Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Mechanistic Insight into Silver-catalyzed Cycloaddition Synthesis of 1,4-Disubstituted-1,2,3-triazoles: the Key Role of Silver

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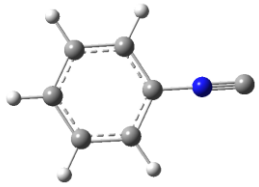
Table of Contents

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. Cartesian Coordinates

1



B3LYP electronic energy: -324.457896122 a.u.
B3LYP enthalpy: -324.351981 a.u.
B3LYP free energy: -324.389475 a.u.
M06 SCF energy in solution: -324.297553516 a.u.
M06 enthalpy in solution: -324.191637516 a.u.
M06 free energy in solution: -324.229132516 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-3.20352500	0.00003300	0.00000000
N	-2.02210400	-0.00006000	0.00000000
C	-0.63652400	-0.00015700	0.00000000
C	0.05704000	1.21732300	0.00000000
C	0.05713600	-1.21735800	0.00000000
C	1.44997100	1.20931800	0.00000000
H	-0.50129100	2.14758800	0.00000000
C	1.45024100	-1.20916400	0.00000000
H	-0.50080500	-2.14786100	0.00000000
C	2.14923200	0.00005500	0.00000000
H	1.98991900	2.15176900	0.00000000
H	1.99010900	-2.15165500	0.00000000
H	3.23536700	0.00027500	0.00000000

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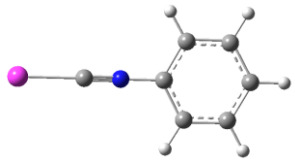

B3LYP electronic energy: -470.018717029 a.u.
B3LYP enthalpy: -469.909157 a.u.
B3LYP free energy: -469.953757 a.u.

M06 SCF energy in solution: -471.179012185 a.u.
M06 enthalpy in solution: -471.069452185 a.u.
M06 free energy in solution: -471.114052185 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.70959900	-0.00018700	-0.00003300
N	0.45291700	-0.00025600	-0.00002300
C	1.84142800	-0.00033400	-0.00001000
C	2.51869800	1.22788000	-0.00000400
C	2.51915400	-1.22811300	-0.00000400
C	3.90998800	1.21517900	0.00000800
H	1.96196900	2.15889000	-0.00000900
C	3.91052300	-1.21476100	0.00000800
H	1.96307100	-2.15951400	-0.00000900
C	4.60330500	0.00030400	0.00001400
H	4.45328800	2.15443800	0.00001200
H	4.45406200	-2.15388500	0.00001200
H	5.68881100	0.00057700	0.00002300
Ag	-2.83516200	0.00003100	0.00000600

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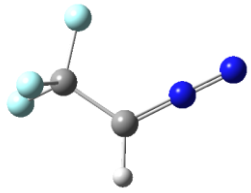

B3LYP electronic energy: -485.773091806 a.u.
B3LYP enthalpy: -485.727345 a.u.
B3LYP free energy: -485.766611 a.u.
M06 SCF energy in solution: -485.715682944 a.u.
M06 enthalpy in solution: -485.669936944 a.u.
M06 free energy in solution: -485.709202944 a.u.

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

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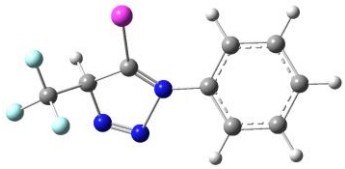

B3LYP electronic energy: -955.796902747 a.u.
B3LYP enthalpy: -955.638677 a.u.
B3LYP free energy: -955.699473 a.u.
M06 SCF energy in solution: -956.899311381 a.u.
M06 enthalpy in solution: -956.741085381 a.u.
M06 free energy in solution: -956.801881381 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.56914800	-0.97193400	-0.76794400
N	-1.11306600	-2.40477800	-0.81083800
C	-2.74195100	-0.82965600	0.22273000
C	-0.34271500	-0.16678600	-0.40524300
N	0.01572000	-2.65863300	-0.65776200
F	-3.74078400	-1.63814900	-0.11108100
F	-3.18237700	0.44965600	0.18474600
F	-2.34096500	-1.10129600	1.46949600
H	-1.94074100	-0.73880200	-1.77260400
N	0.69775600	-0.86943600	-0.32987000
C	2.06635400	-0.62353800	-0.12270200
C	2.69213900	0.48519600	-0.71601300
C	2.79293000	-1.53509500	0.65520500
C	4.05015000	0.69509600	-0.49288100
H	2.12827800	1.14281200	-1.37170000
C	4.14927200	-1.30607000	0.87440600
H	2.29549400	-2.39874200	1.08367100
C	4.77724100	-0.19451100	0.30524700
H	4.54506500	1.54446400	-0.95341200
H	4.71751100	-2.00091700	1.48435500
H	5.83689200	-0.02776500	0.47158400
Ag	-0.56710400	1.94256900	0.05196000

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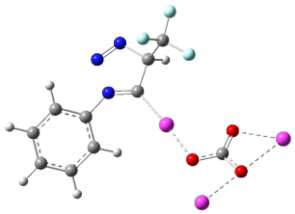

B3LYP electronic energy: -1511.22239962 a.u.
B3LYP enthalpy: -1511.037315 a.u.
B3LYP free energy: -1511.122419 a.u.
M06 SCF energy in solution: -1514.74730582 a.u.
M06 enthalpy in solution: -1514.56222082 a.u.
M06 free energy in solution: -1514.64732482 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.78121000	2.32060300	-0.35159100
N	-4.26014800	2.46391000	-0.34725200
C	-2.16976900	3.10043000	0.82638600
C	-2.51624300	0.83746400	-0.32224300
N	-4.83711500	1.40511000	-0.36825700
F	-2.51892500	4.38596900	0.76884300
F	-0.82824300	3.01324000	0.77275200
F	-2.58370100	2.58518600	1.99410200
H	-2.40930900	2.77827800	-1.27740500
N	-3.67029200	0.27360600	-0.36074600
C	-4.09286700	-1.08352200	-0.41320100
C	-3.41816900	-1.99677100	-1.23173300
C	-5.20437100	-1.46650400	0.34465300
C	-3.85148700	-3.32065500	-1.26501400
H	-2.58460600	-1.66690200	-1.84356200
C	-5.62404200	-2.79495600	0.30050400
H	-5.72382100	-0.73908400	0.95882000
C	-4.94965300	-3.72140500	-0.49883400
H	-3.33924900	-4.03557900	-1.90152800
H	-6.48101300	-3.10392100	0.89060000
H	-5.28606100	-4.75308800	-0.53301700
Ag	-0.58068900	-0.01575600	-0.16176900
C	2.30037600	-0.18214400	-0.14352500
O	2.07445700	0.99604500	-0.57329500
O	1.31692700	-1.00896600	0.11388500
O	3.51638900	-0.60609900	0.05946700
Ag	4.27439200	1.58536700	-0.62040500
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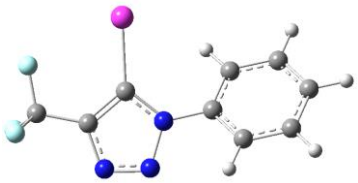

