Electronic Supplementary Information

Mechanistic insight into the ANRORC-like rearrangement between methylhydrazine and 1,2,4-oxadiazole derivatives.

Sebastián Gallardo-Fuentes and Renato Contreras

Departamento de Química, Facultad de Ciencias, Universidad de Chile, Casilla 653, Santiago, Chile.

Contents

Computational Details

All of the TS structures included in this study were fully optimized at the M06-2x/6-31+G(d,p) level of theory. Structures were optimized with the SMD corrections to mimic solvation effects by N,N-dimethylformamide (DMF) used as reaction medium in the experimental study by Palumbo-Piccionello et al. After the optimization procedure, frequency calculations were performed in order to verify the presence of one and only one anomalous vibration associated with the bond-forming/bond-breaking processes. Efforts to locate transition structure associated with the inter and intra nucleophilic attack of NHMe end on C(5) site (**TS-8** and **TS-6´**) and the catalyzed proton transfer (**TS-PT2**) in DMF cavity, were unsuccessful. However, reliable first order saddle point could be located in water cavity for **TS-8** and **TS-PT2**. For **TS-6´** only was feasible locate a first order saddle point by means of M06-HF/6-31+G(d,p) in water cavity. Thereby, the activation barriers for these processes were obtained following the Simón and Goodman recomendation.[1] With this information at hand, an IRC[2,3] calculation was performed to obtain the reaction profile that smoothly connects reactants and the proposed intermediates. In order to keep the same Hamiltonian along the reaction pathway, we re-optimized the corresponding reactive and product complex obtained in each IRC calculation and we use this structure to obtain all Gibbs free energies reported herein. It is worth mentioning that this approach avoid the inclusion of a cratic correction of 1.9 kcal/mol to obtain the corresponding 298 K and 1 M standard state.[4] All of the calculations were performed using the Gaussian 09 suite of programs.[5] 3D structures were generated by using CYLView program.[6]

References:

[1] Simón L, Goodman J. M. *Org. Biomol. Chem*. 2011, **9**, 689

[2] Gonzalez, C.; Schlegel, H. B. *J. Chem. Phys*. 1989, **90**, 2154.

[3] Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* 1990, **94**, 5523.

[4] Vayner, G.; Houk, K. N.; Jorgensen, W. L.; Brauman, J. I *J. Am Chem. Soc.* 2004, **126**, 9054

[5] 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, T. Keith, 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

[6] CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org).

Cartesian coordinates, energies (u.a.) and number of imaginary frequencies (NIMAG) for the Transition State, intermediates, reactive and products structures calculated at the M06-2X/6–31+G(d,p) level of theory with the SMD solvation model in DMF.

Reactive Complex1 (1m + methylhydrazine)

C	-1.20126400	-0.98241900	0.00874300
C	0.87320500	-1.25019700	-0.04351500
C	-2.96017200	0.73207300	-0.43217300
N	-0.11738000	-0.32573900	-0.28484200
N	1.78157700	3.04252000	0.68091500
H	2.57648600	2.76861100	0.10954100
N	0.61865300	2.88470900	-0.13259400
N	0.42397900	-2.40655500	0.36866700
O	-0.94855700	-2.23449500	0.40836100
H	0.28321800	1.91725700	-0.09946100
C	2.30294100	-0.95277700	-0.22289300
C	3.27804700	-1.79634400	0.32230200
C	2.68093200	0.18895000	-0.93653700
C	4.62583100	-1.49333200	0.15348800
H	2.98021600	-2.67734100	0.88314500
C	4.03245400	0.48756400	-1.09974400
H	1.91977900	0.83582000	-1.36460800
C	5.00517100	-0.35092000	-0.55489800
H	5.38132600	-2.14576500	0.58009100
H	4.32357000	1.37493800	-1.65372300
H	6.05759600	-0.11521500	-0.68081200
C	-2.59802200	-0.55654400	-0.03277900
C	-3.62392000	-1.44219600	0.33205000
C	-4.95266900	-1.04058200	0.29101800
C	-4.27818000	1.15198100	-0.48035000
C	-5.27886200	0.25511800	-0.11525400
H	-3.37030000	-2.44920400	0.64657200
H	-5.73392300	-1.73686100	0.57547800
H	-6.31625800	0.57190700	-0.14850700
H	-4.50027500	2.16488400	-0.79892000
F	-2.00275900	1.60962000	-0.78514700
C	1.75147900	2.21772100	1.88409700
H	2.72017400	2.28529700	2.38842500
H	0.97936900	2.59439700	2.56290200
H	1.53668600	1.15862400	1.66917700
H	-0.11399900	3.46889400	0.26378600

Energy -974.30503382 a.u NIMAG = 0

TS-1

C	-0.64124000	0.19546100	-0.26094100
C	1.46643100	0.09487100	-0.47052100
N	-0.96205700	1.55287300	0.75829000

H	-0.05929400	2.03593900	0.87394200
C	-1.95843400	-0.52492400	-0.31959500
C	-2.52884000	-1.06959500	0.82644900
C	-2.63865900	-0.70361900	-1.52589600
C	-3.71839800	-1.77503200	0.81961200
C	-3.84051000	-1.40863000	-1.56621100
H	-2.21332800	-0.29058100	-2.43463800
C	-4.37827500	-1.94519600	-0.39706900
H	-4.10902600	-2.17493000	1.74955800
H	-4.35386700	-1.53963200	-2.51314500
H	-5.31213000	-2.49753400	-0.42552500
N	1.12380500	0.86788400	-1.47580800
O	-0.30706600	0.80634900	-1.44823500
N	0.46183200	-0.43131400	0.26718500
H	-1.24942000	1.20881300	1.67952000
C	2.89060700	-0.18977000	-0.18122400
C	3.22776600	-0.91682200	0.96462700
C	3.90191600	0.25969300	-1.03920900
C	4.56410000	-1.19365200	1.24970500
H	2.43981100	-1.26115500	1.62705100
C	5.23565500	-0.01582200	-0.74952100
H	3.64076900	0.82192200	-1.93074800
C	5.56989100	-0.74345800	0.39497600
H	4.81887600	-1.76082700	2.13994700
H	6.01535600	0.33630400	-1.41834500
H	6.61083300	-0.95883900	0.61771300
C	-2.03636200	3.66344500	0.96905700
H	-1.06816200	4.18181200	0.99653400
H	-2.77325600	4.30018300	0.47587000
H	-2.36992600	3.46834600	1.99148900
N	-1.97668700	2.39902200	0.23243500
H	-1.70203800	2.58062500	-0.73371500
F	-1.89786800	-0.88691000	2.01447100

Energy -974.27883536 a.u NIMAG = 1, ν_I (cm^{-1}) = 116i

Int-1

C	0.00229100	0.25681600	0.06772900
C	0.03256500	0.16314000	2.34574700
N	0.85286200	0.35989300	1.25603300
N	0.04029500	-1.02318900	-0.60108300
N	0.99888700	-1.15033400	-1.62999200
N	-1.22150400	0.21589400	2.05971000
O	-1.30352600	0.40403200	0.66632400
H	0.64165900	-1.84966500	-2.27315200
C	0.53797700	-0.06158500	3.71151500
C	-0.33749400	-0.51767300	4.70575900
C	1.88149500	0.17271400	4.02083300
C	0.12986600	-0.73084100	5.99775800
H	-1.37702200	-0.71058200	4.45849500
C	2.34471300	-0.04606600	5.31755000

H	2.56463800	0.53736400	3.25890500
C	1.47227000	-0.49698900	6.30672500
H	-0.55178400	-1.08734300	6.76397100
H	3.38816100	0.14004400	5.55268500
H	1.83609300	-0.66740900	7.31563000
H	0.11797200	-1.77057800	0.09467200
C	0.21710500	1.39500600	-0.91424400
C	-0.63571600	1.55746700	-2.00390900
C	1.23562900	2.33392000	-0.75473700
C	-0.51134100	2.59232600	-2.91344100
C	1.39332900	3.38510000	-1.66023300
C	0.52015000	3.51525900	-2.73726900
F	-1.64039800	0.67205800	-2.19340900
H	1.90850900	2.23960000	0.09182200
H	2.19460100	4.10272200	-1.51698500
H	-1.21237300	2.66421200	-3.73866000
H	0.63316900	4.33283500	-3.44225700
C	2.33384500	-1.52449000	-1.17111200
H	2.92563300	-1.82582800	-2.03931900
H	2.83004600	-0.66278800	-0.71125000
H	2.31562200	-2.35357800	-0.44698200
H	1.74974900	-0.11591200	1.23437200

