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Supporting Information

Models of the ox1 State of Methylcoenzyme M Reductase: Where are the Electrons?

Emmanuel Gonzalez[a] and Abhik Ghosh[a]*

[a] Department of Chemistry and Center for Theoretical and Experimental Chemistry
University of Tromsø, 9037 Tromsø, Norway

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Optimized coordinates (Å) for lowest-energy states

1. $[Ni^{III}(oxaP)(SMe)(AcNH_2)]^+$

Ni	0.109685000	0.060417000	0.000000000
S	0.058041000	-2.207875000	0.000000000
O	-0.655236000	2.062217000	0.000000000
O	-2.174667000	-0.230486000	0.000000000
N	0.019682000	0.054307000	-1.952462000
N	2.087076000	0.374227000	0.000000000
N	0.019682000	0.054307000	1.952462000
N	-1.261774000	4.220215000	0.000000000
C	-0.309342000	3.262019000	0.000000000
C	-2.422099000	-0.273710000	-2.383273000
C	1.103818000	0.166337000	-2.791732000
C	-2.422099000	-0.273710000	2.383273000
C	2.427356000	0.365538000	2.407275000
C	2.427356000	0.365538000	-2.407275000
C	-0.678277000	-0.097156000	4.145726000
C	0.669667000	0.072659000	4.167420000
C	4.266247000	0.647474000	-0.682505000
C	-4.311683000	-0.487834000	0.689880000
C	-1.085118000	-0.115437000	-2.756914000
C	-1.085118000	-0.115437000	2.756914000
C	-2.976723000	-0.330890000	1.118200000
C	-0.678277000	-0.097156000	-4.145726000
C	1.118304000	3.739601000	0.000000000
C	-4.311683000	-0.487834000	-0.689880000
C	1.747341000	-2.848004000	0.000000000
C	4.266247000	0.647474000	0.682505000
C	2.893406000	0.463320000	-1.098981000
C	0.669667000	0.072659000	-4.167420000
C	1.103818000	0.166337000	2.791732000
C	2.893406000	0.463320000	1.098981000
C	-2.976723000	-0.330890000	-1.118200000

H	5.112689000	0.755083000	-1.351850000
H	2.298690000	-2.574124000	0.905583000
H	3.161773000	0.442512000	-3.206962000
H	1.326513000	0.139088000	5.027427000
H	1.309131000	4.356912000	-0.887394000
H	1.326513000	0.139088000	-5.027427000
H	2.298690000	-2.574124000	-0.905583000
H	-3.134236000	-0.374882000	3.200027000
H	1.608230000	-3.939825000	0.000000000
H	-1.356599000	-0.203167000	-4.985218000
H	-5.163320000	-0.592897000	-1.351482000
H	1.309131000	4.356912000	0.887394000
H	-5.163320000	-0.592897000	1.351482000
H	5.112689000	0.755083000	1.351850000
H	-1.356599000	-0.203167000	4.985218000
H	-2.237461000	3.947879000	0.000000000
H	-3.134236000	-0.374882000	-3.200027000
H	-1.026109000	5.205350000	0.000000000
H	1.794032000	2.883638000	0.000000000
H	3.161773000	0.442512000	3.206962000

2. $[Ni^{III}(pyriP)(SMe)(AcNH_2)]^+$

Ni	-0.132477000	-0.147107000	0.000000000
S	-0.133632000	-2.412763000	0.000000000
O	0.568604000	1.908811000	0.000000000
N	1.134783000	4.079920000	0.000000000
N	2.162361000	-0.447208000	0.000000000
N	-0.158636000	-0.152274000	-1.959963000
N	-0.158636000	-0.152274000	1.959963000
N	-2.191498000	0.208257000	0.000000000
C	-0.840967000	-0.164841000	4.171825000
C	-1.243224000	-0.036341000	-2.781612000
C	-3.005690000	0.318169000	1.091730000
C	-1.836544000	-3.020160000	0.000000000
C	-4.381597000	0.540551000	-0.678971000
C	-3.005690000	0.318169000	-1.091730000
C	2.868217000	-0.528634000	-1.158844000
C	2.868217000	-0.528634000	1.158844000
C	4.277166000	-0.665028000	1.180352000
C	4.995934000	-0.727873000	0.000000000
C	4.277166000	-0.665028000	-1.180352000
C	-1.235056000	3.555838000	0.000000000
C	2.248442000	-0.493287000	-2.443798000
C	-2.564653000	0.200221000	-2.398449000
C	-2.564653000	0.200221000	2.398449000