B3LYP electronic energy: -955.454410517 a.u.
B3LYP enthalpy: -955.306773 a.u.
B3LYP free energy: -955.366114 a.u.
M06 SCF energy in solution: -956.501017675 a.u.
M06 enthalpy in solution: -956.353379675 a.u.
M06 free energy in solution: -956.412720675 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.44842700	-1.08823100	-0.09993000
N	-0.98806800	-2.37166900	-0.16245000
C	-2.91168700	-0.80956800	-0.06319300
C	-0.39223500	-0.19372000	-0.06165100
N	0.30695900	-2.34502200	-0.16764400
F	-3.54906000	-1.26628400	-1.15948900
F	-3.15597300	0.53274600	0.00544600
F	-3.51318200	-1.36958000	1.00585600
N	0.68821600	-1.02586700	-0.10864900
C	2.07730400	-0.71249900	-0.08912100
C	2.56947000	0.37696200	-0.81459700
C	2.94523100	-1.52315800	0.64907400
C	3.93268600	0.67233400	-0.77359400
H	1.89353300	0.96515500	-1.42684100
C	4.30744300	-1.22698600	0.67051800
H	2.54437400	-2.37186600	1.19128400
C	4.80488500	-0.12627800	-0.03136300
H	4.31397000	1.51780100	-1.33958800
H	4.98069900	-1.85667200	1.24521400
H	5.86639400	0.10280500	-0.00648300
Ag	-0.48920900	1.88416200	0.17924300

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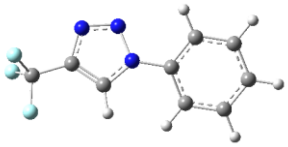

B3LYP electronic energy: -810.31163001 a.u.
B3LYP enthalpy: -810.154416 a.u.
B3LYP free energy: -810.207317 a.u.
M06 SCF energy in solution: -810.095813457 a.u.
M06 enthalpy in solution: -809.938599457 a.u.
M06 free energy in solution: -809.991500457 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.68526200	0.18171200	-0.04975600
N	-1.31898800	1.44563700	-0.40447100
C	-3.11211300	-0.23398200	0.08195200
C	-0.55592800	-0.57399600	0.15612300
N	-0.02320800	1.51406700	-0.43273600
F	-3.76581200	0.49080600	1.00956800
F	-3.17920700	-1.53569500	0.45226700
F	-3.78600500	-0.10223200	-1.07647300
N	0.46542300	0.28560700	-0.09123000
C	1.87062900	0.05487800	-0.03090200
C	2.37878500	-1.22271700	-0.27922500
C	2.72266000	1.11968100	0.27501500
C	3.75450600	-1.43698700	-0.20219400
H	1.71305300	-2.03589200	-0.55103900
C	4.09622100	0.89336900	0.33361100
H	2.30360200	2.10198200	0.45853800
C	4.61613300	-0.38218000	0.10235400
H	4.15091300	-2.42967900	-0.39444600
H	4.76133000	1.71887500	0.56971300
H	5.68741900	-0.55235700	0.15560200
H	-0.41347100	-1.59467800	0.47056800

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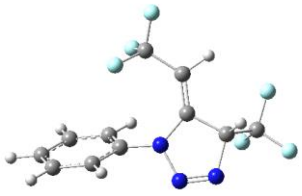

B3LYP electronic energy: -1186.61762092 a.u.
B3LYP enthalpy: -1186.423387 a.u.
B3LYP free energy: -1186.488031 a.u.
M06 SCF energy in solution: -1186.3806644 a.u.
M06 enthalpy in solution: -1186.1864304 a.u.
M06 free energy in solution: -1186.2510744 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.09219800	-0.52856300	0.75898400
N	1.73910200	-1.95656600	0.92874900
C	3.11589600	-0.38600500	-0.37061400
C	0.76284600	0.16087500	0.50457200
N	0.51137700	-2.10511500	0.76876400
F	4.21937200	-1.09992600	-0.10655300
F	3.48313100	0.90878800	-0.50517000
F	2.61252100	-0.79789300	-1.54569400
H	2.57749900	-0.17328500	1.67393200
N	-0.13984700	-0.90026100	0.50972200
C	-1.50840000	-0.97632800	0.10089600
C	-1.87836000	-0.56991500	-1.18279900
C	-2.44691900	-1.52155900	0.97890900
C	-3.20975800	-0.68917100	-1.57814800
H	-1.13405400	-0.15980300	-1.85661500
C	-3.77197500	-1.65402900	0.56681700
H	-2.13346600	-1.83923300	1.96792700
C	-4.15649100	-1.23295000	-0.70782900
H	-3.50325000	-0.36663200	-2.57284600
H	-4.50476400	-2.08040500	1.24575200
H	-5.19148500	-1.33004500	-1.02302700
C	0.60455300	1.49277300	0.39982200
C	-0.65477200	2.27888800	0.25757500
F	-1.09857300	2.35862200	-1.02420200
F	-0.43968800	3.54956000	0.66753000
F	-1.67410300	1.78474800	0.99481400
H	1.49824200	2.10380200	0.41860800

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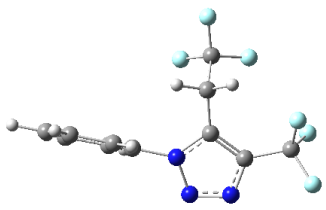


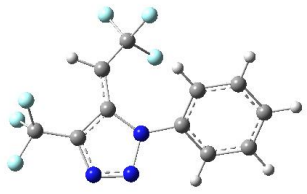
B3LYP electronic energy: -1186.66378448 a.u.
B3LYP enthalpy: -1186.468018 a.u.
B3LYP free energy: -1186.533251 a.u.
M06 SCF energy in solution: -1186.43015198 a.u.
M06 enthalpy in solution: -1186.23438498 a.u.

M06 free energy in solution: -1186.29961898 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.50535900	-1.07827700	0.01402000
N	1.06830200	-2.22369000	-0.57604100
C	2.96596700	-0.79169500	0.15532300
C	0.42059600	-0.29295400	0.35681400
N	-0.22853300	-2.20929200	-0.61873800
F	3.65571800	-1.90113000	0.46360200
F	3.18342700	0.11813500	1.14068300
F	3.49675000	-0.28376300	-0.97452600
N	-0.64582900	-1.03942700	-0.05415300
C	-2.04554100	-0.75345400	0.03429800
C	-2.79201800	-0.66390900	-1.14137900
C	-2.64737900	-0.59982500	1.28513600
C	-4.15978400	-0.40686500	-1.05902500
H	-2.29927800	-0.79665300	-2.09840900
C	-4.01420600	-0.32919700	1.35503200
H	-2.05667500	-0.71502900	2.18905300
C	-4.77008400	-0.23286700	0.18523000
H	-4.74744800	-0.33765900	-1.96958000
H	-4.48852300	-0.20855000	2.32450800
H	-5.83507500	-0.02763200	0.24330200
C	0.32193700	1.08420300	0.93276700
C	0.45050100	2.16628400	-0.13205100
F	1.63776900	2.10451700	-0.76346800
F	0.34083300	3.38813500	0.42713100
F	-0.51757400	2.05206900	-1.06635100
H	1.12103600	1.24341500	1.65870500
H	-0.63602400	1.23863500	1.43431700

10



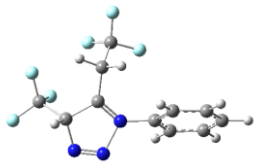
B3LYP electronic energy: -1186.08889812 a.u.
B3LYP enthalpy: -1185.908507 a.u.
B3LYP free energy: -1185.972736 a.u.
M06 SCF energy in solution: -1185.92805339 a.u.

