Electronic Supplementary Material (ESI) for Catalysis Science & Technology.
This journal is © The Royal Society of Chemistry 2024

Supporting Information

Mechanistic Evidence for the Enantioselectivity of Mannich Reactions with Fluorinated Aromatic Ketones

Cheng Peng, Jian Zhang, Yong Wang,* and Wei Liu*

Suzhou Key Laboratory of Novel Semiconductor-Optoelectronics Materials and Devices, College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou, P. R. China

CONTENTS

Computational Details. ……S2
Figure S1. The investigated Mannich reactions of fluorinated aromatic ketones and the results with Zn/(*R*,*R*)-prophenol. ……S3
Figure S2. Four models for the reaction with Zn/(*R*,*R*)-prophenol between α-fluoroketone and pivalaldehyde and Boc-aldimine, and the resulting products, respectively. ……S3
Figure S3. EDA for the lowest energy **TS**s (reaction with Zn/(*R*,*R*)-prophenol between α-fluoroketone and pivalaldehyde and Boc-aldimine) calculated at M06L(D3)/6-311+G(2d,p)/PCM(diethylether) level of theory. ……S4
Figure S4. IRI vs sign(λ2)ρ scatter plots of transition states. ……S5
Figure S5. IRI analyses of transition states (M06L(D3)/6-311+G(2d,p)/PCM(diethylether) level). The blue, green, and red surfaces indicate strong attraction, weak interaction, and steric effects, respectively. ……S6
Figure S6. Intrinsic reaction coordinate (IRC) for transition states. ……S7
SAPT results of transition states. ……S8-S13
Cartesian coordinates of transition states. ……S14-S29

Total: 29 Pages

1. **Computational Details.**

All calculations were carried out with the Gaussian09 package[S1] at the density functional theory (DFT) B3LYP-D3 functional[S2] level of the theory with zero damping. Considering the solvent effect (solvent = diethylether), geometry optimizations performed using the on polarizable continuum model[S3] (PCM) were employed by using 6-31G(d) basis set[S4] for all atoms without any symmetry constraint. Frequency calculations were employed at the same level of the theory for each transition state. Key transition states were performed to connect corresponding intermediates. For the single point calculations, the energies were obtained by using the M06L functional with zero Becke-Johnson damping and 6-311++G(2d,p) basis set[S5] was utilized. The symmetry-adapted perturbation theory (SAPT) is performed at the SAPT0 + def2-SVP level of theory on the lowest energy geometries. The data of IRI isosurfaces are produced towards the Multiwfn program[S6] and are showed by the VMD program.[S7] The interaction strength is indicated by the color of the isosurface. The blue, green, and red colors represent strong, weak, and repulsive interaction, respectively.

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.;Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, revision D.01 Gaussian, Inc.: Wallingford, CT, 2013

S2 (a) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200. (b) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623. (c) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (d) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B.* **1988**, *37*, 785. (d) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.

S3 Miertuš, S.; Scrocco, E.; Tomasi. *J. Chem. Phys*. **1981**, *55*, 117.

S4 (a) Ditchfield, R.; Hehre, W. J.; Pople, J. A. *J. Chem. Phys.* **1971**, *54*, 724. (b) Hariharan, P. C., Pople, J. A. *Theor. Chim. Acta* **1973**, *28*, 213. (c) Hehre, W. J., Ditchfield, R., Pople, J. A. *J. Chem. Phys*. **1972**, *56*, 2257. (d) Rassolov, Vitaly A., Pople, John A., Ratner, Mark A., Windus, Theresa L. *J. Chem. Phys*. **1998**, *109*, 1223.

S5 (a) Clark, Timothy, Chandrasekhar, Jayaraman, Spitznagel, Günther W., Schleyer, P. Von Ragué

J. Comput. Chem. **1983**, *4*, 294. (b) Krishnan, R., Binkley, J. S., Seeger, R., Pople, J. A. *J. Chem. Phys*. **1980**, *72*, 650.

S6 Lu, T.; Chen, F. W. *J. Comput. Chem.* **2012**, *33*, 580.

S7 Humphrey, W.; Dalke, A.; Schulten, K. *J. Mol. Graphics* **1996**, *14*, 33.

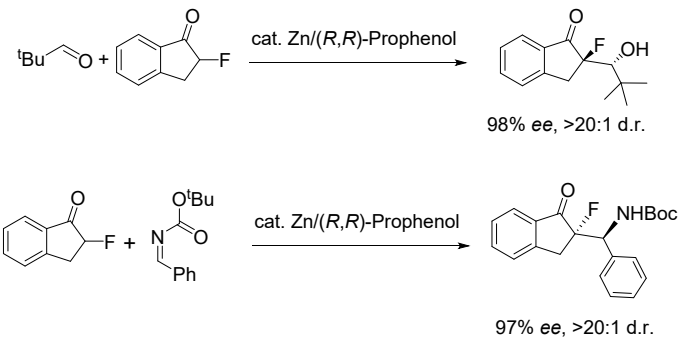


Figure S1. The investigated Mannich reactions of fluorinated aromatic ketones and their results with Zn/(*R*,*R*)-prophenol.

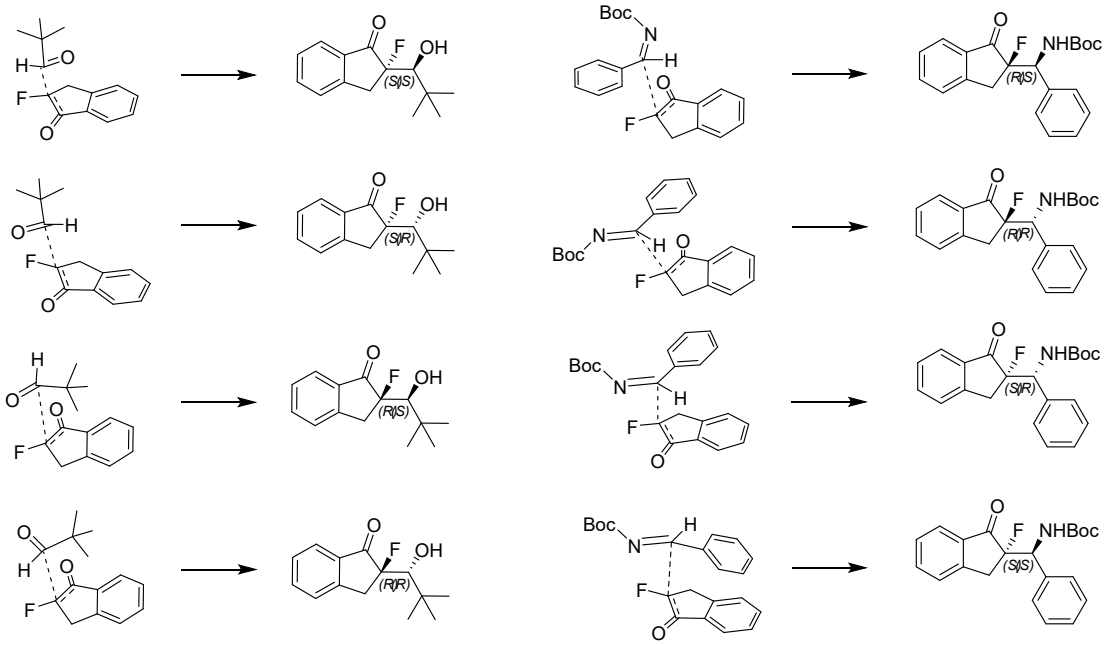


Figure S2. Four models for the reaction with Zn/(*R*,*R*)-prophenol between α-fluoroketone and pivalaldehyde and Boc-aldimine, and the resulting products, respectively.

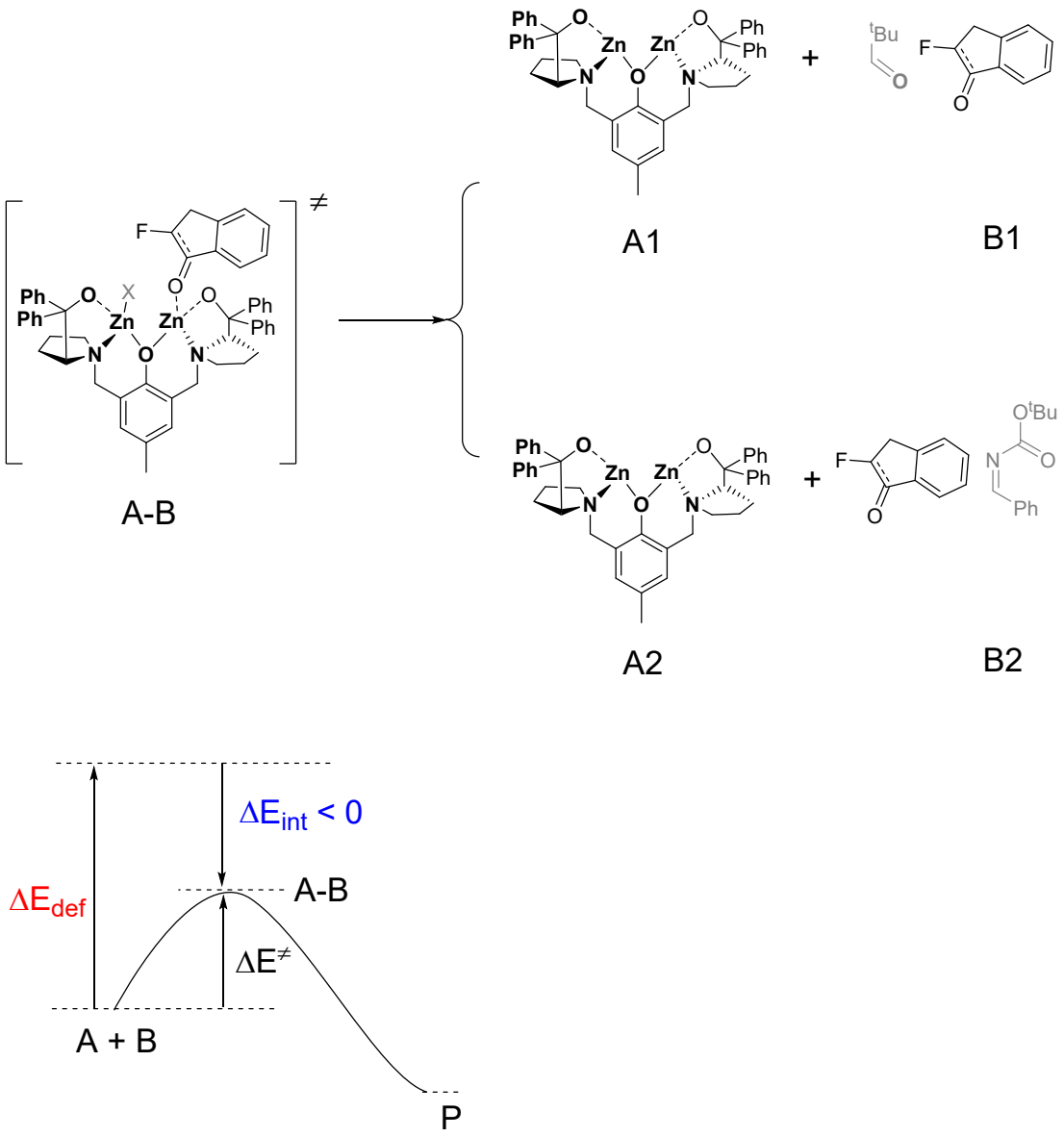


Figure S3. ASM for the lowest energy **TS**s (reaction with Zn/(*R*,*R*)-prophenol between α-fluoroketone and pivalaldehyde and Boc-aldimine) calculated at M06L(D3)/6-311+G(2d,p)/PCM(diethylether) level of theory.

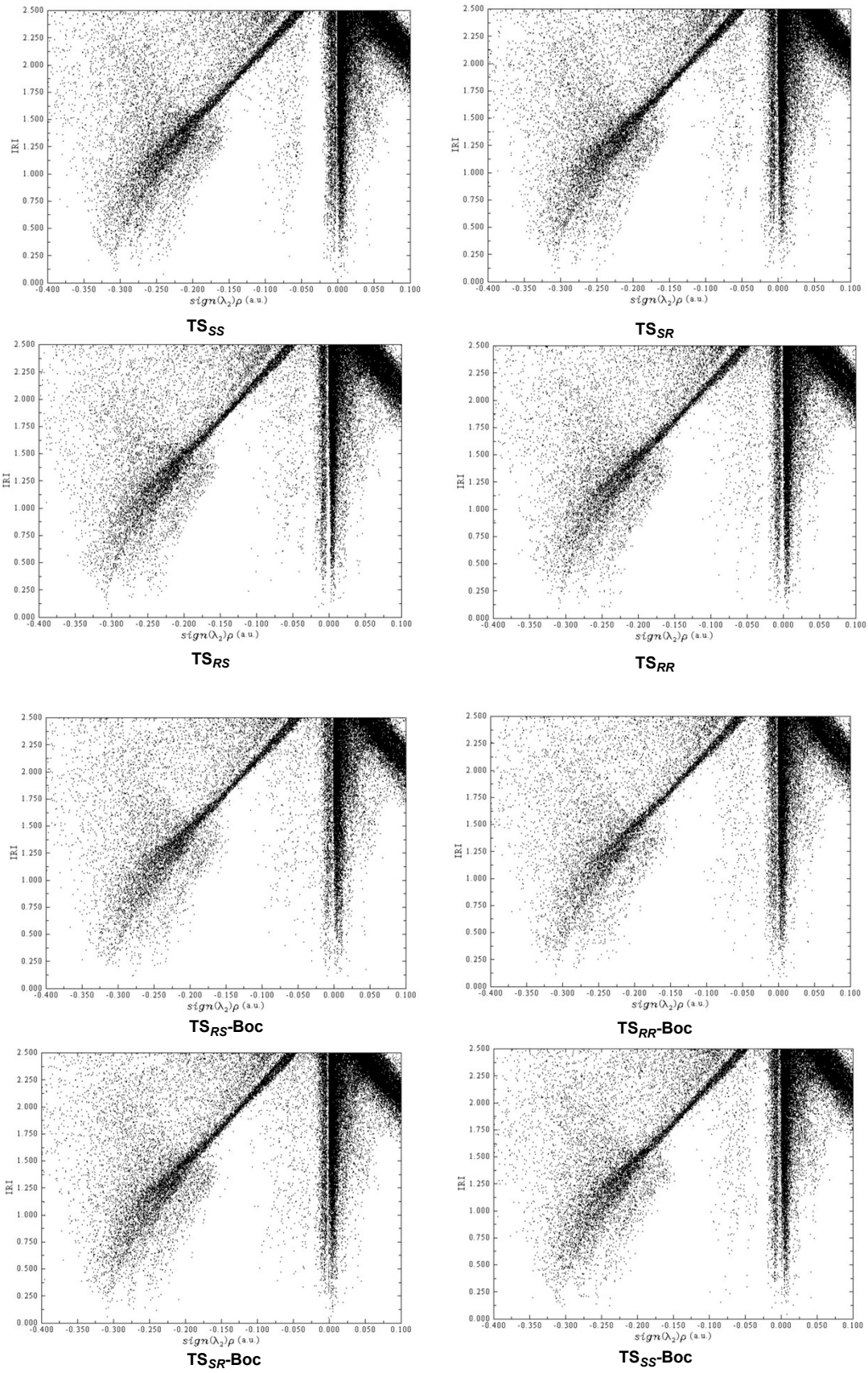


Figure S4. IRI vs sign(λ2)ρ scatter plots of transition states.

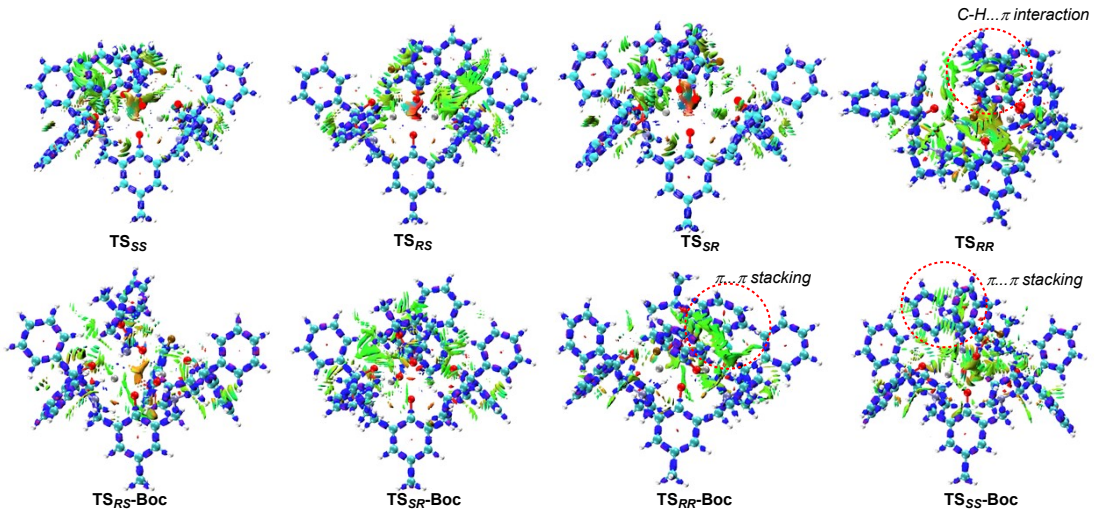
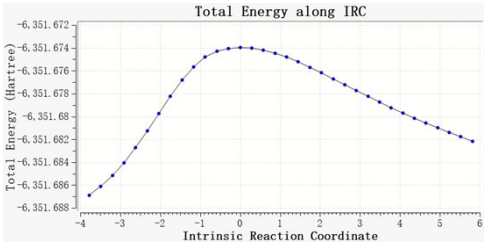
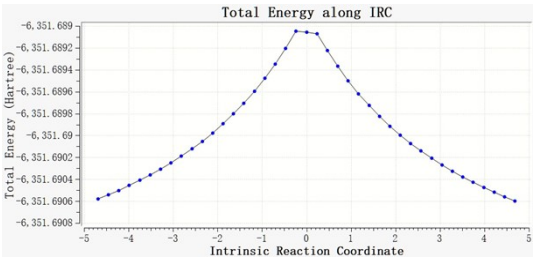


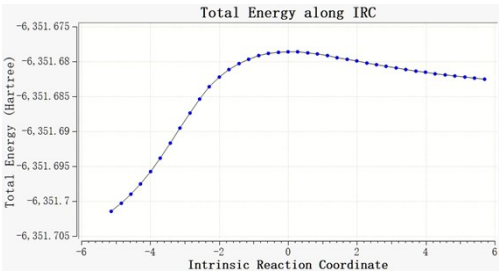
Figure S5. IRI analyses of transition states (M06L(D3)/6-311+G(2d,p)/PCM(diethylether) level). The blue, green, and red surfaces indicate strong attraction, weak interaction, and steric effects, respectively.



