Mechanisms for C(sp^2)-Si Activation of Aryltrimethylsilyl Groups in Palladium-catalysed Couplings

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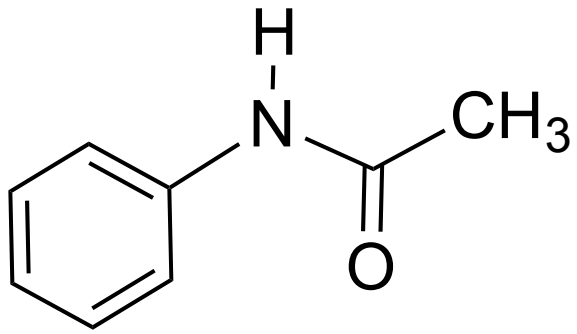
Methods

DFT calculations were carried out on Arcus-B (Oxford University supercomputer) or on the NSCCS Slater cluster facility at the Rutherford Appleton Laboratory using the Gaussian 09 (rev D-01)or Gaussian16 programs.[1] We utilized the B3LYP functional with dispersion corrections applied as recommended by Grimme,[2] and the 6-31g(d,p) basis set for all light atoms together with the Stuttgart-Dresden (SDD) electron core potential for Pd.[3] Alternatively, calculations were conducted with the B3PW91 functional,[4] or with the ωB97-xD functional.[5] Solvent effects were corrected for by the SCRF (Polarized Continuum Model) using the IEFPCM model,[6] in acetic acid had been used in experimental work; Truhlar's SDM model was used for thermodynamic equilibrium calculations.[7] Reported transition states were characterized by a single negative frequency, checked to represent the desired reaction coordinate (> -75 cm^{-1} in all cases), and ground states possessed all positive vibrational frequencies. Reported standard state Gibbs free energies, as derived computationally and adjusted to 298 K within Gaussian 09 or Gaussian 16, were not further corrected.

1) Gaussian 09, Revision D.01: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford, CT, USA, 2009
2) (a) S. Grimme, A. Hansen, J. G. Brandenburg and C. Bannwarth, *Chem. Rev*., 2016, **116**, 5105-5154; (b) M. Steinmetz and S. Grimme, *ChemistryOpen*, 2013, *2*, 115-124.
3) D. Andrae, U. Haeussermann, M. Dolg, H. Stoll, and H. Preuss, *Theor. Chem. Acc.,* 1990, **77**, 123-41.
4) J. P. Perdew and Y, Wang, *Phys. Rev. B*., 1992, **45**, 13244
5) Chai, J-D. and M. Head-Gordon, *Phys. Chem. Chem. Phys.,* 2008, **10**, 6615
6) E, Cances, B. Mennucci and J. Tomasi, *J. Phys. Chem. A*. 1997, **107**, 3032
7) A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.

Scheme 3

Acetanilide series



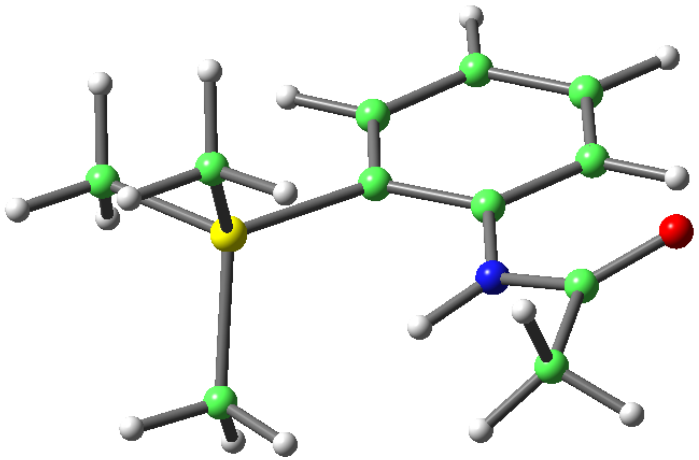
A AASiMe3b

- Zero-point correction= 0.257522 (Hartree/Particle)
- Thermal correction to Energy= 0.274470
- Thermal correction to Enthalpy= 0.275414
- Thermal correction to Gibbs Free Energy= 0.211143
- Sum of electronic and zero-point Energies= -848.778243
- Sum of electronic and thermal Energies= -848.761296
- Sum of electronic and thermal Enthalpies= -848.760352
- Sum of electronic and thermal Free Energies= -848.824623

- # freq rb3lyp/6-31g(d,p) scrf=check guess=tcheck
- geom=(connectivity,allcheck) genchk

- AASiMe3b

- 0 1
- C 1.41117600 1.93416100 -0.13209800
- C 0.69811600 0.72773600 -0.13839400
- C -0.71626000 0.71452400 -0.06036600
- C -1.36649500 1.95792700 0.00390700
- C -0.66745500 3.16508200 0.00852700
- C 0.72405700 3.14390900 -0.05420600
- H 2.48983700 1.91062100 -0.17837700
- H -2.44989700 1.98531200 0.06172100
- H -1.20368500 4.10715100 0.06480800
- H 1.28680300 4.07260700 -0.04918800
- Si -1.76065200 -0.86502200 0.03724700
- C -3.58048500 -0.39747700 0.17150200
- H -4.18668500 -1.30768900 0.23086400
- H -3.78467000 0.19663300 1.06763100
- H -3.92061500 0.17146400 -0.69951300
- C -1.25579100 -1.86149300 1.56007900
- H -1.82953800 -2.79263500 1.62002800
- H -0.19290900 -2.12037100 1.55381200
- H -1.44955900 -1.28681700 2.47159000
- C -1.54901700 -1.91687700 -1.52489500
- H -0.54315200 -2.32173000 -1.68010700
- H -2.23108100 -2.77305600 -1.47796800
- H -1.80543300 -1.33268800 -2.41465800
- N 1.37257200 -0.51169900 -0.24608600
- C 2.68555900 -0.80839500 0.02731900
- H 0.80369000 -1.29319100 -0.53163600
- C 3.03272600 -2.27974000 -0.11867700

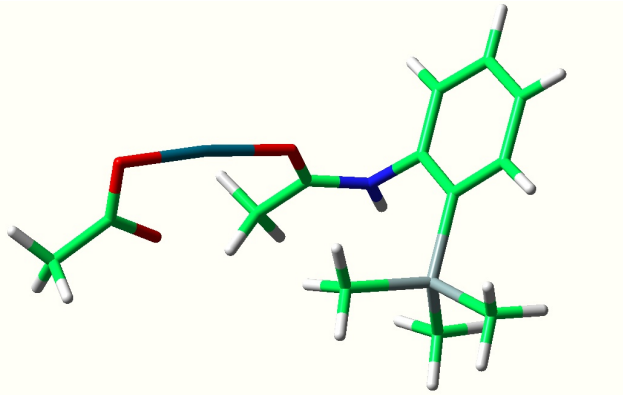


B MePdP1 initial complex

- Zero-point correction= 0.311390 (Hartree/Particle)
- Thermal correction to Energy= 0.334844
- Thermal correction to Enthalpy= 0.335788
- Thermal correction to Gibbs Free Energy= 0.256674
- Sum of electronic and zero-point Energies= -1204.989092
- Sum of electronic and thermal Energies= -1204.965639
- Sum of electronic and thermal Enthalpies= -1204.964695
- Sum of electronic and thermal Free Energies= -1205.043808

- MeOAc2P1

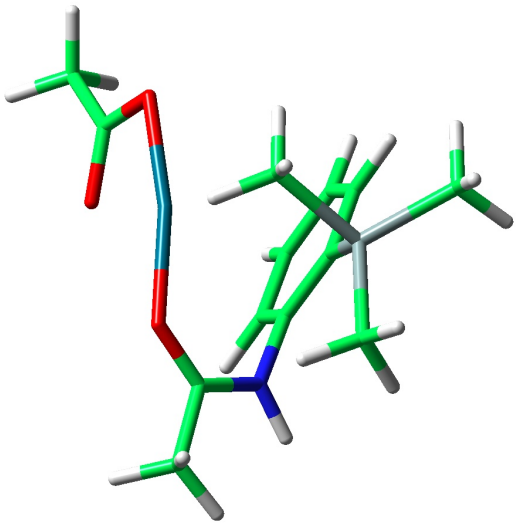
- 1 1
- H 2.28062100 3.07639000 -1.19520300
- C 2.72634600 2.35906800 -0.51370000
- C 2.37976200 1.01274200 -0.60525000
- C 3.64612900 2.76283900 0.45387000
- C 4.20365700 1.81347400 1.30980900
- H 3.92409800 3.80851200 0.53398800
- N 1.42872000 0.63203200 -1.62576600
- H 1.77618900 0.37513700 -2.54141500
- C 0.11445100 0.63615900 -1.44016000
- O -0.33515000 1.01288800 -0.31184600
- Pd -2.19316300 0.79767200 0.41105500
- H 4.92201100 2.11764000 2.06462400
- C 2.91599700 0.02534800 0.23696200
- O -3.13384400 -0.81420700 -0.46473900
- C 3.84191400 0.46952300 1.19767900
- H 4.29302500 -0.24861800 1.87421600
- O -4.05439400 0.36014200 1.10158300
- C -0.78315800 0.19580700 -2.55459100
- H -0.22056800 -0.08016700 -3.44665800
- H -1.38006600 -0.65806200 -2.22464000
- H -1.47371100 1.00847600 -2.79638700
- Si 2.45292600 -1.81673500 0.13429600
- C 0.63492500 -2.07094000 0.58958400
- H 0.35311000 -1.46341100 1.45541500
- H -0.04027100 -1.82203500 -0.23320100
- H 0.46528100 -3.12305100 0.84359500
- C 2.77925800 -2.47686100 -1.60394400
- H 2.65872100 -3.56576000 -1.61298400
- H 2.08605700 -2.06687400 -2.34467700
- H 3.80004800 -2.25263100 -1.92967100
- C 3.52659200 -2.75226100 1.36710400
- H 4.59396000 -2.61670600 1.16551600
- H 3.33307300 -2.44128000 2.39888700
- H 3.30949900 -3.82365300 1.29932700
- C -4.15713100 -0.63395600 0.29526200
- C -5.34146200 -1.52528900 0.25488100
- H -5.54139300 -1.83320100 -0.77335800
- H -5.12648500 -2.42171000 0.84657900
- H -6.20627900 -1.01634800 0.68271100



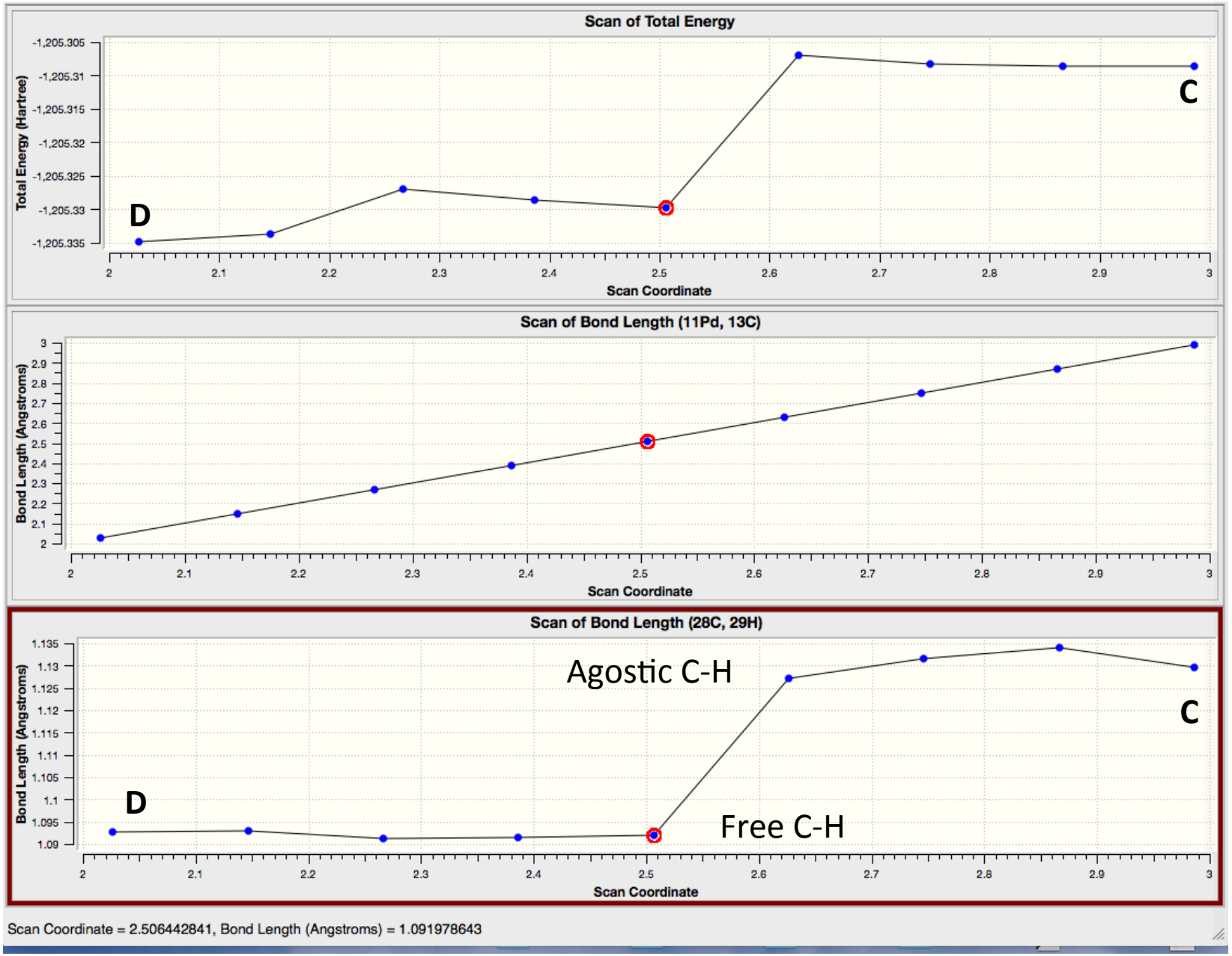
C MePdP7M Agostic new conformer MM

- Zero-point correction= 0.310739 (Hartree/Particle)
- Thermal correction to Energy= 0.333947
- Thermal correction to Enthalpy= 0.334891
- Thermal correction to Gibbs Free Energy= 0.256907
- Sum of electronic and zero-point Energies= -1204.997679
- Sum of electronic and thermal Energies= -1204.974470
- Sum of electronic and thermal Enthalpies= -1204.973526
- Sum of electronic and thermal Free Energies= -1205.051511
-
- MePdN7M

- 1 1
- H 0.46602500 -0.55250400 3.35369300
- C 0.29759500 0.27219300 2.66917400
- C -0.67500500 0.15043800 1.67504300
- C 1.04713000 1.44258000 2.76284200
- C 0.81457100 2.48236600 1.86211800
- H 1.80439300 1.53868800 3.53356200
- N -1.41889200 -1.08635200 1.65362800
- H -2.06021300 -1.24138100 2.42198400
- C -1.26831800 -2.09845300 0.80339300
- O -0.49174500 -2.09140500 -0.19864900
- Pd 0.77910300 -0.64987700 -0.85983900
- H 1.38970400 3.40018600 1.92849200
- C -0.94460200 1.17989900 0.75248800
- O 2.54418900 -0.98564700 0.16860700
- C -0.16483600 2.34690000 0.87901500
- H -0.32640400 3.17108700 0.19190400
- O 2.35975700 0.52040200 -1.38149200
- C -2.07633500 -3.34369900 1.02428200
- H -2.73593200 -3.26554400 1.88883800
- H -2.66917600 -3.54680600 0.12919900
- H -1.38871200 -4.18170700 1.16463900
- Si -2.14544100 1.08673700 -0.71646100
- C 3.10370100 -0.03694400 -0.49069400
- C 4.49229500 0.41035000 -0.21968000
- H 5.12357800 -0.45059900 0.00920300
- H 4.88380000 0.96146700 -1.07573500
- H 4.48077800 1.07007000 0.65458000
- C -1.07503000 0.56602400 -2.20307500
- H -0.60800100 -0.46314600 -2.15205500
- H -1.69384800 0.40132800 -3.09434500
- H -0.32169500 1.31334400 -2.46149900
- C -2.82156400 2.80213300 -1.06947800
- H -3.51096800 2.75683300 -1.91901200
- H -3.37505300 3.18784700 -0.20752200
- H -2.03533000 3.52013600 -1.31825200
- C -3.56049800 -0.13274900 -0.50055300
- H -3.26417100 -1.16494100 -0.70294000
- H -3.99304400 -0.08573800 0.50280100
- H -4.34830300 0.12286500 -1.21683900

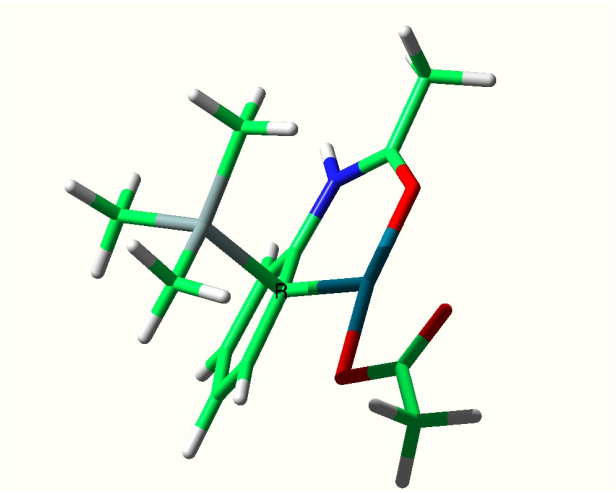


DFT scan (Pd–C bond) from Wheland **D** to agostic intermediate **C**



D MePdP3 Wheland

- Zero-point correction= 0.311758 (Hartree/Particle)
- Thermal correction to Energy= 0.335036
- Thermal correction to Enthalpy= 0.335980
- Thermal correction to Gibbs Free Energy= 0.258271
- Sum of electronic and zero-point Energies= -1205.022812
- Sum of electronic and thermal Energies= -1204.999534
- Sum of electronic and thermal Enthalpies= -1204.998590
- Sum of electronic and thermal Free Energies= -1205.076299
- MePdP3
- 1 1
- H -3.81284000 0.04114400 -1.90276900
- C -2.91095100 -0.49677700 -1.62887700
- C -1.92194200 0.13496300 -0.87184900
- C -2.71726500 -1.80201600 -2.07084300
- C -1.53348600 -2.49591300 -1.77971300
- H -3.48861700 -2.27487200 -2.66937100
- N -2.16140000 1.46716500 -0.50294200
- H -3.12141900 1.77975300 -0.58592300
- C -1.26291300 2.42599800 -0.18083700
- O -0.02606300 2.23523000 -0.14120500
- Pd 0.99529000 0.48268500 -0.26191400
- H -1.37921900 -3.49885300 -2.16057300
- C -0.74885800 -0.57324100 -0.45041300
- O 3.10827700 1.03193100 -0.23360600
- C -0.56848100 -1.88374500 -1.00214900
- H 0.34790200 -2.41088200 -0.76129500
- O 2.37249300 -1.02242900 -0.38252500
- C -1.79224400 3.78791800 0.15208600
- H -2.84293700 3.90839800 -0.11301400
- H -1.67299400 3.95217200 1.22755900
- H -1.19016500 4.53495600 -0.36830600
- Si -0.91550900 -0.94703000 1.58049000
- C -0.95170000 0.64537000 2.57215000
- H -0.00835800 1.19458800 2.54062800
- H -1.76552100 1.30908400 2.27011600
- H -1.14471100 0.35645200 3.61248400
- C -2.57932700 -1.80391300 1.72169100
- H -2.71400400 -2.13042700 2.75910500
- H -3.40571200 -1.13288500 1.47251600
- H -2.64394100 -2.68634400 1.08007100
- C 0.47340300 -2.08501200 2.10996000
- H 0.40777800 -3.06181800 1.62388800
- H 1.46252600 -1.66631900 1.91571800
- H 0.36833400 -2.24175100 3.18990600
- C 3.37501300 -0.20515100 -0.32756500
- C 4.77080600 -0.73532600 -0.34679700
- H 5.47392500 0.06064500 -0.59338600
- H 5.01214800 -1.12995300 0.64586400
- H 4.85143300 -1.55512000 -1.06379400

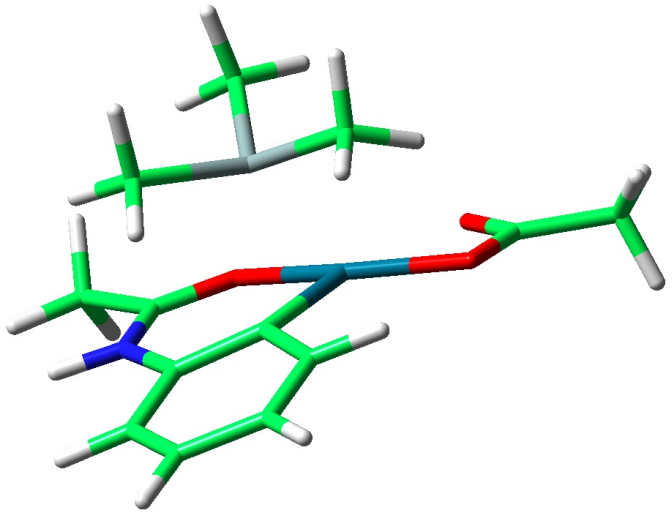


DE MePdP21T2 ν = -129 cm^{-1}

- Zero-point correction= 0.312070 (Hartree/Particle)
- Thermal correction to Energy= 0.334421
- Thermal correction to Enthalpy= 0.335365
- Thermal correction to Gibbs Free Energy= 0.260811
- Sum of electronic and zero-point Energies= -1205.017999
- Sum of electronic and thermal Energies= -1204.995648
- Sum of electronic and thermal Enthalpies= -1204.994704
- Sum of electronic and thermal Free Energies= -1205.069258

