DFT Calculations on Ruthenium(IV) Bis(amido) Porphyrins: Search for a Broader Perspective of Heme Protein Compound II Intermediates

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$Ru^{IV}P(NH_2)_2$, C_{2v}, $S = 0$, PW91 optimized geometry

Ru	0.000000000	0.000000000	-0.032391169
N	0.000000000	-1.489397644	1.426644789
N	0.000000000	1.489397644	1.426644789
N	0.000000000	-1.469499385	-1.459497541
N	0.000000000	1.469499385	-1.459497541
N	-1.929173056	0.000000000	0.210269515
N	1.929173056	0.000000000	0.210269515
C	0.000000000	1.257477328	2.781145812
C	0.000000000	3.506889863	2.519221453
C	0.000000000	2.845023641	1.233723792
C	0.000000000	-2.524703359	-3.498974021
C	0.000000000	0.000000000	3.390721542
C	0.000000000	0.000000000	-3.431248178
C	0.000000000	2.528096691	3.471513325
C	0.000000000	3.467517725	-0.018838731
C	0.000000000	-3.467517725	-0.018838731
C	0.000000000	-3.498801927	-2.543719742
C	0.000000000	-3.506889863	2.519221453
C	0.000000000	-2.528096691	3.471513325
C	0.000000000	1.251444641	-2.815418974
C	0.000000000	-1.257477328	2.781145812
C	0.000000000	-2.845023641	1.233723792
C	0.000000000	2.835192414	-1.260333020
C	0.000000000	2.524703359	-3.498974021

C	0.000000000	-1.251444641	-2.815418974
C	0.000000000	3.498801927	-2.543719742
C	0.000000000	-2.835192414	-1.260333020
H	0.000000000	0.000000000	-4.520419032
H	0.000000000	-4.582016678	2.665122589
H	0.000000000	4.582016678	2.665122589
H	0.000000000	-2.648188977	4.550119168
H	0.000000000	-4.574630968	-2.685174072
H	0.000000000	-2.648461751	-4.577164964
H	0.000000000	2.648188977	4.550119168
H	0.000000000	0.000000000	4.480399721
H	0.000000000	4.574630968	-2.685174072
H	0.000000000	2.648461751	-4.577164964
H	0.000000000	4.556677679	-0.024898320
H	0.000000000	-4.556677679	-0.024898320
H	-2.419236071	-0.837001030	0.536826742
H	-2.419236071	0.837001030	0.536826742
H	2.419236071	-0.837001030	0.536826742
H	2.419236071	0.837001030	0.536826742

$Ru^{IV}P(NPh_2)_2$, D_{2h}, S = 0, PW91 optimized geometry

Ru	0.000000000	0.000000000	0.000000000
N	0.000000000	1.448137000	1.474150000
N	0.000000000	1.448137000	-1.474150000
N	0.000000000	-1.448137000	1.474150000
N	0.000000000	-1.448137000	-1.474150000
C	0.000000000	2.802298000	-1.254110000
C	0.000000000	2.527757000	-3.501277000
C	0.000000000	1.246351000	-2.835259000
C	0.000000000	-3.485785000	2.528705000
C	0.000000000	3.417915000	0.000000000
C	0.000000000	-3.417915000	0.000000000
C	0.000000000	3.485785000	-2.528705000
C	0.000000000	0.000000000	-3.461809000
C	0.000000000	0.000000000	3.461809000
C	0.000000000	-2.527757000	3.501277000
C	0.000000000	2.527757000	3.501277000
C	0.000000000	3.485785000	2.528705000
C	0.000000000	-2.802298000	-1.254110000
C	0.000000000	2.802298000	1.254110000
C	0.000000000	1.246351000	2.835259000
C	0.000000000	-1.246351000	-2.835259000
C	0.000000000	-3.485785000	-2.528705000
C	0.000000000	-2.802298000	1.254110000

