

Supplementary Information

Metal-Free Catalytic Hydroboration of Imine with Pinacolborane by Pincer-Type Phosphorus Compound: Mechanistic Insights and Improvement of Reaction

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1. Complete Representation of Reference 17

Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc, Wallingford CT, 2016.

2. Computational Details

2.1 Computational Details of the Evaluation of Gibbs Free Energy in Solution

In this work, the Gibbs energy was evaluated under experimental conditions (323.15 K, 1 atm and in the benzene solvent) based on the optimized geometry structures. We provided the electronic energy (E_{sol}) with zero-point energy correction as well as the Gibbs energy (G_{sol}^0) in solution to discuss the reaction profile. For each species, the E_{sol} is defined through eq S1:

$$E_{sol} = E_{sol}^{pot} + E_{gas}^{v_0} \quad (S1)$$

where E_{sol}^{pot} is the electronic potential energy calculated by DLPNO-CCSD(T)/cc-pVDZ method and $E_{gas}^{v_0}$ represents the zero-point vibrational energy in the gas phase. In a bimolecular process, such as the reaction of the **1NP** and HBpin, the entropy change must be taken into consideration because the entropy considerably decreases in the process. In this case, the Gibbs energy (G_{sol}^0) must be calculated as follows:

$$\begin{aligned} G_{sol}^0 &= H^0 - T(S_r^0 + S_v^0 + S_t^0) \\ &= E^T + P\Delta V - T(S_r^0 + S_v^0 + S_t^0) \\ &= E_{sol} + E_{therm} - T(S_r^0 + S_v^0 + S_t^0) \end{aligned} \quad (S2)$$

where ΔV is 0 in solution, E_{therm} is the thermal correction by translational, vibrational, and rotational movements, and S_r^0 , S_v^0 and S_t^0 are rotational, vibrational, and translational entropies, respectively. In general, the Sackur-Tetrode equation is used to evaluate translational entropy S_t^0 . In solution phase, however, the usual Sackur-Tetrode equation cannot be directly applied to the evaluation of S_t^0 , because S_t^0 is suppressed very much in solution.^[S1] In this context, the translational entropy was evaluated using the method developed by Whitesides *et al.*^[S2]

2.2 Functional Evaluation

Table S1. Comparison of the geometrical parameters of the **1NP** optimized by various DFT functionals with the experimental molecular crystal structure.

Functionals	P-N1 (Å)	P-N2 (Å)	P-N3 (Å)	N2-P-N3 (°)
B3LYP-D3	1.742	1.734	1.783	115.4
B3PW91-D3	1.745	1.717	1.774	115.0
BMK-D3	1.742	1.698	1.758	112.7
BP86-D3	1.758	1.754	1.800	118.7
M05-2X	1.760	1.702	1.772	112.0
M06	1.754	1.711	1.768	112.7
M06-2X	1.753	1.702	1.768	112.3
PBE0-D3	1.758	1.754	1.795	119.7
TPSS-D3	1.749	1.746	1.791	118.7
ω B97XD	1.740	1.701	1.762	113.1
LC-wPBE	1.737	1.694	1.756	112.3
Exp.	1.720	1.701	1.761	115.2

2.3 Examination of Basis Set and Theoretical Methods

In our previous work^[S3], the BS-I basis set system was employed for the hydrogen generation from ammonia borane catalyzed by the pincer-type triamide phosphorus compound **1NP**; see Table S2 for details of the BS-I. In our present work, however, the employment of BS-I for imine hydroboration reaction was hindered due to the large size of **Acr^{Dipp}-1NP**-catalyzed reaction system. It is difficult to use the same basis set in the present work. Therefore, we made effort to reduce the number of basis sets by using BS-II. The corresponding examination of the basis set effects was shown in Table S3, where the imine hydroboration reaction by **1NP** was employed as the model system. As shown in Table S3, the energy changes evaluated by BS-II was similar to those by BS-I. It is concluded that the use of BS-II is a reasonable choice for energy evaluation. In addition, a comparison of B3PW91-D3 and DLPNO-CCSD(T) methods on the reaction energies and energy barriers for the whole reaction cycles was performed, and the calculated results are presented in Table S4.

Table S2 Details of BS-I and BS-II.

	Phosphorus	Hydride of HBpin	methyl (Me) groups	other atoms
BS-I	6-311+G(2d)	6-311++G(d,p)	6-311G(d)	6-311+G(d)
BS-II	6-31+G(2d)	6-31++G(d,p)	6-31G(d)	6-31+G(d)

Table S3. Basis set effects on energy changes of the hydroboration reaction of imine.

Species	ΔG (kcal/mol)	
	BS-I	BS-II
1NP + HBpin + 2	0.0	0.0
TS_{1NP/2NP} + 2	20.2	19.5
2NP + 2	-19.9	-19.8
2NP' + 2	-19.0	-18.6
TS_{2NP'/3NP}	5.1	4.6
3NP	-44.1	-45.2
TS_{1NP/3NP}	-24.1	-25.5
TS_{2NP/1NP} + 2	-11.0	-12.3
1NP + 4	-37.4	-38.6

Table S4. Electronic energy changes calculated by B3PW91-D3 and DLPNO-CCSD(T) methods, respectively, for hydroboration reaction of imine.

Species	ΔE (kcal/mol)		Species	ΔE (kcal/mol)	
	B3PW91-D3	DLPNO-CCSD(T)		B3PW91-D3	DLPNO-CCSD(T)
1NP + HBpin + 2	0.0	0.0	Acr^{Dipp}-1NP+ HBpin + 2	0.0	0.0
TS_{1NP/2NP} + 2	10.2	16.1	Acr^{Dipp}-TS_{1NP/2NP} + 2	17.1	14.4
2NP + 2	-27.7	-24.9	Acr^{Dipp}-2NP + 2	-15.4	-18.5
2NP' + 2	-26.2	-24.3	Acr^{Dipp}-2NP' + 2	-14.2	-14.4
TS_{2NP'/3NP}	-10.4	1.9	Acr^{Dipp}-TS_{2NP'/3NP}	6.8	13.2
3NP	-62.2	-56.1	Acr^{Dipp}-3NP	-53.7	-54.3
TS_{1NP/3NP}	-46.0	-38.3	Acr^{Dipp}-TS_{1NP/3NP}	-42.1	-42.0
TS_{2NP/1NP} + 2	-31.0	-17.7	Acr^{Dipp}-TS_{2NP/1NP} + 2	-14.8	-6.9
1NP + 4	-47.8	-42.7	Acr^{Dipp}-1NP + 4	-46.5	-42.7

3. Details of Distortion/Interaction Analysis

Here, we applied the distortion/interaction analysis to investigate the key transition states, $\text{TS}_{2\text{NP}'/3\text{NP}}$ and $\text{TS}_{2\text{NP}/1\text{NP}}$. Each transition state structure has been separated into two fragments, followed by single-point calculation. For each fragment, the distortion energy refers to the electronic energy change for the distortion process of **2NP**, **2NP'** and imine as they go from the equilibrium structure to transition state, which were represented by $\Delta E_{2\text{NP}}^{\text{dis}}$, $\Delta E_{2\text{NP}'},$ and $\Delta E_{\text{imine}}^{\text{dis}}$, respectively. The interaction energy ΔE_{int} refers to the energy releasing when these fragments form a complete transition state. The activation energy ΔE is the sum of the total ΔE_{dist} and ΔE_{int} .

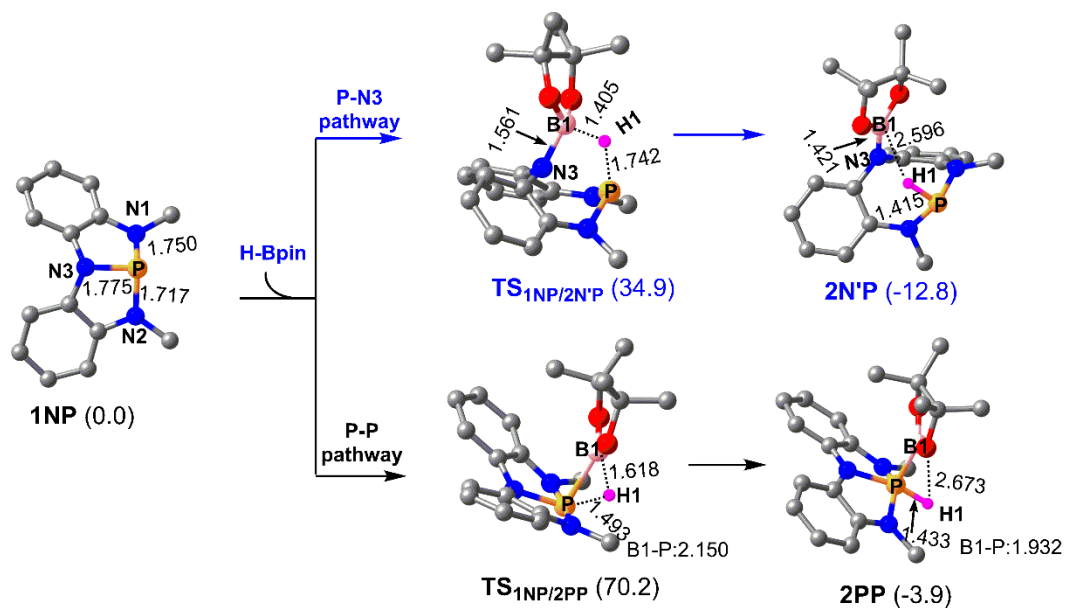


Fig. S1 Changes in geometry and the Gibbs energy in PN3 and PP pathways for the H-Bpin bond activation by **1NP**. Distances are given in Å. Gibbs energy changes are written next to each species (in kcal/mol).

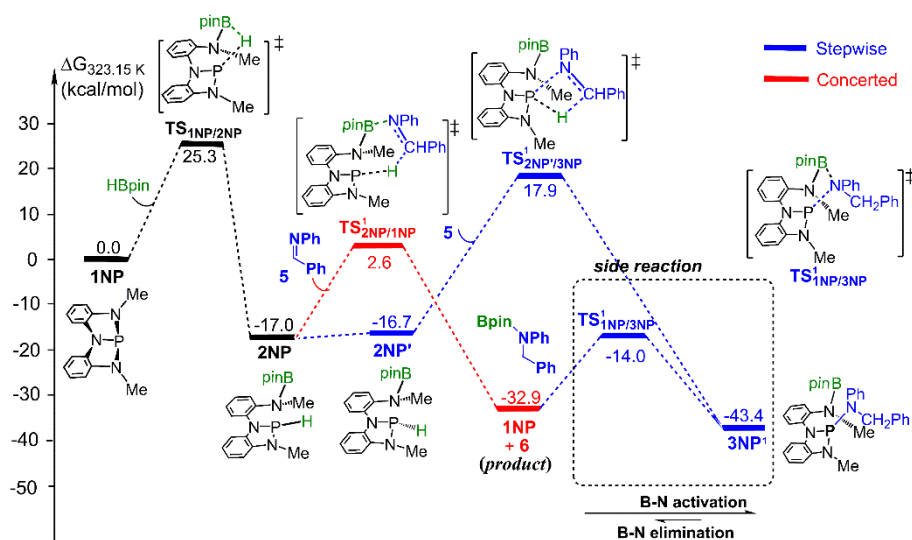


Fig. S2 Gibbs energy profile of the concerted and stepwise pathways for hydroboration reaction of PhCH=NPh catalysed by **1NP**.

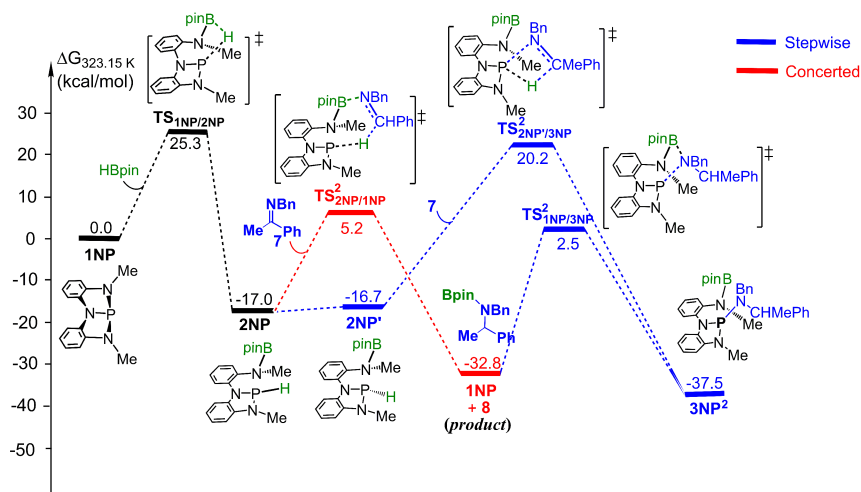


Fig. S3 Gibbs energy profile of the concerted and stepwise pathways for hydroboration reaction of PhCMe=NBn catalysed by **1NP**.

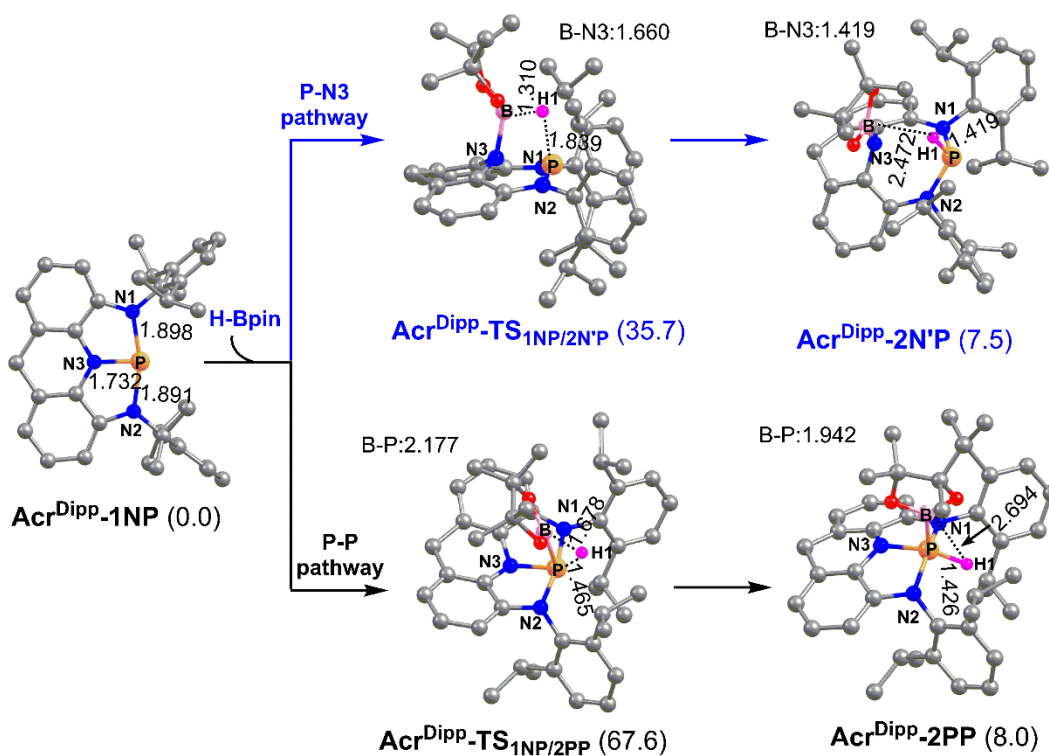


Fig. S4 Changes in geometry and the Gibbs energy in PN3 and PP pathways for the H-Bpin bond activation by **Acr^{Dipp}-1NP**. Distances are given in Å. Gibbs energy changes are written next to each species (in kcal/mol).

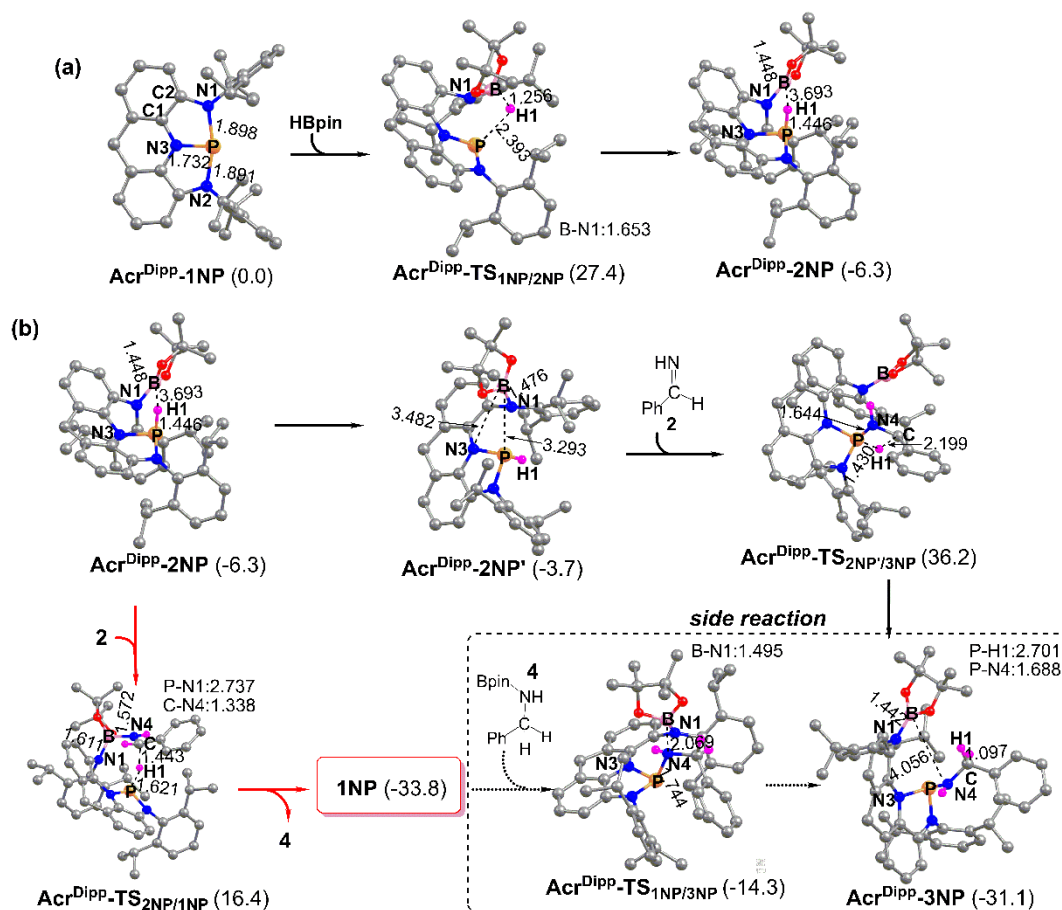


Fig. S5 Changes in geometry and the Gibbs energy involved in the catalytic hydroboration of benzylamine by $\text{Acr}^{\text{Dipp-1NP}}$. (a) B-H bond activation step; (b) concerted and stepwise pathways for hydroboration reaction. Distances are given in Å. Gibbs energy changes are written next to each species (in kcal/mol).

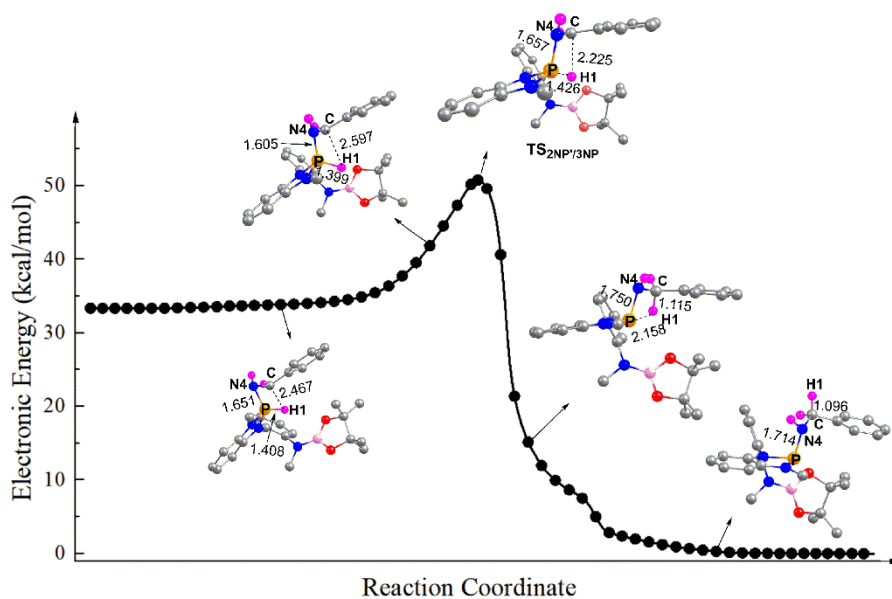


Fig. S6 IRC profile of $\text{TS}_{2\text{NP}'/3\text{NP}}$. Distances are given in Å.

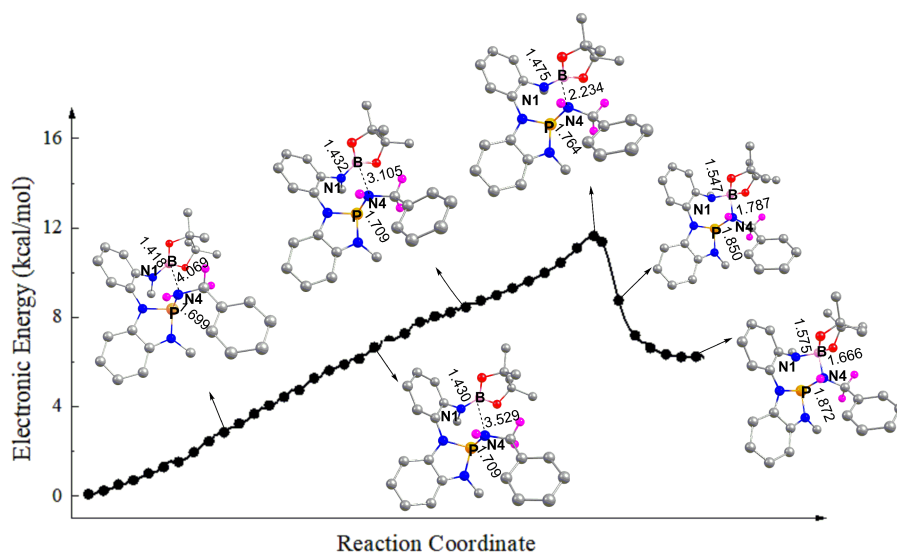


Fig. S7 IRC profile of $TS_{1NP/3NP}$. Distances are given in Å.

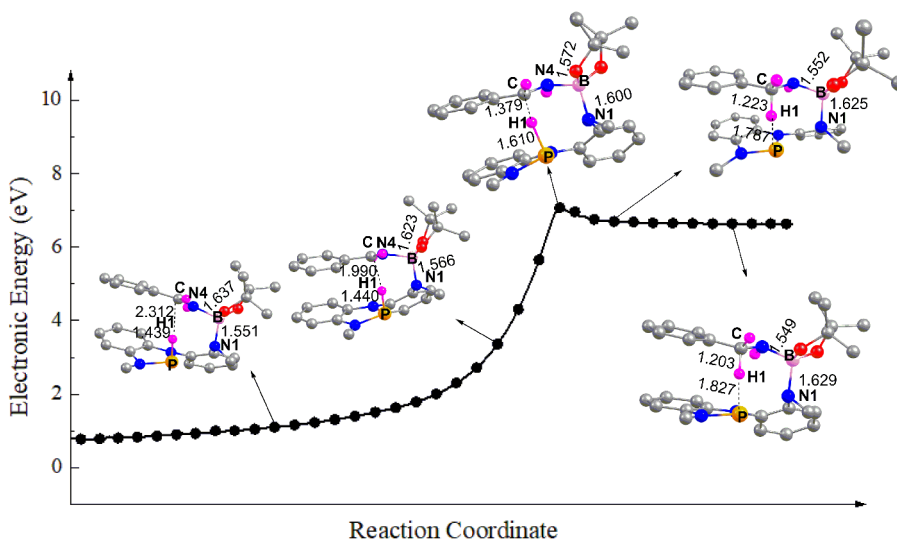


Fig. S8 IRC profile of $TS_{2NP/1NP}$. Distances are given in Å.