- MePdP21T2

- 1 1
- H -4.13072400 -0.44840700 -1.36872400
- C -3.15088800 -0.89254900 -1.22179600
- C -2.08905200 -0.10057100 -0.77421100
- C -2.94988500 -2.24319300 -1.48963900
- C -1.68435000 -2.81708200 -1.33116600
- H -3.78285800 -2.84505300 -1.83618400
- N -2.37898300 1.25550700 -0.51712500
- H -3.36149600 1.49873000 -0.54455600
- C -1.53622100 2.27862400 -0.30924200
- O -0.28275400 2.15858000 -0.28183500
- Pd 0.82377300 0.46816700 -0.38474500
- H -1.52371200 -3.86455100 -1.56057500
- C -0.81276300 -0.67129300 -0.55219200
- O 2.92988500 1.13765700 -0.44852700
- C -0.62802100 -2.03196300 -0.88525300
- H 0.35865800 -2.46557200 -0.77014700
- O 2.28131200 -0.95038800 -0.56477600
- C -2.11920900 3.64345600 -0.09802500
- H -3.20782400 3.65110100 -0.15729500
- H -1.80447900 4.01319800 0.88139100
- H -1.70837500 4.31736400 -0.85408800
- Si -0.31731700 -0.66457500 1.76285400
- C 0.23314500 0.87878900 2.68166800
- H 1.28523000 1.12035900 2.51588000
- H -0.37179100 1.75266400 2.43064600
- H 0.08947100 0.66452800 3.74922900
- C -2.09811300 -1.03970000 2.20352800
- H -2.11743100 -1.30786200 3.26704100
- H -2.74872100 -0.17262200 2.06706100
- H -2.49735300 -1.87811900 1.62878300
- C 0.80492100 -2.13137600 2.03040900
- H 0.34260400 -3.06003000 1.68882200
- H 1.77187400 -2.01194200 1.53969600
- H 0.96929000 -2.20749300 3.11227900
- C 3.24619900 -0.08145900 -0.57195400
- C 4.65410500 -0.54747200 -0.74563900
- H 5.34998600 0.24030200 -0.45616800
- H 4.82624500 -1.44918300 -0.15395700
- H 4.81644100 -0.79964900 -1.79875300

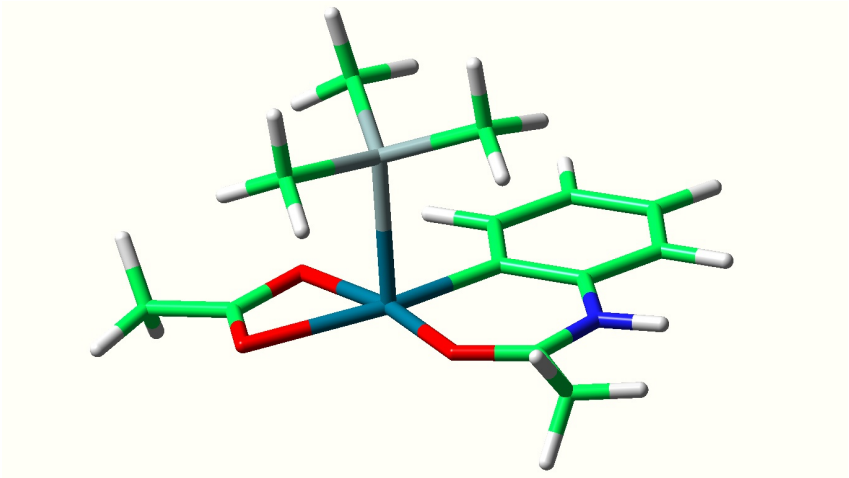


E SiOGS7 Pd-Si complex

- Zero-point correction= 0.311626 (Hartree/Particle)
- Thermal correction to Energy= 0.335091
- Thermal correction to Enthalpy= 0.336036
- Thermal correction to Gibbs Free Energy= 0.258289
- Sum of electronic and zero-point Energies= -1205.027762
- Sum of electronic and thermal Energies= -1205.004297
- Sum of electronic and thermal Enthalpies= -1205.003352
- Sum of electronic and thermal Free Energies= -1205.081099

- SiOGS7

- 1 1
- H 4.44339600 0.95074300 -0.25905500
- C 3.42796400 1.33607800 -0.25280000
- C 2.35061000 0.44724900 -0.38669600
- C 3.19697500 2.69904900 -0.11302900
- C 1.88996000 3.19146700 -0.11158200
- H 4.03853100 3.37499100 -0.00848100
- N 2.67620100 -0.92269500 -0.51906200
- H 3.66618600 -1.13425900 -0.49751400
- C 1.86617800 -1.96888900 -0.67183600
- O 0.60352900 -1.88067700 -0.72250400
- Pd -0.54042400 -0.22719600 -0.61853700
- H 1.70329100 4.25509800 -0.00905800
- C 1.03832400 0.93739500 -0.37299400
- O -2.69614400 -0.82926800 -1.05115800
- C 0.81635100 2.31074000 -0.24125200
- H -0.19968100 2.68857600 -0.23754700
- O -1.98800900 1.20632000 -0.64383700
- C 2.46993800 -3.33572900 -0.78399700
- H 3.55834300 -3.31871300 -0.72340800
- H 2.06995600 -3.96295300 0.01699100
- H 2.16427600 -3.77749500 -1.73582700
- Si -0.62795500 -0.32872200 1.82656700
- C -1.90952000 -1.68210000 1.97794500
- H -2.87574200 -1.38502700 1.56700700
- H -1.58147000 -2.59506900 1.47436400
- H -2.03092300 -1.90259300 3.04645700
- C 1.04077200 -0.84742500 2.48988800
- H 0.91366300 -0.99813900 3.56962400
- H 1.38327500 -1.79322600 2.06588900
- H 1.80376600 -0.08121500 2.34135600
- C -1.17368500 1.34791400 2.43357700
- H -0.36656900 2.07971100 2.35872800
- H -2.03890800 1.71615300 1.88000100
- H -1.45087600 1.24188500 3.48978900
- C -2.96164700 0.39751900 -0.95607800
- C -4.32772100 0.96950000 -1.15937100
- H -5.00401500 0.20559200 -1.54224400
- H -4.70319500 1.34608500 -0.20261300
- H -4.27780300 1.81423100 -1.85093800

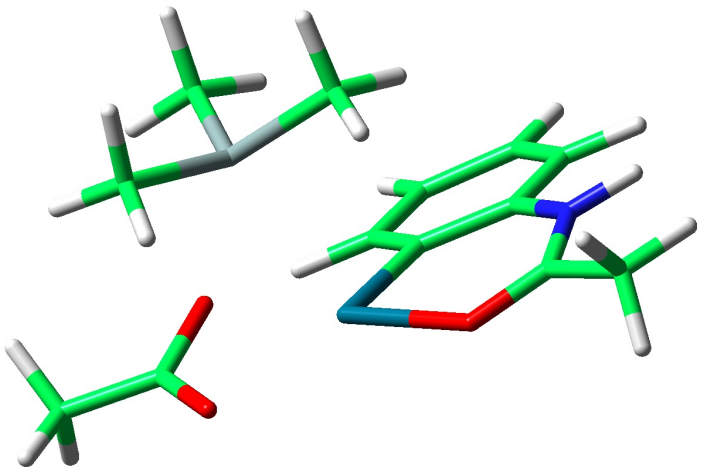


EF MePdP22T TS Pd---O migration (C-H side) ν = -163 cm^{-1}

- Zero-point correction= 0.311079 (Hartree/Particle)
- Thermal correction to Energy= 0.333768
- Thermal correction to Enthalpy= 0.334713
- Thermal correction to Gibbs Free Energy= 0.259460
- Sum of electronic and zero-point Energies= -1205.016198
- Sum of electronic and thermal Energies= -1204.993508
- Sum of electronic and thermal Enthalpies= -1204.992564
- Sum of electronic and thermal Free Energies= -1205.067817

- MePdP22T

- 1 1
- H 4.40695800 1.32582000 0.27430500
- C 3.38957000 1.55352100 −0.03104600
- C 2.44427500 0.51879400 −0.10264600
- C 3.03153800 2.85381300 −0.36469700
- C 1.72869800 3.13443700 −0.78164900
- H 3.77234900 3.64375800 −0.30845600
- N 2.90170700 −0.78069100 0.21731300
- H 3.84330000 −0.83336400 0.58499500
- C 2.29093700 −1.94569700 −0.00600700
- O 1.12197600 −2.03782900 −0.47687800
- Pd −0.26595200 −0.57738700 −0.62118600
- H 1.44395900 4.14487700 −1.05514300
- C 1.12809800 0.80401600 −0.48624000
- O −2.45869300 −1.38095600 −1.16805400
- C 0.78222800 2.11068400 −0.84108800
- H −0.23452600 2.33146100 −1.14485700
- O −1.90584800 0.68161900 −0.59059800
- C 3.02079200 −3.21409600 0.31857500
- H 4.04441700 −3.03615800 0.64874300
- H 2.47219900 −3.74429800 1.10196900
- H 3.02954000 −3.85017100 −0.56985600
- Si −1.34233100 0.36102600 1.56898800
- C −2.95948800 −0.49891400 1.92911600
- H −3.82315700 0.04812100 1.54436000
- H −2.98071100 −1.51898700 1.53859600
- H −3.05085500 −0.55859200 3.02012400
- C 0.04093500 −0.46047800 2.54770600
- H −0.20393700 −0.31417400 3.60890900
- H 0.10178700 −1.53484500 2.35919100
- H 1.01120900 −0.00013100 2.35323800
- C −1.32877700 2.20723000 1.80404700
- H −0.36834200 2.64523800 1.52662100
- H −2.12294500 2.69478000 1.23658600
- H −1.49154400 2.39560000 2.87263700
- C −2.78929300 −0.19128000 −1.08595100
- C −4.10312000 0.37093500 −1.51902400
- H −4.81644100 −0.43256400 −1.69906300
- H −4.48201200 1.06408600 −0.76451700
- H −3.95462600 0.93934500 −2.44319700

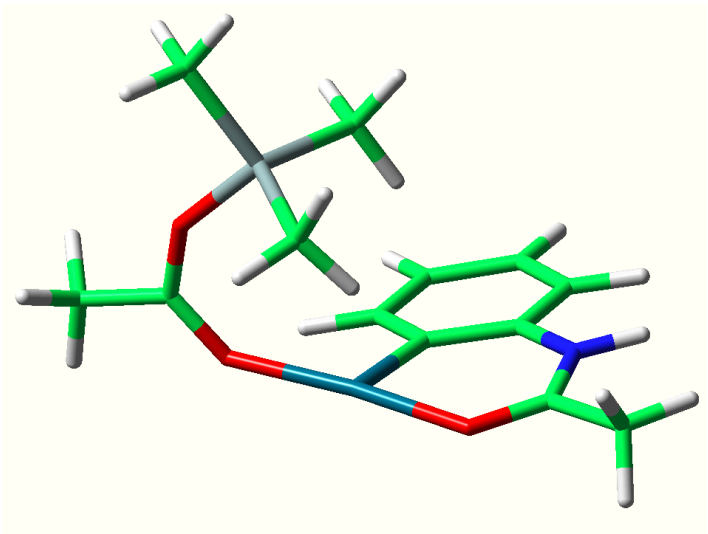


F SiOGS for silyl transfer product

- Zero-point correction= 0.312205 (Hartree/Particle)
- Thermal correction to Energy= 0.335639
- Thermal correction to Enthalpy= 0.336583
- Thermal correction to Gibbs Free Energy= 0.257450
- Sum of electronic and zero-point Energies= -1205.057292
- Sum of electronic and thermal Energies= -1205.033858
- Sum of electronic and thermal Enthalpies= -1205.032914
- Sum of electronic and thermal Free Energies= -1205.112047

- SiOGS
- 1 1

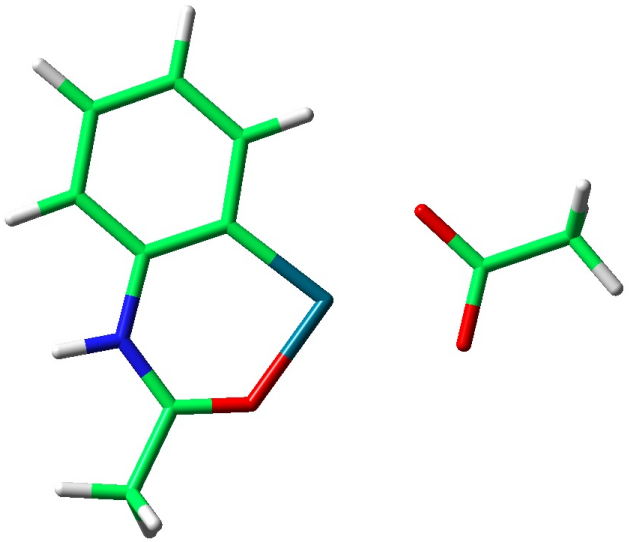
H	3.89595900	1.39035700	2.03525600
C	3.02930300	1.65347300	1.43496300
C	2.41320300	0.66673700	0.64821200
C	2.54769000	2.95563700	1.43821400
C	1.45024200	3.28943900	0.64319900
H	3.03453500	3.70656100	2.05081200
N	3.00336800	-0.61917100	0.69163900
H	3.77740800	-0.71720500	1.33599100
C	2.73644700	-1.68382900	-0.06758000
O	1.80765500	-1.70853100	-0.92206000
Pd	0.32695500	-0.37232800	-1.15348700
H	1.07380200	4.30698300	0.62369600
C	1.28668700	0.98970800	-0.12354200
O	-2.91842700	0.26642500	-0.09001200
C	0.82732300	2.31150700	-0.13242400
H	-0.02385900	2.57937100	-0.74412700
O	-1.29680900	0.85027100	-1.56733400
C	3.58310400	-2.91112600	0.09498700
H	4.36288400	-2.78712500	0.84708400
H	2.94049100	-3.75093900	0.37165300
H	4.04436300	-3.14758200	-0.86738500
Si	-2.49887900	-0.80563400	1.22779500
C	-4.15900600	-1.00694300	2.05558200
H	-4.55320400	-0.04227600	2.38897000
H	-4.88741800	-1.45995000	1.37602900
H	-4.06622900	-1.65663200	2.93249300
C	-1.88866900	-2.43260500	0.53348700
H	-1.98314700	-3.20153700	1.30897000
H	-2.49633400	-2.74873100	-0.32034300
H	-0.83984800	-2.40081400	0.22469900
C	-1.26845000	0.08215500	2.31596600
H	-0.30260900	0.21844300	1.82513900
H	-1.64929900	1.06589100	2.60785800
H	-1.11294500	-0.50114300	3.23073400
C	-2.45216000	0.93103900	-1.10135600
C	-3.43411600	1.87444100	-1.73187900
H	-4.32687500	1.31868300	-2.03095300
H	-3.74460300	2.61223300	-0.98620100
H	-2.99123400	2.37244600	-2.59229400



G MePdP19 final desilylation

- Zero-point correction= 0.197629 (Hartree/Particle)
- Thermal correction to Energy= 0.211271
- Thermal correction to Enthalpy= 0.212215
- Thermal correction to Gibbs Free Energy= 0.155755
- Sum of electronic and zero-point Energies= -795.996943
- Sum of electronic and thermal Energies= -795.983302
- Sum of electronic and thermal Enthalpies= -795.982357
- Sum of electronic and thermal Free Energies= -796.038817
-
- MePdP19

- 0 1
- H -4.26503300 0.94040900 -0.00510600
- C -3.24331500 1.31245500 -0.00318100
- C -2.17402500 0.40265300 -0.00159900
- C -2.99815100 2.68026300 -0.00233800
- C -1.68125300 3.14686700 0.00011900
- H -3.83112300 3.37573200 -0.00356600
- N -2.52587300 -0.97108100 -0.00277500
- H -3.51895800 -1.16277900 -0.00381600
- C -1.72774400 -2.04403600 -0.00252100
- O -0.47031500 -1.98796100 -0.00065700
- Pd 0.71432900 -0.33612900 0.00324800
- H -1.47847600 4.21358500 0.00081300
- C -0.84379100 0.85297500 0.00089900
- O 2.90209000 -1.02454400 0.00672700
- C -0.62244200 2.23864500 0.00171800
- H 0.40014100 2.60151800 0.00377300
- O 2.23841100 1.07765300 0.00742300
- C -2.37535300 -3.40058200 -0.00424400
- H -3.46467500 -3.34738800 -0.01194500
- H -2.03442700 -3.95334500 -0.88344400
- H -2.04679200 -3.94997600 0.88183000
- C 3.19046700 0.20520400 0.00486900
- C 4.61247500 0.69468900 -0.01565600
- H 5.30501300 -0.13663500 0.11799200
- H 4.81227500 1.18383100 -0.97422600
- H 4.76133100 1.43856900 0.77137800



Mulliken Charges for the reaction centre for trimethylsilyl migration from C to Pd in Scheme 3

Stage	Si	Pd	C(Ar)
B	0.667	0.643	-0.058
D	0.774	0.374	-0.321
DE	0.747	0.347	-0.200
E	0.727	0.295	0.048

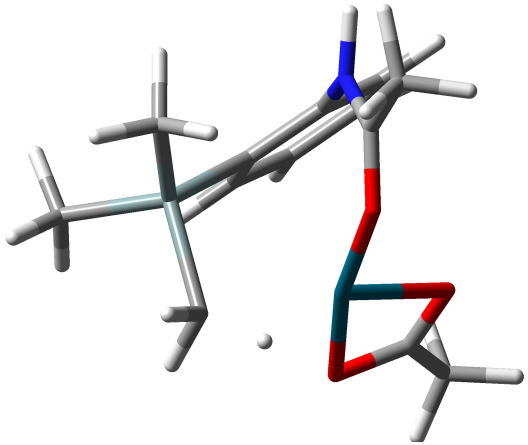
Single point recalculations from the optimized geometries as Scheme 3; B3LYP-D3,6-31G (d,p); def2-QZVP for Pd

Alternative Functionals for AA; first B3PW91-D3(1) then ωB97-xD(2)

C1 MePdP46

- Zero-point correction= 0.312294 (Hartree/Particle)
- Thermal correction to Energy= 0.334971
- Thermal correction to Enthalpy= 0.335915
- Thermal correction to Gibbs Free Energy= 0.260867
- Sum of electronic and zero-point Energies= -1204.691504
- Sum of electronic and thermal Energies= -1204.668826
- Sum of electronic and thermal Enthalpies= -1204.667882
- Sum of electronic and thermal Free Energies= -1204.742931
- MePdP46
-

- 1 1
- H -0.49538600 1.30811400 3.28954700
- C -0.53846100 0.38206400 2.72491000
- C 0.43257100 0.12356600 1.75909300
- C -1.56129500 -0.53530300 2.94143700
- C -1.60411400 -1.70884900 2.19158100
- H -2.31984600 -0.33062500 3.68972500
- N 1.45511000 1.11706900 1.60410900
- H 1.99855900 1.32504300 2.43190700
- C 1.67362600 1.91084600 0.55885200
- O 1.06038300 1.84316900 -0.54398900
- Pd -0.42656500 0.56877300 -1.06311300
- H -2.39574100 -2.43313200 2.35539300
- C 0.42565000 -1.05461000 0.98777700
- O -2.12236300 1.31075700 -0.15887300
- C -0.62262100 -1.95955700 1.23676600
- H -0.67466400 -2.88137700 0.66674100
- O -2.14513300 -0.42135700 -1.46034300
- C 2.72205700 2.96991900 0.68707700
- H 3.32471800 2.85502900 1.58858200
- H 3.36705000 2.94306700 -0.19328400
- H 2.22629000 3.94469600 0.70615900
- Si 1.66818100 -1.48738800 -0.37849300
- C -2.80095400 0.35623400 -0.67406400
- C -4.22835100 0.13454600 -0.35557600
- H -4.73563600 1.09224900 -0.22630000
- H -4.70460000 -0.45444600 -1.14027900
- H -4.28726500 -0.41672100 0.58861000
- C 1.08181300 -0.89134200 -2.11764000
- H 0.68652100 0.11097100 -2.48058100
- H 2.03273700 -0.81823000 -2.66183000
- H 0.45274400 -1.64658000 -2.59171300
- C 1.75546700 -3.35035400 -0.54139400
- H 2.48982000 -3.61396700 -1.30970600
- H 2.07153400 -3.80659100 0.40182400
- H 0.79813500 -3.79108200 -0.83337800
- C 3.37703100 -0.78334000 -0.06277900
- H 3.48230900 0.25529100 -0.38270700
- H 3.64376500 -0.85125100 0.99554200
- H 4.10303300 -1.37354600 -0.63150700
-

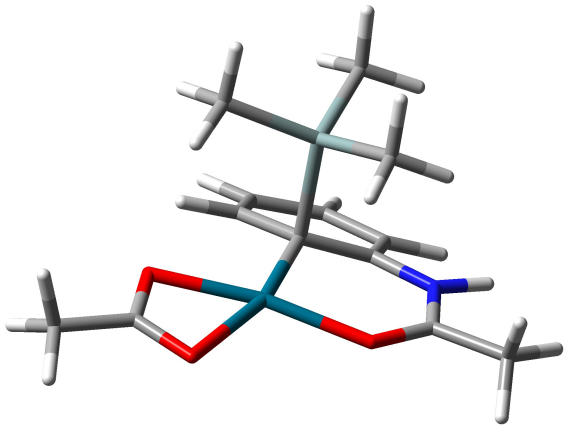


D1 MePdP44

- Zero-point correction= 0.312707 (Hartree/Particle)
- Thermal correction to Energy= 0.335804
- Thermal correction to Enthalpy= 0.336748
- Thermal correction to Gibbs Free Energy= 0.260504
- Sum of electronic and zero-point Energies= -1204.718365
- Sum of electronic and thermal Energies= -1204.695268
- Sum of electronic and thermal Enthalpies= -1204.694324
- Sum of electronic and thermal Free Energies= -1204.770569

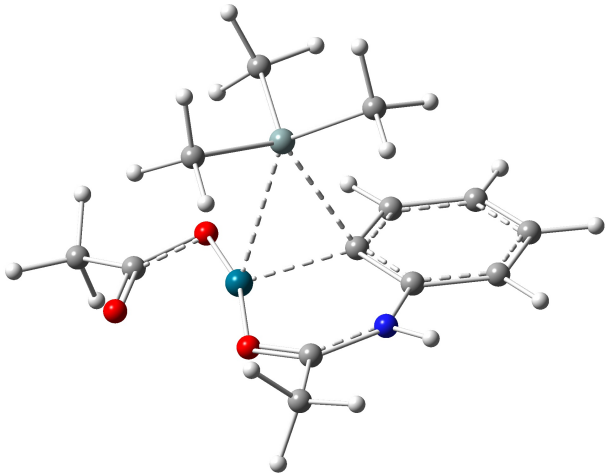
- MePdP44

- 1 1
- H -3.88104000 0.01448700 -1.76575800
- C -2.96137900 -0.51313900 -1.53301800
- C -1.93980000 0.13574000 -0.83839400
- C -2.78221800 -1.82092500 -1.96567500
- C -1.58288400 -2.50336600 -1.72684900
- H -3.58120500 -2.30676100 -2.51628200
- N -2.16533300 1.46530500 -0.47434100
- H -3.12619000 1.77959700 -0.52868100
- C -1.25658600 2.41876500 -0.18197500
- O -0.02232600 2.22196700 -0.16947700
- Pd 0.97891200 0.47540200 -0.27613200
- H -1.44199300 -3.51140700 -2.10027700
- C -0.74433300 -0.55893600 -0.47702000
- O 3.07441500 1.02501700 -0.24039300
- C -0.58361700 -1.87528000 -1.01002400
- H 0.34869800 -2.39218300 -0.80623100
- O 2.34408300 -1.02476800 -0.41164900
- C -1.76569400 3.78302600 0.14825800
- H -2.83144200 3.89855000 -0.04945200
- H -1.57317100 3.97535200 1.20797100
- H -1.20045800 4.51696000 -0.42941100
- Si -0.85247100 -0.92729400 1.56177500
- C -0.91568100 0.66258100 2.54805400
- H 0.00558700 1.24629800 2.49436600
- H -1.76410100 1.29289300 2.27086400
- H -1.06942400 0.36328100 3.59218800
- C -2.48965200 -1.81993700 1.73810700
- H -2.59202100 -2.14485600 2.77967300
- H -3.33659100 -1.16916000 1.50522200
- H -2.54682700 -2.70645500 1.10170200
- C 0.56502800 -2.02867500 2.07578300
- H 0.55946000 -2.98201900 1.54206200
- H 1.53838200 -1.55585400 1.93397300
- H 0.43097800 -2.24170600 3.14285800
- C 3.34259600 -0.20853600 -0.34569600
- C 4.73472100 -0.73455300 -0.36320400
- H 5.43584100 0.05896400 -0.62273000
- H 4.97983100 -1.11262000 0.63475900
- H 4.81527400 -1.56519200 -1.06712700



