Supporting Information

Mechanism of Arylboronic Acid-Catalyzed Amidation Reaction between Carboxylic Acids and Amines

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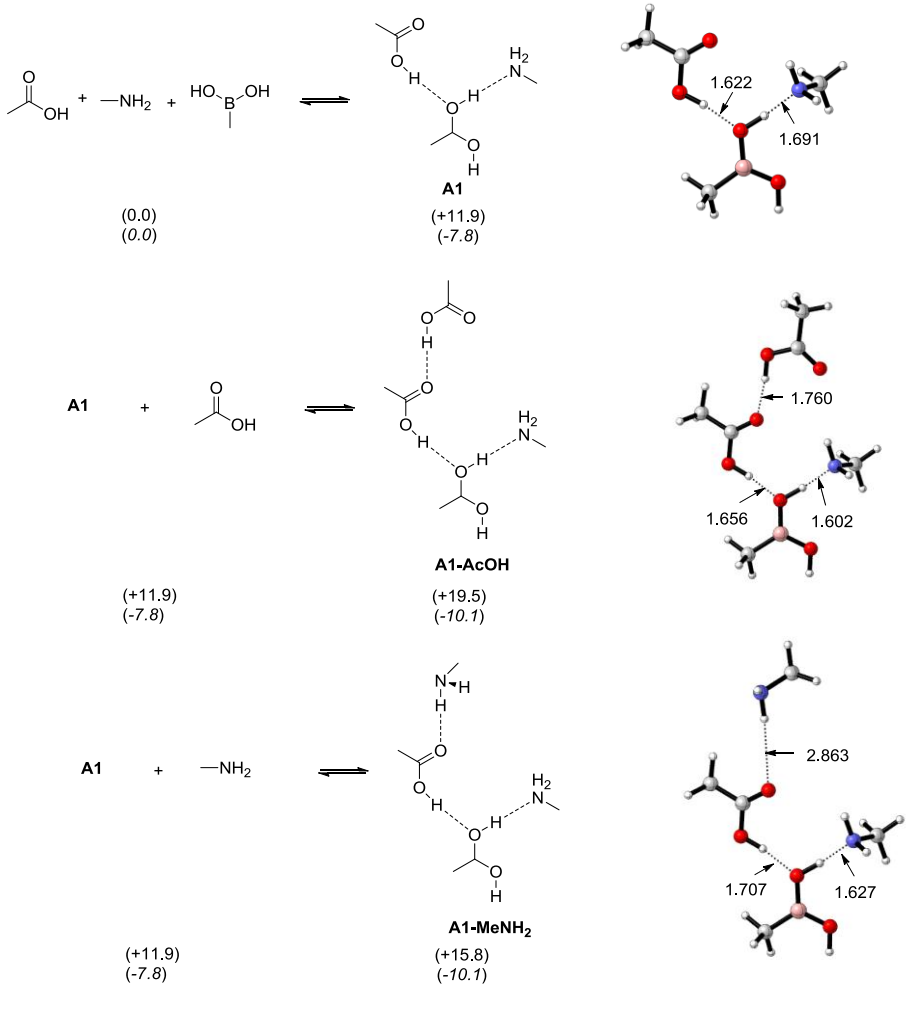
Complete Reference for Ref. 11:

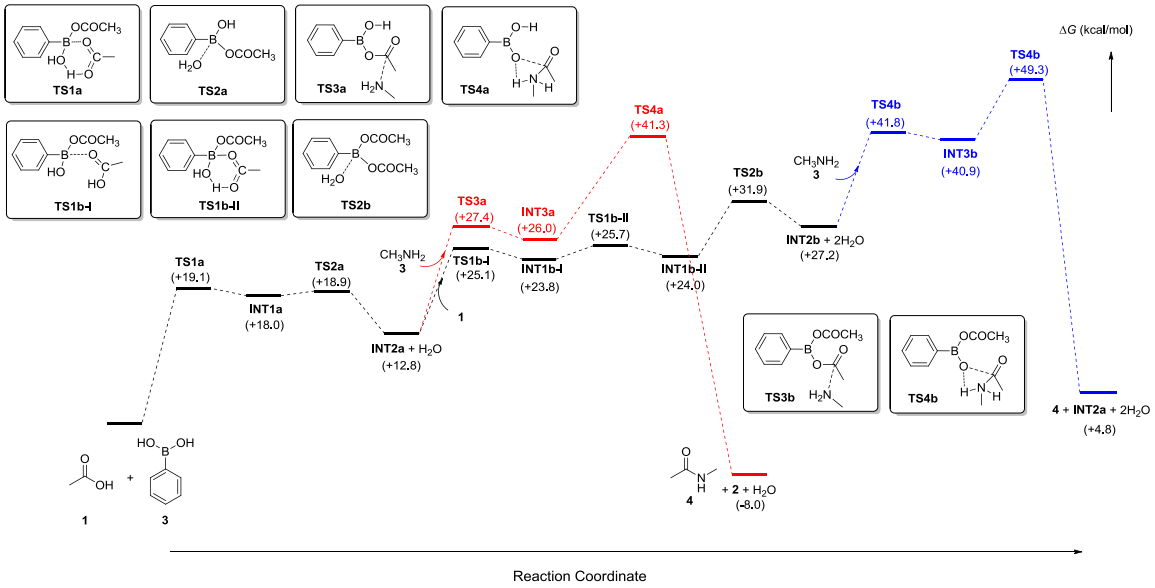
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, 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 09, revision B01; Gaussian, Inc.: Wallingford CT, 2010.

Relative Gibbs free energies (*G*) and zero-point vibrational energy corrected single-point energies (E_{ZPVE}) of the separated reactants and their complexes.



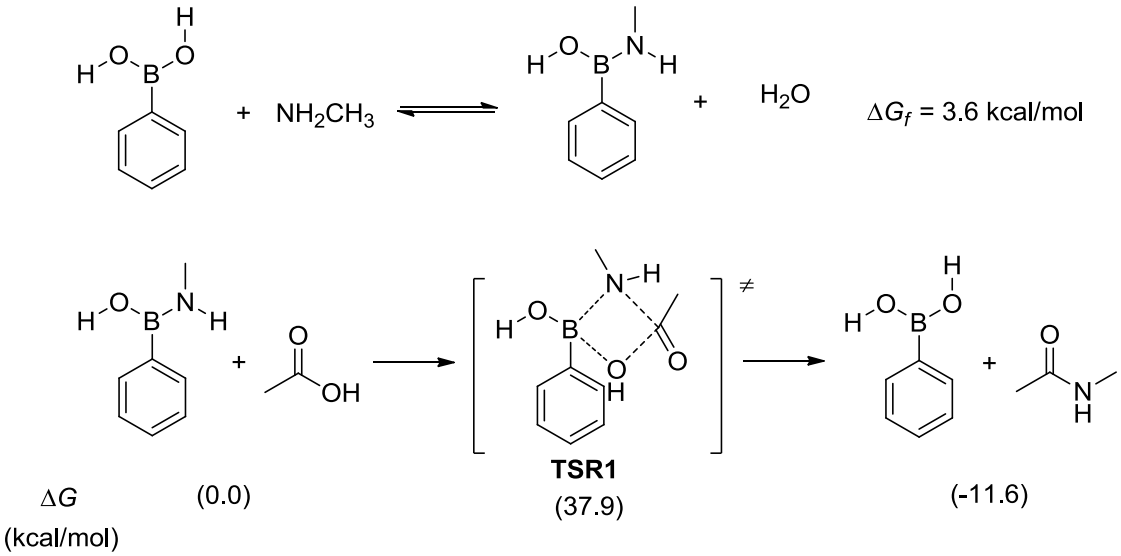
G(M06-2X) E_{ZPVE}(M06-2X) *(*kcal/mol)	(0.0) (*0.0*)	**A1**	(+11.9) (*-7.8*)
G(M06-2X) E_{ZPVE}(M06-2X) *(*kcal/mol)	**A1** + (+11.9) (*-7.8*)	**A1-AcOH**	(+19.5) (*-10.1*)
G(M06-2X) E_{ZPVE}(M06-2X) *(*kcal/mol)	**A1** + (+11.9) (*-7.8*)	**A1-MeNH$_2$**	(+15.8) (*-10.1*)

Overall free energy profile of the catalytic cycle in the case *without the removal of water*



Reaction mechanism invloving $PhB(OH)NHCH_3$

Formation of $PhB(OH)NHCH_3$ and H_2O from $PhB(OH)_2$ and $NHCH_3$ is endergonic by 3.6 kcal/mol (Scheme S1). The transition state for the boronic OH electrophilic assisted nucleophilic addition of the nitrogen to a carboxylic acid was not located. The potential energy surface scan shows that the energy increases continuously as the N1-C1 distance decreases (Figure S1). Instead a four-membered ring transition state **TSR1** is located as shown in Figure S2. The reaction of $PhB(OH)NHCH_3$ with CH_3COOH via **TSR1** has an energy barrier of 37.9 kcal/mol.