Energy -974.29271152 a.u NIMAG = 0

TS-2

C	-0.00029300	-0.04044600	-0.00098600
C	-0.00033100	-0.05004900	2.36835700
N	0.73117500	-0.06141900	1.14059200
N	0.40806900	-0.78096000	-1.02832400
N	0.07683900	-0.47495500	-2.35006000
N	-1.18525600	-0.58290500	2.36203500
O	-1.62966300	-0.97855400	1.20316200
H	-0.43835100	-1.26567400	-2.73239800
C	0.63996100	0.48920900	3.57220900
C	0.04384600	0.33856400	4.83740600
C	1.86703800	1.16267600	3.48314200
C	0.65864400	0.85473500	5.97192600
H	-0.90276500	-0.18611700	4.92101400
C	2.48106400	1.67494700	4.62679300
H	2.34057500	1.29312400	2.51433000
C	1.88205700	1.52559700	5.87572100
H	0.18320900	0.72972500	6.94074000
H	3.43143900	2.19320800	4.53553900
H	2.35953200	1.92445600	6.76564200
H	1.05089400	-1.55286500	-0.85099800
C	-0.92926100	1.09140100	-0.22019800
C	-2.14058800	0.93987200	-0.89542700
C	-0.61120200	2.35326500	0.28640900
C	-3.01532000	1.99285500	-1.08874500
C	-1.47648300	3.43147100	0.10266000

C	-2.67397200	3.25002800	-0.58504300
F	-2.48734600	-0.27315900	-1.36216600
H	0.32798300	2.48475700	0.81645700
H	-1.21158800	4.40771200	0.49519100
H	-3.94711400	1.82102200	-1.61747400
H	-3.35331600	4.08402800	-0.73152300
C	1.28283900	-0.21806000	-3.13688100
H	0.97887900	-0.07905600	-4.17669600
H	1.75217500	0.70179200	-2.77889800
H	2.01070400	-1.03923500	-3.08324500
H	1.53398800	-0.69112400	1.12339300

Energy -974.26268211 a.u NIMAG = 1, ν_I (cm^{-1}) = 167i

Int-2

C	-0.02384500	0.13991400	0.04711400
C	-0.02353200	0.08530200	2.52327200
N	0.60552400	0.15042100	1.28668200
N	0.39027600	0.75926600	3.53714400
O	1.41687600	1.63442200	3.18047100
C	-1.10938700	-0.90087200	2.75598300
C	-2.14265800	-0.61489800	3.65225700
C	-1.07268500	-2.14060400	2.10867100
C	-3.13291400	-1.56470300	3.89947200
H	-2.17600000	0.35339500	4.14259900
C	-2.06222500	-3.08656100	2.35925100
H	-0.26951700	-2.36177100	1.41075100
C	-3.09572500	-2.80039200	3.25373500
H	-3.93787200	-1.33493700	4.59117900
H	-2.02716200	-4.04797200	1.85566300
H	-3.87044100	-3.53751600	3.44272800
C	0.92324200	0.07004800	-1.10628800
C	1.79164800	1.12043100	-1.41322800
C	0.96765000	-1.06771600	-1.90556700
C	2.66330200	1.02546200	-2.49728200
C	1.82085700	-1.18998200	-2.98843600
C	2.67395200	-0.12634200	-3.28347700
H	1.77128100	2.01955300	-0.80244300
H	3.32842800	1.85096400	-2.72835600
H	3.35024700	-0.20432500	-4.12893400
H	1.81362000	-2.10122100	-3.57737100
F	0.15987600	-2.10636000	-1.59789800
H	1.69092200	2.02285300	4.02345200
H	1.54727200	0.52818000	1.29843200
N	-1.29915000	0.17930400	-0.04115900
N	-1.79311800	0.15385700	-1.38113800
H	-2.73679700	-0.21445500	-1.28976700
C	-1.91785900	1.52152800	-1.89755900
H	-2.45603300	1.47673900	-2.84765600
H	-2.45905700	2.18445900	-1.20779600
H	-0.92419800	1.94023500	-2.08039100

Energy -974.28476664 a.u NIMAG = 0

TS-3

C	-0.04463200	0.11812900	0.04247700
C	-0.06729800	0.08415600	2.50518300
N	0.57117100	0.09866100	1.26676400
N	0.37804700	0.75292900	3.50686100
O	1.45387100	1.55964800	3.14315500
C	-1.21123700	-0.83150300	2.74326900
C	-2.26234600	-0.44182000	3.57707700
C	-1.21310300	-2.10562900	2.16561600
C	-3.31035600	-1.32466900	3.83366000
H	-2.26211400	0.55436100	4.00956200
C	-2.25995700	-2.98493000	2.42700500
H	-0.39310100	-2.40720800	1.51914000
C	-3.31128000	-2.59586200	3.25986800
H	-4.12943400	-1.01592500	4.47621700
H	-2.25544600	-3.97516800	1.98136000
H	-4.12950900	-3.28184600	3.45824200
C	0.73876000	0.22631600	-1.19103000
C	1.79707700	1.12052100	-1.37764300
C	-0.02671800	-0.22138700	-2.30442700
C	2.12352400	1.57353000	-2.65209300
C	0.25561800	0.30302600	-3.58628700
C	1.31813800	1.18270300	-3.73498000
H	2.34124200	1.49475900	-0.51265100
H	2.95785200	2.24967700	-2.80087000
H	1.54096300	1.56119400	-4.72959400
H	-0.33954600	-0.01754700	-4.43563200
F	-0.39980200	-1.57937200	-2.30972500
H	1.74374600	1.94825000	3.98103700
H	1.54965400	0.36791600	1.28064200
N	-1.33952300	0.16027900	-0.06625500
N	-1.70786700	0.16620300	-1.44390500
H	-2.34224600	-0.61506200	-1.61284900
C	-2.31115700	1.43969500	-1.82628000
H	-2.70479000	1.34721400	-2.84035800
H	-3.11401600	1.71282600	-1.13546900
H	-1.53013200	2.20634200	-1.80478900

Energy -974.25091943 a.u NIMAG = 1, ν_I (cm^{-1}) = 316i

TS-4

C	-0.00660400	-0.00341600	-0.00243200
C	-0.00531800	0.00045600	2.09535600
C	1.64382300	0.00412900	-1.84426400
N	0.82640800	-0.06758100	1.00655900
N	2.61432900	-1.46057200	-1.03931900
H	2.69048300	-1.23173500	-0.04579600
N	3.93919500	-1.58777900	-1.55716800
N	-1.27338800	0.10150900	1.79182400
O	-1.28115700	0.10330700	0.40152600

H	3.84086300	-1.73952100	-2.56390000
C	0.48492700	-0.04498400	3.48447600
C	-0.40538900	0.07567700	4.55842500
C	1.85227700	-0.20853800	3.72553200
C	0.07442900	0.03124000	5.86379800
H	-1.46695500	0.20582400	4.37009600
C	2.32667700	-0.25321100	5.03527600
H	2.53812100	-0.29951400	2.88889900
C	1.44034300	-0.13332100	6.10506600
H	-0.61830400	0.12623300	6.69442300
H	3.38917300	-0.38100400	5.21880100
H	1.81133000	-0.16686500	7.12509900
C	0.28352000	-0.08562100	-1.41257100
C	-0.72564000	-0.40171400	-2.34019500
C	-0.44788300	-0.56026300	-3.68569400
C	1.89350500	-0.05122000	-3.24745400
C	0.87732000	-0.36414000	-4.12521700
H	-1.74264700	-0.51744000	-1.97508600
H	-1.23669100	-0.79791000	-4.39011500
H	1.10487000	-0.42256300	-5.18665700
H	2.89928700	0.16152400	-3.59651600
F	2.45249000	0.90370400	-1.16310300
C	1.88093800	-2.70881900	-1.22047000
H	0.92459300	-2.63666000	-0.70029700
H	1.70353400	-2.85166800	-2.29208100
H	2.45331100	-3.55319500	-0.82679900
H	4.38682900	-0.67715500	-1.44770400

Energy -974.28060440 a.u NIMAG = 1, ν_I (cm^{-1}) = 288i

Int-3

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.10822656
N	2.79826038	0.00000000	-0.95588551
H	2.58062938	0.24417320	0.02396064
C	0.31073911	0.05039385	-1.39365706
C	1.60480678	0.61068078	-1.79304706
C	-0.62491368	-0.38306273	-2.35756363
C	1.86200550	0.56470907	-3.23086862
C	-0.35054710	-0.36522800	-3.70518921
H	-1.58450723	-0.75028536	-2.00223828
C	0.91976915	0.11975107	-4.11627600
H	2.80902835	0.95858142	-3.58537074
H	-1.07380201	-0.71648328	-4.43152344
H	1.16132017	0.14551098	-5.17645404
N	-1.22820058	-0.32883820	1.80511858
O	-1.23655387	-0.32792789	0.40866348
N	0.80550124	0.21488308	1.02271249
C	0.47497034	0.12030783	3.49859202
C	1.81997118	0.41284967	3.74194896
C	-0.40821864	-0.05653123	4.57052830
C	2.28015341	0.52498757	5.05280418