DE1 MePdP40T n = -106.2 cm^{-1}

- Zero-point correction= 0.313165 (Hartree/Particle)
- Thermal correction to Energy= 0.335265
- Thermal correction to Enthalpy= 0.336209
- Thermal correction to Gibbs Free Energy= 0.262908
- Sum of electronic and zero-point Energies= -1204.714693
- Sum of electronic and thermal Energies= -1204.692593
- Sum of electronic and thermal Enthalpies= -1204.691649
- Sum of electronic and thermal Free Energies= -1204.764949
- MePdP40T
-
- 1 1
- H -4.11446300 -0.47796700 -1.37610600
- C -3.13527500 -0.91788700 -1.21087400
- C -2.07855800 -0.11692900 -0.77394600
- C -2.93241900 -2.27237100 -1.44533700
- C -1.67019700 -2.84164500 -1.26479100
- H -3.76325000 -2.88209900 -1.78431800
- N -2.36700800 1.23748800 -0.54358400
- H -3.34784700 1.48325500 -0.58006100
- C -1.52390600 2.25827200 -0.34660600
- O -0.27325900 2.13618900 -0.31079200
- Pd 0.81943100 0.45060100 -0.37522900
- H -1.50739100 -3.89423600 -1.46932400
- C -0.80656600 -0.68225100 -0.53137500
- O 2.90078000 1.12213200 -0.46896400
- C -0.61826800 -2.04736700 -0.83099000
- H 0.36938400 -2.47636200 -0.69992100
- O 2.26285200 -0.96491700 -0.53899300
- C -2.10128300 3.62359300 -0.16490100
- H -3.19085900 3.63118300 -0.19831800
- H -1.76256200 4.02521500 0.79315800
- H -1.70907700 4.27312800 -0.95175400
- Si -0.30861200 -0.60422700 1.73887800
- C 0.24183100 0.93758100 2.65758500
- H 1.29275900 1.18836000 2.49840000
- H -0.36922900 1.80855500 2.41156400
- H 0.09622700 0.71590100 3.72331000
- C -2.08913300 -0.95181000 2.19282800
- H -2.10672900 -1.19285400 3.26270800
- H -2.73326500 -0.08276000 2.03740300
- H -2.49421900 -1.80214000 1.63930600
- C 0.78475700 -2.07991900 2.05656500
- H 0.29981900 -3.00985400 1.75110000
- H 1.75336300 -2.00063100 1.56023500
- H 0.95062400 -2.11935000 3.13989100
- C 3.22221800 -0.09539300 -0.57520700
- C 4.62437100 -0.55480700 -0.76372300
- H 5.32081000 0.21903300 -0.43989300
- H 4.79486100 -1.48241700 -0.21411400
- H 4.78844200 -0.75646200 -1.82731400
-

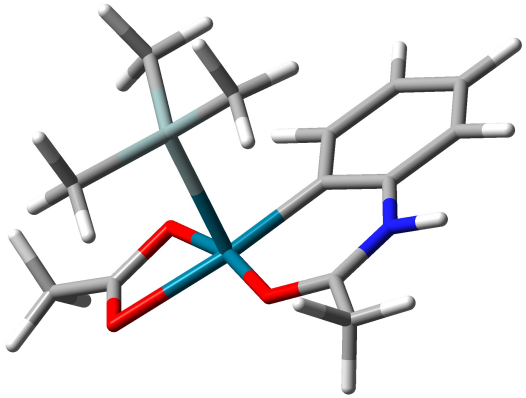


E1 MePdP48

- Zero-point correction= 0.312635 (Hartree/Particle)
- Thermal correction to Energy= 0.335870
- Thermal correction to Enthalpy= 0.336815
- Thermal correction to Gibbs Free Energy= 0.260378
- Sum of electronic and zero-point Energies= -1204.723049
- Sum of electronic and thermal Energies= -1204.699813
- Sum of electronic and thermal Enthalpies= -1204.698869
- Sum of electronic and thermal Free Energies= -1204.775306

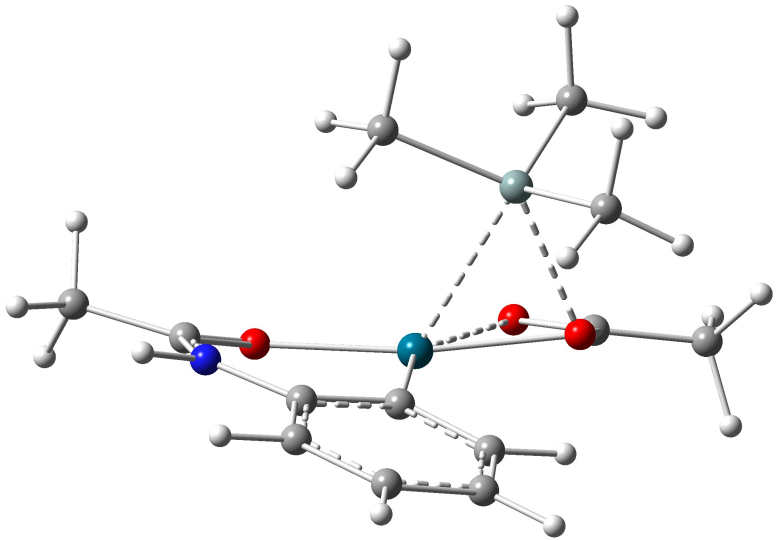
- MePdP48
-

- 1 1
- H 4.41064800 0.96372500 -0.31878300
- C 3.39142200 1.34000500 -0.30857500
- C 2.32201800 0.44111600 -0.41342200
- C 3.15086500 2.70162900 -0.19269100
- C 1.84185400 3.18287800 -0.18626200
- H 3.98838100 3.38622200 -0.11073700
- N 2.65386300 -0.92269800 -0.52202400
- H 3.64400200 -1.13011600 -0.49934800
- C 1.84747600 -1.97193100 -0.64964600
- O 0.58748900 -1.88907100 -0.69986900
- Pd -0.55441900 -0.25039000 -0.60953500
- H 1.64710200 4.24705400 -0.10269600
- C 1.00722600 0.91987100 -0.39200700
- O -2.69350300 -0.86708500 -1.02816600
- C 0.77636000 2.29204100 -0.28562600
- H -0.24401000 2.66015900 -0.27652300
- O -1.99770400 1.16871700 -0.62506400
- C 2.45107100 -3.33498900 -0.73088900
- H 3.54029700 -3.31624500 -0.69162400
- H 2.06766300 -3.93761200 0.09664400
- H 2.12737600 -3.80728400 -1.66155500
- Si -0.55881200 -0.26955500 1.81457600
- C -1.84565800 -1.60391600 2.03710800
- H -2.82336500 -1.30457700 1.65541800
- H -1.54731900 -2.53392600 1.54682500
- H -1.93121000 -1.79564900 3.11462000
- C 1.10729300 -0.78497100 2.47547200
- H 0.98441300 -0.88934000 3.56124800
- H 1.43469200 -1.75285700 2.09095100
- H 1.87811800 -0.03412600 2.29284000
- C -1.08412500 1.41914200 2.39469600
- H -0.26172400 2.13505700 2.33475700
- H -1.92939900 1.79621400 1.81634500
- H -1.39076500 1.32599800 3.44375900
- C -2.96674500 0.35490100 -0.92590400
- C -4.33396800 0.91645400 -1.11149200
- H -5.01761800 0.14190600 -1.45769800
- H -4.68694500 1.32071900 -0.15795700
- H -4.30150300 1.74138700 -1.82755100
-



EF1 MePdP42F $\nu = -152.25\ cm^{-1}$

- Zero-point correction= 0.311910 (Hartree/Particle)
- Thermal correction to Energy= 0.334489
- Thermal correction to Enthalpy= 0.335433
- Thermal correction to Gibbs Free Energy= 0.260418
- Sum of electronic and zero-point Energies= -1204.711451
- Sum of electronic and thermal Energies= -1204.688872
- Sum of electronic and thermal Enthalpies= -1204.687928
- Sum of electronic and thermal Free Energies= -1204.762943
- MePdP42F
-
- 1 1
- H 4.36761200 1.34819900 0.29096100
- C 3.35088300 1.56419500 -0.02604800
- C 2.41725700 0.52221900 -0.10040100
- C 2.98478500 2.85732700 -0.37134100
- C 1.68615100 3.12326200 -0.80382100
- H 3.71816200 3.65444800 -0.31220100
- N 2.87812100 -0.76752300 0.22658900
- H 3.81340900 -0.81495300 0.60885500
- C 2.27809500 -1.93281600 -0.00925000
- O 1.11903900 -2.02999200 -0.49603200
- Pd -0.26992200 -0.58655800 -0.62210700
- H 1.39520300 4.12946600 -1.08745300
- C 1.10381800 0.79417200 -0.49565900
- O -2.45910700 -1.38380600 -1.13915400
- C 0.75038700 2.09260400 -0.86455600
- H -0.26673400 2.30172200 -1.17823300
- O -1.89402000 0.67148300 -0.56123800
- C 3.00765900 -3.19390400 0.31873000
- H 4.02675700 -3.01492100 0.66147800
- H 2.45161100 -3.72869900 1.09351000
- H 3.02834200 -3.82744700 -0.57116000
- Si -1.30245700 0.36663300 1.53513200
- C -2.91572000 -0.47381000 1.94432200
- H -3.78617800 0.07477000 1.57727800
- H -2.95372500 -1.49850400 1.56639400
- H -2.97960600 -0.52240300 3.03758000
- C 0.07605300 -0.46538300 2.50808700
- H -0.16219200 -0.30991000 3.56947400
- H 0.12419200 -1.54188000 2.32694700
- H 1.05031300 -0.01582300 2.30741200
- C -1.26154700 2.20725000 1.78750500
- H -0.28001300 2.62615300 1.55767000
- H -2.01991400 2.71912800 1.19303600
- H -1.46654200 2.38675600 2.85017900
- C -2.78711100 -0.19767700 -1.04428800
- C -4.09836600 0.37176300 -1.45512100
- H -4.83105400 -0.42343800 -1.58748800
- H -4.44172700 1.10082000 -0.71839600
- H -3.96528900 0.90127800 -2.40444900
-

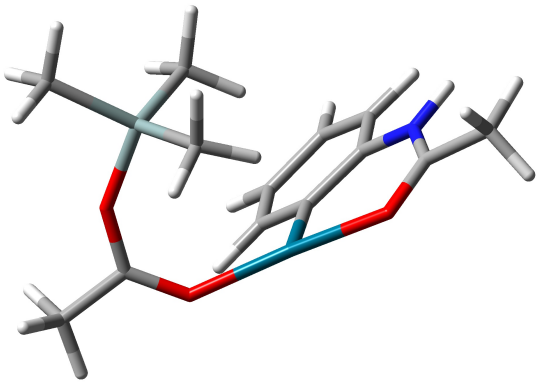


F1 MePdP50

- Zero-point correction= 0.312765 (Hartree/Particle)
- Thermal correction to Energy= 0.336283
- Thermal correction to Enthalpy= 0.337227
- Thermal correction to Gibbs Free Energy= 0.257619
- Sum of electronic and zero-point Energies= -1204.747350
- Sum of electronic and thermal Energies= -1204.723832
- Sum of electronic and thermal Enthalpies= -1204.722888
- Sum of electronic and thermal Free Energies= -1204.802496

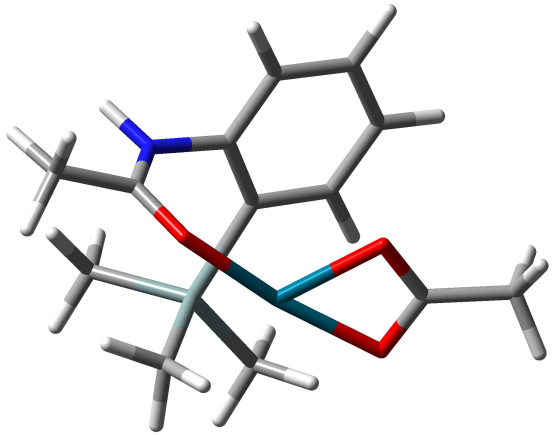
- MePdP50
-

- 1 1
- H 3.71914800 1.43028100 2.11298900
- C 2.87172400 1.68549200 1.48194600
- C 2.30295700 0.69920600 0.66375300
- C 2.36927000 2.97792500 1.48055300
- C 1.29997400 3.30244800 0.64772500
- H 2.82001800 3.72965000 2.11978500
- N 2.90158700 -0.57595900 0.72196000
- H 3.63927400 -0.67800600 1.40607300
- C 2.69242200 -1.62551300 -0.07148600
- O 1.81503500 -1.64379200 -0.97497100
- Pd 0.31624200 -0.34723600 -1.21406600
- H 0.90845000 4.31453500 0.62318400
- C 1.20264800 1.01151600 -0.14685300
- O -2.79643200 0.29209000 0.02516200
- C 0.72506500 2.32450600 -0.16066500
- H -0.10318900 2.58704000 -0.80673700
- O -1.32941000 0.80875100 -1.62093700
- C 3.54584000 -2.83878600 0.10975400
- H 4.24959400 -2.73993400 0.93661500
- H 2.90048000 -3.70356800 0.28143800
- H 4.10069000 -3.01683200 -0.81528700
- Si -2.33885000 -0.86495600 1.25381700
- C -3.95975400 -1.05484100 2.15248700
- H -4.29891800 -0.09798200 2.56029800
- H -4.73746400 -1.44120600 1.48686200
- H -3.84670200 -1.75757900 2.98473900
- C -1.82710500 -2.46927800 0.44720100
- H -1.94515800 -3.27580900 1.17982700
- H -2.46590000 -2.70471900 -0.40954200
- H -0.78351600 -2.46795600 0.12026900
- C -1.03250700 -0.08789100 2.32890000
- H -0.06341200 -0.04002900 1.82958700
- H -1.31949000 0.92692500 2.61984500
- H -0.92561100 -0.68363700 3.24235600
- C -2.43424000 0.90791600 -1.05030900
- C -3.46844900 1.82393200 -1.62195600
- H -4.38199900 1.25727800 -1.82022100
- H -3.71481400 2.58660100 -0.87768500
- H -3.10644100 2.29272100 -2.53485800
-



C2 MePdP45a

- Zero-point correction= 0.314556 (Hartree/Particle)
- Thermal correction to Energy= 0.337106
- Thermal correction to Enthalpy= 0.338050
- Thermal correction to Gibbs Free Energy= 0.262816
- Sum of electronic and zero-point Energies= -1204.634846
- Sum of electronic and thermal Energies= -1204.612297
- Sum of electronic and thermal Enthalpies= -1204.611352
- Sum of electronic and thermal Free Energies= -1204.686587
- MePdP45
-
- 1 1
- H 0.46602500 -0.55250400 3.35369300
- C 0.29759500 0.27219300 2.66917400
- C -0.67500500 0.15043800 1.67504300
- C 1.04713000 1.44258000 2.76284200
- C 0.81457100 2.48236600 1.86211800
- H 1.80439300 1.53868800 3.53356200
- N -1.41889200 -1.08635200 1.65362800
- H -2.06021300 -1.24138100 2.42198400
- C -1.26831800 -2.09845300 0.80339300
- O -0.49174500 -2.09140500 -0.19864900
- Pd 0.77910300 -0.64987700 -0.85983900
- H 1.38970400 3.40018600 1.92849200
- C -0.94460200 1.17989900 0.75248800
- O 2.54418900 -0.98564700 0.16860700
- C -0.16483600 2.34690000 0.87901500
- H -0.32640400 3.17108700 0.19190400
- O 2.35975700 0.52040200 -1.38149200
- C -2.07633500 -3.34369900 1.02428200
- H -2.73593200 -3.26554400 1.88883800
- H -2.66917600 -3.54680600 0.12919900
- H -1.38871200 -4.18170700 1.16463900
- Si -2.14544100 1.08673700 -0.71646100
- C 3.10370100 -0.03694400 -0.49069400
- C 4.49229500 0.41035000 -0.21968000
- H 5.12357800 -0.45059900 0.00920300
- H 4.88380000 0.96146700 -1.07573500
- H 4.48077800 1.07007000 0.65458000
- C -1.07503000 0.56602400 -2.20307500
- H -0.60800100 -0.46314600 -2.15205500
- H -1.69384800 0.40132800 -3.09434500
- H -0.32169500 1.31334400 -2.46149900
- C -2.82156400 2.80213300 -1.06947800
- H -3.51096800 2.75683300 -1.91901200
- H -3.37505300 3.18784700 -0.20752200
- H -2.03533000 3.52013600 -1.31825200
- C -3.56049800 -0.13274900 -0.50055300
- H -3.26417100 -1.16494100 -0.70294000
- H -3.99304400 -0.08573800 0.50280100
- H -4.34830300 0.12286500 -1.21683900
-

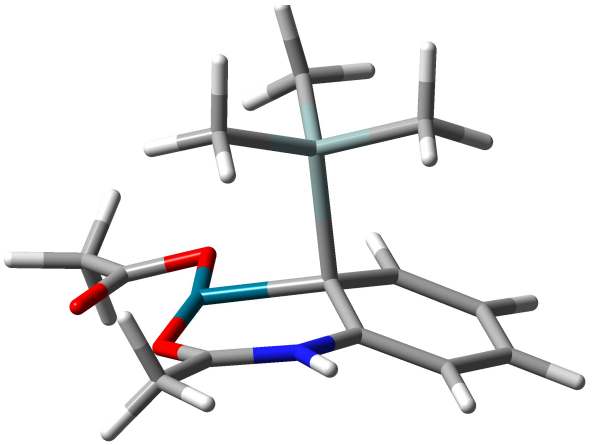


D2 MePdP47

- Zero-point correction= 0.315012 (Hartree/Particle)
- Thermal correction to Energy= 0.337904
- Thermal correction to Enthalpy= 0.338848
- Thermal correction to Gibbs Free Energy= 0.263069
- Sum of electronic and zero-point Energies= -1204.659167
- Sum of electronic and thermal Energies= -1204.636275
- Sum of electronic and thermal Enthalpies= -1204.635331
- Sum of electronic and thermal Free Energies= -1204.711109

- MePdP47
-

- 1 1
- H -3.73188300 0.09316000 -2.01186500
- C -2.85254100 -0.45982400 -1.69851500
- C -1.88867800 0.14939000 -0.89860700
- C -2.66407700 -1.76615300 -2.12938300
- C -1.51236400 -2.48263200 -1.78745900
- H -3.41700300 -2.22418100 -2.76172800
- N -2.12526600 1.48103900 -0.52717900
- H -3.08127200 1.79978800 -0.61687200
- C -1.21877900 2.42850000 -0.20542100
- O 0.00943800 2.22247100 -0.16176800
- Pd 1.01598900 0.45978000 -0.23917700
- H -1.36070600 -3.48810600 -2.16098000
- C -0.74577700 -0.57290900 -0.43359000
- O 3.09968800 1.00330700 -0.19377400
- C -0.57427300 -1.88800400 -0.97051900
- H 0.32055900 -2.43554100 -0.69148400
- O 2.37884500 -1.04836500 -0.31969400
- C -1.73159000 3.79511500 0.12297200
- H -2.77716900 3.93365200 -0.15100000
- H -1.61954300 3.95223400 1.19948200
- H -1.11237700 4.53251400 -0.38911200
- Si -0.98563800 -0.92885500 1.57321000
- C -0.93616800 0.65167500 2.57476100
- H 0.03152200 1.15792900 2.55455700
- H -1.71813900 1.35549200 2.27773900
- H -1.14693300 0.36407600 3.61165600
- C -2.70340600 -1.66575700 1.68966300
- H -2.84617900 -2.05394400 2.70411500
- H -3.47981100 -0.91733900 1.50650500
- H -2.84577600 -2.49468700 0.99064700
- C 0.31570300 -2.15882700 2.10493500
- H 0.09555900 -3.16036500 1.72509000
- H 1.32208200 -1.87837200 1.78595800
- H 0.30207000 -2.20610500 3.19933200
- C 3.37137600 -0.22849600 -0.27599000
- C 4.76913800 -0.74211200 -0.35079100
- H 5.46765500 0.01360400 0.00741800
- H 4.86211300 -1.66005700 0.23161000
- H 5.00040200 -0.97603900 -1.39407000
-

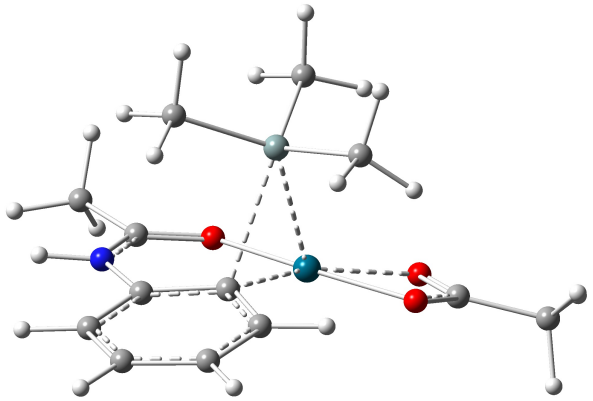


DE2 MePd41T ν = -77.1 cm^{-1}

- Zero-point correction= 0.315374 (Hartree/Particle)
- Thermal correction to Energy= 0.337326
- Thermal correction to Enthalpy= 0.338270
- Thermal correction to Gibbs Free Energy= 0.265412
- Sum of electronic and zero-point Energies= -1204.651645
- Sum of electronic and thermal Energies= -1204.629693
- Sum of electronic and thermal Enthalpies= -1204.628749
- Sum of electronic and thermal Free Energies= -1204.701607

