

Supporting Information for

Hydroxide Anion Attack Governs O–O Bond Formation in Water Oxidation Catalysed by a Mononuclear Manganese Complex

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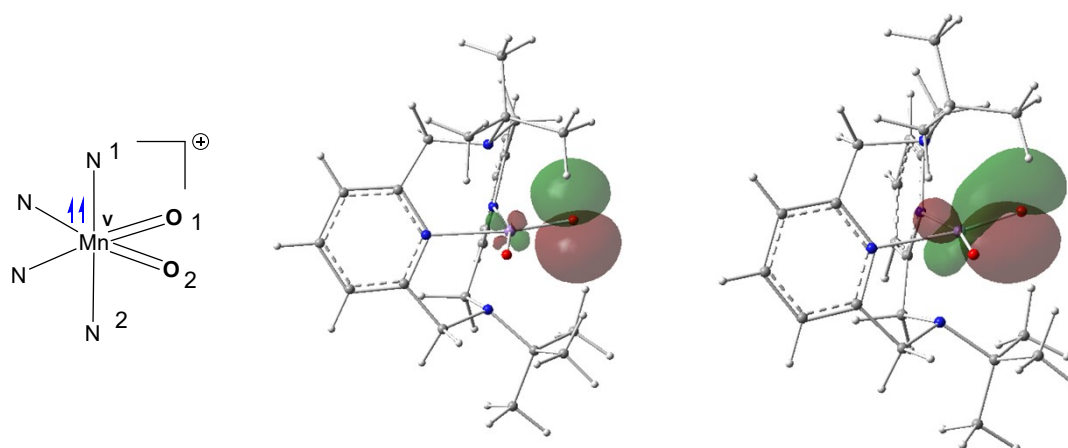


Fig. S1 Spatial plots for the α (left) and β (right) orbitals corresponding to the d_{π} - p_{π} interaction between Mn and O1 in **32**. In the α manifold, no significant interaction is observed apart from a slight antibonding character, because the Mn α d_{π} orbitals are only partially occupied and therefore do not interact effectively with the p_{π} α lone pair on O1. In contrast, in the β manifold, the Mn β d_{π} orbitals are empty and can interact effectively with the p_{π} β lone pair on O1, leading to a clear bonding interaction.

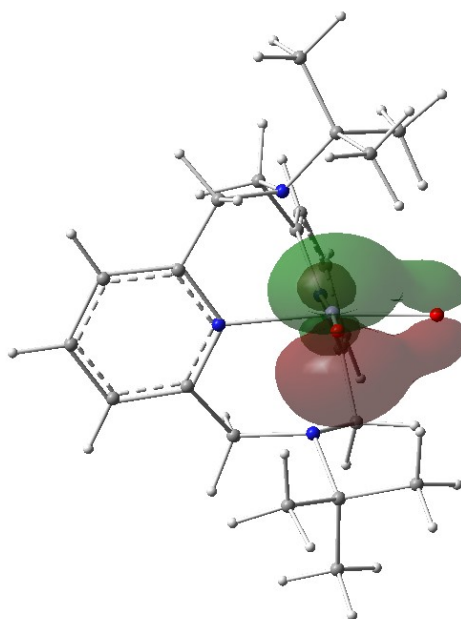


Fig. S2 Spatial plot of the NLMO orbital in **72** showing the π interaction between a β lone pair on O1 and a partially α -occupied orbital centred on O2, consistent with formation of a two-centre three-electron ($2c-3e$) bond between O1 and O2.

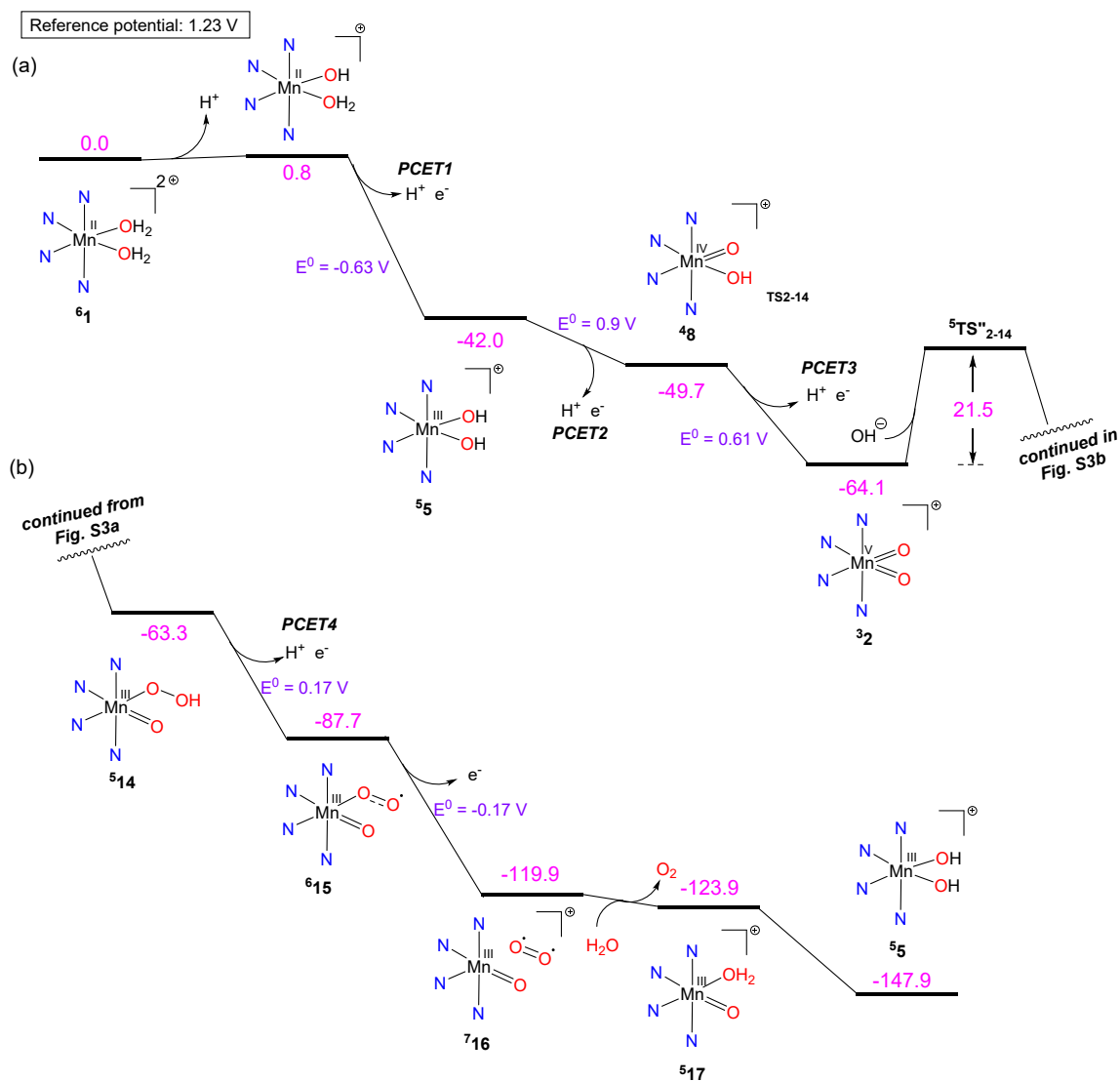


Fig. S3 Free-energy profile for the catalytic cycle shown in Fig. 8, calculated at the SMD/M06-L-D3/def2-TZVP level of theory under an applied potential of 1.23 V and pH 12.2. The relative free energies are given in kcal/mol.

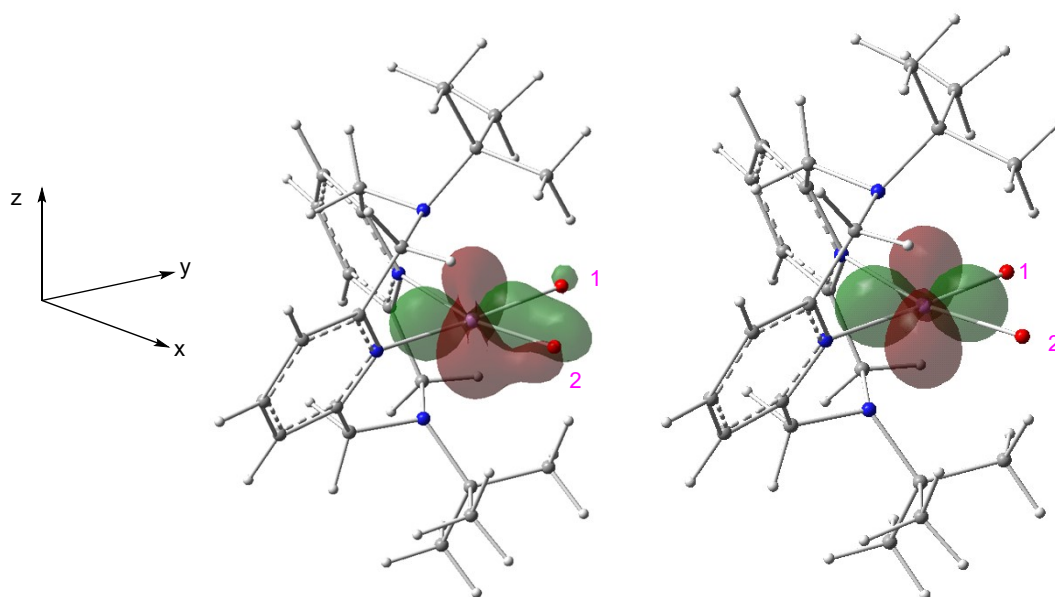


Fig. S4 Spatial plots of the NLMOs corresponding to the Mn d_{xy} orbital with d_{π} character in ${}^5\text{TS}_{2-3}$ (left) and ${}^7\mathbf{2}$ (right). In ${}^5\text{TS}_{2-3}$, antiferromagnetic coupling enables π back-donation from a Mn d_{π} orbital into the vacant α -spin p_{π} orbital of O2. In this transition structure, the unpaired electron on O2 has β spin, whereas the unpaired electrons on the Mn centre are α spin. Consequently, the α -spin p_{π} orbital on O2 remains vacant and is therefore available for interaction with an occupied Mn d_{π} orbital. In contrast, in the ferromagnetically coupled intermediate ${}^7\mathbf{2}$, such interaction is not possible because the relevant orbitals have parallel spin alignment. This interpretation is fully supported by the NLMO analysis of ${}^5\text{TS}_{2-3}$ (left orbital), which shows strong interaction between the Mn d_{xy} orbital and the vacant α -spin p_{π} orbital on O2, with a second-order perturbation stabilisation energy E^2 of 31.9 kcal/mol. By contrast, the corresponding Mn d_{xy} orbital in ${}^7\mathbf{2}$ (right orbital) remains completely nonbonding and cannot participate in π back-donation to the oxyl ligands because of the parallel spin alignment.

Origin of the Energy Difference Between ${}^5\text{TS}_{2-14}$ and ${}^3\text{TS}_{2-14}$. The large difference between the barriers on the quintet and triplet surfaces can be rationalised by the substantially different stability of the resulting Mn(III) hydroperoxide intermediates, consistent with the Hammond postulate, which states that the energy of a transition state generally reflects the stability of the species formed immediately after the transition state along the reaction coordinate. In the case of the triplet surface, O–O coupling leads to the highly unstable low-spin Mn(III) intermediate ${}^3\mathbf{14}$, which lies 31.9 kcal/mol above ${}^3\mathbf{2}$. Consequently, the corresponding transition structure ${}^3\text{TS}_{2-14}$ is also strongly destabilised and exhibits late transition-state character, with a very short O1–O3 distance of 1.59 Å. In contrast, on the quintet surface, the much greater stability of

the high-spin Mn(III) hydroperoxide intermediate **514**, which lies 1.7 kcal/mol below **32**, stabilises **⁵TS₂₋₁₄**, which correspondingly exhibits early transition-state character with a relatively long O1–O3 distance of 1.93 Å. Thus, consistent with the Hammond postulate, the transition structure on the quintet surface (**⁵TS₂₋₁₄**) is substantially lower in energy than that on the triplet surface (**³TS₂₋₁₄**).

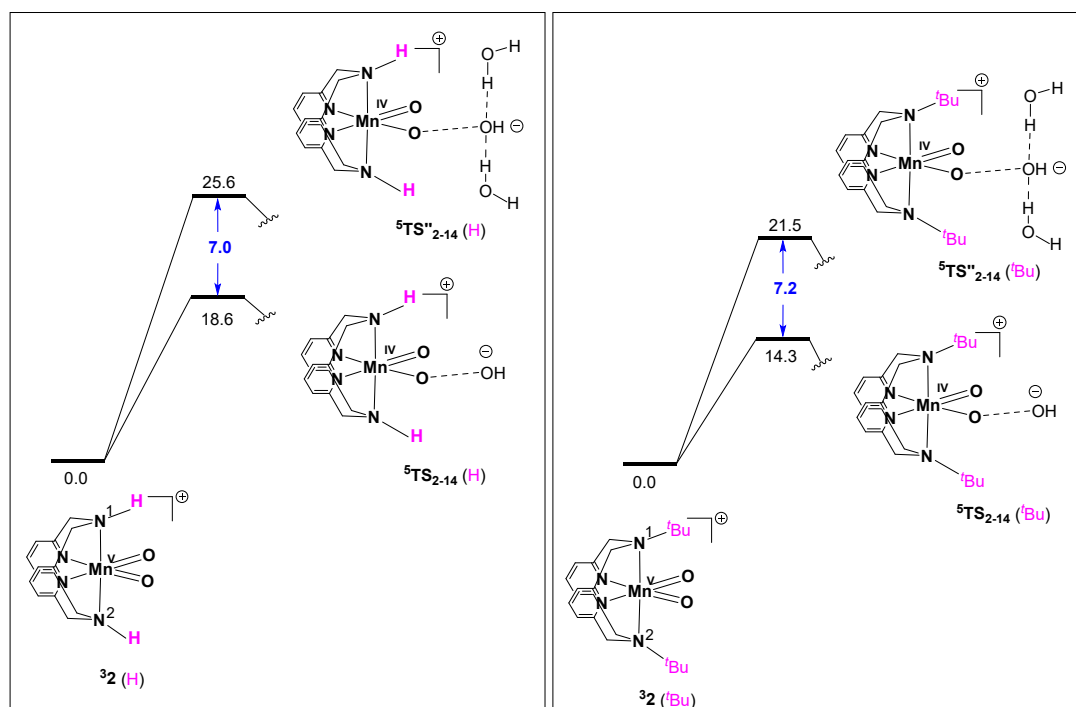


Fig. S5 Comparison of the O–O coupling transition structures for OH[−] and (H₂O)₂OH[−] attack calculated using the original ^tBu-substituted ligand system and the sterically less demanding H-substituted model. To examine whether steric effects have any significant contribution to the increased barrier for (H₂O)₂OH[−] attack relative to OH[−] attack, additional calculations were performed in which the bulky ^tBu substituents of the ligand were replaced by H atoms, thereby minimising steric interactions around the Mn centre. The calculated energy difference between **⁵TS₂₋₁₄(H)** and **⁵TS''₂₋₁₄(H)** is 7.0 kcal/mol, which is very similar to the corresponding difference between **⁵TS₂₋₁₄(^tBu)** and **⁵TS''₂₋₁₄(^tBu)**. This result shows that steric effects contribute insignificantly to the barrier increase upon going from OH[−] to (H₂O)₂OH[−]. Therefore, the reactivity trend is controlled predominantly by the electronic properties of the nucleophile, especially the stabilisation of the hydroxide HOMO through hydrogen bonding, which reduces its nucleophilicity and increases the O–O coupling barrier.

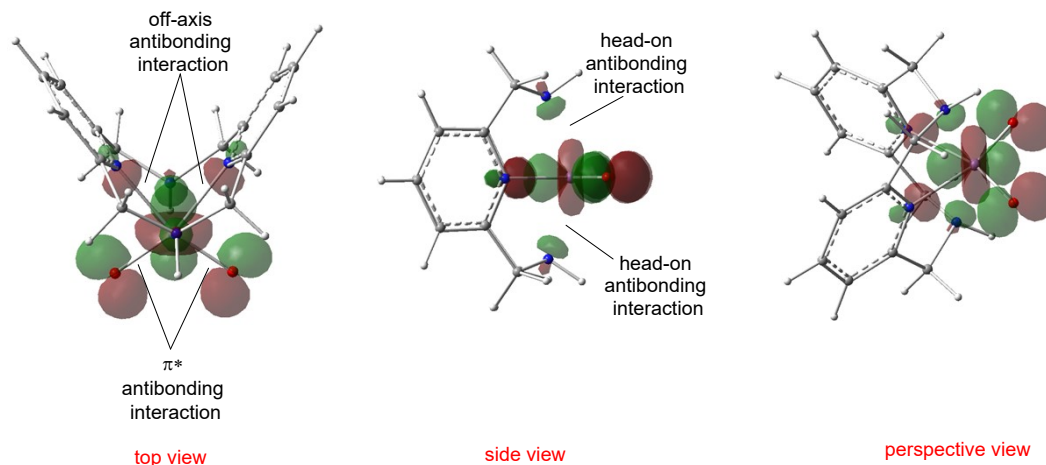


Fig. S6 Top, side, and perspective views of the hybridised Mn d_z^2 orbital in the LUMO of **32**. The orbital shown in this figure a hybridised orbital with predominant Mn d_z^2 character. This hybridised d_z^2 orbital exhibits antibonding interactions with all ligands in the LUMO of **32**. However, the strongest antibonding interactions occur with the axial N1 and N2 donor atoms because they interact with the Mn d_z^2 orbital in a direct head-on fashion. In contrast, antibonding interactions with the remaining N donor atoms are off-axis in nature and therefore considerably weaker. The antibonding interactions with the oxo ligands are primarily π^* -type. Consequently, the energy of this empty d_z^2 orbital is governed primarily by the extent of the axial Mn–N1 and Mn–N2 σ^* -antibonding interactions. The stronger the σ -donor ability of N1 and N2, the greater the σ^* -antibonding interaction and, consequently, the higher the energy of the d_z^2 orbital. Since the X substituents influence the donor ability of the N1 and N2 atoms, they directly modulate the energy of this d_z^2 orbital. Because this hybridised d_z^2 orbital acts as the primary acceptor orbital for the electron transferred during the interaction between OH^- and the oxyl radical ligand in the O–O coupling step, lowering its energy increases the oxidising capability of the Mn centre and facilitates this electron-transfer process. Consequently, the lower the energy of this d_z^2 orbital, the lower the barrier to O–O coupling.

Effect of Hydroxide Solvation Cluster Size on the FHNA Barrier. To assess the effect of larger hydroxide solvation clusters, additional calculations were performed using $(\text{H}_2\text{O})_4\text{OH}^-$. The calculated HOMO energy of this species is -5.49 eV, which is very similar to that of $(\text{H}_2\text{O})_2\text{OH}^-$ (-5.47 eV). Therefore, the nucleophilicity of $(\text{H}_2\text{O})_4\text{OH}^-$ is expected to be very similar to that of $(\text{H}_2\text{O})_2\text{OH}^-$, and consequently the corresponding O–O coupling barriers should also be comparable. Indeed, our calculations show that O–O bond formation via the FHNA mechanism proceeds through transition structure ${}^5\text{TS}''_{2-14}$ with an activation free energy of 20.0 kcal/mol, 1.5 kcal/mol lower than that calculated for $(\text{H}_2\text{O})_2\text{OH}^-$ (21.5 kcal/mol). The lower barrier obtained for $(\text{H}_2\text{O})_4\text{OH}^-$ appears to arise from the greater conformational flexibility of the larger water cluster, which can reorganise during the O–O coupling process and form additional hydrogen-bonding interactions with the oxo ligand, thereby

providing extra stabilisation of the transition structure. It should also be noted that numerous previous benchmark studies have shown that the combination of an implicit solvation model with two explicit water molecules provides one of the most reliable descriptions of the solvation of anions in aqueous solution (ref 12). The very similar HOMO energies and activation barriers obtained for $(\text{H}_2\text{O})_2\text{OH}^-$ and $(\text{H}_2\text{O})_4\text{OH}^-$ therefore suggest that the mechanistic conclusions should not be sensitive to the size of the hydroxide solvation cluster.

Table S1. Cartesian coordinates for all optimised structures, together with total potential energies, enthalpies, and Gibbs free energies calculated at the SMD/M06-L-D3/def2-TZVP level of theory, and single-point potential energies obtained at the SMD/B3LYP*-D3/ def2-TZVP// SMD/M06-L-D3/def2-TZVP level in water.