Scheme S1

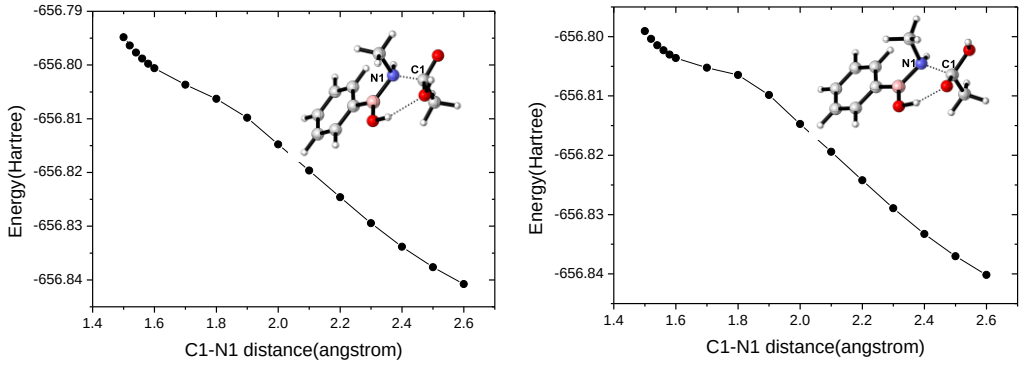


Figure S1 Potential energy surface scan along C1-N1 distance

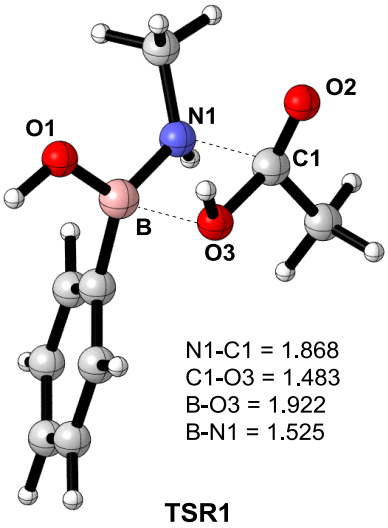
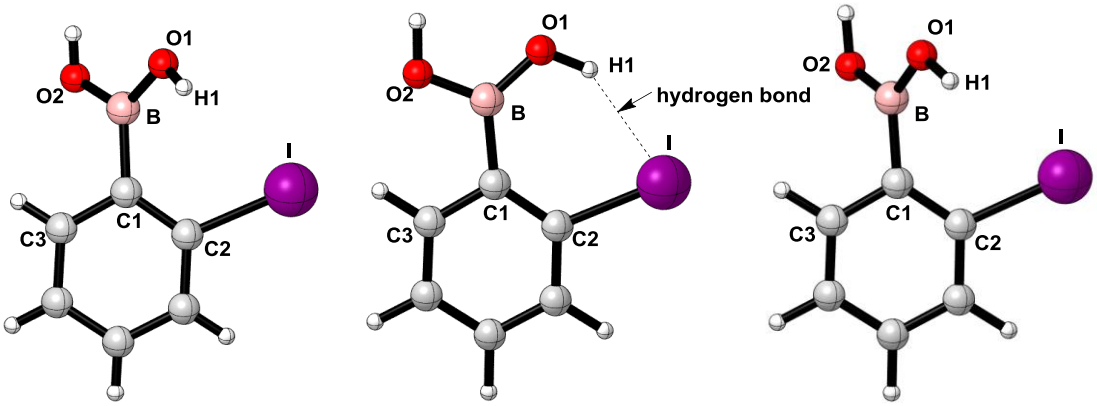


Figure S2 Optimized structure of the transition state for the reaction between PhB(OH)NHCH$_3$ and CH$_3$COOH. Bond lengths are in Å.

X-ray crystal structure and optimized geometry of *ortho*-iodophenylboronic



X-ray crystal structure	geometry optimized in the gas phase	geometry optimized in the solutionphase
B-C1 = 1.570	B-C1 = 1.586	B-C1 = 1.584
C2-I = 2.115	C2-I = 2.146	C2-I = 2.142
I-H1 = 3.029	I-H1 = 2.523	I-H1 = 3.239
∠B-C1-C2 = 126.9°	∠B-C1-C2 = 129.2°	∠B-C1-C2 = 127.5°
∠B-C1-C3 = 117.0°	∠B-C1-C3 = 115.2°	∠B-C1-C3 = 116.3°
∠C1-C2-B-O1 = -39.0°	∠C1-C2-B-O1 = 0.0°	∠C1-C2-B-O1 = -53.8°

*Bond lengths are in Å. The gas phase geometry optimization was performed using B3LYP functional with the 6-31+G(d) basis set for all the atoms except I atom, which was described by the LANL2DZ basis set with an added d-polarization shell.

Cartesian coordinates, thermal correction to Gibbs free energies (TCG), zero-point vibrational energies (ZPVE), and electronic energies (E) of reactants, intermediates and transition states.

CH_3COOH

1

C	-0.089108000	0.114941000	-0.000018000
O	-0.625832000	1.214193000	0.000004000
O	-0.793009000	-1.031465000	0.000000000
H	-1.777140000	-0.806428000	0.000031000
C	1.396219000	-0.125376000	0.000003000
H	1.677801000	-0.710547000	0.885363000
H	1.677818000	-0.710620000	-0.885302000
H	1.929587000	0.828383000	-0.000028000

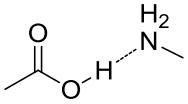
TCG = 0.031136 au
ZPVE = 0.059171 au
E = -229.0960303 au

CH_3NH_2

2

N	0.754794000	-0.000001000	-0.129192000
H	1.149866000	-0.820988000	0.350177000
H	1.149857000	0.820986000	0.350181000
C	-0.711236000	-0.000001000	0.017248000
H	-1.125315000	0.886726000	-0.481401000
H	-1.125362000	-0.886526000	-0.481726000
H	-1.065188000	-0.000183000	1.063625000

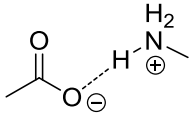
TCG = 0.039552 au
ZPVE = 0.062488 au
E= -95.85165672 au



1-2-complex

C	1.396759000	0.106182000	-0.002998000
O	1.309265000	1.336932000	-0.027804000
O	0.345468000	-0.696937000	0.032889000
H	-0.583163000	-0.154806000	0.036951000
C	2.717177000	-0.629080000	-0.007674000
H	2.808032000	-1.231545000	0.905985000
H	2.757085000	-1.319492000	-0.860255000
H	3.548353000	0.078835000	-0.065131000
N	-1.972132000	0.496943000	0.043186000
H	-2.016544000	1.159835000	-0.741575000
H	-2.059406000	1.063340000	0.896855000
C	-3.083194000	-0.474347000	-0.042683000
H	-4.071064000	0.007247000	-0.039439000
H	-2.977656000	-1.056764000	-0.964935000
H	-3.023023000	-1.161738000	0.808685000

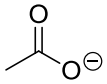
TCG = 0.089326 au
ZPVE = 0.124902 au
E= -324.9547051 au



1-2-complex-salt

C	-1.378785000	0.057671000	-0.003127000
O	-1.223987000	1.309004000	-0.021442000
O	-0.410940000	-0.784414000	0.021956000
H	1.013394000	0.000705000	0.029470000
C	-2.788249000	-0.527096000	-0.005085000
H	-2.901744000	-1.224100000	-0.845555000
H	-2.947882000	-1.102122000	0.917022000
H	-3.546899000	0.258213000	-0.076336000
N	1.969749000	0.494404000	0.034201000
H	2.015160000	1.072391000	0.891980000
H	1.981953000	1.149019000	-0.767881000
C	3.098807000	-0.476804000	-0.032782000
H	4.049046000	0.064305000	-0.027143000
H	3.036776000	-1.140102000	0.834257000
H	3.000727000	-1.058480000	-0.953379000

TCG = 0.089994 au
ZPVE = 0.126995 au
E= -324.9567034 au



1-anion

C	-0.180119000	0.000186000	-0.010769000
O	-0.765056000	1.126505000	0.001993000
O	-0.766479000	-1.125897000	0.002034000
C	1.354213000	-0.000756000	-0.004360000
H	1.701127000	0.001743000	1.039320000
H	1.753366000	-0.898892000	-0.488697000
H	1.753223000	0.895706000	-0.492062000

TCG = 0.020417 au
ZPVE = 0.048354 au
E= -228.6206587 au

2-cation

H	1.086829000	-0.964907000	0.043817000
N	0.703243000	-0.000105000	0.000011000
H	1.087189000	0.444545000	-0.857531000
H	1.087152000	0.520429000	0.813751000
C	-0.794487000	0.000071000	-0.000009000
H	-1.138510000	1.036205000	-0.049651000
H	-1.139153000	-0.560966000	-0.872350000
H	-1.139287000	-0.474997000	0.921942000

TCG = 0.053963 au
ZPVE = 0.077152 au
E= -96.30726218 au

$PhB(OH)_2$

3

C	-2.652579000	-0.019463000	0.009134000
C	-1.964705000	1.197270000	-0.060736000
C	-0.566441000	1.208107000	-0.068766000
C	0.178728000	0.013392000	-0.010842000
C	-0.538001000	-1.199463000	0.050429000
C	-1.935292000	-1.220193000	0.064494000
H	-3.742514000	-0.031955000	0.020480000
H	-2.517489000	2.135466000	-0.107256000
H	0.010426000	-2.139596000	0.092633000

H	-2.465250000	-2.171220000	0.118881000
B	1.751960000	-0.000005000	-0.003260000
O	2.538634000	1.121940000	0.117818000
O	2.392291000	-1.208893000	-0.118200000
H	3.383833000	-1.124035000	-0.095338000
H	-0.053240000	2.169901000	-0.123236000
H	2.046768000	1.979187000	0.210916000

TCG = 0.088688 au
ZPVE = 0.12135 au
E= -408.2750881 au

H_2O

O	0.000000000	0.000000000	0.120333000
H	0.000000000	0.776612000	-0.481333000
H	0.000000000	-0.776612000	-0.481333000

TCG = 0.001886 au
ZPVE = 0.01959 au
E= -76.43895079 au

TS1a

C	3.507718000	0.790258000	-0.397931000
C	2.796628000	1.218526000	0.729952000
C	1.533095000	0.684882000	1.003351000
C	0.942078000	-0.286512000	0.168891000
C	1.676490000	-0.698720000	-0.958387000
C	2.942724000	-0.170513000	-1.242730000
H	4.492757000	1.203236000	-0.615643000
H	3.226650000	1.968798000	1.394089000
H	1.252797000	-1.447043000	-1.627349000
H	3.487578000	-0.510178000	-2.124043000
B	-0.488398000	-0.911062000	0.541979000
O	-1.518718000	0.337959000	0.647331000
O	-0.606571000	-1.631760000	1.759044000
H	0.992849000	1.037329000	1.883782000
C	-2.348712000	0.680265000	-0.267732000
O	-2.540512000	-0.030587000	-1.312058000
C	-3.090639000	1.970133000	-0.105552000
H	-3.246506000	2.192168000	0.954948000
H	-2.477304000	2.775105000	-0.538151000
H	-4.043844000	1.934477000	-0.641805000
O	-1.059503000	-1.754492000	-0.589284000
H	-1.846812000	-1.013801000	-1.129527000
H	-1.539250000	-2.539320000	-0.224056000
H	0.189217000	-1.544326000	2.338424000