- MePdP41T
-

- 1 1
- H -4.13575000 -0.62166100 -1.33286600
- C -3.15049100 -1.03956000 -1.15083400
- C -2.10454700 -0.20526800 -0.75618000
- C -2.93158800 -2.39937600 -1.32002100
- C -1.66277000 -2.93903900 -1.11696300
- H -3.75446500 -3.03602400 -1.62526900
- N -2.42289000 1.15874000 -0.58461600
- H -3.40950400 1.37960800 -0.61270900
- C -1.59929400 2.19960900 -0.43002600
- O -0.34861500 2.09961300 -0.40651000
- Pd 0.78971500 0.43475000 -0.41591300
- H -1.48423600 -3.99714100 -1.26981100
- C -0.82540300 -0.73630000 -0.49914500
- O 2.86469300 1.12280800 -0.62193200
- C -0.62182300 -2.10918600 -0.72763200
- H 0.37068900 -2.52188300 -0.58200600
- O 2.24943300 -0.96620400 -0.51216700
- C -2.19833700 3.55841100 -0.24925900
- H -3.26358300 3.58520300 -0.47827300
- H -2.04460900 3.86373300 0.78933200
- H -1.66573100 4.26345100 -0.88875000
- Si -0.20267900 -0.47488900 1.81404900
- C 0.55204100 1.03545200 2.62901000
- H 1.61820500 1.15101800 2.42023200
- H 0.03668300 1.95942900 2.35559100
- H 0.42803600 0.88602300 3.70947500
- C -1.99705900 -0.59621300 2.31400800
- H -2.01327400 -0.71541200 3.40408600
- H -2.55986300 0.30954000 2.07365700
- H -2.49342000 -1.45831800 1.86261200
- C 0.75530300 -2.03391500 2.15150000
- H 0.17577100 -2.92712700 1.90871700
- H 1.70386700 -2.06149800 1.61127200
- H 0.97071900 -2.04265100 3.22644900
- C 3.19391400 -0.09285900 -0.64127800
- C 4.59840400 -0.55664100 -0.82867600
- H 5.29329200 0.26137500 -0.64185200
- H 4.80526200 -1.39760000 -0.16474600
- H 4.71858200 -0.90173000 -1.85967500
-

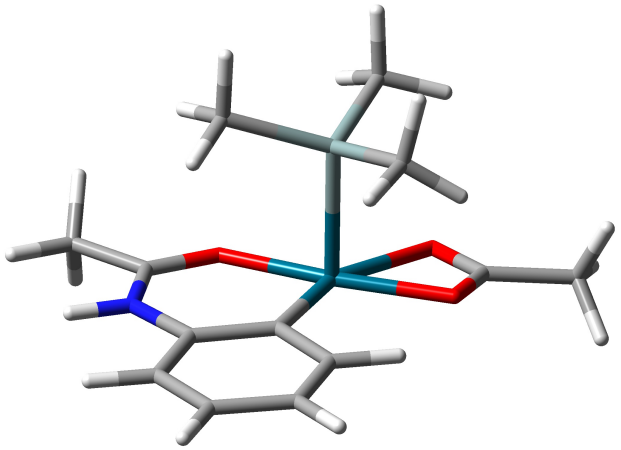


E2 MePdP49

- Zero-point correction= 0.314878 (Hartree/Particle)
- Thermal correction to Energy= 0.338010
- Thermal correction to Enthalpy= 0.338955
- Thermal correction to Gibbs Free Energy= 0.262045
- Sum of electronic and zero-point Energies= -1204.657754
- Sum of electronic and thermal Energies= -1204.634622
- Sum of electronic and thermal Enthalpies= -1204.633678
- Sum of electronic and thermal Free Energies= -1204.710588

- MePdP49
-

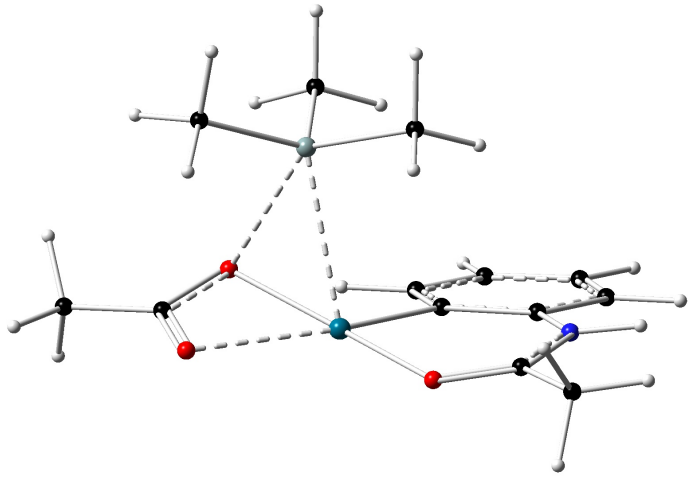
- 1 1
- H 4.43500000 0.94075400 -0.25118500
- C 3.41749100 1.31995600 -0.26910500
- C 2.34555700 0.42619800 -0.37079300
- C 3.18488100 2.68429900 -0.19696900
- C 1.88053600 3.17271100 -0.23058100
- H 4.02472200 3.36545100 -0.11840200
- N 2.67782800 -0.94674400 -0.44671400
- H 3.66548400 -1.15712500 -0.39128500
- C 1.87178600 -1.99079000 -0.61038600
- O 0.61866200 -1.89821300 -0.70354600
- Pd -0.53674500 -0.25858700 -0.61725500
- H 1.69146200 4.23936500 -0.18193300
- C 1.03369500 0.90873800 -0.38486500
- O -2.65585100 -0.87793000 -1.07509000
- C 0.81397700 2.28647400 -0.32377900
- H -0.20285900 2.66416500 -0.34105500
- O -1.98713200 1.15657600 -0.64681000
- C 2.47282000 -3.35854100 -0.68951700
- H 3.55304600 -3.35441700 -0.54665000
- H 2.00558600 -3.98893500 0.06964700
- H 2.23715600 -3.78398000 -1.66758500
- Si -0.63552200 -0.22797900 1.84634000
- C -2.07945100 -1.38865400 2.04870400
- H -3.01445900 -0.95806600 1.68594400
- H -1.91251700 -2.34265000 1.54330200
- H -2.18172700 -1.58291800 3.12393400
- C 0.95038700 -0.93988800 2.51319800
- H 0.83505300 -0.97825200 3.60380900
- H 1.12596600 -1.96069000 2.16673500
- H 1.81814500 -0.31629100 2.28981200
- C -0.97040000 1.51716200 2.38851600
- H -0.06851200 2.13151600 2.35489000
- H -1.74590400 1.98257000 1.77683900
- H -1.32669600 1.47357000 3.42487500
- C -2.93908600 0.33917400 -0.97691000
- C -4.30995900 0.88876500 -1.19234800
- H -4.96029100 0.12517900 -1.61667500
- H -4.71231200 1.21875900 -0.23035900
- H -4.26240400 1.75879400 -1.85010200
-



EF2 MePdP43bT ν= -161.1 cm^{-1}

- Zero-point correction= 0.314066 (Hartree/Particle)
- Thermal correction to Energy= 0.336660
- Thermal correction to Enthalpy= 0.337604
- Thermal correction to Gibbs Free Energy= 0.261887
- Sum of electronic and zero-point Energies= -1204.648958
- Sum of electronic and thermal Energies= -1204.626363
- Sum of electronic and thermal Enthalpies= -1204.625419
- Sum of electronic and thermal Free Energies= -1204.701136

- MePdP43X
- 1 1
- H 4.43755900 1.21413500 0.23966800
- C 3.42492600 1.46577700 -0.06169900
- C 2.44865700 0.46459200 -0.10789700
- C 3.10710100 2.76843800 -0.41342100
- C 1.81365100 3.08365700 -0.82343200
- H 3.87350300 3.53439700 -0.37614600
- N 2.86546200 -0.84333300 0.23440700
- H 3.80325500 -0.92162300 0.60394900
- C 2.21867300 -1.98684100 0.01893100
- O 1.05303400 -2.04381600 -0.44921500
- Pd -0.29018800 -0.55083500 -0.61291300
- H 1.56003500 4.09798500 -1.11122200
- C 1.14168100 0.78091600 -0.48515300
- O -2.39263800 -1.37946500 -1.11970400
- C 0.83913300 2.09188300 -0.85861800
- H -0.17288300 2.34202600 -1.16030200
- O -1.92338400 0.70811500 -0.61566100
- C 2.90632500 -3.27429100 0.34905800
- H 3.92367600 -3.12983500 0.71153700
- H 2.31937600 -3.79723500 1.10739900
- H 2.92409500 -3.89716500 -0.54764600
- Si -1.32304800 0.42606700 1.58310500
- C -2.95675400 -0.38365200 1.95079300
- H -3.80563800 0.19372600 1.57787000
- H -3.01231800 -1.40200800 1.55865300
- H -3.03817700 -0.44562000 3.04220800
- C 0.03934300 -0.41186900 2.56000600
- H -0.20005100 -0.24841900 3.61935000
- H 0.07698800 -1.49012500 2.38668200
- H 1.01937900 0.02660400 2.36070900
- C -1.25932300 2.27132000 1.75839100
- H -0.26263300 2.66512200 1.55045100
- H -1.98696200 2.77086800 1.11742000
- H -1.50052400 2.49585300 2.80486500
- C -2.76614400 -0.20002000 -1.08505200
- C -4.09260400 0.28588600 -1.56028300
- H -4.77608100 -0.55190900 -1.68896300
- H -4.50035200 1.01590200 -0.85902900
- H -3.95322200 0.79065600 -2.52089100
-

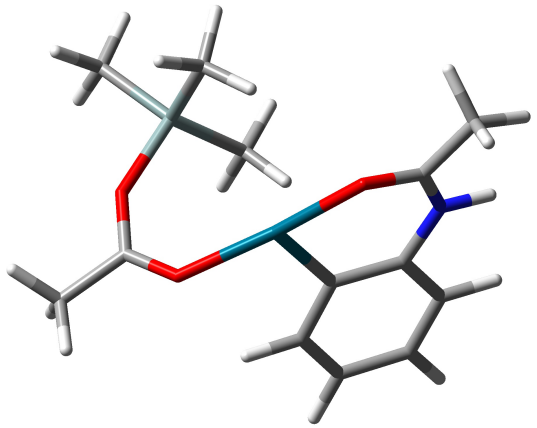


F2 MePdP51

- Zero-point correction= 0.315207 (Hartree/Particle)
- Thermal correction to Energy= 0.338452
- Thermal correction to Enthalpy= 0.339396
- Thermal correction to Gibbs Free Energy= 0.261018
- Sum of electronic and zero-point Energies= -1204.694459
- Sum of electronic and thermal Energies= -1204.671214
- Sum of electronic and thermal Enthalpies= -1204.670270
- Sum of electronic and thermal Free Energies= -1204.748648

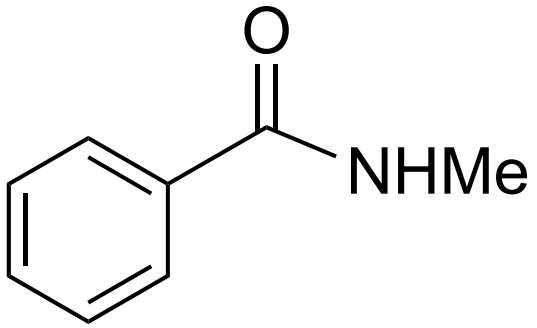
- MePdP51
-

- 1 1
- H 3.83558900 1.35870200 2.10945500
- C 2.98837500 1.62841100 1.48515800
- C 2.38526600 0.65299800 0.68177000
- C 2.52107200 2.93255400 1.47884100
- C 1.45188400 3.27887200 0.65700200
- H 2.99873800 3.67656300 2.10641700
- N 2.95853600 -0.64051400 0.73920600
- H 3.69483200 -0.75980500 1.42123300
- C 2.72910600 -1.67688600 -0.06533900
- O 1.85093600 -1.66870500 -0.96271100
- Pd 0.34756500 -0.35077900 -1.18148400
- H 1.08687600 4.30002400 0.63084300
- C 1.28730100 0.98615200 -0.11908700
- O -2.92941700 0.23479400 -0.10472800
- C 0.84350800 2.31144400 -0.13520400
- H 0.01025800 2.58962300 -0.76848700
- O -1.30248500 0.85970900 -1.54235100
- C 3.56230500 -2.91041900 0.09921400
- H 4.28004000 -2.83183600 0.91563300
- H 2.90015500 -3.76041900 0.27604800
- H 4.09826200 -3.09202200 -0.83508100
- Si -2.50025400 -0.81682400 1.22345700
- C -4.15500800 -1.04505800 2.04453700
- H -4.57026400 -0.08706800 2.36994000
- H -4.87063600 -1.51888400 1.36633200
- H -4.04994700 -1.68616800 2.92595100
- C -1.85832900 -2.43464500 0.54819300
- H -1.92530600 -3.19128900 1.33795700
- H -2.46919200 -2.77980500 -0.29145900
- H -0.81401000 -2.38625700 0.22551200
- C -1.29342600 0.09890900 2.30646600
- H -0.32399900 0.23830000 1.82204600
- H -1.68653600 1.08199000 2.58221300
- H -1.13858700 -0.47102200 3.22917800
- C -2.45865700 0.92301300 -1.09203600
- C -3.44054100 1.86832300 -1.71420500
- H -4.32688100 1.31188500 -2.02725700
- H -3.75841600 2.59337500 -0.96058600
- H -2.99457700 2.38068500 -2.56400900
-



Scheme 4

N-methylbenzamide series

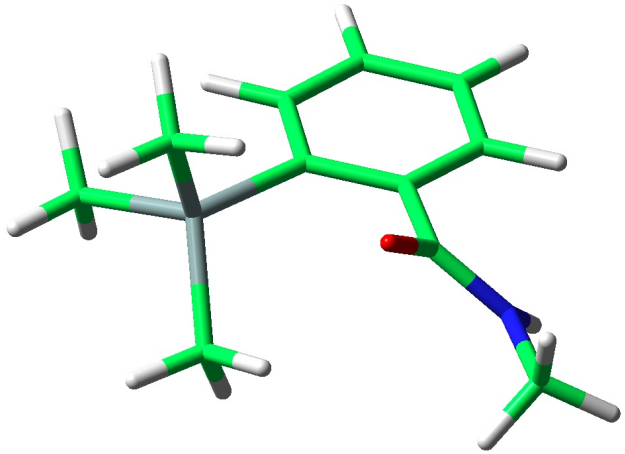


A1 MBZB silyl-Mebenzamide

- Zero-point correction= 0.257742 (Hartree/Particle)
- Thermal correction to Energy= 0.274786
- Thermal correction to Enthalpy= 0.275731
- Thermal correction to Gibbs Free Energy= 0.213237
- Sum of electronic and zero-point Energies= -848.775253
- Sum of electronic and thermal Energies= -848.758210
- Sum of electronic and thermal Enthalpies= -848.757265
- Sum of electronic and thermal Free Energies= -848.819759

- MBZB

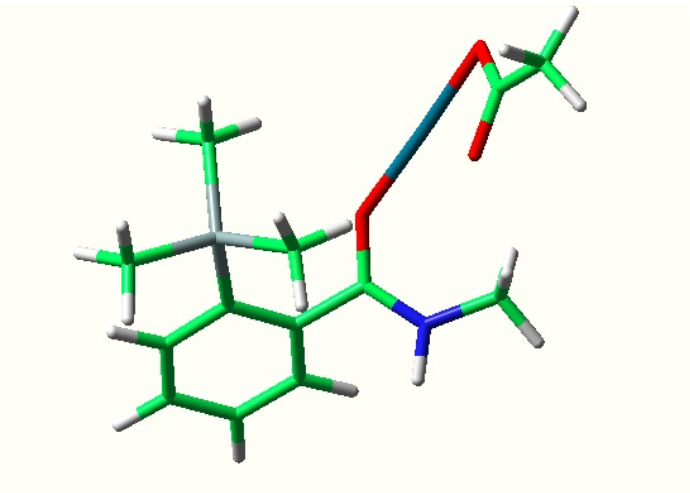
- 0 1
- C 0.74955600 3.22325600 0.06127800
- C 1.46341100 2.02990500 0.15258600
- C 0.80028800 0.79532500 0.13534000
- C -1.29454400 1.94889700 -0.08600000
- C -0.63707300 3.18066800 -0.06068000
- H 1.27296900 4.17372400 0.09034000
- H 2.54235500 2.05743200 0.26966200
- H -2.37392900 1.94555700 -0.19429900
- H -1.20828800 4.10105100 -0.13640100
- C 3.65491800 -1.65127400 -0.34744900
- H 3.24761800 -2.47012200 -0.95227400
- H 4.63911500 -1.38041400 -0.73169300
- H 3.75279500 -2.00574300 0.68013100
- C 1.60854300 -0.46011600 0.28118500
- O 1.22985600 -1.41642700 0.96592800
- N 2.79652700 -0.47957500 -0.37708800
- H 2.98285000 0.24042600 -1.05817100
- Si -1.63159200 -0.88160900 -0.05479500
- C -0.60830100 0.72701600 0.02054800
- C -1.91033800 -1.60327100 1.66458100
- C -3.32922500 -0.42045800 -0.75970400
- C -0.87291400 -2.13389300 -1.24720200
- H -0.65415000 -1.66726800 -2.21395100
- H 0.04936500 -2.56070400 -0.85053800
- H -1.58319900 -2.94867800 -1.42741400
- H -3.92291800 -1.33268300 -0.88734700
- H -3.89438100 0.24356800 -0.09749000
- H -3.25193800 0.06408400 -1.73872800
- H -0.95638500 -1.86169300 2.12687400
- H -2.42651500 -0.88097000 2.30649700
- H -2.53354200 -2.50294000 1.60722200



B1 MePdOAcL1

- Zero-point correction= 0.312423 (Hartree/Particle)
- Thermal correction to Energy= 0.335814
- Thermal correction to Enthalpy= 0.336758
- Thermal correction to Gibbs Free Energy= 0.257748
- Sum of electronic and zero-point Energies= -1204.983708
- Sum of electronic and thermal Energies= -1204.960317
- Sum of electronic and thermal Enthalpies= -1204.959373
- Sum of electronic and thermal Free Energies= -1205.038384
- MePdOAcL1

- 1 1
- C -4.99386800 -0.72419400 -0.31243300
- C -4.15451200 0.38477100 -0.17737300
- C -2.76637200 0.26131300 -0.00675600
- C -2.25868100 -1.05991900 0.04355300
- C -3.09551500 -2.17967100 -0.07417000
- C -4.46580700 -2.01241800 -0.25806700
- H -6.05975200 -0.57839400 -0.45705700
- H -4.60128300 1.37269400 -0.20262000
- H -2.67070200 -3.17865000 -0.05844700
- H -5.10891400 -2.87941800 -0.36491100
- Si -1.75344800 1.86151800 0.25223300
- C -2.96060400 3.20596400 0.79781500
- H -2.39880000 4.11568700 1.03702400
- H -3.68052600 3.46608400 0.01542300
- H -3.52013600 2.91550400 1.69275200
- C -0.93452800 2.42719100 -1.34944200
- H -0.32288000 3.31705900 -1.16225500
- H -0.29791000 1.65270800 -1.78235700
- H -1.69260900 2.69501700 -2.09301500
- O -0.04211400 -0.65541200 -0.62122700
- C -0.80097600 -1.31086700 0.16373100
- N -0.38291900 -2.21960500 1.03274800
- H -1.09175600 -2.59585300 1.64830700
- C 0.98049100 -2.72470200 1.18794000
- H 0.92830400 -3.64908300 1.76154900
- H 1.41504200 -2.94292800 0.20946200
- H 1.61129300 -2.00779900 1.71612000
- C -0.50159900 1.62842400 1.64671300
- H -0.98097500 1.19513900 2.53099500
- H 0.34885700 1.00034000 1.37595100
- H -0.10705400 2.60912000 1.93515500
- Pd 1.91252200 -0.25629500 -0.83596800
- O 3.86268900 0.35094800 -0.86214900
- C 3.90369000 0.37060500 0.42013000
- C 5.09830600 0.79255900 1.19040700
- H 5.98970800 0.72620300 0.56536100
- H 4.96112600 1.83116600 1.51014200
- H 5.20275100 0.17194000 2.08281400
- O 2.80801800 0.01379800 0.99604600