M06 enthalpy in solution: -1185.74766139 a.u.
M06 free energy in solution: -1185.81189139 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.84161300	-0.92211600	0.06222500
N	-1.48639000	-2.21420700	-0.13171200
C	-3.25109100	-0.51642200	0.15836600
C	-0.69640300	-0.06782100	0.03283100
N	-0.21273200	-2.31953000	-0.25748000
F	-4.08738100	-1.57467900	0.26173200
F	-3.69315700	0.21626700	-0.91442100
F	-3.50375800	0.28953500	1.23935600
N	0.32260000	-1.00259000	-0.14173600
C	1.72121700	-0.92455900	-0.00060900
C	2.33222200	-0.02519900	0.88379500
C	2.51883300	-1.83918300	-0.70904200
C	3.71746200	-0.02977200	1.03433800
H	1.72677600	0.68242800	1.43464800
C	3.90103200	-1.84225300	-0.53875000
H	2.03378100	-2.54414700	-1.37364600
C	4.51342000	-0.93554300	0.32981100
H	4.17533600	0.68204900	1.71775500
H	4.50395300	-2.55664900	-1.09589100
H	5.59397600	-0.93351000	0.45380300
C	-0.69506600	1.32278800	0.11903000
C	0.33294800	2.27856000	-0.23654300
F	1.10746700	2.79279300	0.81654700
F	-0.20693500	3.41553400	-0.78422000
F	1.26594800	1.82184100	-1.12426200
H	-1.65558600	1.78161600	0.31453300

11



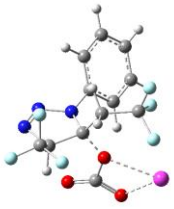
B3LYP electronic energy: -1186.9705696 a.u.
B3LYP enthalpy: -1186.763975 a.u.
B3LYP free energy: -1186.828673 a.u.
M06 SCF energy in solution: -1186.79798311 a.u.
M06 enthalpy in solution: -1186.59138811 a.u.

M06 free energy in solution: -1186.65608611 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.66783600	-1.11534300	-0.76468500
N	1.16759400	-2.39666500	-0.27222000
C	2.90134900	-0.66654000	0.07110500
C	0.45447600	-0.21225100	-0.71983900
N	-0.01343900	-2.38803700	-0.00817600
F	2.56554400	-0.53490200	1.35496200
F	3.33325400	0.51247500	-0.40223400
F	3.86482400	-1.57153000	-0.05121200
H	-0.36851600	1.48639100	-1.74565900
N	-0.54670300	-0.92328400	-0.32251100
C	-1.93992000	-0.70234400	-0.15910000
C	-2.68198700	-0.08863600	-1.17712700
C	-2.53880600	-1.16769100	1.01836900
C	-4.04884500	0.08821700	-0.98877700
H	-2.21542700	0.20493500	-2.11187000
C	-3.90579000	-0.97115200	1.19104900
H	-1.94460900	-1.65691700	1.78263400
C	-4.65811500	-0.34357000	0.19411600
H	-4.64083600	0.55155600	-1.77126700
H	-4.38339000	-1.31382400	2.10301000
H	-5.72519000	-0.20117200	0.33277000
C	0.45804900	1.24626900	-1.07426000
C	0.32215600	2.15771800	0.16227600
F	-0.85578000	1.95183400	0.77669000
F	0.39315300	3.43053500	-0.22671100
F	1.30192400	1.91104500	1.04613500
H	1.39372700	1.50401000	-1.57188700
H	2.02337400	-1.26223900	-1.79481500

12



B3LYP electronic energy: -1596.7856958 a.u.

B3LYP enthalpy: -1596.554992 a.u.

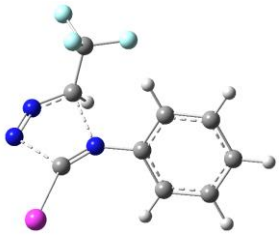
B3LYP free energy: -1596.634191 a.u.

M06 SCF energy in solution: -1597.79797208 a.u.
M06 enthalpy in solution: -1597.56726808 a.u.
M06 free energy in solution: -1597.64646708 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-2.31120400	-0.81657300	-1.52316900
C	-2.39185300	-0.10457200	-0.69804200
N	-2.82823400	1.18355400	-1.26977900
C	-3.47160700	-0.62497100	0.23570800
C	-0.94714900	0.13773000	-0.13209400
N	-1.88411100	2.00047400	-1.23592100
F	-4.61628700	-0.82179000	-0.42915100
F	-3.72785800	0.21853500	1.26060300
F	-3.10437300	-1.81648700	0.78007200
N	-0.74545700	1.48966400	-0.67577500
C	0.33978700	2.38170900	-0.44295600
C	1.61518500	2.08661400	-0.94027100
C	0.11448400	3.58140600	0.24343100
C	2.66412900	2.97899100	-0.72065500
H	1.77609800	1.17905200	-1.51172200
C	1.16499100	4.47763200	0.44013600
H	-0.88526900	3.81026800	0.59944700
C	2.44341700	4.17457700	-0.03246400
H	3.65203200	2.74962600	-1.11059100
H	0.98333800	5.41071900	0.96608600
H	3.26162500	4.87186300	0.12417700
C	-0.83653200	0.10378300	1.42378500
C	0.50813100	-0.21673400	2.05438000
F	0.78569000	-1.57146500	2.01053900
F	0.48980200	0.10404200	3.35874200
F	1.57604600	0.38937800	1.50110200
H	-1.50876400	-0.65092600	1.83019300
H	-1.15501600	1.07020200	1.82140100
C	0.25024300	-1.02670800	-2.03114900
O	-0.52920000	-0.57618500	-2.84266900
O	0.00019800	-0.81018900	-0.59604700
O	1.31971800	-1.70302300	-2.15879800
Ag	2.05786200	-2.16684200	-0.14641200

13

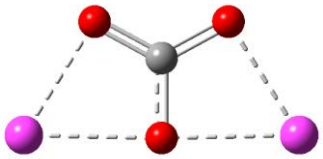


B3LYP electronic energy: -955.794232761 a.u.
B3LYP enthalpy: -955.634937 a.u.
B3LYP free energy: -955.693628 a.u.
M06 SCF energy in solution: -956.907367911 a.u.
M06 enthalpy in solution: -956.748071911 a.u.
M06 free energy in solution: -956.806762911 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.46568300	-1.16424500	0.75061200
N	0.82681000	-2.46644700	0.81903600
C	2.55616400	-1.15946300	-0.35680700
C	-0.74448800	-0.96897200	0.31763700
N	-0.39856800	-2.35660400	0.56157800
F	3.46266300	-2.08790900	-0.07640300
F	3.14459000	0.04145400	-0.39880800
F	1.99550100	-1.41121000	-1.54569300
H	1.93951400	-0.93022900	1.71000500
N	0.34805300	-0.25695000	0.44450500
C	0.48393400	1.16544700	0.26980100
C	0.03913200	1.74813300	-0.92190400
C	1.06305400	1.92705800	1.28904400
C	0.16645200	3.12747300	-1.08336300
H	-0.34833500	1.12638000	-1.72325900
C	1.17886800	3.30472100	1.11254100
H	1.39265200	1.46257400	2.21353900
C	0.73157900	3.90436600	-0.06858200
H	-0.15976200	3.59042900	-2.00927100
H	1.61681000	3.90900300	1.90039000
H	0.83197700	4.97694000	-0.20122900
Ag	-2.76114800	-0.39921700	-0.09216500

