079801 1.621661 -0.572361
H -1.365861 1.940125 -0.847514
H -2.022866 2.009655 0.786585
H -3.729738 -0.622187 -0.696036
H 0.462373 1.462982 0.513608
H 0.566058 0.580222 2.024287
H -0.376705 -1.497323 0.620602
H -2.590680 -1.994202 -0.197198

CBS-QB3 (0 K)=        -538.604577
CBS-QB3 Energy=          -538.595995
CBS-QB3 Enthalpy=        -538.595051
CBS-QB3 Free Energy=        -538.640082


**i2**
C -2.745446 0.144407 0.000000
C -1.231802 0.205157 0.000000
C -0.570818 -1.155872 0.000000
Si 1.428499 -1.247976 0.000000
N 1.563664 0.365248 0.000000
C 0.900028 1.610353 0.000000
C -0.607237 1.384843 0.000000
H -3.113703 -0.396667 -0.878977
H -3.192835 1.140239 0.000000

H -3.113703 -0.396667 0.878977
H -0.887703 -1.741002 0.874239
H 1.167480 2.213504 -0.881350
H 1.167480 2.213504 0.881350
H -1.195875 2.299455 0.000000
H -0.887703 -1.741002 -0.874239

CBS-QB3 (0 K)=        -538.594071
CBS-QB3 Energy=        -538.586306
CBS-QB3 Enthalpy=       -538.585362
CBS-QB3 Free Energy=      -538.627103

H 3.241353 0.639608 -0.316946
H 0.711574 -2.093686 -0.221461
H -2.562478 1.125623 -0.142985
H -0.925984 2.677317 0.132465
H 1.427120 2.100592 -0.003417
H 0.348763 -1.460771 1.352478

CBS-QB3 (0 K)=        -538.635445
CBS-QB3 Energy=        -538.627903
CBS-QB3 Enthalpy=       -538.626959
CBS-QB3 Free Energy=      -538.668260

**i3**
C 2.771937 -0.091163 0.000000
C 1.256270 -0.093104 0.000000
C 0.588620 1.167271 0.000000
Si -1.198943 1.087506 0.000000
N -1.824673 -0.408058 0.000000
C -0.908317 -1.524327 0.000000
C 0.581226 -1.295994 0.000000
H 3.157386 0.431586 -0.880814
H 3.178616 -1.103927 0.000000
H 3.157386 0.431586 0.880814
H -2.060544 2.277246 0.000000
H -1.142781 -2.177363 -0.862531
H -1.142781 -2.177363 0.862531
H 1.175608 -2.207099 0.000000
H 1.190993 2.070273 0.000000

CBS-QB3 (0 K)=        -538.608898
CBS-QB3 Energy=        -538.601389
CBS-QB3 Enthalpy=       -538.600445
CBS-QB3 Free Energy=      -538.641110

**i5**
C 2.692850 -0.331250 0.026739
C 1.195138 -0.122632 0.000571
C 0.331497 -1.181751 0.028633
Si -1.488225 -0.986262 -0.122085
N -1.620630 0.777092 0.061036
C -0.558580 1.636531 0.007079
C 0.746438 1.251785 -0.031582
H 3.140664 0.168397 0.892359
H 3.158963 0.099547 -0.866354
H 2.950421 -1.390292 0.069605
H 0.763317 -2.179861 0.049602
H -2.525330 1.225191 0.090211
H -0.804868 2.694153 0.003843
H 1.493999 2.035347 -0.063522
H -2.262129 -1.613965 1.001018

CBS-QB3 (0 K)=        -538.648719
CBS-QB3 Energy=        -538.641332
CBS-QB3 Enthalpy=       -538.640388
CBS-QB3 Free Energy=      -538.680748

**i4**
C 2.669375 -0.279252 -0.166795
C 1.204720 -0.010027 0.024898
C 0.313898 -1.199513 0.277233
Si -1.571573 -1.042586 -0.137028
N -1.646647 0.706370 -0.037769
C -0.632946 1.635313 0.088896
C 0.718978 1.278851 0.048425
H 2.837050 -0.928820 -1.035213
H 3.090184 -0.809816 0.697886

**i6**
C -2.675744 -0.209334 0.078722
C -1.180159 0.014030 -0.027235
C -0.382995 -1.195861 -0.213062
Si 1.329890 -1.040668 0.057752
N 1.667817 0.569071 0.520485
C 0.791830 1.591289 -0.114898
C -0.665308 1.260236 0.096410
H -3.059603 -0.662158 -0.841680
H -3.207431 0.729912 0.243530

H -2.913790 -0.893428 0.899101
H 2.544448 0.905643 0.887083
H 1.021229 1.669711 -1.193398
H 1.027551 2.560926 0.330653
H -1.328158 2.088922 0.320605
H -0.863464 -2.113808 -0.524114

CBS-QB3 (0 K)=    -538.592390
CBS-QB3 Energy=    -538.584719
CBS-QB3 Enthalpy=    -538.583775
CBS-QB3 Free Energy=    -538.624759

