Electronic supporting information (ESI)

Role of Anation on mechanism of proton reduction involving pentapyridine cobalt complex: A Theoretical study

Panneerselvam Murugesan[1,2] *and Jaccob Madhavan**[1,2]

[1]Department of Chemistry, Loyola College, Chennai – 600 034, Tamil Nadu, India
[2]Computational Chemistry Laboratory, Loyola Institute of Frontier Energy (LIFE), Loyola College, Chennai – 600 034, Tamil Nadu, India
Email: madhavanjack05@gmail.com

Table S1: Relative energies of all possible spin states.

Complexes	Relative energy (in kcal/mol)		
	HS	IS	LS
$[Co^{I}(PY5Me_2)]^{+}$	0.00	-	24.52
$[Co^{II}(PY5Me_2)(NCMe_2)]^{2+}$	0.00	-	3.04
$[Co^{I}(PY5Me_2)(CH_3COO^{-})]^{0}$	0.00	-	13.23
$[Co^{II}(PY5Me_2)(CH_3COO^{-})]^{1+}$	0.00	-	5.80
$[Co^{II}(PY5Me_2)H]^{1+}$	15.79	-	0.00
$[Co^{III}(PY5Me_2)H]^{2+}$	49.44	37.34	0.00

Table S2: Computed bond orders of Co^{III}-H and Co^{II}-H species.

Bond Order	Co^{III}-H	Co^{II}-H
Wiberg	0.8141	0.8549
NAO	0.6285	0.6506
MO	0.6849	0.4708
NBO	0.4484	0.4556

Table S3 : Computed relative free energies for the formation of Co(III)-hydride species **(Scheme 1)** at B3LYP and B3LYP-D3 functionals. All energies are given in kcal/mol.

Species	PCM(CH_3CN)/B3LYP/ TZVP//B3LYP/LANL2DZ (6-31G(d))	PCM(CH_3CN)/B3LYP-D3/TZVP//B3LYP-D3/ LANL2DZ (6-31G(d))	PCM (CH_3CN)/B3LYP-D3/TZVP//B3LYP/LANL2DZ (6-31G(d))
Co^{II}-CH_3CN	0	0	0
$Int1_{SBP}$	-51.1	-57.7	-61.3
$TS2_{SBP}$	-36.3	-52.0	-55.4
$TS1_{AP}$	29.5	46.8	49.3
$Int1_{AP}$	5.7	16.8	21.7
$Int2_{AP}$	-59.4	-52.0	-52.4
$TS1_{AP}$	-57.4	-59.1	-59.1
$Co^{III}H$	-88.0	-94.7	-98.3

Table S4: Computed relative free energies for proton reduction from Co(III)-hydride intermediate **(Scheme 2)** at B3LYP and B3LYP-D3 functionals. All energies are given in kcal/mol.

Species	PCM(CH_3CN)/B3LYP/TZVP// B3LYP/LANL2DZ(6-31G(d))	PCM(CH_3CN)/B3LYP-D3/TZVP// B3LYP/LANL2DZ(6-31G(d))
$Co^{III}H$	0	0
$Int1_{BMHP}$	-8.8	-12.3
$Int1_{RPP}$	-64.9	-63.9
$Int2_{RPP}$	-123.0	-128.5
$Int3_{RPP}$	-15.2	18.2
$TS1_{UMHP}$	102.0	89.2
$Int1_{UMHP}$	113.2	110.7
$TS1_{FHEP}$	38.0	20.3
$Int1_{HEP}$	-10.4	-12.1
$Int2_{HEP}$	-114.7	-127.8