14

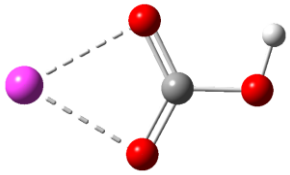


B3LYP electronic energy: -555.334361183 a.u.
B3LYP enthalpy: -555.310250 a.u.
B3LYP free energy: -555.352420 a.u.
M06 SCF energy in solution: -557.798890547 a.u.
M06 enthalpy in solution: -557.774779547 a.u.
M06 free energy in solution: -557.816949547 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.00000800	0.98598600	0.00179500
O	-1.12796800	1.59614800	-0.00063100
O	1.12767800	1.59642100	-0.00012800
O	0.00005500	-0.35325000	0.00606300
Ag	-2.32040600	-0.30458900	-0.00054500
Ag	2.32044700	-0.30457000	-0.00058700

15

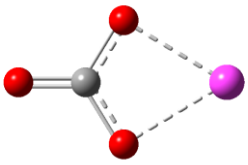


B3LYP electronic energy: -410.165638369 a.u.
B3LYP enthalpy: -410.131446 a.u.
B3LYP free energy: -410.168169 a.u.
M06 SCF energy in solution: -411.397795753 a.u.
M06 enthalpy in solution: -411.363602753 a.u.
M06 free energy in solution: -411.400325753 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	3.16971300	0.85299800	0.00009400
C	1.52811300	-0.04391800	-0.00009500
O	2.88378000	-0.07591900	0.00028200
O	0.96929500	1.10133400	-0.00024600
O	0.93057600	-1.15560600	-0.00023900
Ag	-1.07675700	0.00961800	0.00004500

16

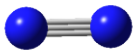


B3LYP electronic energy: -409.580159359 a.u.
B3LYP enthalpy: -409.559934 a.u.
B3LYP free energy: -409.596811 a.u.
M06 SCF energy in solution: -410.899565232 a.u.
M06 enthalpy in solution: -410.879340232 a.u.
M06 free energy in solution: -410.916217232 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.60850300	-0.00023000	-0.00006900
O	-2.85428000	-0.00006900	0.00034500
O	-0.90848900	1.14131900	-0.00031300
O	-0.90818400	-1.14112700	-0.00031300
Ag	1.00039700	0.00000800	0.00005700

17

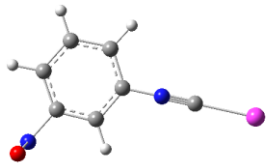


B3LYP electronic energy: -109.524129072 a.u.
B3LYP enthalpy: -109.515225 a.u.
B3LYP free energy: -109.536980 a.u.
M06 SCF energy in solution: -109.484558642 a.u.
M06 enthalpy in solution: -109.475654642 a.u.
M06 free energy in solution: -109.497409642 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.00000000	0.00000000	0.55275100
N	0.00000000	0.00000000	-0.55275100

18-a

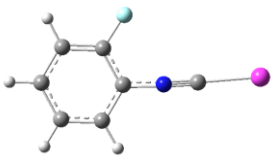


B3LYP electronic energy: -674.4901393 a.u.
B3LYP enthalpy: -674.376891 a.u.
B3LYP free energy: -674.426758 a.u.
M06 SCF energy in solution: -675.63839848 a.u.
M06 enthalpy in solution: -675.52515048 a.u.
M06 free energy in solution: -675.57501748 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.64389300	0.17389200	-0.00011500
N	0.50756500	0.41880500	-0.00009800
C	-0.85127900	0.70780500	-0.00006400
C	-1.76174300	-0.35681200	-0.00005600
C	-1.26437100	2.04713400	-0.00004000
C	-3.10993500	-0.03310700	-0.00002000
H	-1.42563900	-1.38754600	-0.00007900
C	-2.62977000	2.32273800	-0.00000600
H	-0.53024400	2.84520300	-0.00004800
C	-3.56386000	1.28423400	0.00000600
H	-2.96938100	3.35296600	0.00001200
Ag	3.72686900	-0.28732800	0.00005800
H	-4.62849700	1.49332200	0.00003600
N	-4.09473300	-1.13622000	-0.00001000
O	-4.45471900	-1.54087400	-1.09755900
O	-4.45484500	-1.54074100	1.09754600

19-b



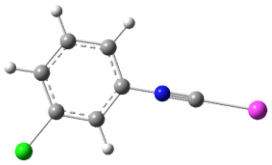
B3LYP electronic energy: -569.2458083 a.u.
B3LYP enthalpy: -569.143584 a.u.
B3LYP free energy: -569.190411 a.u.
M06 SCF energy in solution: -570.414826462 a.u.
M06 enthalpy in solution: -570.312601462 a.u.
M06 free energy in solution: -570.359428462 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.84226900	-0.22122300	0.00001700
N	0.31839700	-0.28735800	-0.00000500

C	1.69864400	-0.30269000	-0.00000900
C	2.41231900	-1.51142100	-0.00001200
C	2.37579000	0.92797300	-0.00001000
C	3.80121200	-1.46829300	-0.00001600
H	1.87357700	-2.45288600	-0.00001100
C	3.76085000	0.96818400	-0.00001400
C	4.46827800	-0.23608300	-0.00001700
H	4.36651800	-2.39384200	-0.00001900
H	4.26239400	1.92973600	-0.00001500
Ag	-2.96193400	-0.04813700	0.00001100
H	5.55333700	-0.21130900	-0.00002100
F	1.65304100	2.05150400	-0.00000600

20-c

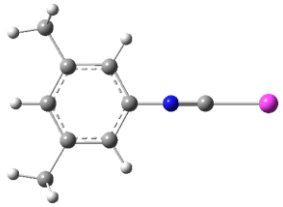


B3LYP electronic energy: -929.6044544 a.u.
B3LYP enthalpy: -929.503493 a.u.
B3LYP free energy: -929.551526 a.u.
M06 SCF energy in solution: -930.771291686 a.u.
M06 enthalpy in solution: -930.670329686 a.u.
M06 free energy in solution: -930.718362686 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.40727600	0.14654400	0.00000900
N	-0.26184200	0.34424500	-0.00000100
C	1.10727500	0.57977700	-0.00000700
C	1.97273900	-0.52225000	-0.00000900
C	1.56944800	1.90229200	-0.00001000
C	3.34313300	-0.27324500	-0.00001500
H	1.58799800	-1.53527000	-0.00000600
C	2.94547200	2.11454000	-0.00001600
H	0.86866800	2.72963500	-0.00000800
C	3.83437700	1.03745600	-0.00001800
H	3.33167200	3.12847300	-0.00001800
Ag	-3.50401500	-0.22111800	0.00001600
H	4.90554200	1.20756300	-0.00002300
Cl	4.44921700	-1.61519100	-0.00001800