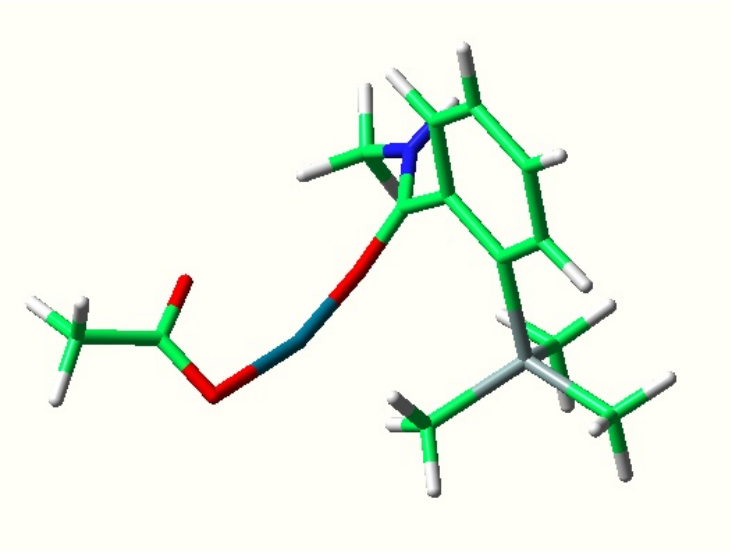


C1 MePdN10

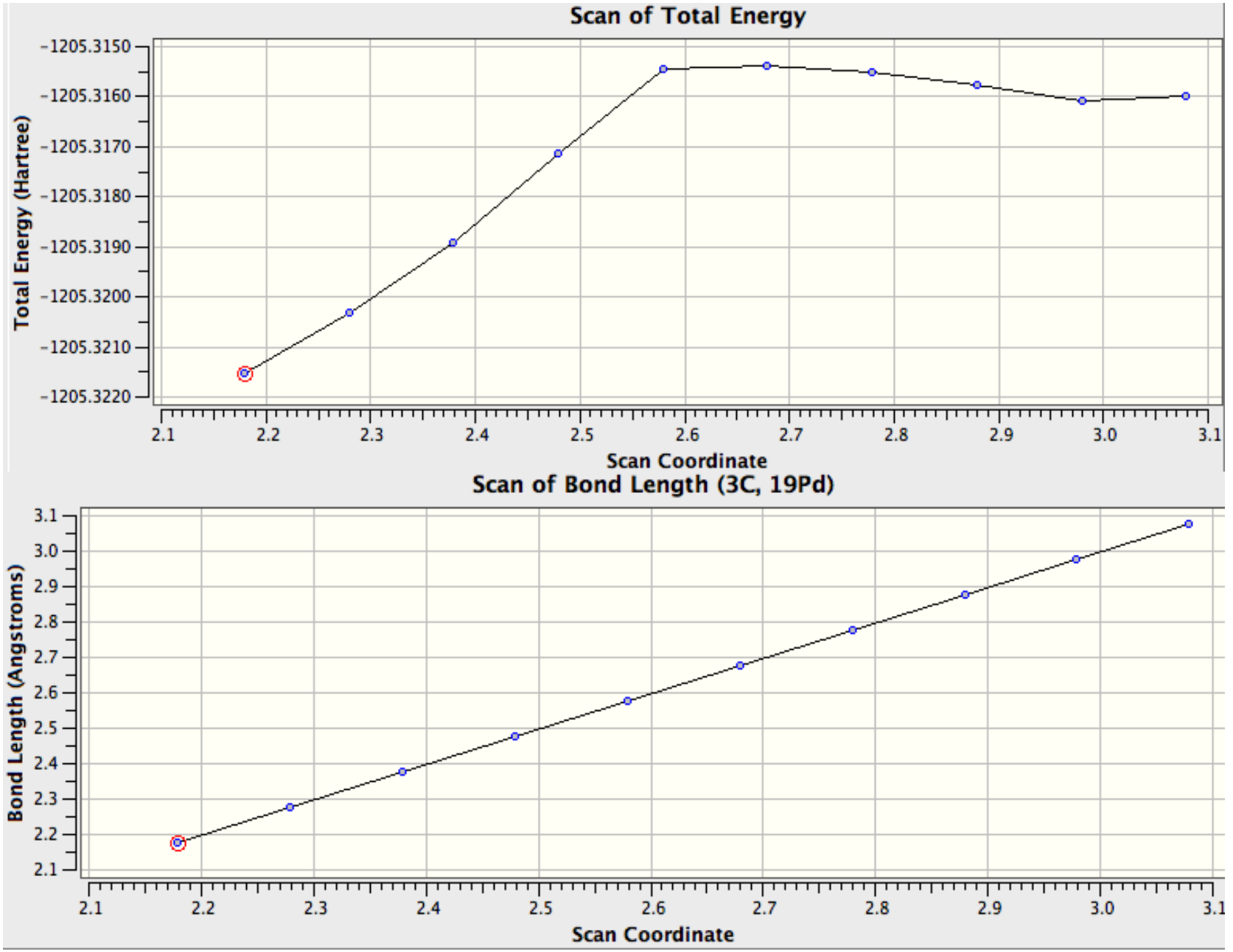
- Zero-point correction= 0.311285 (Hartree/Particle)
- Thermal correction to Energy= 0.334853
- Thermal correction to Enthalpy= 0.335797
- Thermal correction to Gibbs Free Energy= 0.255506
- Sum of electronic and zero-point Energies= -1204.994946
- Sum of electronic and thermal Energies= -1204.971378
- Sum of electronic and thermal Enthalpies= -1204.970434
- Sum of electronic and thermal Free Energies= -1205.050725

- MePdN10

- 1 1
- C 2.54491300 0.47850900 3.06975800
- C 2.57763000 -0.42936500 2.00780900
- C 1.99615800 -0.14234500 0.76280300
- C 1.38743400 1.12919800 0.62695900
- C 1.36756600 2.05244500 1.68090500
- C 1.93736500 1.72201300 2.90916700
- H 2.99852100 0.21271400 4.01923800
- H 3.07267500 -1.38255600 2.15935400
- H 0.88551400 3.01543800 1.54523200
- H 1.90712300 2.43166400 3.72897600
- O -0.14251900 0.83532200 -1.24491000
- C 0.74488600 1.53497100 -0.64920400
- N 1.12050400 2.67698300 -1.20521900
- H 1.91227600 3.15578500 -0.79650400
- C 0.52614200 3.21488400 -2.42684400
- H 0.94306900 2.72193600 -3.30958900
- H -0.55173600 3.05285300 -2.40542200
- H 0.73979600 4.28165900 -2.47239100
- Pd -1.43072700 -0.44878300 -0.32750400
- O -3.02612200 0.78174700 0.15224400
- C -3.66777800 -0.23510700 0.60066000
- C -5.01888400 -0.12653600 1.20568800
- H -5.55219100 0.72541400 0.78117600
- H -5.57492800 -1.05191300 1.04587100
- H -4.90828500 0.03151500 2.28398100
- O -3.04443900 -1.35831900 0.51069900
- Si 2.09652800 -1.45352100 -0.61029900
- C 3.19116000 -2.86912000 -0.04661900
- H 3.25075400 -3.61927800 -0.84204400
- H 4.20882500 -2.52819400 0.16775200
- H 2.79877000 -3.36391100 0.84704500
- C 0.31500300 -2.10813500 -0.82796500
- H -0.18986000 -1.88709300 0.14870400
- H -0.14025800 -1.67167400 -1.72813000
- H 0.19170100 -3.19033700 -0.92178000
- C 2.72352900 -0.72189100 -2.22356400
- H 3.72928100 -0.30976600 -2.09415700
- H 2.77883400 -1.50545000 -2.98692600
- H 2.07255000 0.06849800 -2.60606400



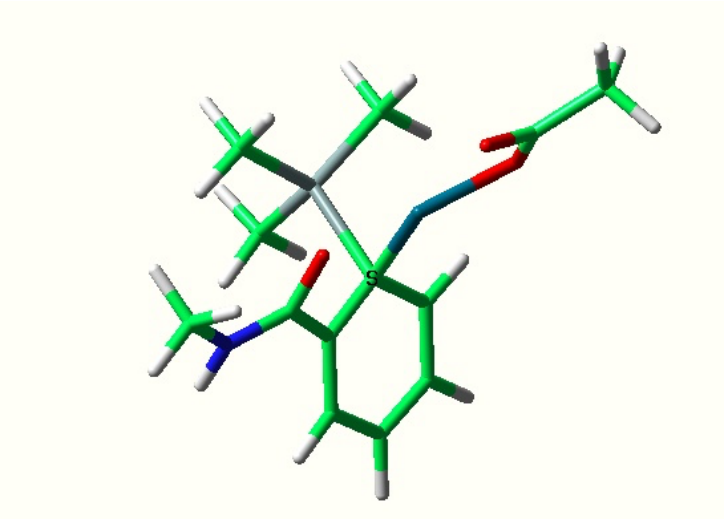
MePdN10aS scanning from **C1** to **D1**



D1 MePdOAcL2 (Si Wheland)

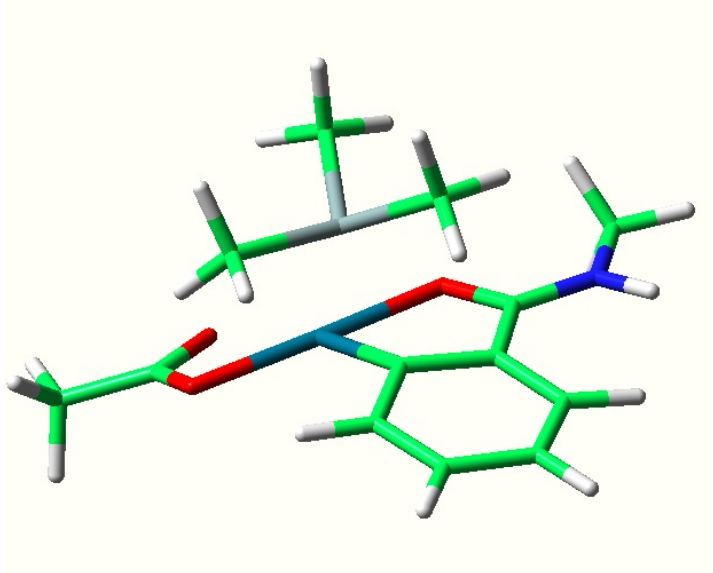
- Zero-point correction= 0.312050 (Hartree/Particle)
- Thermal correction to Energy= 0.335608
- Thermal correction to Enthalpy= 0.336553
- Thermal correction to Gibbs Free Energy= 0.257734
- Sum of electronic and zero-point Energies= -1205.009815
- Sum of electronic and thermal Energies= -1204.986257
- Sum of electronic and thermal Enthalpies= -1204.985313
- Sum of electronic and thermal Free Energies= -1205.064132
- MePdOAcL2

- 1 1
- C -1.37533400 -2.26300000 2.25572800
- C -0.49047900 -1.94265900 1.22960100
- C -0.67700400 -0.78911500 0.42640600
- C -1.74854000 0.09487200 0.79912000
- C -2.62385800 -0.21786100 1.82889300
- C -2.45022200 -1.41644900 2.53586800
- H -1.22696000 -3.16316800 2.84174700
- H 0.34074900 -2.60549100 1.01278200
- H -3.40209100 0.47471900 2.13193500
- H -3.13893100 -1.66537500 3.33608700
- Si -0.64097500 -1.35867700 -1.52189000
- C -2.14462400 -2.48578400 -1.58918200
- H -2.29708300 -2.83207800 -2.61728900
- H -2.01787200 -3.36244600 -0.94761700
- H -3.04992100 -1.95816800 -1.27322400
- C 0.93553800 -2.30604700 -1.87350900
- H 0.83560400 -2.76521900 -2.86378700
- H 1.81176800 -1.65450600 -1.88171600
- H 1.11283000 -3.11058400 -1.15478100
- O -0.54512200 1.86536100 -0.17436200
- C -1.69540100 1.43244200 0.16282000
- N -2.78011500 2.16667400 -0.02026200
- H -3.67836500 1.75449300 0.19288000
- C -2.74384500 3.51399400 -0.58840800
- H -3.65823100 4.03169300 -0.30333100
- H -1.87909600 4.04838800 -0.19514000
- H -2.67202600 3.46997600 -1.67861500
- C -0.88714100 0.07425400 -2.70607900
- H -1.80241700 0.63678100 -2.50324500
- H -0.04494400 0.76906400 -2.71310300
- H -0.98616600 -0.35740800 -3.70935600
- Pd 0.96491000 0.51040300 0.17556500
- O 2.86661400 1.51731900 0.12887700
- C 3.41745800 0.39534900 0.36958900
- C 4.88978200 0.24038400 0.54590700
- H 5.41558300 1.05913400 0.05309900
- H 5.12111100 0.26654000 1.61619400
- H 5.21697300 -0.72274000 0.14954000
- O 2.62977300 -0.62264100 0.48282300



DE1 MePdL6b; TS v = -92 cm^{-1}; Si-C = 2.269 Å, Si-Pd = 2.721 Å, C-Pd = 2.018Å.

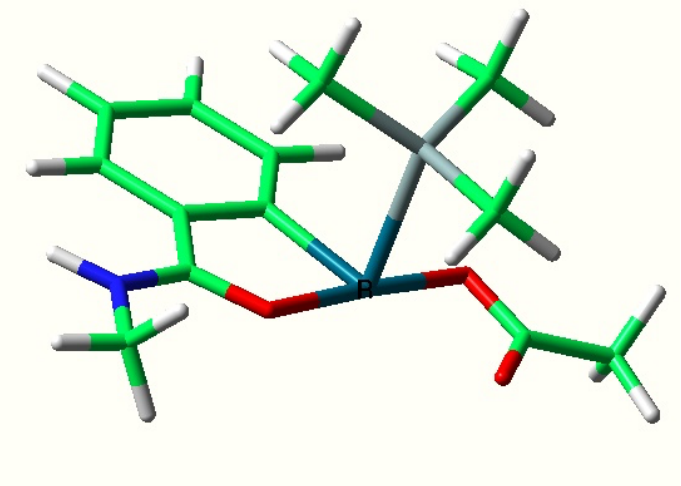
- Zero-point correction= 0.311199 (Hartree/Particle)
- Thermal correction to Energy= 0.334330
- Thermal correction to Enthalpy= 0.335274
- Thermal correction to Gibbs Free Energy= 0.257907
- Sum of electronic and zero-point Energies= -1205.008782
- Sum of electronic and thermal Energies= -1204.985651
- Sum of electronic and thermal Enthalpies= -1204.984707
- Sum of electronic and thermal Free Energies= -1205.062073
- MePdL6b
- 1 1
- C 1.64860000 -2.63623500 -1.74230300
- C 0.54419000 -2.02798800 -1.14076900
- C 0.67023200 -0.75423500 -0.56587800
- C 1.90524000 -0.05461900 -0.70414000
- C 2.99699200 -0.66119500 -1.31624900
- C 2.86976100 -1.96309200 -1.81411700
- H 1.55292300 -3.63071700 -2.16451800
- H -0.40685700 -2.54635300 -1.09734600
- H 3.93960000 -0.13778400 -1.44147400
- H 3.72361200 -2.44040900 -2.28203200
- Si 0.16720000 -1.10878000 1.61828500
- C 1.89250400 -1.71243500 2.03590100
- H 1.84698700 -2.19099200 3.02161700
- H 2.26290500 -2.44428900 1.31455900
- H 2.60544900 -0.88575900 2.09770400
- C -1.10553900 -2.47525400 1.60476000
- H -1.36644600 -2.67851000 2.65028900
- H -2.01477800 -2.18401300 1.07491800
- H -0.71292500 -3.39606900 1.16740000
- O 0.70078200 1.82953700 0.04693700
- C 1.85115400 1.34058400 -0.22569000
- N 2.93247800 2.08725600 -0.07469500
- H 3.83549200 1.67927000 -0.26985100
- C 2.87109800 3.48190200 0.36170200
- H 3.88881400 3.85684900 0.45061400
- H 2.32064600 4.08232500 -0.36637000
- H 2.36764900 3.55018600 1.32844700
- C -0.27408600 0.30703200 2.76944400
- H 0.37788000 1.17159400 2.62619800
- H -1.31142000 0.62929200 2.65449800
- H -0.13372700 -0.06231500 3.79377400
- Pd -0.86293200 0.53006400 -0.29345000
- O -2.80465400 1.56159800 -0.34401100
- C -3.32674800 0.43320500 -0.58765600
- C -4.78744900 0.24535300 -0.82955800
- H -4.95781000 0.15464000 -1.90752300
- H -5.13147400 -0.67611600 -0.35516800
- H -5.34486700 1.10342000 -0.45293500
-



E1 MePdOAcL4

- Zero-point correction= 0.312033 (Hartree/Particle)
- Thermal correction to Energy= 0.335464
- Thermal correction to Enthalpy= 0.336408
- Thermal correction to Gibbs Free Energy= 0.259191
- Sum of electronic and zero-point Energies= -1205.020442
- Sum of electronic and thermal Energies= -1204.997011
- Sum of electronic and thermal Enthalpies= -1204.996067
- Sum of electronic and thermal Free Energies= -1205.073284
- MePdOAcL4

- 1 1
- C 1.78838600 -3.29663500 -0.02869600
- C 0.66029500 -2.47354400 -0.14468000
- C 0.85335000 -1.11162200 -0.31529500
- C 2.14529300 -0.55475400 -0.38107100
- C 3.26342200 -1.38861200 -0.27189800
- C 3.07750000 -2.75852900 -0.09213300
- H 1.65620800 -4.36493800 0.10972700
- H -0.34035800 -2.89011700 -0.10281700
- H 4.27138800 -0.98847800 -0.32423800
- H 3.93977000 -3.40963100 -0.00238600
- Si -0.72651500 0.39045200 1.81787600
- C 0.97791800 0.46563900 2.58135600
- H 0.83373800 0.68424200 3.64736400
- H 1.51389900 -0.48150700 2.49735700
- H 1.58622900 1.26783200 2.15828400
- C -1.71763700 -1.08066000 2.39423900
- H -1.86360000 -0.97908700 3.47700100
- H -2.69371600 -1.12981200 1.90957200
- H -1.18398900 -2.01562200 2.20846600
- O 1.00073200 1.49511300 -0.60907100
- C 2.14238500 0.90301900 -0.53966400
- N 3.24311300 1.63170800 -0.59566200
- H 4.13720200 1.16377400 -0.54365500
- C 3.22031500 3.08696700 -0.74022800
- H 4.24824600 3.44126600 -0.78341900
- H 2.69634500 3.36677000 -1.65661800
- H 2.71063300 3.54198400 0.11226700
- C -1.61807200 2.03333500 1.87179300
- H -1.01919900 2.82211300 1.40887900
- H -2.58791700 1.98866600 1.37334600
- H -1.77234200 2.29431300 2.92692700
- Pd -0.58543600 0.19862100 -0.61355900
- O -2.64638100 1.07492000 -1.14484900
- C -3.05897600 -0.10902900 -1.04340400
- C -4.47997700 -0.51441200 -1.27345500
- H -5.05923500 0.33253700 -1.64025600
- H -4.51965000 -1.33936200 -1.98938200
- H -4.90645400 -0.87322200 -0.33147500
- O -2.20096900 -1.02797700 -0.69770800

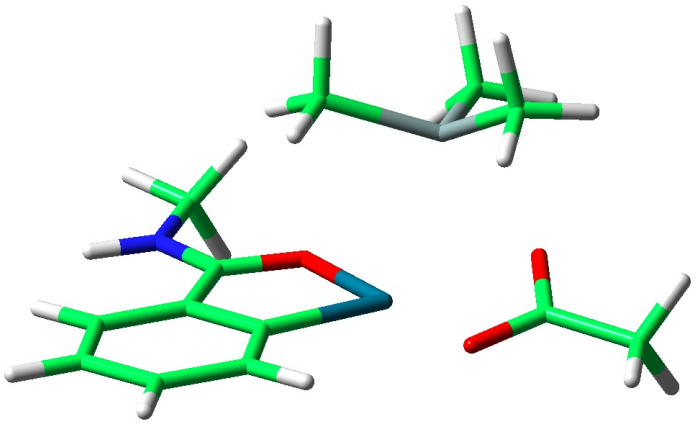


EF1 MePdN33 2nd silyl transfer TS; Si-Pd 2.60 Å, Si-O 2.29 Å, n = 145.4 cm^{-1}

- Zero-point correction= 0.311009 (Hartree/Particle)
- Thermal correction to Energy= 0.334070
- Thermal correction to Enthalpy= 0.335014
- Thermal correction to Gibbs Free Energy= 0.258190
- Sum of electronic and zero-point Energies= -1205.007229
- Sum of electronic and thermal Energies= -1204.984168
- Sum of electronic and thermal Enthalpies= -1204.983224
- Sum of electronic and thermal Free Energies= -1205.060047

- MePdN33

- 1 1
- H -4.54512200 -0.42155100 0.45828500
- C -3.62050000 -0.99029000 0.42365500
- C -2.42510700 -0.40386600 -0.00812800
- C -3.62220200 -2.32785400 0.81427400
- C -2.44219400 -3.07740200 0.77586300
- H -4.54463400 -2.78820800 1.15028800
- O -1.03729600 1.32177600 -0.80125100
- Pd 0.33331900 -0.19520400 -0.66494900
- H -2.45541200 -4.11863800 1.08224600
- C -1.24368000 -1.17185800 -0.03969700
- O 2.59225900 0.36675900 -0.77423200
- C -1.23747200 -2.50321700 0.34721600
- H -0.32297400 -3.08620100 0.32117700
- O 1.79264700 -1.67348800 -0.60895600
- Si 1.64919800 1.04476800 1.20655900
- C 1.83948600 2.79224600 0.59320000
- H 2.77087200 2.93082000 0.04234000
- H 0.99681700 3.06348200 -0.04909900
- H 1.82945700 3.46315100 1.46048700
- C 0.14876300 0.87282400 2.33416600
- H 0.42512200 1.36797300 3.27595000
- H -0.73464400 1.37006000 1.93172000
- H -0.09167500 -0.16919100 2.55453700
- C 3.09790500 0.20310800 2.03181000
- H 2.98050300 -0.88487200 2.01565400
- H 4.04903600 0.46629200 1.56598400
- H 3.11859300 0.51124200 3.08309900
- C 2.78006500 -0.90724100 -0.85302000
- C 4.11160100 -1.45738200 -1.24121500
- H 4.14775500 -2.53367800 -1.07616800
- H 4.28060300 -1.24683600 -2.30231100
- H 4.89712600 -0.95239400 -0.67491700
- C -2.22383300 0.97992100 -0.44499900
- N -3.18880800 1.88514900 -0.47617500
- H -4.12375800 1.60563500 -0.21581200
- C -2.96610100 3.26295400 -0.91113700
- H -2.77781700 3.30163500 -1.98743700
- H -3.85597600 3.84446800 -0.67634900
- H -2.10494100 3.68138100 -0.38699600

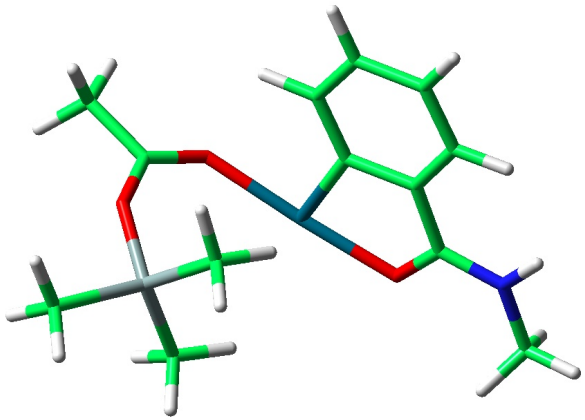


F1 MePdN31 – non-agostic post Si-O transfer

- Zero-point correction= 0.312029 (Hartree/Particle)
- Thermal correction to Energy= 0.335762
- Thermal correction to Enthalpy= 0.336706
- Thermal correction to Gibbs Free Energy= 0.257009
- Sum of electronic and zero-point Energies= -1205.050253
- Sum of electronic and thermal Energies= -1205.026521
- Sum of electronic and thermal Enthalpies= -1205.025576
- Sum of electronic and thermal Free Energies= -1205.105274

