Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.


# Supporting Information

# Using Traceless Directing Group for the Silver-Mediated Synthesis of 3-Trifluoromethylpyrazoles: Computational Study on Mechanism and Origins of Regioselectivity

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# Table of Contents

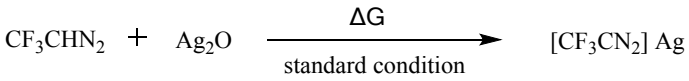
## I. Complete Gaussian 09 Reference

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.;Dapprich, S.;Daniels,A.D.; Farkas,Ö .; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, 2010.

## II. Computational screening of theoretical methods

In order to define the best theoretical calculation method for this reaction, by using the substitution of $CF_3CHN_2$ with $Ag_2O$ to produce silver trifluorodiazoethylide as the calculation model, we carried out a large number of calculations at different theoretical levels. As shown in Table S1, the results demonstrated that the M06/def2tzvpp//b3lyp/6-31G* is particularly suitable for describing this silver-containing system. In addition, the solvation model density (SMD) continuum method for the solvent effect and dispersion correction DFT-D3 method were used in all single-point energy calculations. Tetrahydrofuran (THF) was applied in this calculation to ensure consistency with the experimental condition.

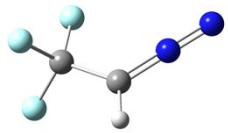
Table S1. Computational Screening of Theoretical Methods




| Theoretical methods | ΔG(kcal/mol) | Theoretical methods | ΔG(kcal/mol) |
|---|---|---|---|
| b2plyp/def2qzvpp// M062x/def2tzvp | 3.22 | b3lyp/def2tzvpp//b3lyp/6-31G* | 1.0731 |
| M06/def2tzvpp//b3lyp/6-31G* | 3.57 | M06-2x/def2tzvpp//b3lyp/6-31G* | -6.6456 |
| M06/6-311++G**//b3lyp/6-31G* | 0.5122 | M06-2x/6-311++G**//b3lyp/6-31G* | -9.8336 |
| b3lyp/6-311++G**//b3lyp/6-31G* | -6.8147 | M06-2x/6-311++G**//m062x/6-31G** | -3.3516 |

## III. Cartesian Coordinates

1

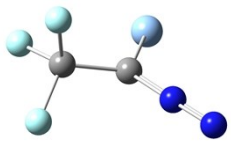


B3LYP electronic energy: -485.7730918 a.u.
B3LYP enthalpy: -485.727345 a.u.
B3LYP free energy: -485.766611 a.u.
M06 SCF energy in solution: -485.782607111 a.u.
M06 enthalpy in solution: -485.736861111 a.u.
M06 free energy in solution: -485.776127111 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| H | 0.49024800 | -1.91400400 | 0.08326500 |
| C | 0.52856700 | -0.83651700 | 0.01268000 |
| C | -0.70563300 | -0.00711500 | -0.00230500 |
| F | -1.38195100 | -0.06180400 | 1.16955800 |
| F | -0.41471500 | 1.28749200 | -0.24341500 |
| F | -1.56790700 | -0.43422400 | -0.95098100 |
| N | 1.69119000 | -0.26069200 | 0.01174300 |
| N | 2.71642600 | 0.23963700 | -0.00059600 |

2



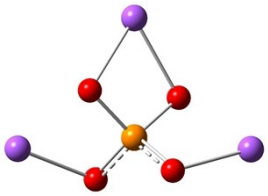
B3LYP electronic energy: -630.9300028 a.u.
B3LYP enthalpy: -630.893000 a.u.
B3LYP free energy: -630.938247 a.u.
M06 SCF energy in solution: -632.186290803 a.u.
M06 enthalpy in solution: -632.149287803 a.u.
M06 free energy in solution: -632.194534803 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|

| | | | |
|---|---|---|---|
| C | 0.42925200 | 0.47499700 | -0.01157400 |
| C | 1.47891100 | -0.57487400 | -0.00258200 |
| F | 2.43976000 | -0.37992400 | -0.94041500 |
| F | 2.13756800 | -0.68216800 | 1.18184600 |
| F | 0.92395100 | -1.79167200 | -0.24328500 |
| N | 0.81889300 | 1.70577400 | 0.00170800 |
| N | 1.11568300 | 2.81393800 | 0.00640600 |
| Ag | -1.58516000 | -0.11393300 | 0.00095400 |

3

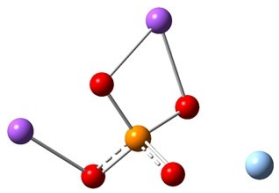


B3LYP electronic energy: - 1129.4100666 a.u.
B3LYP enthalpy: -1129.380938 a.u.
B3LYP free energy: -1129.425631 a.u.
M06 SCF energy in solution: -1129.4671627 a.u.
M06 enthalpy in solution: -1129.4380347 a.u.
M06 free energy in solution: -1129.4827267 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | -0.00015400 | -0.32972600 | -0.00049900 |
| O | -0.86839200 | -1.17727200 | -0.97205800 |
| O | -1.02407700 | 0.65716000 | 0.77018000 |
| O | 0.86705700 | -1.18024300 | 0.96946200 |
| O | 1.02496300 | 0.65753000 | -0.76914000 |
| Na | -2.66245200 | -0.58791300 | 0.01553800 |
| Na | 0.00055100 | 2.38438200 | 0.00014000 |
| Na | 2.66243700 | -0.58842500 | -0.01386600 |

4



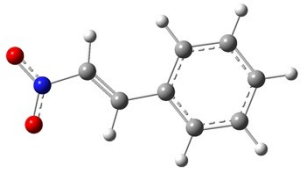
B3LYP electronic energy: -1112.8216025 a.u.
B3LYP enthalpy: -1112.792858 a.u.

B3LYP free energy: -1112.840018 a.u.
M06 SCF energy in solution: -1114.12044793 a.u.
M06 enthalpy in solution: -1114.09170393 a.u.
M06 free energy in solution: -1114.13886293 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | -0.87234400 | -0.28108700 | -0.03093300 |
| O | -1.64210700 | -1.27522800 | -0.93153300 |
| O | -1.97985900 | 0.58919700 | 0.74962200 |
| O | 0.13065200 | -0.97801200 | 0.95970600 |
| O | 0.00043800 | 0.80859600 | -0.84830200 |
| Na | -3.48916400 | -0.84847600 | 0.05506600 |
| Na | -1.12988500 | 2.43183600 | 0.01417300 |
| Ag | 1.95365300 | -0.13525700 | 0.00566900 |

5



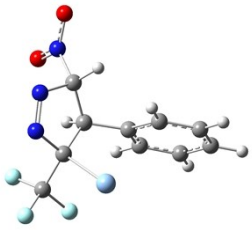
B3LYP electronic energy: -514.1518105 a.u.
B3LYP enthalpy: -514.004658 a.u.
B3LYP free energy: -514.050477 a.u.
M06 SCF energy in solution: -514.019897706 a.u.
M06 enthalpy in solution: -513.872744706 a.u.
M06 free energy in solution: -513.918563706 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.61446700 | -0.44188100 | 0.00025100 |
| H | -0.91759000 | -1.48635200 | 0.00036400 |
| C | -1.60696800 | 0.45956400 | -0.00006700 |
| H | -1.52244800 | 1.53685200 | -0.00086100 |
| N | -2.99317100 | 0.03109300 | -0.00002500 |
| O | -3.83355100 | 0.93574500 | -0.00130300 |
| O | -3.25502000 | -1.17425100 | 0.00121400 |
| C | 0.81996000 | -0.17153400 | 0.00019600 |
| C | 1.70492200 | -1.26532400 | -0.00042900 |
| C | 1.36048500 | 1.12966400 | 0.00065000 |
| C | 3.08414500 | -1.06996700 | -0.00065000 |
| H | 1.30009800 | -2.27418900 | -0.00075500 |

| | | | |
|---|---|---|---|
| C | 2.73678500 | 1.32353100 | 0.00047400 |
| H | 0.70048800 | 1.99194300 | 0.00132000 |
| C | 3.60372900 | 0.22510300 | -0.00019700 |
| H | 3.75157100 | -1.92693900 | -0.00122000 |
| H | 3.13827100 | 2.33290400 | 0.00092300 |
| H | 4.67883500 | 0.38124200 | -0.00025900 |

6



B3LYP electronic energy: -1145.1042371 a.u.
B3LYP enthalpy: -1144.916678 a.u.
B3LYP free energy: -1144.983303 a.u.
M06 SCF energy in solution: -1146.24334564 a.u.
M06 enthalpy in solution: -1146.05578664 a.u.
M06 free energy in solution: -1146.12241164 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.14433300 | -1.04226100 | 0.07309600 |
| N | 0.44692200 | -2.04719100 | -0.76364500 |
| C | -0.73048100 | -1.65016100 | 1.32688100 |
| C | 0.94323200 | 0.03648100 | 0.30753500 |
| H | 1.45662700 | -0.19916100 | 1.24809500 |
| N | 1.53969500 | -1.70869600 | -1.27264400 |
| Ag | -1.90439700 | -0.31092200 | -1.03962100 |
| F | -1.66942100 | -2.58206200 | 1.05996100 |
| F | -1.31138900 | -0.69061700 | 2.09320200 |
| F | 0.21039800 | -2.24177800 | 2.09874800 |
| C | 1.90705300 | -0.32780000 | -0.82303000 |
| H | 1.90352100 | 0.33749900 | -1.68752600 |
| N | 3.36823100 | -0.37874200 | -0.40483400 |
| O | 4.18377900 | -0.10712400 | -1.27688800 |
| O | 3.62586400 | -0.72102900 | 0.74383700 |
| C | 0.47263700 | 1.47783100 | 0.35556600 |
| C | 0.38818100 | 2.13365300 | 1.58965700 |
| C | 0.08059100 | 2.17735000 | -0.79857700 |
| C | -0.07958200 | 3.44642400 | 1.67460500 |
| H | 0.68595600 | 1.60767600 | 2.49278100 |

| | | | |
|---|---|---|---|
| C | -0.38465000 | 3.49236300 | -0.71697100 |
| H | 0.16382400 | 1.71042600 | -1.77800500 |
| C | -0.46910600 | 4.13057900 | 0.52211300 |
| H | -0.13663800 | 3.93404500 | 2.64385400 |
| H | -0.66729800 | 4.02003400 | -1.62408700 |
| H | -0.82797600 | 5.15382900 | 0.58690100 |

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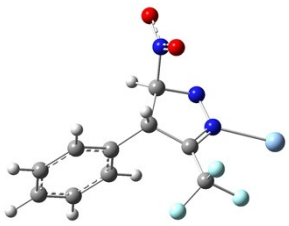