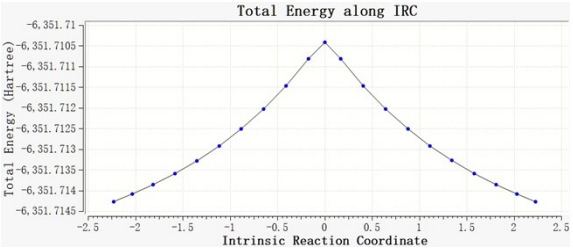
TS_{SS}



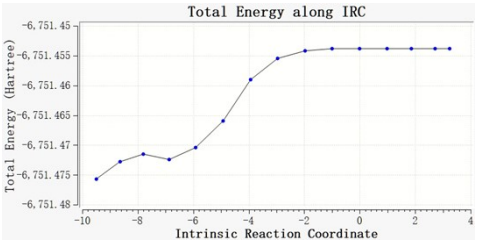
TS_{SR}



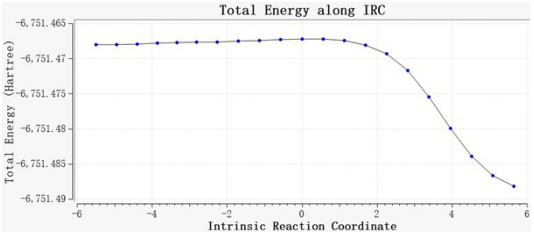
TS_{RS}



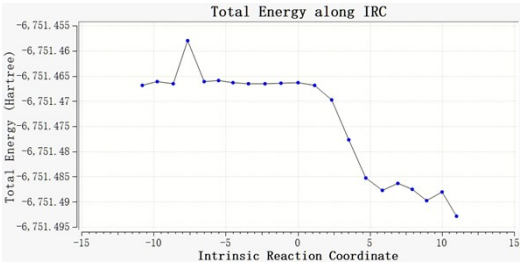
TS_{RR}



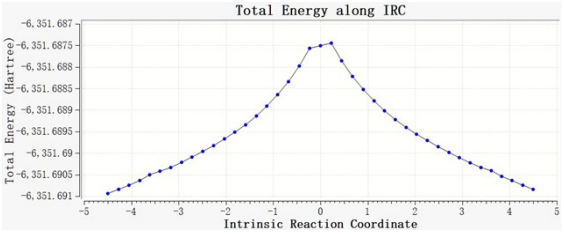
TS_{RS}-Boc



TS_{RR}-Boc



TS_{SR}-Boc



TS_{SS}-Boc

Figure S6. Intrinsic reaction coordinate (IRC) for transition states.

SAPT results of transition states.

TS_{RS} SAPT Results

Electrostatics	-353.05480470 [mEh]	-221.54523471 [kcal/mol]	-926.94526203 [kJ/mol]
Elst10,r	-353.05480470 [mEh]	-221.54523471 [kcal/mol]	-926.94526203 [kJ/mol]
Exchange	213.03781471 [mEh]	133.68324700 [kcal/mol]	559.33070546 [kJ/mol]
Exch10	213.03781471 [mEh]	133.68324700 [kcal/mol]	559.33070546 [kJ/mol]
Exch10(S^2)	209.74866293 [mEh]	131.61927310 [kcal/mol]	550.69503867 [kJ/mol]
Induction	-132.22890520 [mEh]	-82.97489072 [kcal/mol]	-347.16694278 [kJ/mol]
Ind20,r	-480.37943237 [mEh]	-301.44264482 [kcal/mol]	-1261.23602593 [kJ/mol]
Exch-Ind20,r	354.64456106 [mEh]	222.54282189 [kcal/mol]	931.11916678 [kJ/mol]
delta HF,r (2)	-6.49403389 [mEh]	-4.07506779 [kcal/mol]	-17.05008363 [kJ/mol]
Dispersion	-59.51542343 [mEh]	-37.34649204 [kcal/mol]	-156.25772268 [kJ/mol]
Disp20	-73.59468203 [mEh]	-46.18136019 [kcal/mol]	-193.22281105 [kJ/mol]
Exch-Disp20	14.07925860 [mEh]	8.83486816 [kcal/mol]	36.96508837 [kJ/mol]
Disp20 (SS)	-36.79734102 [mEh]	-23.09068010 [kcal/mol]	-96.61140553 [kJ/mol]
Disp20 (OS)	-36.79734102 [mEh]	-23.09068010 [kcal/mol]	-96.61140553 [kJ/mol]
Exch-Disp20 (SS)	7.01326003 [mEh]	4.40088711 [kcal/mol]	18.41331166 [kJ/mol]
Exch-Disp20 (OS)	7.06599858 [mEh]	4.43398105 [kcal/mol]	18.55177671 [kJ/mol]
Total HF	-272.24589519 [mEh]	-170.83687843 [kcal/mol]	-714.78149935 [kJ/mol]
Total SAPT0	-331.76131862 [mEh]	-208.18337047 [kcal/mol]	-871.03922203 [kJ/mol]

Special recipe for scaled SAPT0 (see Manual):

Electrostatics sSAPT0	-353.05480470 [mEh]	-221.54523471 [kcal/mol]	-926.94526203 [kJ/mol]
Exchange sSAPT0	213.03781471 [mEh]	133.68324700 [kcal/mol]	559.33070546 [kJ/mol]
Induction sSAPT0	-115.28194472 [mEh]	-72.34051247 [kcal/mol]	-302.67270417 [kJ/mol]
Dispersion sSAPT0	-58.84263533 [mEh]	-36.92431113 [kcal/mol]	-154.49131778 [kJ/mol]
Total sSAPT0	-314.14157004 [mEh]	-197.12681131 [kcal/mol]	-824.77857852 [kJ/mol]

TS_{SS} SAPT Results

Electrostatics	-372.24417296 [mEh]	-233.58674509 [kcal/mol]	-977.32694147 [kJ/mol]
Elst10,r	-372.24417296 [mEh]	-233.58674509 [kcal/mol]	-977.32694147 [kJ/mol]
Exchange	222.73773134 [mEh]	139.77003658 [kcal/mol]	584.79783306 [kJ/mol]
Exch10	222.73773134 [mEh]	139.77003658 [kcal/mol]	584.79783306 [kJ/mol]
Exch10(S^2)	218.70914583 [mEh]	137.24206101 [kcal/mol]	574.22078326 [kJ/mol]
Induction	-123.99323520 [mEh]	-77.80692977 [kcal/mol]	-325.54419417 [kJ/mol]

Ind20,r	-571.10271285 [mEh]	-358.37236281 [kcal/mol]	-1499.42996600 [kJ/mol]
Exch-Ind20,r	442.13663670 [mEh]	277.44492824 [kcal/mol]	1160.82957974 [kJ/mol]
delta HF,r (2)	4.97284094 [mEh]	3.12050480 [kcal/mol]	13.05619209 [kJ/mol]
Dispersion	-53.48924001 [mEh]	-33.56500485 [kcal/mol]	-140.43598029 [kJ/mol]
Disp20	-67.26730573 [mEh]	-42.21087162 [kcal/mol]	-176.61028687 [kJ/mol]
Exch-Disp20	13.77806572 [mEh]	8.64586677 [kcal/mol]	36.17430657 [kJ/mol]
Disp20 (SS)	-33.63365287 [mEh]	-21.10543581 [kcal/mol]	-88.30514343 [kJ/mol]
Disp20 (OS)	-33.63365287 [mEh]	-21.10543581 [kcal/mol]	-88.30514343 [kJ/mol]
Exch-Disp20 (SS)	6.60542991 [mEh]	4.14496985 [kcal/mol]	17.34255384 [kJ/mol]
Exch-Disp20 (OS)	7.17263581 [mEh]	4.50089692 [kcal/mol]	18.83175273 [kJ/mol]
Total HF	-273.49967683 [mEh]	-171.62363828 [kcal/mol]	-718.07330258 [kJ/mol]
Total SAPT0	-326.98891684 [mEh]	-205.18864313 [kcal/mol]	-858.50928288 [kJ/mol]

Special recipe for scaled SAPT0 (see Manual):

Electrostatics sSAPT0	-372.24417296 [mEh]	-233.58674509 [kcal/mol]	-977.32694147 [kJ/mol]
Exchange sSAPT0	222.73773134 [mEh]	139.77003658 [kcal/mol]	584.79783306 [kJ/mol]
Induction sSAPT0	-99.10818772 [mEh]	-62.19132673 [kcal/mol]	-260.20851102 [kJ/mol]
Dispersion sSAPT0	-52.71376069 [mEh]	-33.07838423 [kcal/mol]	-138.39995961 [kJ/mol]
Total sSAPT0	-301.32839003 [mEh]	-189.08641946 [kcal/mol]	-791.13757904 [kJ/mol]

TS$_{SR}$ SAPT Results

Electrostatics	-377.06235702 [mEh]	-236.61020123 [kcal/mol]	-989.97708196 [kJ/mol]
Elst10,r	-377.06235702 [mEh]	-236.61020123 [kcal/mol]	-989.97708196 [kJ/mol]
Exchange	213.28844615 [mEh]	133.84052061 [kcal/mol]	559.98873823 [kJ/mol]
Exch10	213.28844615 [mEh]	133.84052061 [kcal/mol]	559.98873823 [kJ/mol]
Exch10(S^2)	209.26534971 [mEh]	131.31598947 [kcal/mol]	549.42609996 [kJ/mol]
Induction	-129.13217007 [mEh]	-81.03166009 [kcal/mol]	-339.03646582 [kJ/mol]
Ind20,r	-540.86224806 [mEh]	-339.39618467 [kcal/mol]	-1420.03363665 [kJ/mol]
Exch-Ind20,r	411.55756465 [mEh]	258.25627082 [kcal/mol]	1080.54423712 [kJ/mol]
delta HF,r (2)	0.17251334 [mEh]	0.10825376 [kcal/mol]	0.45293371 [kJ/mol]
Dispersion	-51.37006397 [mEh]	-32.23520181 [kcal/mol]	-134.87208438 [kJ/mol]
Disp20	-64.40049215 [mEh]	-40.41191894 [kcal/mol]	-169.08346885 [kJ/mol]
Exch-Disp20	13.03042818 [mEh]	8.17671713 [kcal/mol]	34.21138447 [kJ/mol]
Disp20 (SS)	-32.20024608 [mEh]	-20.20595947 [kcal/mol]	-84.54173443 [kJ/mol]
Disp20 (OS)	-32.20024608 [mEh]	-20.20595947 [kcal/mol]	-84.54173443 [kJ/mol]
Exch-Disp20 (SS)	6.25609618 [mEh]	3.92575962 [kcal/mol]	16.42537826 [kJ/mol]
Exch-Disp20 (OS)	6.77433200 [mEh]	4.25095751 [kcal/mol]	17.78600621 [kJ/mol]

Total HF	-292.90608093 [mEh]	-183.80134071 [kcal/mol]	-769.02480954 [kJ/mol]
Total SAPT0	-344.27614491 [mEh]	-216.03654253 [kcal/mol]	-903.89689393 [kJ/mol]

Special recipe for scaled SAPT0 (see Manual):

Electrostatics sSAPT0	-377.06235702 [mEh]	-236.61020123 [kcal/mol]	-989.97708196 [kJ/mol]
Exchange sSAPT0	213.28844615 [mEh]	133.84052061 [kcal/mol]	559.98873823 [kJ/mol]
Induction sSAPT0	-104.93651064 [mEh]	-65.84865457 [kcal/mol]	-275.51077073 [kJ/mol]
Dispersion sSAPT0	-50.60399908 [mEh]	-31.75448883 [kcal/mol]	-132.86078128 [kJ/mol]
Total sSAPT0	-319.31442058 [mEh]	-200.37282403 [kcal/mol]	-838.35989574 [kJ/mol]

TS$_{RR}$ SAPT Results

Electrostatics	-365.02499848 [mEh]	-229.05664471 [kcal/mol]	-958.37300148 [kJ/mol]
Elst10,r	-365.02499848 [mEh]	-229.05664471 [kcal/mol]	-958.37300148 [kJ/mol]
Exchange	221.11643406 [mEh]	138.75265718 [kcal/mol]	580.54111766 [kJ/mol]
Exch10	221.11643406 [mEh]	138.75265718 [kcal/mol]	580.54111766 [kJ/mol]
Exch10(S^2)	217.72389501 [mEh]	136.62380679 [kcal/mol]	571.63400760 [kJ/mol]
Induction	-121.29796805 [mEh]	-76.11562410 [kcal/mol]	-318.46777125 [kJ/mol]
Ind20,r	-509.44163696 [mEh]	-319.67945353 [kcal/mol]	-1337.53883356 [kJ/mol]
Exch-Ind20,r	388.68945035 [mEh]	243.90631245 [kcal/mol]	1020.50401131 [kJ/mol]
delta HF,r (2)	-0.54578145 [mEh]	-0.34248303 [kcal/mol]	-1.43294899 [kJ/mol]
Dispersion	-53.05507894 [mEh]	-33.29256466 [kcal/mol]	-139.29609055 [kJ/mol]
Disp20	-67.52137875 [mEh]	-42.37030485 [kcal/mol]	-177.27735548 [kJ/mol]
Exch-Disp20	14.46629981 [mEh]	9.07774018 [kcal/mol]	37.98126492 [kJ/mol]
Disp20 (SS)	-33.76068937 [mEh]	-21.18515242 [kcal/mol]	-88.63867774 [kJ/mol]
Disp20 (OS)	-33.76068937 [mEh]	-21.18515242 [kcal/mol]	-88.63867774 [kJ/mol]
Exch-Disp20 (SS)	7.05940485 [mEh]	4.42984342 [kcal/mol]	18.53446488 [kJ/mol]
Exch-Disp20 (OS)	7.40689496 [mEh]	4.64789676 [kcal/mol]	19.44680004 [kJ/mol]
Total HF	-265.20653247 [mEh]	-166.41961163 [kcal/mol]	-696.29965508 [kJ/mol]
Total SAPT0	-318.26161141 [mEh]	-199.71217630 [kcal/mol]	-835.59574563 [kJ/mol]

Special recipe for scaled SAPT0 (see Manual):

Electrostatics sSAPT0	-365.02499848 [mEh]	-229.05664471 [kcal/mol]	-958.37300148 [kJ/mol]
Exchange sSAPT0	221.11643406 [mEh]	138.75265718 [kcal/mol]	580.54111766 [kJ/mol]
Induction sSAPT0	-102.84389214 [mEh]	-64.53551664 [kcal/mol]	-270.01660162 [kJ/mol]
Dispersion sSAPT0	-52.36825249 [mEh]	-32.86157456 [kcal/mol]	-137.49282796 [kJ/mol]
Total sSAPT0	-299.12070905 [mEh]	-187.70107873 [kcal/mol]	-785.34131341 [kJ/mol]

TS$_{SR}$-Boc SAPT Results

Electrostatics	-390.38090958 [mEh]	-244.96771914 [kcal/mol]	-1024.94493690 [kJ/mol]
Elst10,r	-390.38090958 [mEh]	-244.96771914 [kcal/mol]	-1024.94493690 [kJ/mol]
Exchange	239.92424187 [mEh]	150.55473476 [kcal/mol]	629.92101025 [kJ/mol]
Exch10	239.92424187 [mEh]	150.55473476 [kcal/mol]	629.92101025 [kJ/mol]
Exch10(S^2)	236.15093514 [mEh]	148.18694904 [kcal/mol]	620.01419478 [kJ/mol]
Induction	-136.01213461 [mEh]	-85.34890302 [kcal/mol]	-357.09981022 [kJ/mol]
Ind20,r	-575.12106671 [mEh]	-360.89391793 [kcal/mol]	-1509.98015263 [kJ/mol]
Exch-Ind20,r	439.49101585 [mEh]	275.78477609 [kcal/mol]	1153.88350315 [kJ/mol]
delta HF,r (2)	-0.38208375 [mEh]	-0.23976117 [kcal/mol]	-1.00316074 [kJ/mol]
Dispersion	-67.81940112 [mEh]	-42.55731671 [kcal/mol]	-178.05981312 [kJ/mol]
Disp20	-83.72356682 [mEh]	-52.53733136 [kcal/mol]	-219.81619441 [kJ/mol]
Exch-Disp20	15.90416570 [mEh]	9.98001465 [kcal/mol]	41.75638130 [kJ/mol]
Disp20 (SS)	-41.86178341 [mEh]	-26.26866568 [kcal/mol]	-109.90809721 [kJ/mol]
Disp20 (OS)	-41.86178341 [mEh]	-26.26866568 [kcal/mol]	-109.90809721 [kJ/mol]
Exch-Disp20 (SS)	7.94983544 [mEh]	4.98859706 [kcal/mol]	20.87229008 [kJ/mol]
Exch-Disp20 (OS)	7.95433026 [mEh]	4.99141759 [kcal/mol]	20.88409121 [kJ/mol]
Total HF	-286.46880232 [mEh]	-179.76188740 [kcal/mol]	-752.12373687 [kJ/mol]
Total SAPT0	-354.28820344 [mEh]	-222.31920411 [kcal/mol]	-930.18354999 [kJ/mol]

Special recipe for scaled SAPT0 (see Manual):

Electrostatics sSAPT0	-390.38090958 [mEh]	-244.96771914 [kcal/mol]	-1024.94493690 [kJ/mol]
Exchange sSAPT0	239.92424187 [mEh]	150.55473476 [kcal/mol]	629.92101025 [kJ/mol]
Induction sSAPT0	-114.60667605 [mEh]	-71.91677498 [kcal/mol]	-300.89978652 [kJ/mol]
Dispersion sSAPT0	-67.04478697 [mEh]	-42.07123899 [kcal/mol]	-176.02606395 [kJ/mol]
Total sSAPT0	-332.10813073 [mEh]	-208.40099835 [kcal/mol]	-871.94977711 [kJ/mol]

TS$_{SS}$-Boc SAPT Results

Electrostatics	-382.38891304 [mEh]	-239.95266560 [kcal/mol]	-1003.96195287 [kJ/mol]
Elst10,r	-382.38891304 [mEh]	-239.95266560 [kcal/mol]	-1003.96195287 [kJ/mol]
Exchange	235.79193696 [mEh]	147.96167428 [kcal/mol]	619.07164520 [kJ/mol]
Exch10	235.79193696 [mEh]	147.96167428 [kcal/mol]	619.07164520 [kJ/mol]
Exch10(S^2)	230.72506781 [mEh]	144.78216589 [kcal/mol]	605.76858208 [kJ/mol]
Induction	-128.90050272 [mEh]	-80.88628663 [kcal/mol]	-338.42822326 [kJ/mol]
Ind20,r	-640.74579727 [mEh]	-402.07405807 [kcal/mol]	-1682.27785897 [kJ/mol]
Exch-Ind20,r	500.74098276 [mEh]	314.21971059 [kcal/mol]	1314.69526912 [kJ/mol]
delta HF,r (2)	11.10431179 [mEh]	6.96806085 [kcal/mol]	29.15436659 [kJ/mol]

Dispersion	-59.77677555 [mEh]	-37.51049297 [kcal/mol]	-156.94390259 [kJ/mol]
Disp20	-74.36289295 [mEh]	-46.66341982 [kcal/mol]	-195.23974854 [kJ/mol]
Exch-Disp20	14.58611740 [mEh]	9.15292685 [kcal/mol]	38.29584595 [kJ/mol]
Disp20 (SS)	-37.18144647 [mEh]	-23.33170991 [kcal/mol]	-97.61987427 [kJ/mol]
Disp20 (OS)	-37.18144647 [mEh]	-23.33170991 [kcal/mol]	-97.61987427 [kJ/mol]
Exch-Disp20 (SS)	7.05402031 [mEh]	4.42646457 [kcal/mol]	18.52032777 [kJ/mol]
Exch-Disp20 (OS)	7.53209709 [mEh]	4.72646228 [kcal/mol]	19.77551818 [kJ/mol]
Total HF	-275.49747880 [mEh]	-172.87727795 [kcal/mol]	-723.31853093 [kJ/mol]
Total SAPT0	-335.27425435 [mEh]	-210.38777092 [kcal/mol]	-880.26243352 [kJ/mol]

Special recipe for scaled SAPT0 (see Manual):

Electrostatics sSAPT0	-382.38891304 [mEh]	-239.95266560 [kcal/mol]	-1003.96195287 [kJ/mol]
Exchange sSAPT0	235.79193696 [mEh]	147.96167428 [kcal/mol]	619.07164520 [kJ/mol]
Induction sSAPT0	-95.18095223 [mEh]	-59.72694925 [kcal/mol]	-249.89755565 [kJ/mol]
Dispersion sSAPT0	-58.79455652 [mEh]	-36.89414122 [kcal/mol]	-154.36508688 [kJ/mol]
Total sSAPT0	-300.57248483 [mEh]	-188.61208179 [kcal/mol]	-789.15295021 [kJ/mol]