TCG = 0.139549 au
ZPVE = 0.180005 au
E= -637.3573313 au

INT1a

C	-3.381775000	-0.973970000	-0.183012000
C	-2.374013000	-1.633619000	0.529251000
C	-1.128717000	-1.021270000	0.710145000
C	-0.850042000	0.258043000	0.190273000
C	-1.882489000	0.902093000	-0.519676000
C	-3.131698000	0.298670000	-0.707907000
H	-4.352280000	-1.448245000	-0.329280000
H	-2.557155000	-2.625937000	0.942228000
H	-1.708385000	1.891921000	-0.942072000
H	-3.908625000	0.820670000	-1.267142000
B	0.556758000	0.970936000	0.489428000
O	1.707628000	0.029124000	0.639221000
O	0.633345000	1.884973000	1.568137000
H	-0.357353000	-1.553103000	1.268238000
C	2.211426000	-0.707842000	-0.337709000
O	1.929995000	-0.542571000	-1.530143000
C	3.175026000	-1.763273000	0.139415000
H	3.933765000	-1.312372000	0.791547000
H	2.631070000	-2.508302000	0.736299000
H	3.653481000	-2.255439000	-0.711316000
O	0.908465000	1.873736000	-0.857241000
H	1.233079000	1.264478000	-1.580954000
H	1.640290000	2.521505000	-0.659243000
H	-0.253446000	2.235069000	1.830087000

TCG = 0.142867 au
ZPVE = 0.183577 au
E= -637.3624935 au

TS2a

C	3.794490000	0.662483000	-0.001645000
C	2.784488000	1.590466000	0.274526000
C	1.441036000	1.202081000	0.211504000
C	1.071401000	-0.113891000	-0.125763000
C	2.106178000	-1.029535000	-0.401052000
C	3.451158000	-0.651867000	-0.340566000
H	4.841843000	0.961440000	0.043363000
H	3.042853000	2.617323000	0.534095000
H	1.852663000	-2.054670000	-0.669704000
H	4.231780000	-1.380675000	-0.559984000
B	-0.442463000	-0.574867000	-0.206320000
O	-1.390062000	0.534725000	-0.218649000
O	-0.718552000	-1.723342000	-0.925237000
H	-1.684232000	-1.927547000	-1.010772000
H	0.666773000	1.940151000	0.420092000
C	-2.717296000	0.418735000	-0.135079000
O	-3.285641000	-0.640282000	0.121507000
C	-3.435445000	1.720662000	-0.375023000
H	-3.064055000	2.486725000	0.318168000
H	-3.223738000	2.072731000	-1.393905000
H	-4.512860000	1.589748000	-0.245442000
H	-1.660431000	-1.408845000	1.790277000
H	-0.462284000	-0.522540000	2.300666000
O	-0.704753000	-1.207891000	1.630295000

TCG = 0.14035 au
ZPVE = 0.181926 au
E= -637.3585451 au

INT2a

C	-3.688855000	-0.611441000	-0.033214000
C	-2.664944000	-1.565664000	-0.035744000
C	-1.329303000	-1.155011000	-0.010399000
C	-0.986145000	0.212300000	0.018053000
C	-2.033985000	1.156043000	0.019976000
C	-3.371256000	0.752109000	-0.005470000
H	-4.731447000	-0.929323000	-0.053349000
H	-2.908115000	-2.627941000	-0.057687000
H	-1.796058000	2.219100000	0.041118000
H	-4.166376000	1.497581000	-0.004015000
B	0.503807000	0.680897000	0.042416000
O	1.471128000	-0.353155000	0.036637000
O	0.806347000	2.001928000	0.081629000
H	1.779494000	2.211285000	0.075045000
H	-0.540644000	-1.906179000	-0.012847000
C	2.818695000	-0.234308000	-0.035181000
O	3.386731000	0.835099000	-0.185510000
C	3.510280000	-1.562154000	0.081943000
H	3.247069000	-2.031219000	1.039667000
H	3.163433000	-2.231042000	-0.717138000
H	4.593034000	-1.428960000	0.015299000

TCG = 0.121875 au
ZPVE =0.160041 au
E= -560.9156786 au

TS1b-I

C	-4.019907000	-0.693000000	-0.296520000
C	-3.566856000	0.075534000	0.781551000
C	-2.195329000	0.181821000	1.037418000
C	-1.243346000	-0.467086000	0.227461000
C	-1.723784000	-1.237567000	-0.849143000
C	-3.092737000	-1.352072000	-1.112109000
H	-5.087654000	-0.780572000	-0.497868000
H	-4.281858000	0.588651000	1.425020000
H	-1.015436000	-1.759184000	-1.492328000
H	-3.436779000	-1.957375000	-1.951049000
B	0.310081000	-0.328512000	0.517045000
O	0.791956000	1.016829000	-0.722755000
O	1.099435000	-1.408644000	-0.035212000
H	-1.861668000	0.776787000	1.887464000
C	0.829478000	2.234674000	-0.469961000
O	0.656293000	2.725817000	0.744432000
C	1.055360000	3.261932000	-1.533947000
H	1.824969000	3.974594000	-1.213333000
H	1.346044000	2.777605000	-2.469579000
H	0.122110000	3.823091000	-1.687115000
O	0.671746000	0.227106000	1.756503000
H	0.543352000	1.973785000	1.399560000
C	2.431200000	-1.512537000	0.048783000
O	3.143385000	-0.655946000	0.562066000
C	2.951541000	-2.792837000	-0.548321000
H	2.511526000	-3.649028000	-0.019150000
H	2.645527000	-2.865722000	-1.600146000
H	4.041290000	-2.830232000	-0.472280000
H	1.641935000	0.135694000	1.954032000

TCG = 0.176049 au
ZPVE = 0.221695 au
E= -790.0122144 au

INT1b-I

C	-4.028321000	-0.660840000	-0.299211000
C	-3.571110000	-0.144157000	0.917474000
C	-2.196209000	-0.015552000	1.151921000
C	-1.246442000	-0.393470000	0.185123000
C	-1.731772000	-0.915002000	-1.030473000
C	-3.102034000	-1.048525000	-1.275304000
H	-5.097435000	-0.763951000	-0.485484000
H	-4.284241000	0.155496000	1.685866000
H	-1.024739000	-1.225063000	-1.800629000
H	-3.448563000	-1.456901000	-2.225008000
B	0.323503000	-0.234907000	0.444727000
O	0.813996000	0.959835000	-0.653646000
O	1.068897000	-1.399415000	-0.059041000
H	-1.856752000	0.380220000	2.108730000
C	0.873379000	2.189088000	-0.405149000
O	0.683423000	2.686378000	0.790409000
C	1.141611000	3.178556000	-1.488839000
H	1.847780000	3.940571000	-1.139295000
H	1.523561000	2.671589000	-2.378729000
H	0.195967000	3.683313000	-1.738205000
O	0.663211000	0.234055000	1.752073000
H	0.556644000	1.931102000	1.454635000
C	2.391111000	-1.536426000	0.033576000
O	3.125121000	-0.693659000	0.546024000
C	2.888417000	-2.833718000	-0.550656000
H	2.401022000	-3.677674000	-0.044589000
H	2.618219000	-2.889631000	-1.613512000
H	3.973170000	-2.909322000	-0.438778000
H	1.628886000	0.117510000	1.954042000

TCG = 0.176278 au
ZPVE = 0.222169 au
E= -790.0144127 au

TS1b-II

C	-4.057101000	-0.614799000	-0.217397000
C	-3.537657000	-0.210207000	1.016023000
C	-2.153834000	-0.066681000	1.181942000
C	-1.258394000	-0.318997000	0.127189000
C	-1.805567000	-0.726801000	-1.106081000
C	-3.184551000	-0.874452000	-1.281809000
H	-5.133060000	-0.729200000	-0.349655000
H	-4.208493000	-0.008616000	1.851475000
H	-1.140928000	-0.935371000	-1.945649000
H	-3.579740000	-1.193254000	-2.246621000
B	0.325003000	-0.159644000	0.287524000
O	0.826114000	0.951169000	-0.698629000
O	1.023018000	-1.386216000	-0.121088000
H	-1.767562000	0.243041000	2.152386000
C	0.950868000	2.187507000	-0.348682000
O	0.847361000	2.554427000	0.864622000
C	1.198955000	3.192397000	-1.425723000
H	1.652968000	4.096060000	-1.009100000
H	1.831214000	2.761768000	-2.209667000
H	0.230895000	3.457158000	-1.877674000
O	0.702312000	0.308252000	1.673286000
H	0.747737000	1.499833000	1.494484000
C	2.328970000	-1.606554000	0.037249000
O	3.066612000	-0.859107000	0.678484000
C	2.798585000	-2.867816000	-0.636730000
H	2.196962000	-3.719568000	-0.293808000
H	2.651676000	-2.779125000	-1.721785000
H	3.855480000	-3.043177000	-0.419854000
H	1.632850000	0.038879000	1.888563000

TCG = 0.173745 au
ZPVE = 0.219563 au
E= -790.0089174 au

INT1b-II

C	-4.028473000	-0.669463000	-0.275217000
C	-3.365420000	0.314396000	-1.015710000
C	-1.984141000	0.489322000	-0.869013000
C	-1.232065000	-0.305800000	0.013984000
C	-1.921102000	-1.292874000	0.745964000
C	-3.300833000	-1.475454000	0.608322000
H	-5.104018000	-0.808182000	-0.385381000
H	-3.922852000	0.946652000	-1.707041000
H	-1.371023000	-1.932155000	1.437528000
H	-3.808438000	-2.245955000	1.189027000
B	0.350819000	-0.148530000	0.155739000
O	0.924700000	1.075438000	-0.449519000
O	1.067303000	-1.294435000	-0.438563000
H	-1.486329000	1.260068000	-1.457732000
C	0.813307000	2.291042000	0.075689000
O	0.337968000	2.499779000	1.193624000
C	1.341993000	3.379593000	-0.819929000
H	1.244325000	4.352392000	-0.331170000
H	2.396591000	3.184134000	-1.055543000
H	0.788813000	3.381209000	-1.768411000
O	0.720420000	-0.168649000	1.702098000
H	0.437913000	0.695131000	2.120379000
C	2.357395000	-1.547749000	-0.231019000
O	3.013559000	-1.005259000	0.662717000
C	2.929700000	-2.562670000	-1.181143000
H	2.290084000	-3.453751000	-1.209487000
H	2.943659000	-2.136887000	-2.194361000
H	3.945726000	-2.833896000	-0.883031000
H	1.717695000	-0.243163000	1.792104000