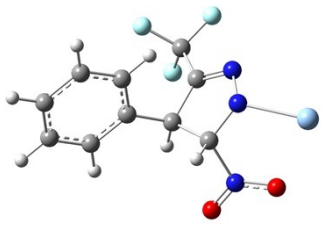
B3LYP electronic energy: - 1145.092699 a.u.
B3LYP enthalpy: -1144.90533 a.u.
B3LYP free energy: -1144.973789 a.u.
M06 SCF energy in solution: -1146.23853981 a.u.
M06 enthalpy in solution: -1146.05117081 a.u.
M06 free energy in solution: -1146.11962981 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 0.11868600 | -0.27733400 | 0.41401000 |
| N | 1.02172900 | 0.33110000 | -0.33241300 |
| C | 0.41240800 | -1.46854300 | 1.22695800 |
| C | -1.14499000 | 0.55534300 | 0.44925200 |
| H | -1.33315300 | 0.91311600 | 1.46845200 |
| N | 0.67659300 | 1.45845400 | -0.92110000 |
| Ag | 3.03928600 | -0.31953500 | -0.67585600 |
| F | 1.55447700 | -2.11190000 | 0.80160900 |
| F | -0.58359200 | -2.37807000 | 1.18901900 |
| F | 0.61925600 | -1.19505500 | 2.54326700 |
| C | -0.65927200 | 1.76608900 | -0.41068300 |
| H | -1.34092800 | 2.07220300 | -1.20526500 |
| N | -0.51292500 | 3.03994700 | 0.44868000 |
| O | -0.69333000 | 4.10630800 | -0.12712100 |
| O | -0.16736300 | 2.90834900 | 1.62138700 |
| C | -2.39396700 | -0.11905400 | -0.09110800 |
| C | -3.60866900 | -0.00806200 | 0.59549900 |
| C | -2.36453500 | -0.83064300 | -1.29857200 |
| C | -4.77086000 | -0.59299200 | 0.08855100 |
| H | -3.64450400 | 0.53871600 | 1.53509100 |

| | | | |
|---|---|---|---|
| C | -3.52388100 | -1.41423100 | -1.80819700 |
| H | -1.42550000 | -0.93066500 | -1.83798600 |
| C | -4.73185400 | -1.29696200 | -1.11565800 |
| H | -5.70475000 | -0.49907600 | 0.63639400 |
| H | -3.48451300 | -1.96281900 | -2.74566700 |
| H | -5.63499000 | -1.75356800 | -1.51147500 |

8



B3LYP electronic energy: -1145.1175068 a.u.
B3LYP enthalpy: -1144.930155 a.u.
B3LYP free energy: -1144.997291 a.u.
M06 SCF energy in solution: -1146.25226395 a.u.
M06 enthalpy in solution: -1146.06491295 a.u.
M06 free energy in solution: -1146.13204795 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 0.50717100 | 1.19496000 | 0.08517400 |
| N | -0.55961000 | 1.12712500 | -0.63792200 |
| C | 1.26045000 | 2.46917500 | 0.26794200 |
| C | 0.92588900 | -0.14070500 | 0.66760500 |
| H | 1.05545900 | -0.09897900 | 1.75162900 |
| N | -1.02545600 | -0.17637700 | -0.68439200 |
| Ag | -3.17526100 | -0.30201700 | -0.72978600 |
| F | 0.58849600 | 3.53498100 | -0.19327600 |
| F | 2.46331100 | 2.44098400 | -0.35670900 |
| F | 1.52059100 | 2.67655900 | 1.58507900 |
| C | -0.35672600 | -0.92409800 | 0.31123500 |
| H | -0.21547400 | -1.97839100 | 0.06471700 |
| N | -1.24422200 | -1.09789600 | 1.69252000 |
| O | -0.63148500 | -1.39833100 | 2.70167800 |
| O | -2.47659000 | -1.02573700 | 1.63256200 |
| C | 2.17645200 | -0.75166000 | 0.04704300 |
| C | 2.40090000 | -0.69768700 | -1.33525400 |
| C | 3.10051800 | -1.41788200 | 0.86015800 |
| C | 3.52854200 | -1.30138000 | -1.89097600 |
| H | 1.69326500 | -0.17643800 | -1.97425700 |
| C | 4.23104200 | -2.02028000 | 0.30442300 |

| | | | |
|---|---|---|---|
| H | 2.93352200 | -1.46538400 | 1.93366700 |
| C | 4.44702200 | -1.96448000 | -1.07311600 |
| H | 3.69189100 | -1.25055900 | -2.96417500 |
| H | 4.94205800 | -2.53008200 | 0.94907700 |
| H | 5.32702700 | -2.43128300 | -1.50733200 |

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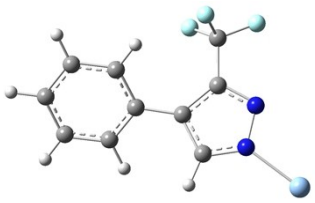

B3LYP electronic energy: -939.4364314 a.u.
B3LYP enthalpy: -939.276535 a.u.
B3LYP free energy: -939.334791 a.u.
M06 SCF energy in solution: -940.579278732 a.u.
M06 enthalpy in solution: -940.419382732 a.u.
M06 free energy in solution: -940.477638732 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.21401400 | 0.97063900 | -0.05662200 |
| N | 1.12317200 | 0.96497800 | -0.02900200 |
| C | -0.92711000 | 2.27920500 | -0.16637300 |
| C | -0.75414900 | -0.34249900 | 0.02425900 |
| N | 1.48059300 | -0.33065400 | 0.08032500 |
| Ag | 3.54840600 | -0.65620800 | 0.06092800 |
| F | -1.47700800 | 2.66350400 | 1.02187700 |
| F | -1.94840300 | 2.21973100 | -1.05256600 |
| F | -0.10964500 | 3.27402600 | -0.55218600 |
| C | 0.38895900 | -1.13562100 | 0.10333700 |
| H | 0.47795200 | -2.20856000 | 0.20652300 |
| C | -2.14602100 | -0.82622700 | 0.03418500 |
| C | -3.17572600 | -0.11874900 | 0.67945200 |
| C | -2.46893500 | -2.04618700 | -0.58775200 |
| C | -4.47837500 | -0.61534600 | 0.69762200 |
| H | -2.95116800 | 0.81741000 | 1.17782100 |
| C | -3.76983900 | -2.54587200 | -0.56021100 |
| H | -1.69221800 | -2.59459400 | -1.11442100 |
| C | -4.78298700 | -1.83126200 | 0.08227500 |
| H | -5.25791600 | -0.05070100 | 1.20276200 |
| H | -3.99424400 | -3.48972900 | -1.05088100 |
| H | -5.79916500 | -2.21617200 | 0.10016300 |

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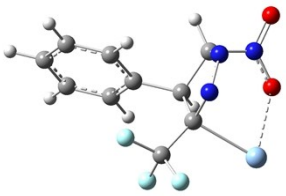
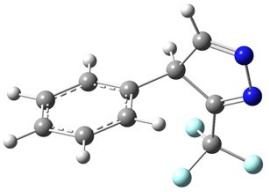


B3LYP electronic energy: -1145.1072376 a.u.
B3LYP enthalpy: -1144.919912 a.u.
B3LYP free energy: -1144.985032 a.u.
M06 SCF energy in solution: -1146.24077877 a.u.
M06 enthalpy in solution: -1146.05345377 a.u.
M06 free energy in solution: -1146.11857377 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 0.32349900 | -0.48903800 | 0.38955600 |
| N | 0.66748500 | -0.02128700 | 1.67410700 |
| C | -0.15568700 | -1.91633100 | 0.36506300 |
| C | -0.49340300 | 0.63754300 | -0.30220700 |
| N | 0.50779700 | 1.22041200 | 1.84333100 |
| Ag | 2.40578500 | -0.53694500 | -0.46104600 |
| F | 0.79675700 | -2.77689800 | 0.80476900 |
| F | -0.47728800 | -2.27756700 | -0.90118600 |
| F | -1.24673900 | -2.14226300 | 1.13130500 |
| C | -0.04750100 | 1.81973900 | 0.57602100 |
| H | -0.80776500 | 2.56171900 | 0.81191400 |
| N | 1.09838400 | 2.61829200 | -0.01902000 |
| O | 1.91154000 | 2.02850900 | -0.75582300 |
| O | 1.19233200 | 3.78788100 | 0.30839200 |
| H | -0.16252600 | 0.79211500 | -1.33006600 |
| C | -2.00676800 | 0.46452800 | -0.30753700 |
| C | -2.75663600 | 0.46360600 | 0.87876900 |
| C | -2.67807800 | 0.32035200 | -1.52792800 |
| C | -4.14396800 | 0.33108400 | 0.83920500 |
| H | -2.25620700 | 0.55607100 | 1.83891300 |
| C | -4.06649200 | 0.18296200 | -1.56845600 |
| H | -2.10932900 | 0.31704200 | -2.45497000 |
| C | -4.80383500 | 0.19098700 | -0.38402500 |
| H | -4.70957100 | 0.33391700 | 1.76689900 |
| H | -4.56947700 | 0.07317300 | -2.52536800 |
| H | -5.88500100 | 0.08729600 | -0.41239600 |

11

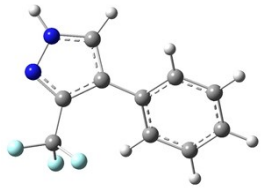


B3LYP electronic energy: -794.2456294 a.u.
B3LYP enthalpy: -794.077401 a.u.
B3LYP free energy: -794.131700 a.u.
M06 SCF energy in solution: -794.129475951 a.u.
M06 enthalpy in solution: -793.961247951 a.u.
M06 free energy in solution: -794.015545951 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.43228300 | 0.37400900 | -0.04063500 |
| N | 2.15565800 | 1.30156000 | 0.47087300 |
| C | 1.78885700 | -1.08143700 | 0.08644200 |
| C | 0.22767200 | 0.88856400 | -0.79210400 |
| N | 1.54341900 | 2.57643400 | 0.15838600 |
| F | 3.00987200 | -1.26917600 | 0.59486100 |
| F | 1.74095300 | -1.66969400 | -1.13332400 |
| F | 0.89986800 | -1.72293200 | 0.87459800 |
| C | 0.48855900 | 2.35025700 | -0.53955000 |
| H | -0.13852300 | 3.16391700 | -0.89188100 |
| H | 0.35989000 | 0.67147900 | -1.86266100 |
| C | -1.13736300 | 0.37801900 | -0.35085700 |
| C | -1.57324600 | 0.57723400 | 0.96606300 |
| C | -1.97311800 | -0.28423700 | -1.25489600 |
| C | -2.82593400 | 0.11894900 | 1.36859100 |
| H | -0.92868400 | 1.08919700 | 1.67651100 |
| C | -3.22826000 | -0.74350100 | -0.85074100 |
| H | -1.64209900 | -0.44587200 | -2.27799200 |
| C | -3.65722000 | -0.54251500 | 0.46096000 |
| H | -3.15291100 | 0.27779900 | 2.39239700 |
| H | -3.86743500 | -1.25839300 | -1.56259300 |
| H | -4.63339600 | -0.89991800 | 0.77654100 |