C	0.000000000	-2.527757000	-3.501277000
C	0.000000000	-1.246351000	2.835259000
H	0.000000000	-4.507574000	0.000000000
H	0.000000000	2.666653000	4.577348000
H	0.000000000	2.666653000	-4.577348000
H	0.000000000	4.564329000	2.653693000
H	0.000000000	-2.666653000	4.577348000
H	0.000000000	-4.564329000	2.653693000
H	0.000000000	4.564329000	-2.653693000
H	0.000000000	4.507574000	0.000000000
H	0.000000000	-2.666653000	-4.577348000
H	0.000000000	-4.564329000	-2.653693000
H	0.000000000	0.000000000	-4.550676000
H	0.000000000	0.000000000	4.550676000
N	-1.990098000	0.000000000	0.000000000
N	1.990098000	0.000000000	0.000000000
C	2.791018000	0.000000000	-1.193758000
C	3.193320000	-1.208620000	-1.778764000
C	3.193320000	1.208620000	-1.778764000
C	3.970600000	-1.205234000	-2.937853000
C	3.970600000	1.205234000	-2.937853000
C	4.358817000	0.000000000	-3.524973000
H	2.887453000	-2.149227000	-1.322486000
H	2.887453000	2.149227000	-1.322486000
H	4.270791000	-2.153438000	-3.383699000
H	4.270791000	2.153438000	-3.383699000
H	4.961983000	0.000000000	-4.433044000
C	2.791018000	0.000000000	1.193758000
C	3.193320000	-1.208620000	1.778764000
C	3.193320000	1.208620000	1.778764000
C	3.970600000	-1.205234000	2.937853000
C	3.970600000	1.205234000	2.937853000
C	4.358817000	0.000000000	3.524973000
H	2.887453000	-2.149227000	1.322486000
H	2.887453000	2.149227000	1.322486000
H	4.270791000	-2.153438000	3.383699000
H	4.270791000	2.153438000	3.383699000
H	4.961983000	0.000000000	4.433044000
C	-2.791018000	0.000000000	-1.193758000
C	-3.193320000	-1.208620000	-1.778764000
C	-3.193320000	1.208620000	-1.778764000
C	-3.970600000	-1.205234000	-2.937853000
C	-3.970600000	1.205234000	-2.937853000
C	-4.358817000	0.000000000	-3.524973000
H	-2.887453000	-2.149227000	-1.322486000
H	-2.887453000	2.149227000	-1.322486000
H	-4.270791000	-2.153438000	-3.383699000

H	−4.270791000	2.153438000	−3.383699000
H	−4.961983000	0.000000000	−4.433044000
C	−2.791018000	0.000000000	1.193758000
C	−3.193320000	−1.208620000	1.778764000
C	−3.193320000	1.208620000	1.778764000
C	−3.970600000	−1.205234000	2.937853000
C	−3.970600000	1.205234000	2.937853000
C	−4.358817000	0.000000000	3.524973000
H	−2.887453000	−2.149227000	1.322486000
H	−2.887453000	2.149227000	1.322486000
H	−4.270791000	−2.153438000	3.383699000
H	−4.270791000	2.153438000	3.383699000
H	−4.961983000	0.000000000	4.433044000

$Ru^{IV}P(NHPh)_2$, C_{2h}, $S = 0$, PW91 optimized geometry

Ru	0.000000000	0.000000000	0.000000000
N	−1.639441000	1.246481000	0.000000000
N	−1.013980000	−1.724299000	0.000000000
N	1.013980000	1.724299000	0.000000000
N	1.639441000	−1.246481000	0.000000000
N	0.000000000	0.000000000	−2.070779000
N	0.000000000	0.000000000	2.070779000
C	3.740355000	4.210065000	0.000000000
C	4.714565000	2.000160000	0.000000000
C	4.875583000	3.390917000	0.000000000
C	3.451312000	1.425447000	0.000000000
C	2.471841000	3.647715000	0.000000000
C	2.289753000	2.235639000	0.000000000
C	−4.875583000	−3.390917000	0.000000000
C	−2.273871000	1.760922000	1.111456000
C	2.273871000	−1.760922000	−1.111456000
C	3.364032000	−2.609900000	0.682362000
C	3.364032000	−2.609900000	−0.682362000
C	2.273871000	−1.760922000	1.111456000
C	−0.878224000	0.674730000	2.879458000
C	−3.364032000	2.609900000	−0.682362000
C	−2.273871000	1.760922000	−1.111456000
C	−3.364032000	2.609900000	0.682362000
C	0.541409000	−0.416545000	4.259576000
C	−0.878224000	0.674730000	−2.879458000
C	−0.541409000	0.416545000	4.259576000
C	0.878224000	−0.674730000	−2.879458000
C	−0.541409000	0.416545000	−4.259576000
C	1.924325000	−1.486769000	−2.432663000