21-d

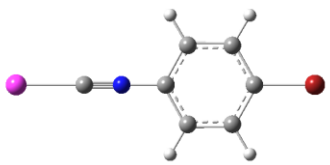


B3LYP electronic energy: -548.657238 a.u.
B3LYP enthalpy: -548.490747 a.u.
B3LYP free energy: -548.540134 a.u.
M06 SCF energy in solution: -549.77073715 a.u.
M06 enthalpy in solution: -549.60424615 a.u.
M06 free energy in solution: -549.65363315 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.36143500	0.00000100	-0.00001300
N	0.19899400	-0.00001000	-0.00001800
C	-1.19022100	-0.00000500	0.00000700
C	-1.86135000	1.22894100	-0.00009000
C	-1.86135800	-1.22894600	0.00008800
C	-3.25836300	1.23341100	-0.00008100
H	-1.29755400	2.15658800	-0.00017700
C	-3.25837300	-1.23340600	0.00006900
H	-1.29757000	-2.15659800	0.00013400
C	-3.92725000	0.00000400	-0.00002500
Ag	3.48341400	0.00000000	-0.00002400
H	-5.01421200	0.00000900	-0.00006700
C	-4.01965700	-2.53768700	0.00011500
H	-3.77420200	-3.13910300	-0.88286800
H	-3.77418600	-3.13904900	0.88313100
H	-5.09935200	-2.36748200	0.00011900
C	-4.01964100	2.53769600	0.00003600
H	-3.77620900	3.13776300	0.88450800
H	-3.77214400	3.14040200	-0.88148400
H	-5.09933300	2.36749800	-0.00265300

22-e



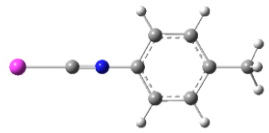
B3LYP electronic energy: -3040.8170756 a.u.

B3LYP enthalpy: -3040.716276 a.u.
B3LYP free energy: -3040.765542 a.u.
M06 SCF energy in solution: -3044.59823344 a.u.
M06 enthalpy in solution: -3044.49743344 a.u.
M06 free energy in solution: -3044.54669944 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.34986700	0.00009900	0.00002500
N	-1.18674900	0.00031200	0.00002000
C	0.19895100	0.00021300	0.00001300
C	0.88209600	-1.22524500	0.00000900
C	0.88226700	1.22557500	0.00000800
C	2.27107800	-1.21914300	-0.00000100
H	0.33190000	-2.16012100	0.00001400
C	2.27124900	1.21927700	-0.00000300
H	0.33220500	2.16053000	0.00001100
C	2.96001900	0.00001900	-0.00000800
H	2.81980100	-2.15387500	-0.00000500
H	2.82010100	2.15393300	-0.00000800
Ag	-4.47598600	-0.00007200	0.00001100
Br	4.84799400	-0.00011500	-0.00002600

23-f



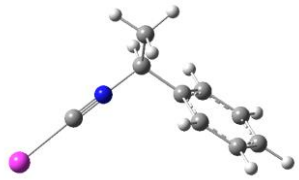
B3LYP electronic energy: -509.3392453 a.u.
B3LYP enthalpy: -509.200339 a.u.
B3LYP free energy: -509.250074 a.u.
M06 SCF energy in solution: -510.475515742 a.u.
M06 enthalpy in solution: -510.336608742 a.u.
M06 free energy in solution: -510.386343742 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.17899800	0.00026100	0.00012900
N	-0.01602200	0.00070800	-0.00131100
C	1.36980200	0.00041800	-0.00207800
C	2.05432600	-1.22378800	-0.00478100
C	2.05481900	1.22432200	-0.00477400
C	3.44304600	-1.20818000	-0.00932300

H	1.50351000	-2.15849900	-0.00687500
C	3.44356100	1.20813800	-0.00931700
H	1.50440000	2.15926600	-0.00686200
C	4.16208100	-0.00015500	-0.00864000
H	3.98154200	-2.15125700	-0.01512500
H	3.98244200	2.15098900	-0.01511300
Ag	-3.30113400	-0.00012100	0.00175200
C	5.66851200	-0.00057900	0.01662100
H	6.07856800	0.88874500	-0.47096400
H	6.03400700	-0.00446600	1.05203200
H	6.07809000	-0.88665500	-0.47730200

24-g



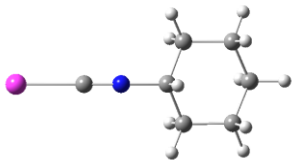
B3LYP electronic energy: -548.645268 a.u.
B3LYP enthalpy: -548.476090 a.u.
B3LYP free energy: -548.528051 a.u.
M06 SCF energy in solution: -549.766289899 a.u.
M06 enthalpy in solution: -549.597112899 a.u.
M06 free energy in solution: -549.649072899 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.07803700	0.07861500	-1.22018400
C	4.05570400	-0.90631500	-1.06673500
C	4.19288700	-1.56893200	0.15353800
C	3.35415500	-1.24388700	1.22369100
C	2.38290600	-0.25492900	1.07574300
C	2.24249000	0.41191600	-0.14892500
H	2.97419000	0.59280800	-2.17274600
H	4.70651100	-1.15365800	-1.89985000
H	4.95227500	-2.33581800	0.27322200
H	3.46125600	-1.75633800	2.17504700
H	1.74085900	-0.00483200	1.91697500
C	1.21055900	1.51539600	-0.32771800
H	1.27003200	1.90148200	-1.35079200
C	1.32429800	2.68355600	0.66442800
H	0.56241400	3.44387500	0.46870300
H	1.23014100	2.33843400	1.69728600

H	2.31172100	3.13603900	0.54162000
N	-0.13327700	0.94687400	-0.23669500
C	-1.18742400	0.47390200	-0.15397500
Ag	-3.11059900	-0.42395800	-0.02535700

25-h

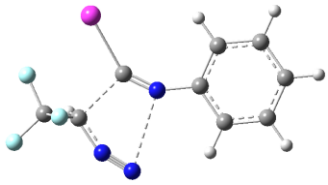


B3LYP electronic energy: -473.6530151 a.u.
B3LYP enthalpy: -473.471393 a.u.
B3LYP free energy: -473.518726 a.u.
M06 SCF energy in solution: -474.812265496 a.u.
M06 enthalpy in solution: -474.630643496 a.u.
M06 free energy in solution: -474.677976496 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.90720000	0.00004700	0.20880500
N	-0.23994900	0.00009100	0.37010400
Ag	3.01540600	-0.00001100	-0.07496000
C	-2.27496900	1.28224800	-0.08452100
C	-3.80444900	1.26920700	0.07945200
C	-4.43039500	-0.00007700	-0.51771700
C	-3.80435200	-1.26930600	0.07947500
C	-2.27486500	-1.28218800	-0.08445900
C	-1.67864900	0.00007800	0.53178700
H	-5.51164700	-0.00010600	-0.34342300
H	-4.05557100	1.34061500	1.14692900
H	-4.21696000	2.16475100	-0.39732600
H	-2.01000700	1.31488400	-1.14919400
H	-1.83632600	2.16440900	0.39459500
H	-4.05549600	-1.34072600	1.14694300
H	-4.21676300	-2.16489100	-0.39731200
H	-1.83612400	-2.16427900	0.39470100
H	-2.00987800	-1.31484000	-1.14912700
H	-1.84439200	0.00010700	1.61627200
H	-4.28839400	-0.00008600	-1.60758400