12

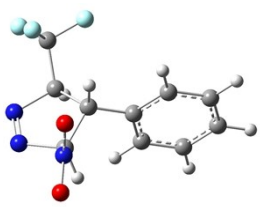


B3LYP electronic energy: -794.2919771 a.u.
B3LYP enthalpy: -794.121656 a.u.
B3LYP free energy: -794.173096 a.u.
M06 SCF energy in solution: -794.178325104 a.u.
M06 enthalpy in solution: -794.008004104 a.u.
M06 free energy in solution: -794.059444104 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.43950000 | 0.36413600 | -0.01843200 |
| N | -2.43744900 | 1.24139900 | -0.11157200 |
| C | -1.77283500 | -1.08322200 | 0.18052100 |
| C | -0.15603200 | 0.98030200 | -0.12642200 |
| N | -1.82039100 | 2.41961600 | -0.27958400 |
| F | -0.97090900 | -1.64760400 | 1.10984100 |
| F | -1.60372000 | -1.79924700 | -0.96462900 |
| F | -3.04467800 | -1.25715200 | 0.56944900 |
| C | -0.46711900 | 2.32193200 | -0.29323700 |
| H | 0.16943900 | 3.18274500 | -0.43848400 |
| H | -2.38401000 | 3.25117400 | -0.37875300 |
| C | 1.20250400 | 0.40757700 | -0.07183300 |
| C | 2.23589800 | 1.11906800 | 0.56149000 |
| C | 1.50804000 | -0.82764500 | -0.66662400 |
| C | 3.53524900 | 0.61635800 | 0.59437600 |
| H | 2.01097500 | 2.06336900 | 1.05051400 |
| C | 2.80677100 | -1.33210400 | -0.62560700 |
| H | 0.72941400 | -1.38902400 | -1.17065200 |
| C | 3.82606200 | -0.61336200 | 0.00116800 |
| H | 4.31829500 | 1.18138400 | 1.09315900 |
| H | 3.02284200 | -2.28950400 | -1.09216000 |
| H | 4.83746800 | -1.00947300 | 0.03013200 |

13



B3LYP electronic energy: -999.9600477 a.u.
B3LYP enthalpy: -999.762300 a.u.
B3LYP free energy: -999.823989 a.u.
M06 SCF energy in solution: -999.839267478 a.u.
M06 enthalpy in solution: -999.641519478 a.u.
M06 free energy in solution: -999.703208478 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.97201500 | -0.78941700 | 0.69663600 |
| N | -2.04452600 | 0.01524100 | 1.34487700 |
| C | -1.59619900 | -1.87380400 | -0.17285600 |
| C | -0.08621800 | 0.21816700 | -0.07519900 |
| H | -0.41320600 | 0.23680900 | -1.11838100 |
| N | -1.83539400 | 1.23229200 | 1.27805900 |
| F | -2.33135100 | -2.72516400 | 0.55927900 |
| F | -0.62431700 | -2.57945500 | -0.78937900 |
| F | -2.38806700 | -1.34460300 | -1.12447100 |
| C | -0.55129400 | 1.53085700 | 0.56002800 |
| H | 0.13943200 | 1.98324900 | 1.27243500 |
| N | -0.85959900 | 2.64337500 | -0.43105600 |
| O | -0.74546500 | 3.78319900 | -0.00203900 |
| O | -1.23146300 | 2.32362900 | -1.55454500 |
| H | -0.42731900 | -1.30071300 | 1.49828000 |
| C | 1.40566300 | -0.03749700 | -0.00798100 |
| C | 2.12934800 | -0.25428000 | -1.18578200 |
| C | 2.08825900 | -0.06197900 | 1.21712200 |
| C | 3.50465900 | -0.48891200 | -1.14351100 |
| H | 1.61280900 | -0.23980300 | -2.14222100 |
| C | 3.46213300 | -0.29547300 | 1.26144100 |
| H | 1.54867400 | 0.10132800 | 2.14854200 |
| C | 4.17479400 | -0.50967200 | 0.07967100 |
| H | 4.05018400 | -0.65494900 | -2.06819600 |
| H | 3.97514700 | -0.31007100 | 2.21901800 |
| H | 5.24517100 | -0.69178500 | 0.11376000 |

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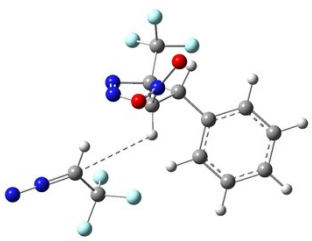

B3LYP electronic energy: -1485.74283878 a.u.
B3LYP enthalpy: -1485.497141 a.u.
B3LYP free energy: -1485.581589 a.u.
M06 SCF energy in solution: -1485.62715825 a.u.
M06 enthalpy in solution: -1485.38146125 a.u.
M06 free energy in solution: -1485.46590825 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.49922100 | -1.06517100 | -0.85813900 |
| N | -0.29733500 | -1.94276200 | -0.82618400 |
| C | -2.75409300 | -1.91819200 | -0.98989100 |
| C | -1.44415700 | -0.20242300 | 0.42821900 |
| H | -2.10605100 | -0.64045800 | 1.17998900 |
| N | 0.49374300 | -1.63535700 | 0.07207300 |
| F | -2.75906600 | -2.61070300 | -2.13906900 |
| F | -3.84822600 | -1.12768700 | -0.96924500 |
| F | -2.85972500 | -2.79363300 | 0.02918000 |
| C | -0.00632300 | -0.46705300 | 0.87151100 |
| H | 0.68290500 | 0.36429600 | 0.72831000 |
| N | 0.17841000 | -0.85032000 | 2.33202100 |
| O | 1.34508700 | -0.92013800 | 2.70543800 |
| O | -0.80992500 | -1.07655400 | 3.01621100 |
| H | -1.42611000 | -0.45916900 | -1.76787700 |
| C | -1.79596900 | 1.25863700 | 0.22473700 |
| C | -2.95191000 | 1.78368400 | 0.81246700 |
| C | -0.99344500 | 2.09864700 | -0.56215700 |
| C | -3.30162500 | 3.12138100 | 0.62249300 |
| H | -3.58271900 | 1.14130500 | 1.42161100 |
| C | -1.34258700 | 3.43556400 | -0.75107700 |
| H | -0.08499500 | 1.71792200 | -1.02456000 |
| C | -2.49798700 | 3.95088400 | -0.15983000 |
| H | -4.20198300 | 3.51308100 | 1.08754500 |
| H | -0.70907400 | 4.07460800 | -1.35986500 |
| H | -2.76830100 | 4.99262700 | -0.30772400 |
| H | 3.26783200 | -0.88710300 | 0.95347200 |
| C | 3.82510900 | -0.35785100 | 0.19162600 |
| C | 3.23375100 | 0.77601000 | -0.55263300 |
| F | 2.64849700 | 1.66062000 | 0.29746800 |
| F | 4.14626300 | 1.43188700 | -1.28935400 |
| F | 2.23045300 | 0.39858200 | -1.40368000 |
| N | 4.99490700 | -0.80331300 | -0.15367900 |
| N | 6.02944300 | -1.19108800 | -0.43505300 |

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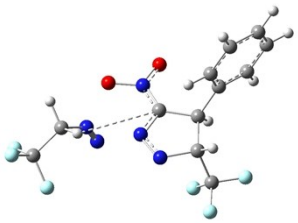

B3LYP electronic energy: -1485.7070136 a.u.
B3LYP enthalpy: -1485.461494 a.u.
B3LYP free energy: -1485.541726 a.u.
M06 SCF energy in solution: -1485.5962841 a.u.
M06 enthalpy in solution: -1485.3507641 a.u.
M06 free energy in solution: -1485.4309961 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.43925600 | -1.43133300 | -0.62367400 |
| N | -0.10261900 | -1.22137800 | -1.26694300 |
| C | -1.42543200 | -2.76803400 | 0.10378800 |
| C | -1.68481700 | -0.21940600 | 0.32363000 |
| H | -1.79036200 | -0.54511100 | 1.36433200 |
| N | 0.43234500 | -0.16420800 | -0.80675900 |
| F | -1.17709200 | -3.78918600 | -0.73269900 |
| F | -2.62028100 | -2.99790400 | 0.69374000 |
| F | -0.48586000 | -2.78839700 | 1.07524600 |
| C | -0.35984900 | 0.46364000 | 0.12337000 |
| H | 2.68160000 | 0.62624200 | -1.16403200 |
| N | 0.06898800 | 1.53965500 | 0.80338600 |
| O | 1.25551200 | 2.04759500 | 0.49987600 |
| O | -0.61394700 | 2.06872600 | 1.69896800 |
| H | -2.19352500 | -1.50671700 | -1.41293700 |
| C | -2.89526200 | 0.62677500 | -0.04368600 |
| C | -3.93348700 | 0.81009100 | 0.87421800 |
| C | -2.99756700 | 1.22063200 | -1.30888100 |
| C | -5.05572900 | 1.56763500 | 0.53620800 |
| H | -3.86032000 | 0.36157200 | 1.86174900 |
| C | -4.11763000 | 1.97834200 | -1.64882000 |
| H | -2.19379300 | 1.09683200 | -2.03172300 |
| C | -5.15161900 | 2.15313000 | -0.72658000 |
| H | -5.85311300 | 1.70189600 | 1.26217800 |
| H | -4.18126300 | 2.43403100 | -2.63337800 |
| H | -6.02439200 | 2.74422900 | -0.99031700 |
| H | 3.44303300 | 2.08685300 | -0.45607300 |

| | | | |
|---|---|---|---|
| C | 3.36282600 | 1.00273600 | -0.39530200 |
| C | 4.73421500 | 0.33155500 | -0.44590900 |
| F | 5.28879600 | 0.63395700 | -1.62976300 |
| F | 5.53353200 | 0.78056900 | 0.53517700 |
| F | 4.63567600 | -0.99926100 | -0.33484700 |
| N | 2.68080500 | 0.69374900 | 0.86348600 |
| N | 2.64167100 | 0.02318700 | 1.76934400 |

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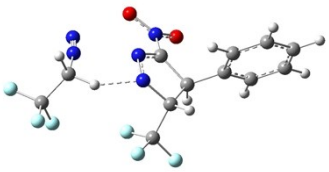

B3LYP electronic energy: -1485.7003554 a.u.
B3LYP enthalpy: -1485.455639 a.u.
B3LYP free energy: -1485.536197 a.u.
M06 SCF energy in solution: -1485.60211387 a.u.
M06 enthalpy in solution: -1485.35739687 a.u.
M06 free energy in solution: -1485.43795487 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 0.67661400 | -1.24093100 | 0.37904300 |
| N | -0.23636400 | -0.45331100 | 1.26589300 |
| C | -0.18779000 | -2.08623400 | -0.54462300 |
| C | 1.54454800 | -0.19602200 | -0.39482000 |
| H | 1.50506400 | -0.35908200 | -1.47657900 |
| N | -0.16439900 | 0.79293000 | 0.91160200 |
| F | -0.95005000 | -2.95685400 | 0.14669500 |
| F | 0.55606300 | -2.79330900 | -1.41913200 |
| F | -1.03465000 | -1.30783300 | -1.27118900 |
| C | 0.75019400 | 1.03101600 | -0.02149200 |
| H | -2.07808300 | -0.20327500 | 1.11014600 |
| N | 0.80315300 | 2.25867400 | -0.66136200 |
| O | -0.02306900 | 3.15833100 | -0.32719600 |
| O | 1.64432100 | 2.41267500 | -1.56496600 |
| H | 1.28025000 | -1.92937100 | 0.97665400 |
| C | 3.00377300 | -0.15715600 | 0.03479700 |
| C | 4.02173800 | -0.20570400 | -0.92237400 |
| C | 3.35184300 | -0.06274100 | 1.38958300 |

| | | | |
|---|---|---|---|
| C | 5.36270100 | -0.17191700 | -0.53693700 |
| H | 3.76177000 | -0.26099000 | -1.97627700 |
| C | 4.69109000 | -0.02980400 | 1.77665300 |
| H | 2.57168300 | -0.00869500 | 2.14576500 |
| C | 5.70123500 | -0.08659700 | 0.81386900 |
| H | 6.14164700 | -0.20986700 | -1.29376700 |
| H | 4.94545700 | 0.04343800 | 2.83076400 |
| H | 6.74493300 | -0.06051100 | 1.11535700 |
| H | -3.24224200 | 0.84262500 | 2.00772600 |
| C | -2.95426100 | 0.49638600 | 1.01152400 |
| C | -4.13887800 | -0.15460600 | 0.29061200 |
| F | -4.50641000 | -1.22403200 | 1.00437200 |
| F | -5.18180300 | 0.68893500 | 0.19997500 |
| F | -3.79588800 | -0.53537100 | -0.94428000 |
| N | -2.52169800 | 1.65614000 | 0.29448400 |
| N | -2.35536400 | 2.59124300 | -0.29711300 |