TCG = 0.17632 au
ZPVE = 0.222473 au
E= -790.0142408 au

TS2b

C	4.338125000	0.028328000	-0.252722000
C	3.639377000	1.235464000	-0.133334000
C	2.243234000	1.230532000	-0.088190000
C	1.516318000	0.024426000	-0.160277000

C	2.240303000	-1.179760000	-0.282138000
C	3.636208000	-1.181026000	-0.326904000
H	5.427614000	0.029893000	-0.289675000
H	4.183308000	2.178164000	-0.076789000
H	1.702845000	-2.125278000	-0.345338000
H	4.178088000	-2.121830000	-0.422046000
B	-0.036344000	0.028094000	-0.134563000
O	-0.701099000	-1.172178000	-0.374278000
O	-0.705761000	1.238664000	0.016945000
H	1.707933000	2.174705000	0.005676000
C	-1.977603000	-1.522852000	-0.057182000
O	-2.596980000	-0.981311000	0.838806000
C	-2.475780000	-2.658666000	-0.900375000
H	-2.511611000	-2.339714000	-1.951382000
H	-1.778232000	-3.504156000	-0.836938000
H	-3.471492000	-2.964636000	-0.569560000
O	-0.281738000	-0.337778000	2.746134000
H	0.197903000	-1.106225000	3.125557000
H	-1.208560000	-0.644747000	2.644728000
C	-1.884031000	1.628972000	-0.540645000
O	-2.323775000	1.111970000	-1.549948000
C	-2.510542000	2.770869000	0.203379000
H	-2.744674000	2.450804000	1.228006000
H	-1.798512000	3.603650000	0.274430000
H	-3.421720000	3.096245000	-0.304801000

TCG = 0.170144 au
ZPVE = 0.218914 au
E= -789.9953331 au

INT2b

C	4.311907000	-0.000006000	-0.000006000
C	3.612009000	1.212249000	0.032720000
C	2.215690000	1.209795000	0.032461000
C	1.490106000	0.000002000	0.000010000
C	2.215683000	-1.209794000	-0.032453000
C	3.612002000	-1.212257000	-0.032725000
H	5.402027000	-0.000009000	-0.000012000
H	4.155798000	2.156306000	0.058366000
H	1.678766000	-2.157314000	-0.059337000
H	4.155785000	-2.156317000	-0.058376000
B	-0.060387000	0.000005000	0.000024000
O	-0.727568000	1.212542000	0.125603000
O	-0.727581000	-1.212520000	-0.125628000
H	1.678779000	2.157317000	0.059352000
C	-1.964210000	1.552248000	-0.344629000
O	-2.470617000	0.979521000	-1.288530000
C	-2.553407000	2.709346000	0.404368000
H	-2.707338000	2.419210000	1.453106000
H	-1.852964000	3.554729000	0.396114000
H	-3.505325000	3.002672000	-0.045282000
C	-1.964211000	-1.552244000	0.344622000
O	-2.470600000	-0.979543000	1.288549000
C	-2.553407000	-2.709344000	-0.404374000
H	-3.505280000	-3.002730000	0.045331000
H	-2.707429000	-2.419168000	-1.453087000
H	-1.852925000	-3.554695000	-0.396208000

TCG = 0.152197 au
ZPVE = 0.19729 au
E= -713.5508782 au

TS3a

C	-4.251527000	0.550070000	0.280518000
C	-3.252384000	1.530340000	0.299850000
C	-1.917241000	1.170684000	0.090661000
C	-1.546889000	-0.168911000	-0.140361000
C	-2.570451000	-1.138267000	-0.155107000
C	-3.907659000	-0.787647000	0.051915000
H	-5.293498000	0.827257000	0.441314000
H	-3.515246000	2.573515000	0.475676000
H	-2.312840000	-2.181616000	-0.334140000
H	-4.681565000	-1.555189000	0.033800000
B	-0.051873000	-0.590317000	-0.385937000
O	0.903864000	0.417744000	-0.378906000
O	0.232505000	-1.907960000	-0.597480000
H	1.199776000	-2.041995000	-0.777670000
H	-1.148568000	1.942591000	0.103635000
C	2.289639000	0.246168000	-0.627222000
O	2.719668000	-0.880691000	-0.970038000
C	2.850120000	1.516671000	-1.242511000
H	2.512387000	2.414282000	-0.714019000
H	3.944390000	1.476312000	-1.248958000
H	2.498124000	1.572327000	-2.282077000
N	2.891287000	0.537879000	1.207387000
H	3.907003000	0.721105000	1.142970000
H	2.441339000	1.391507000	1.578241000
C	2.630129000	-0.622508000	2.072280000
H	3.041529000	-1.518594000	1.592014000
H	3.089388000	-0.501508000	3.063592000
H	1.547422000	-0.745902000	2.194852000

TCG = 0.183068 au
ZPVE = 0.22547 au
E= -656.7627053 au

INT3a

C	-4.239439000	-0.686910000	0.070949000
C	-3.193169000	-1.535361000	0.451862000
C	-1.873122000	-1.075420000	0.414359000
C	-1.562746000	0.234748000	-0.001201000
C	-2.633033000	1.070217000	-0.379111000
C	-3.956358000	0.619200000	-0.345641000
H	-5.269843000	-1.041769000	0.099034000
H	-3.407306000	-2.553174000	0.778505000
H	-2.424022000	2.088840000	-0.704487000
H	-4.766927000	1.284630000	-0.643286000
B	-0.077884000	0.761558000	-0.045644000
O	0.921456000	-0.136045000	0.278912000
O	0.153138000	2.065849000	-0.388110000
H	1.141400000	2.226917000	-0.441716000
H	-1.067855000	-1.744453000	0.715498000
C	2.339238000	0.202397000	0.376145000
O	2.744063000	1.212148000	-0.320532000
C	2.713931000	0.181607000	1.864162000
H	2.374532000	-0.730057000	2.369474000
H	3.799827000	0.281041000	1.976553000
H	2.238220000	1.044294000	2.343708000
N	2.972666000	-1.173255000	-0.232284000
H	4.000231000	-1.116967000	-0.068420000
H	2.619609000	-1.986590000	0.314086000
C	2.711744000	-1.378429000	-1.680887000
H	3.051481000	-0.491930000	-2.221279000
H	3.260709000	-2.262321000	-2.020252000
H	1.639161000	-1.521385000	-1.829190000

TCG = 0.186569 au
ZPVE = 0.227769 au
E= -656.7684143 au

TS4a

C	-4.543338000	-0.607304000	0.045403000
C	-3.537760000	-1.511024000	0.409835000
C	-2.196830000	-1.112458000	0.379140000
C	-1.813963000	0.186732000	-0.009669000
C	-2.847232000	1.075423000	-0.370984000
C	-4.193165000	0.690096000	-0.346598000
H	-5.590091000	-0.911422000	0.067360000
H	-3.800284000	-2.523813000	0.717711000
H	-2.591836000	2.089353000	-0.677002000
H	-4.969389000	1.401055000	-0.631910000
B	-0.267240000	0.606194000	-0.027547000
O	0.716048000	-0.229945000	0.274449000
O	-0.053345000	1.958693000	-0.391307000

H	0.913912000	2.161449000	-0.400795000
H	-1.421968000	-1.823456000	0.665629000
C	3.023166000	0.243834000	0.384172000
O	3.290807000	1.158654000	-0.358673000
C	3.008293000	0.279602000	1.882408000
H	2.431972000	-0.545178000	2.308913000
H	4.052005000	0.212592000	2.230441000
H	2.591960000	1.235231000	2.214060000
N	3.053337000	-1.172590000	-0.181188000
H	3.789033000	-1.726719000	0.322660000
H	2.113589000	-1.565598000	0.075975000
C	3.254582000	-1.258077000	-1.655496000
H	4.211051000	-0.799562000	-1.915207000
H	3.247817000	-2.316510000	-1.930358000
H	2.434473000	-0.730425000	-2.146446000

TCG = 0.182329 au
ZPVE = 0.225004 au
E= -656.7398276 au

TS3b

C	-4.537911000	-0.449419000	0.084029000
C	-4.049048000	0.807999000	-0.288416000
C	-2.671333000	1.043155000	-0.304961000
C	-1.752564000	0.033271000	0.046674000
C	-2.268681000	-1.225345000	0.418744000
C	-3.644255000	-1.467549000	0.438873000
H	-5.611890000	-0.635710000	0.099041000
H	-4.741289000	1.603589000	-0.563738000
H	-1.581420000	-2.022359000	0.699573000
H	-4.021737000	-2.447408000	0.731132000
B	-0.212262000	0.306124000	0.038591000
O	0.212693000	1.550700000	-0.456653000
O	0.631506000	-0.673255000	0.463886000
H	-2.301116000	2.025852000	-0.594865000
C	1.164203000	2.364053000	0.056811000
O	1.450886000	2.356877000	1.241418000
C	1.745838000	3.290632000	-0.971867000
H	2.288173000	2.697869000	-1.720664000
H	0.941330000	3.826280000	-1.492242000
H	2.426549000	4.002275000	-0.497667000
C	2.067166000	-0.739719000	0.333130000
O	2.617111000	-0.087451000	-0.565465000
C	2.688285000	-0.938869000	1.702368000
H	3.739638000	-1.225518000	1.592254000
H	2.642183000	0.019315000	2.236783000
H	2.155777000	-1.693323000	2.290358000
N	2.073598000	-2.617317000	-0.257917000
H	3.051820000	-2.935543000	-0.156132000
H	1.489732000	-3.185365000	0.377512000
C	1.629214000	-2.740980000	-1.653651000
H	1.778996000	-3.758500000	-2.041717000
H	0.564971000	-2.485677000	-1.716412000
H	2.201343000	-2.033519000	-2.26663900