32

E (SMD/M06-L-D3/def2-TZVP) = -2378.273456 au
H (SMD/M06-L-D3/def2-TZVP) = -2377.722901 au
G (SMD/M06-L-D3/def2-TZVP) = -2377.802912 au
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N -2.39811500 0.69668600 0.96787500
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O -1.11952700 -1.01107100 -1.01724400
O -0.19614500 1.52591100 -1.08140800
N -0.58283200 -1.11713400 1.47640300
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C 1.79263600 -1.07106600 1.45145700
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32'

E (SMD/M06-L-D3/def2-TZVP) = -2454.739426 au
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³TS₂₋₁₃

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³13

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G (SMD/M06-L-D3/def2-TZVP) = -2454.225818 au

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C -0.36069300 1.74353600 2.26351800

C -1.67237100 1.04694500 2.36028300

H -3.38163500 -0.93987100 2.18451200

H -3.00659900 -1.46883500 0.54785100

H 2.97304100 -1.99981900 1.58927400

H 2.31454700 -0.59147200 2.35835500

H 3.62781800 0.65709300 0.75947100

H 2.62943500 1.19629600 -0.58706000

H -2.45966600 1.72054100 2.69084300

H -1.57681400 0.29806300 3.14933200

C 2.63367600 -1.45462500 -0.85708000

C -3.11124100 1.17524300 0.31485600
C -4.44219700 1.18141400 1.06079800
C -3.31932800 0.58721200 -1.06815500
C -2.57971200 2.59403500 0.17442300
C 2.24360900 -0.88565500 -2.20797700
C 2.11480100 -2.88246000 -0.76417200
C 4.15249400 -1.43742200 -0.71688300
H -4.35110400 1.49684900 2.09918400
H -5.10454900 1.88875400 0.56439900
H -4.92782900 0.20732400 1.03567800
H -2.41603900 0.65168700 -1.66799400
H -3.65323900 -0.44872500 -1.04362400
H -4.09922900 1.16389100 -1.56420500
H -3.22993100 3.13962900 -0.50705700
H -2.57233100 3.14068600 1.11628500
H -1.57519700 2.59768000 -0.24812000
H 1.18422400 -1.03279600 -2.39830400
H 2.47596500 0.17312400 -2.31090000
H 2.80273700 -1.41801700 -2.97640800
H 2.50846900 -3.42530600 0.09352300
H 1.02599400 -2.90548800 -0.73153900
H 2.43111600 -3.42079300 -1.65586400
H 4.49048700 -1.73531600 0.27484500
H 4.56774400 -2.14905000 -1.42855100
H 4.57354100 -0.46046200 -0.94845100
O -0.76318100 0.29905700 -3.19050400
H 0.17055200 0.46677300 -3.36588700
H -0.91745200 -0.92913300 -1.92404800

³TS₁₃₋₉

E (SMD/M06-L-D3/def2-TZVP) = -2454.691386 au
H (SMD/M06-L-D3/def2-TZVP) = -2454.115749 au
G (SMD/M06-L-D3/def2-TZVP) = -2454.200094 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2454.005923 au
Mn -0.15994100 -0.14649400 0.08529500
N -2.06202300 0.33824600 1.09033000
N 1.97737800 -0.62935500 0.27174300
O -0.90364300 -1.42416800 -1.06947600
O 0.06230400 1.16855700 -1.14727000
N -0.25518800 -1.49070100 1.54929400
C 0.86851600 -2.05907200 1.99473300
C 2.11297800 -1.34455300 1.58678000
C 0.80697400 -3.13389300 2.86184100

H 1.71716800 -3.60389700 3.20746800
C -0.43999900 -3.56956500 3.28742300
H -0.51419100 -4.40717800 3.96786600
C -1.58973400 -2.91309000 2.87179400
H -2.56645900 -3.20454800 3.23183600
C -1.46353100 -1.86126400 1.98361800
C -2.58069800 -1.01415300 1.46460000
N 0.49824900 1.20300800 1.38476000
C 1.78492200 1.56740300 1.32479200
C 2.60395900 0.72343500 0.40267900
C 2.25024600 2.60975700 2.10210500
H 3.29239500 2.89364200 2.05825700
C 1.35386300 3.26992000 2.93223000
H 1.68924100 4.10357600 3.53417000
C 0.03763500 2.83931200 3.01791900
H -0.66640700 3.30845000 3.69116400
C -0.36142500 1.76994500 2.23753200
C -1.66864800 1.06059200 2.34885900
H -3.36717200 -0.93200600 2.21743800
H -3.02001000 -1.47311900 0.58028000
H 2.97976600 -2.00227400 1.58981500
H 2.31144700 -0.59860800 2.35920000
H 3.62669600 0.64326600 0.77528900
H 2.64833700 1.18025800 -0.58529800
H -2.46171000 1.72560500 2.68426700
H -1.55564100 0.31917600 3.14258700
C 2.62487600 -1.45164300 -0.85692700
C -3.11425400 1.15280800 0.31182000
C -4.44811700 1.14872200 1.05240100
C -3.31341200 0.55771500 -1.07043200
C -2.60698900 2.58070400 0.16362500
C 2.21522100 -0.87860900 -2.20099700
C 2.11902500 -2.88474600 -0.76700400
C 4.14461200 -1.42801700 -0.73512100
H -4.36092800 1.46744000 2.09038200
H -5.11778200 1.84828000 0.55450300
H -4.92518500 0.17019000 1.03067400
H -2.41294500 0.63445500 -1.67161600
H -3.62884300 -0.48374700 -1.04349600
H -4.10233000 1.11958800 -1.56965600
H -3.26725100 3.11153100 -0.52024200
H -2.61033100 3.13191800 1.10290500
H -1.60256800 2.60144800 -0.25726400
H 1.15317600 -1.03323100 -2.37532000

H 2.44523100 0.18187400 -2.30001000
H 2.76410900 -1.40241100 -2.98252500
H 2.52575000 -3.42681200 0.08517000
H 1.03105900 -2.91763200 -0.72437100
H 2.43247600 -3.41707200 -1.66353300
H 4.49369900 -1.72920600 0.25200500
H 4.55713900 -2.13410600 -1.45405500
H 4.55966100 -0.44815200 -0.96554500
O -0.41238100 0.91525600 -2.62781100
H 0.45466900 0.79372900 -3.04111100
H -0.96975100 -0.95443100 -1.91404000

³g

E (SMD/M06-L-D3/def2-TZVP) = -2454.691499 au
H (SMD/M06-L-D3/def2-TZVP) = -2454.114538 au
G (SMD/M06-L-D3/def2-TZVP) = -2454.19918 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2454.007214 au
Mn -0.12523000 -0.14324000 0.09855900
N -2.03500900 0.34197200 1.06686200
N 2.00900200 -0.63338600 0.29447100
O -0.87676800 -1.39325400 -1.09191200
O 0.09181800 1.22717500 -1.14440700
N -0.23966400 -1.50333000 1.52261000
C 0.87649500 -2.07197900 1.99143300
C 2.12673600 -1.35491400 1.60709900
C 0.79960300 -3.14418000 2.85900900
H 1.70475900 -3.61223000 3.22046300
C -0.45415400 -3.58045200 3.26639700
H -0.53956600 -4.41722900 3.94636200
C -1.59517100 -2.92001700 2.83367900
H -2.57793800 -3.20625400 3.18157800
C -1.45528500 -1.86943800 1.94612200
C -2.56318300 -1.01388100 1.42209000
N 0.51907500 1.19889400 1.39464200
C 1.80695600 1.56395900 1.34715600
C 2.63819000 0.71765400 0.43763400
C 2.26357400 2.60756400 2.12903700
H 3.30602600 2.89193200 2.09470900
C 1.36043800 3.26636400 2.95203200
H 1.68982200 4.09950700 3.55790500
C 0.04293700 2.83329600 3.02625300
H -0.66717300 3.30037200 3.69461200
C -0.34834100 1.76587300 2.24153900

C -1.65482900 1.05246400 2.33673100
H -3.35809200 -0.93638500 2.16649800
H -2.99297700 -1.45952100 0.52649500
H 2.99388300 -2.01240700 1.62021100
H 2.31282300 -0.61219000 2.38558000
H 3.65481300 0.63439600 0.82651800
H 2.70034700 1.17316800 -0.54996800
H -2.45225100 1.71183200 2.67288600
H -1.54571000 0.30219600 3.12254100
C 2.66465700 -1.45256100 -0.83115500
C -3.07945500 1.16514100 0.28614000
C -4.42073500 1.15592100 1.01373700
C -3.27048500 0.58312500 -1.10269100
C -2.57155200 2.59448400 0.15546900
C 2.28392300 -0.85893900 -2.17357900
C 2.13815400 -2.87917200 -0.76076200
C 4.18262200 -1.44948100 -0.68583800
H -4.34292400 1.46418100 2.05553800
H -5.08422400 1.86179300 0.51644400
H -4.89943300 0.17866800 0.97752900
H -2.36328800 0.65301000 -1.69468100
H -3.59516700 -0.45557700 -1.08879800
H -4.04769900 1.15706000 -1.60629900
H -3.22916200 3.13244900 -0.52549400
H -2.58038000 3.13519500 1.10077600
H -1.56477200 2.62000500 -0.25957400
H 1.21620400 -0.94926900 -2.35051600
H 2.56555300 0.18814400 -2.27061000
H 2.80770600 -1.40861500 -2.95484800
H 2.51599600 -3.43054300 0.09886300
H 1.04910600 -2.89758500 -0.74451100
H 2.46634500 -3.41205800 -1.65169000
H 4.51505600 -1.77149200 0.30040400
H 4.59793800 -2.14752200 -1.41112600
H 4.61195700 -0.47058400 -0.89333800
O -0.17293700 0.92624900 -2.58177600
H -0.84541700 1.59763100 -2.77035100
H -0.97288200 -0.90339200 -1.92086000

52

E (SMD/M06-L-D3/def2-TZVP) = -2378.256883 au

H (SMD/M06-L-D3/def2-TZVP) = -2377.707536 au

G (SMD/M06-L-D3/def2-TZVP) = -2377.789472 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2377.580783 au
Mn -0.47910300 0.22064900 -0.02293500
N -2.38208900 0.68253400 0.96565800
N 1.65378700 -0.27440300 0.17471900
O -1.08595300 -0.87286700 -1.24515300
O -0.36449200 1.37845000 -1.33146700
N -0.59644400 -1.16568200 1.43158600
C 0.52260400 -1.74755800 1.86241200
C 1.77444200 -1.03671900 1.47006600
C 0.44559900 -2.84180200 2.70537600
H 1.34706900 -3.32985800 3.04810300
C -0.80970100 -3.27429900 3.10761800
H -0.89524100 -4.12641000 3.76866500
C -1.95539500 -2.60756400 2.69580200
H -2.93607400 -2.90776000 3.03659800
C -1.81347000 -1.53553000 1.83488800
C -2.91393800 -0.67695500 1.29755200
N 0.17845600 1.53331800 1.35341900
C 1.46303200 1.89081700 1.30501200
C 2.28283700 1.07185000 0.35913400
C 1.92165400 2.91400100 2.11322600
H 2.96259200 3.20336800 2.08952700
C 1.01343700 3.54496800 2.95226000
H 1.34459300 4.35884500 3.58340700
C -0.30682600 3.12324600 3.01340300
H -1.01481600 3.58109300 3.68973300
C -0.69863500 2.07773600 2.19656600
C -2.01504000 1.37727600 2.25175200
H -3.72756900 -0.60978900 2.02210200
H -3.31884800 -1.11961200 0.38768500
H 2.62840800 -1.71001000 1.44998500
H 1.98836600 -0.31978900 2.26582700
H 3.30402000 0.97725800 0.73223800
H 2.33154200 1.56367800 -0.61228900
H -2.81040200 2.04492000 2.57497000
H -1.93414700 0.61957800 3.03421300
C 2.31276500 -1.06450100 -0.97603200
C -3.40839500 1.52511300 0.17626500
C -4.75718800 1.51877000 0.88927800
C -3.58983500 0.96295200 -1.22347300
C -2.87941400 2.94883800 0.07429600
C 1.97973000 -0.42202500 -2.31153600
C 1.76297200 -2.48363200 -0.95659700
C 3.82848300 -1.08842300 -0.80360600

H -4.68870800 1.80834000 1.93696400
H -5.40674500 2.24013500 0.39611600
H -5.24526300 0.54728600 0.82986300
H -2.68072800 1.05132000 -1.81083800
H -3.90794100 -0.07819300 -1.22392100
H -4.37389100 1.53769500 -1.71522900
H -3.51098500 3.50226900 -0.61847700
H -2.90592400 3.47985100 1.02468400
H -1.86215600 2.96697600 -0.31541000
H 0.91865900 -0.48854000 -2.53275600
H 2.28446900 0.62172900 -2.36585700
H 2.52643500 -0.95698200 -3.08721800
H 2.12467700 -3.06777500 -0.11173800
H 0.67349300 -2.48465800 -0.94963000
H 2.09094100 -2.99333900 -1.86089800
H 4.14178400 -1.44321500 0.17722200
H 4.24468400 -1.77152000 -1.54226000
H 4.27471100 -0.11045000 -0.97670300

52'

E (SMD/M06-L-D3/def2-TZVP) = -2454.722166 au
H (SMD/M06-L-D3/def2-TZVP) = -2454.146953 au
G (SMD/M06-L-D3/def2-TZVP) = -2454.234691 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2454.025877 au
Mn -0.12264800 -0.08243600 0.07997600
N -2.02989800 0.37560400 1.06053600
N 2.00806700 -0.57885700 0.28268000
O -0.73246900 -1.17471500 -1.14766000
O 0.00932400 1.08842600 -1.22068600
N -0.24728500 -1.47434500 1.52475400
C 0.87007500 -2.05746300 1.95914200
C 2.12329800 -1.34471500 1.57633000
C 0.78897500 -3.15507200 2.79716800
H 1.68906300 -3.64370300 3.14265000
C -0.46809600 -3.59013000 3.19083700
H -0.55658400 -4.44507200 3.84780900
C -1.61191800 -2.92223500 2.77586000
H -2.59429600 -3.22404900 3.11023800
C -1.46637900 -1.84650000 1.92035600
C -2.56406400 -0.98546300 1.38233100
N 0.52868500 1.22350500 1.46148800
C 1.81332600 1.58231300 1.41804100
C 2.63660500 0.76686400 0.47267700

C 2.26824400 2.60310200 2.23112400
H 3.30899200 2.89338100 2.21136400
C 1.35699000 3.23029300 3.06966700
H 1.68549400 4.04231500 3.70455600
C 0.03703600 2.80707800 3.12549000
H -0.67351000 3.26168400 3.80130300
C -0.35171200 1.76428500 2.30386800
C -1.66781200 1.06342500 2.35175400
H -3.38081400 -0.92138600 2.10356500
H -2.96497700 -1.42303400 0.46822300
H 2.97783000 -2.01729300 1.55792100
H 2.33276200 -0.63013600 2.37538000
H 3.65626900 0.67065800 0.84934100
H 2.68888700 1.26120800 -0.49725500
H -2.46442000 1.72951900 2.67500800
H -1.58976700 0.30200300 3.13087300
C 2.67099100 -1.36636900 -0.86794600
C -3.05227700 1.22321100 0.27118800
C -4.40408400 1.21204200 0.97838700
C -3.22569700 0.67037100 -1.13288800
C -2.52282200 2.64744000 0.18008900
C 2.34137200 -0.72170000 -2.20289600
C 2.12125300 -2.78555500 -0.85375000
C 4.18600300 -1.38986900 -0.68960400
H -4.34006600 1.49357900 2.02855600
H -5.05085400 1.93756500 0.48770200
H -4.89230600 0.24129100 0.90917200
H -2.31603300 0.76982700 -1.71778900
H -3.53592800 -0.37323500 -1.14329200
H -4.01213000 1.24340400 -1.62297700
H -3.15096500 3.20444900 -0.51292100
H -2.55409600 3.17330200 1.13318900
H -1.50369400 2.66790100 -0.20471000
H 1.28226900 -0.79519700 -2.43171800
H 2.63835500 0.32466200 -2.25283500
H 2.89610000 -1.25035800 -2.97729700
H 2.48066300 -3.37238600 -0.00976300
H 1.03170500 -2.78683200 -0.84983400
H 2.45147600 -3.29237900 -1.75884800
H 4.49573600 -1.74454700 0.29240800
H 4.60476800 -2.07295400 -1.42680200
H 4.63251200 -0.41179200 -0.86132100
O -0.82577900 0.03625800 -3.74781700
H -0.96807400 -0.67879700 -3.10614600

H -0.46058700 0.71228700 -3.15352200

⁵TS₂₋₈

E (SMD/M06-L-D3/def2-TZVP) = -2454.694841 au

H (SMD/M06-L-D3/def2-TZVP) = -2454.124246 au

G (SMD/M06-L-D3/def2-TZVP) = -2454.210762 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2453.998003 au

Mn -0.17130200 -0.14392000 0.04618100

N -2.06784500 0.33484700 1.09465900

N 1.98607500 -0.61729200 0.26611000

O -0.84373900 -1.27678000 -1.12223500

O 0.06611400 1.20578800 -1.15422700

N -0.26342000 -1.49698100 1.53284000

C 0.86355300 -2.05720400 1.97622600

C 2.10536000 -1.33425300 1.58457600

C 0.80096300 -3.14079300 2.83333500

H 1.71035400 -3.60923000 3.18208700

C -0.44699400 -3.58701200 3.24099000

H -0.52085100 -4.43189200 3.91254200

C -1.60022500 -2.93741900 2.82454500

H -2.57683900 -3.24016200 3.17440400

C -1.47464200 -1.87425900 1.95109800

C -2.58828900 -1.02564300 1.43227400

N 0.50169600 1.19515200 1.40692100

C 1.77813700 1.57892100 1.31929600

C 2.60568100 0.73663300 0.40389100

C 2.23064200 2.64226800 2.07690800

H 3.26487100 2.95015200 2.01897300

C 1.32803300 3.28643500 2.91103600

H 1.65440900 4.13163400 3.50215000

C 0.02019200 2.83625600 3.02030100

H -0.68286200 3.30182100 3.69640100

C -0.36706100 1.75403600 2.25236500

C -1.66254300 1.02674000 2.36689200

H -3.38583600 -0.96104900 2.17461400

H -3.01089700 -1.46845900 0.53092100

H 2.97387200 -1.98902700 1.59616900

H 2.29140000 -0.58916900 2.36121800

H 3.62330500 0.65583100 0.79013800

H 2.66335300 1.19540200 -0.58211100

H -2.45857100 1.67366200 2.72868500

H -1.52811200 0.26673500 3.13948500

C 2.65198100 -1.44311400 -0.85291300

C -3.11595800 1.18075800 0.33884800
C -4.44818400 1.15161000 1.08192600
C -3.31188100 0.63427800 -1.06185800
C -2.60399100 2.61077600 0.24065000
C 2.29590200 -0.85599000 -2.20458900
C 2.11871600 -2.86655500 -0.78201000
C 4.16828300 -1.43920700 -0.68497100
H -4.35836100 1.42312000 2.13290300
H -5.11147200 1.87796900 0.61516100
H -4.93180300 0.17853400 1.01500700
H -2.41817300 0.76253300 -1.66374900
H -3.59631400 -0.41653900 -1.07439700
H -4.12115900 1.19271800 -1.53111200
H -3.25637900 3.16196300 -0.43432500
H -2.61599400 3.13443700 1.19539200
H -1.59603200 2.64283000 -0.17210500
H 1.23779500 -0.98592500 -2.40660900
H 2.54830400 0.19885000 -2.29633100
H 2.85541100 -1.39259700 -2.96946100
H 2.48921600 -3.41850700 0.08029300
H 1.02907200 -2.87944300 -0.77205400
H 2.44879200 -3.40207200 -1.67037800
H 4.48902500 -1.75035700 0.30812000
H 4.58907300 -2.14670300 -1.39749700
H 4.60070400 -0.46350900 -0.89994500
O -0.86505800 0.08222200 -3.14942500
H 0.00010200 -0.01426300 -3.56546500
H -0.86289700 -0.70215500 -2.09821700

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E (SMD/M06-L-D3/def2-TZVP) = -2454.701941 au
H (SMD/M06-L-D3/def2-TZVP) = -2454.126544 au
G (SMD/M06-L-D3/def2-TZVP) = -2454.213421 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2454.002251 au
Mn -0.16311900 -0.13182200 0.04246100
N -2.06596600 0.33513100 1.09634400
N 1.98223400 -0.62677700 0.26873800
O -0.89290100 -1.39466600 -1.05566900
O 0.05741100 1.15499400 -1.14827800
N -0.25833600 -1.49665600 1.54758800
C 0.86631100 -2.06292200 1.98603700
C 2.10915700 -1.34481800 1.58544700
C 0.80441100 -3.14536700 2.84477300