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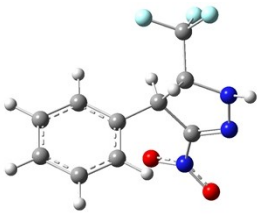

B3LYP electronic energy: -999.9670289 a.u.
B3LYP enthalpy: -999.768557 a.u.
B3LYP free energy: -999.829271 a.u.
M06 SCF energy in solution: -999.855844062 a.u.
M06 enthalpy in solution: -999.657372062 a.u.
M06 free energy in solution: -999.718086062 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.32918300 | -0.27393000 | 0.60141500 |
| N | -1.94502000 | 0.99126400 | 1.03613900 |
| C | -2.34812600 | -1.14325500 | -0.12082300 |
| C | -0.15002300 | 0.20251600 | -0.30762500 |
| H | -0.42541400 | 0.09077400 | -1.36250700 |
| N | -1.13437100 | 2.05296500 | 0.81575600 |
| F | -3.38721200 | -1.42370400 | 0.69485900 |
| F | -1.78243600 | -2.30935300 | -0.49341100 |
| F | -2.83571600 | -0.54814500 | -1.22278300 |
| C | -0.16816700 | 1.67245600 | 0.05898900 |

| | | | |
|---|---|---|---|
| H | -2.45488200 | 1.03776700 | 1.90952300 |
| N | 0.75593400 | 2.64073800 | -0.48987100 |
| O | 0.79328200 | 3.76839500 | -0.00809700 |
| O | 1.44649700 | 2.23015400 | -1.42907000 |
| H | -0.95504400 | -0.85737100 | 1.45173500 |
| C | 1.15617900 | -0.53063800 | -0.05857200 |
| C | 1.63171800 | -1.44868100 | -0.99983400 |
| C | 1.87880200 | -0.33419800 | 1.12529600 |
| C | 2.80976100 | -2.15830600 | -0.76530000 |
| H | 1.07830500 | -1.60739400 | -1.92193600 |
| C | 3.05866400 | -1.03994200 | 1.35945700 |
| H | 1.52724500 | 0.38262300 | 1.86452800 |
| C | 3.52640200 | -1.95535500 | 0.41472700 |
| H | 3.16809400 | -2.86677700 | -1.50694800 |
| H | 3.61382600 | -0.87124800 | 2.27806000 |
| H | 4.44593700 | -2.50470400 | 0.59634500 |

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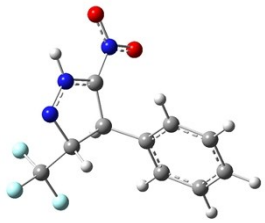


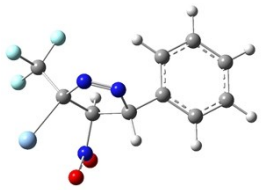
B3LYP electronic energy: -999.9443513 a.u.
B3LYP enthalpy: -999.745703 a.u.
B3LYP free energy: -999.806329 a.u.
M06 SCF energy in solution: -999.830723515 a.u.
M06 enthalpy in solution: -999.632075515 a.u.
M06 free energy in solution: -999.692701515 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.15252300 | -0.57980700 | 0.66014200 |
| N | -1.86983700 | 0.48843100 | 1.39635700 |
| C | -2.16438800 | -1.43681400 | -0.09410300 |
| C | -0.09810600 | 0.09599000 | -0.31078100 |
| H | -0.37005200 | -0.10302600 | -1.35408600 |
| N | -1.35304600 | 1.57904500 | 0.93754900 |
| F | -3.04095900 | -2.01785400 | 0.73797400 |
| F | -1.52077200 | -2.41358100 | -0.77376000 |
| F | -2.85499300 | -0.70436900 | -0.99085700 |
| C | -0.38109500 | 1.52944000 | 0.02466000 |

| | | | |
|---|---|---|---|
| H | -1.69151200 | 2.48451400 | 1.27262300 |
| N | 0.09018500 | 2.71715000 | -0.53892100 |
| O | -0.35837400 | 3.78840700 | -0.07480500 |
| O | 0.91748400 | 2.62305300 | -1.45435300 |
| H | -0.66009300 | -1.23588200 | 1.38600800 |
| C | 1.32620900 | -0.38630400 | -0.08537000 |
| C | 1.81979600 | -1.44037700 | -0.86272600 |
| C | 2.13758700 | 0.15801400 | 0.91631900 |
| C | 3.10316700 | -1.94093200 | -0.64422700 |
| H | 1.19352900 | -1.87325500 | -1.63872300 |
| C | 3.42295200 | -0.33899600 | 1.13301600 |
| H | 1.77058800 | 0.98206400 | 1.52349900 |
| C | 3.90869600 | -1.39045700 | 0.35403400 |
| H | 3.47441100 | -2.75760400 | -1.25718600 |
| H | 4.04537900 | 0.09882600 | 1.90851600 |
| H | 4.91048400 | -1.77602000 | 0.52172400 |

19



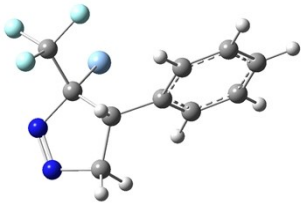
B3LYP electronic energy: -1145.1146577 a.u.
B3LYP enthalpy: -1144.927097 a.u.
B3LYP free energy: -1144.993184 a.u.
M06 SCF energy in solution: -1146.24699372 a.u.
M06 enthalpy in solution: -1146.05943272 a.u.
M06 free energy in solution: -1146.12551972 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 0.83890300 | 0.52720700 | -0.17131300 |
| N | 0.37040300 | 0.77790900 | -1.51484500 |
| C | 1.23767000 | 1.80313800 | 0.52054900 |
| C | -1.21723700 | -0.61504500 | -0.65115500 |
| H | -1.10074000 | -1.67389200 | -0.91112600 |
| N | -0.67860800 | 0.17076600 | -1.81052400 |
| Ag | 2.66443100 | -0.68136700 | -0.50934900 |
| F | 2.18704300 | 2.48244900 | -0.14877900 |
| F | 1.70738300 | 1.54566500 | 1.76713900 |
| F | 0.18294000 | 2.65235600 | 0.68111500 |
| C | -0.27034400 | -0.25237400 | 0.53345900 |

| | | | |
|---|---|---|---|
| H | -0.77825300 | 0.30808000 | 1.31807900 |
| N | 0.17087200 | -1.51751800 | 1.23846500 |
| O | -0.29166900 | -1.71820900 | 2.35109400 |
| O | 0.92392500 | -2.30381000 | 0.64483400 |
| C | -2.67699000 | -0.29914600 | -0.41953000 |
| C | -3.63467700 | -1.31820100 | -0.40198900 |
| C | -3.08488100 | 1.02792700 | -0.22114700 |
| C | -4.98112900 | -1.02071300 | -0.18287500 |
| H | -3.32688400 | -2.34922200 | -0.55999200 |
| C | -4.42912900 | 1.32521800 | -0.00356200 |
| H | -2.34734400 | 1.82649300 | -0.23766300 |
| C | -5.38042700 | 0.30141300 | 0.01630000 |
| H | -5.71539800 | -1.82146400 | -0.16926100 |
| H | -4.73511900 | 2.35677000 | 0.14723100 |
| H | -6.42808300 | 0.53475800 | 0.18533900 |

20



B3LYP electronic energy: -940.6143879 a.u.
B3LYP enthalpy: -940.431820 a.u.
B3LYP free energy: -940.491377 a.u.
M06 SCF energy in solution: -941.747236362 a.u.
M06 enthalpy in solution: -941.564668362 a.u.
M06 free energy in solution: -941.624225362 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.03954200 | 0.37022800 | -0.34229900 |
| N | 2.01400300 | 0.23415400 | -1.40851900 |
| C | 1.66942000 | 0.99985600 | 0.87624400 |
| C | -0.15860000 | 1.14835700 | -0.93670200 |
| H | -0.01545000 | 2.21089800 | -0.69443200 |
| N | 1.55655800 | 0.53886400 | -2.53247300 |
| Ag | 0.56791500 | -1.68501600 | 0.27866800 |
| F | 2.71705900 | 0.29362900 | 1.35109600 |
| F | 0.76635700 | 1.11640700 | 1.88514600 |
| F | 2.12248500 | 2.25561400 | 0.62606200 |
| C | 0.13289700 | 0.95514800 | -2.43991800 |

| | | | |
|---|---|---|---|
| H | -0.46738600 | 0.16107200 | -2.90292900 |
| C | -1.54020000 | 0.75399100 | -0.44451700 |
| C | -2.18322400 | 1.54866700 | 0.51403200 |
| C | -2.19993800 | -0.40362600 | -0.89067000 |
| C | -3.43781500 | 1.20066600 | 1.01752500 |
| H | -1.68810900 | 2.44562500 | 0.87708100 |
| C | -3.45644500 | -0.75449000 | -0.39068800 |
| H | -1.74578700 | -1.03234000 | -1.65243600 |
| C | -4.08042200 | 0.04601500 | 0.56807200 |
| H | -3.91250600 | 1.83436800 | 1.76193500 |
| H | -3.95129700 | -1.64857700 | -0.76147400 |
| H | -5.05898800 | -0.22409400 | 0.95522100 |
| H | -0.01081000 | 1.85796300 | -3.04064700 |

21. $Ag_2O$

B3LYP electronic energy: -366.7041346 a.u.
B3LYP enthalpy: -366.696701 a.u.
B3LYP free energy: -366.731589 a.u.
M06 SCF energy in solution: -369.173801558 a.u.
M06 enthalpy in solution: -369.166367558 a.u.
M06 free energy in solution: -369.201255558 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| O | 0.00000000 | 0.00000000 | 1.25422500 |
| Ag | 0.00000000 | -1.51416500 | -0.10674300 |
| Ag | 0.00000000 | 1.51416500 | -0.10674300 |

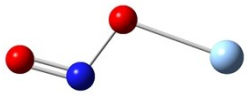
22. AgOH

B3LYP electronic energy: -221.5552675 a.u.
B3LYP enthalpy: -221.539714 a.u.
B3LYP free energy: -221.568641 a.u.
M06 SCF energy in solution: -222.808277364 a.u.
M06 enthalpy in solution: -222.792723364 a.u.
M06 free energy in solution: -222.821650364 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| O | 0.01677100 | 1.70720300 | 0.00000000 |
| Ag | 0.01677100 | -0.33228300 | 0.00000000 |
| H | -0.92238400 | 1.95966000 | 0.00000000 |