C	-1.924325000	1.486769000	-2.432663000
C	1.924325000	-1.486769000	2.432663000
C	-1.924325000	1.486769000	2.432663000
C	0.541409000	-0.416545000	-4.259576000
C	-3.451312000	-1.425447000	0.000000000
C	-2.289753000	-2.235639000	0.000000000
C	-3.740355000	-4.210065000	0.000000000
C	-4.714565000	-2.000160000	0.000000000
C	-2.471841000	-3.647715000	0.000000000
C	0.878224000	-0.674730000	2.879458000
H	-1.588399000	-4.289515000	0.000000000
H	-3.341935000	-0.346601000	0.000000000
H	-4.036120000	3.139569000	1.349673000
H	-5.591113000	-1.352629000	0.000000000
H	1.588399000	4.289515000	0.000000000
H	-5.872174000	-3.829979000	0.000000000
H	-3.849050000	-5.294126000	0.000000000
H	4.036120000	-3.139569000	-1.349673000
H	-1.071079000	0.823794000	-5.114647000
H	4.036120000	-3.139569000	1.349673000
H	1.071079000	-0.823794000	5.114647000
H	-4.036120000	3.139569000	-1.349673000
H	1.071079000	-0.823794000	-5.114647000
H	-1.071079000	0.823794000	5.114647000
H	3.341935000	0.346601000	0.000000000
H	5.872174000	3.829979000	0.000000000
H	5.591113000	1.352629000	0.000000000
H	3.849050000	5.294126000	0.000000000
H	-0.344265000	-2.500627000	0.000000000
H	0.344265000	2.500627000	0.000000000
H	2.532210000	-1.959198000	3.202698000
H	2.532210000	-1.959198000	-3.202698000
H	-2.532210000	1.959198000	-3.202698000
H	-2.532210000	1.959198000	3.202698000

$Ru^{IV}P(NCH_2)_2$, D_{2h}, $S = 0$, PW91 optimized geometry

Ru	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	2.068647000
N	0.000000000	-2.083355000	0.000000000
N	0.000000000	2.083355000	0.000000000
N	0.000000000	0.000000000	-2.068647000
N	-1.881790000	0.000000000	0.000000000
N	1.881790000	0.000000000	0.000000000
C	3.133641000	0.000000000	0.000000000
C	-3.133641000	0.000000000	0.000000000
C	0.000000000	-4.266856000	0.683607000
C	0.000000000	-4.266856000	-0.683607000
C	0.000000000	2.885362000	1.109209000
C	0.000000000	2.885362000	-1.109209000
C	0.000000000	-2.885362000	1.109209000
C	0.000000000	-0.681843000	-4.260271000
C	0.000000000	2.432918000	-2.432077000
C	0.000000000	2.432918000	2.432077000
C	0.000000000	-2.432918000	2.432077000
C	0.000000000	-2.432918000	-2.432077000
C	0.000000000	0.681843000	-4.260271000
C	0.000000000	-1.109420000	-2.875716000
C	0.000000000	4.266856000	0.683607000
C	0.000000000	4.266856000	-0.683607000
C	0.000000000	-2.885362000	-1.109209000
C	0.000000000	-0.681843000	4.260271000
C	0.000000000	1.109420000	2.875716000
C	0.000000000	0.681843000	4.260271000
C	0.000000000	1.109420000	-2.875716000
C	0.000000000	-1.109420000	2.875716000
H	0.000000000	5.122249000	1.350676000
H	0.000000000	-1.350143000	-5.114672000
H	0.000000000	1.350143000	5.114672000
H	0.000000000	-1.350143000	5.114672000
H	0.000000000	-5.122249000	-1.350676000
H	0.000000000	3.200754000	-3.204182000
H	0.000000000	5.122249000	-1.350676000
H	0.000000000	-5.122249000	1.350676000
H	0.000000000	3.200754000	3.204182000
H	0.000000000	-3.200754000	-3.204182000
H	0.000000000	-3.200754000	3.204182000
H	0.000000000	1.350143000	-5.114672000
H	3.710655000	-0.941574000	0.000000000
H	3.710655000	0.941574000	0.000000000
H	-3.710655000	0.941574000	0.000000000
H	-3.710655000	-0.941574000	0.000000000