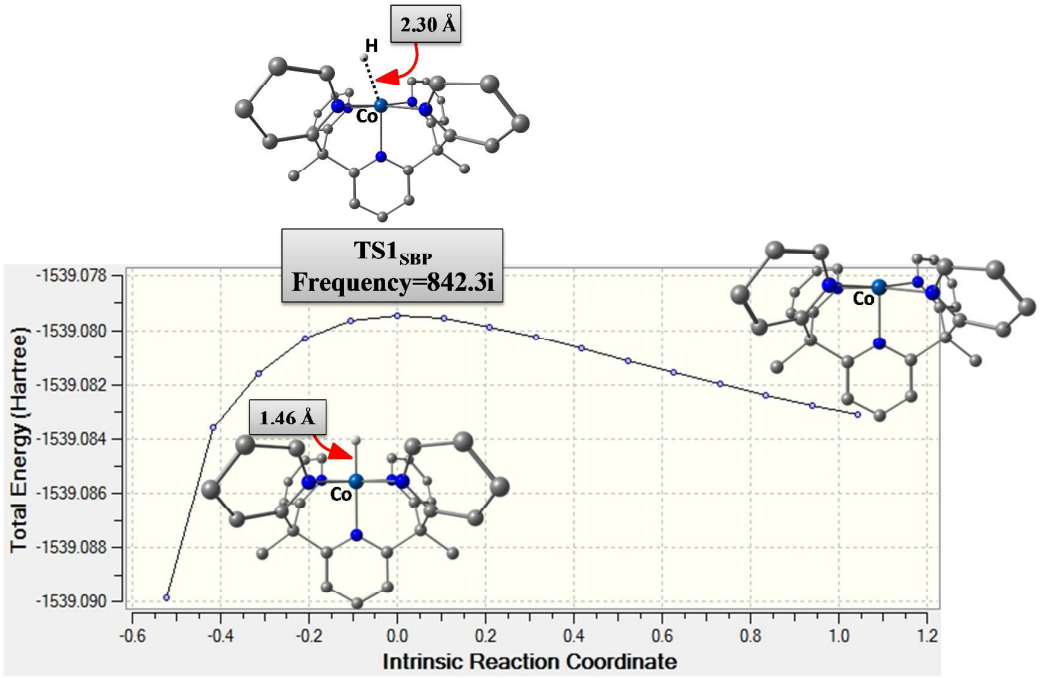


Fig. S1: Intrinsic reaction coordinate (IRC) analysis of $TS2_{SBP}$ and its imaginary frequency is -842.3 cm^{-1}.