TS1

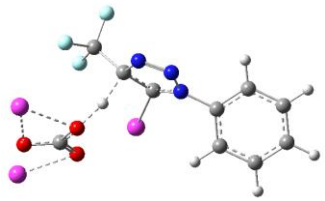


B3LYP electronic energy: -955.769281672 a.u.
B3LYP enthalpy: -955.613209 a.u.
B3LYP free energy: -955.675673 a.u.
M06 SCF energy in solution: -956.871741688 a.u.
M06 enthalpy in solution: -956.715668688 a.u.
M06 free energy in solution: -956.778133688 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.50998100	-1.30617300	-0.76236600
N	-0.75560600	-2.42019600	-0.65468400
C	-2.61531700	-1.17469900	0.27156600
C	-0.07109100	0.09732100	-0.35551000
N	0.20655700	-3.00083500	-0.50836200
F	-3.58274000	-2.07834200	0.11282400
F	-3.16862200	0.05813200	0.11980600
F	-2.12940300	-1.27249400	1.51328000
H	-1.82528900	-1.11808200	-1.78723400
N	1.00721600	-0.42354100	-0.27667600
C	2.38843400	-0.28659900	-0.08466600
C	2.96452800	0.99442700	-0.03136400
C	3.17852900	-1.43458600	0.05038900
C	4.33571900	1.11521500	0.16381200
H	2.34154900	1.87575100	-0.14982600
C	4.55043900	-1.29829700	0.25237900
H	2.71561200	-2.41360100	-0.00039300
C	5.12929800	-0.02856200	0.30821800
H	4.78774400	2.10141400	0.20357100
H	5.16688400	-2.18477600	0.36178500
H	6.19929900	0.07279100	0.46120800
Ag	-1.12275400	1.96052200	-0.07657400

TS2

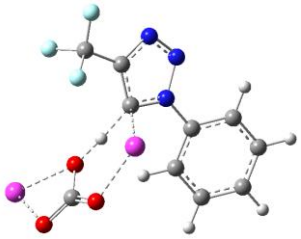


B3LYP electronic energy: -1511.18985698 a.u.
B3LYP enthalpy: -1511.010183 a.u.
B3LYP free energy: -1511.092264 a.u.
M06 SCF energy in solution: -1514.73457558 a.u.
M06 enthalpy in solution: -1514.55490158 a.u.
M06 free energy in solution: -1514.63698258 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.08605200	1.49297800	0.58400600
N	-1.79832500	2.56652100	-0.01027600
C	-0.10978100	1.86813200	1.66834900
C	-1.95395200	0.33840500	0.61945000
N	-2.90932000	2.15177500	-0.42093700
F	0.79359000	2.78186300	1.20058900
F	0.60897300	0.78405200	2.06190400
F	-0.68075900	2.39607100	2.75076200
H	-0.21213500	0.98359500	-0.31539900
N	-3.01516900	0.76029500	-0.05318900
C	-4.18487500	0.04674800	-0.47355900
C	-4.05806500	-1.19173600	-1.10652900
C	-5.43713000	0.62492200	-0.25567000
C	-5.20806800	-1.87452000	-1.50194700
H	-3.07224000	-1.59872700	-1.31283700
C	-6.57879000	-0.06508500	-0.66195500
H	-5.51055700	1.59369200	0.22639600
C	-6.46759300	-1.31366900	-1.27878300
H	-5.11780300	-2.83592800	-1.99848400
H	-7.55679800	0.37416900	-0.49185200
H	-7.36071900	-1.84532900	-1.59250600
Ag	-0.99339700	-1.57351100	0.80678000
C	1.58789100	-0.36437400	-0.60189400
O	0.80635300	0.61994300	-0.99192700
O	1.16277200	-1.49675200	-0.18289500
O	2.86243500	-0.13820800	-0.67656400
Ag	2.61451900	2.17714500	-1.05626900
Ag	3.45802100	-2.26172200	-0.01394700

TS3

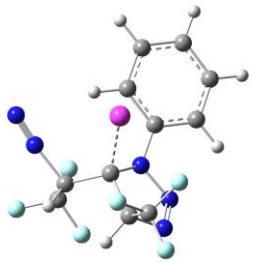


B3LYP electronic energy: -1365.62842761 a.u.
B3LYP enthalpy: -1365.450522 a.u.
B3LYP free energy: -1365.527381 a.u.
M06 SCF energy in solution: -1367.88877436 a.u.
M06 enthalpy in solution: -1367.71086936 a.u.
M06 free energy in solution: -1367.78772836 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.41930500	1.78116600	-0.97630500
N	2.56899000	1.69955900	-1.70002100
C	0.64909000	3.05674100	-0.88472000
C	1.06285000	0.54425200	-0.43134500
N	2.98920600	0.47028600	-1.64320400
F	1.40613500	4.12901300	-1.14841000
F	0.12873400	3.22512900	0.37355700
F	-0.40745800	3.08039600	-1.72744000
N	2.10839800	-0.23392500	-0.88080200
C	2.35981300	-1.61763600	-0.62858500
C	1.31402800	-2.45998200	-0.23698200
C	3.66046400	-2.11422500	-0.77120700
C	1.58154900	-3.80439300	0.02310200
H	0.30578500	-2.07267100	-0.14472200
C	3.90844100	-3.46221700	-0.51717900
H	4.45539300	-1.44552800	-1.07828500
C	2.87478500	-4.31146400	-0.11560600
H	0.76890000	-4.45619300	0.33141200
H	4.91873300	-3.84610900	-0.62727900
H	3.07566000	-5.35941300	0.08777600
Ag	0.75478100	0.84950800	1.86611200
H	-0.26480400	0.06669300	-0.16941100
C	-1.88791500	-0.44364700	1.19298600
O	-1.18498200	-0.17952700	2.21094000
O	-3.09665500	-0.84559400	1.27391600
O	-1.39621300	-0.31864900	-0.06534600
Ag	-3.59104000	-0.90505000	-0.87870100

TS4



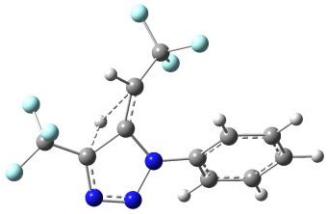
B3LYP electronic energy: -1441.54469355 a.u.
B3LYP enthalpy: -1441.338941 a.u.
B3LYP free energy: -1441.413387 a.u.
M06 SCF energy in solution: -1442.61943074 a.u.
M06 enthalpy in solution: -1442.41367774 a.u.
M06 free energy in solution: -1442.48812474 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.86280500	0.09269200	0.86722100
N	1.38300500	0.02635400	2.26948100
C	2.62896900	-1.20218700	0.56407900
C	0.58447900	0.33492000	0.01692100
N	0.14095100	0.05462100	2.30568900
F	3.65881100	-1.35509700	1.38659900
F	3.09070400	-1.17385400	-0.71060900
F	1.82370300	-2.28836200	0.66918500
H	2.60911700	0.89174800	0.79654400
N	-0.43672300	0.20828300	1.05085700
C	-1.73892700	-0.32133400	0.87867400
C	-2.39805000	-0.20043800	-0.36066300
C	-2.38537600	-0.98349600	1.93903400
C	-3.67223300	-0.75674100	-0.54050400
H	-1.98485000	0.41268500	-1.15257900
C	-3.65377500	-1.51843500	1.74487500
H	-1.88765100	-1.08168500	2.89519300
C	-4.30230000	-1.41889200	0.50682000
H	-4.17067600	-0.64212600	-1.49839300
H	-4.13816400	-2.03141100	2.57015100
H	-5.29147400	-1.84387800	0.37110100
Ag	0.13344900	-1.38737600	-1.41913300
C	0.68678400	1.76272100	-0.53814900
N	-0.01011800	1.91288000	-1.89670900
C	0.12444700	2.97288000	0.27137800
N	-0.52779100	1.88285100	-2.87461100
F	0.41644100	4.10787900	-0.38124700