23. $AgNO_2$

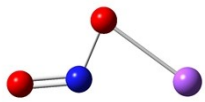


B3LYP electronic energy: -350.8563762 a.u.
B3LYP enthalpy: -350.876690 a.u.
B3LYP free energy: -350.841576 a.u.
M06 SCF energy in solution: -352.101032577 a.u.
M06 enthalpy in solution: -352.086232577 a.u.
M06 free energy in solution: -352.121345577 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Ag | 0.95751800 | -0.03947000 | -0.00005500 |
| N | -1.83621100 | -0.40654100 | 0.00071000 |
| O | -1.02402000 | 0.67416700 | 0.00028100 |
| O | -2.99471500 | -0.08655700 | -0.00058000 |

24. $NaNO_2$

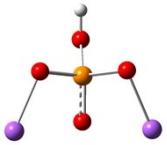


B3LYP electronic energy: -367.4410566 a.u.
B3LYP enthalpy: -367.425792 a.u.
B3LYP free energy: -367.458119 a.u.
M06 SCF energy in solution: -367.449403607 a.u.
M06 enthalpy in solution: -367.434138607 a.u.
M06 free energy in solution: -367.466465607 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| N | -0.56017300 | -0.24232400 | 0.00004500 |
| O | -0.04665800 | 0.95648800 | -0.00000300 |
| O | -1.77337900 | -0.34070700 | -0.00002500 |
| Na | 1.68013700 | -0.29363500 | -0.00000900 |

25. $Na_2HPO_4$

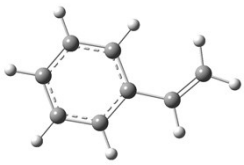


B3LYP electronic energy: -967.6659331 a.u.
B3LYP enthalpy: -967.628029 a.u.
B3LYP free energy: -967.670456 a.u.
M06 SCF energy in solution: -967.732818704 a.u.
M06 enthalpy in solution: -967.694914704 a.u.
M06 free energy in solution: -967.737341704 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | -0.00003500 | 0.48582600 | 0.11854100 |
| O | -1.32062600 | 0.61596900 | 0.89621200 |
| O | 0.00042000 | -0.88323300 | -0.68730400 |
| O | 0.00006100 | 1.62400100 | -1.09526200 |
| O | 1.31996900 | 0.61582100 | 0.89712300 |
| Na | -2.09472300 | -1.16257900 | -0.05374800 |
| Na | 2.09502600 | -1.16194300 | -0.05386800 |
| H | -0.00141100 | 2.50189500 | -0.68048200 |

26. $PhCH=CH_2$



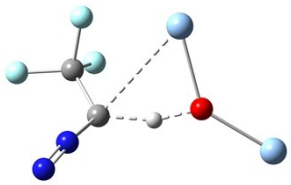
B3LYP electronic energy: -309.6482589 a.u.
B3LYP enthalpy: -309.506814 a.u.
B3LYP free energy: -309.546006 a.u.
M06 SCF energy in solution: -309.516289991 a.u.
M06 enthalpy in solution: -309.374844991 a.u.
M06 free energy in solution: -309.414036991 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.95471800 | -0.52927100 | -0.00022500 |
| H | 2.18626000 | -1.59464700 | -0.00073700 |
| C | 2.97740200 | 0.33497300 | 0.00029500 |
| H | 2.84080300 | 1.41304900 | 0.00083000 |

| | | | |
|---|---|---|---|
| C | 0.51518800 | -0.22049100 | -0.00009200 |
| C | -0.40647400 | -1.28137400 | 0.00000100 |
| C | 0.00885300 | 1.09243700 | -0.00018900 |
| C | -1.78089400 | -1.04613800 | 0.00012600 |
| H | -0.03501300 | -2.30384300 | -0.00000200 |
| C | -1.36221500 | 1.32960500 | -0.00005900 |
| H | 0.69403100 | 1.93525500 | -0.00039900 |
| C | -2.26534300 | 0.26183600 | 0.00011700 |
| H | -2.47205800 | -1.88494300 | 0.00024400 |
| H | -1.73037500 | 2.35233600 | -0.00013300 |
| H | -3.33547100 | 0.45048900 | 0.00019000 |
| H | 4.00440800 | -0.01716700 | 0.00016500 |

TS1

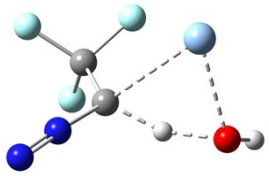


B3LYP electronic energy: -852.481158773 a.u.
B3LYP enthalpy: -852.432109 a.u.
B3LYP free energy: -852.488586 a.u.
M06 SCF energy in solution: -854.964266469 a.u.
M06 enthalpy in solution: -854.915216469 a.u.
M06 free energy in solution: -854.971693469 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| H | -0.12243200 | -0.83008800 | 0.04956200 |
| C | -1.42860000 | -1.19186100 | 0.07023200 |
| C | -2.42829700 | -0.48351700 | -0.73090200 |
| F | -2.05387400 | -0.34564000 | -2.01973500 |
| F | -3.66780400 | -1.01260200 | -0.70450800 |
| F | -2.62435600 | 0.86739900 | -0.30785900 |
| N | -1.86332200 | -1.89622700 | 1.06395100 |
| N | -2.14140600 | -2.56896600 | 1.95033500 |
| O | 0.87066300 | -0.15185700 | 0.18663800 |
| Ag | 2.82219700 | -0.58598400 | -0.23088600 |
| Ag | -0.28079500 | 1.60239200 | 0.41408300 |

TS2

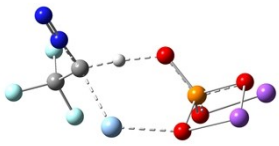


B3LYP electronic energy: -707.329355978 a.u.
B3LYP enthalpy: -707.270775 a.u.
B3LYP free energy: -707.320226 a.u.
M06 SCF energy in solution: -708.588412362 a.u.
M06 enthalpy in solution: -708.529831362 a.u.
M06 free energy in solution: -708.579282362 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| H | 0.08580800 | 0.56558600 | 1.23561400 |
| C | -0.77716600 | 0.54575800 | 0.26701100 |
| C | -1.60612300 | -0.66864800 | 0.04326200 |
| F | -2.49832100 | -0.91681700 | 1.03238500 |
| F | -2.31247100 | -0.63751700 | -1.11159900 |
| F | -0.79506100 | -1.76949100 | -0.01090700 |
| N | -1.32625300 | 1.68204200 | -0.07777300 |
| N | -1.72005200 | 2.71652100 | -0.34956800 |
| O | 1.30287000 | 0.50071900 | 1.78115800 |
| Ag | 1.57906200 | -0.09555600 | -0.33994800 |
| H | 1.35186000 | -0.21836100 | 2.43351100 |

TS3



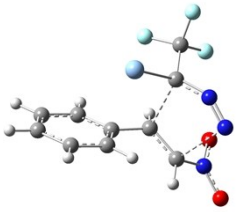
B3LYP electronic energy: -1598.6108746 a.u.
B3LYP enthalpy: -1598.538587 a.u.
B3LYP free energy: -1598.605058 a.u.
M06 SCF energy in solution: -1599.91618101 a.u.
M06 enthalpy in solution: -1599.84389301 a.u.
M06 free energy in solution: -1599.91036401 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.82022300 | 0.13364300 | 0.59888400 |
| C | -2.62405800 | 1.06439200 | -0.25870800 |

| | | | |
|---|---|---|---|
| F | -3.81561800 | 0.52512300 | -0.62932900 |
| F | -2.91204800 | 2.23896800 | 0.34752600 |
| F | -1.93776000 | 1.35265700 | -1.38290300 |
| N | -2.50325500 | -0.40319400 | 1.59671200 |
| N | -3.01466400 | -0.90301500 | 2.47791100 |
| P | 1.83516200 | 0.44244900 | 0.20153900 |
| O | 1.87648100 | 1.60816800 | -0.81003600 |
| O | 3.27412700 | 0.33963700 | 0.89099300 |
| O | 0.71073700 | 0.57551000 | 1.27733700 |
| O | 1.67245900 | -0.99754700 | -0.54213800 |
| Na | 3.75191300 | 2.29493500 | -0.02689700 |
| Na | 3.45076900 | -1.75796400 | 0.42634500 |
| Ag | -0.49068000 | -1.28340500 | -0.64798600 |
| H | -0.68546200 | 0.47497700 | 0.92800200 |

TS4



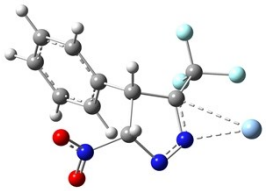
B3LYP electronic energy: -1145.0521397 a.u.
B3LYP enthalpy: -1144.867888 a.u.
B3LYP free energy: -1144.935483 a.u.
M06 SCF energy in solution: -1146.19321033 a.u.
M06 enthalpy in solution: -1146.00895933 a.u.
M06 free energy in solution: -1146.07655333 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 0.64544500 | -0.91844700 | -0.24065200 |
| N | 1.49794100 | -0.74954900 | -1.25263300 |
| C | 1.09563200 | -1.88419800 | 0.82113800 |
| C | 0.68275800 | 1.08407100 | 0.45463900 |
| H | 1.13183800 | 0.82030000 | 1.40782600 |
| N | 2.07714200 | 0.03907300 | -1.87597500 |
| Ag | -1.46131500 | -1.12594100 | -0.79894700 |
| F | 0.92704200 | -3.18038000 | 0.45871100 |
| F | 0.34387400 | -1.68465300 | 1.93306900 |
| F | 2.38529000 | -1.73495300 | 1.17038400 |
| C | 1.52970100 | 1.76999100 | -0.42031500 |
| H | 1.21082300 | 2.47654500 | -1.17232500 |

| | | | |
|---|---|---|---|
| N | 2.91631400 | 1.92789300 | -0.07745500 |
| O | 3.55408900 | 2.78253100 | -0.70194200 |
| O | 3.39236500 | 1.20155200 | 0.80694600 |
| C | -0.76885800 | 1.39985500 | 0.49774800 |
| C | -1.45085300 | 1.38041300 | 1.72457300 |
| C | -1.51625900 | 1.67366900 | -0.67135200 |
| C | -2.82248100 | 1.63725300 | 1.79191600 |
| H | -0.89690000 | 1.16209700 | 2.63332400 |
| C | -2.89242300 | 1.92517500 | -0.60202600 |
| H | -1.00975800 | 1.73207600 | -1.63238200 |
| C | -3.55122700 | 1.90646800 | 0.63194300 |
| H | -3.32185300 | 1.62529500 | 2.75683700 |
| H | -3.44100200 | 2.15557500 | -1.51173500 |
| H | -4.61720700 | 2.10716000 | 0.68621200 |