H 1.71291100 -3.61741900 3.19119400
C -0.44426500 -3.58574900 3.25754000
H -0.51911800 -4.42897100 3.93116800
C -1.59657300 -2.93356500 2.84257100
H -2.57314000 -3.23434900 3.19449100
C -1.46838600 -1.87105600 1.96773200
C -2.58299700 -1.02316400 1.44726500
N 0.50633700 1.18111900 1.41767300
C 1.78312900 1.56372700 1.32624400
C 2.60669600 0.72448800 0.40523500
C 2.23646000 2.63090100 2.07735300
H 3.27109500 2.93690600 2.01652400
C 1.33432200 3.28402200 2.90517600
H 1.66145200 4.13362400 3.48947900
C 0.02513800 2.83948400 3.01272600
H -0.68049400 3.31530800 3.67893300
C -0.36365800 1.75068000 2.25394600
C -1.66721700 1.03915200 2.36375800
H -3.37689100 -0.95046300 2.19291700
H -3.01071600 -1.47337600 0.55267500
H 2.97633800 -2.00153200 1.58893500
H 2.30392100 -0.60051200 2.36064700
H 3.62648800 0.64188400 0.78541000
H 2.65690200 1.18691100 -0.57974300
H -2.45892000 1.70137800 2.70690400
H -1.55189100 0.28822500 3.14838900
C 2.63151100 -1.45429900 -0.85861800
C -3.11346300 1.16524300 0.32451800
C -4.44591200 1.15570800 1.06806100
C -3.31388400 0.58520100 -1.06325400
C -2.59731600 2.59097500 0.19564000
C 2.23742500 -0.88222400 -2.20685000
C 2.11790300 -2.88422700 -0.76847600
C 4.15036300 -1.43363700 -0.72069200
H -4.35691100 1.46057000 2.10990500
H -5.11145400 1.86507400 0.57884300
H -4.92681100 0.17961400 1.03224600
H -2.41060200 0.66430200 -1.66083600
H -3.63567700 -0.45472700 -1.04721600
H -4.09960500 1.15659000 -1.55631000
H -3.25145900 3.13296700 -0.48505600
H -2.60147400 3.13133100 1.14123200
H -1.59105900 2.60905100 -0.22244400
H 1.17878800 -1.03914000 -2.39375000

H 2.46113600 0.17885700 -2.30529000
H 2.79857800 -1.40729500 -2.97874500
H 2.51580500 -3.42772600 0.08685900
H 1.02940000 -2.91192700 -0.73424800
H 2.43495700 -3.41863600 -1.66228500
H 4.49042000 -1.73362800 0.26971000
H 4.56549800 -2.14289600 -1.43477200
H 4.56927200 -0.45542200 -0.95063700
O -0.73382400 0.40219900 -3.18905700
H 0.21499000 0.45395900 -3.36677100
H -0.92368000 -0.93772700 -1.92494100

⁵TS₈₋₉

E (SMD/M06-L-D3/def2-TZVP) = -2454.694316 au
H (SMD/M06-L-D3/def2-TZVP) = -2454.120273 au
G (SMD/M06-L-D3/def2-TZVP) = -2454.207125 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2453.998547 au
Mn -0.16742800 -0.07582200 -0.01075100
N -2.08752500 0.38445800 1.15077300
N 2.10426100 -0.62928100 0.34156600
O -0.89239600 -1.34087000 -1.11811500
O 0.07894700 1.25206000 -1.16140400
N -0.25098100 -1.48381100 1.51659700
C 0.86144000 -2.06919700 1.96567200
C 2.14085100 -1.37167200 1.62926700
C 0.77845700 -3.16709000 2.80482700
H 1.68082200 -3.65041400 3.15276500
C -0.47545800 -3.60598700 3.19903400
H -0.56499700 -4.46152100 3.85525000
C -1.61359300 -2.92725600 2.79063300
H -2.59718400 -3.21574200 3.13387900
C -1.46523400 -1.85036500 1.93604700
C -2.58757700 -0.98166400 1.45861500
N 0.53564800 1.19020300 1.45356800
C 1.82455200 1.54578400 1.42001500
C 2.69305700 0.71835400 0.52445800
C 2.27907500 2.58078200 2.21659200
H 3.32320000 2.85952700 2.19560000
C 1.37263800 3.23133900 3.03954600
H 1.70149500 4.05653800 3.65709900
C 0.05590800 2.80319900 3.10422400
H -0.65613000 3.26350900 3.77492400
C -0.33433300 1.74626400 2.30182200

C -1.65360300 1.05466000 2.41095500
H -3.37068800 -0.94894900 2.21995300
H -3.03054900 -1.40226100 0.55666400
H 2.98413700 -2.06050800 1.67175300
H 2.31653600 -0.65486600 2.43558600
H 3.69820100 0.66209700 0.95126900
H 2.78399800 1.19669200 -0.45072800
H -2.42160300 1.72908500 2.78641400
H -1.53706600 0.28989400 3.18259200
C 2.76128500 -1.42138200 -0.78467800
C -3.11785800 1.23175300 0.39540100
C -4.45331800 1.22761800 1.13321600
C -3.31660800 0.67609200 -1.00415200
C -2.58528000 2.65337700 0.28630800
C 2.41109700 -0.78825800 -2.11961000
C 2.20574700 -2.83923600 -0.76698300
C 4.27589500 -1.45020500 -0.60746900
H -4.35994200 1.53316800 2.17481200
H -5.12105900 1.93575000 0.64495900
H -4.93252400 0.25032600 1.10065300
H -2.39407800 0.71600400 -1.57842900
H -3.68244900 -0.34923300 -1.00769000
H -4.06243000 1.28613300 -1.51212900
H -3.23376100 3.21695500 -0.38222600
H -2.57587000 3.17744500 1.24095200
H -1.57930000 2.66434300 -0.13447700
H 1.34133500 -0.84204400 -2.30701300
H 2.72142800 0.25314700 -2.19247500
H 2.92447200 -1.33481100 -2.90985200
H 2.54265500 -3.41889000 0.09119300
H 1.11570500 -2.83471700 -0.78422300
H 2.55006100 -3.35900200 -1.65946500
H 4.57287500 -1.81647500 0.37507900
H 4.70464100 -2.12248100 -1.34920800
H 4.72193100 -0.46816600 -0.75881000
O -0.30130000 0.77505400 -3.04707100
H -1.03798200 1.40215600 -3.01621200
H -0.89685100 -0.87348800 -1.97496400

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E (SMD/M06-L-D3/def2-TZVP) = -2454.732535 au
H (SMD/M06-L-D3/def2-TZVP) = -2454.155731 au
G (SMD/M06-L-D3/def2-TZVP) = -2454.244143 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2454.042699 au
Mn -0.18412900 -0.14738900 -0.13541000
N -2.18637100 0.39477000 1.14794800
N 2.15845800 -0.67773300 0.29781700
O -0.87195900 -1.47751000 -1.27980800
O 0.11916600 1.28325400 -1.36311100
N -0.27211300 -1.48072900 1.46068400
C 0.84421200 -2.06962200 1.90955200
C 2.14572400 -1.39502700 1.58605900
C 0.76226600 -3.15898000 2.75983200
H 1.66810400 -3.64235900 3.09944500
C -0.48680500 -3.58766000 3.17784800
H -0.57342000 -4.43932600 3.83966700
C -1.62075700 -2.89547300 2.78679000
H -2.60147600 -3.16515600 3.15349600
C -1.48236400 -1.82724400 1.91722200
C -2.63547100 -0.96816500 1.48306200
N 0.49975700 1.18198500 1.32458600
C 1.79570700 1.52422500 1.30905500
C 2.70331000 0.67977600 0.46391300
C 2.25501800 2.56993100 2.09088400
H 3.30401400 2.83099400 2.07288300
C 1.35463700 3.24767800 2.89519200
H 1.68748400 4.08063300 3.50035300
C 0.03792100 2.82429100 2.96098700
H -0.67353100 3.29265600 3.62728100
C -0.36189600 1.75745700 2.17491100
C -1.69520700 1.09296000 2.34811100
H -3.38954400 -0.97763900 2.27738100
H -3.10449700 -1.40973400 0.60289500
H 2.97179000 -2.10184100 1.67917000
H 2.30629100 -0.66990800 2.38936700
H 3.69746800 0.67868000 0.92333700
H 2.81548400 1.13642600 -0.52010600
H -2.42233800 1.80343400 2.74458000
H -1.55619700 0.35953900 3.14775600
C 2.83689200 -1.46517000 -0.80329400
C -3.21586300 1.20265800 0.38673900
C -4.54333000 1.25298800 1.13483500
C -3.42205500 0.58429700 -0.98741100
C -2.67095300 2.61239300 0.19120800
C 2.48658900 -0.84377300 -2.14710000
C 2.29470500 -2.88918900 -0.78528000
C 4.34983200 -1.48406300 -0.61485900

H -4.42837700 1.63806700 2.14847000
H -5.23315900 1.91360400 0.61081200
H -5.01160400 0.27078800 1.19346600
H -2.48046100 0.52679400 -1.53228100
H -3.84914100 -0.41664400 -0.94495900
H -4.11219500 1.20486900 -1.55776100
H -3.33864300 3.16144300 -0.47093700
H -2.60793000 3.17619400 1.12119600
H -1.68307400 2.58873500 -0.27134100
H 1.41153100 -0.87601400 -2.31879600
H 2.81886700 0.18952800 -2.23894800
H 2.97559100 -1.41025400 -2.93902100
H 2.62626100 -3.45794400 0.08257000
H 1.20468200 -2.89504700 -0.81215600
H 2.65281300 -3.41488300 -1.66909100
H 4.63352500 -1.85005400 0.37247800
H 4.80141400 -2.14740400 -1.35165600
H 4.78815900 -0.49596400 -0.75228000
O -0.26084300 0.99056000 -2.72567100
H -1.10553000 1.46193300 -2.79923200
H -0.93578100 -1.04504300 -2.14349800

³TS₂₋₃

E (SMD/M06-L-D3/def2-TZVP) = -2378.202578 au
H (SMD/M06-L-D3/def2-TZVP) = -2377.65482 au
G (SMD/M06-L-D3/def2-TZVP) = -2377.736265 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2377.534201 au
Mn 0.00957100 -0.01389000 0.71296700
N 2.08025800 -0.41927600 0.11266400
N -2.06793500 0.43163600 0.16921800
O -0.16716100 -1.09348500 2.27302800
O 0.13205700 0.59782500 2.34045100
N -0.20707600 -1.33839000 -0.74669300
C -1.37110900 -1.39923800 -1.39962000
C -2.24915700 -0.21311100 -1.18164800
C -1.61438600 -2.43190300 -2.28429500
H -2.56119900 -2.49059500 -2.80260300
C -0.60985100 -3.36590800 -2.50223000
H -0.77601900 -4.18212100 -3.19224900
C 0.61709700 -3.23940100 -1.86702400
H 1.42648600 -3.92881700 -2.06151700
C 0.79199200 -2.19729200 -0.97581900
C 2.04635100 -1.87752600 -0.22707100

N 0.21216200 1.44054000 -0.58689600
C -0.79729000 2.30947100 -0.74590700
C -2.03539500 1.91979800 -0.01012300
C -0.63707400 3.41861500 -1.55180200
H -1.45570900 4.11222100 -1.68308400
C 0.58368900 3.61010200 -2.18501800
H 0.73911000 4.48191600 -2.80565200
C 1.59230600 2.66461500 -2.05326200
H 2.53311000 2.76798800 -2.57587000
C 1.36645900 1.55996400 -1.25625400
C 2.25566800 0.36714900 -1.16155800
H 2.92113000 -2.16191500 -0.81497500
H 2.07809000 -2.44556000 0.70214400
H -3.29408300 -0.45040600 -1.36498800
H -1.97743900 0.52002300 -1.94366100
H -2.92121000 2.27131300 -0.54179200
H -2.04027400 2.37831200 0.97917800
H 3.29801800 0.63703000 -1.31122600
H 1.99954600 -0.28689000 -1.99738100
C -3.20753600 -0.00167000 1.11871900
C 3.21722300 -0.08684500 1.10279300
C 4.56187200 -0.56625600 0.56198300
C 2.97645900 -0.76065400 2.44315900
C 3.23357500 1.42235100 1.29477800
C -2.94284800 0.48533900 2.53342400
C -3.26396900 -1.52267900 1.11982400
C -4.54158700 0.57575500 0.65142800
H 4.79986000 -0.17493400 -0.42551700
H 5.34071300 -0.22024900 1.23974000
H 4.62149200 -1.65298700 0.52746100
H 2.05621600 -0.41927100 2.90484900
H 2.95473300 -1.84669700 2.37083700
H 3.80813000 -0.50391400 3.09798900
H 3.92592200 1.66628300 2.09857800
H 3.57118600 1.95758100 0.40799500
H 2.24851900 1.79414700 1.57768100
H -2.06395200 0.01305300 2.95926200
H -2.82975000 1.56633700 2.59510000
H -3.80674900 0.22112900 3.14210300
H -3.63442100 -1.93444700 0.18193200
H -2.28587800 -1.95270700 1.33476200
H -3.94851900 -1.84463000 1.90270700
H -4.77128200 0.35414500 -0.38943900
H -5.33178500 0.13336700 1.25593400

H -4.59036200 1.65424900 0.79354900

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E (SMD/M06-L-D3/def2-TZVP) = -2378.218702 au

H (SMD/M06-L-D3/def2-TZVP) = -2377.669552 au

G (SMD/M06-L-D3/def2-TZVP) = -2377.752494 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2377.555927 au

Mn -0.46856200 0.21935600 0.01288100

N -2.39988600 0.66301400 0.97965200

N 1.66666900 -0.25016800 0.17828600

O -0.90212800 -0.47269900 -1.65697200

O -0.67131100 0.96123900 -1.67605100

N -0.59161000 -1.17341300 1.38663400

C 0.53202200 -1.73798300 1.84925100

C 1.77873800 -1.01149200 1.47286400

C 0.46570000 -2.82071100 2.70200800

H 1.37613800 -3.28338900 3.05702000

C -0.78358400 -3.27696400 3.10633800

H -0.85866500 -4.12401300 3.77447900

C -1.93144600 -2.62163200 2.68488400

H -2.91097100 -2.92208400 3.02987400

C -1.80440100 -1.55562200 1.81511500

C -2.91577600 -0.70801900 1.29139700

N 0.15126100 1.54621900 1.31676500

C 1.44254500 1.91275500 1.29548000

C 2.27568300 1.10796400 0.35412300

C 1.89411600 2.92257500 2.12286400

H 2.93623200 3.20941800 2.10360600

C 0.98988400 3.53790400 2.97660000

H 1.31646500 4.34105700 3.62296100

C -0.32624300 3.09423300 3.03120300

H -1.03628700 3.52192000 3.72543100

C -0.71566700 2.06739400 2.19552300

C -2.02186500 1.35117600 2.26305900

H -3.73838600 -0.67076700 2.00850000

H -3.30361800 -1.13688700 0.36751000

H 2.63514800 -1.68079200 1.45983700

H 1.98010600 -0.29282200 2.26975000

H 3.30337500 1.03994100 0.71590300

H 2.30165400 1.59011500 -0.62289200

H -2.81538800 2.01238100 2.60283600

H -1.92572200 0.58862700 3.03852500

C 2.34901200 -1.03577600 -0.96077800

C -3.43739500 1.50207000 0.20943500
C -4.73302900 1.64716500 1.00430500
C -3.77500800 0.83885500 -1.11672500
C -2.82230200 2.87124900 -0.03741700
C 2.17726200 -0.30974100 -2.28599900
C 1.68913800 -2.40478600 -1.03033900
C 3.84626000 -1.19136300 -0.70400700
H -4.60403600 2.14065100 1.96554400
H -5.41696700 2.26202900 0.42097000
H -5.22187100 0.68815000 1.16844100
H -2.88741000 0.61925800 -1.69992400
H -4.35138000 -0.07587000 -0.98715500
H -4.39903700 1.52545700 -1.68704600
H -3.49360300 3.45301000 -0.66669200
H -2.67837000 3.43511100 0.88388900
H -1.86534000 2.78677600 -0.55086500
H 1.13592600 -0.10733700 -2.50952200
H 2.73743700 0.62310100 -2.32402800
H 2.57830900 -0.94856300 -3.07161800
H 1.91099200 -3.01850900 -0.15770100
H 0.60843400 -2.31805200 -1.13372500
H 2.06975800 -2.93696900 -1.90040700
H 4.08230600 -1.71396200 0.22088100
H 4.26492500 -1.78191000 -1.51768100
H 4.36265600 -0.23287900 -0.70291800

⁵TS₂₋₃

E (SMD/M06-L-D3/def2-TZVP) = -2378.22093 au
H (SMD/M06-L-D3/def2-TZVP) = -2377.675916 au
G (SMD/M06-L-D3/def2-TZVP) = -2377.760278 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2377.54715 au
Mn -0.02510500 -0.02051400 0.94567300
N 0.15434500 -1.31850900 -0.69241700
N 2.22237900 0.39854600 0.09312100
N -0.19547500 1.43409100 -0.53136700
N -2.25849200 -0.37931600 0.03567000
O -0.04182300 0.69243800 2.54868500
O 0.19945500 -1.32072100 2.26048400
C -0.87872300 -2.12709300 -0.97328700
C -0.73834700 -3.15324400 -1.89052100
C 0.48323700 -3.32402900 -2.51978900
C 1.50943200 -2.42530600 -2.28305400
C 1.30456300 -1.40287800 -1.37307500

C 2.26077300 -0.25837400 -1.22631200
C 2.12349500 1.86608300 -0.03946800
C 0.85218700 2.25034500 -0.72965700
C 0.74321200 3.33682600 -1.57692400
C -0.46159400 3.55912400 -2.22460500
C -1.49995400 2.65785200 -2.07275800
C -1.32870200 1.57255000 -1.22904900
C -2.31672000 0.44463100 -1.18308300
C -2.17500800 -1.81256400 -0.28908200
C -3.35847800 -0.03244600 1.01797700
C -4.73283200 -0.39892800 0.46650900
C -3.13514500 -0.76958500 2.33042700
C -3.27537300 1.46352400 1.29165400
C 3.36448600 -0.05221300 0.98426900
C 4.69986100 0.48387700 0.47314100
C 3.38312200 -1.57588500 0.99558900
C 3.14420900 0.43560900 2.40758900
H 3.10574200 1.52094300 2.48474800
H 2.22959000 0.02316700 2.82871800
H 3.98073800 0.10325500 3.02113300
H -1.58152100 -3.79331800 -2.10989900
H 0.62220100 -4.13327700 -3.22438900
H 2.45213200 -2.49211400 -2.80847000
H 3.26753500 -0.57081100 -1.50454400
H 1.96953000 0.46860600 -1.98971200
H 2.96685900 2.29254000 -0.59102400
H 2.14188100 2.30496200 0.95889900
H 1.59631600 3.98217700 -1.73219600
H -0.57563200 4.41298400 -2.87922500
H -2.42872700 2.76960400 -2.61511300
H -3.31955800 0.82825200 -1.37474900
H -2.08876900 -0.18497000 -2.04801400
H -2.99990900 -2.14913900 -0.92567400
H -2.23796500 -2.38490300 0.63676500
H -5.50026200 -0.09558600 1.17769000
H -4.95195400 0.09843800 -0.47782300
H -4.83018700 -1.47419800 0.31823200
H -3.27326900 -1.84604400 2.24152500
H -2.14031200 -0.57601700 2.72719500
H -3.86674700 -0.41631100 3.05593300
H -3.98189500 1.72642800 2.07713700
H -2.27520400 1.73853900 1.63332600
H -3.52384300 2.06904900 0.42054600
H 5.50869200 0.04977400 1.05926200

H 4.87880700 0.22543200 -0.57028800
H 4.76636500 1.56650900 0.57503900
H 4.08962200 -1.91646700 1.75076200
H 2.40113000 -1.97703700 1.25053000
H 3.69967500 -2.00230800 0.04450900