F	0.72123400	2.96905600	1.45766300
F	-1.19867200	2.88891500	0.40801700
H	1.71537300	1.99948600	-0.83030100

TS5



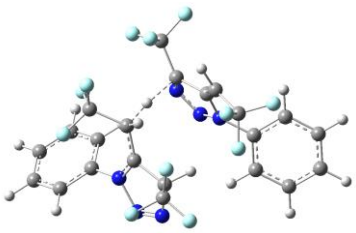
B3LYP electronic energy: -1186.50896066 a.u.
B3LYP enthalpy: -1186.320691 a.u.
B3LYP free energy: -1186.385151 a.u.
M06 SCF energy in solution: -1186.28034094 a.u.
M06 enthalpy in solution: -1186.09207094 a.u.
M06 free energy in solution: -1186.15653094 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.86289200	-0.93957300	0.08468300
N	-1.49310000	-2.23561400	0.02779900
C	-3.29040000	-0.48782400	0.09097900
C	-0.68262500	-0.05162200	0.09059800
N	-0.19807700	-2.30734700	-0.01491900
F	-4.12644100	-1.50448100	-0.12891600
F	-3.49401000	0.45295900	-0.86388700
F	-3.61011400	0.08000700	1.27432900
H	-1.10416600	-0.09998100	-1.01636100
N	0.34285300	-1.06779600	0.05476000
C	1.76464300	-0.95085900	0.06397100
C	2.38572400	-0.06293200	0.94579100
C	2.51452100	-1.79910300	-0.75706800
C	3.77753500	-0.02297600	0.99378100
H	1.79409800	0.59312400	1.57189400
C	3.90499600	-1.75160000	-0.69206200
H	2.00797800	-2.48647500	-1.42522100
C	4.53920600	-0.86364200	0.17951400
H	4.26539000	0.66879000	1.67387000
H	4.49213900	-2.40688800	-1.32868500
H	5.62382400	-0.82415800	0.22116200
C	-0.63246300	1.33496700	0.39549600
C	0.33945600	2.27539500	-0.18687300

F	1.24568900	2.77799600	0.70870500
F	-0.27390600	3.36802500	-0.70891100
F	1.07921400	1.71086800	-1.18377200
H	-1.57106500	1.78112100	0.69907600

TS6



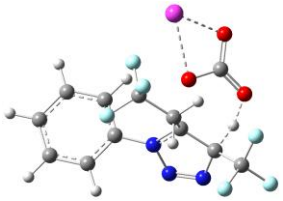
B3LYP electronic energy: -2373.1989188 a.u.
B3LYP enthalpy: -2372.814189 a.u.
B3LYP free energy: -2372.920886 a.u.
M06 SCF energy in solution: -2372.73911242 a.u.
M06 enthalpy in solution: -2372.35438342 a.u.
M06 free energy in solution: -2372.46107942 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.05227500	-1.91236900	-0.61060300
N	0.44589000	-3.06028800	0.22044300
C	-0.26934200	-2.39597300	-2.03689000
C	1.22108100	-0.96579700	-0.49697400
N	1.55895900	-2.86139800	0.73418700
F	0.81790500	-2.94182400	-2.61049400
F	-0.67091500	-1.36404700	-2.80410100
F	-1.24312600	-3.30767400	-2.00950400
H	0.65796900	1.12694100	-0.29572200
N	2.07527900	-1.58824000	0.33415800
C	3.29858100	-1.16367800	0.95433100
C	3.27161000	-0.12532300	1.88710100
C	4.47269400	-1.85750900	0.65732200
C	4.46195200	0.23072700	2.52059800
H	2.34546500	0.39713900	2.10853000
C	5.65164100	-1.49360900	1.30437100
H	4.45596900	-2.66431900	-0.06811400
C	5.64641100	-0.45005300	2.23327900
H	4.45714300	1.03970600	3.24462400
H	6.57254500	-2.02366300	1.08093900
H	6.56789200	-0.16819100	2.73456700
C	1.25842600	0.32981400	-1.08140100

C	2.57230000	1.01447800	-1.42532000
F	3.10685600	1.68317000	-0.38629100
F	2.35588900	1.90870100	-2.40761000
F	3.50477100	0.13812700	-1.86553300
H	0.57736700	0.39101000	-1.93235500
C	-0.27935100	2.01376600	0.57183800
N	0.09984500	1.55076700	1.82689200
C	0.11724000	3.39602800	0.16214500
C	-1.53758800	1.35429300	0.20067100
N	-0.66969300	0.60985200	2.19865700
F	1.33891700	3.71194000	0.62091700
F	-0.74389400	4.34320200	0.59813100
F	0.14677800	3.49801400	-1.19628100
N	-1.68597400	0.43308200	1.24480300
C	-2.84877600	-0.26721600	1.70247400
C	-2.69100300	-1.54815000	2.23815500
C	-4.10328000	0.34570700	1.68185500
C	-3.80064600	-2.22212000	2.74578400
H	-1.70590500	-2.00236500	2.26934800
C	-5.20880600	-0.34477200	2.17634600
H	-4.21423400	1.34302900	1.27221300
C	-5.06247600	-1.62610600	2.71087100
H	-3.67632100	-3.21712000	3.16333200
H	-6.18616000	0.12859200	2.15201000
H	-5.92717900	-2.15671900	3.09890400
C	-2.20947600	1.48068400	-0.98006600
C	-3.21988900	0.56241800	-1.55035300
F	-3.03387900	-0.73430500	-1.15246000
F	-3.14021500	0.57111500	-2.90124000
F	-4.51320200	0.85908500	-1.25049500
H	-1.91183900	2.28200800	-1.64356000
H	-0.87730700	-1.48345900	-0.20725300

TS7



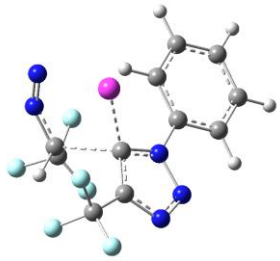
B3LYP electronic energy: -1596.75072 a.u.
B3LYP enthalpy: -1596.525591 a.u.
B3LYP free energy: -1596.604407 a.u.
M06 SCF energy in solution: -1597.75609127 a.u.