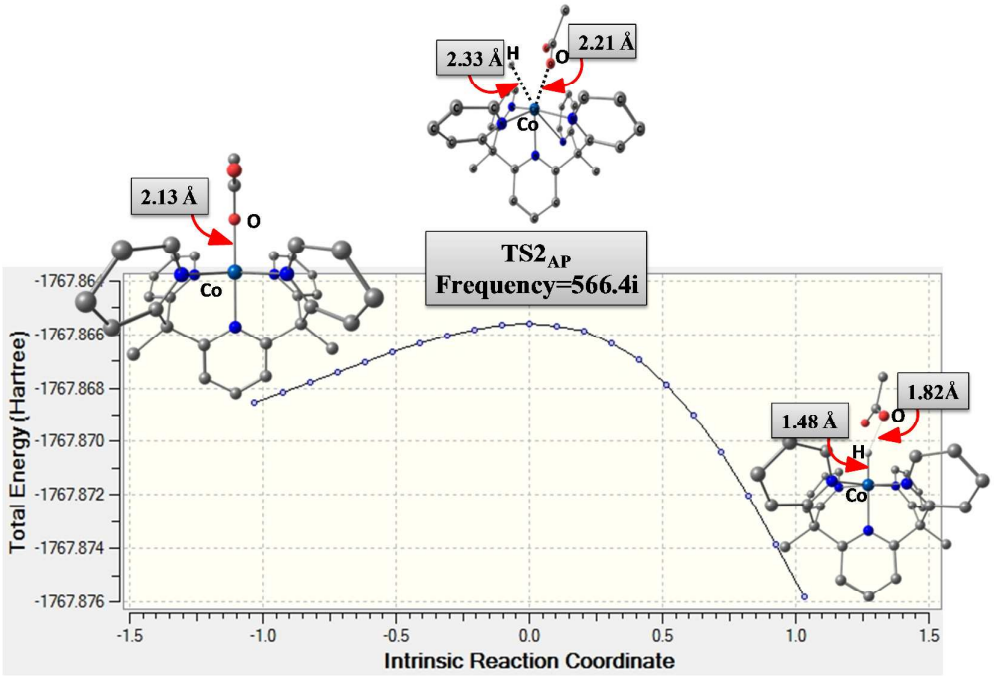


Fig. S2: IRC analysis of $TS2_{AP}$ and its imaginary frequency is -566.4 cm^{-1}.

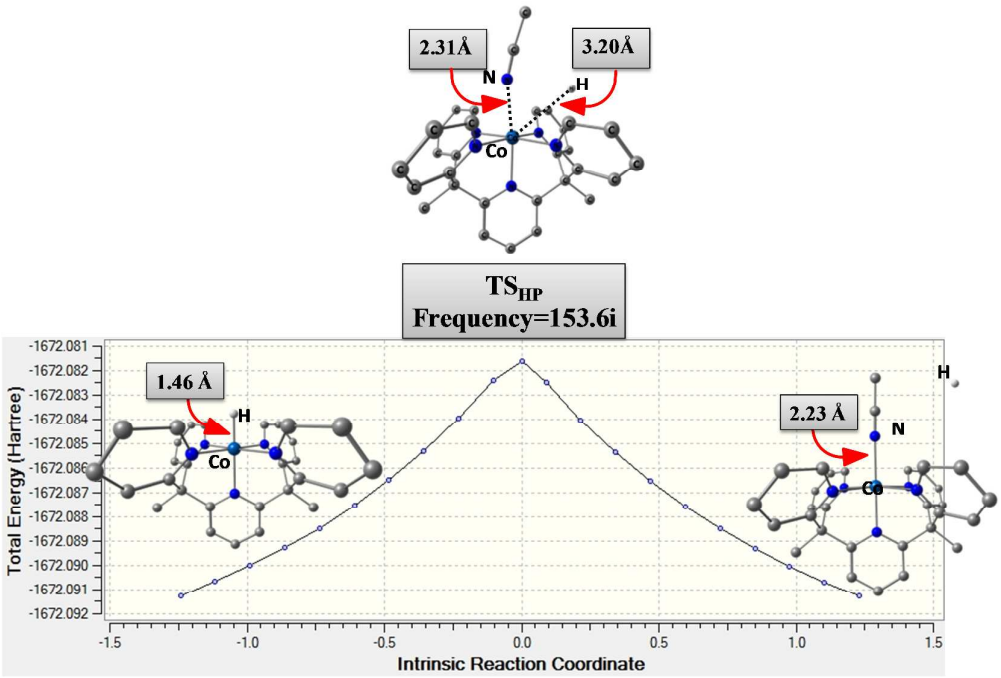


Fig. S3: IRC analysis of TS_{HP} and its imaginary frequency is -153.6 cm^{-1}.