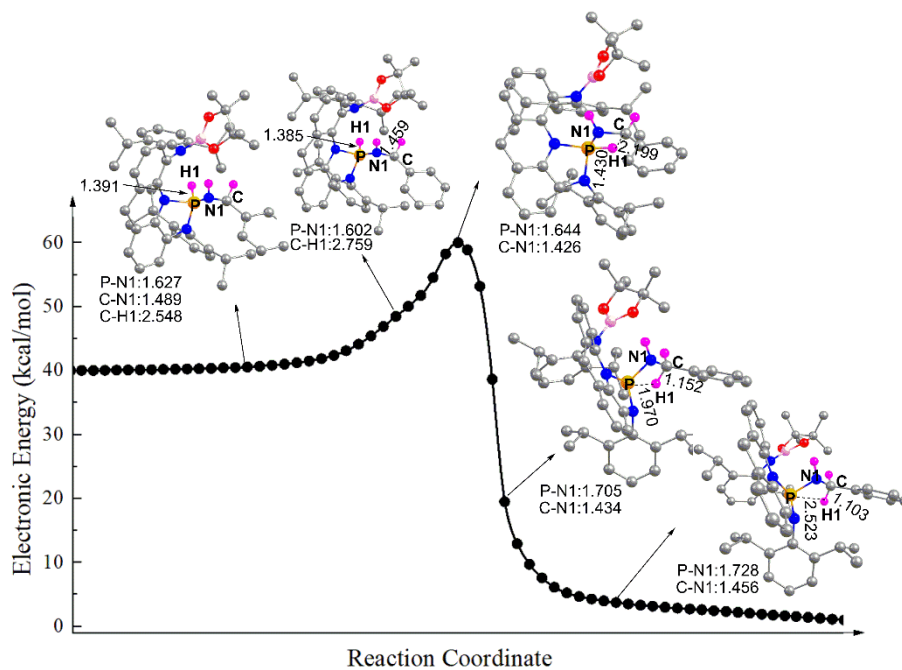


Fig. S9 IRC profile of $\text{Acr}^{\text{Dipp}}\text{-TS}_{1\text{NP}/3\text{NP}}$. Distances are given in Å.

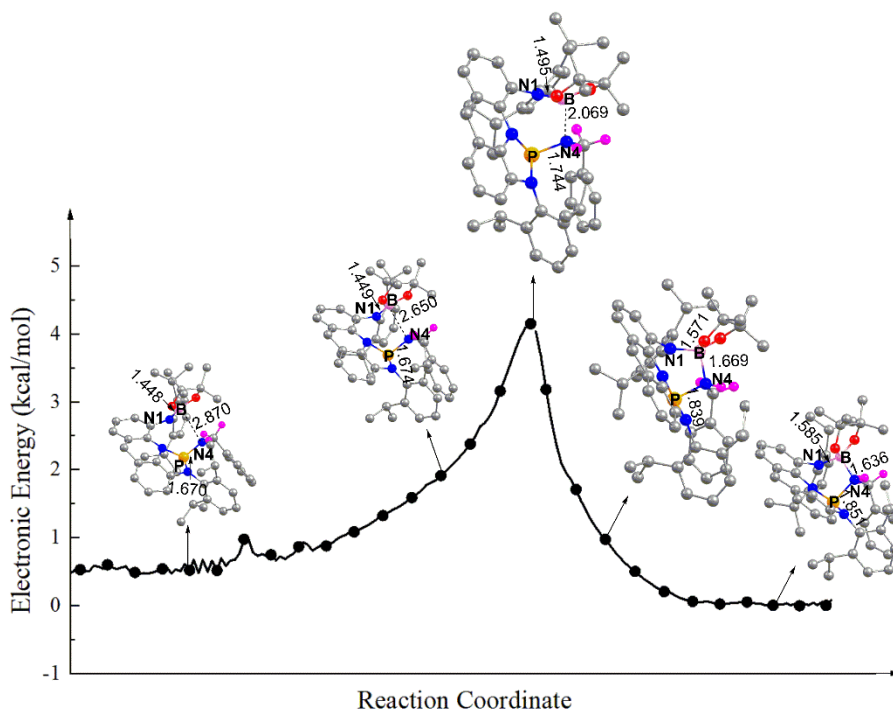


Fig. S10 IRC profile of $\text{Acr}^{\text{Dipp}}\text{-TS}_{2\text{NP}/3\text{NP}}$. Distances are given in Å.

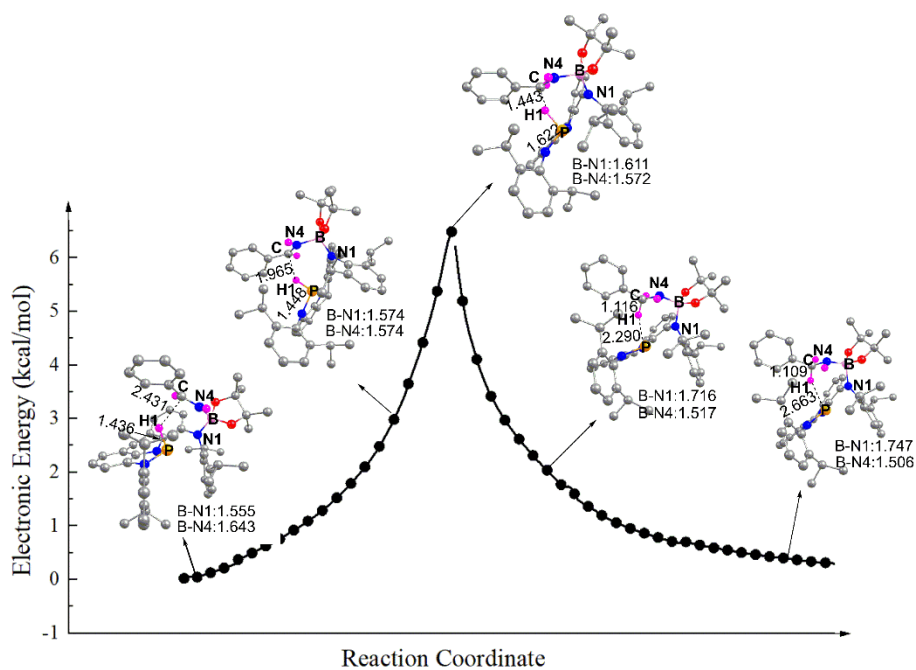


Fig. S11 IRC profile of Acr^{Dipp}-TS_{2NP/1NP}. Distances are given in Å.

References:

- [S1] S. Sakaki, Y. Y. Ohnishi and H. Sato, *Chem. Rec.*, **2010**, *10*, 29–45.
- [S2] M. Mammen, E. I. Shakhnovich, J. M. Deutch and G. M. Whitesides, *J. Org. Chem.*, **1998**, *63*, 3821–3830.
- [S3] D. Yang, P. Bao, Z. Yang, Z. Chen, S. Sakaki, S. Maeda and G. Zeng, *ChemCatChem*, **2021**, *13*, 3925–3929.

Cartesian Coordinates

HBpin

E(B3PW91-D3) = -411.752009 au

E(DLPNO-CCSD(T)) = -411.046719 au

G_{cont} = 0.167108 au

G = -410.879676 au

B	0.000000000	1.938748000	0.000000000
O	-1.068156000	1.192859000	-0.415149000
O	1.068156000	1.192859000	0.415149000
C	-0.781984000	-0.190839000	-0.054015000
C	0.781984000	-0.190839000	0.054015000
H	0.000000000	3.129434000	0.000000000
C	-1.347279000	-1.104939000	-1.128070000
H	-1.065868000	-2.145095000	-0.929240000
H	-2.440126000	-1.040657000	-1.129588000
H	-0.989786000	-0.828473000	-2.122726000
C	-1.478759000	-0.443407000	1.281456000
H	-2.546426000	-0.230136000	1.170137000
H	-1.364390000	-1.484508000	1.599991000
H	-1.082012000	0.209518000	2.065867000
C	1.347279000	-1.104939000	1.128071000
H	1.065869000	-2.145094000	0.929240000
H	2.440126000	-1.040657000	1.129588000
H	0.989786000	-0.828473000	2.122726000
C	1.478759000	-0.443407000	-1.281456000
H	2.546426000	-0.230136000	-1.170137000
H	1.364390000	-1.484509000	-1.599991000
H	1.082012000	0.209518000	-2.065867000

2

E(B3PW91-D3) = -325.595033 au

E(DLPNO-CCSD(T)) = -324.995652 au

G_{cont} = 0.100543 au

G = -324.895109 au

C	1.970999000	0.480140000	0.000147000
C	0.523200000	0.208935000	0.000069000
C	-0.374875000	1.285169000	0.000009000
C	0.021790000	-1.102685000	0.000063000
C	-1.751628000	1.059941000	-0.000062000
H	0.007466000	2.304538000	0.000025000
C	-1.350856000	-1.326987000	0.000001000
H	0.722574000	-1.932734000	0.000120000

C	-2.241204000	-0.246777000	-0.000067000
H	-2.439573000	1.901644000	-0.000112000
H	-1.732843000	-2.344935000	0.000012000
H	-3.313616000	-0.426164000	-0.000120000
N	2.849128000	-0.449164000	-0.000128000
H	2.238726000	1.546993000	0.000200000
H	3.788811000	-0.051612000	-0.000188000

4

E(B3PW91-D3) = -737.423187 au

E(DLPNO-CCSD(T)) = -736.110391 au

G_{cont} = 0.281694 au

G = -735.828697 au

C	-1.537121000	-1.546226000	0.753315000
C	-2.630389000	-0.584521000	0.330312000
C	-2.329766000	0.770251000	0.133304000
C	-3.941704000	-1.019607000	0.121500000
C	-3.318650000	1.668018000	-0.263105000
H	-1.311244000	1.116410000	0.295300000
C	-4.937734000	-0.122904000	-0.277117000
H	-4.188713000	-2.069754000	0.269651000
C	-4.628278000	1.223033000	-0.471133000
H	-3.070807000	2.717118000	-0.408489000
H	-5.952931000	-0.478433000	-0.438165000
H	-5.400450000	1.922756000	-0.781918000
N	-0.446261000	-1.640972000	-0.202783000
B	0.740662000	-0.889870000	-0.129196000
O	1.096653000	-0.139566000	0.980065000
O	1.673872000	-0.824643000	-1.149609000
C	2.226627000	0.671220000	0.574089000
C	2.844329000	-0.180297000	-0.588011000
C	3.141545000	0.876121000	1.770030000
H	4.057405000	1.395962000	1.466634000
H	2.634996000	1.488133000	2.523657000
H	3.414218000	-0.075157000	2.233352000
C	1.667351000	2.011029000	0.095291000
H	1.068457000	2.451738000	0.898891000
H	2.467535000	2.712195000	-0.163473000
H	1.021796000	1.879652000	-0.779819000
C	3.528641000	0.631335000	-1.675643000
H	4.354005000	1.216535000	-1.254619000
H	3.939309000	-0.040645000	-2.436393000
H	2.829626000	1.312435000	-2.167182000

C	3.771623000	-1.286026000	-0.084508000
H	3.994791000	-1.964768000	-0.913761000
H	4.715214000	-0.878719000	0.293386000
H	3.296332000	-1.867194000	0.712957000
H	-1.112125000	-1.214504000	1.706504000
H	-1.967759000	-2.539501000	0.927053000
H	-0.672181000	-2.102986000	-1.071692000

1NP

E(B3PW91-D3) = -1047.288346 au

E(DLPNO-CCSD(T)) = -1045.588302 au

G_{cont} = 0.220938 au

G = -1045.367364 au

P	-0.065218000	1.539159000	-0.890861000
N	-1.608988000	1.433921000	-0.146122000
N	1.295170000	1.538225000	0.210256000
N	0.015927000	-0.233047000	-0.958386000
C	-2.050024000	0.139113000	0.102136000
C	-1.152688000	-0.821549000	-0.402737000
C	-1.451854000	-2.173679000	-0.307982000
C	-2.648867000	-2.565550000	0.309192000
C	-3.533022000	-1.613191000	0.812422000
C	-3.238632000	-0.246851000	0.715941000
H	-0.772865000	-2.920676000	-0.702992000
H	-2.883778000	-3.623628000	0.388482000
H	-4.461650000	-1.926776000	1.282476000
H	-3.922007000	0.497299000	1.114976000
C	1.962104000	0.319438000	0.236974000
C	1.282587000	-0.683158000	-0.486487000
C	1.846188000	-1.935794000	-0.663349000
C	3.088989000	-2.214178000	-0.072507000
C	3.749659000	-1.233859000	0.664203000
C	3.196786000	0.044696000	0.822828000
H	1.342600000	-2.684989000	-1.265397000
H	3.536428000	-3.195708000	-0.203004000
H	4.714755000	-1.452980000	1.114474000
H	3.721299000	0.806310000	1.392691000
C	-2.455437000	2.589198000	0.062811000
H	-3.434896000	2.441252000	-0.408947000
H	-2.604641000	2.792632000	1.130814000
H	-1.978528000	3.464531000	-0.390136000
C	1.969466000	2.768164000	0.570140000
H	1.373268000	3.616682000	0.216763000

H	2.075155000	2.859682000	1.657980000
H	2.966850000	2.828467000	0.112977000

TS_{1NP/2N'P}

E(B3PW91-D3) = -1459.004029 au

E(DLPNO-CCSD(T)) = -1456.590920 au

G_{cont} = 0.399490 au

G = -1456.191429 au

P	-1.136391000	0.543047000	-1.825834000
N	-2.459321000	-0.481288000	-1.349415000
N	-1.023881000	2.085379000	-1.052706000
N	-0.458281000	-0.049624000	0.203731000
C	-2.401901000	-1.325961000	-0.245869000
C	-1.287892000	-1.147619000	0.590086000
C	-1.043585000	-2.007612000	1.649217000
C	-1.956872000	-3.028326000	1.935089000
C	-3.090100000	-3.180565000	1.137489000
C	-3.317546000	-2.344778000	0.039886000
H	-0.136678000	-1.892495000	2.233404000
H	-1.776426000	-3.700065000	2.769669000
H	-3.806455000	-3.968405000	1.357768000
H	-4.196646000	-2.492345000	-0.579388000
C	-0.801757000	2.278491000	0.308223000
C	-0.491569000	1.115392000	1.031666000
C	-0.239113000	1.169087000	2.391645000
C	-0.290111000	2.401816000	3.055699000
C	-0.586227000	3.559944000	2.341481000
C	-0.843475000	3.508883000	0.966622000
H	0.000332000	0.261900000	2.936336000
H	-0.092070000	2.448803000	4.123034000
H	-0.623272000	4.519244000	2.851810000
H	-1.082556000	4.419578000	0.426393000
C	-1.099474000	3.241367000	-1.932114000
H	-1.987434000	3.849058000	-1.715912000
H	-0.202946000	3.865023000	-1.831032000
H	-1.170453000	2.889146000	-2.965824000
C	-3.458531000	-0.728784000	-2.378286000
H	-4.464808000	-0.514601000	-1.998456000
H	-3.263914000	-0.062048000	-3.223984000
H	-3.423081000	-1.766823000	-2.735058000
B	0.868678000	-0.400867000	-0.538841000
O	1.464002000	-1.658389000	-0.304037000
O	1.827869000	0.631423000	-0.497051000

C	2.846617000	-1.402765000	0.024916000
C	3.105174000	-0.015325000	-0.651871000
C	3.703402000	-2.540308000	-0.507308000
H	4.767721000	-2.320964000	-0.361727000
H	3.468234000	-3.465576000	0.029534000
H	3.521694000	-2.710953000	-1.571407000
C	2.939034000	-1.333890000	1.550858000
H	2.534482000	-2.260828000	1.970327000
H	3.974469000	-1.223375000	1.891437000
H	2.350666000	-0.494703000	1.937107000
C	4.164251000	0.836245000	0.031073000
H	5.126944000	0.312281000	0.048831000
H	4.295480000	1.775172000	-0.517314000
H	3.876512000	1.081287000	1.056482000
C	3.405145000	-0.133761000	-2.147589000
H	3.352271000	0.863358000	-2.596777000
H	4.405577000	-0.542100000	-2.326724000
H	2.671111000	-0.772811000	-2.649326000
H	0.306308000	-0.432855000	-1.825540000

2N'P

E(B3PW91-D3) = -1459.076357 au

E(DLPNO-CCSD(T)) = -1456.669684 au

G_{cont} = 0.402303 au

G = -1456.267381 au

P	1.097955000	-0.475767000	-2.128088000
N	2.333484000	0.311395000	-1.232750000
N	0.594895000	-1.819938000	-1.120841000
N	0.239381000	0.360032000	0.674433000
C	2.108720000	1.467014000	-0.459874000
C	1.037174000	1.515357000	0.462970000
C	0.784085000	2.687083000	1.175332000
C	1.599313000	3.808717000	1.026575000
C	2.693112000	3.746760000	0.163249000
C	2.941566000	2.589496000	-0.574353000
H	-0.052321000	2.694460000	1.869459000
H	1.394238000	4.710937000	1.596773000
H	3.351281000	4.604674000	0.048676000
H	3.777547000	2.567162000	-1.267390000
C	1.003907000	-1.935002000	0.215030000
C	0.903296000	-0.833238000	1.092525000
C	1.413708000	-0.908067000	2.386516000
C	1.984217000	-2.085199000	2.867616000

C	2.025568000	-3.201717000	2.032129000
C	1.548734000	-3.127979000	0.724412000
H	1.327988000	-0.028101000	3.019938000
H	2.366329000	-2.135912000	3.883678000
H	2.445648000	-4.138591000	2.390905000
H	1.623970000	-4.004920000	0.089931000
C	0.363118000	-3.052069000	-1.869081000
H	1.281448000	-3.626830000	-2.064319000
H	-0.341837000	-3.686133000	-1.320927000
H	-0.089605000	-2.804165000	-2.832461000
C	3.708670000	-0.047220000	-1.566335000
H	4.339426000	0.048790000	-0.676326000
H	3.735800000	-1.092077000	-1.889357000
H	4.132591000	0.569650000	-2.371453000
B	-1.159085000	0.333621000	0.424882000
O	-1.828521000	1.349394000	-0.224389000
O	-1.966642000	-0.726890000	0.772871000
C	-3.239260000	1.022740000	-0.136090000
C	-3.204827000	-0.533531000	0.045251000
C	-3.930683000	1.500481000	-1.401860000
H	-4.975624000	1.170505000	-1.414213000
H	-3.916156000	2.594525000	-1.442162000
H	-3.431472000	1.121482000	-2.296951000
C	-3.791955000	1.752784000	1.086797000
H	-3.589590000	2.823264000	0.980931000
H	-4.873516000	1.612014000	1.183415000
H	-3.309320000	1.403044000	2.005705000
C	-4.350850000	-1.105190000	0.862584000
H	-5.311137000	-0.877634000	0.386031000
H	-4.250964000	-2.193474000	0.929407000
H	-4.357734000	-0.702521000	1.878357000
C	-3.064005000	-1.284056000	-1.278934000
H	-2.828967000	-2.331347000	-1.066511000
H	-3.988772000	-1.244567000	-1.863851000
H	-2.246494000	-0.873457000	-1.880083000
H	0.098682000	0.484175000	-1.840799000

TS_{1NP/2PP}

E(B3PW91-D3) = -1458.956451 au

E(DLPNO-CCSD(T)) = -1456.534058 au

G_{cont} = 0.398878 au

G = -1456.135180 au

P	-0.447436000	-0.521728000	1.842135000
N	-0.883520000	-1.524292000	0.402239000

N	1.058412000	-1.495902000	1.868937000
N	-2.009543000	0.315253000	1.579030000
C	1.366062000	-2.056316000	0.652009000
C	0.237118000	-2.109849000	-0.203736000
C	0.378339000	-2.629638000	-1.488771000
C	1.624722000	-3.117774000	-1.906372000
C	2.729431000	-3.066786000	-1.060185000
C	2.609607000	-2.515845000	0.220798000
H	-0.448532000	-2.646293000	-2.184388000
H	1.719363000	-3.531993000	-2.906872000
H	3.692169000	-3.447448000	-1.392779000
H	3.473899000	-2.441552000	0.874211000
C	-2.641121000	0.009509000	0.407358000
C	-3.777126000	0.620640000	-0.126482000
C	-4.373634000	0.077666000	-1.271645000
C	-3.841163000	-1.059009000	-1.872761000
C	-2.676637000	-1.654375000	-1.361623000
C	-2.048083000	-1.099134000	-0.251237000
H	-4.201105000	1.496536000	0.355935000
H	-5.268036000	0.543100000	-1.678981000
H	-4.323169000	-1.499055000	-2.741738000
H	-2.306766000	-2.564920000	-1.815011000
B	0.559588000	1.070112000	0.804882000
O	1.863655000	0.965756000	0.439877000
O	-0.160683000	2.014969000	0.147504000
C	1.969713000	1.710117000	-0.822095000
C	0.803447000	2.746232000	-0.684456000
C	3.358456000	2.314069000	-0.911583000
H	4.100845000	1.515376000	-1.005250000
H	3.433632000	2.956704000	-1.796046000
H	3.601139000	2.905696000	-0.025609000
C	1.191079000	3.994442000	0.101817000
H	1.864163000	4.632954000	-0.479508000
H	0.286634000	4.565295000	0.333257000
H	1.682423000	3.733406000	1.044992000
C	0.123476000	3.114812000	-1.990165000
H	-0.673235000	3.840840000	-1.800483000
H	0.846169000	3.568918000	-2.677399000
H	-0.320243000	2.240875000	-2.471845000
C	1.743549000	0.690087000	-1.933651000
H	1.899971000	1.140378000	-2.919451000
H	2.444455000	-0.140025000	-1.805760000
H	0.733980000	0.270798000	-1.891276000
C	2.084458000	-1.139654000	2.814883000

H	2.630481000	-2.036263000	3.132227000
H	2.800438000	-0.413437000	2.401953000
H	1.611593000	-0.702535000	3.701727000
C	-2.362150000	1.444659000	2.392094000
H	-2.144972000	2.398914000	1.890387000
H	-3.426790000	1.411488000	2.656448000
H	-1.784719000	1.403569000	3.323907000
H	0.211337000	0.719701000	2.345268000

2PP

E(B3PW91-D3) = -1459.055741 au

E(DLPNO-CCSD(T)) = -1456.641180 au

G_{cont} = 0.400438 au

G = -1456.240742 au

P	-0.476289000	0.192927000	1.527364000
N	-1.217795000	0.396163000	-0.133163000
N	-1.518876000	-1.177494000	1.676305000
N	-0.479417000	1.921350000	1.590764000
C	-2.081568000	-1.633787000	0.489425000
C	-1.921634000	-0.710305000	-0.574325000
C	-2.445383000	-1.006634000	-1.829686000
C	-3.123241000	-2.220871000	-2.024304000
C	-3.271852000	-3.126967000	-0.979878000
C	-2.748048000	-2.836874000	0.290276000
H	-2.327378000	-0.324837000	-2.661817000
H	-3.524006000	-2.450213000	-3.008493000
H	-3.789487000	-4.069143000	-1.141350000
H	-2.861016000	-3.547929000	1.103161000
C	-0.665285000	2.563215000	0.371710000
C	-0.469417000	3.912152000	0.099773000
C	-0.726567000	4.393996000	-1.193663000
C	-1.167786000	3.530037000	-2.190248000
C	-1.360399000	2.165210000	-1.922915000
C	-1.110991000	1.677943000	-0.642454000
H	-0.118935000	4.587406000	0.874574000
H	-0.570756000	5.447545000	-1.411509000
H	-1.358897000	3.904021000	-3.192958000
H	-1.687869000	1.508799000	-2.718693000
B	1.198433000	-0.387556000	0.757549000
O	1.389783000	-1.667692000	0.320885000
O	2.181148000	0.486057000	0.393546000
C	2.428335000	-1.581251000	-0.704717000
C	3.221715000	-0.308580000	-0.258779000