TCG = 0.213576 au
ZPVE = 0.262499 au
E= -809.3980366 au

INT3b

C	-4.561822000	-0.415091000	0.071994000
C	-4.049817000	0.842867000	-0.265418000
C	-2.667487000	1.051912000	-0.281398000
C	-1.766287000	0.015633000	0.036073000
C	-2.306162000	-1.242657000	0.373560000
C	-3.686097000	-1.459702000	0.392919000
H	-5.639093000	-0.581440000	0.085875000
H	-4.727557000	1.659387000	-0.514431000
H	-1.633456000	-2.060881000	0.627281000
H	-4.080796000	-2.440677000	0.657662000
B	-0.216225000	0.256035000	0.023428000
O	0.224109000	1.504373000	-0.457730000
O	0.604364000	-0.750508000	0.405841000
H	-2.279909000	2.035441000	-0.544609000
C	1.167596000	2.313721000	0.070377000
O	1.414020000	2.328275000	1.264885000
C	1.793613000	3.216198000	-0.954397000
H	2.358708000	2.604017000	-1.669386000
H	1.012733000	3.746848000	-1.514403000
H	2.461618000	3.932916000	-0.469782000
C	2.086652000	-0.856192000	0.281770000
O	2.644295000	-0.108357000	-0.583273000
C	2.644938000	-0.886716000	1.707257000
H	3.712731000	-1.132382000	1.675613000
H	2.530992000	0.112994000	2.136649000
H	2.122556000	-1.607642000	2.346438000
N	2.138285000	-2.434974000	-0.214059000
H	3.137663000	-2.720733000	-0.147930000
H	1.605748000	-3.026507000	0.456206000
C	1.650212000	-2.653195000	-1.598616000
H	1.833218000	-3.693512000	-1.885771000
H	0.580140000	-2.436868000	-1.635776000
H	2.191506000	-1.977265000	-2.264872000

TCG = 0.216952 au
ZPVE = 0.264801 au
E= -809.4029056 au

TS4b

C	-4.630994000	-0.829500000	0.021624000
C	-4.164702000	0.420160000	-0.401103000
C	-2.789395000	0.676574000	-0.438211000
C	-1.846625000	-0.298469000	-0.056270000
C	-2.343364000	-1.548637000	0.366182000
C	-3.714608000	-1.816448000	0.406608000
H	-5.701447000	-1.033612000	0.052329000
H	-4.871931000	1.193970000	-0.700624000
H	-1.637639000	-2.321104000	0.670688000
H	-4.071430000	-2.791699000	0.738825000
B	-0.284324000	-0.028747000	-0.078186000
O	0.091957000	1.282819000	-0.624631000
O	0.623860000	-0.909817000	0.261532000
H	-2.442069000	1.654700000	-0.769582000
C	0.493344000	2.311806000	0.109444000
O	0.473942000	2.311790000	1.339036000
C	0.962318000	3.483907000	-0.717994000
H	1.866135000	3.197099000	-1.272342000
H	0.196736000	3.758375000	-1.454672000
H	1.184507000	4.338835000	-0.073857000
C	2.665618000	-0.584737000	0.369599000
O	3.013010000	0.344864000	-0.332902000
C	2.716937000	-0.611177000	1.874364000
H	3.774738000	-0.643552000	2.177912000
H	2.270268000	0.310339000	2.257761000
H	2.192702000	-1.473972000	2.293908000
N	2.832764000	-2.003246000	-0.232722000
H	3.739946000	-2.392321000	0.122593000
H	2.068870000	-2.598627000	0.156282000
C	2.814076000	-2.050129000	-1.721680000
H	2.943420000	-3.091821000	-2.029071000
H	1.852558000	-1.663832000	-2.064749000
H	3.629125000	-1.433679000	-2.105074000

TCG = 0.214681 au
ZPVE = 0.263343 au
E= -809.3871582 au

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C	-0.479409000	0.148446000	-0.000065000
O	-0.393260000	1.393137000	0.000010000
C	-1.828248000	-0.542865000	0.000017000
H	-2.392735000	-0.223951000	-0.885395000
H	-1.749683000	-1.635802000	-0.000063000
H	-2.392553000	-0.224113000	0.885607000

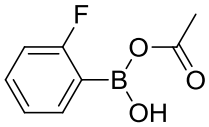
N	0.611693000	-0.642665000	-0.000013000
H	0.488663000	-1.674190000	-0.000038000
C	1.966978000	-0.102453000	0.000017000
H	2.141223000	0.516817000	0.890891000
H	2.671951000	-0.940390000	0.000289000
H	2.141441000	0.516421000	-0.891095000

TCG = 0.070031 au
ZPVE = 0.099861 au
E= -248.5226999 au

Acetic anhydride

C	-1.216239000	0.088428000	0.133778000
O	-1.302825000	1.205781000	0.582121000
O	-0.000016000	-0.576276000	-0.000102000
C	1.216265000	0.088424000	-0.133803000
O	1.302903000	1.205788000	-0.582087000
C	-2.344669000	-0.799388000	-0.296697000
H	-2.261838000	-0.991981000	-1.375688000
H	-2.280537000	-1.767115000	0.217413000
H	-3.300135000	-0.316000000	-0.076706000
C	2.344606000	-0.799441000	0.296780000
H	2.261343000	-0.992588000	1.375632000
H	2.280779000	-1.766927000	-0.217842000
H	3.300112000	-0.315868000	0.077377000

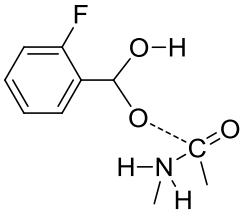
TCG = 0.063889 au
ZPVE = 0.097239 au
E= -381.724333361 au



F-INT2a

C	3.709124000	-0.249293000	0.000125000
C	2.775798000	-1.288729000	0.000044000
C	1.423795000	-0.965532000	-0.000050000
C	0.927289000	0.343871000	-0.000068000
C	1.908516000	1.362504000	0.000016000
C	3.274507000	1.081575000	0.000111000
H	4.773629000	-0.482199000	0.000199000
H	3.081463000	-2.336522000	0.000052000
H	1.575594000	2.398763000	0.000006000
H	3.998525000	1.895313000	0.000174000
B	-0.583625000	0.761633000	-0.000171000
O	-1.561916000	-0.252655000	-0.000139000
O	-0.874694000	2.083462000	-0.000106000
H	-1.842748000	2.305150000	-0.000234000
C	-2.908267000	-0.078256000	-0.000043000
O	-3.437340000	1.021895000	0.000201000
C	-3.643151000	-1.386559000	0.000137000
H	-3.354253000	-1.970435000	-0.884301000
H	-3.353850000	-1.970437000	0.884441000
H	-4.722208000	-1.213573000	0.000382000
F	0.549767000	-2.019258000	-0.000127000

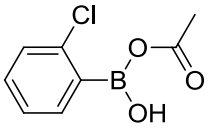
TCG = 0.111545 au
ZPVE = 0.151624 au
E= -660.162593 au



F-TS4a

C	4.512041000	0.258004000	0.011721000
C	3.580548000	1.279493000	0.214893000
C	2.225961000	0.965761000	0.147973000
C	1.708898000	-0.307811000	-0.108931000
C	2.692180000	-1.304574000	-0.305709000
C	4.063820000	-1.041555000	-0.250212000
H	5.577875000	0.480062000	0.058453000
H	3.889334000	2.305690000	0.422363000
H	2.355234000	-2.318764000	-0.509965000
H	4.780720000	-1.846486000	-0.410399000
B	0.141687000	-0.670759000	-0.190463000
O	-0.850176000	0.194407000	-0.083918000
O	-0.058505000	-2.058470000	-0.398407000
H	-1.023907000	-2.252000000	-0.484200000
C	-3.090840000	-0.399625000	0.383852000
O	-3.459138000	-1.229604000	-0.413415000
C	-2.811599000	-0.618920000	1.840394000
H	-2.208040000	0.184178000	2.270915000
H	-3.780509000	-0.665391000	2.363858000
H	-2.302037000	-1.578219000	1.968892000
N	-3.258451000	1.070621000	0.018795000
H	-3.923937000	1.516333000	0.698219000
H	-2.308425000	1.489154000	0.176527000
C	-3.698949000	1.326780000	-1.382209000
H	-4.670667000	0.855975000	-1.545306000
H	-3.768744000	2.410094000	-1.514174000
H	-2.953089000	0.906127000	-2.059467000
F	1.365235000	2.019634000	0.360035000

TCG = 0.171138 au
ZPVE = 0.216416 au
E= -755.9894779 au

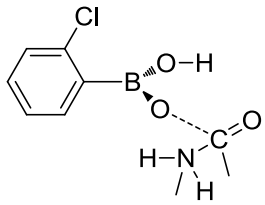


Cl-INT2a

C	3.665128000	-0.104284000	0.376019000
C	2.820151000	0.968376000	0.079932000
C	1.458729000	0.730756000	-0.116827000
C	0.890013000	-0.552935000	-0.034045000
C	1.784086000	-1.611035000	0.244220000
C	3.147312000	-1.400030000	0.454987000
H	4.727529000	0.078866000	0.535287000
H	3.215344000	1.981816000	-0.004322000
H	1.386533000	-2.623410000	0.302338000
H	3.802027000	-2.241980000	0.676772000
B	-0.630390000	-0.922742000	-0.195186000
O	-1.577358000	-0.014092000	0.311698000
O	-0.941703000	-2.124696000	-0.733739000
H	-1.918550000	-2.314324000	-0.802268000
C	-2.929929000	-0.072787000	0.201038000
O	-3.506631000	-0.916347000	-0.464412000
C	-3.603309000	1.020255000	0.978206000
H	-3.323891000	0.944545000	2.037806000
H	-3.253531000	1.996847000	0.617123000
H	-4.688223000	0.945921000	0.869321000
Cl	0.471598000	2.142153000	-0.545040000