H	2.50004917	0.55080014	2.90689272
C	0.05702268	0.05660105	5.87711495
H	-1.45335041	-0.28076536	4.37867116
C	1.40140231	0.34706299	6.12076687
H	3.32557434	0.75117926	5.23928567
H	-0.63041973	-0.08108751	6.70613827
H	1.76177543	0.43471632	7.14142640
N	2.86456250	-1.42382592	-1.01049236
H	2.95648363	-1.67175136	-1.99875518
F	1.75828268	1.97473518	-1.29125369
H	1.96075908	-1.78288074	-0.69876817
C	4.13553756	0.55152384	-1.29755357
H	4.07745279	1.63769874	-1.30238692
H	4.83467758	0.20311608	-0.53867344
H	4.43076710	0.17176083	-2.27574175

Energy -974.28714330 a.u NIMAG = 0

TS-4´

C	-0.22762100	-1.16218300	0.02604300
C	1.84357100	-0.83739900	-0.07495900
C	-2.29066800	0.09161600	0.60868700
N	0.65390100	-0.20229800	0.17423100
N	-1.92616300	1.42101500	-0.62826000
H	-0.90962800	1.48030900	-0.72929800
N	-2.45367500	2.71367300	-0.31635600
N	1.72202300	-2.10790500	-0.36043000
O	0.35152400	-2.33077600	-0.29362900
C	3.14963100	-0.15521300	-0.02917200
C	4.32406500	-0.85100600	-0.34191800
C	3.21423500	1.19240100	0.33734500
C	5.55186600	-0.19906800	-0.28729500
H	4.27351400	-1.89760800	-0.62743800
C	4.44719800	1.84003600	0.39078600
H	2.30159400	1.72715000	0.58150800
C	5.61661400	1.14713200	0.07959400
H	6.46014400	-0.74181600	-0.53073900
H	4.49247900	2.88627600	0.67773100
H	6.57648700	1.65321500	0.12356000
C	-1.66232200	-1.10665500	0.13140500
C	-2.46059800	-2.16350200	-0.35254000
C	-3.83838000	-2.12111900	-0.29156300
C	-3.71104500	0.04990000	0.80501700
C	-4.44941500	-1.00329400	0.32346700
H	-1.96210800	-3.03256600	-0.77344600
H	-4.43669200	-2.94555100	-0.66180500
H	-5.52872000	-0.98599600	0.45198300
H	-4.17767100	0.89275300	1.30686300
F	-1.62238800	0.78518100	1.61134300
H	-2.75459800	2.67103100	0.65730800
C	-3.59808900	3.04220700	-1.16674200
H	-4.03307900	3.97125500	-0.79289400

H	-3.24972100	3.20835700	-2.18993400
H	-4.37089700	2.26169100	-1.17196900
H	-2.31865000	1.07656200	-1.50771300

Energy -974.26996582 a.u NIMAG = 1, ν_I (cm^{-1}) = 365i

TS-5

C	0.00180200	0.00576800	0.00096800
C	-0.00169400	-0.00241000	2.10561300
N	2.77769900	-0.03930300	-0.93407600
H	2.57160300	0.38488400	-0.01736000
C	0.30901500	0.03565900	-1.40865100
C	1.63024200	0.38842000	-1.84415900
C	-0.71836400	-0.15194800	-2.35184700
C	1.88614700	0.29967200	-3.24453100
C	-0.46852100	-0.11724400	-3.70935700
H	-1.72377300	-0.34380100	-1.98782300
C	0.85506900	0.09719000	-4.13723000
H	2.89178600	0.46651700	-3.61208500
H	-1.26548100	-0.27856000	-4.42601900
H	1.08463000	0.08952400	-5.19954200
N	-1.26007300	-0.16826600	1.79459500
O	-1.26396400	-0.16514100	0.40304200
N	0.82507500	0.11006000	1.01639500
C	0.48564600	0.05730400	3.49391300
C	1.84715800	0.26368600	3.73411800
C	-0.40174700	-0.09137700	4.56655600
C	2.31945300	0.32154200	5.04398300
H	2.53017000	0.37834000	2.89784300
C	0.07636100	-0.03319200	5.87191300
H	-1.45873100	-0.25334200	4.37735700
C	1.43660900	0.17333100	6.11311100
H	3.37712600	0.48290600	5.22831100
H	-0.61334000	-0.14934100	6.70229900
H	1.80606800	0.21817600	7.13325700
N	2.84796500	-1.45209200	-0.70768900
H	2.90228300	-1.89424300	-1.62738600
F	1.86253100	2.02850600	-1.36060200
H	1.96747600	-1.74102700	-0.28076000
C	4.12954800	0.42248900	-1.36126500
H	4.07424000	1.48009700	-1.60354500
H	4.79966200	0.24194700	-0.52243200
H	4.44489200	-0.16809100	-2.22109600

Energy -974.28400854 a.u NIMAG = 1, ν_I (cm^{-1}) = 323i

Int-4 (Int-4(N1))

C	0.02496900	0.05521800	0.00105600
C	0.02745000	0.05601100	2.09550300
N	2.69545800	0.12367900	-1.19150800
H	2.48678000	1.21596900	-0.17923900

C	0.24071200	-0.09686000	-1.44183500
C	1.52475600	-0.07501300	-2.02396300
C	-0.88969200	-0.26785300	-2.25001100
C	1.63840300	-0.23221000	-3.40499300
C	-0.76121300	-0.42785700	-3.62431900
H	-1.87308700	-0.28681400	-1.79099500
C	0.50676200	-0.41004100	-4.19886200
H	2.61483600	-0.20962100	-3.87509400
H	-1.64495100	-0.56676200	-4.23827400
H	0.62395800	-0.53377300	-5.27107100
N	-1.10407600	0.63364600	1.78538800
O	-1.10944900	0.63956600	0.40253100
N	0.76468900	-0.32467300	0.99872200
C	0.47086100	-0.17142800	3.48006500
C	1.71837600	-0.75814400	3.71348100
C	-0.34576800	0.19569800	4.55660300
C	2.14731800	-0.97688200	5.02107100
H	2.34808300	-1.03746400	2.87405800
C	0.08866800	-0.02605100	5.85937400
H	-1.31479800	0.65034000	4.37301000
C	1.33466000	-0.61213400	6.09409600
H	3.11681300	-1.43183200	5.19949500
H	-0.54479400	0.25774500	6.69410200
H	1.67025600	-0.78327100	7.11267100
N	3.13561300	-1.07785200	-0.53446600
H	3.16600800	-1.83169000	-1.22430600
F	2.45908600	2.03868700	0.40444700
H	2.43633400	-1.31111000	0.16966300
C	3.85449500	0.69783600	-1.89727000
H	3.54328200	1.59983700	-2.42767700
H	4.59665900	0.95479000	-1.14017500
H	4.29921100	-0.01514100	-2.59929400

Energy -974.33772579 a.u NIMAG = 0

Int-4′ (Int-4(N2))

C	-0.59892900	-0.99479300	-0.04617600
C	1.49573900	-0.92928400	-0.04485800
N	-1.86588700	1.58988500	0.65001000
H	-0.88997800	1.31942400	1.77599200
C	-2.04831000	-0.78487100	-0.08725200
C	-2.64490000	0.44733400	0.24123900
C	-2.86079000	-1.87314000	-0.43619100
C	-4.03520300	0.55379900	0.22501900
C	-4.24459000	-1.75151700	-0.45481900
H	-2.39827000	-2.81994000	-0.69624500
C	-4.83337700	-0.53478800	-0.11553800
H	-4.48934700	1.50677400	0.48486800
H	-4.85733600	-2.60319300	-0.73060300
H	-5.91339700	-0.42637100	-0.12332200
N	1.22486100	-2.20079000	0.09376500