C	3.229829000	-2.869966000	-0.704491000
H	2.593532000	-3.700056000	-1.027275000
H	4.072041000	-2.792819000	-1.401396000
H	3.617194000	-3.103858000	0.290077000
C	4.279630000	-0.597508000	0.802390000
H	5.132688000	-1.135248000	0.376049000
H	4.638746000	0.350938000	1.213790000
H	3.864717000	-1.191413000	1.623574000
C	3.807580000	0.508097000	-1.397255000
H	4.346395000	1.371527000	-0.994237000
H	4.514006000	-0.098026000	-1.975545000
H	3.028385000	0.877266000	-2.067933000
C	1.692319000	-1.396215000	-2.030805000
H	2.389156000	-1.380758000	-2.875032000
H	0.994953000	-2.228114000	-2.166960000
H	1.110322000	-0.468350000	-2.034589000
C	-1.585137000	-1.996547000	2.865211000
H	-2.627472000	-2.246007000	3.099794000
H	-1.016627000	-2.929350000	2.747055000
H	-1.168057000	-1.445803000	3.712815000
C	-0.017134000	2.672242000	2.735897000
H	0.999522000	3.059901000	2.583179000
H	-0.690039000	3.515209000	2.936580000
H	-0.008713000	2.026140000	3.618022000
H	-0.244859000	0.155672000	2.941154000

TS_{1NP/2NP}

E(B3PW91-D3) = -1459.055741 au

E(DLPNO-CCSD(T)) = -1456.609410 au

G_{cont} = 0.402798 au

G = -1456.206612 au

P	0.841906000	-1.207877000	0.300041000
N	-0.702827000	0.418687000	1.127963000
N	2.337950000	-2.043222000	0.156583000
N	1.711779000	0.245073000	-0.064903000
C	-0.124834000	1.618265000	0.677971000
C	1.048132000	1.495670000	-0.094391000
C	1.500490000	2.586944000	-0.845845000
C	0.887938000	3.828548000	-0.700936000
C	-0.184153000	3.986410000	0.181318000
C	-0.699621000	2.880398000	0.851218000
H	2.307735000	2.464619000	-1.558709000
H	1.245818000	4.671461000	-1.286054000

H	-0.656290000	4.958334000	0.299085000
H	-1.594277000	2.973969000	1.458794000
C	3.451450000	-1.277481000	-0.107457000
C	3.096086000	0.083993000	-0.200337000
C	4.107267000	1.046072000	-0.310650000
C	5.431912000	0.623177000	-0.406931000
C	5.768336000	-0.736464000	-0.384745000
C	4.778026000	-1.700421000	-0.221370000
H	3.884907000	2.104770000	-0.289884000
H	6.215458000	1.371279000	-0.491776000
H	6.807809000	-1.040566000	-0.471738000
H	5.027155000	-2.755576000	-0.161848000
C	-1.171390000	0.370727000	2.507198000
H	-2.014769000	1.052476000	2.685034000
H	-0.358447000	0.634679000	3.193145000
H	-1.511691000	-0.644656000	2.718394000
C	2.415841000	-3.480513000	0.348476000
H	1.415621000	-3.860440000	0.576368000
H	3.084754000	-3.723134000	1.181579000
H	2.779652000	-3.971582000	-0.560546000
B	-1.580992000	-0.193682000	-0.000392000
O	-2.519572000	0.673999000	-0.674919000
O	-2.294428000	-1.349286000	0.472806000
C	-3.819957000	0.092132000	-0.540259000
C	-3.496411000	-1.420901000	-0.299689000
C	-4.507948000	0.736576000	0.667405000
H	-5.551387000	0.415279000	0.766465000
H	-4.491164000	1.824454000	0.541305000
H	-3.977348000	0.490525000	1.592219000
C	-4.625249000	0.373609000	-1.802255000
H	-4.828596000	1.447494000	-1.881316000
H	-5.585980000	-0.155082000	-1.778516000
H	-4.077340000	0.068305000	-2.697559000
C	-3.196646000	-2.167851000	-1.603718000
H	-4.102480000	-2.327170000	-2.199252000
H	-2.768013000	-3.145452000	-1.357783000
H	-2.469750000	-1.619466000	-2.211575000
C	-4.549354000	-2.176781000	0.498738000
H	-4.255067000	-3.227348000	0.601664000
H	-5.520694000	-2.142215000	-0.008774000
H	-4.662288000	-1.758202000	1.502348000
H	-0.642763000	-0.534324000	-0.862765000

2NP

E(B3PW91-D3) = -1459.084453 au

E(DLPNO-CCSD(T)) = -1456.674689 au

G_{cont} = 0.400671 au

G = -1456.274017 au

P	1.180985000	0.285563000	1.962276000
N	-1.291777000	1.531177000	0.962113000
N	2.539519000	-0.776767000	1.721305000
N	1.303688000	0.747380000	0.292234000
C	-0.481326000	2.392342000	0.177819000
C	0.806658000	1.964490000	-0.202473000
C	1.590137000	2.777413000	-1.029960000
C	1.119153000	4.016393000	-1.455451000
C	-0.136097000	4.465316000	-1.038345000
C	-0.927269000	3.654472000	-0.226563000
H	2.582202000	2.435992000	-1.312871000
H	1.742106000	4.639738000	-2.091837000
H	-0.504604000	5.438024000	-1.353916000
H	-1.916334000	3.987956000	0.075874000
C	2.662669000	-1.126371000	0.373458000
C	1.984691000	-0.214029000	-0.465092000
C	2.017187000	-0.354531000	-1.845311000
C	2.730157000	-1.429656000	-2.397029000
C	3.383955000	-2.344429000	-1.573514000
C	3.351947000	-2.202658000	-0.176857000
H	1.474604000	0.342186000	-2.476839000
H	2.753642000	-1.554374000	-3.476628000
H	3.921195000	-3.182560000	-2.010239000
H	3.858235000	-2.921810000	0.460582000
C	2.940895000	-1.698566000	2.762538000
H	4.002669000	-1.948510000	2.655927000
H	2.357739000	-2.633019000	2.741542000
H	2.806184000	-1.223130000	3.738821000
C	-1.958170000	2.096860000	2.131847000
H	-1.251671000	2.713802000	2.696023000
H	-2.303342000	1.282510000	2.772876000
H	-2.827949000	2.712079000	1.864601000
B	-1.748879000	0.299771000	0.401369000
O	-1.367874000	-0.159040000	-0.837581000
O	-2.631875000	-0.536424000	1.053522000
C	-1.866658000	-1.517009000	-0.947836000
C	-3.063216000	-1.512151000	0.067879000
C	-2.258554000	-1.767641000	-2.395163000
H	-2.737819000	-2.747747000	-2.498861000

H	-1.361439000	-1.757228000	-3.022684000
H	-2.941805000	-0.999891000	-2.766488000
C	-0.738299000	-2.461751000	-0.540457000
H	0.139684000	-2.261729000	-1.160703000
H	-1.033563000	-3.507895000	-0.673552000
H	-0.447556000	-2.309219000	0.503109000
C	-3.309596000	-2.837573000	0.768527000
H	-3.542703000	-3.618787000	0.036343000
H	-4.160629000	-2.743065000	1.451055000
H	-2.439450000	-3.150227000	1.350582000
C	-4.359864000	-0.981019000	-0.541603000
H	-5.087015000	-0.814938000	0.259600000
H	-4.787372000	-1.692052000	-1.256066000
H	-4.193440000	-0.027486000	-1.054240000
H	0.135627000	-0.709152000	1.871412000

2NP'

E(B3PW91-D3) = -1459.082060 au

E(DLPNO-CCSD(T)) = -1456.673711 au

G_{cont} = 0.400097 au

G = -1456.273614 au

P	1.557649000	-0.072437000	2.039234000
N	-0.732460000	2.026512000	0.769726000
N	1.405917000	-1.756785000	1.714761000
N	1.403074000	0.231440000	0.330901000
C	0.429741000	2.457204000	0.093750000
C	1.491584000	1.558842000	-0.149286000
C	2.639231000	2.001553000	-0.817614000
C	2.751921000	3.322784000	-1.242717000
C	1.716140000	4.221435000	-0.981269000
C	0.570398000	3.788134000	-0.317305000
H	3.449548000	1.297052000	-0.985264000
H	3.649756000	3.650742000	-1.760205000
H	1.793713000	5.256977000	-1.302989000
H	-0.245019000	4.482573000	-0.133716000
C	1.750724000	-2.059138000	0.396543000
C	1.736168000	-0.904002000	-0.418151000
C	1.916561000	-1.008891000	-1.791024000
C	2.139759000	-2.276853000	-2.349395000
C	2.178002000	-3.413514000	-1.544314000
C	1.980916000	-3.313107000	-0.157962000
H	1.861249000	-0.125434000	-2.419475000
H	2.287267000	-2.364924000	-3.422757000

H	2.362571000	-4.388987000	-1.986966000
H	1.995011000	-4.200878000	0.467758000
C	1.365735000	-2.767344000	2.747428000
H	2.361185000	-3.183657000	2.962231000
H	0.702909000	-3.586514000	2.443522000
H	0.964387000	-2.329545000	3.665823000
C	-1.122706000	2.770913000	1.961906000
H	-0.269412000	2.869874000	2.643387000
H	-1.918596000	2.228254000	2.475682000
H	-1.494203000	3.775493000	1.720526000
B	-1.524272000	0.954981000	0.277999000
O	-1.361003000	0.371536000	-0.960124000
O	-2.592932000	0.438281000	0.988274000
C	-2.255769000	-0.769363000	-0.998190000
C	-3.350446000	-0.364024000	0.048565000
C	-2.764830000	-0.936941000	-2.420536000
H	-3.523935000	-1.726382000	-2.465141000
H	-1.935070000	-1.222949000	-3.075114000
H	-3.197402000	-0.010217000	-2.805730000
C	-1.458525000	-1.999338000	-0.573508000
H	-0.607186000	-2.126581000	-1.246873000
H	-2.073427000	-2.904455000	-0.617056000
H	-1.066576000	-1.884533000	0.442081000
C	-3.980089000	-1.527043000	0.797025000
H	-4.472941000	-2.211106000	0.097024000
H	-4.733833000	-1.152087000	1.497421000
H	-3.233396000	-2.085067000	1.367051000
C	-4.433200000	0.539333000	-0.541124000
H	-5.037711000	0.948526000	0.274692000
H	-5.092729000	-0.014361000	-1.217509000
H	-3.991114000	1.376694000	-1.091729000
H	3.009451000	0.032599000	2.104972000

TS_{2NP}/3NP

E(B3PW91-D3) = -1784.651987 au

E(DLPNO-CCSD(T)) = -1781.627595 au

G_{cont} = 0.512019 au

G = -1781.115576 au

P	1.180377000	1.240105000	-0.477109000
N	0.257333000	-2.117441000	0.157744000
N	2.452858000	1.413519000	-1.605925000
N	2.086073000	0.057237000	0.343114000
C	0.646656000	-1.603476000	1.419189000

C	1.594049000	-0.570115000	1.521886000
C	2.017663000	-0.115840000	2.772979000
C	1.479771000	-0.659774000	3.936588000
C	0.505540000	-1.656209000	3.844764000
C	0.101953000	-2.126916000	2.596790000
H	2.748281000	0.687652000	2.815214000
H	1.805242000	-0.295157000	4.907218000
H	0.067113000	-2.076115000	4.746527000
H	-0.643753000	-2.912941000	2.515126000
C	3.608774000	0.706480000	-1.269038000
C	3.403236000	-0.066067000	-0.109685000
C	4.418777000	-0.855128000	0.411042000
C	5.657832000	-0.865567000	-0.245772000
C	5.864415000	-0.101526000	-1.394051000
C	4.836146000	0.695603000	-1.919835000
H	4.246712000	-1.451919000	1.302199000
H	6.462417000	-1.480168000	0.149215000
H	6.830416000	-0.119195000	-1.891773000
H	4.996160000	1.291013000	-2.814157000
C	2.381849000	2.287039000	-2.759741000
H	2.581913000	1.729910000	-3.682401000
H	3.103513000	3.108954000	-2.675348000
H	1.374169000	2.710160000	-2.823037000
C	1.265911000	-2.882818000	-0.569566000
H	2.126680000	-2.260001000	-0.835204000
H	0.822316000	-3.273251000	-1.487771000
H	1.622414000	-3.726419000	0.035971000
B	-1.073475000	-2.001565000	-0.311368000
O	-2.054819000	-1.290301000	0.346979000
O	-1.510350000	-2.575528000	-1.491790000
C	-3.155657000	-1.166001000	-0.592737000
C	-2.955380000	-2.429914000	-1.492922000
C	-4.457624000	-1.125260000	0.188312000
H	-5.314332000	-1.141753000	-0.495129000
H	-4.501211000	-0.199241000	0.770653000
H	-4.539768000	-1.970106000	0.876986000
C	-2.956642000	0.139229000	-1.358160000
H	-2.893660000	0.965521000	-0.647533000
H	-3.792315000	0.333460000	-2.038499000
H	-2.030308000	0.118997000	-1.943115000
C	-3.431312000	-2.273934000	-2.927199000
H	-4.503823000	-2.050364000	-2.950811000
H	-3.263367000	-3.205554000	-3.477834000
H	-2.894878000	-1.472984000	-3.441466000

C	-3.537363000	-3.698554000	-0.871106000
H	-3.181529000	-4.567586000	-1.433728000
H	-4.631959000	-3.690714000	-0.900135000
H	-3.216934000	-3.809948000	0.170384000
C	-0.246786000	2.208830000	1.209717000
N	0.884071000	2.577880000	0.455245000
C	-1.546910000	2.696081000	0.881997000
C	-1.800077000	3.458863000	-0.287813000
C	-3.093645000	3.863698000	-0.619045000
C	-4.179503000	3.535992000	0.193848000
C	-3.946237000	2.788942000	1.360307000
C	-2.666038000	2.380840000	1.699846000
H	-0.977751000	3.720344000	-0.950085000
H	-3.252822000	4.441015000	-1.528283000
H	-5.185619000	3.853463000	-0.068075000
H	-4.780381000	2.521236000	2.006543000
H	-2.506280000	1.785445000	2.597178000
H	-0.121511000	0.664768000	-0.387755000
H	-0.064433000	1.674411000	2.135238000
H	1.073618000	3.524606000	0.140823000

3NP

E(B3PW91-D3) = -1784.734507 au

E(DLPNO-CCSD(T)) = -1781.720097 au

G_{cont} = 0.515183 au

G = -1781.204915 au

P	1.059127000	0.375475000	-0.934559000
N	0.002942000	-2.429177000	0.267315000
N	2.426953000	0.861192000	-1.850202000
N	2.155213000	-0.579399000	0.086914000
C	0.522076000	-1.802526000	1.428237000
C	1.632073000	-0.933394000	1.354491000
C	2.114985000	-0.339220000	2.529073000
C	1.512975000	-0.590721000	3.758668000
C	0.400166000	-1.431164000	3.830090000
C	-0.081430000	-2.031323000	2.669287000
H	2.952091000	0.350091000	2.462392000
H	1.900844000	-0.113222000	4.655136000
H	-0.083900000	-1.625569000	4.783742000
H	-0.940636000	-2.695690000	2.703709000
C	3.653154000	0.567872000	-1.263094000
C	3.502708000	-0.260549000	-0.129002000
C	4.621482000	-0.707236000	0.565439000

C	5.896055000	-0.314534000	0.129406000
C	6.042410000	0.511426000	-0.983720000
C	4.917510000	0.961339000	-1.691883000
H	4.506095000	-1.357407000	1.427987000
H	6.773065000	-0.663225000	0.668716000
H	7.033828000	0.813810000	-1.311425000
H	5.031489000	1.605498000	-2.559231000
C	2.318892000	1.669493000	-3.045103000
H	2.930024000	1.246967000	-3.852619000
H	2.639736000	2.704959000	-2.866024000
H	1.276196000	1.685680000	-3.374988000
C	0.876647000	-3.379266000	-0.414327000
H	1.788481000	-2.888748000	-0.772719000
H	0.345222000	-3.802134000	-1.269305000
H	1.158594000	-4.194421000	0.264523000
B	-1.296530000	-2.133476000	-0.208067000
O	-2.153859000	-1.236482000	0.406409000
O	-1.843873000	-2.720215000	-1.333479000
C	-3.272573000	-1.049901000	-0.499577000
C	-3.253789000	-2.384798000	-1.321541000
C	-4.528543000	-0.822329000	0.325678000
H	-5.410326000	-0.775954000	-0.323498000
H	-4.447575000	0.130069000	0.860078000
H	-4.675620000	-1.615214000	1.063191000
C	-2.977829000	0.178931000	-1.358152000
H	-2.860543000	1.055133000	-0.714329000
H	-3.798984000	0.380460000	-2.053859000
H	-2.052229000	0.049944000	-1.928112000
C	-3.737126000	-2.257748000	-2.756538000
H	-4.773035000	-1.901110000	-2.781961000
H	-3.699774000	-3.235995000	-3.247160000
H	-3.112501000	-1.566924000	-3.327934000
C	-3.980394000	-3.527871000	-0.613182000
H	-3.754201000	-4.465907000	-1.130008000
H	-5.065338000	-3.380013000	-0.621363000
H	-3.647961000	-3.622758000	0.426229000
C	-0.440545000	1.704236000	0.872851000
N	0.723070000	1.758630000	-0.004933000
C	-1.415444000	2.849138000	0.709594000
C	-1.371355000	3.711006000	-0.388445000
C	-2.329132000	4.716834000	-0.541500000
C	-3.347411000	4.868436000	0.400212000
C	-3.399137000	4.008571000	1.501172000
C	-2.438355000	3.010147000	1.653712000

H	-0.581710000	3.582644000	-1.124044000
H	-2.280098000	5.381224000	-1.401529000
H	-4.094060000	5.649854000	0.280398000
H	-4.187630000	4.118560000	2.242373000
H	-2.484511000	2.340079000	2.511289000
H	-0.977431000	0.767448000	0.668904000
H	-0.127056000	1.624509000	1.922138000
H	1.511395000	2.278401000	0.369861000

TS_{3NP/1NP}

E(B3PW91-D3) = -1784.70869 au

E(DLPNO-CCSD(T)) = -1781.691684 au

G_{cont} = 0.520694512 au

G = -1781.17099 au

P	-0.856722000	-0.348780000	1.420303000
N	1.096453000	-1.763224000	1.015842000
N	-2.420678000	0.429521000	1.446168000
N	-1.529077000	-1.505625000	0.242016000
C	0.606738000	-2.625375000	-0.006367000
C	-0.710986000	-2.409018000	-0.460085000
C	-1.104722000	-3.062598000	-1.642479000
C	-0.268374000	-3.990323000	-2.259362000
C	0.992455000	-4.278759000	-1.737999000
C	1.430348000	-3.561472000	-0.627609000
H	-2.048660000	-2.824192000	-2.112579000
H	-0.611365000	-4.481689000	-3.166807000
H	1.639196000	-5.010488000	-2.214489000
H	2.441058000	-3.686940000	-0.248041000
C	-3.392630000	-0.167095000	0.669273000
C	-2.915564000	-1.340778000	0.038487000
C	-3.836592000	-2.195901000	-0.565684000
C	-5.186428000	-1.819924000	-0.652027000
C	-5.624896000	-0.611104000	-0.121562000
C	-4.726036000	0.221669000	0.557789000
H	-3.540312000	-3.167552000	-0.938552000
H	-5.887839000	-2.491636000	-1.140006000
H	-6.668272000	-0.318618000	-0.208283000
H	-5.064046000	1.147209000	1.015002000
C	-2.760437000	1.391069000	2.471325000
H	-3.683753000	1.099668000	2.990018000
H	-2.891596000	2.400169000	2.057842000
H	-1.949829000	1.425279000	3.208161000
C	1.427586000	-2.378728000	2.298535000

H	0.567338000	-2.949890000	2.664813000
H	1.658572000	-1.591684000	3.020467000
H	2.292992000	-3.052348000	2.224776000
B	1.925153000	-0.650342000	0.514541000
O	2.441604000	-0.682872000	-0.774841000
O	2.675981000	0.150755000	1.366784000
C	3.514927000	0.275650000	-0.844424000
C	3.907248000	0.455904000	0.670117000
C	4.621783000	-0.313917000	-1.710094000
H	5.502795000	0.338239000	-1.708736000
H	4.268348000	-0.408621000	-2.742141000
H	4.917586000	-1.306942000	-1.363776000
C	2.982739000	1.545286000	-1.506554000
H	2.183963000	2.006425000	-0.925342000
H	2.570298000	1.283456000	-2.486283000
H	3.777742000	2.284223000	-1.653255000
C	4.358541000	1.858394000	1.044261000
H	5.262491000	2.130536000	0.487678000
H	4.588512000	1.900620000	2.114047000
H	3.586780000	2.602974000	0.833833000
C	4.936382000	-0.571114000	1.145836000
H	5.019579000	-0.506184000	2.235492000
H	5.925063000	-0.392114000	0.710698000
H	4.619020000	-1.588141000	0.891567000
C	0.264601000	2.022500000	0.776939000
N	0.109003000	0.636531000	0.320874000
C	-0.355850000	3.057525000	-0.130596000
C	-1.621934000	2.868463000	-0.700471000
C	-2.188003000	3.849219000	-1.514676000
C	-1.497569000	5.035496000	-1.772750000
C	-0.235130000	5.232246000	-1.210851000
C	0.330023000	4.247701000	-0.398866000
H	-2.170251000	1.951454000	-0.502390000
H	-3.171688000	3.684691000	-1.948206000
H	-1.937974000	5.797982000	-2.410550000
H	0.315125000	6.148662000	-1.410901000
H	1.318864000	4.404253000	0.028628000
H	1.329675000	2.232978000	0.922627000
H	-0.175796000	2.110864000	1.781073000
H	-0.178458000	0.577190000	-0.654126000