TS$_{RS}$-Boc SAPT Results

Electrostatics	-399.09198745 [mEh]	-250.43400304 [kcal/mol]	-1047.81586870 [kJ/mol]
Elst10,r	-399.09198745 [mEh]	-250.43400304 [kcal/mol]	-1047.81586870 [kJ/mol]
Exchange	255.51593510 [mEh]	160.33866998 [kcal/mol]	670.85699519 [kJ/mol]
Exch10	255.51593510 [mEh]	160.33866998 [kcal/mol]	670.85699519 [kJ/mol]
Exch10(S^2)	249.48159607 [mEh]	156.55206507 [kcal/mol]	655.01384024 [kJ/mol]
Induction	-150.00345563 [mEh]	-94.12858951 [kcal/mol]	-393.83401851 [kJ/mol]
Ind20,r	-622.91803864 [mEh]	-390.88697063 [kcal/mol]	-1635.47108512 [kJ/mol]
Exch-Ind20,r	475.69017968 [mEh]	298.50009433 [kcal/mol]	1248.92439469 [kJ/mol]
delta HF,r (2)	-2.77559668 [mEh]	-1.74171321 [kcal/mol]	-7.28732807 [kJ/mol]
Dispersion	-67.78035203 [mEh]	-42.53281303 [kcal/mol]	-177.95728973 [kJ/mol]
Disp20	-84.77157995 [mEh]	-53.19496952 [kcal/mol]	-222.56775249 [kJ/mol]
Exch-Disp20	16.99122792 [mEh]	10.66215649 [kcal/mol]	44.61046276 [kJ/mol]
Disp20 (SS)	-42.38578997 [mEh]	-26.59748476 [kcal/mol]	-111.28387624 [kJ/mol]
Disp20 (OS)	-42.38578997 [mEh]	-26.59748476 [kcal/mol]	-111.28387624 [kJ/mol]
Exch-Disp20 (SS)	8.28815701 [mEh]	5.20089705 [kcal/mol]	21.76055324 [kJ/mol]
Exch-Disp20 (OS)	8.70307091 [mEh]	5.46125944 [kcal/mol]	22.84990952 [kJ/mol]
Total HF	-293.57950798 [mEh]	-184.22392257 [kcal/mol]	-770.79289202 [kJ/mol]
Total SAPT0	-361.35986001 [mEh]	-226.75673560 [kcal/mol]	-948.75018175 [kJ/mol]

Special recipe for scaled SAPT0 (see Manual):

Electrostatics sSAPT0	-399.09198745 [mEh]	-250.43400304 [kcal/mol]	-1047.81586870 [kJ/mol]
Exchange sSAPT0	255.51593510 [mEh]	160.33866998 [kcal/mol]	670.85699519 [kJ/mol]
Induction sSAPT0	-114.64455170 [mEh]	-71.94054231 [kcal/mol]	-300.99922901 [kJ/mol]
Dispersion sSAPT0	-66.51736359 [mEh]	-41.74027582 [kcal/mol]	-174.64131405 [kJ/mol]
Total sSAPT0	-324.73796764 [mEh]	-203.77615119 [kcal/mol]	-852.59941657 [kJ/mol]

TS$_{RR}$-Boc SAPT Results

Electrostatics	-385.14012955 [mEh]	-241.67908002 [kcal/mol]	-1011.18527081 [kJ/mol]
Elst10,r	-385.14012955 [mEh]	-241.67908002 [kcal/mol]	-1011.18527081 [kJ/mol]
Exchange	241.94976904 [mEh]	151.82577225 [kcal/mol]	635.23903109 [kJ/mol]
Exch10	241.94976904 [mEh]	151.82577225 [kcal/mol]	635.23903109 [kJ/mol]
Exch10(S^2)	238.30671918 [mEh]	149.53972395 [kcal/mol]	625.67420501 [kJ/mol]
Induction	-136.04874144 [mEh]	-85.37187415 [kcal/mol]	-357.19592144 [kJ/mol]
Ind20,r	-543.53955587 [mEh]	-341.07622068 [kcal/mol]	-1427.06290732 [kJ/mol]
Exch-Ind20,r	412.30217003 [mEh]	258.72351775 [kcal/mol]	1082.49919827 [kJ/mol]
delta HF,r (2)	-4.81135560 [mEh]	-3.01917122 [kcal/mol]	-12.63221238 [kJ/mol]
Dispersion	-62.27738157 [mEh]	-39.07964694 [kcal/mol]	-163.50924279 [kJ/mol]
Disp20	-77.26179139 [mEh]	-48.48250606 [kcal/mol]	-202.85080536 [kJ/mol]
Exch-Disp20	14.98440982 [mEh]	9.40285912 [kcal/mol]	39.34156257 [kJ/mol]
Disp20 (SS)	-38.63089570 [mEh]	-24.24125303 [kcal/mol]	-101.42540268 [kJ/mol]
Disp20 (OS)	-38.63089570 [mEh]	-24.24125303 [kcal/mol]	-101.42540268 [kJ/mol]
Exch-Disp20 (SS)	7.31513517 [mEh]	4.59031662 [kcal/mol]	19.20588473 [kJ/mol]
Exch-Disp20 (OS)	7.66927466 [mEh]	4.81254251 [kcal/mol]	20.13567784 [kJ/mol]
Total HF	-279.23910195 [mEh]	-175.22518192 [kcal/mol]	-733.14216117 [kJ/mol]
Total SAPT0	-341.51648352 [mEh]	-214.30482886 [kcal/mol]	-896.65140395 [kJ/mol]

Special recipe for scaled SAPT0 (see Manual):

Electrostatics sSAPT0	-385.14012955 [mEh]	-241.67908002 [kcal/mol]	-1011.18527081 [kJ/mol]
Exchange sSAPT0	241.94976904 [mEh]	151.82577225 [kcal/mol]	635.23903109 [kJ/mol]
Induction sSAPT0	-116.84932861 [mEh]	-73.32406071 [kcal/mol]	-306.78786999 [kJ/mol]
Dispersion sSAPT0	-61.57961209 [mEh]	-38.64178998 [kcal/mol]	-161.67724927 [kJ/mol]
Total sSAPT0	-321.61930121 [mEh]	-201.81915846 [kcal/mol]	-844.41135899 [kJ/mol]

Cartesian coordinates of transition states.

Int$_{RS}$
G_{gas} = -6350.754978 a.u.

E_{solv} = -6352.12865 a.u.

Zn	-1.53612000	0.08123400	0.39663900
Zn	1.13916700	0.09403800	-0.80477600
O	-0.40924100	1.40073200	-0.57511400
O	-2.95960400	-1.02841000	-0.11978600
O	2.75074300	-0.88463500	-0.84673700
N	-2.84538500	1.45469600	1.19738200
N	2.21499700	1.74187400	-1.55778400
C	-0.31739400	2.67420100	-0.13542600
C	0.91716600	3.36164100	-0.12259500
C	0.95280400	4.69689600	0.28758800
H	1.91201200	5.21259600	0.28681000
C	-0.18377400	5.38426000	0.71910200
C	-1.38872400	4.67736900	0.73416700
H	-2.29413600	5.17517500	1.07826200
C	-1.47737200	3.35198200	0.30776000
C	-0.11743400	6.83613900	1.13099300
H	0.86566000	7.09253600	1.54152000
H	-0.29842700	7.50662300	0.27958500
H	-0.86964400	7.07141300	1.89247500
C	-2.81113200	2.64663400	0.30228400
H	-3.03950300	2.30267500	-0.70527500
H	-3.61088800	3.33831700	0.60487500
C	-2.64256100	1.80401200	2.62371600
H	-3.35640900	2.59270400	2.91262800
H	-1.62895800	2.17430700	2.77287800
C	-2.94796700	0.48972200	3.33370300
H	-2.06493000	-0.16028600	3.28440400
H	-3.19311700	0.63250500	4.38983300
C	-4.11306800	-0.10641100	2.50963100
H	-3.96734500	-1.17340400	2.33138500
H	-5.07284500	0.01485600	3.01800500
C	-4.12186100	0.66062000	1.15736000
H	-4.95732500	1.37125300	1.11422700
C	-4.15865900	-0.32205200	-0.08226400
C	-5.33658000	-1.30746100	0.07373200
C	-6.57326100	-0.95353000	0.63149400
H	-6.73467100	0.04646700	1.02311500
C	-7.61750000	-1.87684600	0.71272600
H	-8.56432900	-1.57853000	1.15604400
C	-7.44577300	-3.17551600	0.23344800
H	-8.25755000	-3.89550000	0.29585900
C	-6.21749800	-3.54004600	-0.32122300
H	-6.06737700	-4.55032100	-0.69449400
C	-5.17567500	-2.61613800	-0.39657600
H	-4.21845200	-2.89974500	-0.81472300
C	-4.37869000	0.46441800	-1.40469100
C	-5.52406300	1.24247500	-1.62693300
H	-6.31265900	1.27333600	-0.88166600
C	-5.67574600	1.97910400	-2.80121000
H	-6.57116600	2.57803600	-2.94808400
C	-4.68517100	1.94659700	-3.78592000
H	-4.80222300	2.52201300	-4.70047300
C	-3.54841000	1.16480500	-3.58246600
H	-2.76804100	1.12614800	-4.33851400
C	-3.39858800	0.42964400	-2.40445500
H	-2.50347900	-0.15807100	-2.24465100
C	2.23451400	2.66880900	-0.40594200
H	2.53077200	2.09190800	0.47726800
H	3.01998600	3.42611500	-0.55630200
C	1.68238600	2.34819700	-2.79531600
H	0.62116900	2.56876200	-2.67071800
H	2.21521400	3.28847400	-3.01341800
C	1.97074700	1.27939200	-3.84430700
H	1.18397100	0.51654600	-3.80417700
H	1.98951600	1.68582000	-4.85958700
C	3.32321600	0.68000300	-3.39840500
H	3.31609400	-0.40895800	-3.46872400
H	4.15226300	1.03903000	-4.01396300
C	3.52703700	1.12770200	-1.92373000
H	4.30251900	1.90313900	-1.87830500
C	3.87673000	-0.08415300	-0.97670600
C	5.02576400	-0.88752800	-1.63102200
C	6.24398000	-0.29305800	-1.98712100
H	6.41427300	0.76080000	-1.78700400
C	7.25641000	-1.04044300	-2.58826300
H	8.19242100	-0.55851200	-2.86008400
C	7.07191100	-2.40296300	-2.83475200
H	7.86162100	-2.98747000	-3.29980800
C	5.86633600	-3.00521100	-2.47340100
H	5.71247300	-4.06634700	-2.65570600
C	4.85184900	-2.25190300	-1.87882600
H	3.90830400	-2.70382600	-1.59622700
C	4.39816100	0.35197200	0.41835600
C	5.19528400	1.48265300	0.64752300
H	5.43471000	2.16115400	-0.16573200
C	5.68677200	1.77119500	1.92235400
H	6.29189600	2.66147900	2.07570000
C	5.40919600	0.91861700	2.99188400
H	5.80179300	1.13553400	3.98214000
C	4.62924000	-0.21897200	2.77302200
H	4.40987100	-0.90193500	3.58906400
C	4.12015000	-0.49005800	1.50290000
H	3.50652000	-1.36599100	1.33065400
O	-0.09277100	-1.20337400	-1.94102400
C	0.09677600	-2.37739300	-1.61601600
C	-0.83275600	-3.50687900	-1.94654000
C	-1.40211800	-3.98232700	-0.58136200
C	0.00873400	-4.63301000	-2.58744700
C	-1.96987500	-3.05213000	-2.86642300
H	0.99335100	-2.62607800	-1.02461500
H	-2.61212700	-3.90513600	-3.11170100
H	-1.58246200	-2.63287700	-3.80114500
H	-2.57442600	-2.29083900	-2.37033700
H	-0.62328300	-5.51391300	-2.74371100
H	0.84714200	-4.92905700	-1.94557800
H	0.41149900	-4.32647900	-3.55956300
H	-2.07598700	-4.82821600	-0.76127800
H	-1.96396200	-3.17920400	-0.09519700
H	-0.60889600	-4.32418500	0.09207700
C	0.66397000	-0.74037600	2.09374000
C	0.86776900	0.35050300	2.86595700
C	1.16766200	-1.89741900	2.84879500
C	1.49265600	0.05129400	4.19250900
C	1.65301100	-1.45409300	4.09744000
H	0.86084900	0.35513400	5.03924000
H	2.46113500	0.55685200	4.30527200
F	0.57516800	1.62382300	2.49231300
C	2.19751600	-2.35623900	4.99795300
C	1.23471800	-3.23961300	2.48975200
C	2.26326700	-3.71301800	4.64178200
C	1.78946700	-4.14651700	3.40037000
H	2.57445300	-2.02203900	5.96194600
H	2.69118300	-4.43057700	5.33649200
H	1.85441500	-5.19959100	3.13900900
H	0.87084700	-3.56162900	1.51988000
O	0.14214600	-0.81792000	0.86016000

TS$_{RS}$
G_{gas} = -6350.730024 a.u.

E_{solv} = -6352.11367 a.u.

Zn	1.23770300	0.31916300	-0.51871200
Zn	-1.62964900	0.16661400	0.43000900
O	-0.35243100	1.49864300	-0.25813700
O	2.84742500	-0.43390600	0.08729900
O	-3.06038100	-0.98203700	0.17823300
N	2.40109800	2.01760300	-1.09815900
N	-3.09596300	1.71961100	0.78231200
C	-0.46008200	2.84032000	-0.30462200
C	-1.72899400	3.45056400	-0.38163200
C	-1.82480600	4.84165100	-0.44013100
H	-2.81436700	5.29251100	-0.49471600
C	-0.69635200	5.66638400	-0.44287800
C	0.55164800	5.04309800	-0.35675700
H	1.45115600	5.65636700	-0.33801500
C	0.69096800	3.65584300	-0.27513500
C	-0.81861000	7.16776900	-0.55816800
H	-0.79341000	7.49521400	-1.60656000
H	-1.76093500	7.52746500	-0.13008300
H	0.00108500	7.67821800	-0.04015200
C	2.05737900	3.04676700	-0.08488100
H	2.11795100	2.57122700	0.89755400
H	2.82250900	3.83769800	-0.09962300
C	2.25294900	2.50531500	-2.48568700
H	2.76831400	3.47319600	-2.60196000
H	1.19577900	2.65184500	-2.71808200
C	2.92825800	1.41092100	-3.30587000
H	2.21473600	0.59381200	-3.46644900
H	3.24650800	1.76475000	-4.29049900
C	4.10301400	0.95119300	-2.41174100
H	4.19705700	-0.13473000	-2.38437600
H	5.05861500	1.34275700	-2.76994500
C	3.80311400	1.50604000	-0.99376400
H	4.46109200	2.36013000	-0.78627800
C	3.92825400	0.42655200	0.15525500
C	5.23591800	-0.37601200	-0.04259400
C	6.47369500	0.22679400	-0.30853600
H	6.55090000	1.30628100	-0.39844300
C	7.62431700	-0.54288800	-0.48342600
H	8.57198000	-0.05325500	-0.69438100
C	7.55822300	-1.93500200	-0.39419800
H	8.45368100	-2.53584000	-0.53170600
C	6.32970700	-2.54399500	-0.13619800
H	6.25661600	-3.62739900	-0.08084300
C	5.18060700	-1.77106900	0.03630200
H	4.21819700	-2.23684200	0.20682600
C	3.99531100	1.11542300	1.54904700
C	4.87762200	2.16243800	1.85268400
H	5.57355900	2.52831200	1.10476800
C	4.88229100	2.75779700	3.11476800
H	5.57266500	3.57196300	3.32143900
C	4.00643500	2.31356800	4.10751700
H	4.00880100	2.77863600	5.08983500
C	3.13205000	1.26459000	3.82196200
H	2.44707400	0.90108400	4.58449700
C	3.13060800	0.67465800	2.55720100
H	2.44488600	-0.12643000	2.32185200
C	-2.96465700	2.59146200	-0.41631900
H	-2.94309500	1.94575800	-1.29595500
H	-3.86229600	3.22207000	-0.50312400
C	-3.08075300	2.50011300	2.03924800
H	-2.07655700	2.88779100	2.22583300
H	-3.76305200	3.36121300	1.94598900
C	-3.57791100	1.51171700	3.09392400
H	-2.73244900	0.95879500	3.51611200
H	-4.07401000	2.02396100	3.92334400
C	-4.51949000	0.55946200	2.31662900
H	-4.23317400	-0.48403000	2.46408100
H	-5.56132500	0.65874500	2.62902000
C	-4.36536900	0.92687900	0.82057600
H	-5.18712200	1.58229300	0.49996600
C	-4.25977500	-0.34824100	-0.09925900
C	-5.41926500	-1.31870800	0.20843200
C	-6.73399400	-0.89605000	0.44466200
H	-6.97770600	0.16267400	0.45197100
C	-7.75085100	-1.82020500	0.69132100
H	-8.76270600	-1.46944200	0.87954600
C	-7.46889300	-3.18690300	0.70067100
H	-8.25941100	-3.90807700	0.89207900
C	-6.16138000	-3.61683900	0.46525400
H	-5.92943700	-4.67930600	0.47189800
C	-5.14537900	-2.69177100	0.22360600
H	-4.12456600	-3.01278100	0.04967500
C	-4.34889000	0.02057800	-1.60472900
C	-5.40200800	0.77572700	-2.13964000
H	-6.21784400	1.10419700	-1.50245400
C	-5.42346800	1.11730900	-3.49180700
H	-6.24634300	1.71007100	-3.88409600
C	-4.39376900	0.70038700	-4.33913200
H	-4.40832500	0.96993400	-5.39207200
C	-3.35234500	-0.06967700	-3.82045400
H	-2.54770400	-0.40873800	-4.46831500
C	-3.33247700	-0.41157000	-2.46630700
H	-2.51802800	-1.00036500	-2.05876600
O	0.07658900	-0.61318000	1.23439100
C	0.44053700	-1.76974200	1.63473100
C	-0.23337200	-2.36542000	2.86865800
C	0.57358800	-1.71780100	4.03383000
C	-0.09977700	-3.88918700	2.96662500
C	-1.70464200	-1.94544100	2.98545800
H	1.49372200	-2.02381800	1.47275100
H	-2.14325700	-2.38454000	3.88860900
H	-2.28874500	-2.25066500	2.11674000
H	-1.78729200	-0.85848000	3.07592200
H	-0.38500100	-4.22089000	3.97130200
H	0.93211700	-4.21625600	2.79164000
H	-0.75872200	-4.38342800	2.24964200
H	0.15906700	-2.05649200	4.99049500
H	0.50637700	-0.62559300	3.99347000
H	1.63295100	-1.99789600	4.00310400
C	0.40263300	-2.26236000	-1.08676800
C	-0.17679900	-3.17485000	-0.18428100
C	1.64056600	-2.89215800	-1.58163400
C	0.51532700	-4.51991000	-0.26105900
C	1.73416400	-4.20405600	-1.09194900
H	-0.14171300	-5.24170300	-0.76827300
H	0.77404400	-4.95487300	0.70780400
F	-1.50138400	-3.17370700	0.12800700
C	2.83912300	-4.99038400	-1.39829600
C	2.60573800	-2.37607200	-2.44231500
C	3.82273400	-4.46472300	-2.24472300
C	3.69982400	-3.17263200	-2.77330500
H	2.93063900	-6.00013600	-1.00552000
H	4.68813700	-5.06895000	-2.50316000
H	4.47331000	-2.78482200	-3.42990700
H	2.49756200	-1.37346300	-2.83444600
O	0.02347700	-1.05903000	-1.36436500

Int*SS*

G_{gas} = -6350.759101 a.u.

E_{solv} = -6352.132348 a.u.