O	-0.15720800	-2.25007400	0.09870600
N	0.37438300	-0.13882900	-0.13806300
C	2.86387500	-0.39156900	-0.11186400
C	3.05006900	0.98204400	-0.29312600
C	3.96973100	-1.24285500	-0.00053100
C	4.34065500	1.50232400	-0.36550900
H	2.18755700	1.63686600	-0.37537500
C	5.25555600	-0.71622200	-0.07249100
H	3.82138900	-2.30932000	0.14149600
C	5.44319900	0.65568900	-0.25581400
H	4.48400000	2.56912100	-0.50709400
H	6.11270800	-1.37699500	0.01323500
H	6.44837500	1.06256300	-0.31293300
N	-1.17652700	2.32859600	-0.37272500
F	-0.28812900	1.21901100	2.57359400
H	-0.36819100	1.76513800	-0.62610700
C	-1.99892800	2.61846800	-1.54398500
H	-1.38338000	3.19674700	-2.23718700
H	-2.36800100	1.72369500	-2.06367700
H	-2.85398200	3.23334700	-1.24634300
H	-2.50191500	2.25589100	1.09175800

Energy -974.3391197 a.u NIMAG = 0

TS-6

C	0.54348500	0.16731900	0.05718600
C	-1.57650900	0.30427200	0.12296200
N	1.13801300	0.22889500	-1.62302100
H	1.42189600	1.18732800	-1.87192000
C	1.85595700	-0.27708200	0.61785700
C	2.75693100	-0.71560900	-0.34987400
C	2.17477000	-0.31384200	1.96930100
C	4.01497200	-1.19208400	0.01796900
C	3.43057900	-0.78698000	2.34949900
H	1.45651300	0.02944200	2.70897500
C	4.33447500	-1.22090500	1.37562800
H	4.72777000	-1.53464100	-0.72440400
H	3.70587000	-0.81466500	3.39855400
H	5.31210500	-1.58496900	1.67732000
N	-1.22903100	1.56579700	0.22028000
O	0.19342400	1.47870000	0.32232000
N	-0.56961900	-0.60411200	0.11153200
H	0.40531900	-0.08633700	-2.26367800
C	-3.00239200	-0.08675100	0.07727200
C	-3.34497500	-1.43838600	-0.01901400
C	-4.00955600	0.88409400	0.14329700
C	-4.68655300	-1.81688000	-0.04531300
H	-2.56011300	-2.18666600	-0.06964600
C	-5.34713500	0.50186700	0.11170800
H	-3.74321200	1.93414400	0.22000800
C	-5.68861000	-0.84923700	0.01903000

H	-4.94771500	-2.86853000	-0.11614400
H	-6.12466400	1.25822000	0.16347500
H	-6.73326500	-1.14545400	-0.00166900
C	3.16637100	-0.39674400	-2.76424800
H	3.68095900	0.56628200	-2.64162000
H	3.89782800	-1.20461100	-2.80730500
H	2.59843900	-0.39911500	-3.69605300
N	2.24428800	-0.66013200	-1.66262800
F	1.71232200	3.54768500	0.19837100
H	1.12757500	2.79935300	0.23751600

Energy -974.30191670 a.u NIMAG = 1, ν_I (cm^{-1}) = 209i

TS-6´

C	-0.71841000	0.04671300	0.19265700
C	1.38359500	0.35077900	0.09401800
N	-1.19190200	-1.07808100	1.54497800
H	-1.46611100	-0.47410800	2.32839600
C	-2.06897400	0.02339200	-0.44393800
C	-2.91383300	-0.96475300	0.04740900
C	-2.47551700	0.86475900	-1.47463500
C	-4.19644500	-1.13266300	-0.47118200
C	-3.75820900	0.71357200	-1.99861900
H	-1.80023800	1.62666900	-1.85537500
C	-4.60540900	-0.28028900	-1.49510700
H	-4.85394200	-1.90429100	-0.08252800
H	-4.09937100	1.36558400	-2.79582800
H	-5.60360200	-0.39255600	-1.90778100
N	1.02083400	1.32167400	0.89515900
O	-0.40175300	1.20589400	0.88847900
N	0.38552400	-0.40783500	-0.43146800
C	2.80828900	0.10841500	-0.21807700
C	3.16241700	-1.01538400	-0.97089800
C	3.80206700	0.98463800	0.23537700
C	4.50170400	-1.26105000	-1.26925200
H	2.38714600	-1.69148600	-1.31767700
C	5.13819100	0.73386700	-0.06316400
H	3.52649600	1.85884500	0.81764300
C	5.49081500	-0.38889900	-0.81599900
H	4.77163500	-2.13500800	-1.85424900
H	5.90543400	1.41563700	0.29107600
H	6.53410400	-0.58198200	-1.04776700
N	-2.32331400	-1.77267300	1.03932200
F	-1.79506100	3.34847800	1.14039100
H	-1.28314900	2.55345100	1.03892600
H	-2.95312100	-2.06367500	1.78595100
C	-0.11408900	-1.98490800	1.94612000
H	0.26322700	-2.48471400	1.05294400
H	0.67686400	-1.38953900	2.40698800
H	-0.49095500	-2.71701200	2.66372300

Energy -974.3071133 a.u NIMAG = 1, ν_I (cm^{-1}) = 138i

Int-5

C	-0.10718800	0.04785600	-0.03175200
C	-0.10787000	-0.00123700	2.24286300
N	1.20120400	-0.03727700	-0.63685300
H	1.78196800	-0.75924300	-0.20878900
C	-0.96995700	0.41761500	-1.19307500
C	-0.24391000	0.15452300	-2.35243500
C	-2.27835900	0.87914200	-1.23212500
C	-0.80455300	0.38777900	-3.61059600
C	-2.85277000	1.10414800	-2.48238900
H	-2.82741400	1.06940700	-0.31366600
C	-2.11551500	0.85980400	-3.65043900
H	-0.24888200	0.20352100	-4.52415100
H	-3.87022300	1.47406000	-2.55485900
H	-2.57610800	1.04548700	-4.61654200
N	-0.36028800	-1.23073800	1.94239700
O	-0.57702400	-1.22673600	0.53480000
N	-0.13935500	0.85337700	1.16659200
C	0.14602700	0.44694500	3.62261000
C	0.03844800	1.80104500	3.95388000
C	0.48721400	-0.49239900	4.60327100
C	0.26751200	2.21233000	5.26563600
H	-0.23629800	2.53190100	3.19854000
C	0.71407500	-0.07449700	5.90999600
H	0.58022600	-1.54087400	4.33660000
C	0.60443200	1.27749100	6.24334200
H	0.18039000	3.26369800	5.52163400
H	0.98141800	-0.80301800	6.66927900
H	0.78395400	1.60046600	7.26450900
N	1.02920600	-0.33694000	-2.04078400
H	0.43418000	1.69127300	1.17063600
C	2.14690600	0.17468500	-2.82716000
H	1.99245400	-0.10418800	-3.87107200
H	2.23483700	1.26619900	-2.73923300
H	3.06747500	-0.29679700	-2.47794500
F	0.36122600	-3.34781300	-0.41724200
H	-0.01318200	-2.53466500	-0.05968200

Energy -974.32368381 a.u NIMAG = 0

TS-7

C	-0.19614900	-0.11580000	0.07212400
C	-0.11755700	0.02071600	2.44103500
N	0.73194500	-0.02720400	-0.90152000
H	1.72847100	-0.02987000	-0.69741400
C	-1.41788500	-0.55185500	-0.59073300
C	-1.03973600	-0.91457700	-1.88753400
C	-2.73411600	-0.68439000	-0.14713300
C	-1.98006900	-1.38685400	-2.80950500

C	-3.67048400	-1.16663600	-1.05077700
H	-3.01057100	-0.41351800	0.86784800
C	-3.28980400	-1.50882000	-2.36374300
H	-1.69989700	-1.65424200	-3.82283800
H	-4.70659500	-1.27979300	-0.74924600
H	-4.04440900	-1.87893800	-3.05144300
N	-0.02052900	-1.25868400	2.43030400
O	0.12765500	-1.71902800	1.15449100
N	-0.10314800	0.69596400	1.20433200
C	-0.21980000	0.81012300	3.68173800
C	-0.64931100	2.14127700	3.63723400
C	0.11072900	0.23000900	4.91449900
C	-0.75183200	2.88249900	4.81423400
H	-0.91593100	2.59519900	2.68728800
C	0.00113900	0.97272900	6.08509300
H	0.45747400	-0.79818400	4.94683800
C	-0.42919100	2.30138600	6.03891500
H	-1.08786100	3.91409400	4.77102900
H	0.25917300	0.51679000	7.03634800
H	-0.50801500	2.87946600	6.95483500
N	0.32716400	-0.72007700	-2.05671900
H	0.59398900	1.43453300	1.13063400
C	0.83462900	-0.14272200	-3.29989200
H	0.52713200	-0.79098700	-4.12096500
H	0.44717100	0.87128000	-3.45403800
H	1.92487100	-0.12661000	-3.25774400
F	-1.17297700	-3.67230300	0.77560600
H	-0.61772600	-2.82481800	0.95463300