TS5



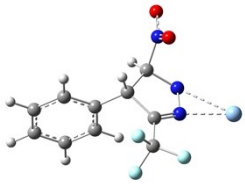
B3LYP electronic energy: -1145.0769945 a.u.
B3LYP enthalpy: -1144.890715 a.u.
B3LYP free energy: -1144.954934 a.u.
M06 SCF energy in solution: -1146.22031651 a.u.
M06 enthalpy in solution: -1146.03403651 a.u.
M06 free energy in solution: -1146.09825651 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.54726400 | -0.25565800 | 0.26102100 |
| N | -1.05161000 | 0.63567700 | -0.65250200 |
| C | -0.74434200 | -1.71725000 | 0.04797800 |
| C | 0.73870900 | 0.32325700 | 0.85389800 |
| N | -0.51227500 | 1.80516400 | -0.64998600 |
| Ag | -3.18200500 | 0.28270200 | 0.02796300 |
| F | -2.07784800 | -2.06475100 | -0.09302000 |
| F | -0.27150100 | -2.41252100 | 1.09863400 |
| F | -0.15211300 | -2.21321900 | -1.06383500 |
| C | 0.47051300 | 1.81374500 | 0.43504900 |
| H | 0.08267700 | 2.38209200 | 1.28829800 |
| N | 1.72792500 | 2.56176700 | 0.04746700 |
| O | 2.40343500 | 2.96664700 | 0.99126300 |

| | | | |
|---|---|---|---|
| O | 1.99804800 | 2.68330800 | -1.13733900 |
| H | 0.73160200 | 0.25876800 | 1.94392400 |
| C | 2.03711900 | -0.30171400 | 0.35746900 |
| C | 2.31602700 | -0.43900300 | -1.01071800 |
| C | 2.98440400 | -0.74555200 | 1.28835100 |
| C | 3.51809900 | -1.00603100 | -1.43146600 |
| H | 1.59830200 | -0.09426300 | -1.74808700 |
| C | 4.18616200 | -1.31632500 | 0.86768300 |
| H | 2.78041800 | -0.64069400 | 2.35144700 |
| C | 4.45562200 | -1.44748000 | -0.49510500 |
| H | 3.72255500 | -1.10047800 | -2.49434500 |
| H | 4.90998000 | -1.65469300 | 1.60412600 |
| H | 5.39140700 | -1.88916000 | -0.82683700 |

TS6



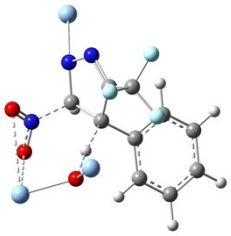
B3LYP electronic energy: -1145.0898447 a.u.
B3LYP enthalpy: -1144.903292 a.u.
B3LYP free energy: -1144.969981 a.u.
M06 SCF energy in solution: -1146.23567891 a.u.
M06 enthalpy in solution: -1146.04912591 a.u.
M06 free energy in solution: -1146.11581591 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.03974600 | -0.54824400 | 0.40772200 |
| N | 0.93347200 | -0.18556100 | -0.37836700 |
| C | -0.12403900 | -1.90964800 | 0.98106800 |
| C | -1.05168200 | 0.57305200 | 0.53415600 |
| H | -1.17300800 | 0.86331400 | 1.58266600 |
| N | 0.87357900 | 1.07014200 | -0.87464900 |
| Ag | 3.08397700 | -0.25837100 | -0.64696600 |
| F | 1.09956800 | -2.49891100 | 1.04235400 |
| F | -0.91819600 | -2.75176800 | 0.27124400 |
| F | -0.62992300 | -1.87845300 | 2.23545500 |
| C | -0.27482800 | 1.69447700 | -0.22834400 |
| H | -0.87656400 | 2.29639300 | -0.90950400 |
| N | 0.28921900 | 2.73266200 | 0.76724000 |
| O | 0.26278200 | 3.90614200 | 0.41506400 |

| | | | |
|---|---|---|---|
| O | 0.77866100 | 2.31154400 | 1.81483600 |
| C | -2.41194400 | 0.26005300 | -0.06824900 |
| C | -2.51954900 | -0.27361500 | -1.36046500 |
| C | -3.58158000 | 0.52019900 | 0.65502200 |
| C | -3.77075200 | -0.53437200 | -1.91756100 |
| H | -1.61817400 | -0.48723700 | -1.92950500 |
| C | -4.83549300 | 0.25616200 | 0.10001400 |
| H | -3.51050000 | 0.92990100 | 1.66000800 |
| C | -4.93318700 | -0.27068400 | -1.18842000 |
| H | -3.83841200 | -0.94710800 | -2.92062700 |
| H | -5.73388200 | 0.46128400 | 0.67606700 |
| H | -5.90806500 | -0.47740800 | -1.62161200 |

TS7



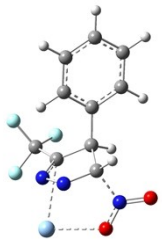
B3LYP electronic energy: -1511.8262095 a.u.
B3LYP enthalpy: -1511.636284 a.u.
B3LYP free energy: -1511.719448 a.u.
M06 SCF energy in solution: -1515.42317605 a.u.
M06 enthalpy in solution: -1515.23325105 a.u.
M06 free energy in solution: -1515.31641505 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 0.85434100 | 0.89470500 | -0.91455100 |
| N | 1.86505200 | 0.22310000 | -1.39292700 |
| C | 0.21644500 | 1.92844300 | -1.77952100 |
| C | 0.37448200 | 0.46161100 | 0.41811600 |
| H | -0.97275900 | 0.06795600 | 0.34232400 |
| N | 2.21223200 | -0.76554500 | -0.50917600 |
| Ag | 4.31703100 | -1.05028700 | -0.46744600 |
| F | -0.52988000 | 2.79891800 | -1.05911500 |
| F | -0.66722100 | 1.37544600 | -2.69586000 |
| F | 1.09450300 | 2.63309200 | -2.50697100 |
| C | 1.31168400 | -0.74501100 | 0.61346800 |
| H | 1.75661800 | -0.83436800 | 1.60360500 |
| N | 0.43050900 | -2.06761400 | 0.54537200 |
| O | 0.16772000 | -2.55827700 | -0.53945800 |

| | | | |
|---|---|---|---|
| O | -0.07663600 | -2.43848200 | 1.61931400 |
| Ag | -2.48650500 | -2.18823700 | 0.83418000 |
| O | -2.15803100 | -0.15839600 | 0.36796900 |
| Ag | -2.95074800 | 0.73478000 | -1.33353800 |
| C | 0.43530700 | 1.49131300 | 1.52861100 |
| C | 1.55298700 | 2.33343000 | 1.66566800 |
| C | -0.60605600 | 1.61379500 | 2.46186100 |
| C | 1.63511400 | 3.25903600 | 2.70648200 |
| H | 2.36263200 | 2.26281800 | 0.94199300 |
| C | -0.52418000 | 2.53830500 | 3.50515400 |
| H | -1.49006400 | 0.99514900 | 2.33544500 |
| C | 0.59604700 | 3.36181000 | 3.63408300 |
| H | 2.50879500 | 3.90084500 | 2.79171300 |
| H | -1.34373900 | 2.62072800 | 4.21504500 |
| H | 0.65632800 | 4.08275400 | 4.44550300 |

TS8



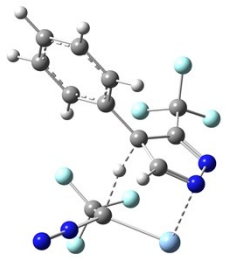
B3LYP electronic energy: -1145.0962964 a.u.
B3LYP enthalpy: -1144.910642 a.u.
B3LYP free energy: -1144.975344 a.u.
M06 SCF energy in solution: -1146.2309732 a.u.
M06 enthalpy in solution: -1146.0453182 a.u.
M06 free energy in solution: -1146.1100202 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.05576100 | 0.58877400 | -0.00865900 |
| N | -0.65898700 | 0.33012700 | 1.15850900 |
| C | -0.03338300 | 1.96413600 | -0.56234200 |
| C | 0.86057300 | -0.55937900 | -0.38358800 |
| N | -0.47407500 | -0.91095300 | 1.60539500 |
| Ag | -2.73024500 | 0.15762500 | 0.19995400 |
| F | -1.27823400 | 2.54477500 | -0.53462000 |
| F | 0.37560000 | 1.95288800 | -1.84951400 |
| F | 0.77680000 | 2.82202600 | 0.10269300 |
| C | 0.22339300 | -1.61167700 | 0.57733200 |
| H | 0.88957200 | -2.40214200 | 0.91857000 |

| | | | |
|---|---|---|---|
| N | -0.82740300 | -2.44834500 | -0.31146500 |
| O | -2.01932800 | -2.09114300 | -0.37948600 |
| O | -0.38332000 | -3.39868300 | -0.92600000 |
| H | 0.75373700 | -0.86306800 | -1.42832800 |
| C | 2.34238200 | -0.33975500 | -0.09702700 |
| C | 2.77361800 | 0.39638800 | 1.01468000 |
| C | 3.29884100 | -0.91555700 | -0.94299600 |
| C | 4.13593400 | 0.55074400 | 1.27229900 |
| H | 2.04390900 | 0.85529300 | 1.67491000 |
| C | 4.66168100 | -0.76026400 | -0.68587700 |
| H | 2.97401400 | -1.48815200 | -1.80891200 |
| C | 5.08358000 | -0.02662600 | 0.42418300 |
| H | 4.45658900 | 1.12541000 | 2.13698700 |
| H | 5.39135800 | -1.20884600 | -1.35464700 |
| H | 6.14411600 | 0.09803100 | 0.62531300 |

TS9



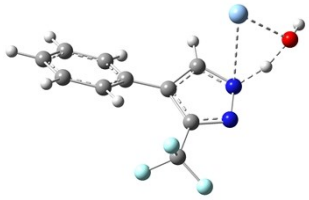
B3LYP electronic energy: -1425.1722138 a.u.
B3LYP enthalpy: -1424.970300 a.u.
B3LYP free energy: -1425.046386 a.u.
M06 SCF energy in solution: -1426.31732652 a.u.
M06 enthalpy in solution: -1426.11541352 a.u.
M06 free energy in solution: -1426.19149852 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.50243600 | -1.57265600 | -0.01308300 |
| N | 0.43155300 | -2.21973300 | -0.65967700 |
| C | -0.86359800 | -1.92664900 | 1.40181500 |
| C | -1.02024900 | -0.43677900 | -0.78448700 |
| H | -0.08408900 | 0.39078200 | -0.40105500 |
| N | 0.51647900 | -1.66744200 | -1.96554200 |
| F | -2.11216300 | -2.43695200 | 1.45215500 |
| F | -0.84953000 | -0.82654200 | 2.18960900 |
| F | -0.02531300 | -2.82699900 | 1.92946200 |
| C | -0.38472900 | -0.71334600 | -2.06243700 |

| | | | |
|---|---|---|---|
| H | -0.47690100 | -0.12511400 | -2.96936200 |
| C | 1.27788100 | 1.24562900 | -0.04949500 |
| C | 1.49024600 | 1.42242700 | 1.42171100 |
| F | 1.72817700 | 0.22101800 | 1.99453700 |
| F | 2.54082300 | 2.22657500 | 1.72135700 |
| F | 0.41591300 | 1.96143200 | 2.05823000 |
| N | 1.18276100 | 2.37547500 | -0.71147300 |
| N | 1.04807400 | 3.30110100 | -1.36334800 |
| Ag | 2.42438900 | -0.43670700 | -0.95803400 |
| C | -2.36298000 | 0.21239700 | -0.62798300 |
| C | -3.39226000 | -0.08172400 | -1.53507600 |
| C | -2.61104100 | 1.12380900 | 0.40849000 |
| C | -4.64283300 | 0.52285800 | -1.40955300 |
| H | -3.21319400 | -0.79474400 | -2.33572100 |
| C | -3.86433400 | 1.72394700 | 0.53419100 |
| H | -1.82266200 | 1.36848500 | 1.11241200 |
| C | -4.88270900 | 1.42730000 | -0.37322600 |
| H | -5.42980800 | 0.28327600 | -2.11948200 |
| H | -4.04154700 | 2.42886600 | 1.34177800 |
| H | -5.85703900 | 1.89781400 | -0.27402000 |