Zn	-1.52506100	0.22923100	0.30412200
Zn	1.19374700	-0.57915700	-0.52983300
O	-0.30704300	0.67117700	-1.20769100
O	-3.00658600	-0.91173600	0.45249500
O	2.78575400	-1.38069900	0.08964900
N	-2.76399600	1.86783800	0.10111300
N	2.30244900	0.19861300	-2.13700500

C	-0.13225600	1.95068900	-1.59613000
C	1.13993800	2.44207500	-1.97222300
C	1.26582700	3.77583700	-2.37461700
H	2.25371800	4.13801100	-2.65516200
C	0.18700200	4.66090700	-2.40945600
C	-1.06130700	4.16028200	-2.02841000
H	-1.92744100	4.82007400	-2.04297800
C	-1.24137100	2.83253800	-1.64251900
C	0.35455800	6.09010500	-2.86929800
H	1.37126200	6.45410200	-2.68459800
H	0.16325400	6.19254100	-3.94620600
H	-0.34086500	6.76156000	-2.35294600
C	-2.62207300	2.32178100	-1.31122500
H	-2.85273600	1.46987700	-1.94919600
H	-3.37467800	3.09835500	-1.51113900
C	-2.59753200	2.96887500	1.07945200
H	-3.27103900	3.80007700	0.81360800
H	-1.57070400	3.33516900	1.06595700
C	-3.01136400	2.31452000	2.39146000
H	-2.17153000	1.72555900	2.78136100
H	-3.28058800	3.04782300	3.15641200
C	-4.18400700	1.39370700	1.98105300
H	-4.10688900	0.41421200	2.45688900
H	-5.15062700	1.82082000	2.25963700
C	-4.09189300	1.24098600	0.43706200
H	-4.87272000	1.82816100	-0.06310300
C	-4.15157300	-0.27269800	-0.01343200
C	-5.40378400	-0.94399200	0.58931400
C	-6.63097400	-0.28615600	0.75241900
H	-6.73319000	0.76315100	0.49096200
C	-7.74324300	-0.95451100	1.26801700
H	-8.68152100	-0.41923000	1.39102500
C	-7.65008600	-2.29884900	1.62829700
H	-8.51473600	-2.82065400	2.02995900
C	-6.43219900	-2.96337000	1.47172600
H	-6.34348200	-4.01022700	1.75214900
C	-5.32245900	-2.29139200	0.96028700
H	-4.37419900	-2.80166000	0.84915800
C	-4.25918500	-0.39104600	-1.55948300
C	-5.32349000	0.17252100	-2.27775300
H	-6.12898300	0.67386600	-1.75015600
C	-5.37104300	0.09478100	-3.66924700
H	-6.20427700	0.54312400	-4.20476100
C	-4.35551100	-0.55770900	-4.37320800
H	-4.39118700	-0.61633600	-5.45787700
C	-3.30056500	-1.13624700	-3.66787900
H	-2.50338600	-1.65073300	-4.19886300
C	-3.25555400	-1.05648100	-2.27429800
H	-2.42395300	-1.49069400	-1.73356200
C	2.41678500	1.63669400	-1.81968300
H	2.76232700	1.71396400	-0.78411600
H	3.20781700	2.08794900	-2.43920700
C	1.74964400	-0.07226600	-3.47983800
H	0.70495600	0.24011200	-3.51763500
H	2.31688300	0.49077000	-4.23929800
C	1.94637000	-1.57871300	-3.63000800
H	1.11621600	-2.10090200	-3.14109700
H	1.96597500	-1.89101100	-4.67802700
C	3.27232800	-1.85781700	-2.88348200
H	3.18202300	-2.72411400	-2.22473900
H	4.09669700	-2.05832000	-3.57239700
C	3.57270100	-0.58438400	-2.04754200
H	4.37190000	0.00078200	-2.52151800
C	3.92845800	-0.91705800	-0.54545100
C	5.02581800	-2.00312800	-0.50114800
C	6.12397000	-2.02303400	-1.37180000
H	6.22109200	-1.27079900	-2.14930000
C	7.10379600	-3.01172100	-1.26908200
H	7.94271500	-3.01123400	-1.96083700
C	7.00637900	-3.99738400	-0.28565800
H	7.76934300	-4.76728000	-0.20370300
C	5.91799200	-3.98421500	0.58849100
H	5.83004400	-4.74690600	1.35878400
C	4.93743600	-2.99777400	0.47886300
H	4.08352900	-2.98114700	1.14609900
C	4.50000300	0.33093500	0.18203100
C	5.52949900	1.11979600	-0.35276700
H	5.98760200	0.85317600	-1.30033600
C	5.98097100	2.25778000	0.31512900
H	6.77310200	2.85986800	-0.12378400
C	5.41642900	2.62538000	1.53914400
H	5.75776800	3.51965900	2.05421600
C	4.41205600	1.83266200	2.09362500
H	3.95627900	2.10942300	3.03957600
C	3.96650500	0.69115100	1.42363900
H	3.18347600	0.07151100	1.84417200
O	-0.06721900	-2.26406500	-0.74540800
C	0.03604700	-2.99466000	0.24399500
C	-0.95458900	-4.05157300	0.62482900
C	-1.60181500	-3.53906900	1.94276700
C	-0.16778200	-5.35294400	0.89803100
C	-2.02195300	-4.24726300	-0.45607900
H	0.89561000	-2.85888800	0.91977700
H	-2.71837100	-5.03567000	-0.14978600
H	-1.57341200	-4.53752700	-1.41250000
H	-2.58555800	-3.32396700	-0.60340900
H	-0.85505200	-6.11862800	1.27376100
H	0.61402600	-5.20182900	1.65156900
H	0.30271400	-5.73622700	-0.01482400
H	-2.26731100	-4.32087000	2.32794500
H	-2.18760300	-2.63491200	1.75337800
H	-0.85071700	-3.31595100	2.70543000
C	0.52544600	0.19678300	2.41662600
C	0.74750000	-0.45980800	3.57674600
C	0.87712500	1.60706900	2.64084400
C	1.22330300	0.43485800	4.68575700
C	1.27410700	1.77809900	3.98235800
H	2.21155200	0.13573400	5.06271000
H	0.53930100	0.43214700	5.54619500
C	1.66958200	3.02572800	4.43966400
C	0.90099300	2.66879700	1.74170400
C	1.67792600	4.10651100	3.54090800
C	1.30520100	3.92607400	2.20623800
H	1.97921100	3.16862600	5.47243300
H	1.99045000	5.08819900	3.88613900
H	1.33906300	4.76379600	1.51480500
H	0.63609400	2.51910500	0.70079900
O	0.09869100	-0.28871300	1.24427500
F	0.58308100	-1.78518300	3.77840300

TS_{SS}

G_{gas} = -6350.72766 a.u.

E_{solv} = -6352.099668 a.u.

Zn	1.67963900	0.24674900	-0.82792500
Zn	-1.26778700	0.27290500	0.29156900
O	0.29845500	1.44593700	-0.06497900
O	3.09980400	-0.69292400	-0.06961600
O	-2.96196100	0.06228400	-0.48870200
N	2.97808400	1.72395300	-1.41436600
N	-2.19074600	1.81116700	1.35725200
C	0.28849800	2.80044200	-0.14189200
C	-0.89447400	3.54644600	0.07467500
C	-0.85414300	4.94000300	-0.03701000
H	-1.77515900	5.49496400	0.13331500
C	0.30617100	5.64186600	-0.36544900
C	1.47202600	4.89251000	-0.53277400
H	2.40921900	5.40555300	-0.74230300
C	1.49037000	3.50255700	-0.40462800

C	0.30127800	7.14240800	-0.53594100
H	-0.48531800	7.61170100	0.06515300
H	1.25932100	7.58373000	-0.23865000
H	0.12375800	7.42742600	-1.58190000
C	2.82278900	2.79349900	-0.39901700
H	2.96486800	2.32557800	0.57667300
H	3.63620000	3.52324000	-0.52302100
C	2.87498900	2.19278800	-2.81167400
H	3.56791300	3.03446600	-2.97274300
H	1.85831900	2.54070600	-3.01078500
C	3.29126000	0.95576200	-3.61104300
H	2.41920900	0.30770900	-3.75739200
H	3.67989600	1.21608000	-4.59917600
C	4.33611500	0.25185700	-2.70534500
H	4.08522100	-0.80232600	-2.56509800
H	5.34655000	0.29419700	-3.11729800
C	4.28062200	0.98203500	-1.33976300
H	5.08960500	1.72075200	-1.26880500
C	4.30817800	-0.01334700	-0.11160900
C	5.45824900	-1.02604800	-0.32070900
C	6.77531200	-0.63161800	-0.59326000
H	7.02775800	0.42157300	-0.67203100
C	7.78336100	-1.57914900	-0.77303200
H	8.79763700	-1.25175300	-0.98813600
C	7.49093800	-2.94117300	-0.67701000
H	8.27578400	-3.68062800	-0.81429000
C	6.18155600	-3.34163100	-0.40783400
H	5.93999700	-4.39953100	-0.33668700
C	5.17215800	-2.39265500	-0.23468700
H	4.14763900	-2.69131700	-0.05000700
C	4.55725900	0.71629900	1.23528700
C	5.54806200	1.69037900	1.42379800
H	6.19327600	1.98557700	0.60221900
C	5.71658800	2.31427200	2.66069900
H	6.48611400	3.07324700	2.77857500
C	4.90122700	1.97024800	3.74045800
H	5.03098900	2.45804200	4.70292200
C	3.91940800	0.99335100	3.56855100
H	3.27844600	0.71122800	4.40046200
C	3.75251700	0.37399200	2.32947500
H	2.98677300	-0.37824700	2.18081500
C	-2.23690800	2.90650600	0.36678500
H	-2.65595500	2.48392300	-0.55044100
H	-2.94040000	3.67895700	0.71238500
C	-1.65518100	2.19843100	2.67552200
H	-0.57877700	2.36992600	2.59744500
H	-2.12692700	3.13743500	3.00645400
C	-2.03707700	1.02064100	3.59562500
H	-1.17364700	0.37335700	3.77599700
H	-2.38291700	1.38394600	4.56759200
C	-3.14290600	0.25333300	2.82372600
H	-2.75492400	-0.70256000	2.46124800
H	-4.02411400	0.03160000	3.42909000
C	-3.50019600	1.15787900	1.62868900
H	-4.21369900	1.92323200	1.96027000
C	-4.03433100	0.42269100	0.31836600
C	-4.80448600	-0.85224800	0.75518400
C	-6.07903600	-0.81627100	1.33430900
H	-6.60075700	0.12912100	1.44446700
C	-6.70647100	-1.99010700	1.75739000
H	-7.69840900	-1.93917300	2.20012900
C	-6.06924900	-3.22310000	1.60548100
H	-6.55929900	-4.13719700	1.93150800
C	-4.80009100	-3.26813100	1.02594100
H	-4.29013800	-4.21913300	0.89260100
C	-4.17468900	-2.09416400	0.60557700
H	-3.18935100	-2.12471500	0.15894400
C	-4.98572000	1.34170500	-0.49001400
C	-5.89623300	2.24153100	0.08180200
H	-5.96362700	2.34913400	1.16044200
C	-6.73977500	3.02264700	-0.71309800
H	-7.43125300	3.71573200	-0.24007700
C	-6.69341600	2.91718600	-2.10231800
H	-7.34668000	3.52573600	-2.72222800
C	-5.79590600	2.02000800	-2.68587700
H	-5.74784800	1.92532100	-3.76822400
C	-4.95528000	1.24542000	-1.88837800
H	-4.24721300	0.55816000	-2.33393400
O	-0.63787100	-1.34330100	1.12589800
C	0.34532400	-2.17203800	1.03439300
C	0.35352200	-3.29795000	2.07586700
C	0.62444600	-2.55673100	3.41615900
C	1.50232800	-4.29444500	1.85040300
C	-1.01745800	-3.98727900	2.17282600
H	1.34624200	-1.77613700	0.81555000
H	-1.02528200	-4.69711000	3.00809800
H	-1.26809500	-4.53767200	1.26253900
H	-1.80835700	-3.24964200	2.33385000
H	1.56850600	-4.98074500	2.70255300
H	2.46088000	-3.77120000	1.76071100
H	1.37208300	-4.89550400	0.94874100
H	0.67606600	-3.28190000	4.23690900
H	-0.17477700	-1.84109400	3.62949900
H	1.57748700	-2.01405300	3.38631000
C	-0.07525600	-1.99684400	-1.63472800
C	0.57078600	-3.05606600	-0.92528700
C	-1.38535300	-2.48503400	-2.05296700
C	-0.15162700	-4.35846800	-1.24178800
C	-1.46707300	-3.86542400	-1.79251000
H	-0.27036500	-5.03594000	-0.39392900
H	0.41950300	-4.90310600	-2.00777800
C	-2.65255300	-4.54775200	-2.03508600
C	-2.45160900	-1.77666100	-2.60957500
C	-3.72906200	-3.83834700	-2.58313200
C	-3.62763000	-2.47180400	-2.87880100
H	-2.74339100	-5.60853300	-1.81636700
H	-4.66349100	-4.35686100	-2.77983500
H	-4.48572300	-1.94529600	-3.28564300
H	-2.36336800	-0.71204400	-2.78234200
O	0.29619100	-0.77860600	-1.77296800
F	1.94081000	-3.12397800	-0.93060400

Int$_{SR}$

G_{gas} = -6350.756603 a.u.

E_{solv} = -6352.127169 a.u.

Zn	-1.51107000	0.38880100	0.17363000
Zn	1.21178900	-0.34722000	-0.55607300
O	-0.37873100	0.68796200	-1.43982700
O	-2.89644200	-0.80084900	0.58312800
O	2.81155600	-1.17830700	0.05037300
N	-2.86258600	1.90156200	-0.18104500
N	2.31366300	0.35775400	-2.20332700
C	-0.27094100	1.95214900	-1.89563500
C	0.97524100	2.50607800	-2.27787500
C	1.01359400	3.79578300	-2.81854900
H	1.98005400	4.20205500	-3.11385500
C	-0.12566800	4.58610900	-2.97769100
C	-1.34300500	4.03855600	-2.56381400
H	-2.25306200	4.62894100	-2.66013400
C	-1.43628900	2.74824200	-2.04415600
C	-0.05087000	5.96361600	-3.59326900
H	-0.80881600	6.63322700	-3.17082900
H	0.93012100	6.42369800	-3.43036300
H	-0.21794000	5.93080500	-4.67870400
C	-2.78074300	2.19168700	-1.64058200
H	-2.96905700	1.25775700	-2.16881600
H	-3.58274100	2.89504900	-1.90935200
C	-2.68488200	3.10909400	0.65758300

H	-3.36927600	3.90301800	0.31631600
H	-1.66040900	3.47664200	0.56343500
C	-3.05254200	2.61268300	2.05037800
H	-2.19715200	2.08331000	2.48604500
H	-3.31033100	3.42951200	2.73015600
C	-4.22242300	1.63869900	1.78866800
H	-4.14277200	0.74621800	2.41147800
H	-5.18842000	2.10444400	2.00205600
C	-4.13841400	1.25430000	0.28446800
H	-4.96748500	1.69903800	-0.28029800
C	-4.09593000	-0.31457200	0.06985800
C	-5.27749000	-0.97090400	0.81454400
C	-6.55450100	-0.39774200	0.89588100
H	-6.74849400	0.57857700	0.46115700
C	-7.59784900	-1.05419900	1.55138300
H	-8.57719300	-0.58510600	1.60582300
C	-7.38345300	-2.30117100	2.13911000
H	-8.19453700	-2.81396300	2.64959700
C	-6.11360200	-2.87737300	2.07114600
H	-5.93018900	-3.84501300	2.53225400
C	-5.07258900	-2.21654600	1.41933300
H	-4.07998800	-2.64845100	1.38166300
C	-4.23676900	-0.65924900	-1.44009700
C	-5.36030000	-0.28812900	-2.19302000
H	-6.19382200	0.21666700	-1.71498500
C	-5.43374900	-0.56342800	-3.55832600
H	-6.31399600	-0.26164100	-4.12069600
C	-4.38399200	-1.22426100	-4.20122100
H	-4.43926400	-1.43569900	-5.26592900
C	-3.26817500	-1.61103700	-3.45923400
H	-2.44110500	-2.12602300	-3.94248300
C	-3.19868600	-1.33492200	-2.09213900
H	-2.32424700	-1.62291700	-1.52479100
C	2.30866200	1.82528900	-2.02141600
H	2.62567200	2.02834100	-0.99387800
H	3.07503500	2.27584700	-2.67270500
C	1.80790800	-0.06200900	-3.52875200
H	0.73941300	0.14497800	-3.59667000
H	2.33081400	0.49656200	-4.32252900
C	2.15125800	-1.54663400	-3.57071800
H	1.38778900	-2.10574400	-3.01771700
H	2.18055000	-1.93969000	-4.59108200
C	3.51038000	-1.62749600	-2.84387800
H	3.55619800	-2.48958200	-2.17588900
H	4.34071700	-1.71767000	-3.54957200
C	3.64309500	-0.30965200	-2.03140600
H	4.41156800	0.33639900	-2.47489200
C	3.93728000	-0.58758300	-0.50664000
C	5.14335400	-1.54209000	-0.37241300
C	6.29114800	-1.44800200	-1.17109100
H	6.35546000	-0.69650400	-1.95271500
C	7.36541500	-2.32031800	-0.98921900
H	8.24257400	-2.23311200	-1.62581300
C	7.31369300	-3.30133900	0.00239300
H	8.15015700	-3.98050500	0.14581800
C	6.17615300	-3.40079100	0.80560800
H	6.12385900	-4.16027300	1.58235600
C	5.10187600	-2.53066700	0.61711400
H	4.21129900	-2.59906600	1.23143800
C	4.31679700	0.71808600	0.24547500
C	5.28477600	1.61677200	-0.22742300
H	5.81637900	1.41280000	-1.15211900
C	5.58109900	2.78456300	0.47519600
H	6.32786400	3.47185900	0.08470600
C	4.92314800	3.07149500	1.67424900
H	5.15095600	3.98430300	2.21873600
C	3.97725600	2.17300000	2.16787100
H	3.45752100	2.37765100	3.09958900
C	3.68315900	1.00586300	1.45883100
H	2.95305700	0.30077400	1.83550700
O	0.02462900	-2.08501100	-0.70121800
C	0.47530400	-3.09579200	-0.16007000
C	-0.31106300	-4.36557500	0.00520500
C	0.40234100	-5.41507200	-0.88629700
C	-1.77128700	-4.17170700	-0.41827200
C	-0.21569200	-4.80117600	1.48533800
H	-0.66724500	-5.79303600	1.59688500
H	-0.74427200	-4.09945400	2.13468800
H	0.82485800	-4.85766000	1.82422100
H	-2.34711600	-5.07792500	-0.20093700
H	-1.85065000	-3.96785000	-1.49038200
H	-2.22191800	-3.32470200	0.10835500
H	-0.10292500	-6.38083700	-0.77581700
H	1.45230700	-5.54637600	-0.59938000
H	0.36473400	-5.13034100	-1.94385900
C	0.45675000	0.26838100	2.36136400
C	0.63577200	-0.87775100	3.04903700
C	0.62657200	1.37863300	3.30705900
C	0.94849900	-0.66239900	4.50060800
C	0.92010400	0.85384000	4.58192600
H	1.93189500	-1.06941000	4.77561700
H	0.20899900	-1.13081000	5.16516100
C	1.14931100	1.70539100	5.65117900
C	0.55888000	2.75110500	3.08695100
C	1.07833700	3.09209500	5.43841500
C	0.78568700	3.60680100	4.17146000
H	1.38416800	1.31252800	6.63765100
H	1.25625000	3.77118300	6.26780000
H	0.74287500	4.68311300	4.02595400
H	0.35774200	3.13558400	2.09105500
O	0.21401800	0.45238100	1.05817500
H	1.52099400	-3.07967200	0.18729000
F	0.56683400	-2.12291700	2.51740800

TS_{SR}

G_{gas} = -6350.736692 a.u.

E_{solv} = -6352.11081 a.u.