Energy -974.30720031 a.u NIMAG = 1, ν_I (cm^{-1}) = 322i

TS-7zw

C	0.00133900	0.11466300	-0.00343600
C	0.04735000	-0.04109100	2.22682500
N	0.98303700	-0.10795100	-1.16375900
H	1.52639900	0.76369900	-1.30189700
C	-1.26175700	0.32821100	-0.71761600
C	-1.08351100	0.03194600	-2.06681800
C	-2.48991500	0.76230400	-0.22845800
C	-2.12195100	0.17507400	-2.98257200
C	-3.54015500	0.90439100	-1.13078000
H	-2.61449400	0.99068900	0.82598800
C	-3.35057800	0.61387900	-2.48901400
H	-1.98714300	-0.04662500	-4.03567500
H	-4.50924300	1.24740200	-0.78407800
H	-4.17829700	0.73634100	-3.18093400
N	-0.41529200	-1.25401500	2.12432900
O	-0.58547800	-1.62351000	0.83133800
N	0.53090000	0.56059600	1.08691800
C	0.24718500	0.59152800	3.54769200
C	0.94914900	1.79750000	3.64159900

C	-0.27555900	0.00615600	4.70893800
C	1.14118700	2.40349400	4.88308400
H	1.34403900	2.25636200	2.74029900
C	-0.08293700	0.61467500	5.94542600
H	-0.83543600	-0.92122700	4.63612500
C	0.62705900	1.81448000	6.03730600
H	1.68992100	3.33856600	4.94602400
H	-0.49359600	0.15599900	6.84012800
H	0.77171400	2.28883200	7.00352600
N	0.22061900	-0.44666500	-2.33199800
C	0.88495800	-0.04178400	-3.57011300
H	0.28480500	-0.40994800	-4.40244200
H	0.98864400	1.04903800	-3.63542700
H	1.86479200	-0.51980700	-3.61190800
H	1.64310700	-0.86156000	-0.93173700
F	0.27442900	-3.82140600	0.56674600
H	-0.10187100	-2.85945900	0.68251800

Energy -974.26257133 a.u NIMAG = 1, ν_I (cm^{-1}) = 315i

TS-PT1

C	0.13642300	-0.04050500	-0.08472600
C	0.06103000	-0.05851600	2.12273400
N	1.61320300	-0.01456300	-0.50269100
H	2.09668500	-0.90866600	-0.35833700
C	-0.52498200	0.45710700	-1.32586800
C	0.43841300	0.70016600	-2.30231200
C	-1.87722700	0.67237000	-1.56903500
C	0.07244900	1.15779100	-3.56817800
C	-2.25420600	1.13045200	-2.82944900
H	-2.61683800	0.48644600	-0.79476300
C	-1.28375000	1.36374300	-3.81326800
H	0.81607100	1.34645100	-4.33545300
H	-3.30130900	1.30855000	-3.05100400
H	-1.59372700	1.71720700	-4.79215800
N	-0.32083100	-1.26725600	1.82132300
O	-0.35488800	-1.27557500	0.38104200
N	0.30175800	0.79651000	1.08518500
H	1.54333800	0.77385400	0.53502800
C	0.23887300	0.35224600	3.53116900
C	0.40587200	1.70615000	3.83658300
C	0.24239200	-0.60172200	4.55601000
C	0.56830800	2.10467600	5.16238600
H	0.40044300	2.44094800	3.03716200
C	0.40546100	-0.19821100	5.87753000
H	0.12444800	-1.65392800	4.31497100
C	0.56795500	1.15491700	6.18336600
H	0.69494900	3.15741300	5.39624400
H	0.41026300	-0.94033300	6.67032200
H	0.69619700	1.46651200	7.21582700
C	2.58910500	-0.42330300	-2.67498400

H	2.14191900	-1.42076800	-2.78219300
H	2.70299900	0.03736600	-3.65702600
H	3.57624600	-0.50129200	-2.21561900
N	1.75624900	0.45537000	-1.85034500
F	-2.38568000	-2.56667800	-0.45602400
H	-1.63267800	-2.06077500	-0.15903100

Energy -974.2562584 a.u NIMAG = 1, ν_I (cm^{-1}) = 1768i

Product Complex (2m +HF)

C	-0.01523900	0.09549200	0.00971300
C	-0.01239000	0.05934200	2.48335600
N	0.60098000	0.12742600	1.24531800
N	0.48726100	0.62756200	3.52467100
O	1.61998800	1.37745500	3.19147800
C	-1.22296400	-0.77673500	2.68573300
C	-2.23782100	-0.33166000	3.53615100
C	-1.33007300	-2.02643900	2.06527600
C	-3.35516400	-1.13285800	3.76662200
H	-2.15282500	0.64348600	4.00629900
C	-2.44684400	-2.82350600	2.29856200
H	-0.54121200	-2.37390700	1.40312200
C	-3.46217800	-2.37804100	3.14805100
H	-4.14369100	-0.78061500	4.42483100
H	-2.52633700	-3.79308700	1.81593400
H	-4.33452500	-3.00016200	3.32581800
C	0.71153600	0.02548600	-1.24279700
C	2.06356400	-0.00462200	-1.60336900
C	-0.29385700	-0.00416700	-2.21328900
C	2.36421500	-0.03542800	-2.95719900
C	-0.00268100	-0.03292900	-3.58000600
C	1.34157800	-0.04210700	-3.92836200
H	2.84720500	0.00190200	-0.85081800
H	3.40054700	-0.05232300	-3.27890000
H	1.61349600	-0.05634000	-4.97956000
H	-0.78660800	-0.04523700	-4.33068800
F	-2.22975400	-2.59120500	-1.49646100
H	1.95301100	1.68280700	4.04695800
H	1.54398800	0.50248700	1.24942800
N	-1.30502900	0.12079400	-0.17574500
N	-1.52249300	-0.04720000	-1.54688100
H	-1.97089700	-1.66460400	-1.54825400
C	-2.70031900	0.64439100	-2.07367500
H	-2.86984000	0.30569200	-3.09690400
H	-3.55848200	0.37342200	-1.45742500
H	-2.55232600	1.72863200	-2.05588800

Energy -974.33845664 a.u NIMAG = 0

TS-2a

C	0.08253900	0.11061400	-0.00328700
C	0.03665200	0.02461100	2.09380700
C	1.78746000	0.09277800	-1.78720600
N	0.89138200	-0.01800200	1.02183300
N	2.60291600	-1.39691600	-1.02538000
H	2.51554300	-1.20950700	-0.02212000
N	3.99272100	-1.43140800	-1.34048300
N	-1.22051900	0.17635900	1.76813800
O	-1.19720100	0.23645700	0.37786300
C	0.48863600	-0.09605500	3.49155500
C	-0.44425100	-0.19239800	4.53126700
C	1.85727600	-0.11119200	3.77688100
C	-0.00632600	-0.29878200	5.84750500
H	-1.50674700	-0.18773800	4.30666300
C	2.28982900	-0.21731000	5.09759400
H	2.57653200	-0.03472500	2.96714800
C	1.36089100	-0.31028200	6.13347400
H	-0.73199800	-0.37492400	6.65155100
H	3.35335300	-0.22557000	5.31623900
H	1.70032400	-0.39237200	7.16178100
C	0.40158100	0.07840500	-1.40408200
C	-0.60067200	-0.10939200	-2.37276600
C	-0.32422300	-0.21562300	-3.71932400
C	2.01460300	0.09093100	-3.19235500
C	1.02579400	-0.09857600	-4.13531400
F	2.61601900	0.95585500	-1.09234000
H	4.06716500	-1.52112000	-2.35397100
F	3.30295700	0.25464000	-3.60297000
O	1.43214800	-0.12431200	-5.42014500
C	0.43461100	-0.28576000	-6.42722800
H	-0.28746100	0.53608000	-6.40079800
H	0.97045800	-0.27045300	-7.37576400
H	-0.08366400	-1.24322600	-6.31467700
H	4.38134300	-2.28843700	-0.94239000
C	1.86490600	-2.60645500	-1.39910500
H	0.84057800	-2.53171800	-1.02898400
H	1.86161200	-2.68355200	-2.49092400
H	2.34724900	-3.48741300	-0.96712300
H	-1.11864100	-0.36470400	-4.43786600
H	-1.63204600	-0.17289000	-2.03820000

Energy -1187.96567535 a.u NIMAG = 1, ν_I (cm^{-1}) = 295i

TS-3a

C	0.12813300	0.14103300	0.01704100
C	0.06212900	0.04240300	2.11250200
C	1.84195900	0.12881700	-1.76196100
N	0.92755100	0.00938400	1.04892000
N	2.58654800	-1.41888300	-1.07624700
H	2.37471100	-1.38264700	-0.07374800
N	3.99272400	-1.56468300	-1.23804200