**i7**
H -2.448004 0.734630 0.390441
C -2.130273 -0.288227 0.194052
C -3.117250 -1.253079 0.199915
Si 1.462314 1.379856 -2.551231
N 0.802794 1.030563 -1.184585
C 0.170408 0.716975 0.059761
C -0.766321 -0.469916 -0.027262
H -4.149319 -0.984819 0.385857
H -0.383658 1.591690 0.419587
H 0.948888 0.509391 0.810848
H -2.907383 -2.300734 0.023964
C -0.140054 -1.799879 -0.318021
H 0.334263 -2.214380 0.582490
H -0.861094 -2.534452 -0.678370
H 0.645191 -1.697012 -1.072087

CBS-QB3 (0 K)=    -538.608314
CBS-QB3 Energy=    -538.599596
CBS-QB3 Enthalpy=    -538.598652
CBS-QB3 Free Energy=    -538.643751

**i8**
C 2.838119 -0.092341 -0.000000
C 1.336489 0.024087 -0.000000
C 0.604052 -1.325476 -0.000000
N -0.790573 -1.128059 -0.000000
Si -2.021924 -0.077898 -0.000000
C -0.774146 1.490400 -0.000000
C 0.700072 1.197097 -0.000000
H 3.191213 -0.642650 0.879777
H 3.315222 0.889154 -0.000000
H 3.191213 -0.642650 -0.879777

H 0.935592 -1.896320 -0.881587
H -1.061645 2.087112 0.875860
H -1.061645 2.087112 -0.875860
H 1.330138 2.088299 -0.000000
H 0.935592 -1.896320 0.881587

CBS-QB3 (0 K)=    -538.595526
CBS-QB3 Energy=    -538.587706
CBS-QB3 Enthalpy=    -538.586762
CBS-QB3 Free Energy=    -538.628579

**i9**
C -2.746917 -0.265334 0.000000
C -1.259749 -0.054975 0.000000
C -0.433968 -1.328569 0.000000
N 1.009674 -1.281469 0.000000
Si 1.748821 0.157500 0.000000
C 0.640694 1.566512 0.000000
C -0.733423 1.222378 0.000000
H -3.064674 -0.841369 0.877943
H -3.064674 -0.841369 -0.877943
H -3.292595 0.680023 0.000000
H -0.769359 -1.933448 0.863752
H 3.213273 0.268875 0.000000
H 0.913283 2.615757 0.000000
H -1.453148 2.040131 0.000000
H -0.769359 -1.933448 -0.863752

CBS-QB3 (0 K)=    -538.610541
CBS-QB3 Energy=    -538.603045
CBS-QB3 Enthalpy=    -538.602101
CBS-QB3 Free Energy=    -538.642774

**i10**
C 2.767108 0.016572 0.030684
C 1.253169 -0.037730 -0.005408
C 0.567643 1.186539 -0.124276
N -0.800642 1.299720 0.032532
Si -2.034710 0.072037 0.237493
C -0.875774 -1.434900 -0.113516
C 0.594742 -1.239539 0.105196
H 3.175929 0.310262 -0.941863
H 3.183921 -0.960865 0.280041
H 3.131019 0.737250 0.769069

H -1.114048 2.261271 0.086821
H -1.069668 -1.679366 -1.175935
H -1.242682 -2.313112 0.430866
H 1.193590 -2.124537 0.309062
H 1.120100 2.112227 -0.241406

H 0.726332 2.390791 0.000000
H 1.592297 -2.177944 0.000000
H -1.358235 1.592388 -0.873617
H -0.801169 -2.379119 0.000000
H -1.358235 1.592388 0.873617

CBS-QB3 (0 K)=        -538.632669
CBS-QB3 Energy=        -538.624866
CBS-QB3 Enthalpy=      -538.623922
CBS-QB3 Free Energy=     -538.666084

CBS-QB3 (0 K)=        -538.629359
CBS-QB3 Energy=        -538.621828
CBS-QB3 Enthalpy=      -538.620884
CBS-QB3 Free Energy=     -538.661941

**i11**
C 2.627642 -0.412704 -0.023733
C 1.164566 -0.056850 0.083117
C 0.228433 -1.039369 0.226476
N -1.123080 -0.830723 0.328669
Si -1.904900 0.751790 0.524101
C -0.476899 1.832577 0.106595
C 0.787486 1.335702 0.006143
H 3.208938 0.027809 0.794069
H 3.061618 -0.043818 -0.959745
H 2.780905 -1.493770 0.008497
H 0.545342 -2.078020 0.253436
H -3.024411 0.826018 -0.473386
H -0.602834 2.909169 0.027269
H 1.607879 2.031731 -0.169231
H -1.667158 -1.677509 0.414877

CBS-QB3 (0 K)=        -538.645300
CBS-QB3 Energy=        -538.637919
CBS-QB3 Enthalpy=      -538.636975
CBS-QB3 Free Energy=     -538.677246

**i12**
C -2.754613 -0.584051 0.000000
C -1.275039 -0.335196 0.000000
C -0.882440 1.112759 0.000000
N 0.549476 1.394043 0.000000
Si 1.949359 0.376477 0.000000
C 1.027069 -1.247987 0.000000
C -0.369670 -1.377272 0.000000
H -3.235391 -0.135135 0.878721
H -2.980385 -1.651660 0.000000
H -3.235391 -0.135135 -0.878721