⁵3

E (SMD/M06-L-D3/def2-TZVP) = -2378.268444 au
H (SMD/M06-L-D3/def2-TZVP) = -2377.719884 au
G (SMD/M06-L-D3/def2-TZVP) = -2377.805278 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2377.598553 au
Mn -0.54190400 0.22913900 -0.28011700
N -2.54560300 0.71598500 1.00914300
N 1.82060700 -0.29778300 0.15674900
O -0.99251700 -0.46962700 -1.97094800
O -0.72103900 0.93189300 -2.01636300
N -0.60587400 -1.14324500 1.32007300
C 0.51662800 -1.69598200 1.79141900
C 1.81857100 -1.03729600 1.43399400
C 0.45156500 -2.74734900 2.69199200
H 1.36428300 -3.20374400 3.05012700
C -0.78931500 -3.17224800 3.13436600
H -0.86250500 -3.99341700 3.83528900
C -1.93464000 -2.51392300 2.71504800
H -2.91063800 -2.78012800 3.09642800
C -1.81023700 -1.48687600 1.79732100
C -2.96869600 -0.66522000 1.31248100
N 0.13444700 1.54676500 1.21729600
C 1.43873600 1.85793900 1.25328900
C 2.32613400 1.07627600 0.33193500
C 1.91278600 2.80620700 2.14092900
H 2.96771400 3.04164200 2.16273400
C 1.01640700 3.41931000 3.00218000
H 1.36030700 4.17628900 3.69467400
C -0.30829900 3.02068300 3.01150800
H -1.01599600 3.43160700 3.71856700
C -0.72100500 2.04683400 2.11550900
C -2.07175000 1.40160000 2.22716000
H -3.76820900 -0.70823100 2.05953700
H -3.36412100 -1.11235400 0.39915200
H 2.62240900 -1.77214300 1.48557200
H 2.02949900 -0.33769500 2.24839400
H 3.34970200 1.10653400 0.72006300

H 2.34224300 1.56215300 -0.64472500
H -2.79419400 2.12825700 2.59920800
H -1.97998000 0.66748300 3.03321600
C 2.52026300 -1.06447400 -0.94422900
C -3.59356300 1.52588500 0.27442800
C -4.87470200 1.67147000 1.09049200
C -3.92623100 0.85438700 -1.04986000
C -2.99072000 2.89491800 -0.01371200
C 2.36443000 -0.32190400 -2.26370100
C 1.83766400 -2.42122900 -1.05971700
C 4.00782700 -1.24594000 -0.65449500
H -4.71282800 2.15741200 2.05208000
H -5.58537100 2.28365600 0.53624100
H -5.34781000 0.70632300 1.27023000
H -3.02682500 0.65906100 -1.62998700
H -4.47297600 -0.07864200 -0.92141800
H -4.56678600 1.51926000 -1.62800200
H -3.67858700 3.47170600 -0.62988600
H -2.80745100 3.47336900 0.89139800
H -2.05017300 2.79829000 -0.55887500
H 1.32468700 -0.06606400 -2.45667200
H 2.96169100 0.58814300 -2.30225200
H 2.71423700 -0.96340300 -3.07149700
H 1.99166000 -3.04381300 -0.17852900
H 0.76435700 -2.30457200 -1.21755800
H 2.24700200 -2.96263500 -1.91120200
H 4.19559000 -1.79605300 0.26691400
H 4.46531700 -1.81107700 -1.46593200
H 4.52467000 -0.28840600 -0.59329000

32''

E (SMD/M06-L-D3/def2-TZVP) = -2454.233732 au
H (SMD/M06-L-D3/def2-TZVP) = -2453.669913 au
G (SMD/M06-L-D3/def2-TZVP) = -2453.757842 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2453.543131 au
Mn -0.15219900 -0.15540900 -0.02147500
N -2.06872300 0.35175900 1.09776500
N 1.98817600 -0.64809300 0.26594900
O -0.81071700 -1.39399800 -0.88901600
O 0.12419200 1.12520900 -1.03057600
N -0.24418600 -1.45166800 1.60872100
C 0.87139700 -2.04262300 2.02600300
C 2.12859800 -1.38636800 1.57146400

C 0.80383500 -3.11446300 2.90057500
H 1.70913800 -3.60494800 3.22998300
C -0.44408100 -3.52165500 3.34511400
H -0.52422800 -4.35257300 4.03334400
C -1.59022500 -2.85959600 2.92819900
H -2.56900000 -3.14532000 3.28710200
C -1.45552700 -1.81554200 2.03167200
C -2.57382300 -1.00038300 1.46512000
N 0.52028300 1.12740900 1.48628600
C 1.79509100 1.50858200 1.39472800
C 2.61103700 0.69785600 0.43912800
C 2.25764900 2.57082300 2.14909500
H 3.29415900 2.87135700 2.08797100
C 1.35735300 3.23479000 2.97030400
H 1.68876600 4.08182800 3.55612500
C 0.03983900 2.81284600 3.05439200
H -0.67229500 3.30927500 3.69878300
C -0.35221100 1.72375300 2.29348700
C -1.68760700 1.06615200 2.36219000
H -3.39200600 -0.93044700 2.18525100
H -2.96160300 -1.48473800 0.56906500
H 2.95423200 -2.09293800 1.52687600
H 2.40677400 -0.66519500 2.34286200
H 3.63611500 0.60349900 0.80246400
H 2.64690600 1.19496700 -0.52960200
H -2.46132400 1.77101800 2.65955200
H -1.64051600 0.33141700 3.16897400
C 2.62869200 -1.44661100 -0.88499800
C -3.09215900 1.16575500 0.29341600
C -4.44541400 1.17082000 0.99763600
C -3.24929900 0.56588200 -1.09249000
C -2.57017600 2.58939200 0.15428000
C 2.23411100 -0.82934000 -2.21440600
C 2.10590500 -2.87510400 -0.82865600
C 4.14827200 -1.44163400 -0.75383700
H -4.38013500 1.49795900 2.03491400
H -5.10218000 1.86700400 0.47831700
H -4.92223100 0.19212100 0.97298400
H -2.32707700 0.63758000 -1.66687100
H -3.56200300 -0.47691300 -1.07022700
H -4.02140300 1.12335400 -1.62163800
H -3.19740500 3.11993100 -0.56012300
H -2.60508800 3.14860200 1.08818700
H -1.54900000 2.59693100 -0.22602800

H 1.16533700 -0.92435600 -2.39642200
H 2.50558400 0.22234200 -2.29118100
H 2.76088700 -1.35948700 -3.00714200
H 2.50970700 -3.44235700 0.00855300
H 1.01773200 -2.89430200 -0.77938100
H 2.40850800 -3.38934000 -1.73916000
H 4.48909800 -1.77727500 0.22508500
H 4.55736400 -2.12888300 -1.49263000
H 4.57336300 -0.45887600 -0.95118300
O -0.79368500 0.14275000 -3.81060400
H -0.44990600 0.54106500 -3.00137600

³TS₂₋₁₄

E (SMD/M06-L-D3/def2-TZVP) = -2454.182205 au
H (SMD/M06-L-D3/def2-TZVP) = -2453.620098 au
G (SMD/M06-L-D3/def2-TZVP) = -2453.706492 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2453.500389 au
Mn -0.08366600 -0.16991700 -0.04747000
N -2.12218800 0.35288500 1.06537400
N 2.04241300 -0.63144000 0.24943800
O -0.69512200 -1.28155600 -1.25839900
O 0.31886600 1.16731300 -1.29787800
N -0.26857700 -1.49463600 1.47252500
C 0.84665000 -2.06203800 1.93572100
C 2.11247700 -1.36481700 1.55863100
C 0.77640700 -3.13646600 2.80647700
H 1.68184100 -3.61004900 3.16032000
C -0.47467200 -3.56643000 3.22281400
H -0.55765800 -4.40266200 3.90453100
C -1.61742700 -2.90472200 2.79835800
H -2.59784800 -3.18982600 3.15427900
C -1.47846600 -1.85454000 1.90745500
C -2.60022100 -1.01625800 1.38235300
N 0.51605000 1.16291900 1.39067500
C 1.79693100 1.54117500 1.35118100
C 2.65044300 0.71644200 0.43754100
C 2.24488000 2.59000500 2.13143500
H 3.28437600 2.88600000 2.10373800
C 1.32651000 3.24401900 2.94472400
H 1.64400700 4.08298800 3.54980200
C 0.01349200 2.80619000 3.00541200
H -0.70716700 3.27872300 3.65904600
C -0.36309500 1.72680700 2.21993800

C -1.68690500 1.03801600 2.31880700
H -3.42283600 -1.01139100 2.10391900
H -2.97781700 -1.46370200 0.46216000
H 2.96165300 -2.04483400 1.59118100
H 2.30348100 -0.63244500 2.34670000
H 3.66166300 0.64469100 0.84655000
H 2.72382000 1.19769100 -0.53750500
H -2.44459600 1.73058800 2.68199700
H -1.58929700 0.28559300 3.10612200
C 2.76478100 -1.43340900 -0.84574400
C -3.18060700 1.17767700 0.34247900
C -4.44944500 1.35486300 1.17512800
C -3.56460900 0.49042800 -0.95930900
C -2.56617100 2.53714700 0.04220800
C 2.47192900 -0.83660200 -2.21229000
C 2.24680500 -2.86586800 -0.81599600
C 4.27412400 -1.42819400 -0.61788700
H -4.28215500 1.88471700 2.11158000
H -5.16113700 1.94517600 0.59870800
H -4.92787300 0.40197700 1.39838000
H -2.68733500 0.19503700 -1.52800900
H -4.18486100 -0.38973900 -0.79403600
H -4.14869700 1.18336100 -1.56382800
H -3.24765000 3.11348000 -0.58192100
H -2.39064100 3.11880200 0.94749100
H -1.62045100 2.43036000 -0.48916600
H 1.41512400 -0.91264200 -2.45877500
H 2.77336000 0.20664800 -2.28944200
H 3.04216200 -1.39426900 -2.95513500
H 2.59699100 -3.42576100 0.05019100
H 1.15750800 -2.89163400 -0.83714800
H 2.61076700 -3.38618800 -1.70056700
H 4.55283600 -1.74180500 0.38774700
H 4.73256800 -2.12941100 -1.31376400
H 4.71294500 -0.44958000 -0.80680300
O -0.66721500 1.13808000 -2.54061300
H -0.86364300 0.17874000 -2.42350700

³14

E (SMD/M06-L-D3/def2-TZVP) = -2454.186696 au

H (SMD/M06-L-D3/def2-TZVP) = -2453.622922 au

G (SMD/M06-L-D3/def2-TZVP) = -2453.706863 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2453.504534 au

Mn -0.18965100 -0.17839700 0.04380600
N -2.06958700 0.34767700 1.06522200
N 2.02888900 -0.62824600 0.26225500
O -0.89562400 -1.22158200 -1.17809900
O 0.05275000 1.28362600 -1.29123200
N -0.24594900 -1.49735600 1.47295500
C 0.87334200 -2.04383400 1.97028600
C 2.12415600 -1.32378000 1.58941300
C 0.80106500 -3.11073900 2.84176700
H 1.70943100 -3.56170500 3.21762400
C -0.45307900 -3.57651200 3.22951000
H -0.53340900 -4.41467900 3.90826000
C -1.59765100 -2.93508700 2.77659700
H -2.58023900 -3.23623200 3.11389300
C -1.46598700 -1.87919600 1.89360300
C -2.58502700 -1.02014400 1.39330100
N 0.50421400 1.19614400 1.36635800
C 1.78266600 1.57827700 1.29500400
C 2.62868200 0.73119300 0.39608500
C 2.23573800 2.64237000 2.05671000
H 3.27179400 2.94720100 2.00245900
C 1.33669800 3.28888600 2.89134600
H 1.66257500 4.13209800 3.48570200
C 0.02722800 2.83254000 2.99645700
H -0.67695600 3.29249700 3.67611800
C -0.35578500 1.75402300 2.22286600
C -1.64977600 1.01711400 2.34053900
H -3.37806900 -0.97732600 2.14448400
H -3.01643800 -1.43876900 0.48458800
H 2.99111700 -1.98125700 1.63793000
H 2.29553800 -0.56593700 2.35660400
H 3.64750800 0.68318300 0.79004700
H 2.68568000 1.18082500 -0.59532900
H -2.43943300 1.65179900 2.73895100
H -1.49353700 0.24088000 3.09270300
C 2.72164000 -1.45467600 -0.82315100
C -3.13334300 1.19962500 0.35408000
C -4.45687200 1.16375100 1.11369300
C -3.36423800 0.69072000 -1.05765300
C -2.62385000 2.63281500 0.26832600
C 2.40050000 -0.87608900 -2.18900700
C 2.17679900 -2.87575600 -0.76340000
C 4.23547300 -1.46775300 -0.63009100
H -4.35016700 1.41557400 2.16833000

H -5.13096800 1.89708100 0.67310300
H -4.94226600 0.19151300 1.04047300
H -2.48307400 0.82093600 -1.68092900
H -3.65596500 -0.35767900 -1.08819100
H -4.17977900 1.26619600 -1.49578500
H -3.28856000 3.19986200 -0.38172400
H -2.61097500 3.13921400 1.23258000
H -1.62379300 2.66713400 -0.16439900
H 1.33724700 -0.94594300 -2.40372100
H 2.70560400 0.16435200 -2.29249200
H 2.93981100 -1.44641200 -2.94469300
H 2.50882000 -3.42233000 0.11823600
H 1.08636200 -2.87853100 -0.78940400
H 2.53287800 -3.42476800 -1.63379900
H 4.53460800 -1.78944300 0.36689600
H 4.67195900 -2.16899400 -1.34007200
H 4.67896100 -0.49192200 -0.82347100
O -0.29194400 0.82491800 -2.65052600
H -0.62984800 -0.08103400 -2.38498400

52''

E (SMD/M06-L-D3/def2-TZVP) = -2454.216956 au
H (SMD/M06-L-D3/def2-TZVP) = -2453.654269 au
G (SMD/M06-L-D3/def2-TZVP) = -2453.741763 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2453.523421 au
Mn -0.19829600 -0.11815300 -0.18645300
N -2.14549900 0.39015800 1.10998400
N 2.10037500 -0.64449300 0.26604300
O -0.84254800 -1.38366500 -1.09056600
O 0.10103500 1.26613100 -1.20204100
N -0.25879700 -1.44822300 1.50366800
C 0.85379400 -2.03952500 1.93397900
C 2.13788100 -1.36283900 1.56456100
C 0.78551000 -3.13460000 2.78086400
H 1.69314800 -3.62274500 3.10936400
C -0.46137300 -3.56518300 3.20498500
H -0.54267700 -4.41743800 3.86686100
C -1.60225300 -2.88356000 2.80987400
H -2.58179900 -3.16803900 3.16921500
C -1.46406300 -1.81431200 1.94089800
C -2.60885700 -0.97124100 1.46120300
N 0.51119900 1.18161900 1.37267900
C 1.79504500 1.54151200 1.33078600

C 2.66905100 0.71097300 0.43842700
C 2.25750200 2.59031000 2.10747900
H 3.30191400 2.86898400 2.07669500
C 1.35455900 3.25854800 2.92008800
H 1.68502700 4.09506800 3.52179200
C 0.03749900 2.83308300 2.98999300
H -0.67473500 3.30892200 3.65044600
C -0.35250500 1.75819700 2.20705200
C -1.68146900 1.08105000 2.34044100
H -3.38040700 -0.94814000 2.23696700
H -3.05673600 -1.42817100 0.57856000
H 2.97020200 -2.06489700 1.61624400
H 2.33347000 -0.63438100 2.35577800
H 3.67716500 0.67512900 0.86278600
H 2.75119200 1.18428100 -0.53991400
H -2.43043100 1.77443600 2.72280900
H -1.55949900 0.33418900 3.12910000
C 2.78718200 -1.43925200 -0.83510500
C -3.20322500 1.20541300 0.37866200
C -4.52432600 1.20283900 1.14208600
C -3.42005200 0.62994500 -1.01121200
C -2.69216200 2.63321200 0.22967300
C 2.45865800 -0.82375500 -2.18527500
C 2.24063600 -2.86125000 -0.81322100
C 4.30002000 -1.45930400 -0.63875000
H -4.40826100 1.52531400 2.17689500
H -5.21522100 1.89444000 0.66161500
H -4.99288400 0.21932800 1.14019200
H -2.51481600 0.70193300 -1.61304400
H -3.74213200 -0.41034500 -0.99475900
H -4.20328500 1.20170100 -1.50819100
H -3.35657900 3.17716000 -0.43989900
H -2.67135600 3.17761400 1.17290000
H -1.69219600 2.64623800 -0.20513200
H 1.38983200 -0.87079100 -2.38686800
H 2.77713700 0.21460900 -2.26846600
H 2.97719900 -1.38366500 -2.96294500
H 2.57720800 -3.43244600 0.05099600
H 1.15016500 -2.85945800 -0.83063600
H 2.58949200 -3.38702400 -1.70068000
H 4.58625400 -1.81224300 0.35203100
H 4.74545200 -2.13628200 -1.36666500
H 4.74265400 -0.47605500 -0.79389600
O -0.58643600 0.55906300 -3.31396900

H -0.71598800 -0.17975100 -2.69374200

⁵TS₂₋₁₄

E (SMD/M06-L-D3/def2-TZVP) = -2454.213339 au

H (SMD/M06-L-D3/def2-TZVP) = -2453.651687 au

G (SMD/M06-L-D3/def2-TZVP) = -2453.738905 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2453.519231 au

Mn -0.21537400 -0.14262500 -0.21979500

N -2.18850300 0.39045200 1.12216800

N 2.13221100 -0.66813100 0.25742400

O -0.87062200 -1.37091800 -1.19360500

O 0.07278300 1.23870500 -1.29395700

N -0.26728600 -1.45854500 1.47052300

C 0.84745900 -2.04121000 1.91496900

C 2.14288100 -1.37439400 1.55513900

C 0.77959900 -3.12219000 2.78006600

H 1.68923900 -3.60139700 3.11640300

C -0.46470300 -3.54840100 3.21419400

H -0.54406700 -4.39046400 3.88930400

C -1.60470700 -2.86897100 2.81484700

H -2.58306300 -3.14235300 3.18596800

C -1.47090400 -1.81351700 1.92831300

C -2.62807000 -0.97585700 1.46310700

N 0.49496300 1.17577900 1.32363700

C 1.78432700 1.52659800 1.29527100

C 2.67505400 0.69413200 0.41954200

C 2.24997500 2.56952900 2.07849000

H 3.29712200 2.83836800 2.05247500

C 1.35147500 3.24135500 2.89164800

H 1.68520900 4.07412100 3.49680600

C 0.03465700 2.81703700 2.96060700

H -0.67532200 3.28723100 3.62764100

C -0.36258800 1.74914900 2.17183300

C -1.69531100 1.08015200 2.33274200

H -3.39607000 -0.98098000 2.24416900

H -3.07403700 -1.43146700 0.57803700

H 2.96731900 -2.08467800 1.63247400

H 2.32971100 -0.64335300 2.34687200

H 3.68122200 0.68929000 0.85247700

H 2.75709300 1.15877200 -0.56353600

H -2.42632500 1.78308300 2.73458900

H -1.55892100 0.33758500 3.12379200

C 2.82399100 -1.46136900 -0.83261600

C -3.24582200 1.20147000 0.39881800
C -4.56069300 1.20979100 1.17296500
C -3.47707400 0.62403800 -0.98941500
C -2.72937100 2.62600100 0.23309600
C 2.49312100 -0.85386900 -2.18731400
C 2.28330200 -2.88614200 -0.80911000
C 4.33641900 -1.47669100 -0.63198200
H -4.43149600 1.54363500 2.20286200
H -5.25991900 1.89405600 0.69372000
H -5.02671400 0.22489500 1.18926300
H -2.57611400 0.69195800 -1.59884600
H -3.80164200 -0.41535300 -0.96970300
H -4.26220400 1.19721500 -1.48187500
H -3.40126500 3.17181200 -0.42759400
H -2.68649100 3.17559900 1.17257100
H -1.73695500 2.62961900 -0.21993700
H 1.42324600 -0.90188800 -2.38542900
H 2.81124600 0.18405500 -2.27800000
H 3.00921100 -1.41757800 -2.96404100
H 2.61290400 -3.45087700 0.06212500
H 1.19283000 -2.89099800 -0.83672600
H 2.64273300 -3.41632500 -1.68978200
H 4.61632900 -1.82770300 0.36168700
H 4.79239100 -2.15050500 -1.35652400
H 4.77497300 -0.49056100 -0.78203600
O -0.40001500 0.87597600 -3.13391600
H -0.66589400 0.00159900 -2.79688100

⁵14

E (SMD/M06-L-D3/def2-TZVP) = -2454.237207 au
H (SMD/M06-L-D3/def2-TZVP) = -2453.673638 au
G (SMD/M06-L-D3/def2-TZVP) = -2453.760381 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2453.5502 au
Mn -0.21287800 -0.14759200 -0.21125700
N -2.21616100 0.40157600 1.14369900
N 2.16880500 -0.66888700 0.26266800
O -0.85073700 -1.29769400 -1.38502600
O 0.00454400 1.24822600 -1.54658800
N -0.28039000 -1.47776800 1.42439400
C 0.83708300 -2.04979600 1.88488700
C 2.13989800 -1.37409100 1.55591600
C 0.76686400 -3.12419400 2.75760900
H 1.67698700 -3.59540400 3.10388300