TS_{2NP/1NP}

E(B3PW91-D3) = -1784.684771 au

E(DLPNO-CCSD(T)) = -1781.658904 au

G_{cont} = 0.517765 au

G = -1781.141139 au

P	0.869718000	0.577053000	1.856618000
N	-1.429864000	0.874572000	1.029831000
N	2.580090000	0.269843000	1.854721000
N	1.096694000	1.459461000	0.382893000
C	-1.212012000	2.092011000	0.327263000
C	0.116179000	2.392317000	-0.022913000
C	0.425271000	3.599392000	-0.658653000
C	-0.596727000	4.486805000	-0.992044000
C	-1.921883000	4.184588000	-0.674369000
C	-2.222002000	2.995485000	-0.011343000
H	1.458412000	3.862588000	-0.858980000
H	-0.349698000	5.422708000	-1.486876000
H	-2.719804000	4.873992000	-0.938602000
H	-3.249158000	2.743844000	0.230428000
C	3.223630000	0.594754000	0.677312000
C	2.366701000	1.308981000	-0.188452000
C	2.804813000	1.688996000	-1.454621000
C	4.115316000	1.380688000	-1.832935000
C	4.971196000	0.699326000	-0.964579000
C	4.529217000	0.288041000	0.294701000
H	2.136421000	2.186225000	-2.149128000
H	4.462484000	1.669810000	-2.821408000
H	5.985289000	0.464082000	-1.276989000
H	5.179293000	-0.275516000	0.956792000
C	3.240008000	-0.466520000	2.912660000
H	4.107827000	0.092773000	3.283299000
H	3.573562000	-1.451681000	2.565682000
H	2.540131000	-0.606366000	3.742001000
C	-2.224682000	1.055016000	2.248847000
H	-1.773993000	1.828154000	2.882045000
H	-2.245929000	0.108462000	2.793124000
H	-3.261906000	1.344285000	2.040432000
B	-1.969791000	-0.284567000	0.067700000
O	-2.982016000	0.188318000	-0.848577000
O	-2.551326000	-1.377724000	0.822994000
C	-3.882096000	-0.899392000	-1.060560000
C	-3.871694000	-1.626766000	0.333124000
C	-5.239375000	-0.337956000	-1.468720000
H	-5.990530000	-1.134904000	-1.527049000
H	-5.162390000	0.130956000	-2.456101000
H	-5.586530000	0.420892000	-0.762680000

C	-3.347423000	-1.785432000	-2.193717000
H	-2.385205000	-2.232360000	-1.929910000
H	-3.195935000	-1.160997000	-3.081229000
H	-4.053060000	-2.583892000	-2.450484000
C	-4.089861000	-3.134566000	0.258725000
H	-5.055071000	-3.369407000	-0.206123000
H	-4.086863000	-3.558517000	1.269585000
H	-3.296567000	-3.622324000	-0.313892000
C	-4.878018000	-1.022216000	1.316203000
H	-4.658153000	-1.395827000	2.322125000
H	-5.908444000	-1.296283000	1.062149000
H	-4.804343000	0.068009000	1.335351000
C	0.121778000	-1.590322000	0.081187000
N	-0.685277000	-0.814855000	-0.667695000
C	1.448764000	-2.078992000	-0.371516000
C	2.183515000	-2.894730000	0.499964000
C	3.453147000	-3.345109000	0.150940000
C	4.002892000	-2.988621000	-1.082068000
C	3.271373000	-2.189103000	-1.962068000
C	2.002539000	-1.736644000	-1.610272000
H	1.756380000	-3.162494000	1.464943000
H	4.014526000	-3.972018000	0.839565000
H	4.997543000	-3.331259000	-1.356083000
H	3.695118000	-1.905980000	-2.921509000
H	1.450087000	-1.109403000	-2.304090000
H	-0.439859000	-2.293100000	0.703017000
H	0.484190000	-0.828643000	1.172316000
H	-0.222801000	-0.186853000	-1.315632000

Acr^{Dipp}-1NP

E(B3PW91-D3) = -1940.428670 au

E(DLPNO-CCSD(T)) = -1936.989568 au

G_{cont} = 0.637862 au

G = -1936.351706 au

P	0.030726000	-0.132660000	0.072128000
N	0.005938000	1.587040000	-0.132450000
N	1.899187000	0.157622000	0.037974000
N	-1.849375000	0.096782000	-0.048132000
C	1.183096000	2.293125000	-0.208938000
C	2.303098000	1.449013000	-0.117955000
C	3.584133000	2.021300000	-0.198790000
H	4.469934000	1.396258000	-0.133346000
H	4.652830000	3.863695000	-0.424275000

C	3.670767000	3.400971000	-0.361696000
C	2.528359000	4.222090000	-0.448728000
H	2.649283000	5.295501000	-0.576669000
C	1.247710000	3.677302000	-0.373408000
C	-1.189454000	2.256427000	-0.250300000
C	-1.289759000	3.639402000	-0.408691000
C	-2.582867000	4.149073000	-0.510893000
H	-2.731021000	5.219453000	-0.635313000
C	-3.702836000	3.295482000	-0.451414000
C	-3.580180000	1.917899000	-0.297804000
H	-4.449882000	1.268904000	-0.254894000
H	-4.696474000	3.730353000	-0.529183000
C	-2.285632000	1.377994000	-0.201031000
C	-0.032445000	4.488513000	-0.451001000
H	-0.028894000	5.092691000	-1.368457000
H	-0.054708000	5.211140000	0.377090000
C	2.820426000	-0.917709000	0.133284000
C	3.300619000	-1.300517000	1.401544000
C	4.162418000	-2.399819000	1.475518000
H	4.541527000	-2.719016000	2.443676000
C	4.534859000	-3.098017000	0.329528000
H	5.200681000	-3.954609000	0.406903000
C	4.054799000	-2.699695000	-0.916058000
H	4.349551000	-3.253462000	-1.804248000
C	3.194861000	-1.603792000	-1.040354000
C	2.891179000	-0.559537000	2.661095000
H	2.281998000	0.299206000	2.360569000
C	2.018835000	-1.448010000	3.556967000
H	2.576157000	-2.324536000	3.909745000
H	1.674494000	-0.890271000	4.436051000
H	1.138934000	-1.805182000	3.010893000
C	4.106288000	-0.016078000	3.422369000
H	4.717245000	0.627491000	2.779409000
H	3.780711000	0.574673000	4.286672000
H	4.745049000	-0.825773000	3.795227000
C	2.665613000	-1.188658000	-2.401353000
H	2.167961000	-0.220027000	-2.284311000
C	3.787110000	-1.002864000	-3.429851000
H	3.377031000	-0.613550000	-4.369047000
H	4.542164000	-0.296167000	-3.067598000
H	4.291586000	-1.949106000	-3.658855000
C	1.612802000	-2.188281000	-2.897900000
H	0.792852000	-2.281568000	-2.177818000
H	1.190410000	-1.862756000	-3.856134000

H	2.052458000	-3.183299000	-3.040533000
C	-2.743876000	-0.997706000	0.075247000
C	-3.316230000	-1.274344000	1.333523000
C	-4.189550000	-2.362266000	1.437899000
H	-4.643877000	-2.593939000	2.398609000
C	-4.478770000	-3.157051000	0.332936000
H	-5.159293000	-3.999829000	0.431347000
C	-3.889545000	-2.879147000	-0.898969000
H	-4.120139000	-3.512260000	-1.751191000
C	-3.010561000	-1.802738000	-1.054743000
C	-2.995996000	-0.435528000	2.557797000
H	-2.319566000	0.367817000	2.249189000
C	-4.253962000	0.221129000	3.139628000
H	-4.966246000	-0.528610000	3.504921000
H	-3.990247000	0.869552000	3.983471000
H	-4.762448000	0.832774000	2.386237000
C	-2.259898000	-1.267916000	3.615483000
H	-2.890670000	-2.081720000	3.993496000
H	-1.349961000	-1.712426000	3.198306000
H	-1.974796000	-0.639899000	4.467973000
C	-2.408974000	-1.474912000	-2.410875000
H	-1.466872000	-0.943959000	-2.234016000
C	-3.333259000	-0.523996000	-3.186969000
H	-3.516227000	0.398628000	-2.626869000
H	-2.887090000	-0.254670000	-4.152054000
H	-4.301570000	-1.002809000	-3.380104000
C	-2.081994000	-2.714166000	-3.248555000
H	-2.987717000	-3.224337000	-3.598008000
H	-1.511729000	-2.421479000	-4.137144000
H	-1.481680000	-3.434916000	-2.682649000

Acr^{DiPP}-TS_{1NP/2N'P}

E(B3PW91-D3) = -2352.145575 au

E(DLPNO-CCSD(T)) = -2347.998944 au

G_{cont} = 0.824469 au

G = -2347.174475 au

P	0.268238000	0.494812000	-0.406385000
N	-1.346744000	1.258626000	0.048630000
N	-0.292867000	-0.739177000	0.970684000
N	1.920701000	-0.034034000	0.170376000
C	0.778868000	-1.211574000	1.784522000
C	2.028297000	-0.872540000	1.274120000
C	3.164173000	-1.347132000	1.931288000

H	4.154918000	-1.135559000	1.540360000
C	2.987060000	-2.060729000	3.124300000
C	1.721285000	-2.272762000	3.677488000
H	1.622149000	-2.779461000	4.634464000
C	0.572493000	-1.831470000	3.001815000
C	-1.393001000	-0.286158000	1.750594000
C	-1.725561000	-0.848103000	2.966939000
C	-2.862619000	-0.319035000	3.600066000
H	-3.184398000	-0.723400000	4.556791000
C	-3.577946000	0.722861000	3.003488000
C	-3.168640000	1.313747000	1.798987000
H	-3.715151000	2.144432000	1.363245000
C	-2.025302000	0.814229000	1.176869000
C	-0.842130000	-1.944066000	3.531493000
H	3.864510000	-2.428476000	3.650626000
H	-4.466228000	1.106860000	3.499306000
H	-1.254285000	-2.930650000	3.277425000
H	-0.836447000	-1.893049000	4.626379000
C	3.080739000	0.289745000	-0.596815000
C	3.512295000	-0.638256000	-1.567150000
C	4.674881000	-0.351932000	-2.290303000
H	5.022121000	-1.052629000	-3.045809000
C	5.386886000	0.819592000	-2.061321000
H	6.291047000	1.028795000	-2.628585000
C	4.934391000	1.735345000	-1.114214000
H	5.496012000	2.651470000	-0.962131000
C	3.775322000	1.499048000	-0.366682000
C	2.736842000	-1.908762000	-1.865892000
H	1.934120000	-2.013736000	-1.132523000
C	2.084862000	-1.809711000	-3.251629000
H	2.840680000	-1.688198000	-4.037272000
H	1.509414000	-2.714348000	-3.473044000
H	1.404384000	-0.952025000	-3.303097000
C	3.607931000	-3.163748000	-1.742108000
H	4.074384000	-3.219541000	-0.752144000
H	2.992635000	-4.060798000	-1.878573000
H	4.403925000	-3.188435000	-2.496092000
C	3.300913000	2.511187000	0.665569000
H	2.203447000	2.494008000	0.661516000
C	3.758656000	2.130876000	2.081733000
H	3.415422000	2.880680000	2.804819000
H	3.366612000	1.159317000	2.390669000
H	4.853989000	2.087028000	2.130093000
C	3.744645000	3.942431000	0.349156000

H	3.477910000	4.237602000	-0.671867000
H	3.266624000	4.641866000	1.041441000
H	4.827646000	4.065570000	0.468900000
C	-1.836987000	2.369906000	-0.700523000
C	-2.533779000	2.120298000	-1.903013000
C	-2.984752000	3.216808000	-2.644725000
H	-3.508827000	3.048139000	-3.582215000
C	-2.781904000	4.519697000	-2.197941000
H	-3.146400000	5.360045000	-2.784561000
C	-2.113977000	4.745998000	-0.997888000
H	-1.962714000	5.766914000	-0.655133000
C	-1.622636000	3.683290000	-0.231793000
C	-2.790954000	0.706875000	-2.388741000
H	-2.575614000	0.021651000	-1.567316000
C	-4.255756000	0.477166000	-2.777232000
H	-4.545268000	1.049671000	-3.667004000
H	-4.416265000	-0.583859000	-3.001319000
H	-4.929957000	0.756946000	-1.959791000
C	-1.853025000	0.344473000	-3.547972000
H	-2.043590000	0.978324000	-4.423698000
H	-0.803255000	0.473453000	-3.261937000
H	-1.999825000	-0.701428000	-3.844260000
C	-0.867076000	3.973814000	1.052244000
H	-0.521346000	3.020522000	1.466564000
C	-1.758498000	4.644591000	2.105801000
H	-2.625654000	4.024185000	2.350911000
H	-1.192010000	4.814362000	3.029113000
H	-2.123597000	5.616856000	1.753175000
C	0.370913000	4.833126000	0.771261000
H	0.091741000	5.843976000	0.450955000
H	0.981940000	4.927648000	1.676144000
H	0.986652000	4.392039000	-0.017911000
B	-0.734207000	-1.760824000	-0.261047000
O	-0.184684000	-3.050258000	-0.089461000
O	-2.128945000	-1.835335000	-0.476061000
C	-1.124033000	-3.948305000	-0.714006000
C	-2.498018000	-3.225665000	-0.471599000
C	-0.997110000	-5.310888000	-0.050696000
H	-1.768191000	-5.994351000	-0.424585000
H	-0.016466000	-5.742548000	-0.277365000
H	-1.090102000	-5.235343000	1.035542000
C	-0.765531000	-4.050164000	-2.197126000
H	0.273060000	-4.384120000	-2.283234000
H	-1.404922000	-4.768935000	-2.720400000

H	-0.851985000	-3.077650000	-2.692601000
C	-3.533235000	-3.449857000	-1.565383000
H	-3.768687000	-4.515830000	-1.666347000
H	-4.455960000	-2.917272000	-1.311733000
H	-3.182018000	-3.072440000	-2.528965000
C	-3.106786000	-3.540356000	0.892806000
H	-3.921369000	-2.835982000	1.088310000
H	-3.504771000	-4.560245000	0.935215000
H	-2.364341000	-3.421053000	1.683963000
H	-0.200035000	-1.075553000	-1.241754000

Acr^{Dipp}-2N^P

E(B3PW91-D3) = -2352.188494 au

E(DLPNO-CCSD(T)) = -2348.049008 au

G_{cont} = 0.8295503 au

G = -2347.219458 au

P	-0.740173000	0.007057000	-0.932773000
N	-0.703140000	-1.505076000	-0.016381000
N	1.280530000	0.105138000	1.146489000
N	-0.916960000	1.485929000	0.015856000
C	0.700039000	1.199103000	1.830415000
C	-0.358264000	1.892845000	1.247396000
C	-0.904728000	2.948853000	2.006926000
H	-1.679158000	3.577439000	1.579171000
C	-0.491522000	3.154138000	3.320751000
C	0.419513000	2.291782000	3.949580000
H	0.639552000	2.396565000	5.009362000
C	1.003979000	1.278541000	3.197429000
C	0.862433000	-1.072606000	1.806771000
C	1.197789000	-1.174349000	3.158546000
C	0.827966000	-2.327722000	3.844027000
H	1.075873000	-2.460062000	4.894471000
C	0.116931000	-3.315197000	3.145611000
C	-0.340666000	-3.114514000	1.842823000
H	-0.947611000	-3.875186000	1.363853000
C	-0.052734000	-1.907653000	1.171815000
C	1.809504000	0.098981000	3.735081000
H	-0.939950000	3.966379000	3.888039000
H	-0.139830000	-4.245352000	3.647398000
H	2.858124000	0.182927000	3.410814000
H	1.805737000	0.082803000	4.828961000
C	-1.556818000	2.549354000	-0.731738000
C	-0.727887000	3.554348000	-1.280629000

C	-1.331653000	4.676231000	-1.859053000
H	-0.708398000	5.470387000	-2.262386000
C	-2.713130000	4.790725000	-1.926129000
H	-3.169844000	5.669219000	-2.376339000
C	-3.515436000	3.768699000	-1.426181000
H	-4.592054000	3.870235000	-1.505071000
C	-2.966605000	2.634443000	-0.817011000
C	0.789221000	3.482328000	-1.245335000
H	1.090880000	2.498113000	-0.879972000
C	1.387081000	3.645932000	-2.648071000
H	1.148555000	4.622741000	-3.084322000
H	2.479438000	3.573853000	-2.598052000
H	1.018249000	2.872921000	-3.331982000
C	1.382228000	4.524424000	-0.287112000
H	0.974408000	4.413631000	0.722151000
H	2.470056000	4.402025000	-0.229174000
H	1.170379000	5.544272000	-0.632721000
C	-3.875086000	1.541388000	-0.272492000
H	-3.454388000	0.586604000	-0.614375000
C	-3.903530000	1.511133000	1.262441000
H	-4.589083000	0.729555000	1.610758000
H	-2.919014000	1.306446000	1.687090000
H	-4.254907000	2.471187000	1.660229000
C	-5.305652000	1.633592000	-0.811463000
H	-5.331390000	1.651498000	-1.906974000
H	-5.888772000	0.772473000	-0.477407000
H	-5.819436000	2.528367000	-0.439354000
C	-1.309257000	-2.586988000	-0.760445000
C	-0.477270000	-3.345469000	-1.611730000
C	-1.029773000	-4.445975000	-2.274682000
H	-0.405994000	-5.040672000	-2.937813000
C	-2.361667000	-4.800113000	-2.086662000
H	-2.774878000	-5.664522000	-2.601490000
C	-3.163537000	-4.049163000	-1.232809000
H	-4.198440000	-4.344747000	-1.082169000
C	-2.661573000	-2.931104000	-0.556473000
C	0.997190000	-3.029852000	-1.799062000
H	1.250623000	-2.156755000	-1.191841000
C	1.873495000	-4.180808000	-1.289340000
H	1.722476000	-5.094664000	-1.876835000
H	2.931965000	-3.906750000	-1.353134000
H	1.645003000	-4.404847000	-0.241672000
C	1.309312000	-2.685628000	-3.260410000
H	1.086792000	-3.525872000	-3.928809000

H	0.721108000	-1.823946000	-3.597098000
H	2.371292000	-2.442626000	-3.380635000
C	-3.571814000	-2.160030000	0.382384000
H	-3.066034000	-1.225990000	0.649466000
C	-3.838440000	-2.928247000	1.685927000
H	-2.918809000	-3.100486000	2.250270000
H	-4.523126000	-2.356974000	2.324238000
H	-4.302281000	-3.900480000	1.477216000
C	-4.904555000	-1.815755000	-0.291068000
H	-5.497893000	-2.715299000	-0.491249000
H	-5.502213000	-1.178748000	0.368610000
H	-4.756402000	-1.292528000	-1.241091000
B	2.479406000	0.112784000	0.387864000
O	3.034540000	1.234500000	-0.181950000
O	3.189386000	-1.044091000	0.141570000
C	4.090660000	0.749642000	-1.058387000
C	4.469370000	-0.610025000	-0.386658000
C	5.200304000	1.784861000	-1.095823000
H	6.057737000	1.406335000	-1.663480000
H	4.839434000	2.694796000	-1.586305000
H	5.532992000	2.051092000	-0.089571000
C	3.483057000	0.553539000	-2.444873000
H	3.036365000	1.490555000	-2.780844000
H	4.243908000	0.252262000	-3.172264000
H	2.697589000	-0.208266000	-2.426366000
C	4.997978000	-1.670296000	-1.336341000
H	5.913719000	-1.321616000	-1.826738000
H	5.233435000	-2.582043000	-0.778114000
H	4.263895000	-1.923610000	-2.103523000
C	5.412988000	-0.442287000	0.803773000
H	5.455325000	-1.384764000	1.358486000
H	6.425936000	-0.185089000	0.477019000
H	5.057382000	0.339174000	1.484086000
H	0.636187000	0.116453000	-1.259260000

Acr^{Dipp}-TS_{1NP/2PP}

E(B3PW91-D3) = -2352.20523 au

E(DLPNO-CCSD(T)) = -2347.944797 au

G_{cont} = 0.821098 au

G = -2347.123699 au

P	0.192097000	0.425546000	-0.005993000
N	1.760278000	-0.487692000	0.305699000
N	0.157071000	-0.476341000	-1.519936000

N	-1.341318000	1.181971000	-0.644096000
C	-1.062480000	-0.503038000	-2.170924000
C	-1.932024000	0.490686000	-1.691041000
C	-3.194154000	0.590291000	-2.271101000
H	-3.890254000	1.360144000	-1.953112000
C	-3.545894000	-0.340536000	-3.264696000
C	-2.683491000	-1.366263000	-3.663558000
H	-3.006878000	-2.087164000	-4.411575000
C	-1.397306000	-1.467592000	-3.107011000
C	0.919172000	-1.629090000	-1.518105000
C	0.723253000	-2.665094000	-2.421085000
C	1.598578000	-3.755427000	-2.299070000
H	1.502451000	-4.601027000	-2.976994000
C	2.593125000	-3.764675000	-1.313751000
C	2.738398000	-2.715972000	-0.391709000
H	3.502826000	-2.745500000	0.379837000
C	1.876052000	-1.627809000	-0.489019000
C	-0.368066000	-2.527109000	-3.472213000
H	-4.528036000	-0.265004000	-3.725919000
H	3.265752000	-4.616654000	-1.249475000
H	-0.865651000	-3.493985000	-3.622912000
H	0.091152000	-2.275097000	-4.441587000
C	-1.793129000	2.433833000	-0.150658000
C	-2.974990000	2.511350000	0.619114000
C	-3.423113000	3.769421000	1.036936000
H	-4.334645000	3.844057000	1.625036000
C	-2.706771000	4.923723000	0.739650000
H	-3.067135000	5.893338000	1.075876000
C	-1.515176000	4.829373000	0.027178000
H	-0.946582000	5.732773000	-0.180497000
C	-1.037659000	3.597888000	-0.432043000
C	-3.710083000	1.268869000	1.086540000
H	-3.318465000	0.408054000	0.540056000
C	-3.415988000	1.048606000	2.578670000
H	-3.713889000	1.922718000	3.170247000
H	-3.966268000	0.182280000	2.959719000
H	-2.345794000	0.880948000	2.752649000
C	-5.221819000	1.328250000	0.840811000
H	-5.450590000	1.540946000	-0.208848000
H	-5.681093000	0.366529000	1.098292000
H	-5.707984000	2.097207000	1.453084000
C	0.287281000	3.558409000	-1.173729000
H	0.457636000	2.529926000	-1.513708000
C	0.275676000	4.442105000	-2.426980000

H	1.217831000	4.331659000	-2.976676000
H	-0.546252000	4.165119000	-3.096335000
H	0.163080000	5.502853000	-2.173101000
C	1.434766000	3.941518000	-0.226248000
H	1.488155000	3.252888000	0.624212000
H	2.399778000	3.907788000	-0.743006000
H	1.299377000	4.958086000	0.162529000
C	2.886789000	0.274715000	0.729729000
C	3.028433000	0.563661000	2.104228000
C	4.089483000	1.378067000	2.516073000
H	4.199443000	1.618148000	3.571233000
C	5.009162000	1.876779000	1.600291000
H	5.832494000	2.503462000	1.935744000
C	4.868875000	1.570676000	0.248825000
H	5.590779000	1.965182000	-0.462680000
C	3.807450000	0.789778000	-0.217561000
C	2.065023000	0.010635000	3.136440000
H	1.398108000	-0.682273000	2.618742000
C	2.788534000	-0.801705000	4.217710000
H	3.455035000	-0.175089000	4.822824000
H	2.059531000	-1.261579000	4.895954000
H	3.390881000	-1.601041000	3.771300000
C	1.214554000	1.123068000	3.764869000
H	1.836937000	1.818820000	4.341729000
H	0.692166000	1.707049000	2.998123000
H	0.465755000	0.698181000	4.444960000
C	3.697796000	0.521840000	-1.711097000
H	2.754154000	0.009997000	-1.904978000
C	4.828599000	-0.403984000	-2.180233000
H	4.828914000	-1.340874000	-1.613977000
H	4.708652000	-0.648734000	-3.242393000
H	5.807254000	0.074752000	-2.051214000
C	3.665281000	1.808484000	-2.544351000
H	4.581833000	2.399100000	-2.431282000
H	3.558906000	1.561003000	-3.607226000
H	2.818268000	2.438652000	-2.260200000
B	-0.846598000	-1.177825000	1.038280000
O	-2.030104000	-1.541213000	0.498867000
O	-0.294641000	-2.062108000	1.900910000
C	-2.402233000	-2.829275000	1.091242000
C	-1.059932000	-3.309743000	1.769777000
C	-2.901109000	-3.714044000	-0.039198000
H	-3.135076000	-4.717783000	0.332230000
H	-3.811994000	-3.280332000	-0.463271000