Zn	1.65066500	0.08755700	-0.47264000
Zn	-1.30300400	0.28426000	0.32770900
O	0.28765700	1.43193700	0.07815500
O	3.19791400	-0.71029800	0.17843600
O	-2.98828300	-0.09857100	-0.37635200
N	2.82960900	1.53199700	-1.39614200
N	-2.25215700	1.85429400	1.34305400
C	0.30635200	2.77317200	-0.07599200
C	-0.86501400	3.55043100	0.09403000
C	-0.79086500	4.93873300	-0.05553300
H	-1.70013200	5.52100000	0.08503000
C	0.39089700	5.60122900	-0.39072300
C	1.53570500	4.81722600	-0.55117300
H	2.48093000	5.30019400	-0.79356100
C	1.52012600	3.43158000	-0.38703000
C	0.42728100	7.09763600	-0.59387700
H	-0.35961400	7.59934000	-0.01994000
H	1.38953600	7.52155500	-0.28493300
H	0.27969700	7.36488600	-1.64924200
C	2.82450000	2.67136700	-0.44824000
H	3.05440300	2.26652900	0.54067500
H	3.64466500	3.35807100	-0.70375700
C	2.48855600	1.89513800	-2.78547900
H	3.13377900	2.72236000	-3.12444900
H	1.44925800	2.22827200	-2.83620800
C	2.77152000	0.60113500	-3.55514800
H	1.87681500	-0.03080400	-3.54561500
H	3.03079500	0.79604500	-4.59936400
C	3.91719400	-0.07764700	-2.75751600
H	3.64029000	-1.09422900	-2.46625500
H	4.84841800	-0.14711900	-3.32353900

C	4.11952800	0.78358300	-1.48713700
H	4.93186700	1.50414700	-1.64985700
C	4.37833200	-0.07658600	-0.18779700
C	5.45144500	-1.14020200	-0.52635800
C	6.73218900	-0.79835300	-0.98189300
H	7.01440900	0.24412000	-1.08902600
C	7.66660500	-1.78419300	-1.29955900
H	8.65375000	-1.49590900	-1.65278500
C	7.33747000	-3.13429000	-1.16108500
H	8.06586300	-3.90365600	-1.40449400
C	6.06473000	-3.48302900	-0.70840700
H	5.79454500	-4.53085700	-0.59920100
C	5.12827600	-2.49482800	-0.39709600
H	4.13138800	-2.75484000	-0.06394700
C	4.90616600	0.78549600	0.98919300
C	5.86139700	1.80353700	0.85370000
H	6.27155600	2.05097300	-0.12063400
C	6.29227700	2.53868200	1.95964300
H	7.02691300	3.32898000	1.82532100
C	5.78068400	2.26609500	3.22894400
H	6.11412900	2.83978900	4.08978700
C	4.83534700	1.24975300	3.37787900
H	4.42804000	1.02428100	4.36063300
C	4.40439000	0.51981100	2.26995500
H	3.66120900	-0.26142800	2.37125200
C	-2.23177500	2.94082400	0.34437800
H	-2.62256700	2.52113600	-0.58776800
H	-2.93487500	3.73206600	0.64626000
C	-1.73992300	2.22548400	2.67248200
H	-0.67069100	2.43930800	2.60821700
H	-2.25341200	3.13194800	3.03299600
C	-2.07704400	0.99806800	3.53463900
H	-1.21529900	0.32553700	3.56848500
H	-2.31909300	1.28327900	4.56209500
C	-3.26489900	0.31626400	2.80249200
H	-2.98320600	-0.68307400	2.45575600
H	-4.14889200	0.19360700	3.43098800
C	-3.57349400	1.21774900	1.58654800
H	-4.29443500	1.98989200	1.88540000
C	-4.07395600	0.45017600	0.29511200
C	-5.03475300	-0.68264600	0.73384800
C	-6.21742100	-0.43253400	1.44237000
H	-6.50400200	0.58821700	1.67862900
C	-7.04385500	-1.48153700	1.84590800
H	-7.95580600	-1.26690500	2.39780300
C	-6.70607200	-2.80160000	1.53644900
H	-7.35283200	-3.61867700	1.84604300
C	-5.53563400	-3.05767300	0.82145000
H	-5.26375800	-4.07839400	0.56226900
C	-4.70511400	-2.00675100	0.42687200
H	-3.79813100	-2.19397800	-0.13410300
C	-4.85489100	1.38878700	-0.66353800
C	-5.70495800	2.42128000	-0.24354200
H	-5.84182800	2.63178900	0.81266900
C	-6.39326700	3.21149600	-1.16774200
H	-7.03890500	4.01112300	-0.81282400
C	-6.25200700	2.98028800	-2.53548400
H	-6.78520600	3.59604900	-3.25504200
C	-5.41776400	1.94688200	-2.96732600
H	-5.29971800	1.75063600	-4.03042200
C	-4.73026400	1.16417500	-2.04136200
H	-4.07688600	0.36546900	-2.36723800
O	-0.32125800	-1.08451800	1.32840500
C	-0.42847200	-2.35453100	1.38110500
C	0.38084900	-3.04751400	2.48595800
C	-0.52786700	-2.88639300	3.73853800
C	1.71314600	-2.31789200	2.72522000
C	0.61546600	-4.54762300	2.26179000
H	1.04531700	-4.98619200	3.16934900
H	1.31355500	-4.72647700	1.44194600
H	-0.32257700	-5.07793400	2.05813300
H	2.26733100	-2.81924200	3.52735500
H	1.53612200	-1.28156900	3.02538000
H	2.33076900	-2.29534700	1.82577700
H	-0.02508000	-3.32369200	4.60902400
H	-1.48995500	-3.39805100	3.61131000
H	-0.72472000	-1.83140800	3.95073600
C	-0.17212500	-2.10830800	-1.31738100
C	0.40549800	-3.16075200	-0.58366500
C	-1.41917000	-2.61417800	-1.89607300
C	-0.27263500	-4.47158900	-0.93237500
C	-1.50929900	-3.99673900	-1.66035500
H	-0.51666000	-5.09899400	-0.07122000
H	0.38105200	-5.06525400	-1.58731600
C	-2.63791200	-4.69942300	-2.06719200
C	-2.41156200	-1.92212000	-2.58847700
C	-3.64388500	-4.00725800	-2.75322600
C	-3.52780400	-2.63536900	-3.02038400
H	-2.73409600	-5.76469900	-1.87292500
H	-4.52896500	-4.54258100	-3.08618400
H	-4.32824700	-2.12092800	-3.54417600
H	-2.31575900	-0.85504400	-2.74291700
O	0.18688700	-0.87340100	-1.37472700
H	-1.39658900	-2.81229400	1.12507300
F	1.74187500	-3.17087700	-0.30658700

Int$_{RR}$

G_{gas} = -6350.753215 a.u.

E_{solv} = -6352.128199 a.u.

Zn	1.57250800	0.52033800	-0.64915900
Zn	-1.19575400	0.19352100	0.23623000
O	0.33283600	1.53483900	0.53844100
O	2.94842800	-0.70655800	-0.32039000
O	-2.81906200	-0.75711300	0.00364400
N	2.95787200	2.03118300	-0.87200700
N	-2.33535900	1.59305500	1.37515600
C	0.21247100	2.86549600	0.35046500
C	-1.04400300	3.51532000	0.37749500
C	-1.09628300	4.90440700	0.22535100
H	-2.07101000	5.38954100	0.25204200
C	0.04222300	5.68917000	0.03048300
C	1.27559900	5.03214600	0.01645600
H	2.18815500	5.61199700	-0.11370600
C	1.37914400	3.65233700	0.18833600
C	-0.05825300	7.18175000	-0.17976200
H	-0.17937700	7.43176800	-1.24271800
H	-0.91838700	7.60502200	0.35105300
H	0.84108200	7.69843000	0.17387700
C	2.73242000	2.98857900	0.24591700
H	2.82306800	2.42396000	1.17422500
H	3.53141000	3.74468000	0.23379500
C	2.94052200	2.67743900	-2.20496200
H	3.61329200	3.55065600	-2.20617900
H	1.92993900	3.02170500	-2.43663400
C	3.46050500	1.57361300	-3.11803800
H	2.65251500	0.86056300	-3.32601700
H	3.81941800	1.95715600	-4.07715100
C	4.56425800	0.90238400	-2.27328300
H	4.56798500	-0.17983900	-2.41125500
H	5.55568400	1.27536000	-2.54575400
C	4.25034500	1.26073200	-0.79362600
H	5.01595500	1.93011300	-0.38262600
C	4.08540600	-0.03102700	0.10564100
C	5.31709800	-0.94365000	-0.06272300
C	6.63080800	-0.45924400	-0.12817800
H	6.82514900	0.60914300	-0.09872100
C	7.71213300	-1.33359900	-0.25007800
H	8.72224100	-0.93514000	-0.30527600

C	7.49761700	-2.71138000	-0.30680800
H	8.33864200	-3.39336200	-0.40193600
C	6.19206800	-3.20279600	-0.24901300
H	6.01129600	-4.27378500	-0.30204600
C	5.11310000	-2.32665000	-0.13121000
H	4.09418500	-2.69503500	-0.10786400
C	3.97373800	0.33680600	1.61188600
C	4.94149000	1.09881000	2.28232900
H	5.83223200	1.43179600	1.75870800
C	4.77941000	1.44425600	3.62400500
H	5.53928800	2.04262300	4.12061100
C	3.64705700	1.02579900	4.32793000
H	3.51846600	1.30068600	5.37160600
C	2.68897400	0.24938800	3.67615000
H	1.80134900	-0.08728300	4.20753100
C	2.85547600	-0.09606800	2.33376300
H	2.10721700	-0.69267600	1.82872700
C	-2.36090300	2.76703500	0.47540000
H	-2.65573000	2.41623300	-0.51805600
H	-3.15128400	3.46268600	0.79984200
C	-1.85217300	1.92125300	2.73301300
H	-0.79390800	2.18057100	2.69753900
H	-2.41485400	2.78226500	3.13045100
C	-2.13957500	0.64967400	3.52663900
H	-1.30235800	-0.04534900	3.40443700
H	-2.25197700	0.84861000	4.59628700
C	-3.42203500	0.08273400	2.87535900
H	-3.31823200	-0.98090900	2.64636700
H	-4.29333700	0.18099700	3.52699000
C	-3.63620500	0.88700600	1.56515300
H	-4.42480800	1.63868600	1.70749400
C	-3.96125300	-0.04264800	0.33248400
C	-5.08753600	-1.03103000	0.70844900
C	-6.20770100	-0.67024600	1.46975100
H	-6.30907500	0.34197600	1.85052300
C	-7.20346500	-1.60168900	1.76828100
H	-8.05939400	-1.30008100	2.36714700
C	-7.10019600	-2.91412400	1.30444000
H	-7.87538000	-3.64001500	1.53597700
C	-5.99112000	-3.28280200	0.54091000
H	-5.89997100	-4.30112100	0.17008500
C	-4.99530300	-2.35005600	0.24820100
H	-4.12948800	-2.62440100	-0.34388600
C	-4.45911600	0.79244600	-0.87632800
C	-5.51343900	1.71238900	-0.78539000
H	-6.04260700	1.85018500	0.15278000
C	-5.90524700	2.46184600	-1.89485200
H	-6.72237300	3.17325500	-1.80156500
C	-5.25240900	2.30070500	-3.11968700
H	-5.55512900	2.88871900	-3.98239600
C	-4.21190500	1.37728600	-3.22392700
H	-3.68801800	1.23433100	-4.16382800
C	-3.82508300	0.62777300	-2.11142600
H	-3.01608800	-0.08725400	-2.17899900
O	-0.23645600	-1.31769000	1.41214800
C	-0.91542600	-2.33309100	1.57701700
C	-0.48022600	-3.50530800	2.40795500
C	1.02850700	-3.48567700	2.68023200
C	-0.91709400	-4.79805400	1.68740100
C	-1.28121000	-3.35720100	3.73160400
H	-1.07352200	-4.22168800	4.37179000
H	-2.36187800	-3.32132600	3.55064700
H	-0.98935800	-2.45007000	4.27210300
H	-0.68824300	-5.66419000	2.31804400
H	-0.39486100	-4.91500900	0.73322200
H	-1.99561200	-4.79792100	1.48977500
H	1.30490300	-4.33780900	3.31040900
H	1.33340800	-2.56685300	3.18886500
H	1.59589700	-3.54921400	1.74664800
C	-0.26621700	-1.02241500	-2.37910600
C	-0.91425600	-0.96607600	-3.56285600
C	0.19464100	-2.41036200	-2.19695300
C	-1.01033700	-2.29386900	-4.25366900
C	-0.24830900	-3.18330400	-3.29128000
H	-0.55615300	-2.28394700	-5.25447600
H	-2.05523500	-2.61176600	-4.37999400
C	0.05978700	-4.53213100	-3.37166600
C	0.97613200	-2.97565100	-1.19072200
C	0.83393100	-5.11228300	-2.35421700
C	1.29538200	-4.33649200	-1.28687700
H	-0.28260400	-5.13193600	-4.21186300
H	1.09029800	-6.16694100	-2.40771300
H	1.92106900	-4.79238300	-0.52282200
H	1.37448300	-2.36585100	-0.38851800
O	-0.08696900	-0.02442600	-1.49435700
H	-1.92672500	-2.35533500	1.13710600
F	-1.47398700	0.13877400	-4.10066100

TS_{RR}

G_{gas} = -6350.738924 a.u.

E_{solv} = -6352.119442 a.u.

Zn	1.86680700	0.45907600	0.24733100
Zn	-0.97495300	-0.98897700	-0.03543600
O	0.45731700	-0.69644400	1.22881000
O	2.99175100	-0.20806800	-1.14833200
O	-2.47211000	-0.95905400	-1.15182400
N	3.32780900	-0.38888600	1.60304500
N	-2.25447400	-1.64724900	1.55558400
C	0.34589200	-0.58259700	2.56664400
C	-0.88821000	-0.40461600	3.22415100
C	-0.88881100	-0.22288600	4.61193800
H	-1.84464000	-0.08043100	5.11432100
C	0.28138300	-0.22870300	5.37541000
C	1.48113900	-0.51442700	4.71206700
H	2.40130400	-0.61293000	5.28622700
C	1.52296400	-0.71833000	3.33528400
C	0.25242400	0.03838400	6.86186400
H	0.45396300	1.09518100	7.08428900
H	-0.72471000	-0.20298800	7.29511900
H	1.00928400	-0.55181100	7.39152000
C	2.74487600	-1.26469400	2.64204100
H	2.44044200	-2.18406300	2.14096200
H	3.51938300	-1.52329700	3.38206900
C	4.07569400	0.75274700	2.18894000
H	4.65831200	0.41297000	3.06137600
H	3.37373300	1.52443900	2.51381600
C	4.99876800	1.18950100	1.05939200
H	4.43233900	1.76679600	0.32259700
H	5.82979500	1.80496500	1.41781300
C	5.45225500	-0.15182400	0.46096200
H	5.72509000	-0.06291300	-0.59082800
H	6.32548000	-0.53279000	1.00257500
C	4.25408000	-1.11806400	0.66108700
H	4.58734300	-2.04693300	1.13885400
C	3.51808200	-1.40781800	-0.70788300
C	4.53881400	-1.96654400	-1.71987900
C	5.30999500	-3.10661600	-1.45585100
H	5.19829400	-3.63531400	-0.51325000
C	6.22476500	-3.58422200	-2.39427100
H	6.81590700	-4.46865800	-2.16920200
C	6.37932900	-2.93042700	-3.61886300
H	7.09022800	-3.30270800	-4.35210800
C	5.61248300	-1.79658300	-3.89106700
H	5.72492800	-1.27945900	-4.84113100
C	4.70073700	-1.31810900	-2.94788700
H	4.10352000	-0.43370400	-3.13776800
C	2.37360600	-2.46438900	-0.60260100
C	2.39956500	-3.61356100	0.19376200

H	3.27569500	-3.84402600	0.79319100
C	1.30014800	-4.47875800	0.25533400
H	1.34190800	-5.35247400	0.90089500
C	0.15971000	-4.22779100	-0.50529000
H	-0.69207500	-4.90044200	-0.46076800
C	0.13255800	-3.10673500	-1.34737300
H	-0.72822300	-2.92215800	-1.98634800
C	1.23372300	-2.24628100	-1.39543000
H	1.22343100	-1.36649900	-2.02695800
C	-2.20693300	-0.48727200	2.48196800
H	-2.39295900	0.41734700	1.90349300
H	-3.02378400	-0.57221700	3.21604400
C	-1.85516800	-2.92454100	2.23460800
H	-0.80825200	-3.13274300	1.99779400
H	-1.92980200	-2.81004400	3.32104700
C	-2.80762600	-4.00638900	1.70468000
H	-2.28489200	-4.94093200	1.47874900
H	-3.57572100	-4.23360100	2.45289900
C	-3.44808600	-3.36705000	0.47216500
H	-2.80151400	-3.46666100	-0.40646700
H	-4.42177100	-3.78920100	0.21964900
C	-3.54121800	-1.87709500	0.83214700
H	-4.39105500	-1.71839700	1.51098200
C	-3.68398200	-0.98027300	-0.46388300
C	-4.77996200	-1.62944700	-1.33730900
C	-6.11706900	-1.66247800	-0.91900200
H	-6.40079100	-1.18355900	0.01485000
C	-7.09146000	-2.28607900	-1.69732200
H	-8.12408100	-2.30366200	-1.35748100
C	-6.74394400	-2.87618400	-2.91568100
H	-7.50326300	-3.35760400	-3.52652300
C	-5.41677500	-2.83332700	-3.34470700
H	-5.13751200	-3.28254300	-4.29485000
C	-4.44106900	-2.21548400	-2.55882500
H	-3.40552500	-2.17247800	-2.87673100
C	-4.15302000	0.47252400	-0.20257600
C	-4.74350900	0.94351500	0.97364600
H	-4.88724200	0.28112600	1.82089500
C	-5.15138500	2.27756500	1.09228000
H	-5.59127900	2.62168600	2.02494800
C	-4.99929900	3.15810900	0.02390500
H	-5.31857400	4.19294500	0.11468000
C	-4.44570000	2.68997000	-1.17286000
H	-4.34314200	3.35806700	-2.02499100
C	-4.03094700	1.36578900	-1.27961300
H	-3.61121800	0.99103800	-2.20746600
O	0.07925600	0.55282300	-1.04208100
C	-0.50441200	1.54422800	-1.56937800
C	0.04227700	2.16426300	-2.83911000
C	-0.37691200	1.12392900	-3.92060800
C	1.57258000	2.28870600	-2.82594900
C	-0.64064200	3.50534900	-3.14106600
H	-0.38919200	3.83289700	-4.15599900
H	-0.31694300	4.28556700	-2.44945300
H	-1.73331700	3.41940700	-3.07958600
H	1.92424000	2.59702900	-3.81746900
H	2.04589900	1.33762900	-2.56532400
H	1.90180900	3.04142200	-2.10514800
H	-0.08824500	1.49599400	-4.91040100
H	-1.45972600	0.95061500	-3.92082000
H	0.12169300	0.16562400	-3.74659900
C	0.83536400	3.16165800	0.37361300
C	-0.54017000	2.92973700	0.35298100
C	1.01603500	4.57550300	-0.01156400
C	-1.33532400	4.20076000	0.21953300
C	-0.24195300	5.20215400	-0.09156600
H	-1.84785000	4.42949800	1.16505400
H	-2.10960300	4.16122600	-0.55535300
C	-0.33121800	6.53860200	-0.45837900
C	2.19469400	5.27409100	-0.26227100
C	0.85115400	7.24855700	-0.70965300
C	2.10089400	6.62395600	-0.60993200
H	-1.29741500	7.03023900	-0.54235900
H	0.79710400	8.29886800	-0.98353000
H	3.00344300	7.19511900	-0.81032800
H	3.15229300	4.76706200	-0.18817100
O	1.80131900	2.35749000	0.64143600
H	-1.58003600	1.64493100	-1.39986300
F	-1.09431500	1.87816900	1.02985700

Int$_{SR}$-Boc

G_{gas} = -6750.421925 a.u.