N	-1.19245100	0.19208500	1.77602600
O	-1.15589600	0.26023800	0.38648800
C	0.50120800	-0.08209400	3.51403700
C	-0.44124700	-0.18481600	4.54449800
C	1.86711400	-0.09284900	3.81241800
C	-0.01563800	-0.29261800	5.86464400
H	-1.50156300	-0.18342100	4.30967600
C	2.28729600	-0.20061700	5.13698400
H	2.59376000	-0.01157800	3.00980500
C	1.34880600	-0.29943300	6.16370500
H	-0.74864800	-0.37340600	6.66154700
H	3.34871200	-0.20548400	5.36576400
H	1.67864200	-0.38243300	7.19506600
C	0.45675100	0.12972800	-1.38224800
C	-0.54262300	-0.00218000	-2.36545300
C	-0.25920900	-0.06146500	-3.71254700
C	2.07975800	0.17748400	-3.16382900
C	1.09671000	0.03985500	-4.11850700
F	2.69993600	0.92761100	-1.03007500
H	4.17590900	-1.46339800	-2.23480600
H	2.05743300	-2.19316000	-1.49717300
C	4.43474600	-2.88880000	-0.79641600
H	5.50219100	-2.97534300	-1.01123600
H	4.28669700	-2.97516000	0.28341000
H	3.89809100	-3.70489300	-1.29991300
F	3.38248700	0.28330100	-3.54676100
O	1.51060000	0.03877200	-5.40104000
C	0.51478500	-0.05307200	-6.41872600
H	-0.18088900	0.78989500	-6.36478400
H	1.05676700	-0.01878500	-7.36325000
H	-0.03424900	-0.99712600	-6.34596400
H	-1.57788300	-0.05364800	-2.04129100
H	-1.05227100	-0.16509700	-4.44063700

Energy -1187.95869238 a.u NIMAG = 1, ν_I (cm^{-1}) = 315i

TS-2b

C	0.04590900	0.07859600	-0.01558200
C	0.03131100	0.03675500	2.08087100
C	1.76131400	0.03998900	-1.79154200
N	0.86382400	-0.07239500	0.99527700
N	2.57374700	-1.49057000	-1.02704900
H	2.49107200	-1.30715200	-0.02350100
N	3.95989500	-1.53014800	-1.35178200
N	-1.22154300	0.24583600	1.77107500
O	-1.22004900	0.27512500	0.38178800
C	0.50201500	-0.07627200	3.47136400
C	-0.41530300	-0.10877400	4.52867100
C	1.87347600	-0.14884500	3.73282500
C	0.04156700	-0.21073600	5.83874600
H	-1.48063200	-0.05957600	4.32376500

C	2.32486200	-0.24990500	5.04755900
H	2.58100700	-0.12129600	2.90974400
C	1.41163500	-0.28047500	6.10083800
H	-0.67202300	-0.23792200	6.65676900
H	3.39077300	-0.30295000	5.24781500
H	1.76552100	-0.35941200	7.12460800
C	0.37567100	0.02791400	-1.41619700
C	-0.58775500	-0.19015700	-2.41637800
C	-0.27848200	-0.30028200	-3.74613100
C	2.02200500	0.04676300	-3.19317300
C	1.06532500	-0.15854900	-4.16239500
F	2.58218900	0.88096200	-1.08208700
H	4.02832900	-1.61831100	-2.36593900
F	3.30548400	0.25160300	-3.57730300
F	-1.25587800	-0.58502400	-4.63416600
F	-1.87730400	-0.32482300	-2.07127800
O	1.47960900	-0.21342300	-5.44226200
C	0.60660700	0.28502000	-6.47313600
H	0.09583800	1.19030500	-6.13503300
H	1.25964200	0.52124700	-7.31298500
H	-0.11558600	-0.47788800	-6.76691700
H	4.35046400	-2.38941700	-0.96000000
C	1.81987800	-2.68600400	-1.40974800
H	0.79681400	-2.60253700	-1.03611800
H	1.81308300	-2.75574000	-2.50248200
H	2.28820700	-3.57994000	-0.98775600

Energy -1386.36020184 a.u NIMAG = 1, ν_I (cm^{-1}) = 294i

TS-3b

C	0.05128300	0.17153500	0.00792200
C	0.06263800	0.09790200	2.10305100
C	1.75581400	0.10357400	-1.77645700
N	0.87152500	-0.04473400	1.00514300
N	2.47750100	-1.49464100	-1.10646400
H	2.25389000	-1.46341600	-0.10689900
N	3.88314300	-1.65234700	-1.25291100
N	-1.18004800	0.38317200	1.81306200
O	-1.19397300	0.43606700	0.42294600
C	0.55402400	-0.05637100	3.48352600
C	-0.32286400	0.05062800	4.56964200
C	1.91202600	-0.30691600	3.70132400
C	0.16169500	-0.09403400	5.86613500
H	-1.37728700	0.24532500	4.39755000
C	2.39082500	-0.45113500	5.00209900
H	2.58665900	-0.38467000	2.85420400
C	1.51824700	-0.34512600	6.08463600
H	-0.51987200	-0.01152400	6.70722900
H	3.44590400	-0.64506700	5.16924700
H	1.89338600	-0.45721600	7.09752200
C	0.37335700	0.13666400	-1.39583500

C	-0.60058200	0.00570500	-2.40434900
C	-0.29290800	-0.04987000	-3.73605100
C	2.02060800	0.16437500	-3.17711300
C	1.05827600	0.04873300	-4.15108900
F	2.62203400	0.86352000	-1.03160500
H	4.07812700	-1.56900700	-2.24895900
H	1.94365100	-2.25746800	-1.54176900
C	4.31392500	-2.97160000	-0.78545000
H	5.38258300	-3.06824700	-0.98988900
H	4.15645300	-3.03815800	0.29447600
H	3.77611700	-3.79268200	-1.27941900
F	3.32219500	0.27658100	-3.53386600
F	-1.27401200	-0.24312300	-4.64484000
F	-1.89339600	-0.08889000	-2.05981600
O	1.45336000	0.01326200	-5.43520000
C	0.66349000	0.72952800	-6.40200900
H	0.29604000	1.66744700	-5.97664700
H	1.33944500	0.94248100	-7.23012200
H	-0.16982200	0.11827100	-6.75177600

Energy -1386.35485477 a.u NIMAG = 1, ν_I (cm^{-1}) = 315i

Reactive Complex 2 (5-(2,3-difluoro-4-methoxyphenyl)-3-phenyl-1,2,4-oxadiazole +methylhydrazine)

C	-0.33845600	-1.15220200	0.00990100
C	1.74221500	-1.34225400	-0.07241600
C	-2.13221200	0.55555900	-0.21904700
N	0.71689900	-0.44835200	-0.28049200
N	2.77756600	3.00474600	0.54980400
H	3.45084600	2.78458700	-0.17893500
N	1.48481900	2.75285100	0.00024300
N	1.34182400	-2.52459600	0.31452400
O	-0.03745600	-2.40347600	0.37544400
H	1.24578900	1.75856900	0.06641500
C	3.15801300	-0.98547100	-0.25563800
C	4.16376100	-1.71448800	0.38923200
C	3.48771900	0.11270800	-1.05629200
C	5.49495000	-1.33841000	0.23492900
H	3.90115000	-2.55839200	1.02041100
C	4.82226000	0.48342600	-1.20659900
H	2.70042000	0.67132700	-1.55579100
C	5.82562400	-0.23850600	-0.55955700
H	6.27518600	-1.89761000	0.74203600
H	5.07773200	1.33754200	-1.82672200
H	6.86488500	0.05578300	-0.67214400
C	-1.74364100	-0.77168100	-0.00762200
C	-2.75336400	-1.71993000	0.19214800
C	-4.09755800	-1.37047500	0.17996500
C	-3.46390100	0.91161100	-0.23081900
C	-4.47379200	-0.03914700	-0.03333000
H	-2.48249700	-2.75717600	0.35785100
H	-4.84846700	-2.13508300	0.33432500

F	-1.23011400	1.52543300	-0.40694100
C	3.06847000	2.20076100	1.73145500
H	4.11698700	2.34415900	2.01066600
H	2.43857800	2.53527500	2.56222400
H	2.88889800	1.12519000	1.57087100
H	0.80740500	3.26190200	0.56345800
F	-3.79422900	2.19558600	-0.43028700
O	-5.72774900	0.42749300	-0.06875500
C	-6.78615900	-0.51081500	0.14113700
H	-7.70722700	0.06571500	0.07223300
H	-6.77360400	-1.28488800	-0.63205800
H	-6.70669000	-0.96485700	1.13347600