TCG = 0.109524 au

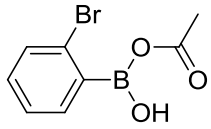
ZPVE = 0.150031 au
E= -1020.517456 au



Cl-TS4a

C	4.271089000	-0.943240000	-0.440327000
C	3.745031000	0.350887000	-0.490292000
C	2.404575000	0.542634000	-0.148243000
C	1.542290000	-0.485913000	0.247100000
C	2.117059000	-1.774015000	0.286581000
C	3.453480000	-2.009316000	-0.050384000
H	5.315121000	-1.111003000	-0.703480000
H	4.367011000	1.196716000	-0.787342000
H	1.494026000	-2.615913000	0.592267000
H	3.857246000	-3.020679000	-0.005761000
B	-0.014934000	-0.276307000	0.606305000
O	-0.966254000	-0.303957000	-0.306868000
O	-0.229680000	-0.107916000	1.991380000
H	-1.196228000	-0.021920000	2.189702000
C	-3.215263000	0.415915000	0.106485000
O	-3.566891000	0.005367000	1.186010000
C	-2.886568000	1.831750000	-0.255803000
H	-2.286482000	1.895596000	-1.167017000
H	-3.837193000	2.368630000	-0.408052000
H	-2.351638000	2.299802000	0.575649000
N	-3.429816000	-0.482725000	-1.105975000
H	-4.092141000	-0.006413000	-1.768293000
H	-2.489154000	-0.526203000	-1.571308000
C	-3.907429000	-1.859958000	-0.794038000
H	-4.868848000	-1.798524000	-0.279957000
H	-4.010727000	-2.396720000	-1.741201000
H	-3.165295000	-2.346004000	-0.157726000
Cl	1.782630000	2.216638000	-0.222814000

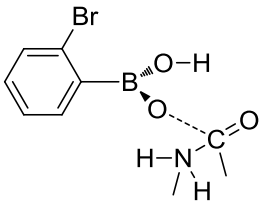
TCG = 0.168295 au
ZPVE = 0.214718 au
E= -1116.344908 au



Br-INT2a

C	-3.581488000	0.619700000	0.493208000
C	-2.776118000	-0.500198000	0.266374000
C	-1.415917000	-0.329004000	0.008490000
C	-0.818975000	0.941394000	-0.024230000
C	-1.663878000	2.052173000	0.184556000
C	-3.026527000	1.901167000	0.446256000
H	-4.643081000	0.482086000	0.697090000
H	-3.211679000	-1.500395000	0.283969000
H	-1.232783000	3.052105000	0.144921000
H	-3.651478000	2.778044000	0.611991000
B	0.709425000	1.222710000	-0.264207000
O	1.619094000	0.432523000	0.461903000
O	1.063628000	2.245750000	-1.072908000
H	2.045097000	2.387184000	-1.178666000
C	2.963449000	0.353051000	0.287636000
O	3.551328000	0.940389000	-0.604742000
C	3.606389000	-0.542585000	1.305369000
H	3.390110000	-0.166922000	2.314715000
H	3.172327000	-1.548962000	1.232276000
H	4.686247000	-0.585570000	1.142957000
Br	-0.391311000	-1.912417000	-0.343091000

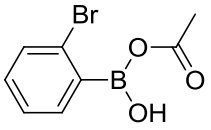
TCG = 0.109001 au
ZPVE = 0.150155 au
E= -3134.483904 au



Br-TS4a

C	4.031842000	-1.257391000	-0.577997000
C	3.455585000	0.014510000	-0.517997000
C	2.126490000	0.145685000	-0.109457000
C	1.327670000	-0.947626000	0.244938000
C	1.950075000	-2.213834000	0.191696000
C	3.275995000	-2.377075000	-0.217679000
H	5.067631000	-1.363732000	-0.899307000
H	4.042222000	0.894685000	-0.785640000
H	1.370564000	-3.091880000	0.478595000
H	3.718897000	-3.372388000	-0.253151000
B	-0.228428000	-0.857773000	0.651268000
O	-1.163534000	-0.445234000	-0.182803000
O	-0.475005000	-1.328557000	1.959414000
H	-1.447206000	-1.323702000	2.150998000
C	-3.375137000	0.151748000	0.300542000
O	-3.895305000	-0.710799000	0.967852000
C	-2.971347000	1.520634000	0.759352000
H	-2.256801000	1.989394000	0.078596000
H	-3.882454000	2.138656000	0.813820000
H	-2.538480000	1.451054000	1.761458000
N	-3.444577000	0.022468000	-1.219641000
H	-3.976415000	0.839998000	-1.608497000
H	-2.444583000	0.109899000	-1.528902000
C	-4.021308000	-1.258839000	-1.715695000
H	-5.047132000	-1.355791000	-1.353887000
H	-3.999367000	-1.231388000	-2.808672000
H	-3.407233000	-2.080241000	-1.341284000
Br	1.415031000	1.935339000	-0.043569000

TCG = 0.168198 au
ZPVE = 0.215013 au
E= -3230.31208 au

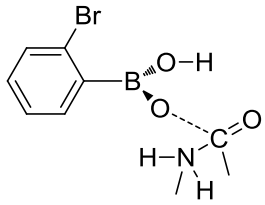


Br-INT2a (LANL2DZ for Br)

C	-3.569186000	0.737949000	0.468288000
C	-2.806147000	-0.415443000	0.262033000
C	-1.434886000	-0.295270000	0.024032000
C	-0.779355000	0.948546000	-0.023576000
C	-1.592593000	2.089322000	0.166643000
C	-2.962483000	1.995910000	0.416724000
H	-4.638194000	0.645078000	0.658974000
H	-3.278157000	-1.398425000	0.280046000
H	-1.125209000	3.072238000	0.121227000
H	-3.552764000	2.899202000	0.566359000
B	0.756628000	1.205626000	-0.244200000
O	1.662090000	0.328838000	0.380506000
O	1.125017000	2.302482000	-0.944953000
H	2.107726000	2.432799000	-1.047231000
C	3.014537000	0.313640000	0.254478000

O	3.616140000	1.027930000	-0.530650000
C	3.652274000	-0.682886000	1.178372000
H	3.386091000	-0.444442000	2.217176000
H	3.260367000	-1.686314000	0.963391000
H	4.738256000	-0.669498000	1.056064000
Br	-0.486863000	-1.951525000	-0.323320000

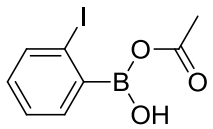
TCG = 0.107258 au
ZPVE = 0.149203 au
E= -573.4402993 au



Br-TS4a (LANL2DZ for Br)

C	-3.856379000	1.632326000	-0.510917000
C	-3.447603000	0.295233000	-0.541215000
C	-2.152886000	-0.020746000	-0.119922000
C	-1.226227000	0.924708000	0.334991000
C	-1.685908000	2.260259000	0.356178000
C	-2.972163000	2.617814000	-0.058682000
H	-4.862293000	1.895013000	-0.837586000
H	-4.127797000	-0.484839000	-0.885330000
H	-1.009011000	3.040388000	0.707870000
H	-3.284725000	3.661475000	-0.027630000
B	0.293047000	0.601091000	0.761445000
O	1.263737000	0.526407000	-0.131096000
O	0.457370000	0.476744000	2.155277000
H	1.411100000	0.339555000	2.388619000
C	3.373931000	-0.312530000	0.178686000
O	3.903389000	0.269095000	1.098341000
C	2.919474000	-1.742805000	0.169802000
H	2.226821000	-1.952416000	-0.649032000
H	3.813801000	-2.377765000	0.061110000
H	2.443365000	-1.976275000	1.126435000
N	3.554190000	0.260875000	-1.228769000
H	4.162465000	-0.393500000	-1.781072000
H	2.597064000	0.245983000	-1.656178000
C	4.109298000	1.643975000	-1.273305000
H	5.094918000	1.648680000	-0.803492000
H	4.181946000	1.940106000	-2.323593000
H	3.426975000	2.304005000	-0.734293000
Br	-1.650982000	-1.905410000	-0.171016000

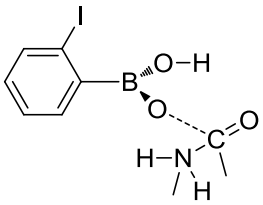
TCG = 0.167104 au
ZPVE = 0.214147 au
E= -669.2681556 au



I-INT2a

C	3.290392000	1.580200000	0.633425000
C	2.728098000	0.310970000	0.458887000
C	1.380298000	0.200281000	0.103142000
C	0.560014000	1.326580000	-0.095564000
C	1.173866000	2.589702000	0.060239000
C	2.514414000	2.723675000	0.427791000
H	4.338308000	1.665489000	0.920817000
H	3.342252000	-0.579789000	0.596732000
H	0.574147000	3.485227000	-0.102598000
H	2.950207000	3.714644000	0.550350000
B	-0.981254000	1.325159000	-0.414874000
O	-1.786252000	0.514975000	0.408570000
O	-1.450293000	2.143695000	-1.383731000
H	-2.442005000	2.146147000	-1.488986000
C	-3.136109000	0.367119000	0.370540000
O	-3.849809000	0.975373000	-0.409260000
C	-3.622037000	-0.617604000	1.393652000
H	-3.139232000	-1.589941000	1.226247000
H	-3.333116000	-0.277976000	2.397602000
H	-4.708365000	-0.720086000	1.330352000
I	0.654364000	-1.781649000	-0.233839000

TCG = 0.106175 au
ZPVE = 0.148833 au
E= -571.6518375 au



I-TS4a

C	3.553215000	2.153878000	-0.650240000
C	3.266197000	0.793670000	-0.496050000
C	1.975475000	0.413418000	-0.109905000
C	0.939649000	1.325603000	0.133231000
C	1.276672000	2.688124000	-0.032252000
C	2.554217000	3.104630000	-0.416166000
H	4.554914000	2.461536000	-0.949932000
H	4.041396000	0.047500000	-0.673563000
H	0.508126000	3.441660000	0.147538000
H	2.770689000	4.166792000	-0.530268000
B	-0.572736000	0.945267000	0.536494000
O	-1.510535000	0.730136000	-0.367458000
O	-0.778691000	0.941651000	1.932209000
H	-1.715473000	0.702196000	2.149173000
C	-3.801870000	0.419558000	0.092646000
O	-3.928807000	-0.164220000	1.143252000
C	-4.111864000	1.862478000	-0.173811000
H	-3.626924000	2.228258000	-1.082460000
H	-5.204773000	1.957051000	-0.281851000
H	-3.794652000	2.461344000	0.684896000
N	-3.677604000	-0.416578000	-1.179067000
H	-4.505356000	-0.221093000	-1.795624000
H	-2.824549000	-0.043231000	-1.662000000
C	-3.533531000	-1.883050000	-0.953965000
H	-4.418297000	-2.254374000	-0.432664000
H	-3.434118000	-2.360554000	-1.932831000
H	-2.638314000	-2.051695000	-0.352275000
I	1.621312000	-1.692001000	0.118074000