TS10



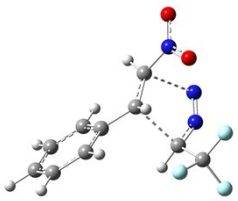
B3LYP electronic energy: -1015.8468474 a.u.
B3LYP enthalpy: -1015.664583 a.u.
B3LYP free energy: -1015.727362 a.u.
M06 SCF energy in solution: -1016.99458824 a.u.
M06 enthalpy in solution: -1016.81232424 a.u.
M06 free energy in solution: -1016.87510224 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 0.42277800 | 1.42574300 | -0.40741200 |
| N | -0.78856100 | 1.84119400 | -0.81347500 |
| C | 1.38392900 | 2.42416700 | 0.15437700 |
| C | 0.58610900 | 0.02732500 | -0.57005500 |
| H | -4.31639800 | -0.15131600 | -1.39030100 |
| N | -1.43153000 | 0.76985400 | -1.27600000 |

| | | | |
|---|---|---|---|
| F | 2.63520200 | 2.24107300 | -0.32623600 |
| F | 1.47950900 | 2.31677900 | 1.51373000 |
| F | 1.02067700 | 3.68610200 | -0.11200100 |
| C | -0.65042000 | -0.35278900 | -1.12215400 |
| H | -0.92777200 | -1.29781200 | -1.57876300 |
| H | -2.69484800 | 0.67997100 | -1.21478000 |
| O | -3.78497000 | 0.32769500 | -0.73460400 |
| Ag | -2.56118900 | -0.90779200 | 0.61718400 |
| C | 1.73542700 | -0.85825100 | -0.30909200 |
| C | 1.99963000 | -1.93627000 | -1.17386800 |
| C | 2.57655900 | -0.67529100 | 0.80275700 |
| C | 3.06276700 | -2.80506700 | -0.93358300 |
| H | 1.38030500 | -2.07595700 | -2.05592700 |
| C | 3.64213400 | -1.54289500 | 1.03814800 |
| H | 2.39019000 | 0.14445400 | 1.48714700 |
| C | 3.88982900 | -2.61216900 | 0.17487800 |
| H | 3.25154600 | -3.62667200 | -1.61963000 |
| H | 4.28006500 | -1.38260500 | 1.90330000 |
| H | 4.72222900 | -3.28532700 | 0.36102300 |

TS11



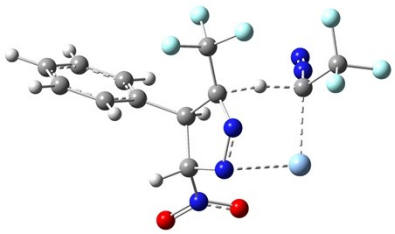
B3LYP electronic energy: -999.8988784 a.u.
B3LYP enthalpy: -999.704981 a.u.
B3LYP free energy: -999.766950 a.u.
M06 SCF energy in solution: -999.778008871 a.u.
M06 enthalpy in solution: -999.584110871 a.u.
M06 free energy in solution: -999.646079871 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 0.64367600 | 0.94254700 | 0.81779900 |
| N | 1.37870500 | 0.14614800 | 1.63405800 |
| C | 1.42276900 | 1.95964800 | 0.01484100 |
| C | -0.17541300 | -0.61680400 | -0.42497200 |
| H | 0.26315900 | -0.17386300 | -1.31418700 |
| N | 1.64557200 | -0.95370000 | 1.85110500 |
| F | 1.73258000 | 3.05782500 | 0.73848200 |

| | | | |
|---|---|---|---|
| F | 0.64829300 | 2.36435600 | -1.01478800 |
| F | 2.55983400 | 1.45086700 | -0.46896000 |
| C | 0.44072600 | -1.78501900 | 0.01473500 |
| H | -0.04232800 | -2.57996400 | 0.56287200 |
| N | 1.66239700 | -2.21944100 | -0.61441400 |
| O | 1.99600200 | -3.39385900 | -0.43375400 |
| O | 2.30819200 | -1.39660100 | -1.27853000 |
| H | -0.22580700 | 1.36591100 | 1.31683900 |
| C | -1.62636600 | -0.37028300 | -0.22560000 |
| C | -2.29778600 | 0.48134600 | -1.11768000 |
| C | -2.35548500 | -0.94646900 | 0.82832400 |
| C | -3.66154600 | 0.73333100 | -0.97505400 |
| H | -1.74276800 | 0.94650600 | -1.92820100 |
| C | -3.71813700 | -0.69234400 | 0.97145400 |
| H | -1.85820000 | -1.59715100 | 1.54278700 |
| C | -4.37747100 | 0.14626500 | 0.06931200 |
| H | -4.16397400 | 1.38891100 | -1.68090800 |
| H | -4.26646600 | -1.15043200 | 1.79004300 |
| H | -5.44003700 | 0.34196400 | 0.18222500 |

TS12



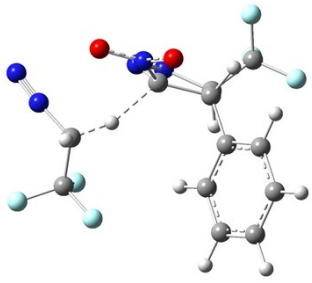
B3LYP electronic energy: -1630.8639642 a.u.
B3LYP enthalpy: -1630.633459 a.u.
B3LYP free energy: -1630.717412 a.u.
M06 SCF energy in solution: -1632.00761879 a.u.
M06 enthalpy in solution: -1631.77711379 a.u.
M06 free energy in solution: -1631.86106579 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.43962800 | -0.65201600 | -0.65499500 |
| N | 0.12329800 | -0.04138100 | -1.76015100 |
| C | -0.76750800 | -2.11183600 | -0.78448300 |
| C | -1.35948300 | 0.36221700 | 0.08145600 |
| H | 0.74356000 | -0.68187900 | 0.13242000 |

| | | | |
|---|---|---|---|
| N | -0.07437800 | 1.22344100 | -1.81789800 |
| F | -1.79220300 | -2.37807200 | -1.63118000 |
| F | -1.10896100 | -2.61407600 | 0.42418100 |
| F | 0.29780900 | -2.80216800 | -1.23666100 |
| C | -1.16352700 | 1.57790800 | -0.87190200 |
| H | -2.06544500 | 1.82263200 | -1.43626000 |
| C | 1.96535400 | -0.49479800 | 0.77497600 |
| C | 2.98040800 | -1.46390600 | 0.22854800 |
| F | 3.02005500 | -1.35803700 | -1.11375700 |
| F | 4.23091100 | -1.21947900 | 0.69529000 |
| F | 2.70176100 | -2.74989800 | 0.53349100 |
| N | 1.86508200 | -0.53228600 | 2.09089700 |
| N | 1.70010500 | -0.53169700 | 3.21702400 |
| Ag | 2.02517500 | 1.51982200 | -0.19659200 |
| C | -2.81321500 | 0.00311800 | 0.32085900 |
| C | -3.69375300 | -0.25040600 | -0.74118300 |
| C | -3.30465200 | -0.05063000 | 1.63072300 |
| C | -5.03318900 | -0.54682100 | -0.49496000 |
| H | -3.33096800 | -0.23640300 | -1.76528900 |
| C | -4.64491400 | -0.35039400 | 1.87905400 |
| H | -2.63409800 | 0.14465100 | 2.46451000 |
| C | -5.51363300 | -0.59731600 | 0.81595500 |
| H | -5.70138200 | -0.74313800 | -1.32876400 |
| H | -5.00779200 | -0.38653200 | 2.90243600 |
| H | -6.55794900 | -0.82873700 | 1.00580900 |
| N | -0.87559100 | 2.85929000 | -0.12295800 |
| O | 0.28836900 | 3.11930400 | 0.23407800 |
| O | -1.82704100 | 3.57893000 | 0.11774000 |
| H | -0.90729600 | 0.59517500 | 1.05544200 |

TS13



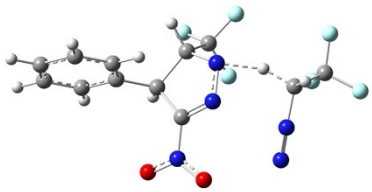
B3LYP electronic energy: -1485.690909 a.u.
B3LYP enthalpy: -1485.449597 a.u.
B3LYP free energy: -1485.527160 a.u.
M06 SCF energy in solution: -1485.59185842 a.u.
M06 enthalpy in solution: -1485.35054642 a.u.

M06 free energy in solution: -1485.42810942 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.71083200 | -0.83315200 | -0.83665200 |
| N | -0.76599700 | -1.99245100 | -0.92742000 |
| C | -3.14267100 | -1.34457500 | -0.86552800 |
| C | -1.34594100 | -0.05832900 | 0.45625600 |
| H | -2.08683700 | -0.25905900 | 1.23860000 |
| N | 0.08796800 | -1.93574300 | -0.00342400 |
| F | -3.40854100 | -2.01111400 | -2.00222800 |
| F | -4.00937700 | -0.30937000 | -0.78076100 |
| F | -3.39600600 | -2.17041100 | 0.17040500 |
| C | -0.06298000 | -0.79167400 | 0.80149500 |
| H | 1.50229300 | -0.28565700 | 0.38909900 |
| N | 0.36221100 | -0.89830300 | 2.14936500 |
| O | 1.39730300 | -1.57046100 | 2.38815400 |
| O | -0.23935800 | -0.24210500 | 3.01135400 |
| H | -1.58036600 | -0.22397200 | -1.73752800 |
| C | -1.20349000 | 1.44594200 | 0.30074200 |
| C | -1.84045200 | 2.30696300 | 1.20072100 |
| C | -0.42077700 | 2.00307800 | -0.72052000 |
| C | -1.70724900 | 3.69105500 | 1.08041500 |
| H | -2.43708600 | 1.88758000 | 2.00609300 |
| C | -0.28547400 | 3.38589800 | -0.84349700 |
| H | 0.08921300 | 1.35539000 | -1.43060900 |
| C | -0.93082000 | 4.23575500 | 0.05701100 |
| H | -2.21136500 | 4.34299600 | 1.78874900 |
| H | 0.32326400 | 3.79837900 | -1.64388100 |
| H | -0.82859100 | 5.31325600 | -0.03888300 |
| H | 3.07421400 | 0.20284700 | 1.25336700 |
| C | 2.71424800 | -0.28180500 | 0.34396600 |
| C | 3.18309400 | 0.42802000 | -0.92691100 |
| F | 2.84784800 | 1.71881600 | -0.82310900 |
| F | 4.51433500 | 0.33813700 | -1.09360900 |
| F | 2.59052400 | -0.09526000 | -2.01093700 |
| N | 3.13070600 | -1.60963100 | 0.36478400 |
| N | 3.35121400 | -2.70551100 | 0.35327900 |