E_{solv} = -6751.94291 a.u.

Zn	-1.50472700	0.12398000	1.00592800
Zn	1.08286200	1.17824300	-0.72217000
O	-0.25276100	1.69888200	0.58542100
O	-2.65150700	-0.26462500	-0.44929900
O	2.70093300	0.23255700	-0.91724700
N	-3.05554900	1.37093400	1.73112500
N	2.18631800	2.93165500	-0.55527900
C	-0.31668200	2.89775700	1.21432100
C	0.84195100	3.67889400	1.41353500
C	0.75096000	4.89408200	2.09771700
H	1.65854200	5.47842000	2.24039500
C	-0.45637500	5.37272600	2.60884300
C	-1.60116200	4.61022200	2.35843600
H	-2.56857800	4.97982800	2.69466900
C	-1.56121300	3.40387500	1.65720300
C	-0.52535500	6.65814700	3.39898400
H	-1.46600600	7.19107900	3.21855900
H	-0.46296900	6.46963700	4.47941900
H	0.29790700	7.33319000	3.13998600
C	-2.85004300	2.74473900	1.22994000
H	-2.85187200	2.69326600	0.14311300
H	-3.70686200	3.37068100	1.52603500
C	-3.25790700	1.32012100	3.19590800
H	-3.97361200	2.10523500	3.49253200
H	-2.30875000	1.51258800	3.70180500
C	-3.82485200	-0.08189900	3.45680100
H	-3.01561400	-0.76152500	3.72973500
H	-4.55121900	-0.06645400	4.27471200
C	-4.45337800	-0.51111300	2.10582900
H	-3.94982200	-1.39746300	1.71491900
H	-5.51570200	-0.75144500	2.18488700
C	-4.23523500	0.66992900	1.13544500
H	-5.09974800	1.35019100	1.16426700
C	-3.94134000	0.22093300	-0.35863900
C	-4.93801500	-0.90686200	-0.73800600
C	-6.32975900	-0.79836900	-0.60569300
H	-6.77476900	0.10520800	-0.20225300
C	-7.17152900	-1.85465200	-0.95745100
H	-8.24729000	-1.74496600	-0.84258500
C	-6.63702600	-3.04828500	-1.44585200
H	-7.29219200	-3.87145900	-1.71958100
C	-5.25216700	-3.17648100	-1.55791800
H	-4.81887700	-4.11075800	-1.90893700
C	-4.41330600	-2.11920900	-1.20165100
H	-3.33591200	-2.21752300	-1.24048600
C	-4.12871000	1.42542400	-1.33081400
C	-5.30794400	2.17773600	-1.42723500
H	-6.17173700	1.92695000	-0.82196000
C	-5.40002800	3.27160000	-2.29035400
H	-6.32779200	3.83645800	-2.34185500
C	-4.31005800	3.64319000	-3.07898100
H	-4.38174600	4.49607500	-3.74911100
C	-3.12682400	2.90889300	-2.98681900
H	-2.26183400	3.18714700	-3.58551400
C	-3.04098600	1.81753500	-2.12188500

H	-2.11773100	1.26585100	-2.01961000
C	2.18103000	3.20709500	0.90715200
H	2.46613100	2.28161800	1.41140300
H	2.96037800	3.94775300	1.13725400
C	1.75975100	4.07335000	-1.39102700
H	0.71119900	4.30789600	-1.19578500
H	2.36407300	4.96213500	-1.14677500
C	2.04115400	3.56911100	-2.80678600
H	1.19300000	2.96686700	-3.15480000
H	2.17692500	4.38840700	-3.51799000
C	3.30094500	2.68047500	-2.64585500
H	3.15813700	1.70411700	-3.11476600
H	4.18598500	3.13347300	-3.09737900
C	3.50228300	2.49792100	-1.11828200
H	4.27125100	3.18889700	-0.74829300
C	3.83465000	1.01148600	-0.71461800
C	5.00068000	0.47736000	-1.57512200
C	6.08653100	1.26151000	-1.98603900
H	6.12873300	2.31831300	-1.73778000
C	7.13089400	0.70566800	-2.72819400
H	7.95906500	1.33506700	-3.04463200
C	7.11318700	-0.64913400	-3.06270700
H	7.92661800	-1.08167900	-3.63949700
C	6.04192000	-1.44135100	-2.64415900
H	6.01549600	-2.50092700	-2.88862200
C	4.99922500	-0.88130700	-1.90796900
H	4.16868200	-1.48882800	-1.57503300
C	4.31740300	0.90715100	0.75796900
C	5.32742200	1.72493000	1.28329800
H	5.80981400	2.46793200	0.65461700
C	5.73661600	1.59386200	2.61046600
H	6.51532500	2.24521100	2.99974800
C	5.15526100	0.62711000	3.43467000
H	5.47561000	0.52439100	4.46816000
C	4.16739300	-0.21019000	2.91500400
H	3.71363700	-0.97998800	3.53326000
C	3.75525100	-0.06753000	1.58911400
H	2.98941700	-0.71097000	1.17721300
O	-0.00903500	0.25260300	-2.32151600
C	-0.24653100	-0.85794200	-1.80797500
C	-0.74375800	-2.18265800	2.58733500
C	-1.41663900	-3.18841700	1.95739700
C	0.26523300	-2.84699200	3.43939800
C	-0.96338900	-4.56623000	2.33822700
C	0.16122900	-4.24616900	3.30410300
H	-0.60636100	-5.14337100	1.47135200
H	-1.75846500	-5.16388400	2.80814500
F	-2.40616900	-3.01590300	1.04525700
C	1.04594700	-5.08207400	3.96957600
C	1.24986100	-2.27183400	4.23870800
C	2.04152800	-4.50888300	4.77855600
C	2.13926000	-3.12008700	4.91055300
H	0.97664300	-6.16288000	3.86626700
H	2.74173500	-5.15177000	5.30519800
H	2.91587700	-2.69501000	5.54199500
H	1.31437000	-1.19116400	4.32449200
O	-0.81768100	-0.87452000	2.48658900
N	0.07867700	-1.01127000	-0.46087700
O	-0.80654100	-1.88689200	-2.38070000
C	-1.24965900	-1.90201000	-3.81167900
C	-1.88257000	-3.28683400	-3.92329000
C	-2.27386500	-0.79952800	-4.05703000
C	-0.01544100	-1.77342300	-4.70385400
H	-2.76861400	-3.35489200	-3.28652900
H	-2.75900200	-0.98025800	-5.02247700
H	-1.16886900	-4.06051700	-3.62347900
H	-2.18412700	-3.46829700	-4.95991500
H	-1.80700100	0.18489500	-4.08138300
H	-3.03561600	-0.80547100	-3.27511400
H	0.68355800	-2.59582900	-4.52342200
H	0.49451200	-0.82174500	-4.53538100
H	-0.32965300	-1.81510800	-5.75210200
C	0.87159900	-1.90548400	0.03147000
C	1.64863500	-2.95050000	-0.62728600
C	2.01955500	-4.06172600	0.15071900
C	2.07302200	-2.86829300	-1.96431300
C	2.74800500	-5.10318000	-0.41960500
H	1.73173600	-4.10537100	1.19747200
C	2.81584300	-3.90217700	-2.52341700
H	1.88703700	-1.96605700	-2.53263200
C	3.14177300	-5.02744000	-1.75750800
H	3.02045500	-5.96402800	0.18389600
H	3.16177700	-3.82143800	-3.55003700
H	3.72223600	-5.83297700	-2.19899000
H	0.99504500	-1.82898700	1.10643600

TS_{SR}-Boc

G_{gas} = -6750.420259 a.u.

E_{solv} = -6751.936398 a.u.

Zn	-1.48468600	0.35738000	0.98439700
Zn	1.04336000	0.88673300	-0.87236900
O	-0.26478400	1.79413800	0.27825600
O	-2.73935000	-0.35388600	-0.22712200
O	2.70970500	0.00847800	-0.77401200
N	-2.99967800	1.70612600	1.58955000
N	2.10984900	2.66684900	-1.20367600
C	-0.31925100	3.09830700	0.61737400
C	0.84212200	3.89823500	0.57263500
C	0.77198700	5.23907600	0.95841300
H	1.67904600	5.84018600	0.91800800
C	-0.41625500	5.82462900	1.40152400
C	-1.56519700	5.02693600	1.39534400
H	-2.51778000	5.46737100	1.68593200
C	-1.54781900	3.69025500	0.99355100
C	-0.46102600	7.25966300	1.87155000
H	-1.41677500	7.73459000	1.62181400
H	-0.33986200	7.33094100	2.96118400
H	0.33816300	7.85606500	1.41747400
C	-2.84772000	2.94492800	0.79513900
H	-2.91137900	2.65911500	-0.25375900
H	-3.69813600	3.61405200	1.00060300
C	-3.09036700	1.96285700	3.04327400
H	-3.78865800	2.79704000	3.22365100
H	-2.10802200	2.25303800	3.42366700
C	-3.62346900	0.64956900	3.63861000
H	-2.79768900	0.05644500	4.03587600
H	-4.32592300	0.84746200	4.45365500
C	-4.28987600	-0.08299200	2.44594500
H	-3.74125800	-0.99712900	2.19914500
H	-5.32477200	-0.37064300	2.64131200
C	-4.20440100	0.88551400	1.24901800
H	-5.08554900	1.54372800	1.22532900
C	-4.02381600	0.14440600	-0.14019200
C	-5.02479800	-1.03772200	-0.21635400
C	-6.40050300	-0.91538500	0.02263500
H	-6.82602600	0.04297200	0.30325200
C	-7.24748600	-2.02096200	-0.07132000
H	-8.31092800	-1.90093500	0.12139800
C	-6.73321900	-3.27526300	-0.40538900
H	-7.39286100	-4.13609100	-0.48042100
C	-5.36179700	-3.41158000	-0.62558800
H	-4.94376400	-4.38741400	-0.86457200
C	-4.51655900	-2.30526800	-0.52554500
H	-3.44556900	-2.39730100	-0.65776700
C	-4.30685800	1.11670300	-1.32208300
C	-5.49263800	1.85249200	-1.45633700
H	-6.28592800	1.75632600	-0.72285200
C	-5.68009400	2.73094100	-2.52500000

H	-6.60913200	3.29075200	-2.60232900
C	-4.68200700	2.89440000	-3.48729100
H	-4.82739300	3.57957900	-4.31856300
C	-3.49436600	2.17233000	-3.36169600
H	-2.70080300	2.29278300	-4.09607500
C	-3.31136200	1.29637200	-2.29092600
H	-2.38027200	0.76090500	-2.16919500
C	2.15959400	3.30312300	0.13937600
H	2.47009200	2.53195400	0.84870600
H	2.94401100	4.07386200	0.14485400
C	1.63115200	3.56045100	-2.27805000
H	0.58370700	3.81917300	-2.10883900
H	2.22039400	4.49224900	-2.27797000
C	1.87858000	2.73494100	-3.54385800
H	1.01245000	2.09207300	-3.73773200
H	2.02338200	3.36910100	-4.42279500
C	3.12063800	1.87093000	-3.20036200
H	2.91188200	0.81037800	-3.36099400
H	3.99559000	2.12274500	-3.80368500
C	3.40944100	2.12232200	-1.70023100
H	4.17713100	2.90074800	-1.59627400
C	3.82604300	0.81538000	-0.91806700
C	4.89920000	0.07361900	-1.75535900
C	6.14716800	0.63200700	-2.06337900
H	6.41107500	1.61825600	-1.69619400
C	7.07487100	-0.06954900	-2.83430800
H	8.03703200	0.38339500	-3.06090400
C	6.77387600	-1.34852000	-3.30799900
H	7.49939600	-1.89698200	-3.90337900
C	5.53257200	-1.91133100	-3.00937300
H	5.28047500	-2.90484700	-3.37337700
C	4.60306900	-1.20268200	-2.24592100
H	3.63126700	-1.62224500	-2.01912300
C	4.43401000	1.14121900	0.47370900
C	5.33284000	2.19174500	0.71191300
H	5.62822900	2.85811000	-0.09281100
C	5.84961700	2.42524300	1.98767800
H	6.53705400	3.25305600	2.14384100
C	5.48308200	1.60731900	3.05730500
H	5.88410200	1.79036700	4.05079900
C	4.59181000	0.55653000	2.83564800
H	4.28772600	-0.09178700	3.65271600
C	4.07514400	0.33241800	1.55962300
H	3.36680500	-0.46819300	1.39085800
O	-0.19215300	-0.21262900	-2.27998100
C	-0.41365400	-1.17757600	-1.51554400
C	-0.32198100	-1.53243000	2.83199100
C	-0.67858700	-2.71383600	2.18403700
C	0.77275100	-1.89307100	3.75316700
C	-0.06945200	-3.92992300	2.82616700
C	0.94010300	-3.29020200	3.75879500
H	0.39847700	-4.61849800	2.11259200
H	-0.82883300	-4.50393300	3.37805500
F	-1.78025400	-2.82456900	1.40046100
C	1.94576000	-3.86773000	4.52124200
C	1.59074800	-1.05720900	4.50928500
C	2.76705500	-3.03442300	5.29447200
C	2.59030400	-1.64540400	5.29066600
H	2.09617900	-4.94447100	4.52286900
H	3.55287400	-3.47324500	5.90344500
H	3.23956700	-1.01994500	5.89793800
H	1.44742800	0.01862800	4.47747400
O	-0.73691400	-0.32926400	2.64820600
N	0.04623600	-1.02095000	-0.21399700
O	-1.01401400	-2.29075300	-1.84773400
C	-1.36461900	-2.63394400	-3.25837500
C	-2.02328700	-4.00393300	-3.10150000
C	-2.35380300	-1.61618600	-3.81962800
C	-0.06561600	-2.72579800	-4.05884900
H	-2.91572200	-3.92906300	-2.47343000
H	-2.75380300	-1.99691300	-4.76592300
H	-1.32843700	-4.71977200	-2.65340500
H	-2.32192400	-4.37929100	-4.08544200
H	-1.87673000	-0.65385300	-4.00285200
H	-3.18261000	-1.46858700	-3.12285700
H	0.62569800	-3.42732100	-3.58015000
H	0.41641900	-1.74909500	-4.13792800
H	-0.28712100	-3.08773400	-5.06858300
C	0.81104500	-1.89815300	0.43105300
C	1.32108300	-3.19558500	-0.05591200
C	2.71687000	-3.35242100	-0.08296800
C	0.50228200	-4.26218500	-0.46281700
C	3.28469300	-4.53143900	-0.56493800
H	3.34992700	-2.52675500	0.22418200
C	1.07464800	-5.44717300	-0.91939800
H	-0.57160400	-4.15986300	-0.38425300
C	2.46567000	-5.58069500	-0.98561700
H	4.36601500	-4.62523400	-0.60982000
H	0.43318700	-6.27152500	-1.21985000
H	2.90658300	-6.50352900	-1.35294200
H	1.43352900	-1.42610300	1.18154300

Int$_{SS}$-Boc

G_{gas} = -6750.433585 a.u.

E_{solv} = -6751.952684 a.u.

Zn	1.79497800	0.30041800	-0.17916800
Zn	-1.13052900	0.62537000	0.63223300
O	0.58140700	1.79860300	0.23074400
O	3.35625500	-0.41686600	0.53912900
O	-2.92916500	0.23822600	0.18734200
N	2.91973900	1.25687900	-1.61711300
N	-1.93624300	2.54275700	1.17581300
C	0.61134900	2.96133400	-0.44968200
C	-0.55002600	3.76340000	-0.55133000
C	-0.48328200	4.99828100	-1.20113200
H	-1.38887800	5.60050700	-1.25935200
C	0.68661500	5.47657100	-1.79439000
C	1.81239300	4.65374900	-1.72744900
H	2.73865000	4.98112700	-2.19704200
C	1.80166300	3.42348800	-1.06741700
C	0.73520600	6.83047400	-2.46246800
H	-0.22818100	7.08910400	-2.91643600
H	0.97933900	7.62651400	-1.74554200
H	1.49588400	6.86147000	-3.25067300
C	3.07273700	2.60879100	-1.01753900
H	3.39537100	2.47153900	0.01793900
H	3.88402800	3.14407800	-1.53126300
C	2.45064100	1.27214200	-3.01920000
H	3.06903000	1.97238400	-3.60337400
H	1.41648400	1.62095600	-3.05796700
C	2.64065000	-0.17901200	-3.49149100
H	1.69948500	-0.73131300	-3.41634500
H	2.95755600	-0.21157400	-4.53761900
C	3.69996900	-0.77388300	-2.52678800
H	3.26189000	-1.56559800	-1.91265300
H	4.56107000	-1.20560700	-3.04057100
C	4.13536200	0.38978200	-1.61294800
H	4.96490100	0.93623500	-2.08054600
C	4.51527800	-0.06688300	-0.14922100
C	5.43571300	-1.30674200	-0.27141500
C	6.72478700	-1.23725100	-0.81628200
H	7.13475000	-0.28226100	-1.12777900
C	7.50727800	-2.38455600	-0.95210700
H	8.50547200	-2.30718800	-1.37631200
C	7.01494500	-3.62433800	-0.53924500
H	7.62546000	-4.51800600	-0.64120800
C	5.73314100	-3.70183000	0.00655200
H	5.33600800	-4.66137300	0.32974300

C	4.94995900	-2.55347200	0.13649200
H	3.94610800	-2.60398700	0.53875700
C	5.27753800	1.04270200	0.62204400
C	6.22356100	1.90085800	0.04212600
H	6.45287700	1.83643900	-1.01716900
C	6.87794400	2.87356600	0.80118100
H	7.59990400	3.53068900	0.32254000
C	6.60323100	3.00687500	2.16213300
H	7.10910500	3.76587400	2.75306700
C	5.66800800	2.15519400	2.75302700
H	5.44185500	2.24639900	3.81282100
C	5.01515800	1.18732100	1.99040500
H	4.27863400	0.53279400	2.43743000
C	-1.91184300	3.28202900	-0.09853500
H	-2.33059800	2.61143200	-0.85708900
H	-2.59548200	4.14299300	-0.03904700
C	-1.32198000	3.26743000	2.30421000
H	-0.23808700	3.27926200	2.17751400
H	-1.68169000	4.30902400	2.31715400
C	-1.79550100	2.49532800	3.55148800
H	-0.99712800	1.85183300	3.93175900
H	-2.07463500	3.18453700	4.35390400
C	-2.99500100	1.64583600	3.06116100
H	-2.71669600	0.58953900	3.01975200
H	-3.87687400	1.72132900	3.70022600
C	-3.29069400	2.15160200	1.63612600
H	-3.92883900	3.04381500	1.70561500
C	-3.92898500	1.07932300	0.66699600
C	-4.96694300	0.27857800	1.49343500
C	-6.22342700	0.80363100	1.82247800
H	-6.51578900	1.78133400	1.45103800
C	-7.11926900	0.07423300	2.60620200
H	-8.09189100	0.49738900	2.84600000
C	-6.77446300	-1.19688300	3.07043300
H	-7.47532300	-1.76870900	3.67358900
C	-5.52307500	-1.72512800	2.74903800
H	-5.24019200	-2.71354600	3.10398600
C	-4.62570200	-0.99148200	1.97161700
H	-3.64670700	-1.38750700	1.73226600
C	-4.67990100	1.70732900	-0.53681100
C	-5.25299200	2.98498000	-0.55825500
H	-5.16632900	3.64349100	0.30000400
C	-5.94480000	3.44981100	-1.68169200
H	-6.36845300	4.45120000	-1.67306400
C	-6.09267600	2.63648200	-2.80317200
H	-6.63242000	2.99509300	-3.67572900
C	-5.54388900	1.35099700	-2.78727800
H	-5.66667200	0.69692800	-3.64758200
C	-4.84628800	0.89696600	-1.67051700
H	-4.41261700	-0.09551100	-1.65972000
O	-0.25929800	-0.28661600	2.29483800
C	-0.37429100	-1.52921800	2.28101300
C	0.01508200	-1.64739200	-1.37567900
C	0.73526400	-2.79760000	-1.42860800
C	-0.96286900	-1.69933600	-2.47004700
C	0.34251900	-3.69804900	-2.55983700
C	-0.78936800	-2.90243900	-3.18351300
H	-0.00197900	-4.68111700	-2.20928800
H	1.17068800	-3.87369100	-3.26130500
F	1.74466400	-3.12161100	-0.58148200
C	-1.61569000	-3.20372000	-4.25405900
C	-1.95236800	-0.78457100	-2.81600200
C	-2.61493300	-2.28509400	-4.61297700
C	-2.77863700	-1.09145000	-3.90249800
H	-1.50017800	-4.13480100	-4.80364700
H	-3.26998700	-2.50676400	-5.45144600
H	-3.55896300	-0.39249000	-4.19009600
H	-2.10739700	0.10895700	-2.22120300
O	0.12651100	-0.63906000	-0.52062700
N	-1.30016500	-2.12401200	1.46098100
O	0.29738500	-2.34027500	3.07713700
C	1.25361700	-1.84672100	4.11148300
C	1.84776900	-3.15334000	4.63397000
C	2.32840000	-0.96661200	3.47902800
C	0.44848400	-1.12128400	5.18899600
H	2.38750400	-3.67276400	3.83597600
H	3.13782900	-0.82871400	4.20513000
H	1.06055000	-3.81273100	5.01293800
H	2.54907500	-2.94152000	5.44713200
H	1.93855300	0.01303800	3.20179000
H	2.74902600	-1.42214100	2.57882300
H	-0.32713700	-1.77662100	5.59884800
H	-0.02226100	-0.22256300	4.78423100
H	1.11762400	-0.82476000	6.00368100
C	-1.09399500	-3.26478300	0.89372600
H	-0.16079200	-3.81718900	1.04913500
C	-2.08852800	-3.85022800	0.00602300
C	-1.97229700	-5.19833400	-0.37627500
C	-3.13408600	-3.06135000	-0.51554300
C	-2.90201800	-5.76158400	-1.24654000
H	-1.15558900	-5.79943900	0.01795800
C	-4.05355900	-3.63118700	-1.38888000
H	-3.18115300	-2.00491000	-0.26666200
C	-3.94245800	-4.97656900	-1.75356200
H	-2.81445200	-6.80545000	-1.53459800
H	-4.84551200	-3.01631700	-1.80543000
H	-4.65991500	-5.41232800	-2.44386000

TS$_{SS}$-Boc

G_{gas} = -6750.420977 a.u.