- MePdN31

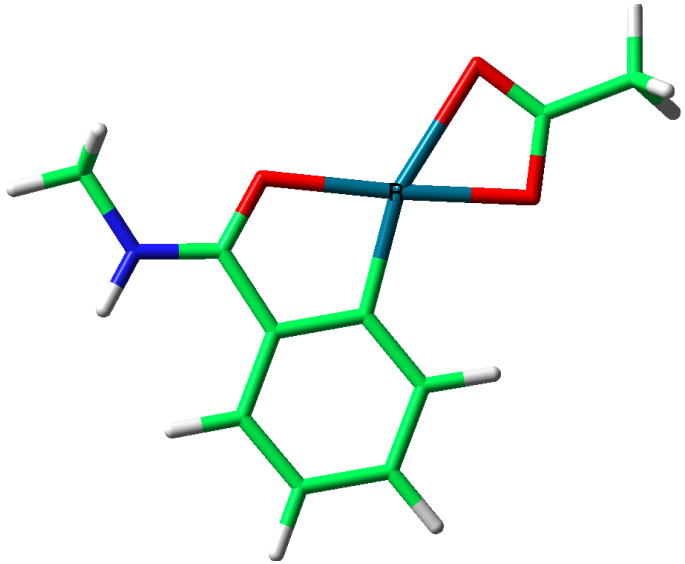
- 1 1
- H 4.03731500 1.33299400 1.62072800
- C 3.07266700 1.59801900 1.19735600
- C 2.35632500 0.68843200 0.40946400
- C 2.54369900 2.86246100 1.44075500
- C 1.30808700 3.22105100 0.89386000
- H 3.09373100 3.56979300 2.05135300
- C 2.77421000 -0.66873900 0.04668600
- O 1.98315500 -1.35308100 -0.69441800
- Pd 0.24665200 -0.37268700 -1.14612500
- H 0.90290700 4.21073800 1.08101400
- C 1.10023500 1.05500400 -0.12656500
- O -2.98072400 0.28376000 -0.01344000
- C 0.57857900 2.32246100 0.10646900
- H -0.37572900 2.61896100 -0.31097200
- O -1.45311100 0.67617600 -1.64689900
- Si -2.58845300 -0.87664500 1.23877800
- C -4.23150400 -1.02152800 2.11077000
- H -4.55221000 -0.05594400 2.51355700
- H -5.00852100 -1.38634600 1.43219600
- H -4.15257200 -1.72682600 2.94504400
- C -2.08891100 -2.48829900 0.43082500
- H -2.15089700 -3.29153200 1.17365800
- H -2.76063000 -2.74459700 -0.39432600
- H -1.06103800 -2.46514000 0.05541400
- C -1.27175600 -0.13148700 2.33248800
- H -0.29204300 -0.12595000 1.85085800
- H -1.52547200 0.89650000 2.60871300
- H -1.20020900 -0.71932300 3.25471100
- C -2.57608600 0.82369700 -1.12020200
- C -3.58439600 1.71614800 -1.78283300
- H -4.49461800 1.14490300 -1.98437700
- H -3.85190100 2.52108700 -1.09191300
- H -3.18381500 2.13078800 -2.70588300
- N 3.91642400 -1.21089000 0.44639900
- C 4.32341200 -2.56211500 0.06932700
- H 3.51050900 -3.26326300 0.26645900
- H 4.57865400 -2.60750500 -0.99304100
- H 5.19357300 -2.83565700 0.66378200
- H 4.54841000 -0.65632800 1.00476600



G1 MePdN32 end product

- Zero-point correction= 0.197518 (Hartree/Particle)
- Thermal correction to Energy= 0.213289
- Thermal correction to Enthalpy= 0.214233
- Thermal correction to Gibbs Free Energy= 0.150441
- Sum of electronic and zero-point Energies= -
- Sum of electronic and thermal Energies= -795.973533
- Sum of electronic and thermal Enthalpies= -795.972589
- Sum of electronic and thermal Free Energies= -796.036381
-
- MePdN32

- 0 1
- H -4.07328800 -0.90447000 0.00562200
- C -3.06475800 -1.31023000 0.00360500
- C -2.88577300 -2.69105200 0.00300900
- C -1.59300900 -3.22888700 0.00031800
- H -3.74863200 -3.34865600 0.00459500
- C -1.95314800 0.99702700 0.00180100
- O -0.83127100 1.60629800 -0.00016100
- Pd 0.79941400 0.31195200 -0.00365500
- H -1.46104600 -4.30721300 -0.00015800
- C -0.63575300 -1.01138700 -0.00113100
- O 2.88012100 1.29491000 -0.00764300
- C -0.46936400 -2.39645600 -0.00178300
- H 0.52975200 -2.82121800 -0.00393800
- O 2.49368700 -0.87665600 -0.00793500
- C 3.32427800 0.11306900 -0.00548200
- C 4.79760900 -0.18867500 0.01803200
- H 5.37603800 0.72091600 -0.14514100
- H 5.06220000 -0.61635400 0.99032400
- H 5.03900700 -0.93142900 -0.74650800
- C -1.94281400 -0.47095400 0.00157300
- N -3.07938300 1.70818500 0.00379500
- C -3.08523600 3.16676700 0.00411800
- H -2.57772000 3.55181900 0.89233000
- H -2.57472600 3.55184300 -0.88230500
- H -4.11992000 3.50686000 0.00239600
- H -3.96150800 1.21907900 0.00590300



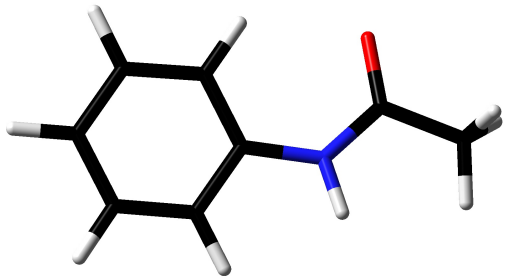
Scheme 5

Reaction equilibria

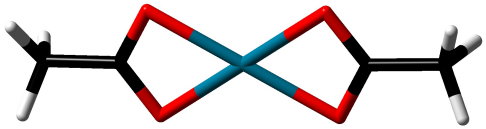
Acetanilide

Activation **X = H**

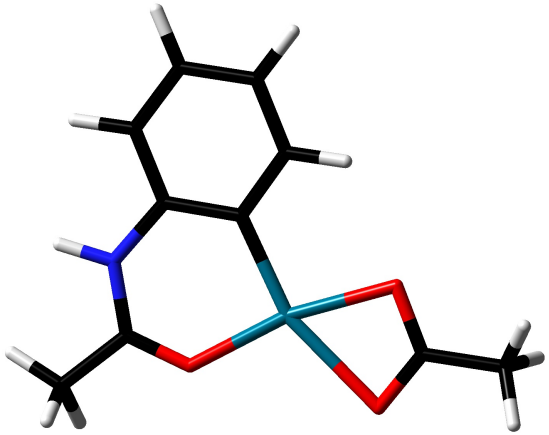
Reactant + $Pd(OAc)_2$ ⇌ Pdcycle + AcOH



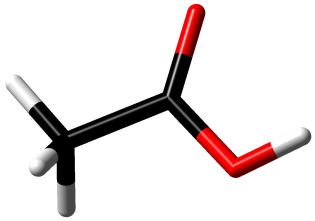
-440.20224 **-440.021332**



-584.894592 **-584.711487**



-796.042297 **-795.757690**

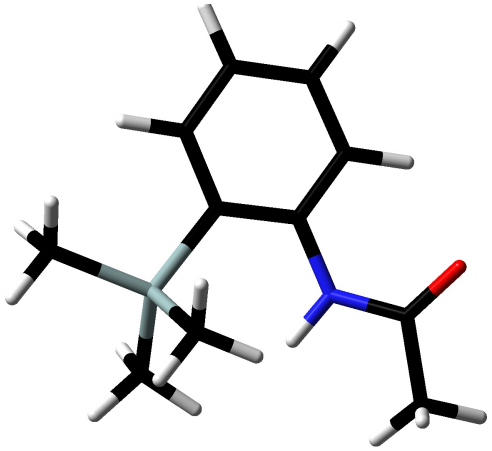


-229.067337 **-228.988434**

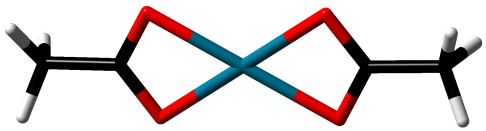
2-Trimethylsilylbenzamide

Activation **X = $SiMe_3$**

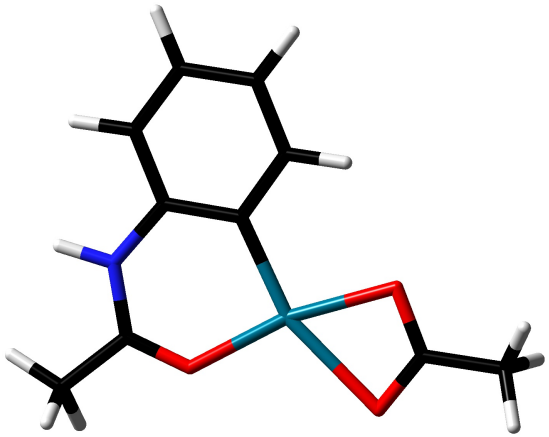
Reactant + $Pd(OAc)_2$ ⇌ Pdcycle + AcOH



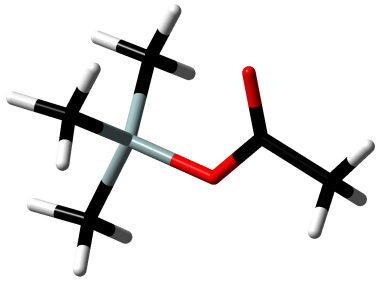
-848.823364 **-848.565369**



-584.894592 **-584.711487**



-796.042297 **-795.757690**

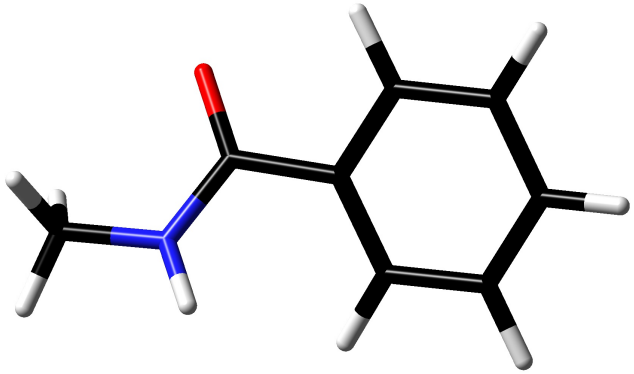


-637.726868 **-637.567871**

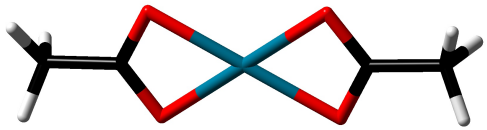
N-Methylbenzanilide

Activation **X = H**

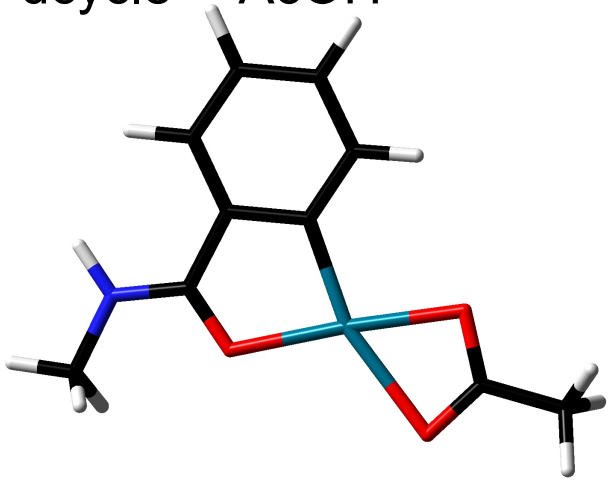
Reactant + $Pd(OAc)_2$ ⇌ Pdcycle + AcOH



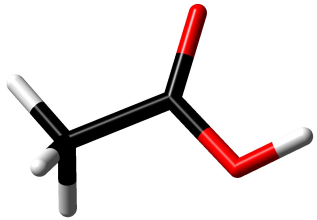
-440.197662 **-440.017761**



-584.894592 **-584.711487**



-796.03241 **-795.750732**

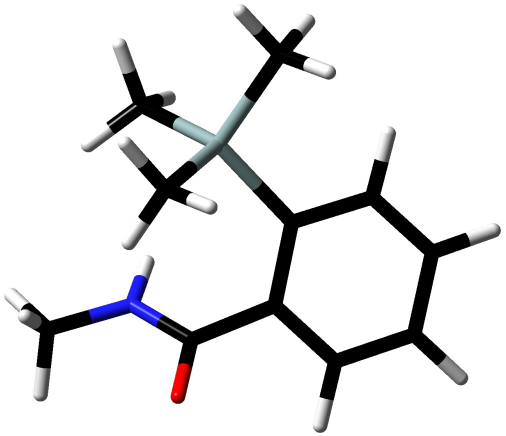


-229.067337 **-228.988434**

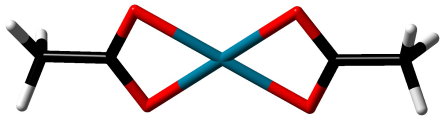
N-Methyl-2-trimethylsilylbenzamide

Activation **X = $SiMe_3$**

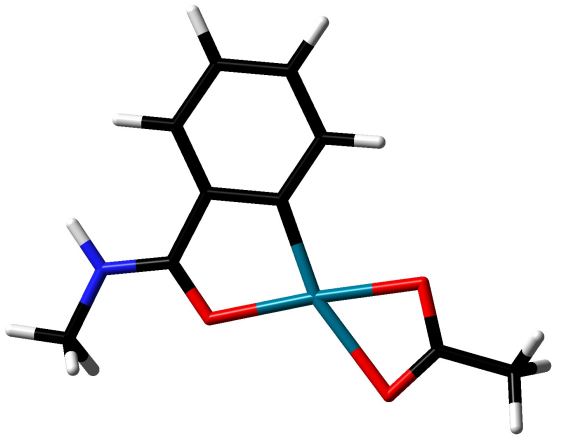
Reactant + $Pd(OAc)_2$ ⇌ Pdcycle + AcOH



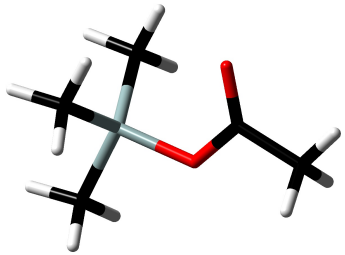
-848.818298 **-848.559082**



-584.894592 **-584.711487**

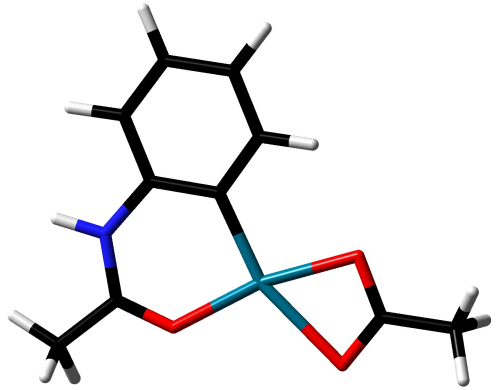


-796.03241 **-795.750732**

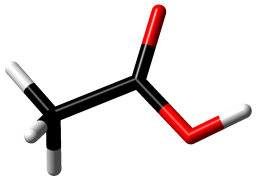


-637.726868 **-637.567871**

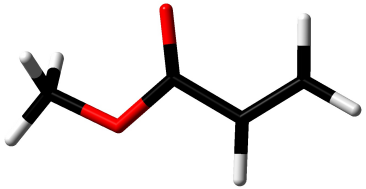
Product formation from acetanilide (H or $SiMe_3$)



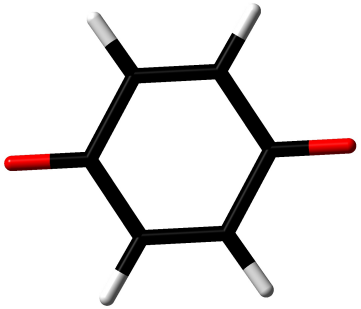
-796.042297 -795.757690



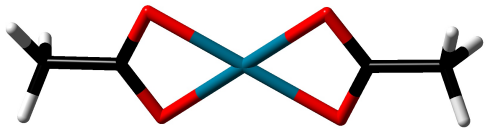
229.067337 -228.988434



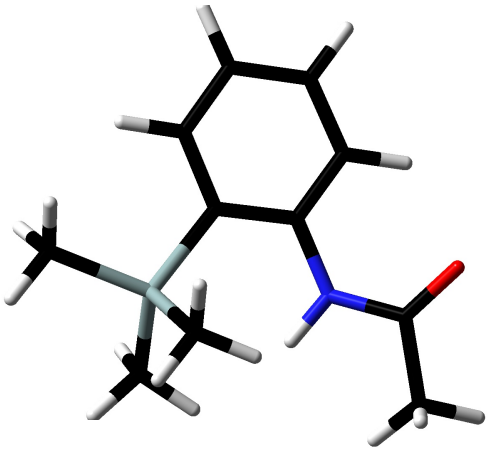
-306.425568 -306.308777



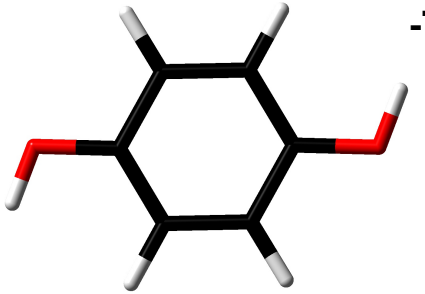
-381.426788 -381.273468



-584.894592 -584.711487

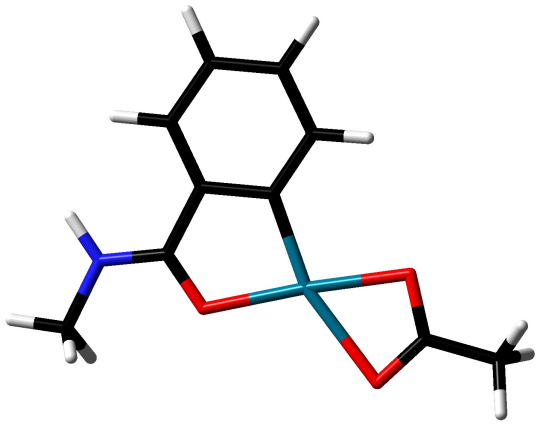


-745.441467 -745.143616

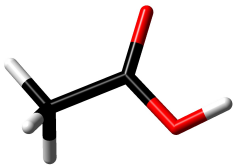


-382.651215 -382.506958

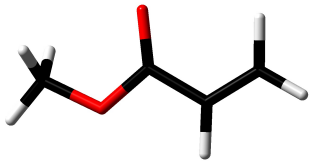
Product formation for N-methylbenzamide



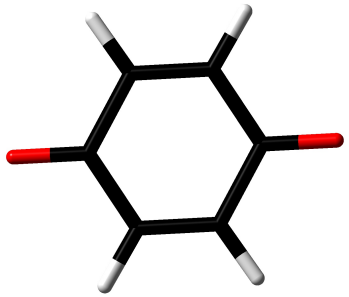
-796.03241 -795.750732



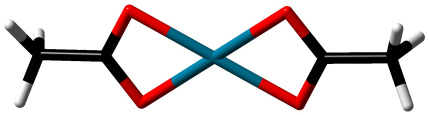
-229.067337 -228.988434



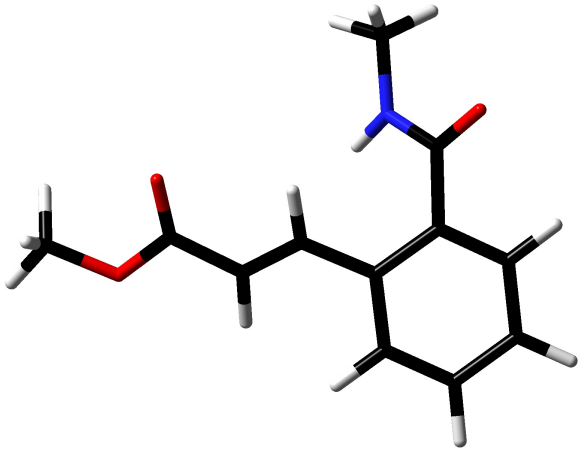
-306.425568 -306.308777



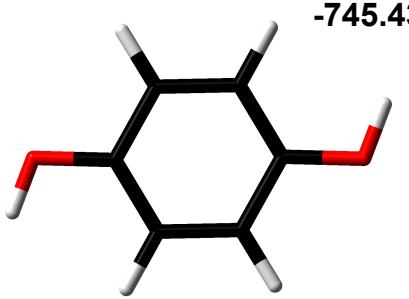
-381.426788 -381.273468



-584.894592 -584.711487



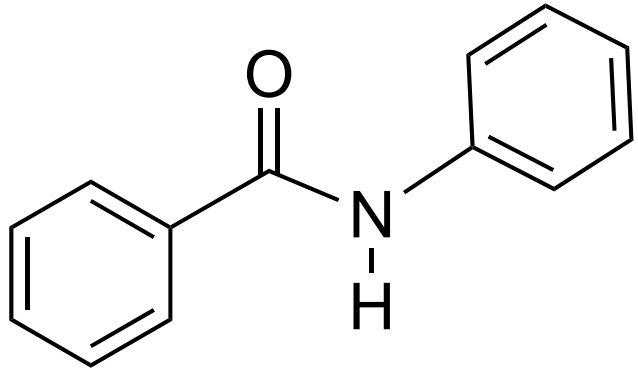
-745.436035 -745.137268



-382.651215 -382.506958

Scheme 6

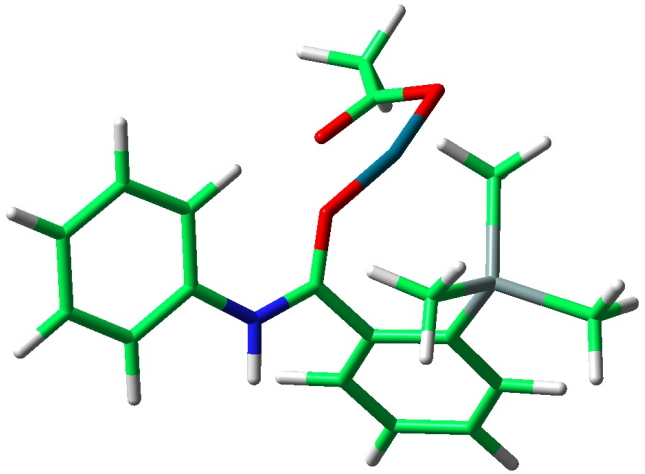
Benzanilide series



BA1 MePdP38 agostic BA precursor

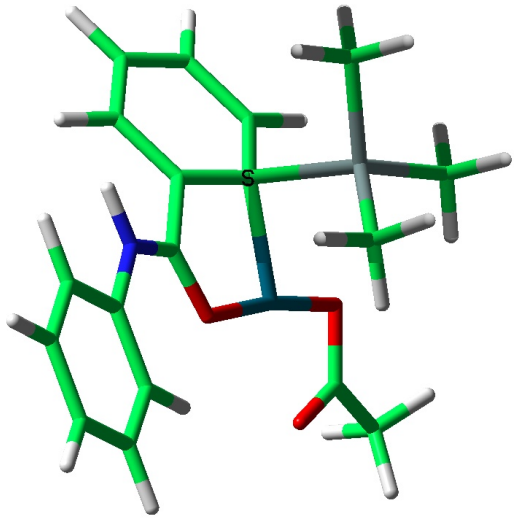
- Zero-point correction= 0.365395 (Hartree/Particle)
- Thermal correction to Energy= 0.391480
- Thermal correction to Enthalpy= 0.392424
- Thermal correction to Gibbs Free Energy= 0.306491
- Sum of electronic and zero-point Energies= -1396.698215
- Sum of electronic and thermal Energies= -1396.672130
- Sum of electronic and thermal Enthalpies= -1396.671186
- Sum of electronic and thermal Free Energies= -1396.757119
- MePdP38