$Ru^{IV}P(NCPh_2)_2$, D_2, $S = 0$, PW91 optimized geometry

Ru	0.000000000	0.000000000	0.000000000
N	0.000000000	2.069100000	0.000000000
N	-2.082900000	0.000000000	0.000000000
N	2.082900000	0.000000000	0.000000000
N	0.000000000	-2.069100000	0.000000000
N	0.000000000	0.000000000	-1.895500000
N	0.000000000	0.000000000	1.895500000
C	2.289400000	0.990000000	-3.525300000
C	1.277300000	0.115900000	-3.942200000
C	-3.676900000	-0.308100000	-5.387400000
C	2.674100000	-0.568800000	-5.807600000
C	3.477700000	1.089500000	-4.247200000
C	1.478600000	-0.658700000	-5.096200000
C	-2.674100000	0.568800000	-5.807600000
C	-1.277300000	-0.115900000	-3.942200000
C	0.000000000	0.000000000	3.164500000
C	0.000000000	0.000000000	-3.164500000
C	-3.477700000	-1.089500000	-4.247200000
C	-1.478600000	0.658700000	-5.096200000
C	-2.289400000	-0.990000000	-3.525300000
C	2.289400000	-0.990000000	3.525300000
C	1.478600000	0.658700000	5.096200000
C	1.277300000	-0.115900000	3.942200000
C	3.676900000	-0.308100000	5.387400000
C	3.477700000	-1.089500000	4.247200000
C	2.674100000	0.568800000	5.807600000
C	-3.676900000	0.308100000	5.387400000
C	-2.289400000	0.990000000	3.525300000
C	-1.277300000	0.115900000	3.942200000
C	3.676900000	0.308100000	-5.387400000
C	-2.674100000	-0.568800000	5.807600000
C	-3.477700000	1.089500000	4.247200000
C	-1.478600000	-0.658700000	5.096200000
C	-4.266600000	0.682600000	-0.024700000
C	-4.266600000	-0.682600000	0.024700000
C	2.885400000	1.107800000	0.036800000
C	2.885400000	-1.107800000	-0.036800000
C	-2.885400000	1.107800000	-0.036800000
C	-0.681700000	-4.260800000	0.017100000
C	2.432900000	-2.431200000	-0.050900000
C	2.432900000	2.431200000	0.050900000
C	-2.432900000	2.431200000	-0.050900000
C	-2.432900000	-2.431200000	0.050900000
C	0.681700000	-4.260800000	-0.017100000
C	-1.109600000	-2.876600000	0.026400000