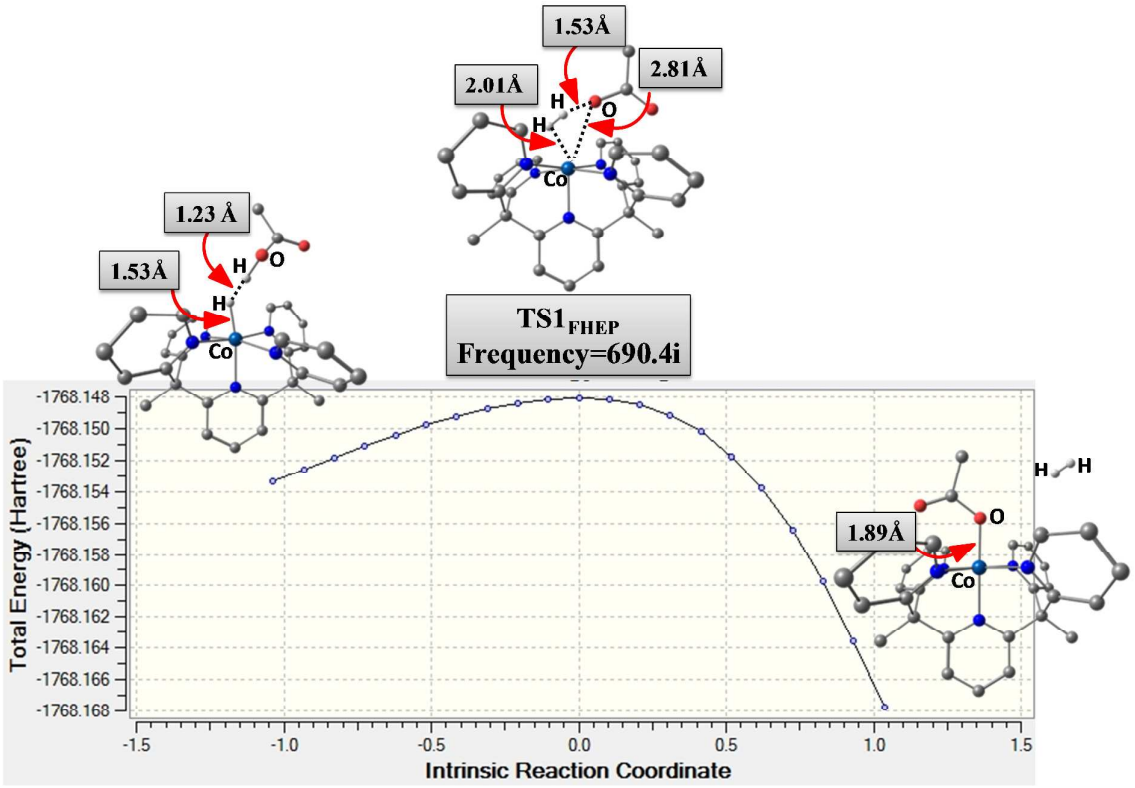


Fig. S4 (a): IRC analysis of $TS1_{FHEP}$ and its imaginary frequency is -690.4 cm^{-1}.