TS14



B3LYP electronic energy: -1485.699674 a.u.
B3LYP enthalpy: -1485.457684 a.u.
B3LYP free energy: -1485.534971 a.u.
M06 SCF energy in solution: -1485.60087082 a.u.
M06 enthalpy in solution: -1485.35888082 a.u.
M06 free energy in solution: -1485.43616782 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.56479000 | -1.16534100 | -0.26461000 |
| N | 0.30207900 | -0.32789700 | -1.14569400 |
| C | 0.32481300 | -1.90017100 | 0.72761300 |
| C | -1.54714700 | -0.16650500 | 0.43663800 |
| H | -1.55446600 | -0.30455200 | 1.52224600 |
| N | 0.13498800 | 0.92863200 | -0.80799000 |
| F | 1.22156200 | -2.68794900 | 0.09597700 |
| F | -0.39271700 | -2.67846700 | 1.56172500 |
| F | 1.03317600 | -1.02964400 | 1.49240200 |
| C | -0.82360000 | 1.10813700 | 0.06865100 |
| H | 1.88146700 | -0.12245400 | -1.10098800 |
| N | -0.97210800 | 2.35453400 | 0.69543500 |
| O | -0.16391300 | 3.26864300 | 0.41482000 |
| O | -1.88249500 | 2.46402800 | 1.53382500 |
| H | -1.08846500 | -1.92317100 | -0.85339500 |
| C | -2.97886800 | -0.24294700 | -0.07224000 |
| C | -4.04220600 | -0.34483800 | 0.82981300 |
| C | -3.25717900 | -0.20021400 | -1.44575500 |
| C | -5.35902000 | -0.41173300 | 0.37215900 |
| H | -3.83808500 | -0.36186800 | 1.89724600 |
| C | -4.57213200 | -0.26782300 | -1.90472200 |
| H | -2.44143000 | -0.10820400 | -2.15943200 |
| C | -5.62765600 | -0.37545800 | -0.99642900 |
| H | -6.17409000 | -0.48948700 | 1.08672100 |
| H | -4.77235600 | -0.23314600 | -2.97238700 |
| H | -6.65252400 | -0.42721200 | -1.35392900 |
| H | 3.13500100 | 0.80267600 | -2.08954700 |
| C | 2.89357800 | 0.51365600 | -1.06363700 |
| C | 4.03579500 | -0.26671400 | -0.41306400 |
| F | 4.19743800 | -1.40117900 | -1.10150400 |

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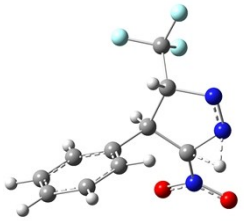
|---|---|---|---|
| F | 5.19318500 | 0.42170000 | -0.44133000 |
| F | 3.75345600 | -0.55144800 | 0.86369400 |
| N | 2.63576800 | 1.70008300 | -0.34656900 |
| N | 2.46095500 | 2.62588400 | 0.25469400 |

TS15



B3LYP electronic energy: -999.8530199 a.u.
B3LYP enthalpy: -999.661097 a.u.
B3LYP free energy: -999.721825 a.u.
M06 SCF energy in solution: -999.744094372 a.u.
M06 enthalpy in solution: -999.552171372 a.u.
M06 free energy in solution: -999.612899372 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.10135900 | -0.74640600 | 0.62660800 |
| N | -1.81898000 | 0.20349100 | 1.53312100 |
| C | -2.11505800 | -1.48315400 | -0.24148000 |
| C | -0.06575300 | 0.07655000 | -0.20928400 |
| H | -0.32308700 | 0.05618700 | -1.27346100 |
| N | -1.45203700 | 1.39003000 | 1.22204800 |
| F | -3.00230800 | -2.16227200 | 0.49932500 |
| F | -1.48024100 | -2.36241900 | -1.04820100 |
| F | -2.79273600 | -0.62375300 | -1.03088300 |
| C | -0.38672700 | 1.45276200 | 0.32336500 |
| H | -0.48565900 | 1.95333300 | 1.67347100 |
| N | -0.18021400 | 2.68290700 | -0.41824000 |
| O | -0.55736300 | 3.74160000 | 0.08170000 |
| O | 0.40154300 | 2.55557600 | -1.49720500 |
| H | -0.60678500 | -1.50035500 | 1.24824000 |
| C | 1.38530600 | -0.33785500 | -0.04324600 |
| C | 2.16227500 | -0.64200300 | -1.16543800 |
| C | 1.96769000 | -0.41845700 | 1.22893100 |
| C | 3.49589000 | -1.02610500 | -1.02034000 |
| H | 1.72246200 | -0.57325400 | -2.15686400 |
| C | 3.30043200 | -0.80173300 | 1.37557400 |
| H | 1.38117900 | -0.18186000 | 2.11491100 |

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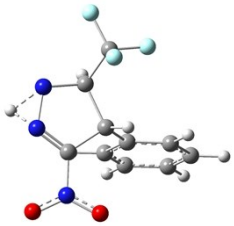
|---|---|---|---|
| C | 4.06784200 | -1.10746400 | 0.24985000 |
| H | 4.08681100 | -1.26077800 | -1.90120800 |
| H | 3.73856500 | -0.85990300 | 2.36804300 |
| H | 5.10603700 | -1.40660000 | 0.36299600 |

TS16



B3LYP electronic energy: -999.8586932 a.u.
B3LYP enthalpy: -999.666623 a.u.
B3LYP free energy: -999.727655 a.u.
M06 SCF energy in solution: -999.751793986 a.u.
M06 enthalpy in solution: -999.559723986 a.u.
M06 free energy in solution: -999.620755986 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.32325600 | -0.29021300 | 0.60469900 |
| N | -2.02370000 | 0.92965400 | 1.09436100 |
| C | -2.32185700 | -1.19602200 | -0.10482600 |
| C | -0.15414700 | 0.19441600 | -0.32074600 |
| H | -0.42634600 | 0.06214900 | -1.37486300 |
| N | -1.23401000 | 1.99359000 | 0.72329100 |
| F | -3.30850000 | -1.57749500 | 0.72169800 |
| F | -1.69501600 | -2.30665100 | -0.55164000 |
| F | -2.87563000 | -0.58345400 | -1.16848800 |
| C | -0.17995300 | 1.66648600 | 0.02394000 |
| H | -1.55880700 | 1.94833500 | 1.85378000 |
| N | 0.69866900 | 2.67034900 | -0.48659700 |
| O | 0.63444400 | 3.80481400 | -0.00929000 |
| O | 1.46722600 | 2.30219700 | -1.38256100 |
| H | -0.93860200 | -0.85385600 | 1.46323600 |
| C | 1.16348300 | -0.51907300 | -0.06631100 |
| C | 1.64777600 | -1.43887400 | -1.00136500 |
| C | 1.88481000 | -0.30694700 | 1.11537100 |
| C | 2.83270200 | -2.13507000 | -0.76182200 |
| H | 1.09428700 | -1.61125200 | -1.92082200 |
| C | 3.07196900 | -0.99860100 | 1.35433400 |
| H | 1.52751300 | 0.41119100 | 1.85080400 |

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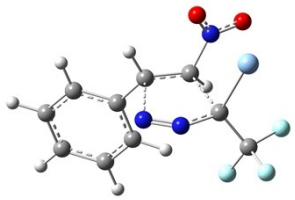
|---|---|---|---|
| C | 3.54821700 | -1.91615400 | 0.41610100 |
| H | 3.19703100 | -2.84620300 | -1.49793600 |
| H | 3.62561900 | -0.81773100 | 2.27148800 |
| H | 4.47308300 | -2.45514400 | 0.60135400 |

TS17



B3LYP electronic energy: -1145.0566628 a.u.
B3LYP enthalpy: -1144.872289 a.u.
B3LYP free energy: -1144.939775 a.u.
M06 SCF energy in solution: -1146.18465368 a.u.
M06 enthalpy in solution: -1146.00027968 a.u.
M06 free energy in solution: -1146.06776568 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.94037600 | -0.62316000 | -0.35296400 |
| N | -0.18005600 | -0.51900400 | -1.43682700 |
| C | -1.03122200 | -1.99971200 | 0.24076400 |
| C | 1.42175200 | 1.04126900 | -0.11485000 |
| H | 1.27207900 | 2.01989000 | -0.56043500 |
| N | 0.75255200 | 0.05412900 | -1.85805300 |
| Ag | -2.75486100 | 0.58454800 | -0.46272200 |
| F | -1.84103500 | -2.82758500 | -0.45715700 |
| F | -1.52047200 | -1.91336500 | 1.49428700 |
| F | 0.17719000 | -2.61566300 | 0.32331800 |
| C | 0.45895300 | 0.64164800 | 0.82959500 |
| H | 0.69799900 | -0.01628300 | 1.65423800 |
| N | -0.55555900 | 1.58291000 | 1.21583600 |
| O | -1.00852600 | 1.50559100 | 2.35790300 |
| O | -0.99030000 | 2.38857300 | 0.35874800 |
| C | 2.80804100 | 0.54303100 | -0.07881400 |
| C | 3.84552500 | 1.37015900 | -0.54246300 |
| C | 3.13687500 | -0.74051500 | 0.39518100 |
| C | 5.17088400 | 0.93981400 | -0.51551600 |
| H | 3.60617400 | 2.36136700 | -0.91992100 |
| C | 4.46212700 | -1.16847400 | 0.42193900 |
| H | 2.35088500 | -1.41664400 | 0.71802400 |

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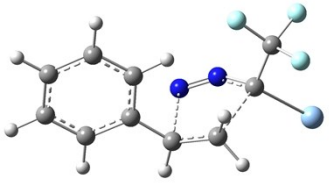
|---|---|---|---|
| C | 5.48575600 | -0.33043200 | -0.02897500 |
| H | 5.95792700 | 1.59798000 | -0.87379100 |
| H | 4.69615100 | -2.16395500 | 0.78968000 |
| H | 6.51827400 | -0.66791600 | -0.00719000 |

TS18



B3LYP electronic energy: -940.5491268 a.u.
B3LYP enthalpy: -940.370341 a.u.
B3LYP free energy: -940.431282 a.u.
M06 SCF energy in solution: -941.676398559 a.u.
M06 enthalpy in solution: -941.497612559 a.u.
M06 free energy in solution: -941.558553559 a.u.

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.30834600 | 0.09053500 | -0.25975000 |
| N | 1.81027800 | 0.74219800 | -1.30304900 |
| C | 2.29158500 | -0.26969300 | 0.80812500 |
| C | 0.01755000 | 1.88248600 | 0.36146800 |
| H | 0.51542800 | 1.98214000 | 1.32274500 |
| N | 1.69461200 | 1.75208700 | -1.89397500 |
| Ag | -0.29063400 | -1.32422800 | -0.66500300 |
| F | 3.12074300 | -1.28991600 | 0.47564800 |
| F | 1.62122700 | -0.65379100 | 1.92275700 |
| F | 3.08452800 | 0.77196000 | 1.16504400 |
| C | 0.36204000 | 2.78708700 | -0.64445300 |
| H | -0.34010300 | 3.02874000 | -1.43718600 |
| C | -1.29434100 | 1.20593800 | 0.41820300 |
| C | -1.85774400 | 0.85202000 | 1.65803300 |
| C | -2.01079000 | 0.83963200 | -0.74843700 |
| C | -3.07926900 | 0.18089300 | 1.73896700 |
| H | -1.32620000 | 1.11245300 | 2.56981700 |
| C | -3.23566600 | 0.16306200 | -0.66479600 |
| H | -1.62462700 | 1.12583400 | -1.72419900 |
| C | -3.77653500 | -0.17145800 | 0.58085800 |
| H | -3.48793000 | -0.06807400 | 2.71494800 |
| H | -3.77218200 | -0.08369000 | -1.57795300 |
| H | -4.72750000 | -0.69216800 | 0.64556100 |

| | | | |
|---|---|---|---|
| H | 1.09914000 | 3.55620000 | -0.43979000 |