C -0.47716200 -3.55151600 3.19110700
H -0.55662600 -4.38999200 3.87068800
C -1.61558200 -2.86990100 2.79257400
H -2.59293300 -3.13376900 3.17309300
C -1.48379100 -1.82020600 1.89892100
C -2.64505300 -0.97061900 1.46135000
N 0.48689300 1.19256300 1.28856200
C 1.78174700 1.53461200 1.27904500
C 2.68924000 0.69908600 0.42270100
C 2.24832600 2.56857200 2.07412800
H 3.29777000 2.82888700 2.05689100
C 1.35205600 3.23698400 2.89110600
H 1.68744100 4.06240700 3.50540800
C 0.03638000 2.80976400 2.95825100
H -0.67114800 3.26761700 3.63635900
C -0.36492700 1.75281700 2.15770300
C -1.69304500 1.07713100 2.34317500
H -3.40647600 -1.00268700 2.24920500
H -3.09775700 -1.40903600 0.57038300
H 2.96348700 -2.08229100 1.66474200
H 2.29652600 -0.64299100 2.35472900
H 3.69125700 0.71898500 0.86651400
H 2.77726700 1.15643300 -0.56365800
H -2.41163600 1.77478700 2.77766900
H -1.53052800 0.32746600 3.12311800
C 2.88202000 -1.45781100 -0.81059000
C -3.27337400 1.22172500 0.44039100
C -4.57934400 1.23986700 1.22939300
C -3.52510600 0.65575100 -0.94942900
C -2.74543000 2.64239400 0.27388300
C 2.59152900 -0.83919900 -2.17058700
C 2.32753200 -2.87774500 -0.80969000
C 4.38899600 -1.49008500 -0.57224000
H -4.43368100 1.57220900 2.25775500
H -5.28190200 1.92807800 0.76044200
H -5.05051300 0.25738000 1.25249700
H -2.62787600 0.71370900 -1.56492600
H -3.86546600 -0.37857000 -0.93396700
H -4.30542700 1.24323400 -1.43293000
H -3.42215900 3.20074900 -0.37128400
H -2.67820000 3.18512800 1.21601700
H -1.76090900 2.63892600 -0.19688900
H 1.52322000 -0.85065900 -2.38342600
H 2.95020700 0.18549400 -2.25923300

H 3.09711700 -1.42178900 -2.94035700
H 2.62335700 -3.44689200 0.07095900
H 1.23813000 -2.87149300 -0.87032700
H 2.70874000 -3.41088300 -1.67939000
H 4.63908400 -1.86034600 0.42257400
H 4.86059900 -2.15468800 -1.29549000
H 4.83905800 -0.50487900 -0.69232800
O -0.41447700 0.78592500 -2.87878100
H -0.68398000 -0.14279000 -2.60994900

⁵TS'₂₋₁₄

E (SMD/M06-L-D3/def2-TZVP) = -2530.678221 au
H (SMD/M06-L-D3/def2-TZVP) = -2530.089474 au
G (SMD/M06-L-D3/def2-TZVP) = -2530.18489 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2529.965296 au
Mn -0.19975900 -0.22048800 -0.21087800
N -2.17611000 0.36219000 1.10890600
N 2.13908500 -0.74217900 0.28654300
O -0.84628100 -1.47316300 -1.15746800
O 0.06893800 1.13770400 -1.33476700
N -0.26481600 -1.48158900 1.51969400
C 0.84689500 -2.04839800 1.99102400
C 2.14509200 -1.40012700 1.60947400
C 0.77435300 -3.09360100 2.89864800
H 1.68219300 -3.56011500 3.25686100
C -0.47181700 -3.49964500 3.34601600
H -0.55512000 -4.31370700 4.05417900
C -1.60884500 -2.83353800 2.91707900
H -2.58881200 -3.08836800 3.29701200
C -1.47016300 -1.81454300 1.98986400
C -2.62272200 -0.98993100 1.49326800
N 0.51010800 1.14638900 1.28143700
C 1.80174300 1.48926700 1.24391300
C 2.68708300 0.62405300 0.39516100
C 2.27189900 2.55387600 1.99414400
H 3.32040100 2.81641900 1.96067800
C 1.37583800 3.25556000 2.78449000
H 1.71305900 4.10566600 3.36298300
C 0.05719300 2.83935200 2.86653100
H -0.65055300 3.33320600 3.51864300
C -0.34511100 1.74899100 2.11188600
C -1.67988600 1.08995300 2.29553000
H -3.39361500 -0.96663000 2.27111500

H -3.06691600 -1.47284400 0.62182500
H 2.96521000 -2.11183500 1.71348500
H 2.33499700 -0.64222900 2.37469300
H 3.69602300 0.63331500 0.82118400
H 2.76176500 1.05328700 -0.60483800
H -2.40814400 1.80842500 2.67408400
H -1.54521800 0.37362200 3.11073800
C 2.82613500 -1.58322800 -0.77070800
C -3.22980800 1.15363800 0.35874200
C -4.54365000 1.19828500 1.13344300
C -3.46624900 0.52679400 -1.00682500
C -2.70511100 2.56820500 0.14176400
C 2.53553000 -0.99985500 -2.14439500
C 2.24677400 -2.99138100 -0.71258300
C 4.33522100 -1.63146300 -0.55007700
H -4.41183000 1.57091200 2.14956900
H -5.23941400 1.86760800 0.62868100
H -5.01538700 0.21751900 1.18787100
H -2.56386800 0.55959000 -1.61655900
H -3.80459600 -0.50668900 -0.94764000
H -4.24352600 1.09037900 -1.52232900
H -3.37387200 3.09373300 -0.53831800
H -2.65946500 3.15115300 1.06085900
H -1.71287200 2.54903400 -0.31085800
H 1.46401500 -0.96577400 -2.33907500
H 2.94228200 0.00161300 -2.26813700
H 2.99920500 -1.62908500 -2.90373000
H 2.53988600 -3.53322300 0.18592700
H 1.15748300 -2.96753300 -0.76692200
H 2.61362900 -3.56193400 -1.56448200
H 4.59647200 -1.98247900 0.44844000
H 4.78387300 -2.32047200 -1.26483400
H 4.79752000 -0.65646000 -0.70172700
O -0.46511900 0.71504000 -3.12538600
H -0.62594500 -0.18419900 -2.78446300
O 1.90895200 1.58736500 -4.20796900
H 1.59142400 2.35203200 -4.69763300
H 1.09242500 1.20842200 -3.81240100

⁵TS''₂₋₁₄

E (SMD/M06-L-D3/def2-TZVP) = -2607.145322 au
H (SMD/M06-L-D3/def2-TZVP) = -2606.529433 au
G (SMD/M06-L-D3/def2-TZVP) = -2606.632017 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2606.413877 au
Mn -0.18549700 -0.16806700 -0.19285500
N -2.17793900 0.37829600 1.11221200
N 2.14793500 -0.68952700 0.31822800
O -0.82577800 -1.39227200 -1.18063200
O 0.11927800 1.20583000 -1.30344900
N -0.26746600 -1.46954400 1.50118700
C 0.84058700 -2.04484500 1.97120200
C 2.13956000 -1.37807800 1.62592400
C 0.75972800 -3.11632700 2.84673600
H 1.66429400 -3.58946000 3.20453400
C -0.49119500 -3.54081400 3.26306700
H -0.58077900 -4.37585400 3.94554200
C -1.62539700 -2.86775000 2.83724500
H -2.60945100 -3.13863500 3.19479700
C -1.47821300 -1.82099100 1.94287300
C -2.62643600 -0.98537800 1.45372000
N 0.49960300 1.17156100 1.33224400
C 1.79025900 1.52006800 1.31959800
C 2.69162200 0.67480500 0.46800200
C 2.24600900 2.56886100 2.10049900
H 3.29363800 2.83647100 2.08644000
C 1.33746900 3.24689400 2.89708800
H 1.66369000 4.08434400 3.49982600
C 0.02047000 2.82126400 2.95531400
H -0.69669800 3.29405400 3.61267000
C -0.36752000 1.74815000 2.16954300
C -1.69777300 1.07335700 2.32466200
H -3.40662300 -0.98407500 2.22245300
H -3.05921200 -1.44442000 0.56381700
H 2.96470300 -2.08453500 1.72593200
H 2.31044600 -0.63595600 2.41084200
H 3.69145500 0.67412500 0.91495700
H 2.78811600 1.12513800 -0.52026000
H -2.43585500 1.77223300 2.72060300
H -1.56127800 0.33314700 3.11776000
C 2.85668600 -1.50062600 -0.74844300
C -3.22506500 1.18756500 0.37280400
C -4.55192800 1.19590500 1.12588100
C -3.43067300 0.60711600 -1.01797200
C -2.71055800 2.61396400 0.21693800
C 2.55692900 -0.90708000 -2.11578700
C 2.30731000 -2.92174400 -0.71665800
C 4.36494900 -1.52103300 -0.51886800

H -4.43914100 1.53465000 2.15614300
H -5.24453600 1.87674700 0.63242700
H -5.01613400 0.21028600 1.13876400
H -2.51056000 0.65218800 -1.60045300
H -3.77631300 -0.42559700 -1.00035500
H -4.18952700 1.19268800 -1.53706300
H -3.39295500 3.16563800 -0.42967500
H -2.66408200 3.15755800 1.15958700
H -1.71882300 2.62593700 -0.23938800
H 1.49074300 -0.94848700 -2.33479900
H 2.88669900 0.12639500 -2.21191000
H 3.08246300 -1.48333700 -2.87681800
H 2.61699600 -3.47666400 0.16815800
H 1.21752000 -2.92090900 -0.76510000
H 2.68050800 -3.46550000 -1.58318900
H 4.62542400 -1.86259700 0.48327100
H 4.83032500 -2.20499900 -1.22768200
H 4.81113100 -0.53880200 -0.67180500
O -0.32080200 0.78385300 -3.09815500
H -0.61967300 -0.08097300 -2.75734100
O 1.77493900 0.65200600 -4.90070200
H 1.38921500 1.11581000 -5.64999800
H 1.06570300 0.67562400 -4.22173100
O -2.07561700 2.89452200 -3.31826900
H -1.50507300 2.10279500 -3.20141800
H -2.44619300 3.03927600 -2.44144700

OH⁻

E (SMD/M06-L-D3/def2-TZVP) = -75.950221 au
H (SMD/M06-L-D3/def2-TZVP) = -75.938202 au
G (SMD/M06-L-D3/def2-TZVP) = -75.95775 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -75.933573 au
O -0.77462500 0.72499200 0.00000000
H -1.09528000 1.63049400 0.00000000

H₂O

E (SMD/M06-L-D3/def2-TZVP) = -76.455734 au
H (SMD/M06-L-D3/def2-TZVP) = -76.430794 au
G (SMD/M06-L-D3/def2-TZVP) = -76.452877 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -76.435028 au
O 0.14302600 -0.00111700 0.00000000
H 1.10412900 0.05003900 0.00000000

H -0.12958700 0.92194800 0.00000000

OH-H₂O

E (SMD/M06-L-D3/def2-TZVP) = -152.42019 au
H (SMD/M06-L-D3/def2-TZVP) = -152.382347 au
G (SMD/M06-L-D3/def2-TZVP) = -152.412147 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -152.385931 au
O -0.28644000 -0.58706200 -0.25638100
H 0.72214300 -0.39956400 -0.24593900
H -0.64725600 0.00267000 0.41108600
O 2.26516800 -0.13117500 -0.30038100
H 2.61638200 -0.69812400 0.39161600

OH-2H₂O

E (SMD/M06-L-D3/def2-TZVP) = -228.88886 au
H (SMD/M06-L-D3/def2-TZVP) = -228.823981 au
G (SMD/M06-L-D3/def2-TZVP) = -228.862359 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -228.835812 au
O -0.15885000 -0.86592500 -0.09709800
H 0.78611600 -0.54924200 0.07460900
H -0.69951600 -0.07968600 0.01853600
O 2.33548600 -0.16183300 0.36786200
H 2.63848400 0.24049300 -0.45113400
O 2.70058600 -2.74319500 -0.01127000
H 3.60251800 -2.94156500 0.25528700
H 2.60879200 -1.74650500 0.13381500

⁴⁸

E (SMD/M06-L-D3/def2-TZVP) = -2378.922927 au
H (SMD/M06-L-D3/def2-TZVP) = -2378.361441 au
G (SMD/M06-L-D3/def2-TZVP) = -2378.442615 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2378.249522 au
Mn 0 -0.0244405710 -0.0903058111 0.6672997135
N 0 -2.0757169405 0.3727192467 0.0773389977
N 0 2.0981651368 -0.3733375534 -0.0246884297
O 0 0.0775704246 1.2285703023 1.9758180062
O 0 -0.1002341173 -1.4507593978 1.6785807024
N 0 0.1792113792 1.4676465064 -0.6562808320
C 0 1.3452761934 1.6693521945 -1.2660642003
C 0 2.2601992471 0.4887708230 -1.2455182518
C 0 1.5734130369 2.8548381000 -1.9425718705
H 0 2.5229485855 3.0333190758 -2.4276500616

C	0	0.5492434374	3.7900560151	-1.9908780039
H	0	0.7018077750	4.7238540863	-2.5156819992
C	0	-0.6771203785	3.5295960044	-1.3954840678
H	0	-1.4952854639	4.2332028179	-1.4585490784
C	0	-0.8303400404	2.3343345602	-0.7160384864
C	0	-2.0752595539	1.8673523955	-0.0282424001
N	0	-0.1719398590	-1.2728785680	-0.9620120163
C	0	0.8491011735	-2.0867179410	-1.2375621654
C	0	2.0885332124	-1.8024643439	-0.4521046717
C	0	0.7052717566	-3.0680080659	-2.2005685626
H	0	1.5332109945	-3.7204980150	-2.4391387264
C	0	-0.5179130217	-3.1844298414	-2.8458725801
H	0	-0.6601087626	-3.9567334684	-3.5899679384
C	0	-1.5496637713	-2.3013627834	-2.5660288245
H	0	-2.4970226561	-2.3562567416	-3.0835131773
C	0	-1.3339297889	-1.3218312067	-1.6124317918
C	0	-2.2534817544	-0.1894100203	-1.3096724066
H	0	-2.9558507965	2.2102505336	-0.5747347827
H	0	-2.1281614815	2.2870513561	0.9750783469
H	0	3.2985818770	0.7839638777	-1.3824785151
H	0	2.0111723881	-0.1149722495	-2.1211075738
H	0	2.9715536716	-2.0413729589	-1.0484990843
H	0	2.1123652472	-2.4307617618	0.4384075853
H	0	-3.2930285665	-0.4519798331	-1.4922934155
H	0	-2.0214903560	0.6013324786	-2.0264016510
C	0	3.2101503805	-0.0807685984	0.9969463926
C	0	-3.1913275580	-0.1331577618	1.0172154231
C	0	-4.5237834722	0.5156077724	0.6555052358
C	0	-2.8454529636	0.2074447224	2.4563522453
C	0	-3.2948865202	-1.6446323603	0.8729918100
C	0	2.8650055800	-0.7147699705	2.3333932013
C	0	3.3172050570	1.4269951274	1.1827009109
C	0	4.5433179504	-0.6368940148	0.5058976212
H	0	-4.7791198737	0.4002811525	-0.3972858116
H	0	-5.3077758475	0.0294755525	1.2338806974
H	0	-4.5445821866	1.5754094793	0.9039104460
H	0	-1.9550556988	-0.3249810699	2.7837404181
H	0	-2.6959174312	1.2739530087	2.6149599302
H	0	-3.6789971059	-0.0995064908	3.0869841706
H	0	-3.9506768961	-2.0213263318	1.6559933523
H	0	-3.7253123708	-1.9508060218	-0.0794381772
H	0	-2.3222423885	-2.1206615732	0.9936974856
H	0	1.9896431753	-0.2497470394	2.7803042657
H	0	2.6877853390	-1.7862854610	2.2607833419

H	0	3.7087675603	-0.5699858488	3.0073161586
H	0	3.7481615693	1.9315269839	0.3192618386
H	0	2.3474178223	1.8696718299	1.4055974745
H	0	3.9745407827	1.6238576272	2.0279822397
H	0	4.7920334097	-0.3065008599	-0.5021920124
H	0	5.3308330777	-0.2811619188	1.1684358144
H	0	4.5653820643	-1.7254171447	0.5274046426
H	0	-0.0147061122	0.7789213970	2.8252910980

⁵17

E (SMD/M06-L-D3/def2-TZVP) = -2379.544901 au

H (SMD/M06-L-D3/def2-TZVP) = -2378.972265 au

G (SMD/M06-L-D3/def2-TZVP) = -2379.058572 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2378.879075 au

Mn	0	-0.2259600567	-0.1669244870	-0.1474746373
N	0	-2.1906709904	0.3835498665	1.1387310887
N	0	2.1367752062	-0.6702293178	0.2760577901
O	0	-0.8895525932	-1.3345260251	-1.2286332449
O	0	-0.0107739969	1.3963215300	-1.6595532774
N	0	-0.2738478772	-1.4765303680	1.4960763619
C	0	0.8450011716	-2.0600909641	1.9285967912
C	0	2.1415713956	-1.3875382030	1.5684929362
C	0	0.7763999464	-3.1442215909	2.7890666954
H	0	1.6849400713	-3.6280025815	3.1217663593
C	0	-0.4687700338	-3.5679414117	3.2253647250
H	0	-0.5474611983	-4.4131248724	3.8966060922
C	0	-1.6104039388	-2.8849547926	2.8355055087
H	0	-2.5869670780	-3.1589343808	3.2108325162
C	0	-1.4790539523	-1.8257244655	1.9534957805
C	0	-2.6351565018	-0.9786936707	1.4938626105
N	0	0.4862483292	1.1972246317	1.3054148078
C	0	1.7819536629	1.5350624372	1.2987144628
C	0	2.6819479934	0.6903486115	0.4457318567
C	0	2.2483576739	2.5692465195	2.0930024159
H	0	3.2983998049	2.8269310595	2.0800052971
C	0	1.3499209839	3.2417937457	2.9046893788
H	0	1.6854646059	4.0671907760	3.5187974029
C	0	0.0321888460	2.8197474602	2.9681621545
H	0	-0.6760742741	3.2816137662	3.6425173860
C	0	-0.3679516427	1.7616360604	2.1693364354
C	0	-1.6925917954	1.0823866316	2.3432666611
H	0	-3.3954273176	-0.9749448278	2.2821691351
H	0	-3.0920655255	-1.4366095473	0.6151693139
H	0	2.9661149976	-2.0980339779	1.6443450944

H	0	2.3248840324	-0.6604716963	2.3648897495
H	0	3.6795947923	0.6841939343	0.8980479799
H	0	2.7974065996	1.1497800329	-0.5366454295
H	0	-2.4271038773	1.7771473292	2.7529551164
H	0	-1.5391953068	0.3429046273	3.1341567717
C	0	2.8236605505	-1.4484955071	-0.8254232327
C	0	-3.2474892361	1.1986601261	0.4162740442
C	0	-4.5600686126	1.2161465471	1.1930055917
C	0	-3.4886012089	0.6255065735	-0.9716004118
C	0	-2.7210169820	2.6192194060	0.2454214944
C	0	2.4909406355	-0.8094089545	-2.1665507450
C	0	2.2760267920	-2.8703078200	-0.8236806233
C	0	4.3361503641	-1.4765478590	-0.6288965386
H	0	-4.4272548054	1.5485972364	2.2227547713
H	0	-5.2557044136	1.9050246901	0.7151791219
H	0	-5.0321911998	0.2341784288	1.2093436134
H	0	-2.5938368905	0.6986762894	-1.5882348016
H	0	-3.8066130096	-0.4158798630	-0.9538550272
H	0	-4.2799309104	1.1976313219	-1.4550043342
H	0	-3.3888075071	3.1670803793	-0.4176422775
H	0	-2.6733448952	3.1729404616	1.1820698974
H	0	-1.7294666211	2.6177331030	-0.2081441283
H	0	1.4149371940	-0.8098109506	-2.3405872720
H	0	2.8573177601	0.2132323023	-2.2530463516
H	0	2.9625094341	-1.3840023747	-2.9631100927
H	0	2.5977416131	-3.4446869731	0.0442506706
H	0	1.1858566390	-2.8710733870	-0.8578013678
H	0	2.6398749944	-3.3929449084	-1.7069819270
H	0	4.6137939783	-1.8568572387	0.3546016242
H	0	4.7887312971	-2.1323634672	-1.3718159732
H	0	4.7801277743	-0.4890100304	-0.7511785550
H	0	0.9267162881	1.5807167502	-1.8087154039
H	0	-0.3008439188	0.9658229788	-2.4761477424