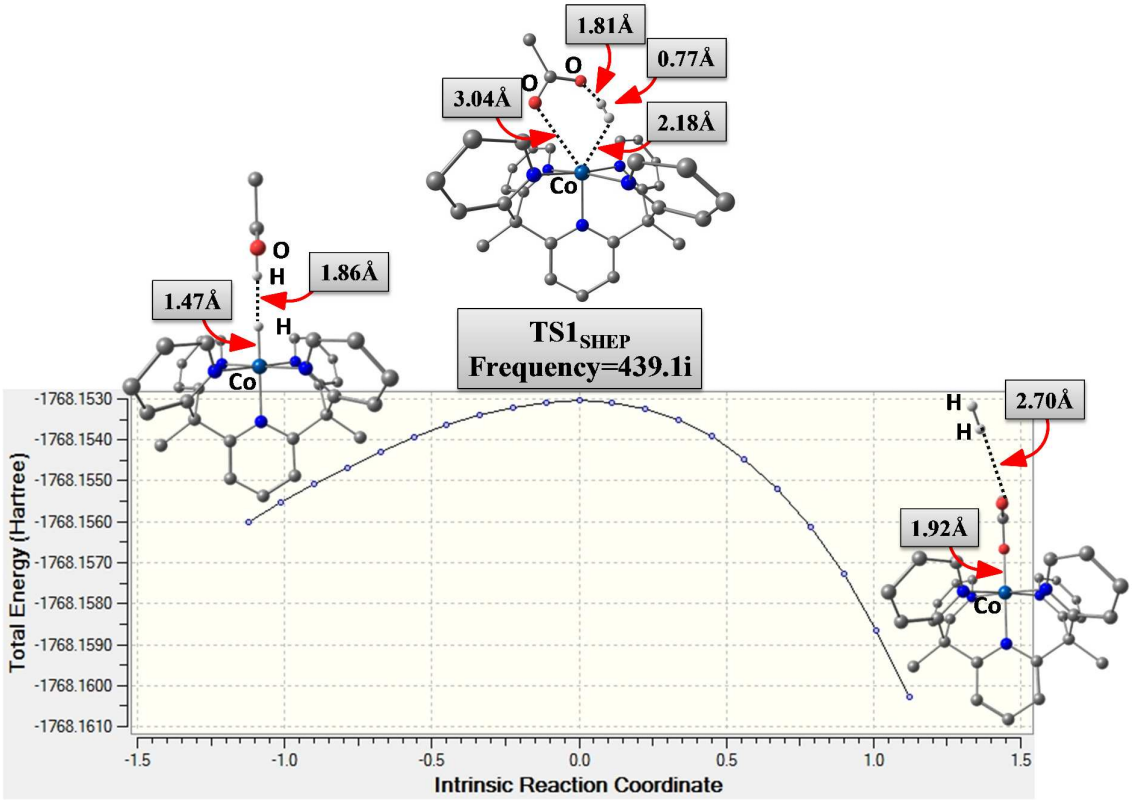


Fig. S4 (b): IRC analysis of $TS1_{SHEP}$ and its imaginary frequency is -439.1 cm^{-1}.

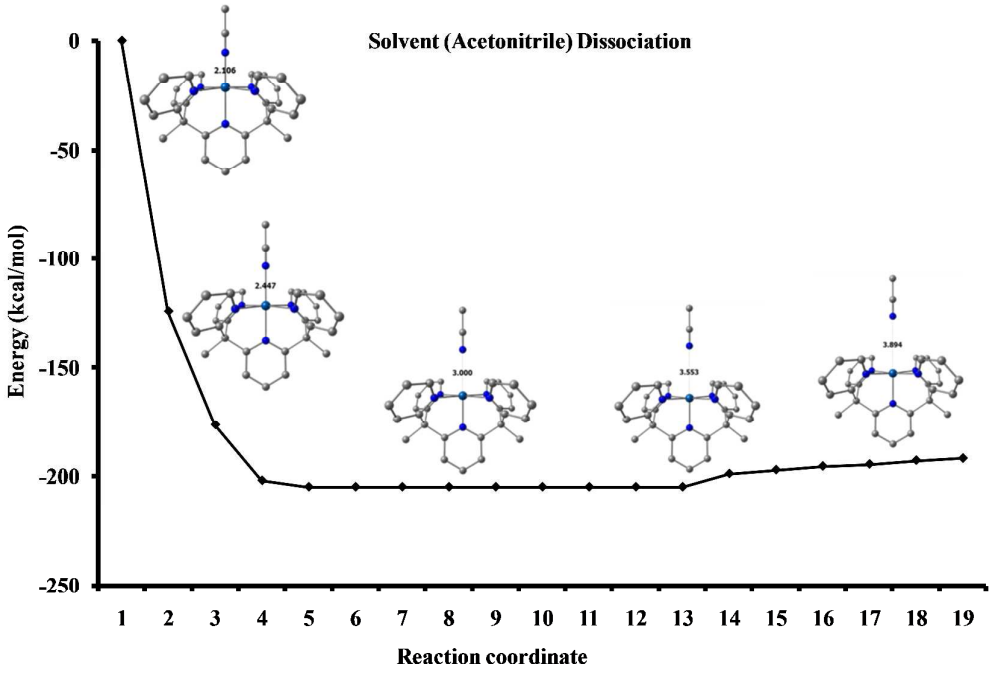


Fig. S5: Geometry scan for Co-N bond breaking mechanism starting from the structure Co(II)(NCMe) on the left hand side and degree of freedom (Co-N) fixed. All data points are represents a full geometry optimization. All data are given in kcal/mol which is likely to be a barrierless process. For clarity, unimportant hydrogen atoms are not shown.