E_{solv} = -6751.938244 a.u.

Zn	-1.62770500	-0.31429200	-0.53833100
Zn	1.50562000	-0.61061500	0.30242300
O	-0.08106700	-1.56463100	-0.50845100
O	-3.23442300	0.01463100	0.38039300
O	3.23147100	-0.07479900	-0.26675000
N	-2.74510800	-1.50122900	-1.80833400
N	2.43509700	-2.38688300	0.86538800
C	-0.18262100	-2.90269600	-0.74059500
C	0.96100400	-3.73528500	-0.65733400
C	0.85836500	-5.10482500	-0.90928600
H	1.75968400	-5.71049000	-0.83283100
C	-0.34086000	-5.71473500	-1.27424300
C	-1.45723900	-4.88661500	-1.36405400
H	-2.41574600	-5.32189400	-1.64099500
C	-1.41334800	-3.51498600	-1.09257000
C	-0.42837900	-7.20057000	-1.52874200
H	-1.27649600	-7.44628000	-2.17717900
H	0.48146100	-7.58003700	-2.00783600
H	-0.56019200	-7.76233800	-0.59394500
C	-2.73945400	-2.78911400	-1.09251200
H	-3.03565400	-2.58107200	-0.06044200
H	-3.51770500	-3.44463100	-1.51015800
C	-2.35917000	-1.56048700	-3.22843100
H	-2.95817700	-2.32729600	-3.74642400
H	-1.30491000	-1.83509600	-3.31309500
C	-2.68118100	-0.14410400	-3.73603200
H	-1.79021400	0.48556400	-3.66456600
H	-3.00619500	-0.15809900	-4.78004100
C	-3.77735200	0.38226100	-2.76888500
H	-3.41791200	1.25912900	-2.22299300
H	-4.69829900	0.67662300	-3.27590000
C	-4.04093100	-0.77214600	-1.77818000
H	-4.82241000	-1.42625200	-2.18647500
C	-4.39652700	-0.33275300	-0.30043900
C	-5.34786500	0.88797500	-0.38371400
C	-6.60506700	0.81802000	-0.99941200
H	-6.96113200	-0.12416400	-1.40428400

C	-7.41916700	1.94669900	-1.09582700
H	-8.39018300	1.87010700	-1.57924500
C	-6.99226300	3.16825200	-0.56982600
H	-7.62710100	4.04778800	-0.64183600
C	-5.74567900	3.24376500	0.05196500
H	-5.40336900	4.18819400	0.47014100
C	-4.92945300	2.11393000	0.14230200
H	-3.95934800	2.16133000	0.61860500
C	-5.13796900	-1.46321400	0.46665200
C	-6.07825700	-2.33120200	-0.10674300
H	-6.32479000	-2.26442100	-1.16209700
C	-6.71477100	-3.31301900	0.65685900
H	-7.43333700	-3.97762700	0.18318600
C	-6.42880800	-3.44403100	2.01550000
H	-6.92153200	-4.20943300	2.60948700
C	-5.50045800	-2.58025200	2.60036400
H	-5.26526700	-2.66802600	3.65855900
C	-4.86550700	-1.60486700	1.83324100
H	-4.13104700	-0.94260500	2.26991000
C	2.33513600	-3.18511500	-0.37633900
H	2.65548300	-2.54183900	-1.20097900
H	3.05812700	-4.01194800	-0.33122400
C	1.96862900	-3.08849500	2.08220500
H	0.87828800	-3.10643300	2.09349000
H	2.33725000	-4.12575200	2.06963400
C	2.58234400	-2.28268900	3.24761700
H	1.81353900	-1.69676600	3.75570500
H	3.03115800	-2.95521200	3.98473900
C	3.64452000	-1.36596900	2.58921500
H	3.28753600	-0.33213600	2.52273500
H	4.59339400	-1.34174000	3.12815000
C	3.81688000	-1.92441600	1.16854300
H	4.48562000	-2.79574900	1.20268800
C	4.30147200	-0.87850800	0.09263600
C	5.42135800	-0.02612900	0.74397100
C	6.66341800	-0.56862500	1.10111900
H	6.88654300	-1.60775900	0.88021100
C	7.63311100	0.21553400	1.72704000
H	8.59025700	-0.22539900	1.99530100
C	7.38051500	1.56229400	1.99959100
H	8.13846800	2.17517400	2.48115300
C	6.14852200	2.11073900	1.64208100
H	5.93500900	3.15863900	1.84019700
C	5.17710600	1.32090000	1.02451200
H	4.21917400	1.73655600	0.74777100
C	4.89465900	-1.55208300	-1.17379900
C	5.63582000	-2.74166400	-1.17531000
H	5.81171300	-3.28478100	-0.25130500
C	6.15303400	-3.26890600	-2.36154100
H	6.71622000	-4.19866100	-2.33423100
C	5.94581300	-2.61055300	-3.57309400
H	6.34604600	-3.02054700	-4.49672700
C	5.21640900	-1.41919700	-3.58406700
H	5.04816800	-0.89349000	-4.52116700
C	4.69781900	-0.90005000	-2.39905900
H	4.11843300	0.01623900	-2.39610800
O	-0.16254800	-0.71830100	2.42242700
C	0.05686600	0.48997600	2.36887900
C	-0.80115000	2.44681600	-0.99700700
C	-1.07576900	3.00326600	0.26256400
C	-0.40008500	3.56278100	-1.86007600
C	-1.09456900	4.50718100	0.22377100
C	-0.55121500	4.77553400	-1.16463600
H	-0.47200900	4.96877900	1.00304500
H	-2.11618300	4.89246900	0.35096100
F	-1.79643000	2.34914400	1.20999700
C	-0.18532500	5.97167400	-1.76657800
C	0.08188900	3.52446700	-3.16751300
C	0.30117300	5.94011000	-3.07988100
C	0.42739900	4.73033600	-3.77661400
H	-0.27552000	6.91543300	-1.23493200
H	0.58217400	6.86966200	-3.56760400
H	0.80689400	4.73506200	-4.79469700
H	0.19164900	2.57204600	-3.67725300
O	-0.74331800	1.21746300	-1.35650400
N	0.77025500	1.00932800	1.28711200
O	-0.28040700	1.37665100	3.30465000
C	-1.21529500	1.04104500	4.39894600
C	-1.52032300	2.42057400	4.98202400
C	-2.48355100	0.39084800	3.84330000
C	-0.48919800	0.14547700	5.40267400
H	-1.99781200	3.04820300	4.22269200
H	-3.25283400	0.38366000	4.62345300
H	-0.59980900	2.91153200	5.31506200
H	-2.19622700	2.32681900	5.83785400
H	-2.29461400	-0.63389700	3.52395200
H	-2.85925200	0.94880400	2.98165300
H	0.43184800	0.62594100	5.74986600
H	-0.24073200	-0.81452800	4.94512600
H	-1.13342100	-0.03566600	6.27017800
C	0.92315400	2.33893600	1.17954800
H	0.58789000	2.92256700	2.03361600
C	1.92029100	3.00136800	0.34012000
C	2.44414100	4.22354800	0.80162400
C	2.35178700	2.50402100	-0.90100500
C	3.40530200	4.91003200	0.06373300
H	2.11114900	4.61966800	1.75822600
C	3.30430300	3.19589300	-1.63879000
H	1.93391200	1.58599600	-1.28646100
C	3.83956900	4.39383700	-1.15911000
H	3.81274100	5.84389200	0.44065600
H	3.63178800	2.79559700	-2.59346100
H	4.59085200	4.92413500	-1.73761000

Int$_{RS}$-Boc

G_{gas} = -6750.410723 a.u.

E_{solv} = -6751.934941 a.u.

Zn	1.35656100	-0.52761600	0.29957500
Zn	-1.40527400	-0.42641500	-0.68315200
O	0.15259600	-1.84069600	-0.55660700
O	2.94273700	-0.19368000	-0.74130100
O	-3.04212800	0.49545700	-0.83917100
N	2.55965900	-1.80720100	1.38944700
N	-2.40959900	-2.07282700	-1.60025700
C	-0.04664400	-3.02314300	0.06196500
C	-1.30127500	-3.67556800	0.03412400
C	-1.43798600	-4.92676500	0.64614100
H	-2.41319600	-5.41121500	0.61288400
C	-0.39049300	-5.56944100	1.30554200
C	0.84598900	-4.91878200	1.31667800
H	1.69682000	-5.39773400	1.79938500
C	1.03799500	-3.68312600	0.70022700
C	-0.58723800	-6.89974700	1.99390300
H	-1.40847500	-7.46709700	1.54209500
H	0.31635900	-7.51793500	1.93954000
H	-0.82849600	-6.77281500	3.05838800
C	2.42381700	-3.08853300	0.64404600
H	2.68302100	-2.87336600	-0.39339600
H	3.16437600	-3.80481000	1.02762300
C	2.33707500	-1.92208100	2.84270900
H	2.96922900	-2.72716700	3.25092400
H	1.29431800	-2.17790300	3.03591700
C	2.76635400	-0.54590900	3.37400900
H	1.89581600	0.11526500	3.44205500
H	3.19170400	-0.61974000	4.37862900
C	3.78742100	-0.02815500	2.32285400
H	3.43189700	0.88744400	1.83912200
H	4.76585300	0.20271900	2.74848800

C	3.89362600	-1.14354000	1.26313800
H	4.66668000	-1.86290000	1.56455900
C	4.13771600	-0.63713000	-0.21904800
C	5.15292400	0.53838500	-0.17346200
C	6.46328100	0.40685700	0.30488200
H	6.82869200	-0.55933500	0.63706400
C	7.32187100	1.50616500	0.35669500
H	8.33442100	1.37978400	0.73247400
C	6.88664500	2.76109000	-0.07487800
H	7.55662900	3.61636100	-0.03736900
C	5.58367100	2.90212300	-0.55424200
H	5.22778000	3.87356700	-0.89102700
C	4.72558000	1.80151200	-0.59967800
H	3.70925300	1.90105200	-0.95896700
C	4.73210200	-1.76848700	-1.10493000
C	5.74309200	-2.64714000	-0.68964700
H	6.15255300	-2.58453100	0.31426200
C	6.23952200	-3.63351500	-1.54476000
H	7.01930900	-4.30506700	-1.19359400
C	5.73445900	-3.76220700	-2.83871900
H	6.11816500	-4.53129300	-3.50404200
C	4.72464000	-2.89668800	-3.26336400
H	4.31371400	-2.98979600	-4.26591700
C	4.23073400	-1.91505900	-2.40468600
H	3.42375900	-1.26189300	-2.71196600
C	-2.57514700	-3.05435200	-0.51240100
H	-3.08670700	-2.54439000	0.30704200
H	-3.25458000	-3.85666300	-0.84634200
C	-1.74791800	-2.62826900	-2.79811500
H	-0.70876800	-2.86443700	-2.56751600
H	-2.26456800	-3.54891000	-3.11794000
C	-1.91559600	-1.50869400	-3.82152200
H	-1.13633700	-0.75454600	-3.65877500
H	-1.82546500	-1.86691900	-4.85121100
C	-3.30669300	-0.91711900	-3.49564600
H	-3.27919300	0.17422600	-3.48297800
H	-4.06172900	-1.21935700	-4.22609600
C	-3.67966200	-1.45261300	-2.08626000
H	-4.44374500	-2.23869200	-2.16302900
C	-4.13765100	-0.29845500	-1.11650500
C	-5.23100700	0.55747000	-1.79441000
C	-6.27856900	0.01511900	-2.55054000
H	-6.33765700	-1.05684200	-2.71693200
C	-7.25499300	0.83723300	-3.11583000
H	-8.05495900	0.39574500	-3.70553700
C	-7.20325000	2.21934000	-2.92814600
H	-7.96375600	2.86065800	-3.36665000
C	-6.16297000	2.76826600	-2.17539100
H	-6.11090000	3.84435500	-2.02501400
C	-5.18459500	1.94518000	-1.61703400
H	-4.36177100	2.35467500	-1.04156100
C	-4.76075600	-0.86567900	0.19095800
C	-5.78129700	-1.82741500	0.20415500
H	-6.19599200	-2.19843900	-0.72848800
C	-6.27606900	-2.32937800	1.40835100
H	-7.06080900	-3.08217600	1.39464300
C	-5.76685800	-1.87174400	2.62661100
H	-6.14825700	-2.26970600	3.56355400
C	-4.76872000	-0.89656400	2.62571000
H	-4.35991500	-0.52534600	3.56264300
C	-4.27929500	-0.39666800	1.41781500
H	-3.50231700	0.35594500	1.40209800
O	-0.06200300	0.90620700	-1.76160800
C	0.75749400	1.70667600	-1.29071700
C	-1.04902300	0.89379700	1.94961100
C	-1.52576100	2.13014100	1.61389900
C	-1.09486200	0.81891000	3.42075400
C	-1.94168600	2.95878700	2.78958500
C	-1.60181200	2.02877700	3.93795200
H	-3.01404300	3.19912900	2.76182300
H	-1.39860600	3.91360300	2.83840800
C	-1.74509500	2.20057500	5.30613600
C	-0.76198500	-0.23794400	4.26352900
C	-1.38710400	1.14664600	6.16179900
C	-0.90753700	-0.06058000	5.64412100
H	-2.13702300	3.12999200	5.71279500
H	-1.49569000	1.26706800	7.23629800
H	-0.65307800	-0.87220700	6.32085900
H	-0.41965400	-1.17848000	3.84486600
O	-0.61110500	-0.08260000	1.17666800
N	1.11288800	1.64515700	0.04399200
O	1.46844700	2.56709300	-1.99281100
C	1.55606300	2.49024700	-3.48116200
C	2.62360800	3.54174600	-3.77760100
C	2.03284100	1.09251200	-3.87523600
C	0.20259700	2.86577300	-4.08190600
H	3.57310300	3.26391500	-3.30929700
H	2.33751000	1.10111400	-4.92713600
H	2.31677000	4.52015800	-3.39396300
H	2.77496300	3.62123600	-4.85873300
H	1.24752700	0.34645100	-3.74213500
H	2.88606800	0.80608700	-3.25466300
H	-0.10793400	3.85925400	-3.73983300
H	-0.56538100	2.14077400	-3.80678400
H	0.28751800	2.89255600	-5.17367700
C	1.18807300	2.57085600	0.93836900
C	0.87185400	3.99749000	0.91010200
C	0.19645500	4.65275800	-0.13701000
C	1.25020800	4.74070900	2.04507900
C	-0.07387800	6.01364300	-0.04733800
H	-0.13285500	4.10240900	-1.00600900
C	0.98276600	6.10416700	2.12805100
H	1.75734800	4.23771800	2.86481400
C	0.32001000	6.74415300	1.07851000
H	-0.60204400	6.50815300	-0.85743000
H	1.28569800	6.66354300	3.00830000
H	0.10436600	7.80728400	1.13894400
H	1.59559600	2.22492400	1.88901500
F	-1.69809700	2.58507500	0.35569100

TS$_{RS}$-Boc

G_{gas} = -6750.408099 a.u.

E_{solv} = -6751.929787 a.u.