- 1 1
- C -2.02308400 -2.50758800 2.72236800
- C -1.90404500 -2.71553600 1.34511200
- C -0.94976500 -2.03889600 0.56918700
- C -0.09572700 -1.14606400 1.26142500
- C -0.19101500 -0.94782300 2.64458900
- C -1.16652500 -1.62371700 3.37594800
- H -2.78212000 -3.04310800 3.28354300
- H -2.57096600 -3.42767200 0.87099600
- H 0.47639500 -0.24793700 3.13822000
- H -1.25291200 -1.45988400 4.44472000
- O 0.59998400 0.40209700 -0.45238200
- C 0.92099600 -0.36244500 0.51557200
- N 2.19367400 -0.49887500 0.88382700
- H 2.34626200 -1.18264100 1.61593400
- Pd -1.29539100 1.14426400 -0.64075100
- O -1.30816600 2.75713300 0.67051800
- C -2.50294000 3.04700900 0.29978700
- C -3.26678900 4.18305800 0.87178300
- H -2.58233800 4.95962700 1.21667500
- H -3.95900500 4.57852500 0.12622000
- H -3.84707700 3.82026400 1.72708000
- O -3.00114800 2.26317400 -0.59260100
- Si -0.83947400 -2.41947300 -1.29374800
- C -1.94804800 -3.88319300 -1.68188000
- H -1.86469700 -4.13134000 -2.74500100
- H -1.65724500 -4.76890600 -1.10844500
- H -3.00100100 -3.66985800 -1.47296500
- C -1.49429300 -0.88359200 -2.21543800
- H -2.25189500 -0.39556900 -1.55184500
- H -0.67656700 -0.22698600 -2.53649500
- H -2.08424400 -1.09094500 -3.11378300
- C 0.93554600 -2.76697400 -1.80757200
- H 1.35274400 -3.59572900 -1.22700300
- H 0.96021500 -3.05336600 -2.86445800
- H 1.58905600 -1.89887800 -1.68730500
- C 3.36921600 0.13701400 0.39928400
- C 4.54314000 -0.10555500 1.12486900
- C 3.39434400 0.94862000 -0.74185800
- C 5.74180700 0.46912800 0.71513100
- H 4.51419500 -0.73751200 2.00785400
- C 4.60520100 1.51785000 -1.13725200
- H 2.49343600 1.12595600 -1.30898100
- C 5.77739200 1.28512800 -0.41793300
- H 6.64649000 0.27857300 1.28268800
- H 4.62602600 2.14578500 -2.02200400
- H 6.71233400 1.73243900 -0.73841400



BA2 Si Wheland for BA (MePd11)

- Zero-point correction= 0.364735 (Hartree/Particle)
- Thermal correction to Energy= 0.391357
- Thermal correction to Enthalpy= 0.392301
- Thermal correction to Gibbs Free Energy= 0.305179
- Sum of electronic and zero-point Energies= -1396.715286
- Sum of electronic and thermal Energies= -1396.688664
- Sum of electronic and thermal Enthalpies= -1396.687720
- Sum of electronic and thermal Free Energies= -1396.774842
- MePdP11
- 1 1
- C 1.84142200 3.05942500 -1.73233600
- C 2.08829900 2.01665500 -0.84317600
- C 1.03191700 1.23235700 -0.31574900
- C -0.28661500 1.47901900 -0.83646400
- C -0.53111800 2.51459600 -1.72776100
- C 0.53459100 3.32131500 -2.15042800
- H 2.66108300 3.66356700 -2.10489500
- H 3.10349100 1.82083800 -0.51421100
- H -1.51864100 2.67711000 -2.14756800
- H 0.34214500 4.13455900 -2.84196100
- Si 1.15953000 1.32489200 1.72444300
- C 0.80364700 3.14762400 2.01738100
- H 0.82979700 3.35287100 3.09333500
- H 1.54628100 3.78528200 1.52975000
- H -0.18720000 3.42695900 1.64625600
- C 2.90072100 0.87880700 2.24938900
- H 2.97721800 1.05601400 3.32848200
- H 3.13783600 -0.16892600 2.05364200
- H 3.65466200 1.50110100 1.76002800
- O -0.82740500 -0.73237300 -0.26388900
- C -1.27733700 0.43385300 -0.49744500
- N -2.57700000 0.72601300 -0.45497700
- H -2.80837300 1.69789400 -0.61972400
- C -0.13732300 0.28929900 2.59954700
- H -1.15472300 0.49270700 2.25640400
- H 0.04920100 -0.78392100 2.51786400
- H -0.09123900 0.56405100 3.66041900
- Pd 1.23086100 -0.85274400 -0.31421300
- O 1.85671800 -2.91699100 -0.42342700
- C 3.05931800 -2.50313300 -0.42092200
- C 4.23041400 -3.42049600 -0.52156800
- H 3.95823700 -4.41660400 -0.17026000
- H 4.53476000 -3.48904000 -1.57144900
- H 5.06997600 -3.02427500 0.05260500
- O 3.23145900 -1.22341000 -0.34997800
- C -3.69253900 -0.11178500 -0.19227400
- C -4.95189300 0.50000200 -0.25740000
- C -3.57695000 -1.47142300 0.12584300
- C -6.09771100 -0.24629900 -0.00360100
- H -5.03111300 1.55469600 -0.50609700
- C -4.73714400 -2.20327100 0.37758300
- H -2.60761300 -1.94357900 0.17612000
- C -5.99479500 -1.60236500 0.31533500
- H -7.06947200 0.23291800 -0.05640900
- H -4.64968500 -3.25630200 0.62416900
- H -6.88826800 -2.18514900 0.51255100



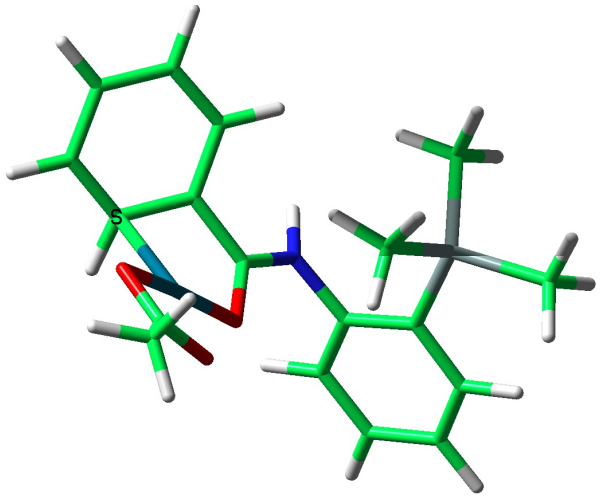
BA3 MePdP15 BA 5C-H Wheland

Zero-point correction=	0.365032 (Hartree/Particle)
Thermal correction to Energy=	0.391369
Thermal correction to Enthalpy=	0.392313
Thermal correction to Gibbs Free Energy=	0.306324
Sum of electronic and zero-point Energies=	-1396.706102
Sum of electronic and thermal Energies=	-1396.679765
Sum of electronic and thermal Enthalpies=	-1396.678821
Sum of electronic and thermal Free Energies=	-1396.764810

MePdP15

1 1

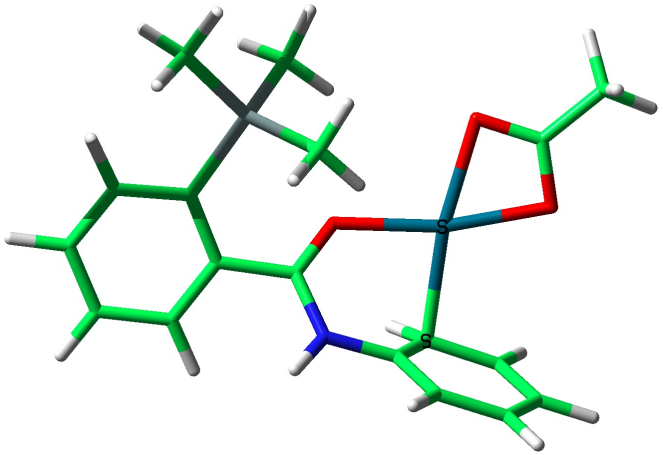
C	-3.11069200	3.08826400	0.70725800
C	-3.15040100	2.41452700	-0.50677000
C	-1.98883200	1.78967200	-1.00751300
C	-0.77787300	1.87450400	-0.25284300
C	-0.74360500	2.57439900	0.95611000
C	-1.90759500	3.18453900	1.42210500
H	-4.00637600	3.55921900	1.09621300
H	-4.06515700	2.37306800	-1.08712300
H	0.16584000	2.61392300	1.54463700
H	-1.88378200	3.72602800	2.36160800
O	0.01623300	-0.13821000	-1.13298000
C	0.34398100	1.02286600	-0.72563400
N	1.60515600	1.41863400	-0.67208600
H	1.79130800	2.38650000	-0.43528900
Pd	-1.92055900	-0.45681000	-0.51989200
O	-2.19756800	-2.51995300	-0.20137200
C	-3.39772400	-2.28047000	0.16597800
C	-4.32353700	-3.34581400	0.63329700
H	-4.03349100	-4.30761400	0.20808000
H	-4.26100500	-3.41030600	1.72500500
H	-5.35070200	-3.09558900	0.36173700
O	-3.75370000	-1.04069600	0.13453900
C	2.70568900	0.56104100	-1.06489300
C	3.11975100	0.62352400	-2.39351100
C	3.29501400	-0.28738600	-0.11416600
C	4.17008900	-0.18920400	-2.81842400
H	2.62163800	1.29879200	-3.08161800
C	4.34782400	-1.09425200	-0.58214000
C	4.78162900	-1.05053500	-1.90853800
H	4.50193200	-0.14932000	-3.85050500
H	4.84417800	-1.77200400	0.10402400
H	5.59806700	-1.68947400	-2.22994700
H	-1.95865700	1.47907600	-2.05147400
Si	2.79036700	-0.35628500	1.71979500
C	3.91673000	-1.59274000	2.58385800
C	1.00181400	-0.92905000	1.93783000
C	3.03981600	1.34782100	2.49302900
H	3.66639700	-1.62966800	3.64947400
H	3.79814300	-2.60389900	2.18131900
H	4.97204800	-1.31407800	2.50095900
H	2.75510300	1.32822800	3.55059300
H	4.09139200	1.64672700	2.43483200
H	2.44739500	2.12782100	2.00577700
H	0.85378400	-1.23119100	2.98069800
H	0.26384700	-0.15270300	1.71942200
H	0.78039100	-1.7920800	1.30239800



BA4 MePdP32 BA 6-ring Wheland

- Zero-point correction= 0.365315 (Hartree/Particle)
- Thermal correction to Energy= 0.391411
- Thermal correction to Enthalpy= 0.392355
- Thermal correction to Gibbs Free Energy= 0.307983
- Sum of electronic and zero-point Energies= -1396.718280
- Sum of electronic and thermal Energies= -1396.692184
- Sum of electronic and thermal Enthalpies= -1396.691239
- Sum of electronic and thermal Free Energies= -1396.775611
-
- MePdP32

- 1 1
- H -1.28083200 1.90989200 -1.71470100
- C -1.82512300 1.90506600 -0.77418300
- C -1.12343100 2.14481500 0.44460700
- C -3.23575400 2.06555700 -0.78914500
- C -3.91485700 2.42092300 0.36414700
- H -3.76670200 1.90752000 -1.72095200
- N 0.28798900 2.05258100 0.46409400
- H 0.79909600 2.68345500 1.06915700
- C 0.98407300 1.08634900 -0.17237900
- O 0.40113300 0.09592500 -0.70357400
- Pd -1.58142500 -0.29815700 -0.42868200
- H -4.99291800 2.52970200 0.35260000
- C -1.81275500 2.52398000 1.59876600
- O -1.70399600 -2.41294400 -0.32372400
- C -3.19777500 2.66364600 1.54742000
- H -3.73039300 2.95410100 2.44667300
- O -3.42994200 -1.10059300 -0.13643200
- C -2.96291500 -2.30417000 -0.14153300
- C -3.84708500 -3.47857300 0.08700200
- H -3.42993600 -4.36190200 -0.39903000
- H -3.90575500 -3.66791600 1.16438400
- H -4.85269100 -3.27090200 -0.28261200
- C 2.44809800 1.18955300 -0.24054600
- C 3.25787600 0.03644200 -0.07462000
- C 2.99800000 2.45388000 -0.51028900
- C 4.64101300 0.23408100 -0.20560600
- C 4.37461100 2.60068900 -0.64567400
- H 2.34590800 3.30974100 -0.65375900
- C 5.19544600 1.48399300 -0.49543500
- H 5.31361200 -0.60563300 -0.07154200
- H 4.79842100 3.57312400 -0.87168600
- H 6.27149400 1.58356900 -0.59778700
- H -1.27007200 2.69906800 2.52084800
- Si 2.64527700 -1.70299100 0.44817700
- C 1.44637900 -1.53738800 1.89898800
- C 4.15440200 -2.64717800 1.07689700
- C 1.91225000 -2.66569700 -0.99382600
- H 4.67561900 -2.11025000 1.87579500
- H 3.82529400 -3.60985400 1.48363900
- H 4.87557600 -2.86058900 0.28138100
- H 0.51878700 -1.01794900 1.64864600
- H 1.17489000 -2.53752200 2.25461300
- H 1.92454400 -1.00930800 2.73099400
- H 2.60717400 -2.67950800 -1.84018600
- H 1.73718300 -3.70362300 -0.68921800
- H 0.96517900 -2.24112500 -1.32871400

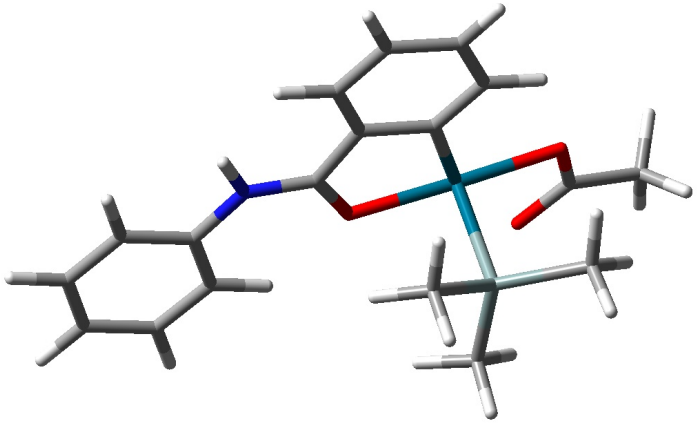


BA5 MePdP33 BA (Pd-$SiMe_3$)

- Zero-point correction= 0.364525 (Hartree/Particle)
- Thermal correction to Energy= 0.391048
- Thermal correction to Enthalpy= 0.391992
- Thermal correction to Gibbs Free Energy= 0.305595
- Sum of electronic and zero-point Energies= -1396.725597
- Sum of electronic and thermal Energies= -1396.699074
- Sum of electronic and thermal Enthalpies= -1396.698129
- Sum of electronic and thermal Free Energies= -1396.784526

- MePdP33

- 1 1
- C 1.48704700 3.87198300 -0.33685500
- C 1.85754100 2.52298700 -0.41345000
- C 0.85726500 1.56418900 -0.42065600
- C -0.50555800 1.91846500 -0.35901900
- C -0.86079000 3.27117700 -0.28712600
- C 0.13966300 4.24125500 -0.27382200
- H 2.25705700 4.63664900 -0.32451900
- H 2.90170900 2.23330000 -0.46351100
- H -1.90013500 3.58291500 -0.23413000
- H -0.13076300 5.28927600 -0.21167600
- Si 1.38010700 -0.44659400 1.85176300
- C 0.17953600 0.73281200 2.66418200
- H 0.27141600 0.57486700 3.74656900
- H 0.41231700 1.77761400 2.45046200
- H -0.85645200 0.52649200 2.38704600
- C 3.16124900 -0.02079200 2.20554000
- H 3.30765200 -0.07991300 3.29139900
- H 3.85477900 -0.70971000 1.72158800
- H 3.39552000 0.99701400 1.88472300
- O -0.86879400 -0.40723000 -0.36507800
- C -1.40386400 0.76057800 -0.33752600
- N -2.72548300 0.90818700 -0.27148000
- H -3.05340000 1.86576600 -0.26820100
- C 0.90395200 -2.23924800 2.07873600
- H -0.11699900 -2.41660100 1.72986300
- H 1.58233300 -2.91118800 1.54987900
- H 0.94469500 -2.46455100 3.15225400
- Pd 1.16807300 -0.37055000 -0.58100200
- O 2.24627800 -2.37235700 -0.97826300
- C 3.28019500 -1.66654600 -1.09762900
- C 4.62503600 -2.21628500 -1.45272900
- H 4.56336100 -3.29281000 -1.60969000
- H 4.99287100 -1.72563500 -2.35822900
- H 5.33218200 -1.99587600 -0.64772600
- O 3.17045100 -0.38341500 -0.89401600
- C -3.76025800 -0.06267800 -0.22430100
- C -5.06930100 0.43763700 -0.19060600
- C -3.52828600 -1.44446700 -0.20628700
- C -6.14672000 -0.44043200 -0.13984100
- H -5.24083300 1.51034000 -0.20604900
- C -4.62112700 -2.30968400 -0.15532100
- H -2.52151600 -1.83212600 -0.23332900
- C -5.92694100 -1.81955300 -0.12230700
- H -7.15655400 -0.04488900 -0.11493800
- H -4.44221400 -3.37988400 -0.14298400
- H -6.76682500 -2.50510500 -0.08410400

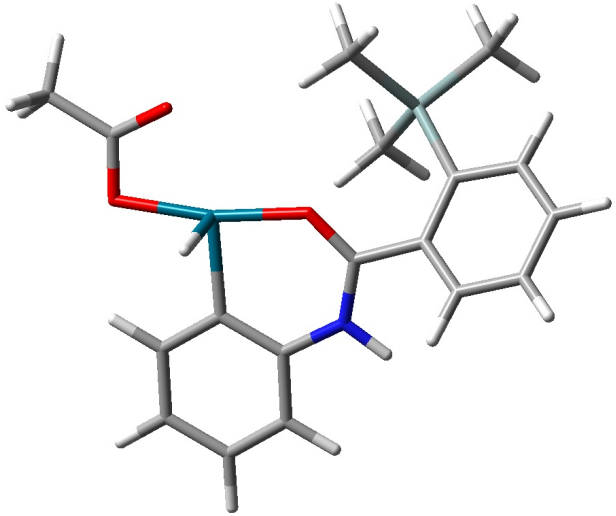


BA6 MePdP34 Pd hydride complex

- Zero-point correction= 0.363001 (Hartree/Particle)
- Thermal correction to Energy= 0.388646
- Thermal correction to Enthalpy= 0.389590
- Thermal correction to Gibbs Free Energy= 0.307200
- Sum of electronic and zero-point Energies= -1396.675053
- Sum of electronic and thermal Energies= -1396.649408
- Sum of electronic and thermal Enthalpies= -1396.648464
- Sum of electronic and thermal Free Energies= -1396.730853

- MePdP34

- 1 1
- H -1.95709000 0.12969200 -1.63895800
- C -1.98678300 1.43426700 0.14773100
- C -0.97594100 2.39385200 0.28760700
- C -3.32149700 1.76257800 0.38594400
- C -3.65316500 3.05085600 0.80424300
- H -4.09293700 1.01243700 0.25529200
- N 0.39179300 2.14373700 0.06135600
- H 1.01685700 2.91213400 0.27386300
- C 0.98605100 1.02111800 -0.34978400
- O 0.35401500 -0.05699600 -0.58521000
- Pd -1.59036300 -0.45504200 -0.31849400
- H -4.69038800 3.30054700 0.99873700
- C -1.32266300 3.68603000 0.71220200
- O -1.90864700 -2.67359200 -0.69469300
- C -2.64958300 4.00880800 0.96692800
- H -2.89948700 5.01252300 1.29240200
- O -3.45741300 -1.21490700 -0.16863800
- C -3.12234000 -2.44676500 -0.45780800
- C -4.19441100 -3.48257000 -0.51523700
- H -3.75802100 -4.47729900 -0.42339800
- H -4.93436400 -3.30934100 0.26841000
- H -4.70103100 -3.40362400 -1.48318700
- C 2.45097500 1.02499200 -0.52950300
- C 3.22978200 -0.07873000 -0.09940100
- C 3.02832700 2.14649400 -1.14680600
- C 4.61289500 0.02244900 -0.32030200
- C 4.40274300 2.19811400 -1.35690000
- H 2.40169700 2.96010000 -1.49899000
- C 5.19541300 1.13047900 -0.94026900
- H 5.26281000 -0.78181800 0.00552400
- H 4.84488000 3.05933000 -1.84582500
- H 6.26940300 1.15757400 -1.09461400
- H -0.54231100 4.43049200 0.83989800
- Si 2.59743800 -1.62571400 0.83652500
- C 1.42041700 -1.12025100 2.22676100
- C 4.09490400 -2.43206200 1.65323600
- C 1.82837700 -2.88029000 -0.33835900
- H 4.63456400 -1.73764200 2.30494600
- H 3.75206600 -3.26944600 2.27086500
- H 4.80251200 -2.83669100 0.92274200
- H 0.50337100 -0.63889500 1.88021800
- H 1.13279200 -2.01396800 2.79184300
- H 1.91885700 -0.43748600 2.92289600
- H 2.53286700 -3.13493800 -1.13734300
- H 1.60086900 -3.80214700 0.20877800
- H 0.90744100 -2.51801200 -0.79761100