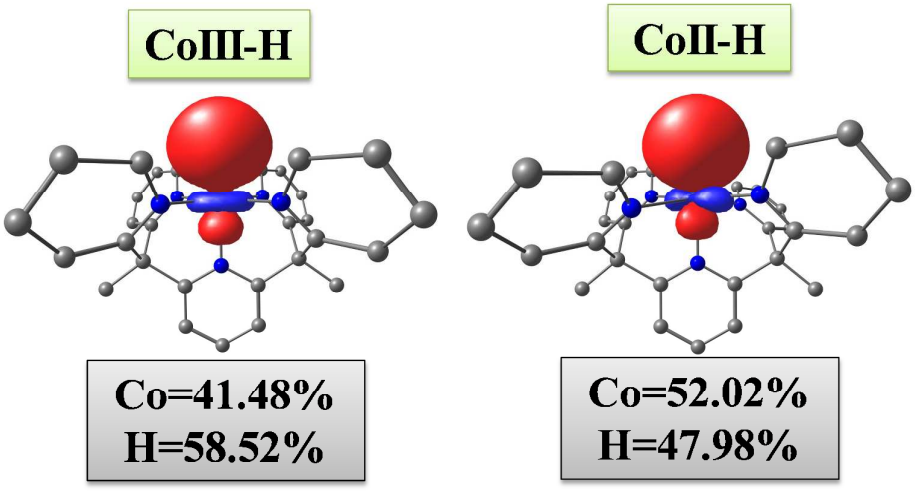


Fig. S6: Bonding orbital contributions for $Co^{III/II}$-H species from NBO Analysis.

Cartesian coordinates of key intermediates and transition states

$[Co^{II}(PY5Me_2)(NCMe)]^{2+}$

7	0.000500000	-1.524858000	-0.008654000
6	-2.503252000	-1.374326000	-0.007716000
7	-1.660505000	0.511475000	-1.403287000
7	1.660711000	0.512646000	-1.402942000
7	-1.660762000	0.495883000	1.408712000
6	3.684739000	0.236871000	3.299785000
1	4.475518000	0.114879000	4.033596000
6	3.604547000	-0.629138000	2.210419000
1	4.345585000	-1.409159000	2.115440000
6	2.586171000	-0.475995000	1.261101000
6	2.504183000	-1.373040000	-0.007699000
6	1.178688000	-2.188971000	-0.013047000
6	-1.177340000	-2.189580000	-0.013048000
6	-3.701575000	-2.349317000	-0.013178000
1	-3.689404000	-2.987343000	-0.898714000
1	-4.646670000	-1.803075000	-0.009002000
1	-3.688214000	-2.998719000	0.864030000
6	-3.686843000	0.274638000	-3.294856000
1	-4.478446000	0.161455000	-4.029192000
6	-3.605883000	-0.603929000	-2.215646000
1	-4.347174000	-1.384696000	-2.128983000
6	-2.586431000	-0.462240000	-1.265699000
6	-1.759623000	1.370471000	-2.433326000
1	-1.016203000	2.157084000	-2.471482000
6	-2.751164000	1.297863000	-3.402930000
1	-2.781511000	2.019488000	-4.212038000
6	1.759524000	1.371902000	-2.432789000
1	1.015889000	2.158336000	-2.470664000
6	2.750981000	1.299743000	-3.402509000
1	2.781089000	2.021542000	-4.211471000
6	3.686903000	0.276702000	-3.294762000
1	4.478435000	0.163848000	-4.029224000
6	3.606296000	-0.602088000	-2.215708000
1	4.347793000	-1.382685000	-2.129277000
6	2.586924000	-0.460823000	-1.265610000
7	1.660389000	0.496314000	1.409078000
6	1.758891000	1.343412000	2.448972000
1	1.015784000	2.129889000	2.495350000
6	2.749466000	1.259273000	3.418613000
1	2.779471000	1.971632000	4.235898000
6	1.200482000	-3.586598000	-0.022294000
1	2.127869000	-4.138676000	-0.025925000
6	0.001214000	-4.286573000	-0.026923000
1	0.001496000	-5.372292000	-0.034112000
6	-1.198415000	-3.587219000	-0.022304000
1	-2.125518000	-4.139771000	-0.025952000
6	-2.585739000	-0.477237000	1.261026000
6	-1.759960000	1.343198000	2.448372000
1	-1.017682000	2.130477000	2.494377000
6	-2.750356000	1.258403000	3.418137000
1	-2.780952000	1.970992000	4.235201000