⁵5

E (SMD/M06-L-D3/def2-TZVP) = -2379.577198 au

H (SMD/M06-L-D3/def2-TZVP) = -2379.006158 au

G (SMD/M06-L-D3/def2-TZVP) = -2379.092936 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2378.910249 au

Mn	0	-0.0125574272	-0.0941085665	0.9019345581
N	0	-2.2492469502	0.4082022206	0.0457377401
N	0	2.2480234807	-0.3890881736	-0.0438157462
O	0	0.1082307590	1.1957438277	2.2607060990
O	0	-0.1116463398	-1.6596144533	1.9441455001

N	0	0.1729704864	1.4429229710	-0.5118420493
C	0	1.3276262304	1.6431346990	-1.1617960700
C	0	2.2856926108	0.4902701842	-1.2222112618
C	0	1.5418660691	2.8168195125	-1.8644073603
H	0	2.4877654649	2.9741621811	-2.3645455363
C	0	0.5238531786	3.7529697553	-1.9307165300
H	0	0.6718070895	4.6785939296	-2.4712483699
C	0	-0.6999921397	3.4783847045	-1.3444906885
H	0	-1.5368858191	4.1563779641	-1.4393600543
C	0	-0.8506684556	2.2985591386	-0.6361398395
C	0	-2.1565898998	1.8749489011	-0.0304625738
N	0	-0.1831838927	-1.2783481385	-0.8165939347
C	0	0.8456565175	-2.0772006629	-1.1320012877
C	0	2.1493611745	-1.8018411768	-0.4415601132
C	0	0.7015151524	-3.0609960061	-2.0949509786
H	0	1.5420221028	-3.6946243898	-2.3422219793
C	0	-0.5195748922	-3.1967485807	-2.7333986900
H	0	-0.6612549906	-3.9721641465	-3.4746597840
C	0	-1.5415639837	-2.3044354952	-2.4572623666
H	0	-2.4839314447	-2.3435324085	-2.9862611864
C	0	-1.3338865816	-1.3243127620	-1.5014091239
C	0	-2.2889435211	-0.1849658820	-1.3016582146
H	0	-2.9681366204	2.3163375282	-0.6189887473
H	0	-2.2418511486	2.2861839468	0.9762459109
H	0	3.2922611645	0.8485853168	-1.4443095214
H	0	1.9948458079	-0.0904911813	-2.1025774980
H	0	2.9626454173	-2.1091570239	-1.1081205557
H	0	2.2248127773	-2.4234751709	0.4516557025
H	0	-3.2966081403	-0.4777743533	-1.6006315583
H	0	-1.9912430638	0.5768693250	-2.0279222536
C	0	3.3720028398	-0.1099797715	0.9297058899
C	0	-3.3747978265	-0.0816498221	0.9319361690
C	0	-4.7056092688	0.5422806913	0.5259737225
C	0	-3.0605130544	0.2612985011	2.3810433438
C	0	-3.4570538666	-1.5990955160	0.8159259681
C	0	3.0696317824	-0.7836946577	2.2605063537
C	0	3.4407500504	1.3936415049	1.1691970170
C	0	4.7062427655	-0.6127831621	0.3884950575
H	0	-4.9249864361	0.3821523037	-0.5301896462
H	0	-5.5128042109	0.0888561277	1.1000991517
H	0	-4.7269846101	1.6141329664	0.7208628614
H	0	-2.1506097373	-0.2411881296	2.7083974465
H	0	-2.9467029672	1.3307427252	2.5520332603
H	0	-3.8812241309	-0.0795422262	3.0115363356

H	0	-4.1510204462	-1.9740455270	1.5665771615
H	0	-3.8242106066	-1.9312984879	-0.1543044985
H	0	-2.4867130351	-2.0615090007	0.9993825469
H	0	2.1527475188	-0.3887874372	2.6974083668
H	0	2.9768095524	-1.8655820274	2.1792721996
H	0	3.8871428324	-0.5828647208	2.9523163450
H	0	3.7950961425	1.9461398423	0.2998821787
H	0	2.4675568269	1.7889717340	1.4621580595
H	0	4.1388422645	1.5916699364	1.9811189468
H	0	4.9242804108	-0.2096952104	-0.6009849105
H	0	5.5117887265	-0.3021283113	1.0529235270
H	0	4.7331583564	-1.7005005859	0.3275637694
H	0	0.1609588515	-1.4556335688	2.8470046856
H	0	-0.1513398964	0.8006572950	3.1017830544

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E (SMD/M06-L-D3/def2-TZVP) = -2380.656254 au

H (SMD/M06-L-D3/def2-TZVP) = -2380.05939 au

G (SMD/M06-L-D3/def2-TZVP) = -2380.148951 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2379.987742 au

Mn	0	-0.5349262857	0.1332274218	-0.3294182917
N	0	-2.5146951116	0.6744246805	1.1034436764
N	0	1.7774173863	-0.3570749912	0.2157971117
O	0	-1.3501227799	-1.1698609977	-2.0154981545
O	0	-0.2167430114	1.8821688578	-1.8842777684
N	0	-0.6182336592	-1.2317138917	1.4010317001
C	0	0.5053835033	-1.7528926011	1.8934531454
C	0	1.7976380055	-1.0885147889	1.5003252669
C	0	0.4582486325	-2.7486128279	2.8587289397
H	0	1.3745272245	-3.1826234848	3.2364431901
C	0	-0.7776813874	-3.1373157715	3.3483944835
H	0	-0.8420104028	-3.9098180779	4.1037936023
C	0	-1.9271840602	-2.4940550561	2.9137015236
H	0	-2.8945501767	-2.7214317973	3.3407833930
C	0	-1.8090762482	-1.5278538640	1.9285335851
C	0	-2.9610166097	-0.6925253438	1.4390036494
N	0	0.1555450229	1.4906263662	1.3068172305
C	0	1.4418771818	1.8408214000	1.2788258369
C	0	2.3261401613	1.0034008032	0.3937733348
C	0	1.9105820772	2.8851682919	2.0604371915
H	0	2.9564622374	3.1600197745	2.0353678952
C	0	1.0086676781	3.5519212538	2.8754563524
H	0	1.3409874713	4.3851096489	3.4811522178
C	0	-0.3084791576	3.1250251759	2.9478057791

H	0	-1.0153811561	3.5952407896	3.6185494607
C	0	-0.7023759814	2.0574935140	2.1553949310
C	0	-2.0361397600	1.3770265097	2.3092577401
H	0	-3.7475296032	-0.7014391447	2.2019211051
H	0	-3.3883263750	-1.1477515653	0.5439024360
H	0	2.6201827696	-1.8038170357	1.5532237541
H	0	2.0055071718	-0.3718356190	2.3001559870
H	0	3.3356477474	0.9908966920	0.8188701498
H	0	2.4102314023	1.4760774152	-0.5860973170
H	0	-2.7771628754	2.0757635117	2.7030152708
H	0	-1.8983183575	0.6401888306	3.1057978184
C	0	2.4548751216	-1.1329920892	-0.8948878388
C	0	-3.5389900791	1.4748145952	0.3355462895
C	0	-4.8868649459	1.4964229084	1.0487586290
C	0	-3.7008148843	0.8790313688	-1.0551946268
C	0	-3.0153424940	2.8980205441	0.1757320460
C	0	2.1455621329	-0.4775213252	-2.2335517065
C	0	1.8680966217	-2.5392709470	-0.9114969640
C	0	3.9656724499	-1.2004193879	-0.6998535457
H	0	-4.7954683956	1.8455303177	2.0779298845
H	0	-5.5672661252	2.1730520548	0.5327341241
H	0	-5.3524576566	0.5112878486	1.0625434100
H	0	-2.7628019666	0.9200085987	-1.6108056886
H	0	-4.0465942860	-0.1533155175	-1.0408616150
H	0	-4.4394032750	1.4570515082	-1.6096883772
H	0	-3.6456956168	3.4343250963	-0.5319537377
H	0	-3.0257882075	3.4608979031	1.1081966181
H	0	-1.9958546364	2.9021581808	-0.2128017402
H	0	1.0711205697	-0.4403735886	-2.4129345084
H	0	2.5441072857	0.5323109879	-2.3165914137
H	0	2.5968225839	-1.0667374848	-3.0309045211
H	0	2.1721157448	-3.1360954892	-0.0526263886
H	0	0.7779198320	-2.5091820549	-0.9327833646
H	0	2.2068100942	-3.0622302788	-1.8042913183
H	0	4.2371551883	-1.6071748137	0.2743387818
H	0	4.4033205889	-1.8497576327	-1.4573766493
H	0	4.4294018527	-0.2197398351	-0.8022988014
H	0	0.2434039927	2.6083253390	-1.4442019242
H	0	-1.0701255973	2.2612282286	-2.1295487706
H	0	-1.4324194497	-0.6039276005	-2.7937711798
H	0	-0.7121201172	-1.8437945136	-2.2824123295

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E (SMD/M06-L-D3/def2-TZVP) = -2453.599719 au

H (SMD/M06-L-D3/def2-TZVP) = -2453.047669 au

G (SMD/M06-L-D3/def2-TZVP) = -2453.136702 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2452.909162 au

Mn	0	-0.2231153479	-0.1669866331	-0.1946401437
N	0	-2.2077241383	0.3815078689	1.1391247836
N	0	2.1527479980	-0.6787399817	0.2669156790
O	0	-0.8631504787	-1.3396367006	-1.3031176965
O	0	0.0621897962	1.4306573288	-1.5312523634
N	0	-0.2759414171	-1.4836629375	1.4635720087
C	0	0.8432525309	-2.0562496933	1.9133792995
C	0	2.1437783042	-1.3860744443	1.5610647751
C	0	0.7773051668	-3.1273019037	2.7909320375
H	0	1.6880588161	-3.6004196412	3.1330590395
C	0	-0.4654993197	-3.5492505390	3.2340672466
H	0	-0.5420883856	-4.3839831004	3.9185755883
C	0	-1.6069374760	-2.8715401399	2.8359116240
H	0	-2.5826815307	-3.1368423294	3.2196924688
C	0	-1.4782761246	-1.8262346549	1.9366658277
C	0	-2.6404405919	-0.9844651773	1.4827496570
N	0	0.4843229877	1.1810325225	1.3000285389
C	0	1.7785702539	1.5229589220	1.2903779769
C	0	2.6770533266	0.6898537354	0.4244575753
C	0	2.2464208554	2.5554427089	2.0862195983
H	0	3.2959824980	2.8151550822	2.0698011037
C	0	1.3492918523	3.2255628675	2.9013797214
H	0	1.6848896845	4.0505592648	3.5160998003
C	0	0.0319179290	2.8030862750	2.9640647512
H	0	-0.6769005745	3.2654710466	3.6376841185
C	0	-0.3690694648	1.7457863523	2.1634720411
C	0	-1.7011771829	1.0774043558	2.3375228936
H	0	-3.4024537008	-0.9975352094	2.2702586817
H	0	-3.0921266781	-1.4399471710	0.5999924428
H	0	2.9661207588	-2.0978957582	1.6522362951
H	0	2.3196819935	-0.6559936164	2.3566454606
H	0	3.6841824612	0.7061278447	0.8558169520
H	0	2.7546210255	1.1491613163	-0.5619063389
H	0	-2.4259889953	1.7838824657	2.7457041713
H	0	-1.5560336799	0.3402821268	3.1325370461
C	0	2.8535411364	-1.4605600667	-0.8203021834
C	0	-3.2582876951	1.1938024559	0.4136126591
C	0	-4.5664864108	1.2384164907	1.1972586269
C	0	-3.5147001446	0.6031032503	-0.9647970493
C	0	-2.7134906468	2.6039367212	0.2160607389
C	0	2.5369923455	-0.8323817893	-2.1705263221

C	0	2.3072288189	-2.8833262891	-0.8172903718
C	0	4.3639220480	-1.4865062934	-0.6050213899
H	0	-4.4251546600	1.5937192373	2.2182463757
H	0	-5.2626629571	1.9192421825	0.7085326868
H	0	-5.0431132201	0.2592004117	1.2401794149
H	0	-2.6208620117	0.6491640618	-1.5858590095
H	0	-3.8545457617	-0.4309029072	-0.9304430355
H	0	-4.2963625253	1.1829071550	-1.4550263897
H	0	-3.3796395112	3.1543305887	-0.4467593399
H	0	-2.6445529952	3.1693255810	1.1446333847
H	0	-1.7266057883	2.5771366594	-0.2492600908
H	0	1.4632888960	-0.8331539645	-2.3568901225
H	0	2.9036952108	0.1891347349	-2.2623204941
H	0	3.0176849661	-1.4152450278	-2.9557116098
H	0	2.6151703863	-3.4518629413	0.0595507816
H	0	1.2175489396	-2.8836903441	-0.8682538733
H	0	2.6844090096	-3.4122635328	-1.6912673977
H	0	4.6297359603	-1.8602825522	0.3843969521
H	0	4.8273691019	-2.1460410413	-1.3380340921
H	0	4.8083981751	-0.4991166310	-0.7272428315
O	0	-0.2518378181	1.2757503972	-2.8005626795

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E (SMD/M06-L-D3/def2-TZVP) = -2380.176815 au

H (SMD/M06-L-D3/def2-TZVP) = -2379.594892 au

G (SMD/M06-L-D3/def2-TZVP) = -2379.68748 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2379.508941 au

Mn	0	-0.5433312043	0.1727096596	-0.4206472961
N	0	-2.5375337680	0.7174319687	1.0708765281
N	0	1.8055450623	-0.3390819582	0.2079963444
O	0	-1.2850901158	-1.1686541002	-1.7682789695
O	0	-0.2089683594	1.9346043327	-2.0297165331
N	0	-0.6231289811	-1.1635169912	1.3810087647
C	0	0.4871478189	-1.7503224132	1.8269944350
C	0	1.7853999859	-1.0609831869	1.4973965316
C	0	0.4149748912	-2.8454658349	2.6753897789
H	0	1.3191556967	-3.3321598351	3.0170113642
C	0	-0.8355036813	-3.2766923471	3.0917757460
H	0	-0.9208949563	-4.1290828476	3.7534569807
C	0	-1.9733117727	-2.5889681271	2.6979378357
H	0	-2.9527863251	-2.8671510398	3.0637470084
C	0	-1.8275947059	-1.5180564977	1.8289835905
C	0	-2.9778129569	-0.6546606141	1.3775716251
N	0	0.1499977433	1.5372061758	1.2453306123

C	0	1.4459648893	1.8553249196	1.2656789217
C	0	2.3378851316	1.0260202289	0.3823074986
C	0	1.9268924682	2.8439678495	2.1101793842
H	0	2.9810498495	3.0867443651	2.1201455417
C	0	1.0301476789	3.4900300673	2.9469152489
H	0	1.3717298222	4.2812385806	3.6018359200
C	0	-0.2929849543	3.0807827612	2.9831503449
H	0	-0.9980800203	3.5184406099	3.6777535126
C	0	-0.6977420535	2.0645502743	2.1294273782
C	0	-2.0333653967	1.3868699793	2.2795413247
H	0	-3.7555587921	-0.6845845872	2.1503420207
H	0	-3.4206116928	-1.0869111647	0.4782528936
H	0	2.6172037489	-1.7620410160	1.5913470427
H	0	1.9426877459	-0.3347111909	2.3002453941
H	0	3.3470031694	1.0303418913	0.8102380388
H	0	2.4163793996	1.4951394627	-0.5996825033
H	0	-2.7614290338	2.0806568308	2.7065110795
H	0	-1.8851162527	0.6317903274	3.0570537905
C	0	2.5132491844	-1.1182632908	-0.8762372999
C	0	-3.5746922601	1.5429350849	0.3505212770
C	0	-4.9029995335	1.5654206002	1.1008990534
C	0	-3.7862313073	0.9881088524	-1.0499494844
C	0	-3.0379592720	2.9623221085	0.2014044075
C	0	2.2284533991	-0.4735855890	-2.2264145847
C	0	1.9391515381	-2.5298035767	-0.8980753630
C	0	4.0203171375	-1.1745813307	-0.6447340734
H	0	-4.7826469030	1.8919314504	2.1344388369
H	0	-5.5898376120	2.2589733396	0.6165674843
H	0	-5.3784997445	0.5848167331	1.1066771570
H	0	-2.8627249303	1.0382340240	-1.6282747909
H	0	-4.1369385944	-0.0427122554	-1.0549522934
H	0	-4.5380525022	1.5874819926	-1.5628770991
H	0	-3.6957099070	3.5278083128	-0.4569896650
H	0	-2.9852139203	3.5013914849	1.1463316564
H	0	-2.0426326368	2.9563770581	-0.2458892021
H	0	1.1551993698	-0.4319329399	-2.4186187431
H	0	2.6357735073	0.5325448497	-2.3131181970
H	0	2.6869347809	-1.0727384393	-3.0124635574
H	0	2.2114692116	-3.1105605080	-0.0175624645
H	0	0.8511210627	-2.5056983069	-0.9764258869
H	0	2.3259772905	-3.0615001066	-1.7662724672
H	0	4.2689752430	-1.5747157395	0.3386185746
H	0	4.4820329844	-1.8251448708	-1.3869178841
H	0	4.4818319604	-0.1920080366	-0.7395355049

H	0	-0.4218077404	2.8063094684	-1.6749141811
H	0	-0.9143587919	1.7604440118	-2.6654395385
H	0	-1.0154420930	-0.8985319136	-2.6517933458

716

E (SMD/M06-L-D3/def2-TZVP) = -2453.449387 au

H (SMD/M06-L-D3/def2-TZVP) = -2452.895941 au

G (SMD/M06-L-D3/def2-TZVP) = -2452.98571 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2452.751217 au

Mn	0	-0.2252773471	-0.1901279258	-0.0994231283
N	0	-2.1705737276	0.3377708810	1.1323530642
N	0	2.0978363543	-0.6712707290	0.2876749817
O	0	-0.8524550232	-1.3415253613	-1.2005673648
O	0	0.6537389166	2.0579749653	-1.8465884196
N	0	-0.2647758953	-1.4962475350	1.5573848086
C	0	0.8599658399	-2.0709726551	1.9783811490
C	0	2.1441705734	-1.3953773842	1.5805052319
C	0	0.8043707246	-3.1451451118	2.8519405701
H	0	1.7160567124	-3.6250063185	3.1815997399
C	0	-0.4370828376	-3.5647111802	3.3048049571
H	0	-0.5066113876	-4.4011518324	3.9879261818
C	0	-1.5871870367	-2.8950492017	2.9142548746
H	0	-2.5591380215	-3.1738774232	3.2978419485
C	0	-1.4659818277	-1.8461144111	2.0186024586
C	0	-2.6220891332	-1.0133567122	1.5310139774
N	0	0.4766606185	1.1954983238	1.3204346015
C	0	1.7731848719	1.5306308359	1.3166293608
C	0	2.6571276303	0.6893285542	0.4472491134
C	0	2.2401432597	2.5557557502	2.1205055695
H	0	3.2901911236	2.8131380621	2.1118394677
C	0	1.3395413260	3.2212739309	2.9369696762
H	0	1.6755833718	4.0393403942	3.5604678090
C	0	0.0197355190	2.8044783510	2.9921466503
H	0	-0.6885064917	3.2639051367	3.6679794018
C	0	-0.3805181916	1.7551487426	2.1815642506
C	0	-1.7085589089	1.0805456929	2.3318600763
H	0	-3.3853345468	-0.9762068919	2.3148477972
H	0	-3.0767162023	-1.4989121090	0.6665729631
H	0	2.9719185985	-2.1041975409	1.6217568971
H	0	2.3537990586	-0.6698182410	2.3713642308
H	0	3.6633577382	0.6722198132	0.8774832884
H	0	2.7474740804	1.1484533236	-0.5373297753
H	0	-2.4575075337	1.7883956294	2.6872128456
H	0	-1.5855333856	0.3674087629	3.1515304642