H	-2.163065000	-3.792601000	-0.840481000
C	-3.521800000	-2.539987000	2.081679000
H	-4.337386000	-2.030588000	1.559663000
H	-3.910751000	-3.466542000	2.516256000
H	-3.177809000	-1.891000000	2.890478000
C	-1.220816000	-3.905631000	3.158324000
H	-1.840142000	-4.808300000	3.114694000
H	-0.237501000	-4.184783000	3.549390000
H	-1.676507000	-3.200201000	3.856844000
C	-0.224457000	-4.231388000	0.891449000
H	0.757769000	-4.370127000	1.351040000
H	-0.703563000	-5.210379000	0.786286000
H	-0.062480000	-3.806535000	-0.101431000
H	-0.284581000	0.366481000	1.377523000

Acr^{Dipp}-2PP

E(B3PW91-D3) = - 2352.197335 au

E(DLPNO-CCSD(T)) = -2348.048225 au

G_{cont} = 0.8296231 au

G = -2347.218602 au

P	-0.061951000	-0.077880000	-0.019678000
N	1.449853000	-1.087862000	0.000210000
N	0.258872000	0.132318000	-1.733167000
N	-0.885195000	1.516541000	-0.169449000
C	-0.065897000	1.335882000	-2.304785000
C	-0.732944000	2.165159000	-1.394680000
C	-1.041805000	3.461321000	-1.798115000
H	-1.539788000	4.151691000	-1.122856000
C	-0.673786000	3.854292000	-3.098779000
C	0.005911000	3.000309000	-3.976886000
H	0.273250000	3.350528000	-4.971734000
C	0.340663000	1.695622000	-3.579615000
C	1.292681000	-0.595353000	-2.261382000
C	1.753605000	-0.406611000	-3.556356000
C	2.853724000	-1.192476000	-3.933958000
H	3.254365000	-1.113470000	-4.942533000
C	3.440140000	-2.077391000	-3.020949000
C	3.011467000	-2.161997000	-1.685259000
H	3.539517000	-2.781071000	-0.965182000
C	1.943759000	-1.365117000	-1.285846000
C	1.059192000	0.643180000	-4.419906000
H	-0.923573000	4.860108000	-3.428152000
H	4.278604000	-2.690937000	-3.341646000

H	1.789598000	1.121552000	-5.083932000
H	0.327413000	0.150072000	-5.080038000
C	-1.489046000	2.149968000	0.953168000
C	-2.894239000	2.104710000	1.091461000
C	-3.475034000	2.751677000	2.186628000
H	-4.555916000	2.749355000	2.300310000
C	-2.692649000	3.396937000	3.140234000
H	-3.162964000	3.886474000	3.990034000
C	-1.309154000	3.415469000	3.002191000
H	-0.703614000	3.924011000	3.748612000
C	-0.684203000	2.808664000	1.907370000
C	-3.778088000	1.408975000	0.072377000
H	-3.130033000	0.789380000	-0.558789000
C	-4.807188000	0.492330000	0.742314000
H	-5.522158000	1.059455000	1.349070000
H	-5.390282000	-0.042027000	-0.016801000
H	-4.315590000	-0.243115000	1.386010000
C	-4.472495000	2.427514000	-0.842644000
H	-3.743220000	3.053455000	-1.365391000
H	-5.080867000	1.912512000	-1.595880000
H	-5.133680000	3.082465000	-0.261513000
C	0.820249000	2.909870000	1.761317000
H	1.101534000	2.355626000	0.859277000
C	1.241385000	4.371025000	1.549260000
H	2.324525000	4.444799000	1.399169000
H	0.743479000	4.797454000	0.671423000
H	0.984054000	4.986533000	2.419488000
C	1.561479000	2.280995000	2.946996000
H	1.291716000	1.227194000	3.075680000
H	2.643586000	2.322492000	2.785545000
H	1.339194000	2.809166000	3.882028000
C	2.347692000	-0.995283000	1.111182000
C	2.023569000	-1.690524000	2.297397000
C	2.848529000	-1.542937000	3.418280000
H	2.598799000	-2.068362000	4.336979000
C	3.984525000	-0.745592000	3.373546000
H	4.618327000	-0.641744000	4.251234000
C	4.303942000	-0.077231000	2.195996000
H	5.191535000	0.550310000	2.169471000
C	3.501351000	-0.166215000	1.054612000
C	0.819849000	-2.608727000	2.396622000
H	0.315673000	-2.597501000	1.427553000
C	1.251514000	-4.056303000	2.664824000
H	1.755437000	-4.151661000	3.633964000

H	0.380122000	-4.721168000	2.676645000
H	1.941463000	-4.409893000	1.890267000
C	-0.180188000	-2.121621000	3.451592000
H	0.262795000	-2.133936000	4.454829000
H	-0.513014000	-1.100126000	3.240492000
H	-1.066938000	-2.764046000	3.466478000
C	3.935622000	0.629039000	-0.172066000
H	3.195061000	0.500018000	-0.962854000
C	5.280954000	0.114308000	-0.706562000
H	5.257565000	-0.964400000	-0.881300000
H	5.523910000	0.605095000	-1.656106000
H	6.091407000	0.328418000	0.001111000
C	4.028097000	2.135201000	0.098857000
H	4.749926000	2.368687000	0.890045000
H	4.350357000	2.656227000	-0.810382000
H	3.060990000	2.545252000	0.391341000
B	-1.421974000	-1.455915000	-0.164832000
O	-1.559278000	-2.090895000	-1.363177000
O	-2.248599000	-1.920301000	0.814129000
C	-2.720521000	-2.963906000	-1.254722000
C	-2.848025000	-3.154037000	0.295275000
C	-2.440654000	-4.237683000	-2.034772000
H	-3.258193000	-4.954749000	-1.899955000
H	-2.361902000	-4.004086000	-3.101106000
H	-1.504967000	-4.706266000	-1.721626000
C	-3.887810000	-2.203403000	-1.876220000
H	-3.632681000	-1.943939000	-2.908173000
H	-4.799706000	-2.809024000	-1.884424000
H	-4.086175000	-1.275410000	-1.334014000
C	-4.270359000	-3.267601000	0.812955000
H	-4.748986000	-4.162590000	0.399873000
H	-4.258930000	-3.357980000	1.903851000
H	-4.872327000	-2.397084000	0.549548000
C	-1.999410000	-4.305723000	0.826033000
H	-1.980628000	-4.261298000	1.918162000
H	-2.417216000	-5.272372000	0.527677000
H	-0.968654000	-4.245117000	0.464435000
H	0.106820000	0.135097000	1.380434000

Acr^{Dipp}-TS_{1NP/2NP}

E(B3PW91-D3) = -2352.153381 au

E(DLPNO-CCSD(T)) = -2348.013341 au

G_{cont} = 0.825602905 au

G = -2347.187738 au

P	0.645999000	0.639592000	-0.036737000
N	-1.694826000	0.518849000	0.023951000
N	0.384616000	-0.011414000	1.517850000
N	2.218009000	-0.063045000	0.024494000
C	1.429000000	-0.737799000	2.042032000
C	2.502696000	-0.816916000	1.149875000
C	3.639572000	-1.554035000	1.487505000
H	4.481539000	-1.621694000	0.805562000
H	4.514284000	-2.760618000	3.028072000
C	3.643822000	-2.181130000	2.732249000
C	2.559352000	-2.077228000	3.624878000
H	2.614940000	-2.574325000	4.590609000
C	1.423347000	-1.339591000	3.298884000
C	-0.869695000	-0.102014000	2.159727000
C	-0.974956000	-0.591673000	3.457879000
C	-2.257044000	-0.619383000	4.024217000
H	-2.379656000	-0.990549000	5.039389000
C	-3.366786000	-0.179653000	3.304620000
C	-3.238797000	0.246222000	1.977195000
H	-4.104196000	0.540365000	1.391271000
H	-4.349927000	-0.198186000	3.767909000
C	-1.981806000	0.263484000	1.389399000
H	0.535817000	-0.345512000	4.968397000
H	-0.011128000	-1.998302000	4.762318000
C	0.245272000	-1.087163000	4.208179000
C	3.202032000	0.193774000	-0.988074000
C	3.198941000	-0.573151000	-2.166207000
C	4.184160000	-0.290419000	-3.120031000
H	4.210605000	-0.863185000	-4.043440000
C	5.128167000	0.708986000	-2.906813000
H	5.884234000	0.910997000	-3.661838000
C	5.104631000	1.454848000	-1.730621000
H	5.841776000	2.239207000	-1.578313000
C	4.141606000	1.215757000	-0.746473000
C	2.185026000	-1.672411000	-2.424873000
H	1.491652000	-1.715228000	-1.579231000
C	1.355432000	-1.370153000	-3.679307000
H	1.980899000	-1.352128000	-4.580125000
H	0.587862000	-2.138844000	-3.820649000
H	0.848418000	-0.403695000	-3.592766000
C	2.871079000	-3.040805000	-2.523847000
H	3.429838000	-3.268293000	-1.608776000
H	2.123353000	-3.827765000	-2.671985000

H	3.570979000	-3.079040000	-3.367264000
C	4.120301000	2.055999000	0.518578000
H	3.322146000	1.684290000	1.168860000
C	5.433307000	1.930191000	1.301158000
H	5.371128000	2.494902000	2.238474000
H	5.645640000	0.883776000	1.546507000
H	6.281833000	2.324409000	0.729671000
C	3.795131000	3.520375000	0.195097000
H	2.844760000	3.602192000	-0.343492000
H	3.716314000	4.106420000	1.118044000
H	4.576186000	3.973589000	-0.426825000
C	-2.247615000	1.736134000	-0.513509000
C	-2.830520000	1.842998000	-1.807684000
C	-3.542702000	3.009379000	-2.126048000
H	-4.021158000	3.069627000	-3.100249000
C	-3.649274000	4.086218000	-1.260069000
H	-4.232210000	4.963936000	-1.528777000
C	-2.928990000	4.042089000	-0.073311000
H	-2.908705000	4.918422000	0.570373000
C	-2.189457000	2.916760000	0.294500000
C	-2.683464000	0.848665000	-2.951410000
H	-2.122918000	-0.013739000	-2.614066000
C	-4.027421000	0.322025000	-3.461695000
H	-4.646037000	1.114305000	-3.901559000
H	-3.861273000	-0.437870000	-4.234901000
H	-4.584303000	-0.147006000	-2.645437000
C	-1.850516000	1.470764000	-4.082766000
H	-2.349908000	2.333370000	-4.540824000
H	-0.876185000	1.807174000	-3.708387000
H	-1.673848000	0.727959000	-4.870813000
C	-1.262173000	3.101180000	1.493059000
H	-0.706937000	2.181814000	1.666447000
C	-1.997639000	3.422575000	2.798476000
H	-2.719385000	2.639180000	3.047052000
H	-1.282671000	3.505008000	3.625951000
H	-2.536743000	4.374818000	2.729907000
C	-0.203608000	4.171643000	1.180993000
H	-0.650240000	5.167072000	1.076071000
H	0.536557000	4.218642000	1.989551000
H	0.322342000	3.939488000	0.248322000
B	-1.486201000	-0.920501000	-0.761727000
O	-0.956327000	-1.899494000	0.174475000
O	-2.694679000	-1.506796000	-1.300315000
C	-1.489842000	-3.170406000	-0.167793000

C	-2.900002000	-2.805805000	-0.746634000
C	-1.516121000	-4.035093000	1.087150000
H	-2.008367000	-4.995659000	0.892875000
H	-0.489774000	-4.235625000	1.415624000
H	-2.036835000	-3.528916000	1.904226000
C	-0.569286000	-3.812021000	-1.210996000
H	0.443541000	-3.861943000	-0.797874000
H	-0.886084000	-4.827064000	-1.475609000
H	-0.533674000	-3.206430000	-2.121272000
C	-3.388379000	-3.734171000	-1.854812000
H	-3.467161000	-4.767750000	-1.495713000
H	-4.380522000	-3.413501000	-2.191840000
H	-2.717946000	-3.711310000	-2.718046000
C	-3.974605000	-2.708743000	0.337844000
H	-4.864639000	-2.235183000	-0.091281000
H	-4.258044000	-3.696661000	0.720218000
H	-3.633082000	-2.092771000	1.172019000
H	-0.621668000	-0.625741000	-1.623167000

Acr^{Dipp}-2NP

E(B3PW91-D3) = -2352.20523 au

E(DLPNO-CCSD(T)) = -2348.065693 au

G_{cont} = 0.824258235 au

G = -2347.241435 au

P	0.741719000	-0.329781000	0.599496000
N	-1.931062000	0.412883000	-0.183328000
N	0.634091000	1.427862000	0.773670000
N	2.461217000	-0.219477000	0.717802000
C	1.811098000	1.882650000	1.405615000
C	2.866929000	0.959900000	1.345651000
C	4.115830000	1.289451000	1.857805000
H	4.939680000	0.584960000	1.784487000
C	4.269934000	2.540584000	2.473483000
C	3.198862000	3.429307000	2.578036000
H	3.330416000	4.383310000	3.084158000
C	1.945323000	3.108463000	2.035203000
C	-0.571728000	2.037812000	1.137157000
C	-0.547417000	3.234955000	1.892932000
C	-1.736638000	3.738861000	2.412520000
H	-1.705553000	4.649694000	3.006982000
C	-2.954967000	3.099675000	2.178212000
C	-2.983514000	1.995597000	1.338060000
H	-3.934344000	1.556227000	1.049333000

C	-1.812487000	1.477388000	0.770062000
C	0.742239000	4.008986000	2.065193000
H	5.236566000	2.812011000	2.890339000
H	-3.876308000	3.491814000	2.599874000
H	0.716114000	4.584890000	2.997791000
H	0.815959000	4.750666000	1.252416000
C	3.334256000	-1.127236000	0.049558000
C	3.517818000	-2.411923000	0.594813000
C	4.297255000	-3.328307000	-0.120848000
H	4.437572000	-4.334213000	0.266601000
C	4.900479000	-2.965212000	-1.320406000
H	5.504904000	-3.687143000	-1.865084000
C	4.738187000	-1.675246000	-1.824780000
H	5.219530000	-1.408451000	-2.761274000
C	3.949807000	-0.732824000	-1.158801000
C	2.868245000	-2.806952000	1.909370000
H	2.550029000	-1.883096000	2.406882000
C	1.619386000	-3.667242000	1.664921000
H	1.888400000	-4.602693000	1.158766000
H	1.130364000	-3.918244000	2.613673000
H	0.888819000	-3.150427000	1.031971000
C	3.842074000	-3.517439000	2.856281000
H	4.749976000	-2.923612000	3.009481000
H	3.368043000	-3.675787000	3.831788000
H	4.140780000	-4.500786000	2.474372000
C	3.700919000	0.644033000	-1.751674000
H	3.512974000	1.338342000	-0.926570000
C	4.896041000	1.197038000	-2.533007000
H	4.707670000	2.241914000	-2.804013000
H	5.817531000	1.158953000	-1.940842000
H	5.066678000	0.647705000	-3.466741000
C	2.440771000	0.620906000	-2.627000000
H	1.558067000	0.300633000	-2.066457000
H	2.228795000	1.617825000	-3.030077000
H	2.565252000	-0.069579000	-3.470218000
C	-1.527421000	0.553953000	-1.560015000
C	-1.103287000	-0.608721000	-2.274422000
C	-0.693573000	-0.476138000	-3.604193000
H	-0.381076000	-1.364622000	-4.145647000
C	-0.637251000	0.753095000	-4.242005000
H	-0.283830000	0.832619000	-5.267100000
C	-1.044096000	1.876591000	-3.541667000
H	-1.018776000	2.843657000	-4.037059000
C	-1.522601000	1.810346000	-2.226845000

C	-1.081395000	-2.034576000	-1.730773000
H	-1.281440000	-2.006731000	-0.653948000
C	-2.159133000	-2.894892000	-2.409669000
H	-1.926483000	-3.028110000	-3.472932000
H	-2.194619000	-3.893107000	-1.954834000
H	-3.146191000	-2.438166000	-2.327474000
C	0.282385000	-2.723817000	-1.906834000
H	0.491558000	-2.934870000	-2.961701000
H	1.105549000	-2.120773000	-1.516006000
H	0.282401000	-3.684169000	-1.377768000
C	-2.036776000	3.133393000	-1.665857000
H	-2.449378000	2.975475000	-0.675529000
C	-3.189224000	3.693256000	-2.512210000
H	-3.999032000	2.960256000	-2.603225000
H	-3.595911000	4.595441000	-2.039095000
H	-2.868118000	3.965950000	-3.524238000
C	-0.900931000	4.156264000	-1.522478000
H	-0.512732000	4.466090000	-2.500473000
H	-1.257266000	5.053164000	-1.001858000
H	-0.067491000	3.736866000	-0.949973000
B	-2.827417000	-0.634511000	0.260571000
O	-2.790389000	-1.095955000	1.556313000
O	-3.826398000	-1.199195000	-0.490538000
C	-3.698008000	-2.222862000	1.630652000
C	-4.666462000	-1.953301000	0.426262000
C	-4.365873000	-2.222478000	2.996385000
H	-5.131240000	-3.004930000	3.048927000
H	-3.618525000	-2.422135000	3.771064000
H	-4.831223000	-1.258739000	3.216023000
C	-2.854217000	-3.484813000	1.456747000
H	-2.060667000	-3.485397000	2.210365000
H	-3.457696000	-4.389297000	1.585074000
H	-2.383016000	-3.518716000	0.470381000
C	-5.175473000	-3.203164000	-0.272135000
H	-5.764307000	-3.810477000	0.424404000
H	-5.820728000	-2.920802000	-1.110352000
H	-4.358812000	-3.812050000	-0.663319000
C	-5.837198000	-1.041409000	0.789683000
H	-6.339805000	-0.726341000	-0.130033000
H	-6.564426000	-1.558501000	1.423861000
H	-5.495328000	-0.144652000	1.315807000
H	0.437549000	-0.603978000	1.986626000

Acr^{Dipp}-2NP'

E(B3PW91-D3) = -2352.203248 au

E(DLPNO-CCSD(T)) = -2348.059300 au

G_{cont} = 0.822033 au

G = -2347.237266 au

P	0.732066000	-0.16018900	-0.067611000
N	-1.740007000	0.40269600	-0.343415000
N	0.369671000	0.73959400	1.420317000
N	2.418868000	-0.13257800	0.414341000
C	1.531958000	1.21079000	2.050664000
C	2.710634000	0.72787000	1.461857000
C	3.946087000	1.09873800	1.982493000
H	4.863013000	0.72566300	1.534815000
C	3.968294000	1.96145000	3.091198000
C	2.788403000	2.42843900	3.670779000
H	2.828497000	3.08891500	4.534338000
C	1.538626000	2.04146000	3.157572000
C	-0.816363000	1.41723100	1.669390000
C	-0.927612000	2.27600300	2.782991000
C	-2.119686000	2.97867100	2.968158000
H	-2.201138000	3.64638100	3.823939000
C	-3.203613000	2.83522300	2.100255000
C	-3.088225000	1.98729500	1.001802000
H	-3.904880000	1.85516800	0.297622000
C	-1.891972000	1.31341200	0.768048000
C	0.211140000	2.40190600	3.774266000
H	4.926589000	2.26577100	3.505076000
H	-4.126281000	3.38065000	2.277593000
H	0.238089000	3.41784500	4.187375000
H	0.018918000	1.73355000	4.630086000
C	3.393959000	-0.89722300	-0.284562000
C	3.657632000	-2.21598400	0.139800000
C	4.578426000	-2.97044300	-0.594085000
H	4.790982000	-3.99507700	-0.299017000
C	5.223946000	-2.43066400	-1.704896000
H	5.935045000	-3.03396600	-2.264924000
C	4.961306000	-1.12140000	-2.099713000
H	5.469406000	-0.71170400	-2.969595000
C	4.043720000	-0.33113600	-1.398867000
C	2.931988000	-2.81620900	1.329795000
H	2.452528000	-1.99384700	1.871440000
C	1.822797000	-3.76796800	0.856578000
H	2.247265000	-4.61427100	0.301697000
H	1.267712000	-4.16722000	1.714380000

H	1.113536000	-3.25057100	0.201443000
C	3.882854000	-3.51660500	2.306336000
H	4.687147000	-2.84486700	2.626289000
H	3.333491000	-3.84073000	3.197818000
H	4.341880000	-4.40822500	1.862544000
C	3.741901000	1.08606100	-1.852375000
H	3.102815000	1.55098900	-1.094141000
C	5.011234000	1.93939400	-1.957168000
H	4.750620000	2.97514400	-2.203771000
H	5.562136000	1.94231400	-1.010069000
H	5.684761000	1.57167600	-2.740491000
C	2.965573000	1.07964100	-3.176688000
H	2.030352000	0.51527800	-3.088247000
H	2.715123000	2.10263600	-3.481355000
H	3.559444000	0.62291300	-3.977961000
C	-1.816909000	0.82869900	-1.706030000
C	-1.936712000	-0.18394400	-2.697506000
C	-2.140864000	0.18912300	-4.027704000
H	-2.255863000	-0.58651900	-4.780549000
C	-2.171793000	1.52259000	-4.415270000
H	-2.352600000	1.79753100	-5.451350000
C	-1.892859000	2.49159300	-3.461837000
H	-1.817458000	3.53010700	-3.774224000
C	-1.663342000	2.18192900	-2.114947000
C	-1.734913000	-1.67067100	-2.424480000
H	-1.589507000	-1.83707400	-1.349615000
C	-2.923544000	-2.52501700	-2.877117000
H	-3.054572000	-2.47415100	-3.963845000
H	-2.758886000	-3.57879000	-2.621893000
H	-3.848255000	-2.18852300	-2.402417000
C	-0.433146000	-2.16051100	-3.078910000
H	-0.488788000	-2.08874900	-4.171449000
H	0.424884000	-1.56996500	-2.742808000
H	-0.248754000	-3.20917800	-2.815812000
C	-1.146080000	3.33279000	-1.252051000
H	-0.941482000	2.97363400	-0.246583000
C	-2.158683000	4.47717400	-1.127295000
H	-3.112386000	4.11957000	-0.727277000
H	-1.775790000	5.25084400	-0.451525000
H	-2.354315000	4.94807800	-2.098166000
C	0.198476000	3.84583600	-1.792776000
H	0.096738000	4.29914500	-2.785613000
H	0.607604000	4.60604400	-1.116359000
H	0.927102000	3.03124800	-1.869191000

B	-2.497953000	-0.76697300	0.141991000
O	-2.005057000	-1.53116400	1.165005000
O	-3.789172000	-1.06374300	-0.203702000
C	-2.995797000	-2.55034500	1.454893000
C	-4.305656000	-1.92683800	0.851607000
C	-3.030771000	-2.77136700	2.958600000
H	-3.834666000	-3.46633200	3.225621000
H	-2.080440000	-3.20421400	3.287075000
H	-3.180428000	-1.83367300	3.498813000
C	-2.540762000	-3.82207600	0.743984000
H	-1.526466000	-4.06681100	1.073511000
H	-3.197777000	-4.66595100	0.978079000
H	-2.520320000	-3.68760700	-0.340482000
C	-5.266134000	-2.93220400	0.240965000
H	-5.621739000	-3.62994000	1.007316000
H	-6.133261000	-2.40836200	-0.174005000
H	-4.797642000	-3.50420800	-0.562571000
C	-5.037047000	-1.01035800	1.829812000
H	-5.820823000	-0.46993000	1.289674000
H	-5.503586000	-1.58081200	2.639299000
H	-4.356533000	-0.27070200	2.263928000
H	0.753001000	0.96569000	-0.964783000