TCG = 0.165751 au
ZPVE = 0.213669 au
E= -667.4795715 au

$CH_3B(OH)_2$

C	1.507032000	-0.179381000	-0.000407000
B	-0.065580000	-0.015673000	-0.001529000
O	-0.693452000	1.213645000	0.000255000
O	-0.872684000	-1.127467000	-0.000317000
H	-1.842764000	-0.901624000	0.003213000
H	1.961842000	0.345014000	-0.853587000
H	1.819582000	-1.229151000	-0.043482000
H	1.946184000	0.264937000	0.905341000
H	-0.070041000	1.986047000	-0.000903000

TCG = 0.038966 au
ZPVE = 0.067247 au
E= -216.5508372 au

A1

C	-1.599112000	-2.833977000	0.154667000
B	-1.869170000	-1.284058000	-0.039411000
O	-3.147385000	-0.766174000	-0.143590000
O	2.299518000	1.140653000	-0.358514000
C	2.646911000	0.006812000	-0.042386000
O	1.781325000	-0.988367000	0.168598000
O	-0.828608000	-0.400179000	-0.132020000
C	4.079825000	-0.420429000	0.148162000
N	-1.322976000	2.184002000	-0.531659000
C	-1.642764000	2.908587000	0.714523000
H	-2.076192000	2.320025000	-1.223142000
H	-0.465996000	2.573051000	-0.955296000
H	-1.072370000	0.599501000	-0.290938000
H	-2.555300000	2.483794000	1.152046000
H	-1.795998000	3.988308000	0.561336000
H	-0.821552000	2.769912000	1.429261000
H	-2.277890000	-3.284002000	0.892825000
H	-0.568984000	-3.046104000	0.464970000
H	-1.770286000	-3.369938000	-0.791993000
H	4.217789000	-0.823894000	1.159811000
H	4.750664000	0.428119000	-0.008282000
H	4.324031000	-1.222113000	-0.561529000
H	0.830341000	-0.686063000	0.031054000
H	-3.859537000	-1.451739000	-0.067039000

TCG = 0.146698 au
ZPVE = 0.194481 au
E= -541.5105254 au

A1-AcOH

C	4.618444000	1.091798000	-0.563641000
B	3.715286000	-0.201432000	-0.403631000
O	4.228806000	-1.477416000	-0.551755000
O	-0.848107000	1.025825000	0.113926000
C	-0.260756000	2.092961000	0.307587000
O	1.062677000	2.179669000	0.320166000
O	2.379577000	-0.092608000	-0.128457000
C	-0.948397000	3.409259000	0.549140000
N	0.875963000	-2.261228000	0.090947000
C	0.953944000	-2.878907000	1.430005000
H	1.110160000	-2.958109000	-0.632774000
H	-0.093232000	-1.959364000	-0.100944000
H	1.826252000	-0.979526000	-0.057516000
H	1.986606000	-3.199618000	1.618120000
H	0.288428000	-3.748672000	1.543417000
H	0.682599000	-2.130540000	2.185467000
H	5.569498000	0.998340000	-0.020160000
H	4.117523000	2.003530000	-0.217071000
H	4.880481000	1.244882000	-1.622089000
H	-0.622224000	3.825256000	1.511397000
H	-2.033605000	3.279937000	0.548570000
H	-0.658786000	4.123593000	-0.233069000
H	1.495644000	1.281213000	0.141618000
H	5.200304000	-1.493296000	-0.748479000
H	-2.567021000	0.684228000	-0.044764000
O	-3.558334000	0.604141000	-0.148528000
C	-3.918824000	-0.671776000	-0.337659000
O	-3.112507000	-1.594529000	-0.368271000
C	-5.407128000	-0.830986000	-0.507889000
H	-5.929163000	-0.419507000	0.365810000
H	-5.740914000	-0.264546000	-1.387583000
H	-5.661316000	-1.886795000	-0.630329000

TCG = 0.195945 au
ZPVE = 0.256052 au
E= -770.6096044 au

A1-$MeNH_2$

C	-4.007183000	-1.764040000	-0.141311000
B	-3.423457000	-0.291836000	-0.213616000
O	-4.236773000	0.812554000	-0.396337000
O	1.419595000	-0.448428000	-0.113938000
C	1.083831000	-1.588198000	0.194890000
O	-0.192483000	-1.961768000	0.318543000
O	-2.076812000	-0.069883000	-0.119471000
C	2.047267000	-2.712638000	0.474620000
N	-1.118580000	2.407722000	-0.324178000
C	-1.286883000	3.204917000	0.907202000
H	-1.536510000	2.904107000	-1.126017000
H	-0.115402000	2.299783000	-0.541209000
H	-1.753508000	0.914447000	-0.207602000
H	-2.358034000	3.311873000	1.120827000
H	-0.840024000	4.209126000	0.838499000
H	-0.820782000	2.671509000	1.745494000
H	-4.956908000	-1.811057000	0.409446000
H	-3.308103000	-2.470842000	0.321944000
H	-4.216128000	-2.136200000	-1.156594000
H	1.885855000	-3.095191000	1.491088000
H	3.077753000	-2.364369000	0.369077000
H	1.861528000	-3.541651000	-0.221087000
H	-0.819562000	-1.196979000	0.130180000
H	-5.200192000	0.586471000	-0.456521000
H	4.208015000	0.060491000	-0.519142000
N	5.229580000	0.151358000	-0.614279000
H	5.412513000	0.211598000	-1.625453000
C	5.676693000	1.392661000	0.041638000
H	6.764259000	1.493706000	-0.074714000
H	5.204117000	2.310828000	-0.350318000
H	5.460827000	1.331961000	1.116769000

TCG = 0.196291 au
ZPVE = 0.257500 au
E= -637.3633408 au

$TS_{A1\text{-}B1}$

C	1.212903000	2.236294000	-0.965445000
B	0.291957000	1.325754000	-0.029569000
O	1.529612000	0.122719000	0.608924000
C	1.668488000	-1.015738000	0.074351000
C	2.798206000	-1.914729000	0.491875000
O	-0.626002000	0.430014000	-0.732116000
O	-0.287763000	1.861845000	1.135408000
O	0.872043000	-1.442765000	-0.849203000
N	-2.844115000	-0.285843000	0.535241000
C	-3.695829000	-1.176185000	-0.279416000
H	-3.363562000	0.569825000	0.786512000
H	-2.604316000	-0.743117000	1.428798000
H	-1.485625000	0.167848000	-0.193745000
H	-3.957796000	-0.664565000	-1.214339000
H	-4.625007000	-1.472020000	0.231881000
H	-3.130608000	-2.082730000	-0.530974000
H	0.604984000	3.022177000	-1.439684000
H	1.685526000	1.663217000	-1.775069000
H	2.014651000	2.736527000	-0.403893000
H	2.433976000	-2.939386000	0.631108000
H	3.267581000	-1.547592000	1.408759000
H	3.547481000	-1.934023000	-0.312584000
H	0.043226000	-0.593904000	-0.934071000
H	0.212781000	2.637516000	1.486167000

TCG = 0.147305 au
ZPVE = 0.190877 au
E= -541.496496725 au

B1

C	-0.913815000	2.330796000	0.424253000
B	-0.114423000	1.012738000	-0.078837000
O	0.815196000	1.236893000	-1.181564000
O	-1.189222000	-0.020129000	-0.653131000
C	-2.002326000	-0.727869000	0.085295000
O	-1.966361000	-0.780181000	1.326570000

O	0.680549000	0.327620000	0.962662000
C	-3.048040000	-1.494855000	-0.702659000
N	2.653469000	-0.956475000	-0.346747000
C	3.992368000	-0.798492000	0.288890000
H	2.585012000	-0.427668000	-1.234592000
H	2.446236000	-1.948203000	-0.557403000
H	1.871051000	-0.564401000	0.260452000
H	4.154245000	0.264022000	0.489447000
H	4.763611000	-1.177297000	-0.387432000
H	4.002680000	-1.361163000	1.226343000
H	-0.211512000	3.089032000	0.803469000
H	-1.621222000	2.111090000	1.237214000
H	-1.493273000	2.802195000	-0.385556000
H	-3.442049000	-2.326098000	-0.109957000
H	-2.637955000	-1.863633000	-1.649480000
H	-3.878092000	-0.814143000	-0.941706000
H	0.088477000	-0.052526000	1.655058000
H	0.480203000	1.929329000	-1.795402000

TCG = 0.154031 au
ZPVE = 0.197220 au
E= -541.5136193 au

$TS_{B1\text{-}C1}$

C	2.642145000	0.214975000	1.202489000
B	1.485587000	-0.154154000	0.164757000
O	0.202569000	-0.365972000	0.766959000
C	-1.002667000	-0.564944000	0.057900000
C	-2.065723000	-1.004619000	1.061771000
O	1.764396000	-1.008021000	-0.934161000
O	1.227595000	1.464364000	-0.771922000
O	-0.917865000	-1.598536000	-0.901023000
N	-1.323452000	0.692616000	-0.674397000
C	-1.924272000	1.779372000	0.123827000
H	-1.965421000	0.444757000	-1.458652000
H	0.234803000	1.326725000	-0.966787000
H	2.681225000	-0.888341000	-1.282881000
H	-2.923446000	1.532248000	0.513260000
H	-2.008875000	2.669236000	-0.513396000
H	-1.268727000	2.021168000	0.970146000
H	2.904294000	-0.668381000	1.804244000
H	2.343998000	1.003637000	1.907320000
H	3.561861000	0.546693000	0.699754000
H	-3.035696000	-1.114779000	0.562445000
H	-2.160714000	-0.277941000	1.874111000
H	-1.772738000	-1.970496000	1.487622000
H	-0.142123000	-1.425267000	-1.490464000
H	1.277329000	2.239825000	-0.164472000