C	0	2.7587494304	-1.4461368727	-0.8370698011
C	0	-3.2112691589	1.1312248330	0.3587298715
C	0	-4.5230809746	1.2275136896	1.1300545808
C	0	-3.4715957715	0.4833799561	-0.9919235108
C	0	-2.6327937257	2.5173738436	0.1033863776
C	0	2.4123764106	-0.7788627423	-2.1604151299
C	0	2.1945733289	-2.8608387220	-0.8387173593
C	0	4.2736219154	-1.4935891899	-0.6685460814
H	0	-4.3929662842	1.6297815406	2.1342824801
H	0	-5.2048023792	1.8916386751	0.6002639263
H	0	-5.0110642462	0.2566361499	1.2122467291
H	0	-2.5751684827	0.4893697045	-1.6091957935
H	0	-3.8253254335	-0.5432816967	-0.9131242243
H	0	-4.2444079673	1.0536154791	-1.5063694150
H	0	-3.2777348935	3.0536467855	-0.5908766013
H	0	-2.5556868522	3.1225600139	1.0058436315
H	0	-1.6422897352	2.4431207473	-0.3501123840
H	0	1.3326302061	-0.6934585593	-2.2843424271
H	0	2.8556557668	0.2104519250	-2.2639847329
H	0	2.7982190973	-1.3865373461	-2.9781977222
H	0	2.5168751446	-3.4422987002	0.0242973482
H	0	1.1045411281	-2.8465971084	-0.8657508669
H	0	2.5474006228	-3.3831668341	-1.7266198813
H	0	4.5674110099	-1.9084704103	0.2958260285
H	0	4.7026367127	-2.1308149688	-1.4409973089
H	0	4.7259294778	-0.5077086223	-0.7705040570
O	0	-0.2319771667	1.6242588444	-2.5409773954

³²(CF3)

E (SMD/M06-L-D3/def2-TZVP) = -2737.965014 au

H (SMD/M06-L-D3/def2-TZVP) = -2737.635287 au

G (SMD/M06-L-D3/def2-TZVP) = -2737.713451 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2737.255255 au

Mn	0	-0.0127598944	-1.4333508673	-0.0172807602
N	0	2.1284006586	-0.8274657717	-0.0200884940
N	0	-2.1311207259	-0.8112478144	0.0026384670
O	0	-0.0369319571	-2.3531099980	-1.3694060864
O	0	-0.0007851357	-2.3934757497	1.3065892281
N	0	-0.0078435112	0.2579716768	-1.2757879473
C	0	-1.1787961120	0.7999208848	-1.6073627172
C	0	-2.3673794043	-0.0286918165	-1.2601857453
C	0	-1.2301462300	2.0053129681	-2.2817063084
H	0	-2.1841081486	2.4411180719	-2.5417569621
C	0	-0.0342193532	2.6310166817	-2.5994000656

H	0	-0.0445099090	3.5809900815	-3.1160912617
C	0	1.1737414413	2.0488466620	-2.2506027434
H	0	2.1177080993	2.5185774442	-2.4873921929
C	0	1.1497251280	0.8406763323	-1.5762895567
C	0	2.3663646038	0.0602031690	-1.2117428880
N	0	0.0125474584	0.2248036385	1.2848845471
C	0	-1.1397618463	0.8119420264	1.5974009976
C	0	-2.3623606451	0.0499469971	1.2161496980
C	0	-1.1539558228	2.0075578768	2.2936896619
H	0	-2.0939639224	2.4810158176	2.5386315769
C	0	0.0589274388	2.5733102073	2.6523576380
H	0	0.0773713311	3.5140343493	3.1855132918
C	0	1.2491666774	1.9433083030	2.3224854184
H	0	2.2069287947	2.3665504659	2.5892468222
C	0	1.1878241738	0.7510315940	1.6257905098
C	0	2.3699467675	-0.0786472475	1.2603528709
H	0	3.2213965083	0.7076039480	-1.0193620793
H	0	2.6217107910	-0.5795485080	-2.0571851029
H	0	-2.5336538473	-0.7452055331	-2.0655093261
H	0	-3.2681505716	0.5744255053	-1.1550359226
H	0	-3.2121289251	0.7080802194	1.0385198712
H	0	-2.6222811206	-0.6085653511	2.0455969300
H	0	2.5283866429	-0.8152899755	2.0488967053
H	0	3.2756152146	0.5199031481	1.1722097438
C	0	3.0318496865	-1.9721740806	-0.0858193934
C	0	-3.0519092056	-1.9456949524	0.0398888666
F	0	-2.8724225419	-2.6587821328	1.1379794351
F	0	-4.3219120152	-1.5260694121	0.0262318332
F	0	-2.8711688233	-2.7285639004	-1.0092001650
F	0	2.8432988936	-2.7770079854	0.9458168309
F	0	2.8389459444	-2.6578172484	-1.1995811625
F	0	4.3089204144	-1.5734514242	-0.0666366830

$^5\text{TS}''_{2-14}(\text{H})$

E (SMD/M06-L-D3/def2-TZVP) = -2292.5906 au

H (SMD/M06-L-D3/def2-TZVP) = -2292.208969 au

G (SMD/M06-L-D3/def2-TZVP) = -2292.291321 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2292.024177 au

Mn	0	-0.3012558353	-0.0643178923	-0.4797174408
N	0	-2.2125412524	0.3556524021	0.7537760726
N	0	1.9489010163	-0.5127127593	-0.1968590138
O	0	-0.8256274647	-1.2842766726	-1.5496268644
O	0	-0.0967111259	1.3574140436	-1.5764358154
N	0	-0.1834875630	-1.4074508631	1.2388788395

C	0	0.9979613786	-1.9429251714	1.5564617918
C	0	2.0835363713	-1.7738624029	0.5342470659
C	0	1.1760672110	-2.6153461379	2.7540787740
H	0	2.1413135908	-3.0386301247	2.9965312505
C	0	0.1064191509	-2.7077812916	3.6296156513
H	0	0.2227476922	-3.2172066938	4.5772006027
C	0	-1.1028426730	-2.1180470918	3.3011201229
H	0	-1.9462979462	-2.1462259060	3.9774722138
C	0	-1.2131680790	-1.4623636434	2.0857008125
C	0	-2.4758951725	-0.7972336597	1.6245715360
N	0	0.3344517489	1.2550476393	1.1073626376
C	0	1.6339228523	1.3249783887	1.4095174991
C	0	2.5653170295	0.6495424210	0.4477302793
C	0	2.0645837975	2.0011007693	2.5389061744
H	0	3.1197228867	2.0411124238	2.7723547961
C	0	1.1205091082	2.5963196671	3.3589245107
H	0	1.4312519489	3.1222039519	4.2521230270
C	0	-0.2251570726	2.4915093113	3.0469999033
H	0	-0.9868461665	2.9204497341	3.6834954214
C	0	-0.5896634874	1.8006365270	1.9038421729
C	0	-2.0107485032	1.6264489150	1.4619094246
H	0	-3.0905563739	-0.5220173125	2.4858773927
H	0	-3.0519422509	-1.5199153247	1.0424943554
H	0	2.0032289238	-2.5851744200	-0.1928583942
H	0	3.0636954239	-1.8695589138	1.0098918111
H	0	3.4990333143	0.3882190314	0.9537461788
H	0	2.8223042078	1.3622557152	-0.3401353680
H	0	-2.2559013452	2.4300404282	0.7628755002
H	0	-2.6860848190	1.7292091452	2.3154842897
O	0	-0.4110047425	0.9090638464	-3.3518430265
H	0	-0.6261588318	0.0096926961	-3.0274016411
O	0	2.3540691054	0.2711372155	-3.1400723491
H	0	2.7554035856	1.0281902753	-2.6997882313
H	0	1.4071692571	0.5187786053	-3.1989558151
O	0	-2.9757036529	1.7577497607	-2.4732145155
H	0	-2.0831337222	1.4939059824	-2.7779670900
H	0	-2.8030122854	2.1539116913	-1.6124324566
H	0	-2.9899488441	0.4656714376	0.1161487502
H	0	2.3127063684	-0.5999893432	-1.1404942764

³²(H)

E (SMD/M06-L-D3/def2-TZVP) = -2063.722238 au

H (SMD/M06-L-D3/def2-TZVP) = -2063.406719 au

G (SMD/M06-L-D3/def2-TZVP) = -2063.468796 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2063.210588 au

Mn	0	-0.5157620857	0.2195529244	-0.2197655615
N	0	-2.3751434238	0.5843282189	0.7455633201
N	0	1.5727238855	-0.1663413799	-0.0169099456
O	0	-0.9396000777	-1.1066031839	-1.1002314702
O	0	-0.4519638515	1.5474756074	-1.1928280289
N	0	-0.4420343533	-1.0811273445	1.4251149747
C	0	0.7072834478	-1.6905505944	1.7060371286
C	0	1.7771969622	-1.4557267299	0.6924944075
C	0	0.7996550251	-2.5204112569	2.8093980315
H	0	1.7335567299	-3.0110507256	3.0445966825
C	0	-0.3310734193	-2.7009446060	3.5919467385
H	0	-0.2834412166	-3.3371941602	4.4655584681
C	0	-1.5243229877	-2.0771860379	3.2598341295
H	0	-2.4192195193	-2.2192588729	3.8490403607
C	0	-1.5477294002	-1.2603007569	2.1434014851
C	0	-2.7529576399	-0.5906460764	1.5727842672
N	0	0.0310104081	1.4725886315	1.3699836742
C	0	1.3231992368	1.6098994060	1.6591043076
C	0	2.2325428667	0.9816402106	0.6570879253
C	0	1.7121363287	2.3434979411	2.7657859735
H	0	2.7602294449	2.4471679889	3.0085265158
C	0	0.7262012144	2.9282937808	3.5464923736
H	0	1.0029417815	3.4952358826	4.4253269856
C	0	-0.6120691810	2.7907107630	3.2095543891
H	0	-1.3936809173	3.2464877093	3.8007083651
C	0	-0.9323470110	2.0426285512	2.0907681833
C	0	-2.2985323805	1.8469968023	1.5246889364
H	0	-3.4654276582	-0.3015122358	2.3457614325
H	0	-3.2589844528	-1.3008189446	0.9163225131
H	0	1.7196724031	-2.2497882062	-0.0544428445
H	0	2.7742029883	-1.4986100965	1.1318325290
H	0	3.1797979255	0.6741828368	1.1010608393
H	0	2.4607246392	1.7223695610	-0.1113511692
H	0	-2.5063793778	2.6675818804	0.8356460150
H	0	-3.0689469756	1.8682189995	2.2960602724
H	0	-3.0886549352	0.7033074718	0.0348104626
H	0	1.9785824172	-0.2550009089	-0.9418323977

³2(Me)

E (SMD/M06-L-D3/def2-TZVP) = -2142.34550212 au

H (SMD/M06-L-D3/def2-TZVP) = -2141.972002 au

G (SMD/M06-L-D3/def2-TZVP) = -2142.039629 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2141.79559162 au

Mn	0	-0.5079435395	0.2233536418	-0.1872676749
N	0	-2.3935820323	0.6721679652	0.7464607848
N	0	1.5838942343	-0.2524828783	-0.0284914772
O	0	-0.9885423684	-1.0809033169	-1.0712474176
O	0	-0.3770462205	1.5525259756	-1.1539041939
N	0	-0.4815503019	-1.0551709156	1.4701821952
C	0	0.6630739567	-1.6539979765	1.7883011815
C	0	1.7103918687	-1.5308288423	0.7343301423
C	0	0.7637096838	-2.3769182053	2.9638284122
H	0	1.6928168401	-2.8619830569	3.2274024335
C	0	-0.3528718609	-2.4534254767	3.7836290108
H	0	-0.2978314990	-3.0013965188	4.7146707536
C	0	-1.5394123085	-1.8335877127	3.4198370009
H	0	-2.4206717419	-1.8911257895	4.0427602354
C	0	-1.5712600845	-1.1284712830	2.2296764757
C	0	-2.7676165421	-0.4821516276	1.6178774378
N	0	0.0839872601	1.4324769065	1.4142809561
C	0	1.3753014432	1.4703587160	1.7329726356
C	0	2.2611518021	0.8632775629	0.6989199080
C	0	1.7846291513	2.1028018806	2.8935204481
H	0	2.8322272138	2.1312804433	3.1575102386
C	0	0.8174066095	2.6842317049	3.7002471360
H	0	1.1091996741	3.1729232400	4.6201946439
C	0	-0.5213534334	2.6411689511	3.3389388764
H	0	-1.2872432708	3.0929363780	3.9531715811
C	0	-0.8612321086	1.9931564078	2.1646545180
C	0	-2.2226816282	1.9112348371	1.5627704725
H	0	-3.4998023521	-0.1660995310	2.3624339188
H	0	-3.2542089573	-1.2209900147	0.9777890844
H	0	1.5634688166	-2.3445243237	0.0209177109
H	0	2.7209993178	-1.6287294340	1.1335623306
H	0	3.2102055414	0.5181548342	1.1116699495
H	0	2.4900071636	1.6345647052	-0.0393414330
H	0	-2.3409773454	2.7600012139	0.8860210065
H	0	-3.0155628258	1.9786243610	2.3092900637
C	0	-3.4514134846	0.8898002147	-0.2575321884
H	0	-3.5638780651	-0.0087530950	-0.8577744910
H	0	-4.4003181024	1.1173521918	0.2329914143
H	0	-3.1699639826	1.7208653694	-0.8982568431
C	0	2.2022151860	-0.4145543367	-1.3570578634
H	0	2.1001331968	0.5126932222	-1.9140221290
H	0	3.2615590319	-0.6604174843	-1.2566552934
H	0	1.6969055344	-1.2145542437	-1.8909334515

O2

E (SMD/M06-L-D3/def2-TZVP) = -150.37011 au
H (SMD/M06-L-D3/def2-TZVP) = -150.363042 au
G (SMD/M06-L-D3/def2-TZVP) = -150.386312 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -150.318089 au
O 0 -1.4277338185 -3.1467661200 0.0000000000
O 0 -2.6318762415 -3.1467661200 0.0000000000

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E (SMD/M06-L-D3/def2-TZVP) = -2378.209725 au
H (SMD/M06-L-D3/def2-TZVP) = -2377.662277 au
G (SMD/M06-L-D3/def2-TZVP) = -2377.74899 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2377.533709 au
Mn 0 0.0342556246 -0.0297470932 0.9198140792
N 0 0.1783668407 -1.3261009756 -0.7255882811
N 0 2.2481003284 0.3897825230 0.0556251481
N 0 -0.1577048440 1.4310095456 -0.5445038754
N 0 -2.2303951856 -0.3820221508 0.0433111764
O 0 -0.1088924567 1.1688556793 2.2828894705
O 0 0.0588592621 -1.0191752586 2.6241699655
C 0 -0.8655261218 -2.1176812760 -1.0135164012
C 0 -0.7482699367 -3.1218368006 -1.9575874669
C 0 0.4637265239 -3.2887799439 -2.6065842026
C 0 1.5022458665 -2.4080468560 -2.3587621070
C 0 1.3205421744 -1.4052866339 -1.4211899644
C 0 2.3016041187 -0.2845888242 -1.2551614649
C 0 2.1805002115 1.8520313990 -0.1078744221
C 0 0.8823569337 2.2522588073 -0.7474387660
C 0 0.7467881974 3.3662587380 -1.5561844827
C 0 -0.4782267620 3.6103532475 -2.1550117046
C 0 -1.5132645571 2.7045426039 -1.9986078166
C 0 -1.3146506079 1.5914348900 -1.1990177151
C 0 -2.2940122355 0.4532481360 -1.1670753860
C 0 -2.1465197009 -1.8123655231 -0.2994451647
C 0 -3.3343169699 -0.0662390725 1.0287929584
C 0 -4.6931980875 -0.5263416438 0.5105812866
C 0 -3.0364705926 -0.7588481359 2.3507445222
C 0 -3.3491665997 1.4401117354 1.2582796370
C 0 3.3439356634 -0.0804593068 0.9897717524
C 0 4.7155020993 0.3861404800 0.5147947589
C 0 3.2808627526 -1.6013703320 1.0461731549
C 0 3.0893895766 0.4426474219 2.3950389969
H 0 3.0978651208 1.5298111188 2.4579054626
H 0 2.1357228762 0.0841377850 2.7802800114

H	0	3.8791312253	0.0778942582	3.0506307928
H	0	-1.6003077262	-3.7487278856	-2.1807301496
H	0	0.5857267407	-4.0812013608	-3.3331747902
H	0	2.4384717779	-2.4738940559	-2.8957679094
H	0	3.3064346523	-0.6280897557	-1.5038890109
H	0	2.0535028080	0.4426600949	-2.0336985750
H	0	3.0043762113	2.2464712438	-0.7116379592
H	0	2.2585127550	2.3182353323	0.8747553461
H	0	1.5950826182	4.0165495190	-1.7185550894
H	0	-0.6132802166	4.4858632169	-2.7762584741
H	0	-2.4588186815	2.8343457333	-2.5071854085
H	0	-3.3008708664	0.8249323824	-1.3622598509
H	0	-2.0522855344	-0.1665212235	-2.0356140297
H	0	-2.9830858214	-2.1473194913	-0.9213545934
H	0	-2.1883097047	-2.3935960478	0.6229682480
H	0	-5.4710427147	-0.2190222799	1.2087137764
H	0	-4.9337995510	-0.0883768151	-0.4583437492
H	0	-4.7453315665	-1.6108473355	0.4191752274
H	0	-3.1180099476	-1.8428020822	2.2896836077
H	0	-2.0372671179	-0.5042279968	2.7095556816
H	0	-3.7534100834	-0.4259608673	3.1004287564
H	0	-4.0403531827	1.6717087185	2.0670341844
H	0	-2.3616175507	1.8029990575	1.5453654132
H	0	-3.6839501202	1.9944670965	0.3821390567
H	0	5.4864659213	-0.0291282574	1.1626988319
H	0	4.9365908660	0.0628210332	-0.5022055417
H	0	4.8037251743	1.4716427294	0.5547275892
H	0	3.9720191186	-1.9619136578	1.8062416652
H	0	2.2773583727	-1.9337510869	1.3229826206
H	0	3.5583786314	-2.0768945004	0.1061201739

⁵TS''₂₋₁₄(CF3)

E (SMD/M06-L-D3/def2-TZVP) = -2966.852922 au

H (SMD/M06-L-D3/def2-TZVP) = -2966.45784 au

G (SMD/M06-L-D3/def2-TZVP) = -2966.556207 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2966.086465 au

Mn -0.05477200 0.64002600 -0.31913900

N -2.34463700 -0.22182900 0.02575200

N 2.29253500 -0.24748000 -0.29460000

O -0.13566500 1.38664000 -1.81388700

O 0.13077000 1.89975500 0.89763200

N -0.10910300 -1.41630600 -1.17875000

C 1.00903100 -2.13817700 -1.29455000

C 2.33635200 -1.45967600 -1.13416400

C 0.97176700 -3.49336700 -1.58879100
H 1.89866600 -4.04414700 -1.67170200
C -0.25143300 -4.11323800 -1.74804900
H -0.30584400 -5.17052500 -1.96968700
C -1.40766100 -3.37102800 -1.58031400
H -2.38625100 -3.82419500 -1.65457900
C -1.29947200 -2.02441800 -1.28640900
C -2.51852600 -1.18188000 -1.08661800
N 0.06840700 -0.77109800 1.36248000
C 1.27663900 -1.22454000 1.72572100
C 2.46853700 -0.52633300 1.14953400
C 1.41655200 -2.28625500 2.60021200
H 2.40528200 -2.63191300 2.86747100
C 0.27740600 -2.89828100 3.09593400
H 0.35876900 -3.73607100 3.77520500
C -0.96339000 -2.44993600 2.68604700
H -1.87489900 -2.92355100 3.02358000
C -1.03408100 -1.38025200 1.80638000
C -2.36628100 -0.85626400 1.36232400
H -3.38828700 -1.81955900 -0.91458600
H -2.70057400 -0.60735200 -1.99512100
H 2.69168500 -1.17928600 -2.12599300
H 3.06239800 -2.17183400 -0.73430600
H 3.36644000 -1.12389000 1.32118100
H 2.59864900 0.42991300 1.65900900
H -2.68841700 -0.10689200 2.08669600
H -3.10635600 -1.65884400 1.38842600
O 0.40216800 3.66738700 0.15285900
H 0.65283800 3.21736800 -0.67075800
O 2.22763400 3.76275900 2.26370000
H 2.34099200 2.84193200 2.52015800
H 1.62724700 3.70934500 1.49154800
O -2.07612200 4.41854600 -0.83579400
H -1.22570800 4.13007500 -0.43792300
H -2.21499700 3.78443800 -1.54637400
C 3.21324900 0.73457700 -0.75391600
C -3.29660100 0.83635200 -0.04752800
F -3.04632300 1.76533300 0.87181900
F -3.27931900 1.41890400 -1.24310800
F -4.56347900 0.41621300 0.16087400
F 3.11128200 1.85804600 -0.05012000
F 3.00145400 1.02965800 -2.03496000
F 4.50132300 0.33372700 -0.65882600