Acr^{Dipp}-TS_{2NP/3NP}

E(B3PW91-D3) = -2677.766759 au

E(DLPNO-CCSD(T)) = -2673.010877 au

G_{cont} = 0.942077 au

G = -2672.0688 au

P	-0.755882000	0.032562000	-0.276175000
N	-0.177533000	-1.275760000	-1.301758000
N	-2.319431000	-0.619497000	-0.300154000
N	2.173984000	-0.197309000	0.034323000
C	-2.492190000	-1.542510000	-1.347347000
C	-1.268541000	-1.892616000	-1.927281000
C	-1.187128000	-2.744764000	-3.017526000
C	-2.382788000	-3.303714000	-3.485142000
C	-3.603696000	-3.008317000	-2.872730000
C	-3.673644000	-2.114367000	-1.797773000
H	-2.354548000	-3.977490000	-4.338955000
H	-4.616613000	-1.877197000	-1.315345000
C	2.212307000	-0.763482000	-1.286441000
C	3.425462000	-0.740049000	-1.983108000
C	3.564987000	-1.366415000	-3.213973000

C	2.485883000	-2.082344000	-3.728772000
C	1.253188000	-2.108246000	-3.077987000
C	1.087953000	-1.361977000	-1.888996000
H	4.288017000	-0.293432000	-1.498351000
H	2.599252000	-2.645309000	-4.653073000
C	0.162886000	-3.011275000	-3.621612000
H	4.517771000	-1.348291000	-3.735380000
H	-4.516148000	-3.467230000	-3.243813000
H	0.455084000	-4.055635000	-3.430552000
H	0.110006000	-2.912332000	-4.713585000
C	-3.101788000	-0.787274000	0.903497000
C	-2.841934000	-1.906809000	1.727216000
C	-4.143847000	0.113720000	1.183222000
C	-3.678297000	-2.114897000	2.828146000
C	-4.952028000	-0.140917000	2.297928000
C	-4.729128000	-1.246534000	3.110596000
H	-3.507226000	-2.973110000	3.472709000
H	-5.770814000	0.536476000	2.526100000
H	-5.371370000	-1.431206000	3.968801000
C	2.221297000	-1.009497000	1.229963000
C	2.603615000	-2.383184000	1.255521000
C	1.880715000	-0.368410000	2.459530000
C	2.696805000	-3.025383000	2.497955000
C	2.035921000	-1.062020000	3.662588000
C	2.453102000	-2.382558000	3.699921000
H	2.974949000	-4.075040000	2.516314000
H	1.797381000	-0.555567000	4.593905000
H	2.556201000	-2.909819000	4.644912000
C	-4.413945000	1.322620000	0.317045000
H	-3.583277000	1.419749000	-0.383968000
C	-1.720840000	-2.894978000	1.453446000
H	-1.061671000	-2.472432000	0.689964000
C	1.315701000	1.042639000	2.596742000
H	1.171084000	1.474411000	1.599384000
C	2.882074000	-3.294662000	0.057917000
H	3.006665000	-2.702769000	-0.839183000
C	-4.463128000	2.610324000	1.143194000
H	-4.553356000	3.473703000	0.477500000
H	-5.317026000	2.619784000	1.832076000
H	-3.545126000	2.733972000	1.726759000
C	-5.695517000	1.153030000	-0.507512000
H	-5.648852000	0.263053000	-1.144898000
H	-6.576181000	1.060165000	0.140516000
H	-5.837774000	2.026629000	-1.154521000

C	-2.269096000	-4.219696000	0.904994000
H	-1.442747000	-4.901016000	0.670097000
H	-2.912936000	-4.709498000	1.646080000
H	-2.853363000	-4.063138000	-0.007192000
C	-0.846070000	-3.133987000	2.686763000
H	0.006428000	-3.765808000	2.419983000
H	-0.443664000	-2.195263000	3.078260000
H	-1.396629000	-3.636571000	3.490669000
C	4.188135000	-4.089647000	0.194162000
H	4.398822000	-4.608955000	-0.748223000
H	5.031312000	-3.424735000	0.412772000
H	4.145734000	-4.851113000	0.981063000
C	1.685839000	-4.226820000	-0.183565000
H	1.530047000	-4.900548000	0.668029000
H	0.762857000	-3.656120000	-0.329547000
H	1.851798000	-4.840638000	-1.077341000
C	2.251819000	1.973242000	3.382221000
H	3.253796000	1.979791000	2.953429000
H	1.856732000	2.996690000	3.383476000
H	2.329304000	1.652598000	4.427537000
C	-0.059608000	1.028848000	3.293355000
H	-0.723919000	0.249917000	2.906308000
H	0.051051000	0.848027000	4.368855000
H	-0.557422000	1.996910000	3.166497000
B	2.826410000	1.107567000	0.019176000
O	3.890310000	1.473280000	0.800133000
O	2.483804000	2.055789000	-0.914067000
C	3.275129000	3.244646000	-0.643545000
C	4.467795000	2.670174000	0.203043000
C	4.966221000	3.587761000	1.307980000
H	5.371295000	4.509981000	0.877042000
H	5.766935000	3.089636000	1.864144000
H	4.176133000	3.852001000	2.012661000
C	5.646999000	2.207198000	-0.650808000
H	6.332182000	1.626341000	-0.025682000
H	6.193078000	3.060369000	-1.065816000
H	5.321041000	1.574881000	-1.481346000
C	3.675345000	3.864416000	-1.973001000
H	4.351091000	4.711808000	-1.812890000
H	2.782180000	4.232190000	-2.487893000
H	4.167711000	3.139139000	-2.624949000
C	2.393040000	4.210688000	0.140721000
H	1.494645000	4.432620000	-0.442189000
H	2.918353000	5.150470000	0.338627000

H	2.081405000	3.778420000	1.096524000
C	-0.771550000	2.460869000	-0.279466000
N	-0.428166000	1.385892000	-1.150901000
C	-1.773835000	3.407222000	-0.684604000
C	-1.927968000	4.622987000	0.029165000
C	-2.619062000	3.213656000	-1.805458000
C	-2.877428000	5.568010000	-0.338729000
H	-1.286222000	4.810136000	0.889604000
C	-3.580017000	4.156086000	-2.157328000
H	-2.506428000	2.306944000	-2.395187000
C	-3.724728000	5.344120000	-1.431786000
H	-2.964825000	6.488991000	0.235264000
H	-4.219267000	3.966642000	-3.018192000
H	-4.471409000	6.081446000	-1.715978000
H	-0.837383000	0.673553000	0.999713000
H	0.051585000	2.861753000	0.308354000
H	0.439038000	1.409515000	-1.686275000

Acr^{Dipp}-3NP

E(B3PW91-D3) = -2677.8632 au

E(DLPNO-CCSD(T)) = -2673.118424 au

G_{cont} = 0.942439 au

G = -2672.175985 au

P	0.765158000	0.021669000	0.088372000
N	-2.221884000	-0.368506000	0.107683000
N	0.348882000	-1.231750000	1.278233000
N	2.377603000	-0.627972000	0.062978000
C	1.523212000	-1.644792000	1.939080000
C	2.688833000	-1.328403000	1.226999000
C	3.937441000	-1.680575000	1.726027000
H	4.835193000	-1.449905000	1.159113000
C	3.997576000	-2.329019000	2.966871000
C	2.835716000	-2.587965000	3.697170000
H	2.901737000	-3.056834000	4.676845000
C	1.575571000	-2.240093000	3.189736000
C	-0.821394000	-1.110829000	2.046642000
C	-0.819291000	-1.553718000	3.393038000
C	-1.887340000	-1.232260000	4.226402000
H	-1.863824000	-1.561291000	5.263267000
C	-2.978020000	-0.509794000	3.745170000
C	-3.039455000	-0.209674000	2.392300000
H	-3.940029000	0.238959000	1.985247000
C	-2.001953000	-0.546194000	1.510769000

C	0.278527000	-2.457710000	3.912810000
H	-3.802111000	-0.244202000	4.401728000
H	4.964556000	-2.614317000	3.373639000
H	-0.046857000	-3.504716000	3.795120000
H	0.412526000	-2.305720000	4.990540000
C	3.217799000	-0.679872000	-1.090144000
C	3.977950000	0.448874000	-1.450921000
C	4.824009000	0.353001000	-2.562407000
H	5.413019000	1.216842000	-2.861596000
C	4.929280000	-0.831528000	-3.282929000
H	5.601466000	-0.893724000	-4.135920000
C	4.162810000	-1.936189000	-2.917999000
H	4.241684000	-2.852780000	-3.496860000
C	3.282621000	-1.881244000	-1.833481000
C	3.883589000	1.754373000	-0.687402000
H	3.249498000	1.582493000	0.186754000
C	3.207832000	2.831927000	-1.544760000
H	3.781277000	3.026036000	-2.459739000
H	3.123306000	3.769801000	-0.985823000
H	2.199601000	2.518739000	-1.841284000
C	5.248059000	2.229144000	-0.176690000
H	5.729540000	1.458463000	0.436351000
H	5.121488000	3.128365000	0.437117000
H	5.927821000	2.480010000	-0.999990000
C	2.423668000	-3.087789000	-1.495480000
H	1.627086000	-2.755685000	-0.819884000
C	3.237273000	-4.172541000	-0.774599000
H	2.592880000	-5.021288000	-0.515422000
H	3.687130000	-3.792563000	0.147013000
H	4.041900000	-4.543019000	-1.422603000
C	1.748684000	-3.673653000	-2.741256000
H	1.227067000	-2.899253000	-3.310882000
H	1.009127000	-4.425430000	-2.446110000
H	2.473601000	-4.161420000	-3.404078000
C	-2.093836000	-1.465344000	-0.823499000
C	-1.588072000	-1.209780000	-2.132437000
C	-1.462600000	-2.279147000	-3.024039000
H	-1.089037000	-2.084213000	-4.025567000
C	-1.781101000	-3.581108000	-2.667492000
H	-1.645718000	-4.397086000	-3.373101000
C	-2.287147000	-3.816916000	-1.399213000
H	-2.571804000	-4.828978000	-1.122664000
C	-2.489462000	-2.783275000	-0.476199000
C	-1.221435000	0.160980000	-2.694021000

H	-1.234453000	0.889399000	-1.875442000
C	-2.235451000	0.599609000	-3.763790000
H	-2.162361000	-0.045706000	-4.647478000
H	-2.026767000	1.626901000	-4.089474000
H	-3.257498000	0.550632000	-3.387976000
C	0.186086000	0.197977000	-3.312828000
H	0.219176000	-0.349546000	-4.262146000
H	0.942590000	-0.230286000	-2.652355000
H	0.471475000	1.235369000	-3.526248000
C	-3.202576000	-3.180666000	0.810669000
H	-3.329486000	-2.305360000	1.440422000
C	-4.617139000	-3.700691000	0.516343000
H	-5.196743000	-2.958775000	-0.045044000
H	-5.144382000	-3.908802000	1.455545000
H	-4.600775000	-4.627254000	-0.069550000
C	-2.389100000	-4.201444000	1.617448000
H	-2.333438000	-5.170011000	1.105816000
H	-2.848578000	-4.366406000	2.599155000
H	-1.365953000	-3.846566000	1.774795000
B	-2.994722000	0.791139000	-0.261907000
O	-2.876487000	1.999026000	0.388219000
O	-3.965469000	0.794495000	-1.234229000
C	-3.682205000	2.953443000	-0.345944000
C	-4.714771000	2.027962000	-1.074755000
C	-4.289277000	3.937242000	0.640724000
H	-4.981119000	4.616113000	0.129632000
H	-3.495685000	4.537369000	1.097775000
H	-4.827130000	3.422715000	1.440605000
C	-2.745795000	3.678375000	-1.310577000
H	-1.940063000	4.143009000	-0.735851000
H	-3.270135000	4.463061000	-1.865272000
H	-2.296528000	2.983263000	-2.026448000
C	-5.163745000	2.525426000	-2.438899000
H	-5.683602000	3.484779000	-2.338129000
H	-5.857979000	1.805107000	-2.883702000
H	-4.323645000	2.653374000	-3.123759000
C	-5.931170000	1.689904000	-0.213715000
H	-6.494029000	0.885112000	-0.696544000
H	-6.591720000	2.555098000	-0.096731000
H	-5.632404000	1.344200000	0.781170000
N	0.765552000	1.325168000	1.160888000
C	0.295315000	2.638220000	0.777076000
C	1.258567000	3.772325000	1.063800000
C	0.992245000	5.040219000	0.530237000

C	2.403786000	3.605978000	1.845189000
C	1.857332000	6.109261000	0.753854000
H	0.106851000	5.186862000	-0.086018000
C	3.272913000	4.675109000	2.075655000
H	2.640614000	2.628010000	2.254785000
C	3.007108000	5.929521000	1.528198000
H	1.639314000	7.081676000	0.318109000
H	4.164743000	4.521084000	2.678811000
H	3.687839000	6.759689000	1.700170000
H	-0.672807000	2.853114000	1.248949000
H	0.092064000	2.608404000	-0.300767000
H	0.872491000	1.159676000	2.155159000

Acr^{Dipp}-TS_{3NP/1NP}

E(B3PW91-D3) = -2677.844646 au

E(DLPNO-CCSD(T)) = -2673.098864 au

G_{cont} = 0.949651 au

G = -2672.149212 au

P	-0.705293000	0.069737000	-0.403039000
N	-0.127333000	-1.490093000	-1.019649000
N	-2.250543000	-0.704184000	-0.047305000
N	2.220118000	0.052769000	-0.426986000
C	-2.396214000	-1.939404000	-0.683207000
C	-1.186014000	-2.386733000	-1.228813000
C	-1.122157000	-3.553748000	-1.975049000
C	-2.300481000	-4.300016000	-2.140584000
C	-3.503975000	-3.863978000	-1.594957000
C	-3.565520000	-2.666341000	-0.868659000
H	-2.265706000	-5.215115000	-2.728290000
H	-4.507972000	-2.290897000	-0.483679000
C	2.236145000	-0.932758000	-1.448219000
C	3.396930000	-1.132562000	-2.192235000
C	3.487785000	-2.169661000	-3.115062000
C	2.417002000	-3.048019000	-3.240628000
C	1.235237000	-2.870454000	-2.514556000
C	1.103563000	-1.752156000	-1.666054000
H	4.235491000	-0.466473000	-2.015663000
H	2.490516000	-3.905286000	-3.907508000
C	0.177011000	-3.946531000	-2.612967000
H	4.395903000	-2.313757000	-3.694656000
H	-4.412916000	-4.439622000	-1.750275000
H	0.008646000	-4.208615000	-3.666677000
H	0.564661000	-4.863211000	-2.140268000

C	2.704123000	1.368904000	-0.739456000
C	3.839568000	1.906254000	-0.079168000
C	2.046857000	2.159329000	-1.728347000
C	4.123782000	3.271209000	-0.221693000
C	2.391993000	3.508655000	-1.848762000
C	3.383000000	4.087406000	-1.064039000
H	4.972637000	3.692670000	0.310443000
H	1.876674000	4.119918000	-2.584728000
H	3.611587000	5.146985000	-1.152957000
C	-3.424173000	0.005713000	0.373638000
C	-4.024160000	0.932561000	-0.515066000
C	-4.020508000	-0.294874000	1.622534000
C	-5.192677000	1.585899000	-0.115355000
C	-5.197129000	0.390070000	1.962032000
C	-5.779492000	1.322368000	1.115431000
H	-5.659191000	2.304192000	-0.782464000
H	-5.666715000	0.175076000	2.920230000
H	-6.687717000	1.841219000	1.413363000
C	4.878728000	1.060070000	0.641710000
H	4.481242000	0.051695000	0.760567000
C	5.237008000	1.600640000	2.029109000
C	6.147233000	0.964074000	-0.223468000
H	5.716413000	2.584722000	1.965368000
H	4.344713000	1.685893000	2.652742000
H	5.946939000	0.931312000	2.528109000
H	6.874057000	0.286502000	0.241576000
H	5.928326000	0.588233000	-1.228716000
H	6.624234000	1.945311000	-0.335930000
C	1.087957000	1.602041000	-2.771166000
H	0.736340000	0.624877000	-2.443529000
C	1.841577000	1.390161000	-4.093994000
C	-0.156179000	2.462161000	-3.002606000
H	2.198707000	2.347243000	-4.494090000
H	2.704982000	0.732118000	-3.957216000
H	1.179785000	0.933313000	-4.840108000
H	-0.846143000	1.932166000	-3.669338000
H	-0.681309000	2.665909000	-2.066265000
H	0.083151000	3.419569000	-3.480060000
C	-3.601853000	-1.353172000	2.649027000
H	-4.018844000	-0.984941000	3.596552000
C	-4.278944000	-2.709690000	2.388476000
C	-2.114371000	-1.560141000	2.915359000
H	-5.343113000	-2.587508000	2.158159000
H	-3.806344000	-3.235219000	1.554679000

H	-4.192101000	-3.343143000	3.279372000
H	-1.647312000	-0.616861000	3.218263000
H	-1.986536000	-2.258492000	3.750662000
H	-1.589804000	-1.979686000	2.052299000
C	-3.498223000	1.174910000	-1.921687000
H	-2.437528000	0.908461000	-1.945751000
C	-4.224355000	0.266476000	-2.925442000
C	-3.594439000	2.640731000	-2.355318000
H	-5.297657000	0.494621000	-2.944004000
H	-3.825082000	0.422351000	-3.935017000
H	-4.104441000	-0.790393000	-2.669262000
H	-3.079674000	2.779398000	-3.311619000
H	-4.633659000	2.958439000	-2.501256000
H	-3.133319000	3.303515000	-1.616722000
B	1.951331000	-0.486104000	0.941647000
O	2.571181000	0.023969000	2.087574000
O	1.710016000	-1.861314000	1.082446000
C	2.446245000	-2.322186000	2.222560000
C	2.603793000	-1.020119000	3.084960000
C	1.454233000	-0.792118000	4.065777000
H	1.497972000	-1.497703000	4.902161000
H	1.526100000	0.223022000	4.469509000
H	0.480122000	-0.904462000	3.588460000
C	3.918496000	-0.946470000	3.848875000
H	3.966482000	-0.020311000	4.430196000
H	3.995111000	-1.790867000	4.543834000
H	4.777468000	-0.968861000	3.177114000
C	3.778348000	-2.868583000	1.702571000
H	4.385555000	-3.306149000	2.502280000
H	3.567877000	-3.644340000	0.959573000
H	4.359689000	-2.084820000	1.206480000
C	1.657068000	-3.435614000	2.896413000
H	1.591338000	-4.297616000	2.224286000
H	2.150746000	-3.758160000	3.820459000
H	0.638769000	-3.117288000	3.133469000
C	0.231699000	1.640014000	1.615539000
N	0.027296000	0.238394000	1.170907000
C	-0.934424000	2.584114000	1.458501000
C	-0.839349000	3.660117000	0.568696000
C	-2.101111000	2.436153000	2.216803000
C	-1.889631000	4.569252000	0.437105000
H	0.065614000	3.780577000	-0.024044000
C	-3.154025000	3.338485000	2.084698000
H	-2.192179000	1.605419000	2.912177000

C	-3.051064000	4.408284000	1.193565000
H	-1.802711000	5.397330000	-0.262585000
H	-4.059384000	3.197599000	2.667704000
H	-3.875893000	5.108452000	1.085129000
H	1.088850000	2.038094000	1.067376000
H	0.541812000	1.580469000	2.661146000
H	-0.418309000	-0.336173000	1.876428000

Acr^{Dipp}-TS_{2NP/1NP}

E(B3PW91-D3) = -2677.801056 au

E(DLPNO-CCSD(T)) = -2673.042952 au

G_{cont} = 0.942656 au

G = -2672.100296 au

P	0.886340000	-0.223515000	-0.112393000
N	0.691329000	-1.163858000	1.320022000
N	-1.837383000	-0.347773000	0.128234000
N	2.592167000	-0.256209000	0.095275000
C	-1.722840000	-0.714641000	1.509416000
C	-0.511234000	-1.216478000	2.053791000
C	-0.444051000	-1.692232000	3.385932000
C	-1.538910000	-1.519347000	4.223754000
C	-2.697586000	-0.909630000	3.746730000
C	-2.787102000	-0.539206000	2.413523000
H	-1.481907000	-1.870667000	5.251782000
H	-3.699300000	-0.103851000	2.030483000
C	2.998793000	-0.780116000	1.319242000
C	4.279947000	-0.857846000	1.857367000
C	4.422944000	-1.439980000	3.120823000
C	3.317070000	-1.935331000	3.821860000
C	2.034181000	-1.880195000	3.267889000
C	1.903501000	-1.300266000	2.015280000
H	5.131570000	-0.472343000	1.304766000
H	3.452190000	-2.374729000	4.807517000
C	0.782303000	-2.421607000	3.891060000
H	-3.552312000	-0.764753000	4.402637000
H	5.411987000	-1.504365000	3.566835000
H	0.688514000	-3.491729000	3.642999000
H	0.833833000	-2.364162000	4.983890000
C	3.494179000	-0.114770000	-1.009977000
C	3.980559000	-1.281965000	-1.635150000
C	3.840938000	1.173411000	-1.454918000
C	4.852997000	-1.124502000	-2.715995000
C	4.699915000	1.277206000	-2.554467000

C	5.208933000	0.140878000	-3.175608000
H	5.244908000	-2.005727000	-3.217914000
H	4.972294000	2.259723000	-2.930323000
H	5.879385000	0.240751000	-4.026035000
C	3.561087000	-2.677148000	-1.204792000
H	2.852775000	-2.589398000	-0.375669000
H	1.962562000	-2.826546000	-2.678407000
C	2.828138000	-3.403719000	-2.339997000
H	2.466862000	-4.378872000	-1.993271000
H	3.486863000	-3.574260000	-3.199880000
C	4.757440000	-3.491352000	-0.696760000
H	5.496403000	-3.651717000	-1.491088000
H	4.424622000	-4.474608000	-0.344711000
H	5.254932000	-2.981796000	0.135359000
C	3.256774000	2.416051000	-0.814021000
H	2.861641000	2.132757000	0.166940000
C	4.293856000	3.517750000	-0.577350000
H	3.840198000	4.325741000	0.006502000
H	4.656292000	3.950614000	-1.517265000
H	5.158789000	3.137138000	-0.022408000
C	2.086257000	2.940687000	-1.658023000
H	1.686307000	3.862515000	-1.225131000
H	1.271330000	2.209419000	-1.715075000
H	2.411953000	3.149954000	-2.684161000
C	-1.765092000	-1.434380000	-0.821876000
C	-2.320799000	-2.706837000	-0.485415000
C	-1.079593000	-1.327843000	-2.083171000
C	-1.944812000	-3.846331000	-1.204863000
C	-0.791137000	-2.503995000	-2.788768000
C	-1.146596000	-3.765369000	-2.335365000
H	-2.334186000	-4.813672000	-0.895901000
H	-0.262656000	-2.421959000	-3.734032000
H	-0.858505000	-4.657705000	-2.886125000
C	-3.446965000	-2.914925000	0.523360000
H	-3.756417000	-1.940742000	0.898529000
C	-3.042416000	-3.785230000	1.717994000
H	-3.867597000	-3.860051000	2.436217000
H	-2.175683000	-3.374450000	2.240530000
H	-2.790978000	-4.801817000	1.390387000
C	-4.681957000	-3.518644000	-0.169306000
H	-4.516287000	-4.561559000	-0.463256000
H	-4.952215000	-2.957294000	-1.069143000
H	-5.538058000	-3.501320000	0.516632000
C	-0.734301000	-0.041283000	-2.836614000