C	4.266600000	0.682600000	0.024700000
C	4.266600000	-0.682600000	-0.024700000
C	-2.885400000	-1.107800000	0.036800000
C	-0.681700000	4.260800000	-0.017100000
C	1.109600000	2.876600000	0.026400000
C	0.681700000	4.260800000	0.017100000
C	1.109600000	-2.876600000	-0.026400000
C	-1.109600000	2.876600000	-0.026400000
H	2.128300000	-1.599500000	2.637800000
H	0.695200000	1.338400000	5.429800000
H	2.821500000	1.184700000	6.694200000
H	4.607900000	-0.384500000	5.948900000
H	4.251600000	-1.782700000	3.918400000
H	-0.695200000	-1.338400000	5.429800000
H	-2.128300000	1.599500000	2.637800000
H	-4.251600000	1.782700000	3.918400000
H	-4.607900000	0.384500000	5.948900000
H	-2.821500000	-1.184700000	6.694200000
H	5.122400000	1.349100000	0.050500000
H	-1.348700000	-5.116300000	0.034600000
H	1.348700000	5.116300000	0.034600000
H	-1.348700000	5.116300000	-0.034600000
H	-5.122400000	-1.349100000	0.050500000
H	3.201000000	-3.202700000	-0.078000000
H	5.122400000	-1.349100000	-0.050500000
H	-5.122400000	1.349100000	-0.050500000
H	3.201000000	3.202700000	0.078000000
H	-3.201000000	-3.202700000	0.078000000
H	-3.201000000	3.202700000	-0.078000000
H	0.695200000	-1.338400000	-5.429800000
H	2.128300000	1.599500000	-2.637800000
H	4.251600000	1.782700000	-3.918400000
H	4.607900000	0.384500000	-5.948900000
H	2.821500000	-1.184700000	-6.694200000
H	-4.607900000	-0.384500000	-5.948900000
H	-2.128300000	-1.599500000	-2.637800000
H	1.348700000	-5.116300000	-0.034600000
H	-0.695200000	1.338400000	-5.429800000
H	-2.821500000	1.184700000	-6.694200000
H	-4.251600000	-1.782700000	-3.918400000

$Ru^{IV}Pz_2$, C_2, $S = 1$, OLYP optimized geometry

Ru	0.000000000	0.000000000	0.009419000
N	0.000000000	0.000000000	-2.043714000
N	-2.060138000	0.053674000	0.015495000
N	-0.065839000	-2.064823000	0.001494000
N	-0.913618000	-2.745245000	-0.818959000
N	0.913618000	2.745245000	-0.818959000
N	0.065839000	2.064823000	0.001494000
N	2.060138000	-0.053674000	0.015495000
N	0.000000000	0.000000000	2.078477000
C	2.432078000	0.051923000	2.445413000
C	-2.425992000	0.151150000	-2.413826000
C	4.247124000	-0.121279000	-0.668561000
C	-2.870370000	0.119416000	-1.092234000
C	0.683130000	0.026609000	4.267089000
C	4.249802000	-0.042033000	0.695692000
C	-0.699614000	-4.035929000	-0.572705000
C	0.303582000	-4.226330000	0.424055000
C	0.676017000	-2.945777000	0.757599000
C	-4.249802000	0.042033000	0.695692000
C	0.680819000	-0.052980000	-4.232177000
C	1.108665000	0.038157000	2.890836000
C	-0.680819000	0.052980000	-4.232177000
C	0.699614000	4.035929000	-0.572705000
C	2.425992000	-0.151150000	-2.413826000
C	-1.104773000	0.079772000	-2.854441000
C	-0.303582000	4.226330000	0.424055000
C	-0.676017000	2.945777000	0.757599000
C	-2.432078000	-0.051923000	2.445413000
C	1.104773000	-0.079772000	-2.854441000
C	-2.873126000	0.001699000	1.121650000
C	2.870370000	-0.119416000	-1.092234000
C	2.873126000	-0.001699000	1.121650000
C	-4.247124000	0.121279000	-0.668561000
C	-0.683130000	-0.026609000	4.267089000
C	-1.108665000	-0.038157000	2.890836000
H	-3.201105000	-0.087650000	3.211526000
H	1.344741000	-0.103981000	-5.086786000
H	-1.344741000	0.103981000	-5.086786000
H	1.407905000	-2.600450000	1.470574000
H	0.686602000	-5.156317000	0.826828000
H	-1.265385000	-4.788288000	-1.112283000
H	-3.191589000	0.208616000	-3.181986000
H	1.347011000	0.052319000	5.122910000
H	5.106156000	-0.012810000	1.358801000
H	5.101134000	-0.168115000	-1.333498000

H	-1.407905000	2.600450000	1.470574000
H	-0.686602000	5.156317000	0.826828000
H	-1.347011000	-0.052319000	5.122910000
H	3.191589000	-0.208616000	-3.181986000
H	1.265385000	4.788288000	-1.112283000
H	3.201105000	0.087650000	3.211526000
H	-5.101134000	0.168115000	-1.333498000
H	-5.106156000	0.012810000	1.358801000