M06 enthalpy in solution: -1597.53096227 a.u.
M06 free energy in solution: -1597.60977827 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	2.21794100	0.61271700	-1.29529100
C	2.31535500	-0.46379600	-0.59278900
N	2.41870600	-1.52017400	-1.54615500
C	3.52578200	-0.28564000	0.28022600
C	0.94445000	-0.55198800	-0.00857500
N	1.32897500	-2.11481000	-1.66925300
F	4.64698300	-0.23295400	-0.44638200
F	3.67895200	-1.28719900	1.19074300
F	3.43082400	0.86507700	0.99591400
N	0.40625200	-1.60447200	-0.69900200
C	-0.91146100	-2.15388600	-0.72583700
C	-2.01010100	-1.36468700	-1.07841900
C	-1.06870500	-3.51924000	-0.47019000
C	-3.27797400	-1.94447100	-1.13755000
H	-1.85187100	-0.32135100	-1.32381700
C	-2.33730300	-4.09154500	-0.54476100
H	-0.19935400	-4.11761600	-0.21809100
C	-3.44493100	-3.30454300	-0.86977300
H	-4.13465100	-1.33528500	-1.41291700
H	-2.46047000	-5.15218600	-0.34579800
H	-4.43310600	-3.75245400	-0.92420500
C	0.73577500	-0.32723100	1.48248200
C	-0.63370900	-0.41840400	2.13476600
F	-1.59133400	0.38779700	1.58489600
F	-0.51629300	-0.03245400	3.42327800
F	-1.13276000	-1.66445100	2.13203200
H	1.14429400	0.65128300	1.73209500
H	1.34881900	-1.06922600	2.00693600
C	0.64788900	1.94031100	-1.31405700
O	1.78990400	1.72985300	-1.83197400
O	0.06624000	1.00348700	-0.53843300
O	-0.00585500	3.01694200	-1.47274400
Ag	-1.68232300	2.59034900	-0.06234700

TS8



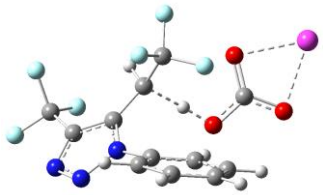
B3LYP electronic energy: -1441.19749611 a.u.
B3LYP enthalpy: -1441.003526 a.u.
B3LYP free energy: -1441.078050 a.u.
M06 SCF energy in solution: -1442.18953163 a.u.
M06 enthalpy in solution: -1441.99556163 a.u.
M06 free energy in solution: -1442.07008563 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.43076400	-0.09125800	-1.39723600
N	-0.92220600	-0.03154200	-2.65401900
C	-2.89777000	-0.02463900	-1.15386600
C	-0.41365800	-0.19659600	-0.43459100
N	0.36881300	-0.10489100	-2.57496100
F	-3.61383200	-0.31573600	-2.24217200
F	-3.29568500	1.21338500	-0.72839200
F	-3.27754700	-0.88303600	-0.16150900
N	0.70278900	-0.21327800	-1.24734100
C	2.07813400	-0.40340900	-0.91364900
C	2.48741000	-0.54775600	0.41673500
C	3.02605300	-0.46103900	-1.94538900
C	3.83565600	-0.75679600	0.71006800
H	1.77079800	-0.47722000	1.22494800
C	4.36833600	-0.66690300	-1.63691900
H	2.70102500	-0.34814000	-2.97131400
C	4.78259200	-0.81877300	-0.31144900
H	4.14025100	-0.86400700	1.74734400
H	5.09454300	-0.71015400	-2.44368800
H	5.83107200	-0.97977300	-0.07846800
Ag	-0.67551900	-1.71747500	1.19348800
C	-0.61674600	1.44067100	0.92948900
N	-0.60446500	0.99353200	2.21370700
C	0.40190000	2.52415700	0.63031400
N	-0.62742400	0.02304300	2.87299900
F	0.02522600	3.71155700	1.15087500
F	0.51661500	2.68171200	-0.69680700
F	1.60994200	2.22698500	1.14106100

H	-1.62015000	1.73279300	0.62602100

TS9



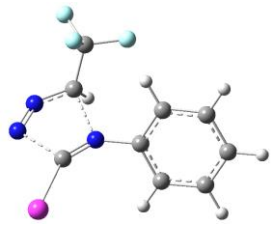
B3LYP electronic energy: -1596.25598541 a.u.
B3LYP enthalpy: -1596.043547 a.u.
B3LYP free energy: -1596.125293 a.u.
M06 SCF energy in solution: -1597.33147707 a.u.
M06 enthalpy in solution: -1597.11903807 a.u.
M06 free energy in solution: -1597.20078407 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.07263300	-1.37991000	-0.42523300
N	4.15462200	-0.72354900	-0.92217400
C	3.06447400	-2.85206700	-0.25774600
C	2.07465500	-0.47065400	-0.04367300
N	3.92855300	0.54793200	-0.90186200
F	4.12567400	-3.43596400	-0.85388800
F	1.94614800	-3.42916700	-0.77434200
F	3.09357000	-3.23435600	1.05217500
N	2.65341800	0.73046200	-0.38090800
C	2.15935600	2.06478700	-0.32635800
C	3.00301600	3.06647300	0.16736800
C	0.89370900	2.38470000	-0.82672500
C	2.57458000	4.39267900	0.16847400
H	3.98540900	2.79146100	0.53467800
C	0.47289100	3.71513800	-0.80735700
H	0.24445600	1.61134800	-1.22457400
C	1.30567700	4.72166200	-0.31474300
H	3.23265300	5.16854000	0.55287100
H	-0.51424100	3.95948700	-1.19101500
H	0.96931000	5.75594400	-0.30787700
C	0.75947400	-0.72789400	0.50556700
C	0.28832300	0.08083200	1.66602400
F	1.29322300	0.71183800	2.36391700
F	-0.36795500	-0.69192800	2.56963300
F	-0.58167500	1.09186800	1.35519900
H	0.64780700	-1.78295900	0.74400900

H	-0.28834000	-0.54299000	-0.59855500
C	-2.25498600	-0.37314800	-0.97402700
O	-1.01822400	-0.25719200	-1.41096000
O	-2.49479700	-1.05197500	0.09223800
O	-3.18435900	0.20954900	-1.64846600
Ag	-4.67910300	-0.40200000	-0.04130000

TS10



B3LYP electronic energy: -955.744846549 a.u.
B3LYP enthalpy: -955.588840 a.u.
B3LYP free energy: -955.650529 a.u.
M06 SCF energy in solution: -956.848300808 a.u.
M06 enthalpy in solution: -956.692293808 a.u.
M06 free energy in solution: -956.753982808 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.60486800	-1.42155200	-0.92506200
N	-0.61399200	-2.30359500	-0.86719100
C	-2.72104000	-1.54448500	0.10110600
C	0.96701100	-0.55193300	-0.22310500
N	0.53941900	-2.33324700	-0.63621900
F	-3.48306600	-2.61495300	-0.14079000
F	-3.47755900	-0.44285100	0.02535000
F	-2.21294700	-1.64784600	1.33935000
H	-1.89753600	-1.09993700	-1.92284300
N	-0.06780700	0.08358500	-0.27127800
C	-0.49297700	1.43645800	-0.16320400
C	-1.43976000	1.78123100	0.80557000
C	0.04821200	2.39066600	-1.03359100
C	-1.82991800	3.11515300	0.91512600
H	-1.84413600	1.02590100	1.46889700
C	-0.36757700	3.71638700	-0.91946700
H	0.76178000	2.09206500	-1.79538900
C	-1.30146600	4.08046300	0.05396900
H	-2.55341100	3.39728700	1.67347100
H	0.03958800	4.46337500	-1.59379400

H	-1.62015500	5.11460700	0.13869000
Ag	3.04525500	-0.39965900	0.25043700