H	-0.820462000	0.803730000	-2.152353000
C	-1.750405000	0.165550000	-3.973154000
H	-1.617928000	-0.599288000	-4.748863000
H	-1.607300000	1.149076000	-4.438096000
H	-2.771191000	0.112726000	-3.598658000
C	0.673112000	-0.014517000	-3.455474000
H	0.876611000	0.983416000	-3.860690000
H	0.769494000	-0.721088000	-4.287514000
H	1.462978000	-0.248526000	-2.736276000
B	-2.508246000	1.081105000	-0.194868000
O	-3.651769000	1.370625000	0.669453000
O	-2.994783000	1.211589000	-1.543961000
C	-4.671112000	1.964614000	-0.126516000
C	-4.419045000	1.296059000	-1.513072000
C	-6.025408000	1.650010000	0.498455000
H	-6.843413000	1.978966000	-0.153906000
H	-6.123108000	2.171959000	1.457200000
H	-6.135259000	0.578287000	0.685224000
C	-4.465381000	3.483760000	-0.164169000
H	-4.412187000	3.857286000	0.864129000
H	-5.289857000	3.993027000	-0.676738000
H	-3.528505000	3.741926000	-0.666878000
C	-4.895804000	2.107921000	-2.709825000
H	-5.971781000	2.307356000	-2.637032000
H	-4.715385000	1.554633000	-3.637806000
H	-4.365573000	3.061861000	-2.777904000
C	-4.993739000	-0.120299000	-1.574193000
H	-4.584831000	-0.640357000	-2.446039000
H	-6.087115000	-0.118956000	-1.650430000
H	-4.702200000	-0.682113000	-0.684265000
C	-0.480120000	2.155157000	0.988732000
C	0.383970000	3.320489000	1.305149000
C	1.468586000	3.148120000	2.178697000
C	0.120629000	4.595389000	0.790979000
C	2.284024000	4.223099000	2.515276000
H	1.679971000	2.156915000	2.577355000
C	0.940144000	5.673683000	1.127565000
H	-0.738200000	4.751942000	0.143451000
C	2.024763000	5.491157000	1.985513000
H	3.127617000	4.072153000	3.183956000
H	0.724854000	6.659269000	0.722404000
H	2.664343000	6.331299000	2.243921000
N	-1.389077000	2.165922000	0.006993000
H	-0.785695000	1.589310000	1.870594000

H	0.514459000	1.181350000	0.606926000
H	-1.192964000	2.762192000	-0.788587000

5

E(B3PW91-D3) = -556.576548 au

E(DLPNO-CCSD(T)) = -555.530804 au

G_{cont} = 0.172649 au

G = -555.358154 au

C	-0.395668000	0.380174000	-0.178969000
H	-0.079913000	1.370376000	-0.540887000
N	0.459048000	-0.525075000	0.121825000
C	1.829085000	-0.229027000	0.070774000
C	2.698352000	-1.216607000	-0.419423000
C	2.366925000	0.982669000	0.538621000
C	4.068453000	-0.977666000	-0.488160000
H	2.278348000	-2.161132000	-0.755414000
C	3.741857000	1.207841000	0.483590000
H	1.709294000	1.730357000	0.975532000
C	4.597577000	0.235227000	-0.037382000
H	4.728133000	-1.745334000	-0.885549000
H	4.146526000	2.144974000	0.858840000
H	5.669016000	0.413947000	-0.077671000
C	-1.842817000	0.168425000	-0.086819000
C	-2.708751000	1.205442000	-0.465313000
C	-2.385248000	-1.044124000	0.371917000
C	-4.090890000	1.038071000	-0.388889000
H	-2.295083000	2.147309000	-0.821165000
C	-3.763639000	-1.209806000	0.446721000
H	-1.710634000	-1.843706000	0.664511000
C	-4.620568000	-0.169884000	0.067172000
H	-4.752607000	1.848218000	-0.684514000
H	-4.176566000	-2.150555000	0.802366000
H	-5.697852000	-0.303346000	0.128134000

6

E(B3PW91-D3) = -968.3978443 au

E(DLPNO-CCSD(T)) = -966.6445412 au

G_{cont} = 0.354333 au

G = -966.2902083 au

C	-1.253799000	-0.356833000	-1.463906000
N	-0.417409000	0.624904000	-0.781431000
C	-1.006272000	1.834542000	-0.353637000

C	-0.227097000	2.996000000	-0.212954000
C	-2.383461000	1.918968000	-0.089499000
C	-0.807032000	4.193180000	0.197336000
H	0.835326000	2.954787000	-0.427253000
C	-2.957883000	3.127067000	0.307153000
H	-3.011529000	1.037146000	-0.170300000
C	-2.177200000	4.272265000	0.458802000
H	-0.181003000	5.076932000	0.298542000
H	-4.026291000	3.163400000	0.507663000
H	-2.627110000	5.210913000	0.771759000
C	-1.939669000	-1.370228000	-0.563891000
C	-2.755364000	-2.350233000	-1.143413000
C	-1.773107000	-1.368887000	0.822493000
C	-3.387664000	-3.310091000	-0.354714000
H	-2.893277000	-2.362448000	-2.223854000
C	-2.404943000	-2.328500000	1.616764000
H	-1.153639000	-0.605373000	1.286452000
C	-3.213080000	-3.303412000	1.032052000
H	-4.016311000	-4.064748000	-0.821822000
H	-2.265230000	-2.310426000	2.695194000
H	-3.705073000	-4.051043000	1.649465000
B	0.905041000	0.215979000	-0.435543000
O	1.743049000	0.875314000	0.436601000
O	1.449607000	-0.949086000	-0.937962000
C	3.031366000	0.212748000	0.345712000
C	2.629643000	-1.220903000	-0.140232000
C	3.701106000	0.259474000	1.708492000
H	4.628087000	-0.324772000	1.697776000
H	3.951535000	1.294405000	1.963209000
H	3.046639000	-0.133520000	2.490161000
C	3.856806000	0.982176000	-0.684368000
H	3.919922000	2.030576000	-0.376107000
H	4.873203000	0.582590000	-0.762331000
H	3.388743000	0.944722000	-1.673906000
C	3.664301000	-1.912456000	-1.011483000
H	4.605023000	-2.033902000	-0.462690000
H	3.303853000	-2.906305000	-1.296159000
H	3.861055000	-1.347658000	-1.925984000
C	2.191318000	-2.136711000	1.001739000
H	1.722431000	-3.030320000	0.578454000
H	3.042894000	-2.447188000	1.615892000
H	1.455405000	-1.643049000	1.644947000
H	-2.004279000	0.173791000	-2.061846000
H	-0.622780000	-0.901536000	-2.173320000

TS¹_{2NP/1NP}

E(B3PW91-D3) = -2015.661172 au

E(DLPNO-CCSD(T)) = -2012.193352 au

G_{cont} = 0.592444 au

G = -2011.600908 au

P	-1.038823000	0.812615000	-2.180756000
N	1.363313000	0.864954000	-1.463782000
N	-2.767370000	0.658710000	-2.030812000
N	-1.065436000	1.761144000	-0.736144000
C	1.299434000	2.134215000	-0.823505000
C	0.029297000	2.595866000	-0.435943000
C	-0.115868000	3.846697000	0.173105000
C	1.011700000	4.621902000	0.436169000
C	2.280499000	4.163245000	0.076087000
C	2.416751000	2.928515000	-0.556601000
H	-1.104619000	4.220993000	0.417870000
H	0.893200000	5.591789000	0.912717000
H	3.160976000	4.764626000	0.287804000
H	3.398475000	2.551219000	-0.823441000
C	-3.277906000	1.098019000	-0.823984000
C	-2.285256000	1.740404000	-0.052943000
C	-2.560354000	2.153153000	1.249092000
C	-3.850420000	1.963810000	1.755486000
C	-4.844349000	1.365501000	0.975919000
C	-4.564732000	0.917306000	-0.317946000
H	-1.780821000	2.578313000	1.870941000
H	-4.072093000	2.278917000	2.771498000
H	-5.842660000	1.228114000	1.383606000
H	-5.321905000	0.406892000	-0.905200000
C	-3.525899000	-0.223503000	-2.894615000
H	-4.445452000	0.267204000	-3.234551000
H	-3.786990000	-1.156245000	-2.376242000
H	-2.924440000	-0.468192000	-3.775216000
C	2.039429000	0.933073000	-2.766039000
H	1.575174000	1.709372000	-3.384978000
H	1.937774000	-0.031889000	-3.267513000
H	3.109596000	1.155864000	-2.685471000
B	1.893991000	-0.291541000	-0.506297000
O	2.851701000	0.154905000	0.466796000
O	2.519892000	-1.361801000	-1.261372000
C	3.800718000	-0.898118000	0.649614000
C	3.853437000	-1.547727000	-0.776270000

C	5.113466000	-0.285096000	1.122134000
H	5.909065000	-1.039249000	1.150443000
H	4.988119000	0.116697000	2.133793000
H	5.428799000	0.534559000	0.471377000
C	3.293876000	-1.875225000	1.716328000
H	2.401753000	-2.410274000	1.382418000
H	3.027505000	-1.312124000	2.616259000
H	4.062445000	-2.611796000	1.977234000
C	4.173877000	-3.038414000	-0.785016000
H	5.146820000	-3.231966000	-0.317536000
H	4.214647000	-3.401442000	-1.818421000
H	3.409810000	-3.613249000	-0.255432000
C	4.827563000	-0.819916000	-1.706706000
H	4.640134000	-1.135853000	-2.738335000
H	5.869800000	-1.049287000	-1.456755000
H	4.691165000	0.263366000	-1.650493000
C	-0.200217000	-1.589018000	-0.664082000
N	0.570446000	-0.906657000	0.206424000
C	0.245635000	-0.706620000	1.564454000
C	-0.175812000	-1.785575000	2.359808000
C	-0.454766000	-1.605586000	3.710682000
C	-0.293696000	-0.350957000	4.304663000
C	0.164115000	0.713943000	3.528072000
C	0.437005000	0.540081000	2.172926000
H	-0.269797000	-2.771229000	1.914382000
H	-0.782673000	-2.454906000	4.305624000
H	-0.506360000	-0.211466000	5.361635000
H	0.313154000	1.693651000	3.976416000
H	0.811641000	1.369519000	1.587556000
C	-1.490854000	-2.275052000	-0.406720000
C	-1.736206000	-3.472692000	-1.093920000
C	-2.966709000	-4.119571000	-0.981981000
C	-3.974327000	-3.565486000	-0.191383000
C	-3.740508000	-2.366202000	0.488436000
C	-2.510938000	-1.726648000	0.383490000
H	-0.956879000	-3.898734000	-1.722677000
H	-3.138890000	-5.049942000	-1.517305000
H	-4.938827000	-4.060543000	-0.109001000
H	-4.523618000	-1.914803000	1.091229000
H	-2.351263000	-0.787610000	0.902122000
H	0.388394000	-2.039317000	-1.465839000
H	-0.706084000	-0.590314000	-1.573748000

TS¹_{2NP/3NP}

E(B3PW91-D3) = -2015.630919 au

E(DLPNO-CCSD(T)) = -2012.165021 au

G_{cont} = 0.588355 au

G = -2011.576667 au

P	-1.860039000	-0.388600000	-1.313473000
N	1.613372000	0.736676000	0.665644000
N	-1.417801000	-1.901290000	-1.947644000
N	-0.255643000	0.159240000	-1.494333000
C	1.073407000	1.751592000	-0.151985000
C	0.154769000	1.488880000	-1.189191000
C	-0.354509000	2.537877000	-1.962550000
C	0.031105000	3.852333000	-1.726983000
C	0.956619000	4.121029000	-0.715774000
C	1.465885000	3.083227000	0.056342000
H	-1.046660000	2.303262000	-2.766995000
H	-0.376197000	4.655835000	-2.334429000
H	1.274367000	5.142019000	-0.520183000
H	2.176195000	3.288461000	0.851399000
C	-0.051860000	-2.030846000	-2.215722000
C	0.629738000	-0.829449000	-1.946065000
C	1.994890000	-0.721946000	-2.174406000
C	2.675208000	-1.842934000	-2.669403000
C	2.003778000	-3.038979000	-2.921720000
C	0.623994000	-3.144790000	-2.697320000
H	2.515575000	0.211391000	-1.983922000
H	3.741619000	-1.771357000	-2.863728000
H	2.548964000	-3.898570000	-3.302292000
H	0.093991000	-4.070172000	-2.903308000
C	-2.373033000	-2.960815000	-2.209688000
H	-2.372212000	-3.227513000	-3.272693000
H	-2.141543000	-3.851441000	-1.614027000
H	-3.372669000	-2.613707000	-1.932402000
C	0.716890000	-0.211407000	1.322204000
H	0.529333000	-1.099593000	0.709467000
H	1.169967000	-0.540384000	2.260228000
H	-0.238530000	0.267202000	1.547001000
B	3.016336000	0.588020000	0.824595000
O	3.956749000	1.391809000	0.210628000
O	3.572760000	-0.397472000	1.615202000
C	5.240322000	0.751017000	0.428068000
C	4.981024000	-0.071149000	1.735811000
C	6.308689000	1.824243000	0.548691000
H	7.271141000	1.376208000	0.820499000

H	6.428748000	2.336447000	-0.411597000
H	6.043576000	2.571127000	1.300933000
C	5.506925000	-0.139182000	-0.783972000
H	5.445188000	0.469339000	-1.691925000
H	6.501796000	-0.593933000	-0.737277000
H	4.760096000	-0.935695000	-0.854233000
C	5.776206000	-1.361322000	1.845515000
H	6.851330000	-1.150129000	1.827299000
H	5.541718000	-1.861364000	2.790887000
H	5.538553000	-2.048901000	1.030338000
C	5.140492000	0.765310000	3.004662000
H	4.744391000	0.199896000	3.853983000
H	6.192245000	0.996751000	3.202391000
H	4.582996000	1.705327000	2.931192000
C	-2.816362000	0.991823000	0.388142000
N	-2.432843000	-0.367090000	0.256015000
C	-2.516883000	-1.370699000	1.246166000
C	-3.286588000	-1.129671000	2.393982000
C	-3.381247000	-2.095695000	3.392144000
C	-2.704085000	-3.312143000	3.277671000
C	-1.918676000	-3.541584000	2.148164000
C	-1.817488000	-2.582594000	1.140991000
H	-3.806612000	-0.182797000	2.494900000
H	-3.990022000	-1.890055000	4.269500000
H	-2.776585000	-4.061231000	4.061688000
H	-1.361110000	-4.470093000	2.048975000
H	-1.170002000	-2.772739000	0.292760000
C	-4.203057000	1.362980000	0.383236000
C	-5.223635000	0.437503000	0.053908000
C	-6.558934000	0.832099000	-0.009315000
C	-6.929501000	2.152924000	0.253888000
C	-5.931270000	3.080351000	0.585558000
C	-4.597797000	2.698106000	0.648510000
H	-4.958029000	-0.600639000	-0.132383000
H	-7.320014000	0.095425000	-0.260615000
H	-7.972648000	2.455590000	0.209230000
H	-6.201156000	4.113333000	0.797681000
H	-3.834123000	3.432034000	0.901862000
H	-2.617676000	0.793520000	-1.599158000
H	-2.052852000	1.692074000	0.716299000

3NP¹

E(B3PW91-D3) = -2015.715642 au

E(DLPNO-CCSD(T)) = -2012.263026 au

G_{cont} = 0.588670 au

G = -2011.674356 au

P	-0.323807000	-0.206886000	-1.091482000
N	2.258946000	-1.853123000	0.088065000
N	-1.434206000	-0.798090000	-2.276293000
N	-0.565527000	-1.704263000	-0.230308000
C	1.399426000	-1.905070000	1.213744000
C	-0.000140000	-1.884589000	1.056615000
C	-0.829681000	-1.990067000	2.179227000
C	-0.284337000	-2.098152000	3.454499000
C	1.102603000	-2.082949000	3.619844000
C	1.932546000	-1.991304000	2.505192000
H	-1.906363000	-1.950412000	2.039289000
H	-0.942205000	-2.168399000	4.316879000
H	1.537930000	-2.153088000	4.613621000
H	3.013348000	-1.993876000	2.616035000
C	-2.077575000	-1.986032000	-1.953570000
C	-1.562107000	-2.528908000	-0.757690000
C	-2.031491000	-3.743086000	-0.273896000
C	-3.045740000	-4.404631000	-0.983779000
C	-3.575556000	-3.855758000	-2.150088000
C	-3.096629000	-2.631818000	-2.644735000
H	-1.624143000	-4.165082000	0.640019000
H	-3.419653000	-5.354903000	-0.611173000
H	-4.364763000	-4.375507000	-2.687366000
H	-3.508768000	-2.201303000	-3.553167000
C	-1.793304000	-0.021794000	-3.441249000
H	-1.734582000	-0.635002000	-4.349166000
H	-2.810933000	0.386356000	-3.359429000
H	-1.095465000	0.814933000	-3.544366000
C	2.198619000	-2.983101000	-0.835546000
H	1.202136000	-3.085719000	-1.277787000
H	2.922578000	-2.826707000	-1.637692000
H	2.445608000	-3.916871000	-0.313692000
B	3.186512000	-0.799980000	-0.086650000
O	3.341391000	0.246526000	0.804405000
O	4.043162000	-0.720950000	-1.170234000
C	4.221369000	1.203115000	0.163871000
C	5.014322000	0.303018000	-0.845071000
C	5.075802000	1.870551000	1.229210000
H	5.823714000	2.524523000	0.766470000
H	4.443288000	2.482136000	1.881097000
H	5.589713000	1.133490000	1.851004000

C	3.338306000	2.236339000	-0.532863000
H	2.717711000	1.765553000	-1.302509000
H	2.677147000	2.693271000	0.209719000
H	3.935299000	3.028455000	-0.996488000
C	5.438290000	1.002490000	-2.125943000
H	6.091525000	1.852808000	-1.899746000
H	5.992764000	0.305016000	-2.762381000
H	4.574329000	1.362271000	-2.689952000
C	6.209054000	-0.400193000	-0.201072000
H	6.585216000	-1.162060000	-0.891133000
H	7.020485000	0.302393000	0.015621000
H	5.918765000	-0.898056000	0.730447000
C	-0.377795000	2.195122000	0.109455000
N	-1.092339000	0.930340000	-0.042254000
C	-2.183088000	0.671066000	0.823819000
C	-2.151607000	1.085259000	2.164323000
C	-3.195806000	0.765220000	3.027878000
C	-4.289023000	0.022100000	2.576928000
C	-4.336626000	-0.369655000	1.238641000
C	-3.304881000	-0.030892000	0.364799000
H	-1.296631000	1.634500000	2.545303000
H	-3.144939000	1.086513000	4.065639000
H	-5.096800000	-0.237252000	3.256467000
H	-5.186574000	-0.933615000	0.861913000
H	-3.371225000	-0.317941000	-0.677823000
C	-1.248506000	3.408818000	-0.123981000
C	-1.018770000	4.587585000	0.591553000
C	-1.787514000	5.728224000	0.352133000
C	-2.804410000	5.698072000	-0.603504000
C	-3.045811000	4.520701000	-1.315779000
C	-2.273044000	3.385067000	-1.076451000
H	-0.234852000	4.612299000	1.347012000
H	-1.598009000	6.636758000	0.919081000
H	-3.409856000	6.582462000	-0.786635000
H	-3.842086000	4.485715000	-2.055837000
H	-2.471865000	2.463661000	-1.618142000
H	0.115671000	2.268238000	1.087481000
H	0.431117000	2.180501000	-0.630053000

$TS_{1NP/3NP}^1$

$E(\text{B3PW91-D3}) = -2015.677567 \text{ au}$

$E(\text{DLPNO-CCSD(T)}) = -2012.224879 \text{ au}$

$G_{\text{cont}} = 0.597417 \text{ au}$

G = -2011.627463 au

P	0.559196000	-0.464044000	-1.615127000
N	-1.155164000	-1.834961000	-0.916445000
N	2.092222000	0.344303000	-1.927379000
N	1.465661000	-1.617965000	-0.623074000
C	-0.587593000	-2.537453000	0.184414000
C	0.801402000	-2.389687000	0.344705000
C	1.400040000	-2.910567000	1.500982000
C	0.634607000	-3.621018000	2.422665000
C	-0.733385000	-3.816616000	2.227465000
C	-1.343908000	-3.251340000	1.109001000
H	2.440357000	-2.711014000	1.721363000
H	1.117672000	-4.007957000	3.316786000
H	-1.321403000	-4.373846000	2.952006000
H	-2.416746000	-3.321713000	0.957405000
C	3.208829000	-0.309135000	-1.428918000
C	2.860465000	-1.473313000	-0.711745000
C	3.860947000	-2.347505000	-0.294000000
C	5.204666000	-2.014002000	-0.518774000
C	5.545386000	-0.833845000	-1.174647000
C	4.543261000	0.023572000	-1.647766000
H	3.616211000	-3.297225000	0.166558000
H	5.980797000	-2.696356000	-0.182017000
H	6.589656000	-0.582081000	-1.341562000
H	4.799834000	0.928511000	-2.191157000
C	2.232764000	1.163813000	-3.114908000
H	2.841188000	0.654925000	-3.876203000
H	2.705822000	2.127105000	-2.889877000
H	1.241337000	1.359539000	-3.536634000
C	-1.587178000	-2.678900000	-2.030007000
H	-0.752067000	-3.309662000	-2.356603000
H	-1.896985000	-2.039021000	-2.859563000
H	-2.426543000	-3.329661000	-1.748578000
B	-1.984225000	-0.626936000	-0.578732000
O	-2.842754000	-0.685681000	0.531482000
O	-2.598724000	0.072546000	-1.628146000
C	-3.991959000	0.138907000	0.280492000
C	-3.987424000	0.256931000	-1.289153000
C	-5.214181000	-0.569498000	0.854030000
H	-6.132020000	-0.026600000	0.600669000
H	-5.133952000	-0.612921000	1.945432000
H	-5.296651000	-1.593400000	0.482080000
C	-3.807494000	1.470188000	1.008470000
H	-2.945976000	2.024240000	0.632801000

H	-3.635183000	1.271831000	2.071371000
H	-4.694180000	2.105938000	0.914348000
C	-4.453739000	1.602496000	-1.824571000
H	-5.491673000	1.795048000	-1.529913000
H	-4.402966000	1.601478000	-2.918466000
H	-3.832092000	2.424004000	-1.459380000
C	-4.763444000	-0.870525000	-1.972805000
H	-4.558776000	-0.836018000	-3.047715000
H	-5.843745000	-0.773058000	-1.821685000
H	-4.444137000	-1.849016000	-1.600902000
C	-0.572045000	1.903674000	-0.769202000
N	-0.311904000	0.511173000	-0.253992000
C	0.294704000	0.467176000	1.066771000
C	-0.447976000	0.052930000	2.174223000
C	0.144076000	-0.010035000	3.435783000
C	1.484748000	0.331217000	3.607640000
C	2.227860000	0.754110000	2.504257000
C	1.634920000	0.833141000	1.247696000
H	-1.480721000	-0.239953000	2.039247000
H	-0.448853000	-0.343749000	4.284269000
H	1.946941000	0.270201000	4.590164000
H	3.273073000	1.031579000	2.618393000
H	2.211566000	1.191119000	0.403964000
C	0.131649000	3.039449000	-0.074335000
C	-0.295350000	3.473435000	1.188190000
C	0.352876000	4.519003000	1.841280000
C	1.438471000	5.157422000	1.236281000
C	1.861536000	4.746459000	-0.027853000
C	1.208933000	3.695760000	-0.674906000
H	-1.123578000	2.966951000	1.676721000
H	0.014025000	4.833295000	2.825573000
H	1.947413000	5.971990000	1.745993000
H	2.699999000	5.241942000	-0.511805000
H	1.543625000	3.379597000	-1.657822000
H	-1.649537000	2.061150000	-0.722046000
H	-0.331207000	1.907900000	-1.837637000