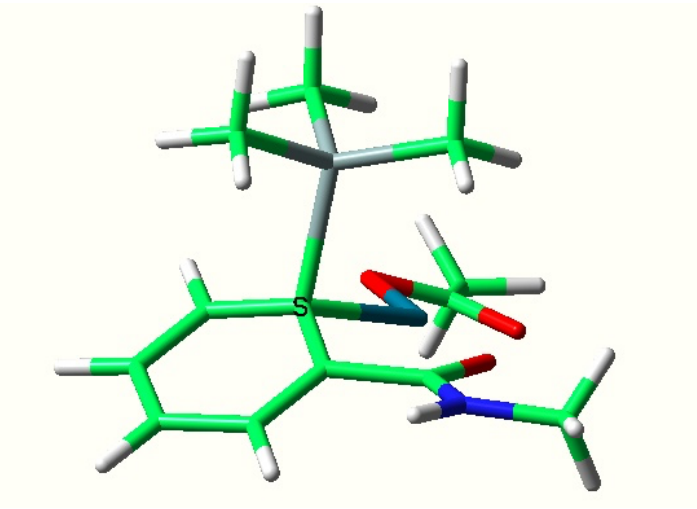


Miscellaneous files

MePdOAcL5 (alt Wheland) for N-Mebenzamide

- Zero-point correction= 0.311929 (Hartree/Particle)
- Thermal correction to Energy= 0.334640
- Thermal correction to Enthalpy= 0.335584
- Thermal correction to Gibbs Free Energy= 0.259579
- Sum of electronic and zero-point Energies= -1205.010008
- Sum of electronic and thermal Energies= -1204.987298
- Sum of electronic and thermal Enthalpies= -1204.986353
- Sum of electronic and thermal Free Energies= -1205.062358
- MePdOAcL5

- 1 1
- C 1.48664600 -2.30275200 -2.16863100
- C 0.52996400 -1.93985600 -1.22356200
- C 0.67137200 -0.76108300 -0.45029200
- C 1.77260200 0.10498700 -0.77365200
- C 2.72239400 -0.25428900 -1.71867700
- C 2.58959000 -1.47630100 -2.39380100
- H 1.37397500 -3.22202200 -2.73252700
- H -0.32110000 -2.58829700 -1.04338500
- H 3.53657900 0.41345700 -1.98006400
- H 3.33672100 -1.76150800 -3.12658100
- Si 0.61841200 -1.33227300 1.51863900
- C 2.13172800 -2.44382100 1.60221300
- H 2.27700100 -2.77931400 2.63498800
- H 2.01733000 -3.32694400 0.96775400
- H 3.03590000 -1.91189500 1.29106900
- C -0.95049400 -2.29615900 1.85425200
- H -0.85237700 -2.75399100 2.84548500
- H -1.83464500 -1.65581400 1.85364000
- H -1.10951000 -3.10245000 1.13343300
- O 0.52146200 1.87806900 0.13920500
- C 1.68309800 1.45577800 -0.17164900
- N 2.74819200 2.21555800 0.02355100
- H 3.65782000 1.84275800 -0.21016000
- C 2.65742200 3.57511400 0.55631200
- H 3.66540000 3.92979200 0.76293400
- H 2.17633600 4.23638700 -0.16873900
- H 2.07104200 3.57262700 1.47707300
- C 0.84369200 0.11045300 2.69420600
- H 1.76056700 0.67320500 2.49964500
- H -0.00047400 0.80245800 2.68622300
- H 0.93094800 -0.31572400 3.70107300
- Pd -0.97296200 0.50440300 -0.19824400
- O -2.89387800 1.48666300 -0.15688500
- C -3.42639600 0.35538600 -0.39167900
- C -4.89705500 0.17417700 -0.56124700
- H -5.43310600 1.01936600 -0.12821500
- H -5.12528700 0.11837400 -1.63090900
- H -5.21522900 -0.76202400 -0.09788200
- O -2.62434900 -0.65196200 -0.50284600

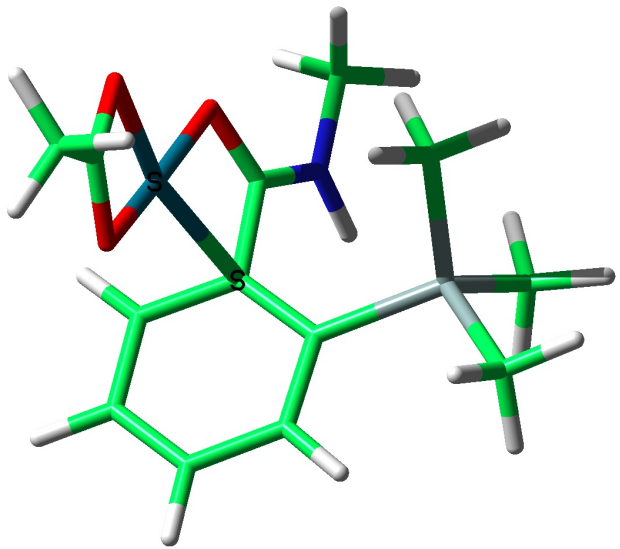


MePdN10a ipso-Wheland for N-Me benzamide

- Zero-point correction= 0.311763 (Hartree/Particle)
- Thermal correction to Energy= 0.335484
- Thermal correction to Enthalpy= 0.336428
- Thermal correction to Gibbs Free Energy= 0.256892
- Sum of electronic and zero-point Energies= -1205.004234
- Sum of electronic and thermal Energies= -1204.980513
- Sum of electronic and thermal Enthalpies= -1204.979569
- Sum of electronic and thermal Free Energies= -1205.059105

- MePdN10a

- 1 1
- C −0.06471800 −1.93779200 2.59233800
- C −0.92286800 −2.04624100 1.48015700
- C −1.28654500 −0.95316200 0.69488200
- C −0.73813400 0.30841100 1.09348900
- C 0.14634600 0.42777500 2.20714700
- C 0.47661200 −0.71578500 2.95359300
- H 0.17574800 −2.82693300 3.16565600
- H −1.29846800 −3.03059000 1.22403900
- H 0.46110400 1.40957800 2.54745700
- H 1.13633700 −0.62495600 3.80857100
- O −0.06122600 2.14672300 −0.16912400
- C −1.06384900 1.60003300 0.39966200
- N −2.27245700 2.11657000 0.38078900
- H −2.98717500 1.65205000 0.92727500
- C −2.60449200 3.36915400 −0.30335800
- H −2.39553600 4.22372700 0.34477200
- H −2.00668400 3.44882300 −1.21096700
- H −3.66297200 3.35294300 −0.55784900
- Pd 1.29375500 0.59786700 0.04924400
- O 2.89397600 0.73166900 −1.31948400
- C 3.34700500 −0.37469500 −0.86919300
- C 4.55772200 −1.03519200 −1.42492200
- H 5.26100200 −0.28316800 −1.78637500
- H 5.02242700 −1.66912600 −0.66825200
- H 4.25684400 −1.66280000 −2.27085700
- O 2.66594000 −0.90594300 0.08863500
- Si −2.29503700 −1.23573900 −0.91038400
- C −2.35651200 −3.09159700 −1.20231600
- H −2.86335500 −3.28456000 −2.15374400
- H −1.35560400 −3.53021600 −1.26348900
- H −2.91558200 −3.61653700 −0.42115100
- C −4.04878700 −0.56151300 −0.75068900
- H −4.49963100 −0.82410900 0.21155100
- H −4.08994400 0.52422000 −0.87168900
- H −4.67168200 −0.99890500 −1.53835700
- C −1.36249700 −0.38834400 −2.31127700
- H −0.31848900 −0.71961300 −2.33273600
- H −1.82136100 −0.64516000 −3.27202800
- H −1.36719000 0.70191100 −2.22449100

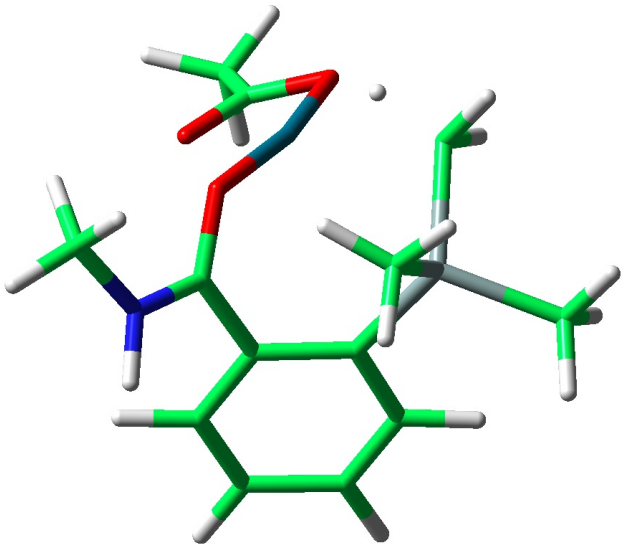


MePdN10M alternative agostic conformer for N-Mebenzamide

- Zero-point correction= 0.311742 (Hartree/Particle)
- Thermal correction to Energy= 0.334936
- Thermal correction to Enthalpy= 0.335880
- Thermal correction to Gibbs Free Energy= 0.257965
- Sum of electronic and zero-point Energies= -1204.996083
- Sum of electronic and thermal Energies= -1204.972890
- Sum of electronic and thermal Enthalpies= -1204.971945
- Sum of electronic and thermal Free Energies= -1205.049860

- MePdN10M

- 1 1
- C 1.43334900 -0.45251100 3.39978400
- C 1.58759900 -1.14109900 2.19316100
- C 1.47609500 -0.49888800 0.95008300
- C 1.21586800 0.89331900 0.97876900
- C 1.08497700 1.59551700 2.18306000
- C 1.18622200 0.91858800 3.39772600
- H 1.51537500 -0.98911300 4.33952800
- H 1.80752400 -2.20242600 2.22885400
- H 0.87077700 2.65937500 2.16788000
- H 1.06964200 1.45966800 4.33052500
- O 0.18023800 1.25157900 -1.17704900
- C 1.00775500 1.64359400 -0.28460100
- N 1.69076300 2.75742200 -0.49251500
- H 2.41929300 2.98582900 0.17074000
- C 1.51984700 3.60498800 -1.67055500
- H 2.06337300 3.19278000 -2.52546900
- H 0.46024300 3.66812100 -1.91913700
- H 1.90544500 4.59690800 -1.43959700
- Pd -1.24421400 -0.13243800 -0.72994400
- O -2.69199200 0.90921800 0.32547300
- C -3.40912400 -0.15435000 0.37720500
- C -4.71687900 -0.20035500 1.07763400
- H -5.21173900 0.76991200 1.00743300
- H -5.34227300 -0.98708300 0.65315500
- H -4.54013900 -0.42334700 2.13543000
- O -2.90040600 -1.18660700 -0.20035000
- Si 1.81742000 -1.50890400 -0.62646700
- C 2.60425700 -3.14300900 -0.13866300
- H 2.83988300 -3.71798200 -1.04014000
- H 3.53715300 -2.98788500 0.41204400
- H 1.94044900 -3.75553400 0.47918100
- C 0.20010200 -1.96329400 -1.52593700
- H -0.40853100 -1.14956400 -2.03587100
- H 0.46904000 -2.47719800 -2.45944900
- H -0.43787500 -2.64961500 -0.96572500
- C 2.93705200 -0.55951500 -1.80096800
- H 3.84483900 -0.22841500 -1.28689700
- H 3.23845500 -1.21573800 -2.62437800
- H 2.44825700 0.31474300 -2.23733800

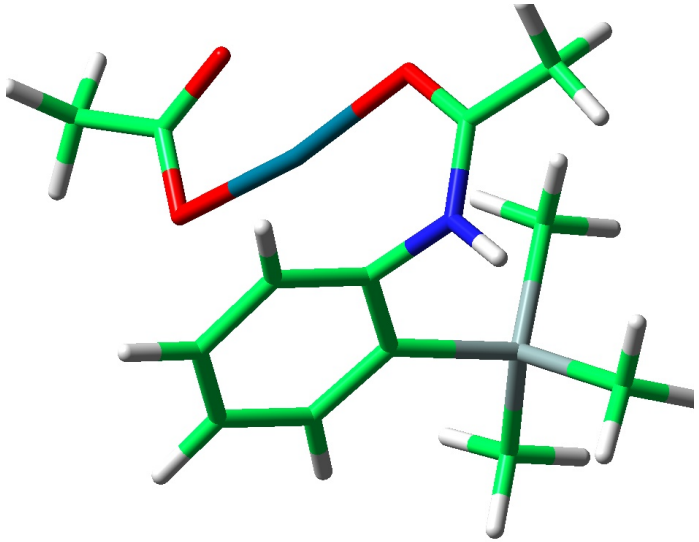


MePdP13 AA ipso-Wheland

- Zero-point correction= 0.311918 (Hartree/Particle)
- Thermal correction to Energy= 0.334953
- Thermal correction to Enthalpy= 0.335897
- Thermal correction to Gibbs Free Energy= 0.259036
- Sum of electronic and zero-point Energies= -1205.019060
- Sum of electronic and thermal Energies= -1204.996024
- Sum of electronic and thermal Enthalpies= -1204.995080
- Sum of electronic and thermal Free Energies= -1205.071942

- MePdP13

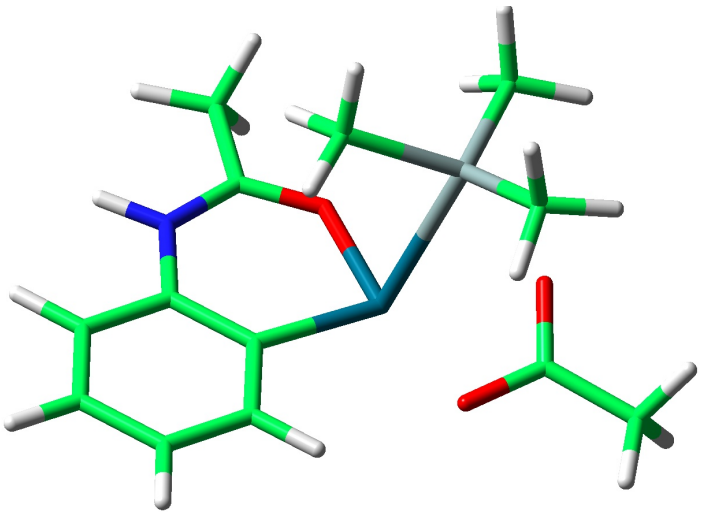
- 1 1
- H -0.37972300 1.14930600 2.84326100
- C -0.18770100 0.20888600 2.33783300
- C 0.70725100 0.18800300 1.22434900
- C -0.74346200 -0.98597800 2.79189100
- C -0.39423800 -2.18317700 2.16828900
- H -1.42610700 -0.97755900 3.63351500
- N 1.50923600 1.37520200 0.99261300
- H 2.39513700 1.45208200 1.47682100
- C 1.08754200 2.38575100 0.23652700
- O -0.03561900 2.31353900 -0.34986200
- Pd -1.06313600 0.58433700 -0.06697200
- H -0.81000300 -3.11726300 2.53129500
- C 1.08913200 -1.03882200 0.58591100
- O -2.79326800 0.73794500 -1.27820000
- C 0.49085600 -2.20203900 1.08099900
- H 0.72802600 -3.15586900 0.62428500
- O -2.33838700 -0.99545600 -0.05096600
- C 1.93965500 3.59868300 0.05571200
- H 2.88952900 3.51640200 0.58469200
- H 2.12530300 3.73895300 -1.01214700
- H 1.39228000 4.47320700 0.41669300
- Si 2.36721700 -1.12121000 -0.84046500
- C -3.15024000 -0.41878100 -0.87368600
- C -4.42712100 -1.06077600 -1.28417200
- H -4.67206000 -0.78293200 -2.31081500
- H -4.35424500 -2.14462200 -1.18314400
- H -5.22736600 -0.69937800 -0.62921000
- C 1.76605200 -0.06861900 -2.28079800
- H 0.74351300 -0.34331300 -2.55986900
- H 1.77799800 1.00141500 -2.05778900
- H 2.41094600 -0.23410500 -3.15060600
- C 2.48997200 -2.91980800 -1.36958500
- H 3.20424600 -3.00121200 -2.19574800
- H 2.84546700 -3.56554100 -0.56055700
- H 1.52977800 -3.30826800 -1.72392700
- C 4.03236200 -0.51517600 -0.19972500
- H 4.03470600 0.55849100 0.00984600
- H 4.32811900 -1.04520700 0.71106000
- H 4.80086300 -0.700665 -0.9577680



MePdP23T Acetanilide Si----O C=O side (ν=-143 cm^{-1})

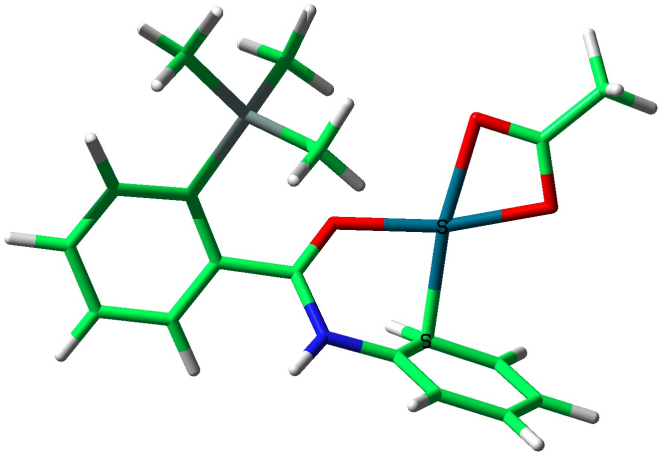
- Zero-point correction= 0.311050 (Hartree/Particle)
- Thermal correction to Energy= 0.333831
- Thermal correction to Enthalpy= 0.334775
- Thermal correction to Gibbs Free Energy= 0.258640
- Sum of electronic and zero-point Energies= -1205.014907
- Sum of electronic and thermal Energies= -1204.992126
- Sum of electronic and thermal Enthalpies= -1204.991182
- Sum of electronic and thermal Free Energies= -1205.067317
- MePdP23T

- 1 1
- H –4.72599500 –0.27567300 0.58928400
- C –3.80481700 –0.84256000 0.48672100
- C –2.64027600 –0.19367000 0.04783000
- C –3.78032400 –2.19941100 0.78416900
- C –2.59461200 –2.92443900 0.64708500
- H –4.68709600 –2.68893200 1.12222500
- N –2.75319600 1.18869400 –0.22925500
- H –3.67288400 1.58535500 –0.08184700
- C –1.82133100 2.03041300 –0.67586500
- O –0.62500100 1.69225900 –0.90786400
- Pd 0.24168300 –0.11373500 –0.67060500
- H –2.56815400 –3.98423400 0.87751600
- C –1.45104500 –0.91910800 –0.08732900
- O 2.54402100 0.10600800 –0.74829900
- C –1.43355300 –2.28336800 0.21257600
- H –0.51139200 –2.84392600 0.10976700
- O 1.46946800 –1.80666800 –0.64105000
- C –2.20081800 3.46099400 –0.91433000
- H –3.25163300 3.65644400 –0.69932600
- H –1.57507900 4.10031100 –0.28614900
- H –1.99073500 3.71044300 –1.95751600
- Si 1.69496300 0.86037500 1.24844300
- C 2.25053700 2.55537400 0.71385300
- H 3.23280900 2.52581400 0.23993000
- H 1.53022900 2.99049100 0.01579300
- H 2.29551200 3.20025000 1.59932000
- C 0.14753700 0.94920700 2.32273000
- H 0.46882000 1.39730800 3.27390400
- H –0.63327300 1.58125500 1.89716200
- H –0.26600500 –0.03951900 2.53137100
- C 2.92567500 –0.27110300 2.08062200
- H 2.60902300 –1.31665100 2.01762500
- H 3.92641900 –0.17424600 1.65570200
- H 2.96573000 –0.00679600 3.14337500
- C 2.55731700 –1.18074200 –0.85104300
- C 3.81125200 –1.89905100 –1.22106800
- H 4.63540200 –1.53635900 –0.60260300
- H 3.68856300 –2.97531000 –1.10590800
- H 4.05404700 –1.66831300 –2.26320700



MePdP32 optimized Wheland BA

- Zero-point correction= 0.365315 (Hartree/Particle)
- Thermal correction to Energy= 0.391411
- Thermal correction to Enthalpy= 0.392355
- Thermal correction to Gibbs Free Energy= 0.307983
- Sum of electronic and zero-point Energies= -1396.718280
- Sum of electronic and thermal Energies= -1396.692184
- Sum of electronic and thermal Enthalpies= -1396.691239
- Sum of electronic and thermal Free Energies= -1396.775611
-
- MePdP32
- 1 1
- H -1.28083200 1.90989200 -1.71470100
- C -1.82512300 1.90506600 -0.77418300
- C -1.12343100 2.14481500 0.44460700
- C -3.23575400 2.06555700 -0.78914500
- C -3.91485700 2.42092300 0.36414700
- H -3.76670200 1.90752000 -1.72095200
- N 0.28798900 2.05258100 0.46409400
- H 0.79909600 2.68345500 1.06915700
- C 0.98407300 1.08634900 -0.17237900
- O 0.40113300 0.09592500 -0.70357400
- Pd -1.58142500 -0.29815700 -0.42868200
- H -4.99291800 2.52970200 0.35260000
- C -1.81275500 2.52398000 1.59876600
- O -1.70399600 -2.41294400 -0.32372400
- C -3.19777500 2.66364600 1.54742000
- H -3.73039300 2.95410100 2.44667300
- O -3.42994200 -1.10059300 -0.13643200
- C -2.96291500 -2.30417000 -0.14153300
- C -3.84708500 -3.47857300 0.08700200
- H -3.42993600 -4.36190200 -0.39903000
- H -3.90575500 -3.66791600 1.16438400
- H -4.85269100 -3.27090200 -0.28261200
- C 2.44809800 1.18955300 -0.24054600
- C 3.25787600 0.03644200 -0.07462000
- C 2.99800000 2.45388000 -0.51028900
- C 4.64101300 0.23408100 -0.20560600
- C 4.37461100 2.60068900 -0.64567400
- H 2.34590800 3.30974100 -0.65375900
- C 5.19544600 1.48399300 -0.49543500
- H 5.31361200 -0.60563300 -0.07154200
- H 4.79842100 3.57312400 -0.87168600
- H 6.27149400 1.58356900 -0.59778700
- H -1.27007200 2.69906800 2.52084800
- Si 2.64527700 -1.70299100 0.44817700
- C 1.44637900 -1.53738800 1.89898800
- C 4.15440200 -2.64717800 1.07689700
- C 1.91225000 -2.66569700 -0.99382600
- H 4.67561900 -2.11025000 1.87579500
- H 3.82529400 -3.60985400 1.48363900
- H 4.87557600 -2.86058900 0.28138100
- H 0.51878700 -1.01794900 1.64864600
- H 1.17489000 -2.53752200 2.25461300
- H 1.92454400 -1.00930800 2.73099400
- H 2.60717400 -2.67950800 -1.84018600
- H 1.73718300 -3.70362300 -0.68921800
- H 0.96517900 -2.24112500 -1.32871400



Alternative scan from Agostic (**C**) to Wheland (**D**) intermediates (←)