TCG = 0.126849 au
ZPVE = 0.195930 au
E= -834.8043292 au

C1

C	3.067977000	-0.046955000	0.861155000
B	1.730729000	0.104209000	0.027680000
O	-1.356363000	2.920865000	-0.136321000
O	0.753834000	-0.851130000	0.200618000
C	-0.553317000	-0.904399000	-0.383975000
N	-1.411651000	0.056913000	0.320419000
C	-1.505223000	-0.096127000	1.783617000
O	1.526902000	1.135853000	-0.855370000
C	-1.000590000	-2.363492000	-0.289773000
O	-0.560911000	-0.572294000	-1.748246000
H	-2.365994000	-0.051498000	-0.092119000
H	-1.281686000	1.940563000	-0.000930000
H	2.281438000	1.779608000	-0.901270000
H	-1.841560000	-1.096016000	2.103028000
H	-2.223026000	0.645320000	2.156291000
H	-0.531379000	0.109926000	2.241391000
H	3.055516000	-0.920484000	1.523006000
H	3.247473000	0.844036000	1.481286000
H	3.939228000	-0.140106000	0.195708000
H	-2.020154000	-2.466375000	-0.679111000
H	-0.974608000	-2.708612000	0.748572000
H	-0.327488000	-2.992697000	-0.883376000
H	-0.394828000	0.404488000	-1.834745000
H	-2.295796000	3.131891000	0.049342000

TCG = 0.151239 au
ZPVE = 0.194407 au
E= -541.4957089 au

$TS_{C1\text{-}D1|cis}$

C	-2.911933000	-0.558184000	-0.719223000
B	-1.597458000	0.152935000	-0.122719000
O	-0.386056000	-0.588785000	-0.655668000
C	0.895351000	-0.405208000	-0.273509000
N	1.400276000	0.877402000	-0.455965000
C	2.766845000	1.202653000	-0.041868000
O	-1.480364000	-0.078078000	1.431358000
O	-1.536373000	1.598351000	-0.261608000
O	0.855961000	-0.643903000	1.441644000
C	1.796976000	-1.535604000	-0.735804000
H	0.714342000	1.614643000	-0.213361000
H	-1.704888000	0.751031000	1.917490000
H	2.955188000	0.976200000	1.019381000
H	2.920195000	2.275877000	-0.205689000
H	3.498062000	0.661311000	-0.654998000
H	-2.979623000	-0.433728000	-1.811087000
H	-3.828992000	-0.131648000	-0.286793000
H	-2.925749000	-1.638926000	-0.518207000
H	2.773144000	-1.506620000	-0.242976000
H	1.943480000	-1.449246000	-1.819998000
H	1.314817000	-2.496133000	-0.526388000
H	0.926539000	-1.611461000	1.621409000
H	-1.954698000	1.902682000	-1.101547000
H	-0.375238000	-0.343113000	1.604730000

TCG = 0.155286 au
ZPVE = 0.192444 au
E= -541.473232 au

$D1_{cis}$*(optimized in gas-phase)

C	-2.991961000	-0.213745000	0.740018000
B	-1.642442000	-0.048984000	-0.111130000
O	-1.273996000	1.309640000	-0.517687000
O	-1.509169000	-0.916517000	-1.284644000
O	-0.448823000	-0.413610000	0.950817000
C	0.775884000	-0.566751000	0.633679000
N	1.148172000	-0.819185000	-0.615795000
C	2.518502000	-0.781301000	-1.114184000
C	1.803590000	-0.448505000	1.721243000
O	1.286403000	2.298821000	-0.150174000
H	0.368460000	-0.904928000	-1.275691000
H	-1.533469000	1.435983000	-1.441648000
H	2.919670000	0.236043000	-1.054308000
H	2.505938000	-1.097991000	-2.158857000
H	3.164376000	-1.466456000	-0.555927000
H	-3.151030000	-1.240564000	1.103247000
H	-3.870075000	0.062736000	0.138576000
H	-2.988170000	0.440602000	1.621420000
H	2.314055000	0.515047000	1.605389000
H	2.549911000	-1.247711000	1.673378000
H	1.299560000	-0.468861000	2.688542000
H	1.258888000	3.219214000	0.147896000
H	-2.076463000	-1.696991000	-1.227553000
H	0.341950000	2.028230000	-0.269280000

TCG = 0.158818 au
ZPVE = 0.199776 au
E= -541.5112926 au

$TS_{D1\text{-}E1|cis}$*(optimized in gas-phase)

C	-2.913793000	-0.020532000	0.925625000
B	-1.755128000	-0.212152000	-0.141768000
O	-1.549438000	-1.470556000	-0.786007000
O	-0.265078000	-0.076062000	1.074993000
C	0.930478000	-0.268084000	0.743928000
C	2.036160000	0.372251000	1.541956000
O	-1.465934000	0.866840000	-1.020587000
N	1.246171000	-1.014605000	-0.329264000
C	2.581019000	-1.198221000	-0.883914000
O	0.829008000	2.489579000	-0.774373000
H	0.443659000	-1.427095000	-0.804480000
H	-1.222017000	0.527253000	-1.895165000
H	3.069508000	-0.235789000	-1.066926000
H	2.482916000	-1.718634000	-1.839212000
H	3.216479000	-1.805399000	-0.227730000
H	-2.905513000	-0.792118000	1.707193000
H	-3.895853000	-0.052115000	0.431652000
H	-2.834705000	0.950711000	1.427944000
H	2.329509000	1.296616000	1.028788000
H	2.914477000	-0.272214000	1.645353000
H	1.648296000	0.633992000	2.528012000
H	0.624334000	3.435579000	-0.771997000
H	-1.969664000	-2.198904000	-0.308839000
H	-0.040628000	2.030221000	-0.758678000

TCG = 0.157459 au
ZPVE = 0.199037 au
E= -541.5096276 au

$E1_{cis}$

C	3.815455000	-1.496787000	0.043015000
B	2.305012000	-1.038355000	-0.013232000
O	1.999686000	0.303725000	-0.019888000
O	1.243633000	-1.917107000	-0.043764000
O	-1.288743000	1.289981000	-0.031372000
C	-2.383534000	0.686186000	-0.007440000
N	-2.442016000	-0.660909000	-0.003773000
C	-3.657297000	-1.471465000	0.026324000
C	-3.698471000	1.438948000	0.017445000
O	3.705203000	2.610140000	0.000329000
H	-1.523515000	-1.154802000	-0.020209000
H	1.018725000	0.496688000	-0.040774000
H	-4.241458000	-1.289405000	0.939736000
H	-3.359890000	-2.525306000	0.008372000
H	-4.294638000	-1.274219000	-0.847267000
H	4.037821000	-2.257506000	-0.718720000
H	4.041124000	-1.956684000	1.017216000
H	4.511559000	-0.661465000	-0.095940000
H	-4.281956000	1.179959000	0.911449000
H	-4.311129000	1.185221000	-0.858433000
H	-3.496166000	2.513121000	0.017006000
H	3.100051000	3.375467000	0.104549000
H	1.515284000	-2.872217000	-0.039549000
H	3.118094000	1.824079000	-0.003372000

TCG = 0.138001 au
ZPVE = 0.190321 au
E= -541.5153323 au

$Ph(OH)NHCH_3$

C	-3.104359000	-0.296535000	0.065703000
C	-2.566680000	0.971207000	0.313234000
C	-1.182536000	1.167349000	0.254420000
C	-0.296207000	0.111086000	-0.041839000
C	-0.865656000	-1.156408000	-0.283806000
C	-2.248156000	-1.361904000	-0.236144000
H	-4.182305000	-0.453202000	0.105946000
H	-3.225018000	1.806370000	0.553119000
H	-0.786863000	2.164408000	0.456219000
H	-0.217446000	-1.998722000	-0.527856000
H	-2.658206000	-2.351972000	-0.436691000
B	1.271036000	0.339987000	-0.095104000
O	1.814955000	1.563159000	-0.474941000
H	1.143015000	2.218632000	-0.786709000
N	2.160226000	-0.697612000	0.252131000
C	3.618540000	-0.642500000	0.236732000
H	4.040366000	-1.464770000	-0.361198000
H	3.946031000	0.305264000	-0.203771000
H	4.037543000	-0.711395000	1.253073000
H	1.776809000	-1.590314000	0.608210000

TCG = 0.125613 au
ZPVE = 0.161395 au
E= -427.6813528 au

TSR1

C	-3.861040000	-0.294765000	-0.359487000
C	-3.203112000	-0.976047000	0.671424000
C	-1.857666000	-0.706569000	0.943672000
C	-1.130989000	0.241403000	0.196988000
C	-1.814602000	0.912072000	-0.836280000
C	-3.162288000	0.653304000	-1.113918000
H	-4.909246000	-0.503017000	-0.573848000
H	-3.738145000	-1.720473000	1.261503000
H	-1.359092000	-1.255024000	1.742921000
H	-1.290928000	1.658753000	-1.436180000
H	-3.664817000	1.190782000	-1.918377000
B	0.368359000	0.642291000	0.546653000
O	0.634931000	1.460308000	1.640664000
H	-0.124623000	1.512776000	2.275494000
N	1.380840000	0.753039000	-0.587870000
C	2.393869000	1.820253000	-0.557906000
H	3.081855000	1.692202000	-1.400577000
H	1.922156000	2.808529000	-0.620453000
H	2.964129000	1.758444000	0.371830000
H	0.944670000	0.700892000	-1.536778000
C	2.135504000	-0.908997000	-0.192183000
O	3.351119000	-0.818082000	0.059510000
O	1.232137000	-1.019598000	0.978500000
C	1.606517000	-1.799409000	-1.300680000
H	0.523182000	-1.706568000	-1.428822000
H	2.112611000	-1.550035000	-2.240149000
H	1.841943000	-2.840286000	-1.040700000
H	1.805979000	-0.858184000	1.786779000

TCG = 0.181942 au
ZPVE = 0.222826 au
E= -656.7390853 au