Energy -1187.98990376 a.u NIMAG = 0

Reactive Complex 3 (3-phenyl-5-(2,3,5,6-tetrafluoro-4-methoxyphenyl)-1,2,4-oxadiazole + methylhydrazine)

C	-0.09854700	-0.98584600	0.06378100
C	1.96561000	-1.28798800	-0.00553800
C	-1.74792900	0.87642800	-0.03514000
N	0.98529200	-0.36802100	-0.29890300
N	3.36123200	3.04139900	0.27632200
H	3.95535000	2.73445700	-0.48914900
N	2.01550000	2.79858000	-0.13137600
N	1.50591000	-2.40345900	0.49818800
O	0.13670900	-2.20715200	0.55141900
H	1.75356100	1.82060400	0.02724200
C	3.39616200	-1.02283700	-0.22311800
C	4.36673000	-1.75199600	0.47404300
C	3.77855900	-0.01272000	-1.11159000
C	5.71504800	-1.46356500	0.28397700
H	4.06493600	-2.52605100	1.17337500
C	5.13024200	0.26926500	-1.29820700
H	3.02003200	0.54920800	-1.65010400
C	6.09851300	-0.45202000	-0.59932000
H	6.46742100	-2.02286100	0.83132700
H	5.42573700	1.05424700	-1.98788700
H	7.15108500	-0.22620000	-0.74112100
C	-1.47058600	-0.49560800	0.01386300
C	-2.57758100	-1.34243800	0.00962100
C	-3.88181700	-0.87391200	-0.04238900
C	-3.03964000	1.35142900	-0.07872600
C	-4.15510000	0.49818000	-0.08419200
F	-0.75897400	1.77098500	-0.02005700
C	3.73288100	2.32627600	1.49226600
H	4.80538900	2.45439100	1.66804600
H	3.18863800	2.75042000	2.34230800
H	3.50947800	1.24831500	1.43996700
H	1.41013900	3.36929700	0.45453700
F	-3.24551100	2.67240500	-0.11070600
O	-5.34179100	1.09938300	-0.13342300

C	-6.55782800	0.33283800	-0.06655100
H	-7.35307400	1.07615500	-0.07394900
H	-6.65051000	-0.31850700	-0.93696800
H	-6.59697800	-0.24317200	0.85997600
F	-2.41453100	-2.66676600	0.03263100
F	-4.86036000	-1.79112800	-0.06051900

Energy -1386.38213879 a.u NIMAG = 0

TS-8

C	-0.38472200	-0.64322600	0.22898200
C	-2.39045400	-0.29694000	-0.35456300
N	-0.30005300	-1.25839600	1.93533900
C	1.06513900	-0.30409000	0.01178000
C	1.60841900	0.82768700	0.61706800
C	1.94543700	-1.04826300	-0.77356400
C	2.92390300	1.22019100	0.43814600
C	3.26012600	-0.65687700	-0.97053500
C	3.78943300	0.49312200	-0.38299500
N	-2.20417100	-1.53991800	-0.72425000
O	-0.82439300	-1.75554400	-0.44058300
N	-1.31627600	0.34626700	0.16652700
H	0.15138900	-0.53262000	2.50050300
C	-3.71178100	0.35237700	-0.49400200
C	-3.91938700	1.61828700	0.06212400
C	-4.75923600	-0.29153500	-1.16499500
C	-5.16344600	2.23723200	-0.05352700
H	-3.10415700	2.11176900	0.58218600
C	-6.00014000	0.32889300	-1.27625400
H	-4.59841200	-1.27325000	-1.60080500
C	-6.20531600	1.59452800	-0.72155500
H	-5.31750400	3.22081600	0.38025100
H	-6.80867000	-0.17416000	-1.79808400
H	-7.17420200	2.07678700	-0.81236400
N	0.48922400	-2.44342100	2.05826700
H	0.14114700	-3.09326100	1.34947600
F	0.86459300	1.56319000	1.45527200
H	1.44792900	-2.20614300	1.80105200
C	-1.64301200	-1.50030500	2.48885100
H	-2.23241800	-0.59027300	2.37232300
H	-2.10150500	-2.32563300	1.94087100
H	-1.55663000	-1.75901900	3.54588600
F	1.56155900	-2.17600100	-1.38136700
F	4.04542100	-1.40626500	-1.75406700
F	3.36231600	2.30199800	1.09795500
O	5.07952600	0.77944600	-0.60718400
C	5.45641700	2.16573400	-0.72143400
H	5.63272100	2.60117100	0.26311000
H	6.38051000	2.16867400	-1.29845700
H	4.68440000	2.72499200	-1.25630600

Energy -1386.36067683 a.u NIMAG = 1, ν_I (cm^{-1}) = 134i

TS-9

C	0.05011100	0.00469700	-0.01312400
C	0.04243700	-0.00184900	2.34720200
N	0.78458500	0.04521000	1.12956100
N	0.47934600	-0.71352300	-1.05225600
N	0.10692600	-0.33077600	-2.34851700
N	-1.09760100	-0.62063600	2.30804600
O	-1.48168900	-1.02451900	1.12635100
H	-0.39080800	-1.10824700	-2.78209700
C	0.62919500	0.55530600	3.57060000
C	0.00109000	0.37547400	4.81546800
C	1.83169500	1.27391500	3.51792100
C	0.56298500	0.90792700	5.96973700
H	-0.92837200	-0.18295500	4.86772100
C	2.39292500	1.80192800	4.68135600
H	2.32593800	1.42856500	2.56332600
C	1.76288000	1.62375300	5.91107400
H	0.06446500	0.76228900	6.92383500
H	3.32473400	2.35690600	4.62098600
H	2.19855300	2.03646200	6.81602600
C	-0.93927800	1.08890300	-0.24568000
C	-2.15591800	0.82398000	-0.87736400
C	-0.73275500	2.39189100	0.19733200
C	-3.11289800	1.80529700	-1.05170000
C	-1.68900400	3.38268400	0.01595000
C	-2.90243700	3.11223700	-0.60712900
F	-2.43243700	-0.40103000	-1.32520700
H	1.64177700	-0.50520000	1.12483400
F	0.41355100	2.75475300	0.78606900
F	-4.26710600	1.49571900	-1.65525100
F	-1.42275200	4.62777500	0.43346600
O	-3.82682800	4.06880800	-0.83816000
C	-4.52512500	4.51410400	0.34156400
H	-3.83017100	4.95501600	1.06092000
H	-5.23527100	5.26716800	0.00177300
H	-5.05930300	3.67530000	0.79752600
H	0.96182500	-0.16957700	-2.88064800
C	1.31492900	-1.89683400	-0.88207400
H	1.06258900	-2.59696800	-1.68047300
H	2.37897500	-1.64536800	-0.94614900
H	1.09944000	-2.36708400	0.08022200

Energy -1386.34341677 a.u NIMAG = 1, ν_I (cm^{-1}) = 176i

TS-10

C	-0.04922300	-0.13206100	-0.06677700
C	0.04900500	0.01339900	2.32258200
N	0.59352800	-0.07295900	1.04954600
N	0.55804700	0.82374000	3.18810000

O	1.54223200	1.65493600	2.68442800
C	-1.01645900	-0.91861600	2.78553900
C	-1.82174000	-0.57466600	3.87945800
C	-1.23624900	-2.13131300	2.12454400
C	-2.82764400	-1.43590600	4.30696600
H	-1.66458100	0.37554500	4.38058600
C	-2.24676600	-2.99101000	2.55492700
H	-0.61543200	-2.41202200	1.27819100
C	-3.04548400	-2.64581800	3.64421600
H	-3.44893200	-1.15856600	5.15336700
H	-2.40706400	-3.93206500	2.03723800
H	-3.83491500	-3.31412300	3.97520200
C	0.61139500	-0.31584900	-1.35550800
C	1.77439500	0.34864000	-1.74406600
C	-0.29647600	-0.78097800	-2.35216500
C	2.07573900	0.58639900	-3.06524700
C	0.01373300	-0.47454600	-3.69738500
C	1.17273500	0.18341400	-4.07282500
F	-0.79508900	-2.09459700	-2.19847100
H	1.71722800	1.36897500	1.76399800
N	-1.79350100	-0.11400100	-1.61272100
H	-2.57233600	-0.77018600	-1.71645000
H	-2.04659000	0.80100300	-2.00700300
C	-2.32162000	0.79737400	0.56866100
H	-1.76446400	1.29004200	1.36430700
H	-2.77483500	1.57013100	-0.05956700
H	-3.10411300	0.16726900	0.99861100
N	-1.41703500	0.00198100	-0.26065400
F	2.59866200	0.85585800	-0.81381500
F	3.20752700	1.25984700	-3.37833900
F	-0.84742300	-0.90020200	-4.65329700
C	2.69027000	0.32611900	-5.91686600
H	3.20899700	1.27812500	-5.79374200
H	3.25115400	-0.47983500	-5.43617700
H	2.56988400	0.10768800	-6.97785600
O	1.35548900	0.39851900	-5.38721500