Zn	1.52120600	-0.52416400	0.03496900
Zn	-1.59255300	-0.31644000	-0.70093000
O	0.10869200	-1.75588800	-0.38502200
O	3.01759500	-0.13710700	-1.04985800
O	-3.17668700	0.55332200	-1.30019600
N	2.72937300	-1.61225900	1.27228800
N	-2.53056300	-2.13765600	-1.22689500
C	-0.05300200	-2.82950500	0.41562700
C	-1.33183900	-3.40355200	0.61940100
C	-1.45528800	-4.53437200	1.43206900
H	-2.44872400	-4.95743900	1.57584900
C	-0.37033000	-5.13528100	2.07310100
C	0.88772200	-4.57710000	1.84248100
H	1.76538500	-5.03372600	2.29779900
C	1.06693300	-3.46365600	1.01983200
C	-0.55511000	-6.32599500	2.98396400
H	0.36317800	-6.91894200	3.06047500
H	-0.82918500	-6.01783400	4.00246600
H	-1.35128800	-6.98783500	2.62404800
C	2.47057500	-2.98027700	0.73708600
H	2.64398600	-2.94455800	-0.34062900
H	3.20936200	-3.67625800	1.15883000
C	2.62432100	-1.54277400	2.74663100
H	3.20811500	-2.36657000	3.18619900
H	1.58557000	-1.66445600	3.05193400

C	3.22797900	-0.17639500	3.10949800
H	2.43424300	0.55132200	3.30867400
H	3.82759900	-0.24597000	4.02135400
C	4.07654700	0.22065400	1.87355100
H	3.62219600	1.06021900	1.33765700
H	5.09649400	0.51747600	2.12445400
C	4.06713900	-1.01393300	0.95193900
H	4.84922700	-1.71591200	1.26876000
C	4.20861500	-0.67132600	-0.58990000
C	5.32483700	0.39642600	-0.73194000
C	6.68481300	0.12103200	-0.54329900
H	7.01368800	-0.89200800	-0.33732200
C	7.64042500	1.13497400	-0.63821100
H	8.69134800	0.89714000	-0.49233200
C	7.25254100	2.44467600	-0.92637500
H	7.99737900	3.23262100	-1.00388900
C	5.89903000	2.72891900	-1.11603500
H	5.58064100	3.74520900	-1.33799300
C	4.94562700	1.71467800	-1.01804000
H	3.89095800	1.92388400	-1.15396700
C	4.58523700	-1.93049400	-1.41384900
C	5.49466200	-2.91022200	-0.98885400
H	5.97900400	-2.83208200	-0.01991400
C	5.78652600	-4.01933100	-1.78600400
H	6.48992600	-4.76713800	-1.42802900
C	5.17396100	-4.17160600	-3.02980200
H	5.39695400	-5.03615500	-3.64950200
C	4.26618900	-3.20390800	-3.46457500
H	3.77630600	-3.31167900	-4.42930100
C	3.97576300	-2.09919800	-2.66438300
H	3.25278000	-1.35742400	-2.98185800
C	-2.62533000	-2.81400200	0.08477300
H	-3.00384800	-2.08605400	0.80757000
H	-3.38033900	-3.61456200	0.02642900
C	-1.89943800	-2.97422100	-2.27302400
H	-0.84515800	-3.12346600	-2.04559400
H	-2.40085400	-3.95547000	-2.31726800
C	-2.14592700	-2.16641800	-3.53967500
H	-1.41764300	-1.34750600	-3.58880000
H	-2.03967800	-2.76678300	-4.44817100
C	-3.56693100	-1.60494000	-3.33517200
H	-3.64058200	-0.57226900	-3.67785900
H	-4.31409200	-2.18940000	-3.87984100
C	-3.84038700	-1.68927600	-1.80757100
H	-4.59051300	-2.46415700	-1.60322600
C	-4.27010400	-0.29255300	-1.22140300
C	-5.43537300	0.26461800	-2.07193100
C	-6.59737400	-0.47279800	-2.33744900
H	-6.70914400	-1.47718500	-1.93947700
C	-7.62716900	0.06557800	-3.10923800
H	-8.51803300	-0.52604600	-3.30668500
C	-7.51618800	1.35914600	-3.62417400
H	-8.31910100	1.78112800	-4.22351800
C	-6.36524300	2.10269000	-3.35960800
H	-6.26766000	3.11181200	-3.75389400
C	-5.33334600	1.55813900	-2.59257400
H	-4.42859200	2.11739800	-2.38387600
C	-4.79940300	-0.39346900	0.23783000
C	-5.61132000	-1.43293600	0.71368400
H	-5.89837000	-2.25009000	0.05913200
C	-6.04440200	-1.45730300	2.04075500
H	-6.66057700	-2.28263700	2.38972700
C	-5.68396600	-0.43265000	2.91771600
H	-6.01393800	-0.45520500	3.95319300
C	-4.89630600	0.61961000	2.44786600
H	-4.60936000	1.42646300	3.11888900
C	-4.46498000	0.63869300	1.12183300
H	-3.84595000	1.44201600	0.74565700
O	-0.23858300	0.88362000	-1.80472800
C	0.56159200	1.63560400	-1.22403500
C	-1.27197500	0.82770000	2.10024300
C	-1.46802900	2.19168800	1.91446600
C	-0.97274500	0.65761900	3.53450100
C	-1.54904200	2.95496100	3.20367600
C	-1.10499200	1.89353700	4.19464500
H	-2.57896000	3.28608700	3.40577900
H	-0.91651900	3.85242100	3.22383600
C	-0.83515400	1.98608100	5.55291700
C	-0.61945100	-0.50318500	4.21751000
C	-0.45654600	0.82560300	6.24569000
C	-0.35735400	-0.40633100	5.58787700
H	-0.92355500	2.93476700	6.07706400
H	-0.24855100	0.88300500	7.31083000
H	-0.07947700	-1.29422200	6.14973700
H	-0.57433200	-1.44983200	3.68614400
O	-1.21991300	-0.12651000	1.25054000
N	0.85003600	1.41746300	0.11379300
O	1.28965600	2.55887900	-1.80846800
C	1.35763900	2.68953000	-3.29580300
C	2.42272700	3.77244800	-3.45809800
C	1.82674900	1.35756900	-3.88360900
C	-0.00267800	3.14764300	-3.81889900
H	3.38491800	3.42571700	-3.06884800
H	2.15226400	1.51828100	-4.91694000
H	2.13160700	4.68006700	-2.91959700
H	2.54195500	4.01548800	-4.51872700
H	1.02785400	0.61380900	-3.87869300
H	2.66363100	0.96965700	-3.29490100
H	-0.29768300	4.09036900	-3.34508500
H	-0.77253400	2.39746000	-3.62899100
H	0.06611300	3.31618700	-4.89905000
C	0.90915600	2.29651600	1.08949900
C	0.82506900	3.75799200	1.06107200
C	0.14119200	4.50954300	0.08612900
C	1.45883600	4.43953300	2.11835600
C	0.11889000	5.89774300	0.16301800
H	-0.39627900	4.01315900	-0.70873700
C	1.44192200	5.83065500	2.18517500
H	1.97508000	3.86772600	2.88573000
C	0.77326300	6.56462100	1.20400500
H	-0.41973200	6.46496300	-0.59084700
H	1.94663400	6.33868900	3.00195500
H	0.75359900	7.64975500	1.25296200
H	1.31145200	1.88877100	2.01344100
F	-1.95058900	2.71534200	0.76042500

Int$_{RR}$-Boc

G_{gas} = -6750.434431 a.u.

E_{solv} = -6751.955398 a.u.

Zn	-1.48796400	-0.61649100	-0.39307000
Zn	1.47785300	-0.55903200	0.12484600
O	-0.03094500	-1.88091300	0.16824200
O	-3.18795000	0.14582000	-0.05170100
O	3.19973500	-0.07570400	-0.47887900
N	-2.51589000	-2.21319900	-1.30165800
N	2.56328300	-1.99846200	1.31928800
C	0.00067200	-3.22616100	0.15561400
C	1.20786500	-3.92429300	0.39389500
C	1.20470800	-5.32089000	0.41937300
H	2.14480000	-5.83632300	0.61032400
C	0.05298300	-6.07430400	0.18436500
C	-1.12152100	-5.36995700	-0.08793300
H	-2.03691700	-5.92397000	-0.29029200
C	-1.17497000	-3.97439400	-0.09618900
C	0.07226900	-7.58366100	0.24290400
H	-0.13431600	-7.95179500	1.25741800
H	-0.68435500	-8.02024500	-0.41887200
H	1.04796300	-7.98476100	-0.05395000
C	-2.51443500	-3.30479700	-0.30073800
H	-2.85360000	-2.87620100	0.64418800

H	-3.26264900	-4.05929500	-0.58881600
C	-1.98348900	-2.60783200	-2.62106400
H	-2.50128600	-3.51208500	-2.98191600
H	-0.91779600	-2.83112900	-2.53631400
C	-2.29469400	-1.38802400	-3.48749000
H	-1.49592100	-0.64873600	-3.36455900
H	-2.35771500	-1.64010200	-4.54968600
C	-3.62592900	-0.84582200	-2.90892800
H	-3.56500400	0.22961900	-2.72441800
H	-4.46789600	-1.01119700	-3.58495800
C	-3.85009400	-1.59992600	-1.57015000
H	-4.58306300	-2.40876000	-1.70101400
C	-4.27622200	-0.64093700	-0.39268800
C	-5.45171800	0.25804000	-0.83769200
C	-6.49506100	-0.18551800	-1.66099600
H	-6.49032200	-1.19759900	-2.05530300
C	-7.54930000	0.66271700	-2.00620500
H	-8.34152700	0.29787100	-2.65532900
C	-7.58424400	1.97221000	-1.52619500
H	-8.40358900	2.63372600	-1.79516000
C	-6.55415300	2.42203200	-0.69769900
H	-6.57004800	3.43925900	-0.31272800
C	-5.50074400	1.57305100	-0.35932000
H	-4.69595700	1.91845100	0.27821600
C	-4.76703100	-1.43830100	0.84612600
C	-5.80442300	-2.37785100	0.78279800
H	-6.31694000	-2.56202100	-0.15686900
C	-6.20269300	-3.08236900	1.91952300
H	-7.00677200	-3.81068100	1.84680300
C	-5.57504300	-2.85289400	3.14607500
H	-5.88471700	-3.40242100	4.03125000
C	-4.54964600	-1.90904700	3.22191600
H	-4.05303800	-1.71829600	4.17070700
C	-4.15169300	-1.20783300	2.08249900
H	-3.34080200	-0.49076400	2.12067700
C	2.53992000	-3.21464600	0.48292600
H	2.84826000	-2.91413400	-0.52214100
H	3.30721600	-3.91970700	0.83992500
C	2.09203500	-2.20777400	2.69885500
H	1.01769300	-2.40538100	2.69222100
H	2.60168400	-3.07776600	3.14605900
C	2.48274000	-0.90490200	3.40949400
H	1.65703200	-0.18788900	3.36217200
H	2.70701100	-1.07506500	4.46640600
C	3.70390300	-0.37707500	2.61230000
H	3.51093400	0.62457400	2.22084800
H	4.60537000	-0.31108900	3.22447600
C	3.90330100	-1.36466200	1.43821800
H	4.63413900	-2.13602000	1.72357700
C	4.30986500	-0.68371600	0.07055600
C	5.40574300	0.38561300	0.29343300
C	6.47250000	0.22850100	1.18664000
H	6.55719900	-0.67570800	1.78304900
C	7.43658200	1.22774100	1.33643200
H	8.24902900	1.08916400	2.04561600
C	7.35851400	2.39902100	0.58169000
H	8.10854200	3.17710100	0.69778100
C	6.31362500	2.55364800	-0.33245600
H	6.25413600	3.45141800	-0.94425000
C	5.34811800	1.55588400	-0.47653100
H	4.54113700	1.65560000	-1.19486800
C	4.90660300	-1.71248900	-0.92750900
C	5.91047800	-2.62470800	-0.57764000
H	6.31402500	-2.63437200	0.43104500
C	6.41488100	-3.52858300	-1.51387400
H	7.18837200	-4.23381600	-1.21915400
C	5.93058200	-3.52642100	-2.82338600
H	6.32089400	-4.23149100	-3.55285900
C	4.94660400	-2.60498800	-3.18687900
H	4.56882400	-2.58670300	-4.20644500
C	4.44102600	-1.70385700	-2.24850000
H	3.67628500	-0.98254900	-2.51490500
O	-1.00890200	0.41662900	1.63122100
C	-0.19009600	1.32040700	1.77166900
C	0.21720700	1.48872800	-1.84855800
C	1.34456900	1.95348100	-2.46440100
C	-0.75494300	2.60632300	-1.86574600
C	1.24518700	3.37560300	-2.91811800
C	-0.16415400	3.72204000	-2.49746100
H	1.40454500	3.47982600	-4.00050300
H	1.98655800	4.01780800	-2.41911500
C	-0.85740200	4.91419500	-2.62994500
C	-2.05686700	2.68394300	-1.36714500
C	-2.16555000	4.99714500	-2.13011900
C	-2.75334100	3.89112600	-1.50982500
H	-0.39280700	5.77388600	-3.10724800
H	-2.72544100	5.92299600	-2.23476000
H	-3.77574300	3.95214700	-1.14560900
H	-2.53903500	1.83261800	-0.89517100
O	0.02941600	0.29082700	-1.30677300
N	1.02059500	1.27320600	1.08274300
O	-0.30206700	2.31663200	2.63959800
C	-1.56571400	2.52558200	3.40309300
C	-1.26585000	3.82498600	4.14872300
C	-2.74160400	2.69778100	2.43647200
C	-1.76477400	1.36008100	4.37345300
H	-1.03888200	4.62766200	3.44020800
H	-3.64873900	2.89034100	3.01981700
H	-0.40630300	3.69999500	4.81483400
H	-2.13428800	4.11782200	4.74728600
H	-2.90531100	1.81093700	1.82126200
H	-2.57885500	3.55584400	1.77588000
H	-0.86796400	1.22168000	4.98684800
H	-1.97814400	0.43216200	3.84176900
H	-2.60544600	1.58527100	5.03837400
C	1.75758500	2.26030900	0.64890000
C	1.57396100	3.70300900	0.59626500
C	0.34130900	4.37988700	0.66348800
C	2.75383500	4.45282100	0.39827100
C	0.29903600	5.76595400	0.56948800
H	-0.58166800	3.82489200	0.73430900
C	2.70760900	5.84177700	0.32636900
H	3.70531600	3.93197300	0.31710500
C	1.47837700	6.50105000	0.41499000
H	-0.66169300	6.27079900	0.59066200
H	3.62479500	6.40761400	0.19088600
H	1.43711200	7.58469900	0.34491700
H	2.70637700	1.89859500	0.25085400
F	2.45684700	1.24599300	-2.72919200

TS$_{RR}$-Boc

G_{gas} = -6750.419762 a.u.

E_{solv} = -6751.941303 a.u.

Zn	1.53323600	-0.07402400	0.48929400
Zn	-1.68599900	-0.70860900	-0.12442000
O	-0.22203300	-0.92094200	1.17752600
O	2.80062000	-0.82780100	-0.73299000
O	-3.21088500	0.11576600	-0.86091600
N	2.78658100	-0.98837800	1.99725600
N	-2.98920300	-1.82300100	1.05242600
C	-0.38524600	-1.28664200	2.47495300
C	-1.65621200	-1.30923900	3.09514800
C	-1.76259500	-1.62362500	4.45343700
H	-2.75310100	-1.62467300	4.90556300
C	-0.65623000	-1.94158200	5.24071800
C	0.57433300	-2.02984500	4.58606200
H	1.44904200	-2.36672300	5.14007400
C	0.72140200	-1.74814800	3.22738200
C	-0.78597500	-2.20698300	6.72126900
H	-0.61904300	-1.29395400	7.30895100
H	-1.78483900	-2.57797600	6.97726000
H	-0.05444600	-2.94851200	7.06235700
C	2.00683900	-2.11885200	2.53640600
H	1.76351300	-2.77146300	1.69780300
H	2.63977900	-2.70077300	3.22598400
C	3.26583800	-0.06797600	3.05050600
H	3.70094700	-0.64821500	3.88237300
H	2.42945200	0.52158800	3.42956100

C	4.32734400	0.76402400	2.33541500
H	3.83389800	1.57656500	1.79698300
H	5.04965500	1.19933800	3.03289800
C	4.96777400	-0.22309000	1.33452600
H	5.09335200	0.23467600	0.35160200
H	5.95674200	-0.55707600	1.66000900
C	4.00129200	-1.43343400	1.24818700
H	4.43269100	-2.29463800	1.77820000
C	3.62255300	-1.81660700	-0.23312800
C	4.90455600	-1.90986800	-1.09086600
C	6.08724300	-2.51736300	-0.64737800
H	6.14804000	-2.93270700	0.35472800
C	7.21240800	-2.58324500	-1.47078200
H	8.12164600	-3.05266300	-1.10275200
C	7.17347400	-2.04389800	-2.75780200
H	8.04935500	-2.09390600	-3.39974700
C	6.00030300	-1.43544600	-3.20802100
H	5.95860700	-1.00684300	-4.20675400
C	4.87865200	-1.36795600	-2.38078900
H	3.96532100	-0.88500600	-2.70923600
C	2.91684300	-3.20150200	-0.30832100
C	3.46116200	-4.37344500	0.23604400
H	4.43218000	-4.35030800	0.72118800
C	2.76967200	-5.58388900	0.17182100
H	3.20804400	-6.47742000	0.60987100
C	1.52161600	-5.65048900	-0.45247800
H	0.98274900	-6.59333200	-0.50165700
C	0.98193000	-4.49450200	-1.01822900
H	0.01928400	-4.53159000	-1.52393600
C	1.67423400	-3.28418500	-0.94796500
H	1.25020600	-2.38196800	-1.36856500
C	-2.92545000	-1.05320400	2.32110300
H	-3.02616400	0.00594200	2.06773300
H	-3.79765700	-1.30077400	2.94266100
C	-2.74088100	-3.27290000	1.18302300
H	-1.71024800	-3.45300700	1.49301800
H	-3.41292100	-3.70149900	1.94378100
C	-3.05949300	-3.79581400	-0.22114100
H	-2.15481000	-3.75254100	-0.83801200
H	-3.39190300	-4.83731900	-0.20214200
C	-4.13635500	-2.82036400	-0.76462400
H	-3.82259800	-2.37482000	-1.71271500
H	-5.09688900	-3.30862000	-0.93933300
C	-4.27057500	-1.70666300	0.30178000
H	-5.09401000	-1.93969200	0.99029200
C	-4.42826000	-0.26596300	-0.31356500
C	-5.51883500	-0.28116000	-1.40942200
C	-6.71969600	-0.99262600	-1.28584200
H	-6.91009000	-1.59787900	-0.40395900
C	-7.68689000	-0.94638900	-2.29111600
H	-8.60719200	-1.51427600	-2.17834800
C	-7.47422500	-0.17634800	-3.43588900
H	-8.22664000	-0.14014100	-4.21945500
C	-6.28738500	0.54814100	-3.56068200
H	-6.11122100	1.15697800	-4.44441600
C	-5.32169200	0.49598300	-2.55519300
H	-4.39671100	1.05223300	-2.63815600
C	-4.90870100	0.76609200	0.74402300
C	-5.96265400	0.51741000	1.63379900
H	-6.48808800	-0.43264300	1.60932600
C	-6.36227600	1.48113500	2.56068700
H	-7.17681000	1.26201600	3.24679400
C	-5.72254000	2.72137600	2.60611000
H	-6.03103900	3.47150500	3.32955600
C	-4.68823100	2.98720600	1.70748700
H	-4.18748900	3.95309000	1.72561300
C	-4.28857200	2.02029000	0.78406100
H	-3.47942100	2.20923100	0.09164600
O	-0.52346700	-0.87293500	-1.72740000
C	0.04251600	0.15606900	-2.18332600
C	0.81042500	2.75294700	1.03574900
C	-0.32600000	2.89896500	0.23666600
C	1.29187400	4.12414200	1.28705200
C	-0.78803400	4.32268200	0.11839000
C	0.37677300	5.05285000	0.75928900
H	-1.72999800	4.48346900	0.66414000
H	-0.96355400	4.64538500	-0.91763700
C	0.64358500	6.41384800	0.83123100
C	2.47084500	4.53467200	1.90338200
C	1.82687700	6.83333600	1.45309300
C	2.73097700	5.90365600	1.98370200
H	-0.04874300	7.14191100	0.41533700
H	2.04656400	7.89536000	1.52419700
H	3.64460700	6.25424900	2.45612600
H	3.16527600	3.79799300	2.29406700
O	1.42274100	1.69507900	1.40631500
N	0.83932100	0.93939500	-1.43139500
O	-0.02103400	0.48632100	-3.47122200
C	-0.80625000	-0.29774100	-4.45836100
C	-0.45539600	0.41003500	-5.76760900
C	-0.32350000	-1.75102100	-4.48507800
C	-2.29221900	-0.16357800	-4.13439400
H	0.61623700	0.33079600	-5.97596200
H	-0.73787500	-2.24646800	-5.36994100
H	-0.72148900	1.47040200	-5.71233400
H	-1.00878400	-0.04498800	-6.59534300
H	-0.63704700	-2.29750000	-3.59595600
H	0.76903700	-1.78668800	-4.55051800
H	-2.59720700	0.88625100	-4.19726300
H	-2.52826000	-0.52075300	-3.13104100
H	-2.88129600	-0.73201700	-4.86251500
C	0.98093200	2.23535300	-1.69915000
C	2.24020400	2.94447900	-1.53230700
C	3.41256100	2.26890200	-1.14291900
C	2.29024300	4.32928900	-1.78421600
C	4.59880600	2.98211700	-0.98553800
H	3.39065400	1.18901400	-1.01480700
C	3.47710400	5.03307000	-1.61930800
H	1.38797100	4.85032300	-2.09384300
C	4.63441600	4.36015300	-1.21352200
H	5.50311600	2.45452100	-0.69427900
H	3.50077400	6.10401600	-1.79784200
H	5.56322200	4.90976500	-1.08512100
H	0.22866000	2.72423400	-2.32307500
F	-1.21089200	1.88596300	0.01677900