⁵TS''₂₋₁₄(Me)

E (SMD/M06-L-D3/def2-TZVP) = -2371.21221426 au
H (SMD/M06-L-D3/def2-TZVP) = -2370.773883 au
G (SMD/M06-L-D3/def2-TZVP) = -2370.861855 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2370.60691442 au
Mn 0.81883100 0.31828900 -0.38510500
N -0.19413400 2.25670900 0.45295700
N 0.36555100 -1.92232300 -0.92223000
O 1.54207500 0.85034000 -1.82299000
O 2.21664200 -0.06107800 0.70559400
N -1.22667700 0.31948400 -1.21545900
C -1.73352300 -0.83757700 -1.64802400
C -0.73685000 -1.92708300 -1.89877700
C -3.09301100 -0.98557000 -1.86944700
H -3.48244900 -1.93249600 -2.21765400
C -3.92852900 0.08941300 -1.61501900
H -4.99561100 -0.00285200 -1.76877400
C -3.39463700 1.27275100 -1.13185500
H -4.02315800 2.11988100 -0.89359700
C -2.02605700 1.35039900 -0.93337300
C -1.33461400 2.57643700 -0.42468800
N -0.43601400 -0.38436700 1.23083900
C -0.79324600 -1.67249300 1.24497100
C -0.00448900 -2.57399300 0.34694200
C -1.81923500 -2.11804400 2.06120100
H -2.09563800 -3.16337800 2.05595700
C -2.48730400 -1.19857200 2.85300000
H -3.29966400 -1.52003600 3.49124900
C -2.13293500 0.13934800 2.79876100
H -2.65747000 0.88608800 3.37868100
C -1.09671300 0.51848700 1.96236000
C -0.61980200 1.93048300 1.82767700
H -2.04346500 3.24436800 0.07475100
H -0.93439100 3.12041000 -1.28372900
H -0.29413600 -1.75711300 -2.88336700
H -1.23197300 -2.90272800 -1.93679400
H -0.54343500 -3.51062800 0.17218800
H 0.92529600 -2.83454900 0.85975100
H 0.25441100 2.05359900 2.47154700
H -1.37970400 2.63232900 2.18472700
O 3.86410100 -0.09667300 -0.10803700
H 3.41833600 -0.12745300 -0.97134600
O 4.10369100 -2.53219600 1.20271800
H 3.20479900 -2.68779700 1.51119100

H 4.02335000 -1.69635300 0.69501300
 O 4.09023900 2.66170600 -0.34416400
 H 4.03329200 1.69032500 -0.21224100
 H 3.27136000 2.86390100 -0.81060700
 C 1.55608500 -2.55487900 -1.49234500
 H 2.37250100 -2.50383700 -0.77371400
 H 1.37914000 -3.60578200 -1.74590800
 H 1.85044600 -2.02420200 -2.39589300
 C 0.75621800 3.37058600 0.47195300
 H 1.08717200 3.57763000 -0.54424400
 H 0.30865700 4.28126900 0.88425100
 H 1.61834700 3.10071900 1.07844100

MECP1

Energy of Triplet State: -2378.2542902900

Energy of Quintet State: -2378.2542928200

25	-0.4783083	0.2213493	-0.0318364
7	-2.3727839	0.6853327	0.9697135
7	1.6458551	-0.2769738	0.1829538
8	-1.1017882	-0.9513707	-1.1421719
8	-0.2905942	1.4594235	-1.2272571
7	-0.5917428	-1.1569599	1.4507953
6	0.5250773	-1.7452894	1.8747218
6	1.7769163	-1.0394259	1.4757277
6	0.4465548	-2.8459437	2.7097163
1	1.3480285	-3.3382062	3.0466327
6	-0.8097532	-3.2806097	3.1063163
1	-0.8975640	-4.1392495	3.7585807
6	-1.9544017	-2.6109426	2.6951017
1	-2.9371836	-2.9169512	3.0245644
6	-1.8097088	-1.5315139	1.8440441
6	-2.9085318	-0.6730617	1.3011045
7	0.1823338	1.5183947	1.3794547
6	1.4634964	1.8837855	1.3204601
6	2.2796635	1.0668911	0.3685480
6	1.9194425	2.9177271	2.1164169
1	2.9576986	3.2158118	2.0805414
6	1.0103982	3.5530122	2.9517242
1	1.3386108	4.3767672	3.5715728
6	-0.3083497	3.1275499	3.0181819
1	-1.0198922	3.5923497	3.6861025
6	-0.6970416	2.0720046	2.2121332
6	-2.0152973	1.3759328	2.2601278
1	-3.7258492	-0.6022332	2.0207983

1	-3.3090093	-1.1177246	0.3902538
1	2.6301009	-1.7135633	1.4479849
1	1.9990687	-0.3227003	2.2687240
1	3.3024791	0.9655425	0.7354173
1	2.3246866	1.5639323	-0.6003202
1	-2.8127935	2.0419758	2.5818381
1	-1.9401407	0.6154204	3.0398155
6	2.2873143	-1.0637866	-0.9781477
6	-3.3864094	1.5261478	0.1671029
6	-4.7494973	1.5150186	0.8513749
6	-3.5320245	0.9617747	-1.2353260
6	-2.8646751	2.9530554	0.0754568
6	1.9172013	-0.4238755	-2.3048272
6	1.7525450	-2.4885286	-0.9488155
6	3.8061534	-1.0765216	-0.8394803
1	-4.7032933	1.8139577	1.8975207
1	-5.3924612	2.2286948	0.3389316
1	-5.2306947	0.5403189	0.7901425
1	-2.6085179	1.0538449	-1.7997896
1	-3.8407994	-0.0818929	-1.2394399
1	-4.3059766	1.5298970	-1.7496327
1	-3.4898970	3.5029450	-0.6257701
1	-2.9078075	3.4838198	1.0251786
1	-1.8427399	2.9767539	-0.3002704
1	0.8499813	-0.4909973	-2.4958076
1	2.2179629	0.6202928	-2.3673687
1	2.4409435	-0.9591326	-3.0957081
1	2.1321029	-3.0684406	-0.1090881
1	0.6637387	-2.5014645	-0.9280013
1	2.0741135	-2.9948957	-1.8572018
1	4.1421017	-1.4322130	0.1334136
1	4.2097613	-1.7550028	-1.5892180
1	4.2420821	-0.0952545	-1.0195434

MECP2

Energy of Quintet State: -2378.2082146400

Energy of Septet State: -2378.2082163000

25	-0.4676116	0.2121057	-0.2840654
7	-2.5258929	0.7128090	1.0309931
7	1.8443691	-0.3254097	0.1725816
8	-1.3533801	-0.3621785	-1.9915515
8	-0.3710477	1.5212439	-1.5481542
7	-0.5839340	-1.1733388	1.2796872
6	0.5323512	-1.7329261	1.7694799

6	1.8388210	-1.0773708	1.4380630
6	0.4568910	-2.7793659	2.6731787
1	1.3674613	-3.2344574	3.0379447
6	-0.7860857	-3.1951604	3.1158199
1	-0.8666174	-4.0087557	3.8244335
6	-1.9218680	-2.5263731	2.6913218
1	-2.9008265	-2.7733152	3.0780599
6	-1.7901365	-1.5049824	1.7678061
6	-2.9472884	-0.6689452	1.3150781
7	0.1851590	1.5078437	1.2297533
6	1.4811511	1.8471463	1.2363519
6	2.3961567	1.0237356	0.3719888
6	1.9330419	2.8677385	2.0543484
1	2.9834891	3.1244981	2.0610648
6	1.0212701	3.5268943	2.8621120
1	1.3471322	4.3437796	3.4922910
6	-0.2969502	3.1050881	2.8992516
1	-1.0154053	3.5581023	3.5689840
6	-0.6880497	2.0569378	2.0826326
6	-2.0247837	1.3852160	2.2390078
1	-3.7312421	-0.7255893	2.0779205
1	-3.3668593	-1.0970890	0.4038380
1	2.6492141	-1.8060122	1.4944625
1	2.0348612	-0.3830477	2.2602996
1	3.3893305	1.0115948	0.8335128
1	2.5082065	1.5061918	-0.5997640
1	-2.7446726	2.0917966	2.6551115
1	-1.8833877	0.6388085	3.0264330
6	2.4827587	-1.1025289	-0.9592677
6	-3.5832373	1.5201058	0.3125224
6	-4.8856922	1.5672837	1.1072024
6	-3.8537624	0.9077366	-1.0540999
6	-3.0496265	2.9327862	0.1068152
6	2.1637177	-0.4295074	-2.2857569
6	1.8502270	-2.4885533	-0.9911025
6	3.9917487	-1.2054763	-0.7754052
1	-4.7356567	1.9565987	2.1145787
1	-5.5966521	2.2239943	0.6069576
1	-5.3485985	0.5841056	1.1867391
1	-2.9373180	0.8514612	-1.6479189
1	-4.2947133	-0.0859274	-1.0016012
1	-4.5540545	1.5404758	-1.5993000
1	-3.7366881	3.4845237	-0.5333908
1	-2.9623742	3.4886378	1.0396957

1	-2.0752135	2.9155274	-0.3825650
1	1.0922780	-0.4474720	-2.4828829
1	2.5035146	0.6034701	-2.3377094
1	2.6631367	-0.9739932	-3.0865617
1	2.1196708	-3.1040263	-0.1336695
1	0.7612471	-2.4127656	-1.0386185
1	2.1852859	-3.0149094	-1.8836500
1	4.2597468	-1.6311627	0.1918133
1	4.4148684	-1.8508894	-1.5442111
1	4.4734071	-0.2317105	-0.8647231

⁵TS₂₋₁₄(H)

E (SMD/M06-L-D3/def2-TZVP) = -2139.65606 au

H (SMD/M06-L-D3/def2-TZVP) = -2139.328869 au

G (SMD/M06-L-D3/def2-TZVP) = -2139.397796 au

E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2139.126153 au

Mn -0.25043300 -0.13149400 -0.37491900

N -2.19516900 0.26290700 0.83670700

N 2.03575400 -0.56003200 -0.00633900

O -0.75235700 -1.36406100 -1.43319400

O -0.11403900 1.31168800 -1.41366400

N -0.15053500 -1.48137700 1.35862700

C 1.02725200 -1.99275700 1.72386100

C 2.15285800 -1.81097300 0.75109800

C 1.17367600 -2.66329000 2.92747100

H 2.13848800 -3.06483100 3.20595700

C 0.07380500 -2.78279100 3.76007200

H 0.16381000 -3.29232400 4.71042200

C -1.13356700 -2.21832100 3.38415700

H -2.00246300 -2.26580000 4.02631800

C -1.21003500 -1.56139200 2.16704500

C -2.46774000 -0.91882700 1.66467900

N 0.34379300 1.17007700 1.27400500

C 1.63395700 1.25142900 1.61192000

C 2.60446200 0.61382800 0.66517100

C 2.02954200 1.90783800 2.76567300

H 3.07852700 1.95533800 3.02416500

C 1.05961200 2.47324400 3.57626500

H 1.34204100 2.98366200 4.48766600

C -0.27580700 2.35586300 3.22940000

H -1.05914100 2.75919600 3.85642100

C -0.60392000 1.68511100 2.06270700

C -2.01610600 1.50714700 1.59502400

H -3.12731300 -0.68268600 2.50421900

H -2.99706600 -1.64002300 1.03809100
H 2.12164500 -2.63205100 0.03134600
H 3.11138700 -1.88381900 1.27277800
H 3.53271800 0.37259400 1.19099900
H 2.85928800 1.34136400 -0.10853300
H -2.26534600 2.33531200 0.92800900
H -2.70146500 1.56721900 2.44500700
O -0.46996400 0.94810800 -3.24570700
H -0.64493900 0.03853500 -2.94283700
H 2.50754200 -0.67848000 -0.89213500
H -2.96932500 0.38804200 0.19902100

(H₂O)₄OH⁻

E (SMD/M06-L-D3/def2-TZVP) = -381.822049 au
H (SMD/M06-L-D3/def2-TZVP) = -381.701873 au
G (SMD/M06-L-D3/def2-TZVP) = -381.751508 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -381.732491 au
O -1.47678000 -1.56711600 0.10438600
H -2.28566600 -1.07234300 -0.05944600
O 0.14057300 -0.39028800 -1.61805800
H -0.07621900 0.53397200 -1.41032300
H -0.48666100 -0.89086600 -0.99768200
O -0.14135300 0.08713700 1.67064300
H -0.67566400 -0.57295400 1.11835200
O -0.72258400 2.03742900 -0.24955500
H -1.65368600 1.89621300 -0.45151300
H -0.54813400 1.41339800 0.49044600
O 2.28563700 -0.34427300 0.15247900
H 2.68346500 0.52525500 0.04112900
H 1.59414100 -0.38115000 -0.54712600
H 0.76448400 -0.03464000 1.33701000

⁵TS^{'''}₂₋₁₄

E (SMD/M06-L-D3/def2-TZVP) = -2760.083327 au
H (SMD/M06-L-D3/def2-TZVP) = -2759.412219 au
G (SMD/M06-L-D3/def2-TZVP) = -2759.523493 au
E (SMD/B3LYP*-D3/def2-TZVP//SMD/M06-L-D3/def2-TZVP) = -2759.312634 au
Mn -0.03631300 0.06563600 -0.03861500
N 1.20195600 2.11949600 0.37803300
N 0.50495200 -2.27309000 -0.37387800
O -1.18167000 0.17622100 1.22200200
O -0.92587700 0.33401200 -1.56685000
N 1.48471600 -0.35002100 1.40046500
C 1.92480500 -1.59651900 1.57626200

C 1.71354300 -2.54569000 0.43333600
C 2.65499000 -1.93028800 2.70582700
H 2.98914800 -2.94884100 2.85061600
C 2.96009100 -0.93264700 3.61725100
H 3.52874000 -1.16785200 4.50739700
C 2.56966200 0.37385600 3.36908100
H 2.84413000 1.18065700 4.03488000
C 1.81900800 0.63676600 2.23549600
C 1.37197100 2.01530800 1.84036400
N 1.66120400 -0.05314000 -1.32908100
C 1.75170300 -1.11416400 -2.13720900
C 0.84758500 -2.26670300 -1.80976400
C 2.66944100 -1.13432000 -3.17372500
H 2.73947400 -2.00116100 -3.81646800
C 3.48977500 -0.03219700 -3.35444500
H 4.19994800 -0.01348900 -4.17065800
C 3.42912200 1.02688000 -2.46338200
H 4.09586300 1.87433000 -2.54836500
C 2.50788100 0.97518200 -1.42965800
C 2.50837400 1.95649100 -0.29526200
H 2.09783900 2.73987200 2.22438700
H 0.41773300 2.23841500 2.31987900
H 1.74776400 -3.57764300 0.78518700
H 2.59188800 -2.43831300 -0.20925600
H 1.33801100 -3.19538700 -2.12001000
H -0.07203900 -2.18590200 -2.39023900
H 2.92705400 2.91052700 -0.61807600
H 3.22783600 1.56805200 0.43116400
C -0.63454000 -3.21548600 -0.03443200
C 0.49379000 3.38980500 -0.05491500
C 1.16324600 4.62345500 0.54252700
C -0.96292500 3.33214900 0.37861000
C 0.52452200 3.46663300 -1.57708000
C -1.92446300 -2.68789300 -0.64334700
C -0.80760400 -3.23775500 1.47994800
C -0.35867400 -4.62425700 -0.54918400
H 2.23191600 4.65649600 0.32795900
H 0.71660100 5.52084100 0.11595800
H 1.02997800 4.67404600 1.62280200
H -1.48022000 2.51304300 -0.11908400
H -1.08487700 3.21318200 1.45455400
H -1.45398900 4.26395400 0.09852500
H -0.12372500 4.27902900 -1.90217800
H 1.51811900 3.67103600 -1.97379200

H 0.15199100 2.54286700 -2.02175700
H -2.16106500 -1.70068400 -0.24840500
H -1.89331200 -2.62338600 -1.73059600
H -2.74060400 -3.36161500 -0.38353300
H 0.01116900 -3.73931500 1.99444500
H -0.90401600 -2.22602000 1.87643600
H -1.71989800 -3.78081100 1.72334100
H 0.59539900 -5.01396600 -0.19328100
H -1.13852100 -5.29816500 -0.19641800
H -0.35988000 -4.66474200 -1.63808100
O -2.79188100 0.62976200 -1.32879000
H -2.62306700 0.38717000 -0.40136700
O -4.89951100 -1.15273800 -0.79348400
H -4.53935500 -1.08722500 0.11521400
H -4.20904700 -0.68149800 -1.29763600
O -4.35903500 2.19872400 0.62027000
H -3.73595900 2.01095900 -0.10066600
O -3.77698400 -0.43747600 1.71381500
H -2.80116100 -0.37668300 1.57481300
H -4.06300200 0.46743100 1.48376600
O -6.64821600 0.99284300 -0.47541700
H -7.23640600 0.76907600 0.25335500
H -6.11278400 0.18030400 -0.61089900
H -5.21207500 1.87537700 0.26255400

⁵a

E (SMD/M06-L-D3/def2-TZVP) = -2380.032598 au
H (SMD/M06-L-D3/def2-TZVP) = -2379.445910 au
G (SMD/M06-L-D3/def2-TZVP) = -2379.530151 au
Mn 0.04757000 0.02567600 0.83562400
N -2.20922500 0.39570700 0.00496600
N 2.19486900 -0.40569500 0.02630300
O 0.14414900 1.65585500 2.21471500
O -0.10163000 -1.37329100 2.02405000
N 0.18443400 1.38176500 -0.68654200
C 1.35101100 1.50728200 -1.33907600
C 2.28824800 0.34604800 -1.24901700
C 1.56994700 2.59697500 -2.16180700
H 2.52083700 2.70436200 -2.66456100
C 0.54786700 3.51442400 -2.34187200
H 0.70052900 4.37630700 -2.97765300
C -0.68532600 3.30240400 -1.74892700
H -1.52141900 3.96276900 -1.93131100
C -0.84720800 2.21020600 -0.91579700

C -2.15493500 1.84393800 -0.28051200
N -0.17571300 -1.37887400 -0.71330000
C 0.84356800 -2.21936800 -0.91287300
C 2.13813600 -1.85563700 -0.24624400
C 0.68782700 -3.32230800 -1.73398300
H 1.52068200 -3.99149300 -1.89963800
C -0.54156800 -3.53140200 -2.33718600
H -0.69289300 -4.39546600 -2.97053300
C -1.56428400 -2.61330400 -2.16323200
H -2.51617600 -2.72519300 -2.66406700
C -1.34118800 -1.51555500 -1.35021800
C -2.29193000 -0.36010900 -1.26086500
H -2.96592000 2.16561600 -0.94128900
H -2.28496000 2.40019600 0.64928200
H 3.31023600 0.65284800 -1.47091200
H 2.00923100 -0.32308500 -2.06744600
H 2.96491300 -2.18349600 -0.88294200
H 2.23060400 -2.39648500 0.69615300
H -3.30932100 -0.68412200 -1.48201100
H -2.02265100 0.30854400 -2.08304400
C 3.30599200 -0.02034900 0.99474500
C -3.30880100 0.01572600 0.98085600
C -4.65488400 0.57460600 0.53526300
C -2.95385000 0.55509300 2.35763200
C -3.37994600 -1.50415500 1.06319600
C 2.96340400 -0.53727200 2.38205500
C 3.38489900 1.49946100 1.06170400
C 4.64327800 -0.59393400 0.54205900
H -4.90903000 0.26844600 -0.47973800
H -5.43707300 0.20105700 1.19488500
H -4.67879200 1.66289900 0.58211300
H -2.00531600 0.14472000 2.70274100
H -2.89699700 1.64329100 2.38369000
H -3.72669100 0.26126500 3.06674800
H -4.05247500 -1.78088300 1.87345100
H -3.77055900 -1.95874800 0.15371000
H -2.40263900 -1.93524800 1.27916200
H 2.06867200 -0.05381500 2.77013200
H 2.81432900 -1.61507800 2.41193600
H 3.78671900 -0.30497300 3.05640700
H 3.78107000 1.94638700 0.15099000
H 2.40891100 1.93773400 1.27112800
H 4.05396400 1.77945900 1.87367200
H 4.88321800 -0.31560000 -0.48422700

H 5.43574700 -0.20450400 1.17956400
H 4.66577300 -1.68047500 0.61721700
H 0.08343800 -1.03795800 2.91170800
H 0.19672100 1.28914100 3.10884900
H -0.68141700 2.15999500 2.21871900