7

E(B3PW91-D3) = -635.177233 au

E(DLPNO-CCSD(T)) = -633.978724 au

G_{cont} = 0.221847 au

G = -633.756877 au

C	-1.102793000	1.079517000	-0.065810000
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N	0.030432000	0.483573000	-0.076459000
C	1.263316000	1.239276000	-0.083500000
C	-2.323448000	0.222463000	-0.050636000
C	-3.562186000	0.718504000	0.382302000
C	-2.244824000	-1.118571000	-0.461041000
C	-4.688811000	-0.104963000	0.414555000
H	-3.655724000	1.748196000	0.716221000
C	-3.370075000	-1.936765000	-0.439347000
H	-1.287246000	-1.502648000	-0.799801000
C	-4.598238000	-1.433793000	0.000928000
H	-5.637743000	0.295130000	0.763459000
H	-3.291907000	-2.969853000	-0.769742000
H	-5.477307000	-2.073440000	0.018520000
C	-1.294992000	2.579523000	-0.047203000
H	-1.457581000	2.929593000	0.980989000
H	-0.422267000	3.106156000	-0.439724000
H	-2.165885000	2.876746000	-0.638863000
C	2.491173000	0.352834000	-0.013155000
C	3.754355000	0.924034000	-0.216054000
C	2.409448000	-1.012240000	0.273573000
C	4.911316000	0.150479000	-0.132929000
H	3.832749000	1.986725000	-0.443142000
C	3.567289000	-1.790344000	0.357342000
H	1.431025000	-1.457943000	0.425149000
C	4.821572000	-1.214159000	0.155106000
H	5.882934000	0.611412000	-0.295930000
H	3.486001000	-2.851836000	0.581011000
H	5.721783000	-1.820837000	0.219071000
H	1.332917000	1.860252000	-0.991629000
H	1.296613000	1.942559000	0.764845000

8

E(B3PW91-D3) = -1047.005747 au

E(DLPNO-CCSD(T)) = -1045.098016 au

G_{cont} = 0.409296023 au

G = -1044.68872 au

C	-0.838871000	0.912314000	0.985791000
N	-0.076886000	0.327784000	-0.130292000
C	-0.790124000	-0.425754000	-1.154052000
C	-2.078770000	1.624126000	0.465075000
C	-3.378666000	1.184071000	0.726202000
C	-1.907068000	2.755874000	-0.344331000
C	-4.482094000	1.856674000	0.192370000

H	-3.542573000	0.305116000	1.342591000
C	-3.001921000	3.430423000	-0.879157000
H	-0.896755000	3.097433000	-0.563078000
C	-4.298585000	2.980443000	-0.611879000
H	-5.486138000	1.496880000	0.405813000
H	-2.846464000	4.307374000	-1.503487000
H	-5.156528000	3.503783000	-1.027212000
B	1.330439000	0.344820000	-0.102210000
O	2.127603000	-0.225712000	-1.084019000
O	2.069329000	0.931489000	0.913610000
C	3.476011000	-0.234529000	-0.556827000
C	3.442359000	0.962070000	0.453415000
C	4.456548000	-0.071302000	-1.706226000
H	5.478980000	0.032929000	-1.325496000
H	4.420940000	-0.954663000	-2.352336000
H	4.217244000	0.803885000	-2.315170000
C	3.679066000	-1.584799000	0.130872000
H	3.477586000	-2.382943000	-0.590848000
H	4.704387000	-1.700561000	0.497382000
H	2.990724000	-1.704978000	0.974553000
C	4.365364000	0.810505000	1.651218000
H	5.406955000	0.718827000	1.322998000
H	4.286068000	1.693065000	2.294481000
H	4.106110000	-0.067721000	2.247570000
C	3.662765000	2.314833000	-0.223014000
H	3.417111000	3.110112000	0.487915000
H	4.703632000	2.441781000	-0.538614000
H	3.014947000	2.427927000	-1.098972000
H	-1.623787000	0.175632000	-1.536779000
H	-0.097252000	-0.576353000	-1.988190000
C	-1.310031000	-1.769575000	-0.684930000
C	-2.676811000	-2.057588000	-0.690484000
C	-0.416330000	-2.737908000	-0.211105000
C	-3.148642000	-3.286551000	-0.221394000
H	-3.379022000	-1.305374000	-1.044980000
C	-0.880779000	-3.965064000	0.257099000
H	0.648670000	-2.515507000	-0.201415000
C	-2.251751000	-4.242306000	0.256750000
H	-4.216513000	-3.493454000	-0.224169000
H	-0.175726000	-4.707779000	0.623934000
H	-2.615962000	-5.198010000	0.626299000
C	-1.101554000	-0.093456000	2.110287000
H	-1.593923000	0.397071000	2.958607000
H	-1.720897000	-0.933224000	1.783873000

H	-0.144791000	-0.499688000	2.453433000
H	-0.187168000	1.688635000	1.403590000

$TS_{2NP/1NP}^2$

E(B3PW91-D3) = -2094.260311au

E(DLPNO-CCSD(T)) = -2090.641542 au

$G_{cont} = 0.646027$ au

G = -2089.995515 au

P	0.679947000	-2.034716000	-1.699387000
N	-1.606037000	-1.504414000	-0.819122000
N	2.414330000	-2.134548000	-1.812996000
N	0.838028000	-2.450959000	-0.030993000
C	-1.541201000	-2.351246000	0.328628000
C	-0.284623000	-2.840230000	0.725013000
C	-0.177233000	-3.741391000	1.792805000
C	-1.314005000	-4.121398000	2.499204000
C	-2.565694000	-3.621785000	2.131667000
C	-2.671284000	-2.752541000	1.049702000
H	0.787563000	-4.170149000	2.044296000
H	-1.221216000	-4.821604000	3.325583000
H	-3.456647000	-3.914134000	2.681705000
H	-3.636201000	-2.352419000	0.760525000
C	3.058187000	-2.135075000	-0.591262000
C	2.136800000	-2.304526000	0.466834000
C	2.560723000	-2.196616000	1.791659000
C	3.917918000	-1.975597000	2.047728000
C	4.834591000	-1.853722000	1.000075000
C	4.411613000	-1.919807000	-0.330054000
H	1.850160000	-2.256851000	2.608701000
H	4.254272000	-1.886823000	3.077132000
H	5.885684000	-1.682604000	1.217476000
H	5.114025000	-1.772893000	-1.144773000
C	3.103676000	-1.750874000	-3.028966000
H	3.926412000	-2.444035000	-3.237758000
H	3.503611000	-0.730676000	-2.954372000
H	2.401267000	-1.792477000	-3.866793000
C	-2.417031000	-2.130212000	-1.877274000
H	-3.472696000	-2.226611000	-1.601679000
H	-2.031236000	-3.130784000	-2.104565000
H	-2.367300000	-1.521191000	-2.782339000
B	-2.026460000	0.014439000	-0.475487000
O	-2.775888000	0.092166000	0.760515000
O	-2.868534000	0.611268000	-1.492999000
C	-3.769491000	1.104354000	0.611098000

C	-4.113718000	1.001163000	-0.912361000
C	-4.925464000	0.793248000	1.553775000
H	-5.764116000	1.478623000	1.382171000
H	-4.595887000	0.910879000	2.592163000
H	-5.279654000	-0.233305000	1.428490000
C	-3.165601000	2.462102000	0.978512000
H	-2.377058000	2.735784000	0.275265000
H	-2.718234000	2.398800000	1.975955000
H	-3.921575000	3.255488000	0.985813000
C	-4.559581000	2.311574000	-1.553259000
H	-5.453543000	2.707106000	-1.056090000
H	-4.803282000	2.143108000	-2.608500000
H	-3.769424000	3.065454000	-1.506629000
C	-5.163449000	-0.076233000	-1.198614000
H	-5.181840000	-0.279733000	-2.274479000
H	-6.164841000	0.243493000	-0.888191000
H	-4.925788000	-1.008690000	-0.679661000
C	0.194999000	0.876312000	-1.407469000
N	-0.631253000	0.797626000	-0.331130000
C	-0.051604000	0.753437000	1.010860000
C	1.519589000	1.600687000	-1.304110000
C	1.673048000	2.824095000	-1.972729000
C	2.865203000	3.541053000	-1.888255000
C	3.935782000	3.040200000	-1.146216000
C	3.798133000	1.818258000	-0.488250000
C	2.600749000	1.112147000	-0.566632000
H	0.849246000	3.238682000	-2.546211000
H	2.955010000	4.494632000	-2.403035000
H	4.867166000	3.597386000	-1.082046000
H	4.618622000	1.406326000	0.093533000
H	2.515907000	0.172596000	-0.036030000
C	-0.444341000	0.996878000	-2.782076000
H	-1.147096000	0.188386000	-2.974119000
H	-1.013806000	1.927755000	-2.859383000
H	0.337274000	0.980174000	-3.546833000
H	-0.869839000	0.451658000	1.670370000
H	0.700686000	-0.044924000	1.078449000
C	0.546021000	2.028276000	1.568078000
C	1.380353000	1.926851000	2.688057000
C	0.278811000	3.294803000	1.047292000
C	1.928838000	3.064136000	3.278551000
H	1.612272000	0.942163000	3.092052000
C	0.829270000	4.436716000	1.630464000
H	-0.341959000	3.383735000	0.161543000

C	1.654539000	4.328132000	2.750407000
H	2.578003000	2.963408000	4.145579000
H	0.616959000	5.413859000	1.202206000
H	2.086133000	5.217738000	3.202998000
H	0.648828000	-0.439215000	-1.578000000

$TS_{2NP/3NP}^2$

E(B3PW91-D3) = -2094.234705 au

E(DLPNO-CCSD(T)) = -2090.614273 au

$G_{cont} = 0.642590$ au

G = -2089.971683 au

P	-1.732792000	-0.109222000	1.034391000
N	2.044029000	-0.875526000	-0.659069000
N	-1.546561000	1.501934000	1.514385000
N	-0.061896000	-0.383592000	1.291150000
C	1.586916000	-1.879437000	0.221184000
C	0.553009000	-1.659197000	1.155687000
C	0.118269000	-2.703279000	1.980015000
C	0.693160000	-3.966278000	1.898064000
C	1.735309000	-4.185716000	0.994891000
C	2.171618000	-3.153876000	0.171655000
H	-0.668215000	-2.505268000	2.703015000
H	0.340512000	-4.766274000	2.543119000
H	2.200487000	-5.165333000	0.921024000
H	2.969719000	-3.323608000	-0.544528000
C	-0.230373000	1.864221000	1.805828000
C	0.640916000	0.767154000	1.677525000
C	1.992479000	0.897400000	1.969467000
C	2.466074000	2.151776000	2.378316000
C	1.606325000	3.244671000	2.486368000
C	0.240407000	3.109571000	2.202922000
H	2.658466000	0.043015000	1.902083000
H	3.518279000	2.266210000	2.623160000
H	1.992181000	4.210564000	2.801552000
H	-0.436549000	3.953537000	2.295622000
C	-2.665600000	2.376182000	1.815329000
H	-2.664840000	2.639788000	2.879820000
H	-2.615551000	3.286071000	1.211711000
H	-3.597881000	1.858933000	1.578104000
C	1.072860000	-0.129242000	-1.449945000
H	0.723000000	0.770390000	-0.930692000
H	1.535565000	0.177928000	-2.390867000
H	0.212453000	-0.763142000	-1.673246000

B	3.421519000	-0.544918000	-0.759877000
O	4.418965000	-1.144078000	-0.017812000
O	3.887729000	0.428573000	-1.620074000
C	5.614926000	-0.350398000	-0.234160000
C	5.332994000	0.295680000	-1.632894000
C	6.825157000	-1.267183000	-0.184965000
H	7.733672000	-0.715238000	-0.451152000
H	6.949217000	-1.661681000	0.828843000
H	6.715054000	-2.113428000	-0.867375000
C	5.675670000	0.681788000	0.889794000
H	5.637981000	0.161645000	1.852278000
H	6.599513000	1.267790000	0.847157000
H	4.823705000	1.366305000	0.836927000
C	5.950142000	1.669070000	-1.836833000
H	7.040413000	1.615840000	-1.740807000
H	5.712810000	2.036293000	-2.840608000
H	5.567842000	2.391870000	-1.112156000
C	5.687571000	-0.628944000	-2.796579000
H	5.275530000	-0.210580000	-3.720235000
H	6.771699000	-0.727175000	-2.914060000
H	5.259351000	-1.626935000	-2.653432000
C	-2.829785000	-1.701006000	-0.498517000
N	-2.366534000	-0.344243000	-0.465178000
C	-2.448536000	0.515723000	-1.662457000
C	-4.255704000	-1.867123000	-0.498106000
C	-5.131161000	-0.811988000	-0.113733000
C	-6.511007000	-0.987193000	-0.056742000
C	-7.095111000	-2.214105000	-0.384616000
C	-6.255755000	-3.266092000	-0.775548000
C	-4.876996000	-3.102746000	-0.837033000
H	-4.709841000	0.154041000	0.148117000
H	-7.139560000	-0.150720000	0.245911000
H	-8.173350000	-2.347149000	-0.345687000
H	-6.686929000	-4.229183000	-1.044569000
H	-4.262572000	-3.942207000	-1.151533000
C	-1.921367000	-2.753501000	-1.075064000
H	-0.869967000	-2.501158000	-0.913115000
H	-2.076337000	-3.731628000	-0.600733000
H	-2.059671000	-2.900928000	-2.162987000
H	-1.560766000	0.346552000	-2.284348000
H	-3.307950000	0.130165000	-2.220363000
C	-2.628789000	1.995921000	-1.431339000
C	-3.914531000	2.541935000	-1.336577000
C	-1.527319000	2.855763000	-1.351899000

C	-4.096811000	3.914384000	-1.163358000
H	-4.778822000	1.885219000	-1.411495000
C	-1.702488000	4.227151000	-1.168191000
H	-0.521805000	2.450957000	-1.431580000
C	-2.990128000	4.761713000	-1.076844000
H	-5.102837000	4.322195000	-1.100778000
H	-0.833646000	4.877372000	-1.101473000
H	-3.129278000	5.831548000	-0.941813000
H	-2.387657000	-1.322424000	1.458922000

3NP²

E(B3PW91-D3) = -2094.318633 au

E(DLPNO-CCSD(T)) = -2090.711381 au

G_{cont} = 0.647707 au

G = -2090.063674 au

P	-1.586259000	-0.497957000	1.628699000
N	2.326480000	-0.961956000	-0.529746000
N	-1.666729000	1.205251000	1.831847000
N	0.162723000	-0.325845000	1.415677000
C	2.041125000	-1.754608000	0.602974000
C	1.005979000	-1.462326000	1.524863000
C	0.793831000	-2.337603000	2.603833000
C	1.576254000	-3.469542000	2.796894000
C	2.614767000	-3.742903000	1.904874000
C	2.832221000	-2.893920000	0.827261000
H	0.007694000	-2.095488000	3.313386000
H	1.387839000	-4.119519000	3.647489000
H	3.244458000	-4.618852000	2.038860000
H	3.624594000	-3.108393000	0.116346000
C	-0.467966000	1.883053000	1.669345000
C	0.613666000	0.998129000	1.455666000
C	1.914083000	1.486392000	1.395863000
C	2.123926000	2.872015000	1.485744000
C	1.051814000	3.747276000	1.642731000
C	-0.258918000	3.256217000	1.745608000
H	2.753529000	0.805377000	1.314398000
H	3.138941000	3.258573000	1.445020000
H	1.226475000	4.818527000	1.705430000
H	-1.096297000	3.931604000	1.894059000
C	-2.864678000	1.876122000	2.290688000
H	-2.696236000	2.348605000	3.268306000
H	-3.187768000	2.639045000	1.573971000
H	-3.671554000	1.144721000	2.384407000

C	1.241511000	-0.538149000	-1.405072000
H	0.936274000	0.493528000	-1.194421000
H	1.568816000	-0.592323000	-2.447482000
H	0.383499000	-1.198352000	-1.273727000
B	3.635808000	-0.488569000	-0.805245000
O	4.736812000	-0.715303000	-0.003451000
O	3.917924000	0.284187000	-1.914910000
C	5.775074000	0.176919000	-0.484041000
C	5.363397000	0.385767000	-1.980555000
C	7.125352000	-0.488351000	-0.278643000
H	7.921415000	0.115646000	-0.728581000
H	7.331601000	-0.583195000	0.792488000
H	7.150886000	-1.488186000	-0.718869000
C	5.678332000	1.460295000	0.339202000
H	5.744475000	1.206596000	1.401797000
H	6.488566000	2.155297000	0.095794000
H	4.722469000	1.964809000	0.167102000
C	5.734512000	1.740626000	-2.560006000
H	6.819340000	1.889821000	-2.518444000
H	5.421755000	1.793576000	-3.607971000
H	5.246325000	2.554782000	-2.019101000
C	5.851030000	-0.738680000	-2.893189000
H	5.357496000	-0.645001000	-3.865668000
H	6.933861000	-0.688588000	-3.047687000
H	5.601783000	-1.720806000	-2.477142000
C	-2.803463000	-2.085021000	-0.158590000
N	-2.298306000	-0.722732000	0.105468000
C	-2.125442000	0.206783000	-1.014822000
C	-4.226757000	-2.032068000	-0.683450000
C	-5.273560000	-1.867819000	0.233777000
C	-6.591132000	-1.729303000	-0.197031000
C	-6.884080000	-1.746808000	-1.563670000
C	-5.852245000	-1.919866000	-2.485715000
C	-4.534008000	-2.068978000	-2.046823000
H	-5.043728000	-1.826741000	1.297152000
H	-7.388982000	-1.602034000	0.530887000
H	-7.909764000	-1.630967000	-1.905216000
H	-6.070552000	-1.939235000	-3.550821000
H	-3.745491000	-2.210499000	-2.781437000
C	-1.840315000	-2.920583000	-1.003628000
H	-0.890941000	-3.034529000	-0.469366000
H	-2.256610000	-3.916933000	-1.190583000
H	-1.625201000	-2.460299000	-1.974441000
H	-1.072438000	0.483738000	-1.099748000

H	-2.381012000	-0.323184000	-1.939272000
C	-2.941843000	1.478855000	-0.938777000
C	-4.332803000	1.455959000	-0.786047000
C	-2.298759000	2.716134000	-1.047360000
C	-5.061707000	2.643650000	-0.738185000
H	-4.847053000	0.505002000	-0.692514000
C	-3.024086000	3.908025000	-0.996888000
H	-1.215333000	2.750505000	-1.139135000
C	-4.410760000	3.875967000	-0.842605000
H	-6.142030000	2.606345000	-0.616799000
H	-2.502302000	4.859684000	-1.067209000
H	-4.979388000	4.801910000	-0.799400000
H	-2.847750000	-2.556418000	0.832697000

$TS_{3NP/1NP}^2$

$E(B3PW91-D3) = -2094.261602$ au

$E(DLPNO-CCSD(T)) = -2090.653885$ au

$G_{cont} = 0.654033$ au

$G = -2089.999852$ au

P	1.304946000	-0.908978000	-1.389836000
N	-0.053208000	-2.344363000	-0.421306000
N	2.569292000	0.278178000	-1.767437000
N	2.336699000	-1.402345000	-0.007445000
C	0.476074000	-2.583452000	0.878686000
C	1.776608000	-2.088730000	1.080665000
C	2.329156000	-2.199070000	2.367109000
C	1.617597000	-2.842536000	3.380489000
C	0.346266000	-3.368687000	3.154206000
C	-0.229989000	-3.218483000	1.892957000
H	3.279650000	-1.745897000	2.609329000
H	2.067623000	-2.913171000	4.367820000
H	-0.197953000	-3.866228000	3.952224000
H	-1.238720000	-3.562486000	1.687994000
C	3.703182000	0.210003000	-0.980361000
C	3.608584000	-0.800433000	0.000685000
C	4.744405000	-1.150967000	0.729100000
C	5.932649000	-0.426967000	0.552216000
C	5.997666000	0.618463000	-0.364854000
C	4.883258000	0.932335000	-1.152203000
H	4.744413000	-2.007528000	1.391243000
H	6.809124000	-0.702447000	1.132807000
H	6.920790000	1.178076000	-0.493258000
H	4.937907000	1.716417000	-1.902092000

C	2.692840000	0.756111000	-3.133360000
H	3.608364000	0.369439000	-3.602958000
H	2.712988000	1.852890000	-3.185553000
H	1.832589000	0.405741000	-3.714484000
C	0.025954000	-3.537645000	-1.277851000
H	1.072095000	-3.857994000	-1.350841000
H	-0.346020000	-3.291903000	-2.273247000
H	-0.562601000	-4.364082000	-0.863866000
B	-1.275428000	-1.442991000	-0.543567000
O	-2.182043000	-1.396633000	0.526058000
O	-1.971594000	-1.541576000	-1.759050000
C	-3.522936000	-1.375637000	-0.008819000
C	-3.314349000	-1.961765000	-1.447667000
C	-4.405651000	-2.211737000	0.907702000
H	-5.410887000	-2.318632000	0.483903000
H	-4.496274000	-1.716433000	1.880410000
H	-3.986854000	-3.207060000	1.074691000
C	-4.036671000	0.058293000	-0.044759000
H	-3.432809000	0.654852000	-0.728522000
H	-3.974370000	0.508894000	0.948735000
H	-5.078987000	0.096896000	-0.378191000
C	-4.258108000	-1.420872000	-2.512324000
H	-5.298824000	-1.650463000	-2.256348000
H	-4.031540000	-1.891843000	-3.474763000
H	-4.159442000	-0.340433000	-2.636206000
C	-3.356974000	-3.491401000	-1.464637000
H	-2.975912000	-3.849680000	-2.425912000
H	-4.379631000	-3.861928000	-1.336039000
H	-2.735527000	-3.916957000	-0.671859000
C	-0.224629000	1.359744000	-1.605899000
N	-0.060727000	0.221005000	-0.610355000
C	0.480395000	0.736793000	0.693810000
C	-0.602275000	2.726323000	-1.059961000
C	-1.882421000	3.057157000	-0.603657000
C	-2.178259000	4.346574000	-0.171603000
C	-1.200188000	5.343086000	-0.206270000
C	0.074426000	5.035443000	-0.678502000
C	0.364800000	3.737206000	-1.100412000
H	-2.647532000	2.294695000	-0.547004000
H	-3.173319000	4.571577000	0.204373000
H	-1.431318000	6.349143000	0.135494000
H	0.846205000	5.801001000	-0.712582000
H	1.367291000	3.499921000	-1.452571000
H	1.408461000	1.284420000	0.476980000

H	0.758842000	-0.133471000	1.283041000
C	-0.369284000	1.588749000	1.614443000
C	0.111128000	2.834431000	2.034422000
C	-1.552039000	1.105233000	2.181490000
C	-0.599611000	3.605923000	2.951925000
H	1.035640000	3.220656000	1.612958000
C	-2.269998000	1.876276000	3.094787000
H	-1.903456000	0.121822000	1.892713000
C	-1.803120000	3.134866000	3.478678000
H	-0.217979000	4.581308000	3.244693000
H	-3.194964000	1.486811000	3.516036000
H	-2.365407000	3.737986000	4.188036000
C	-1.105464000	0.996068000	-2.797174000
H	-1.028184000	1.799229000	-3.538832000
H	-0.793034000	0.055387000	-3.257147000
H	-2.152775000	0.885788000	-2.512986000
H	0.781857000	1.529485000	-1.991456000