Energy -1386.32011789 a.u NIMAG = 1, ν_I (cm^{-1}) = 325i

TS-PT2

C	-0.16961500	0.07270400	-0.31846500
C	-0.04384500	0.31495700	1.81570900
N	1.23317700	0.18090000	-0.96365000
H	1.49422200	-0.77557000	-1.24805500
C	-1.03193600	0.21661600	-1.54138000
C	-0.26186700	0.74435200	-2.57415100
C	-2.38982800	-0.01613200	-1.70048700
C	-0.82299000	1.03204900	-3.81553000
C	-2.96748500	0.26195800	-2.94142700
H	-2.98193700	-0.41078600	-0.87957000

C	-2.18647400	0.77777200	-3.98060200
H	-0.23004700	1.44055200	-4.62724100
H	-4.02455600	0.07721500	-3.10114700
H	-2.64719100	0.98588800	-4.94158200
N	0.07763600	-0.99538300	1.70928000
O	-0.20114300	-1.20861900	0.29624700
N	-0.32496000	1.02349100	0.71414500
H	2.05730100	0.70778300	-0.12708300
C	0.16200700	0.96735600	3.13007300
C	-0.26847500	2.28397700	3.32401400
C	0.83511200	0.30118500	4.16162900
C	-0.03829300	2.92436000	4.53990900
H	-0.77711900	2.80519700	2.51916200
C	1.06751900	0.94613400	5.37463000
H	1.18626300	-0.71460500	4.00870100
C	0.63191900	2.25815400	5.56647800
H	-0.37712700	3.94586600	4.68296300
H	1.59481200	0.42575500	6.16815600
H	0.81710200	2.75982300	6.51143100
C	2.13723600	0.72141700	-3.11002900
H	2.11496300	-0.31896700	-3.46292300
H	2.02196500	1.39851500	-3.95633600
H	3.09631000	0.92682100	-2.63166700
N	1.06934400	0.98399900	-2.14960700
F	-2.15832800	-2.75118700	0.19975100
H	-1.41397500	-2.13092900	0.20453100
N	2.81284700	1.27044000	0.78245900
H	3.78238500	1.29804100	0.46216500
H	2.79258600	0.70371800	1.64121800
N	2.37717700	2.61308600	1.03173900
H	1.35962800	2.54614300	1.09133900
C	2.91061600	3.10233100	2.30165300
H	3.99464800	3.21494600	2.22084700
H	2.47427500	4.08276000	2.50148500
H	2.68409600	2.43228700	3.14444200

Energy -1125.43622134 a.u NIMAG = 1, ν_I (cm^{-1}) = 798i

Ketenimine intermediate

C	0.45003400	0.58494500	0.24900000
C	-1.64488100	-0.45296500	-0.06916200
C	2.79509700	0.03691100	0.53427800
N	-0.69733200	0.38037100	0.59289200
N	2.43524200	-1.37484800	0.33143400
N	3.23427600	-2.28852000	1.07179900
N	-1.14299600	-1.46538300	-0.67050700
O	-2.07263700	-2.26117500	-1.30069300
H	4.23038900	-2.15585100	0.87618100
C	-3.05276600	-0.00678600	0.05752500
C	-4.13942100	-0.89300300	0.01510300

C	-3.29136300	1.36342600	0.24313600
C	-5.43790700	-0.40670100	0.15367400
H	-3.97620900	-1.95552100	-0.10735600
C	-4.59210800	1.84326500	0.36330000
H	-2.45542600	2.05480500	0.29045300
C	-5.66962300	0.95860700	0.31929000
H	-6.27176400	-1.10148000	0.13119400
H	-4.76258500	2.90740100	0.49572200
H	-6.68488600	1.33106000	0.41975000
C	1.70684900	0.92109000	-0.02756600
C	2.01014300	2.09862900	-0.82531400
C	3.28712800	2.38457600	-1.15187000
C	4.16085500	0.44008900	0.07188400
C	4.36947500	1.51911200	-0.70387200
H	1.18213700	2.72110400	-1.15005700
H	3.52089300	3.25614900	-1.75367000
H	5.38259600	1.76273100	-1.01304700
H	4.99145300	-0.18334500	0.39142900
F	2.78000100	0.18479300	1.95123300
C	2.48116800	-1.76887100	-1.07521500
H	1.92568900	-1.05427800	-1.68493900
H	3.51459200	-1.82424600	-1.45162600
H	2.01801200	-2.75294100	-1.16897600
H	3.08299600	-2.10851200	2.05978800
H	-1.53721000	-2.96609100	-1.69487900

Energy -974.20764250 a.u NIMAG = 0

6-membered TS

C	0.05551500	-0.01964700	0.06994400
C	-0.03197400	-0.02995300	2.16538600
C	0.89687200	-0.01120800	-2.28670200
N	-0.81745400	0.03458600	1.04527200
N	1.91502500	-1.59696000	-2.05373500
H	2.32734500	-1.55892900	-1.11816900
N	2.99982600	-1.69867300	-2.97810900
N	1.25037600	-0.11303100	1.91914800
O	1.31610200	-0.10716800	0.52844400
H	2.58159300	-1.73521400	-3.91027400
C	-0.58178100	0.00047900	3.53276000
C	0.24938900	-0.19677900	4.64200300
C	-1.94821800	0.23200800	3.71546300
C	-0.28834100	-0.15983700	5.92504800
H	1.30982700	-0.38160300	4.49745200
C	-2.48081100	0.26836200	5.00272400
H	-2.58628600	0.38482400	2.85055100
C	-1.65327400	0.07322000	6.10792600
H	0.35773900	-0.31559000	6.78369700
H	-3.54223200	0.44983500	5.14166800
H	-2.06928300	0.10123300	7.11066100
C	-0.18747800	-0.03278900	-1.35052100

C	-1.50812800	-0.18609300	-1.81463200
C	-1.80413100	-0.23161100	-3.16250200
C	0.55894100	0.06711100	-3.67503400
C	-0.74668100	-0.07982500	-4.08602600
H	-2.29937100	-0.25847300	-1.07320500
H	-2.82689200	-0.34160800	-3.50412400
H	-0.96508600	-0.04212600	-5.15036800
H	1.36124500	0.24036800	-4.38586400
F	1.99882200	0.76153000	-1.93507700
C	1.04462300	-2.76556600	-2.17195700
H	0.29658500	-2.73000000	-1.37846900
H	0.54802400	-2.72250800	-3.14675100
H	1.62885300	-3.68556300	-2.09406300
H	3.51311500	-0.81808300	-2.92512900

Energy -974.2790464 a.u NIMAG = 1, ν_I (cm^{-1}) = 293i

Thermochemistry (atomic units)

Structure	ZPE	H_{corr}	G_{corr}
React_Complex1 (1m+HF)	0.286596	0.306558	0.236405
TS-1	0.287122	0.305622	0.239543
Int-1	0.287841	0.30646	0.240626
TS-2	0.285361	0.304094	0.238424
Int-2	0.285816	0.305613	0.237271
TS-3	0.285273	0.30385	0.239072
TS-4	0.285984	0.304705	0.238614
Int-3	0.288377	0.306861	0.242131
TS-5	0.287710	0.306029	0.241052
Int-4	0.286397	0.305279	0.238912
Int-4´	0.286106	0.305265	0.237481
TS-6	0.284662	0.303479	0.236203
TS-6´	0.285093	0.303764	0.236633
Int-5	0.285471	0.304262	0.237795
TS-7	0.283322	0.301932	0.236312

TS-7zw	0.283104	0.301794	0.235056
TS-PT1	0.279833	0.298691	0.23009
TS-PT2	0.367196	0.390182	0.315415
2m+HF	0.284202	0.304068	0.235625
React_Complex2	0.311684	0.335209	0.257017
React_Complex3	0.294934	0.320351	0.238225
TS-2a	0.311717	0.33377	0.260515
TS-3a	0.311626	0.333882	0.259649
TS-2b	0.294527	0.317760	0.242908
TS-3b	0.29487	0.319099	0.240879
TS-8	0.296063	0.319759	0.243782
TS-9	0.29453	0.318587	0.242427
TS-10	0.294502	0.318412	0.242075
Ketenimine Intermediate	0.284824	0.304433	0.237278
6-membered TS	0.286050	0.304723	0.238962