C	0.201065000	3.100359000	0.000000000
C	2.248442000	-0.493287000	2.443798000
C	-1.243224000	-0.036341000	2.781612000
C	0.931708000	-0.351458000	2.790584000
C	-4.381597000	0.540551000	0.678971000
C	0.497101000	-0.357040000	4.178148000
C	0.931708000	-0.351458000	-2.790584000
C	-0.840967000	-0.164841000	-4.171825000
C	0.497101000	-0.357040000	-4.178148000
H	-1.895156000	2.687984000	0.000000000
H	0.880389000	5.059080000	0.000000000
H	2.931644000	-0.605841000	3.283114000
H	-3.301222000	0.286417000	-3.194456000
H	4.779453000	-0.722772000	2.143569000
H	4.779453000	-0.722772000	-2.143569000
H	6.078870000	-0.831947000	0.000000000
H	2.115750000	3.824561000	0.000000000
H	-1.520690000	-0.103470000	-5.014485000
H	-1.436811000	4.169729000	0.887312000
H	-1.520690000	-0.103470000	5.014485000
H	-5.222155000	0.667600000	1.352902000
H	-2.383027000	-2.733352000	-0.904825000
H	-3.301222000	0.286417000	3.194456000
H	-2.383027000	-2.733352000	0.904825000
H	-1.436811000	4.169729000	-0.887312000
H	-5.222155000	0.667600000	-1.352902000
H	1.158196000	-0.491229000	-5.026867000
H	2.931644000	-0.605841000	-3.283114000
H	-1.722844000	-4.114803000	0.000000000
H	1.158196000	-0.491229000	5.026867000

3. $[Ni^{III}(isoP)(SMe)(AcNH_2)]^+$

Ni	0.228891000	-0.202058000	0.000000000
S	-0.540253000	-2.328619000	0.000000000
O	0.477969000	1.855083000	0.000000000
N	-1.194841000	0.195279000	-1.434242000
N	2.723852000	2.291752000	0.000000000
N	-1.194841000	0.195279000	1.434242000
N	1.629718000	-0.624621000	-1.432948000
N	1.629718000	-0.624621000	1.432948000
C	0.808751000	-3.529069000	0.000000000
C	-3.086215000	0.803343000	2.580509000
C	-0.963354000	0.104400000	2.813845000
C	3.564781000	-1.278431000	2.517076000
C	1.146883000	4.145163000	0.000000000

C	3.564781000	-1.278431000	-2.517076000
C	2.929486000	-1.045227000	-1.244588000
C	-3.629828000	2.356943000	0.000000000
C	-4.460894000	-0.037151000	0.000000000
C	2.628463000	-1.004019000	3.474211000
C	-2.448993000	0.608319000	-1.284856000
C	-2.448993000	0.608319000	1.284856000
C	1.432036000	-0.605591000	-2.777377000
C	0.217684000	-0.253019000	-3.408354000
C	-3.183070000	0.860434000	0.000000000
C	0.217684000	-0.253019000	3.408354000
C	3.527442000	-1.227930000	0.000000000
C	1.435694000	2.663631000	0.000000000
C	1.432036000	-0.605591000	2.777377000
C	2.628463000	-1.004019000	-3.474211000
C	-0.963354000	0.104400000	-2.813845000
C	2.929486000	-1.045227000	1.244588000
C	-2.162962000	0.483877000	-3.524959000
C	-3.086215000	0.803343000	-2.580509000
C	-2.162962000	0.483877000	3.524959000
H	3.464766000	2.981051000	0.000000000
H	0.066389000	4.299727000	0.000000000
H	-2.267608000	0.507777000	-4.604019000
H	2.970280000	1.306628000	0.000000000
H	4.562719000	-1.567242000	0.000000000
H	-5.070260000	0.170694000	-0.885671000
H	-4.190634000	-1.099406000	0.000000000
H	-5.070260000	0.170694000	0.885671000
H	-4.236565000	2.571010000	-0.886182000
H	-4.236565000	2.571010000	0.886182000
H	-2.758205000	3.021272000	0.000000000
H	-4.104121000	1.137262000	2.746682000
H	-4.104121000	1.137262000	-2.746682000
H	1.581619000	4.620247000	0.888568000
H	2.732010000	-1.069605000	4.551656000
H	-2.267608000	0.507777000	4.604019000
H	1.422637000	-3.479533000	0.905817000
H	0.223508000	-0.272443000	4.497723000
H	1.422637000	-3.479533000	-0.905817000
H	4.588122000	-1.610536000	-2.653501000
H	1.581619000	4.620247000	-0.888568000
H	2.732010000	-1.069605000	-4.551656000
H	0.223508000	-0.272443000	-4.497723000
H	0.277427000	-4.493634000	0.000000000
H	4.588122000	-1.610536000	2.653501000