6	-3.684673000	0.235079000	3.299708000
1	-4.475236000	0.112527000	4.033659000
6	-3.603846000	-0.631095000	2.210520000
1	-4.344203000	-1.411793000	2.115796000
6	3.703003000	-2.347416000	-0.013219000
1	3.690088000	-2.996728000	0.864065000
1	4.647819000	-1.800692000	-0.009244000
1	3.691040000	-2.985548000	-0.898682000
6	-0.001870000	4.002423000	0.021442000
7	-0.000681000	2.843531000	0.016650000
6	-0.003720000	5.460480000	0.026533000
1	-0.932496000	5.835264000	-0.415482000
1	0.074072000	5.829697000	1.054363000
1	0.847247000	5.837730000	-0.549745000
27	-0.000036000	0.608228000	0.003790000

$[Co^{III}(PY5Me_2)(NCMe)]^{3+}$

6	-1.176634000	-2.165947000	-0.012500000
6	-1.197026000	-3.560372000	-0.020620000
1	-2.133958000	-4.096872000	-0.023692000
6	-0.005428000	-4.271352000	-0.024727000
1	-0.007367000	-5.357128000	-0.030998000
6	1.188239000	-3.564458000	-0.020667000
1	2.123902000	-4.103260000	-0.023776000
6	1.170758000	-2.169851000	-0.012572000
6	-1.575240000	1.343084000	2.382184000
1	-0.824081000	2.111725000	2.414137000
6	-2.562663000	1.319109000	3.356378000
1	-2.552575000	2.058338000	4.150154000
6	-3.543526000	0.336903000	3.276510000
1	-4.331650000	0.266219000	4.020015000
6	-3.510158000	-0.545699000	2.198841000
1	-4.287995000	-1.290276000	2.108444000
6	-2.495034000	-0.461463000	1.242380000
6	-2.478688000	-1.361195000	-0.007670000
6	-3.704227000	-2.296732000	-0.013037000
1	-3.710639000	-2.945030000	0.865169000
1	-3.710570000	-2.934917000	-0.898622000
1	-4.632366000	-1.722093000	-0.009768000
6	-1.576565000	1.371919000	-2.364892000
1	-0.826058000	2.141539000	-2.387277000
6	-2.563979000	1.359185000	-3.339316000
1	-2.554315000	2.108026000	-4.124043000
6	-3.544247000	0.375447000	-3.271435000
1	-4.332272000	0.313265000	-4.015804000
6	-3.510442000	-0.520037000	-2.204446000
1	-4.287853000	-1.266098000	-2.123001000
6	-2.495348000	-0.446761000	-1.247024000
6	1.637514000	1.439837000	-2.303286000
1	0.925611000	2.246714000	-2.285141000
6	2.627868000	1.427670000	-3.274924000
1	2.653616000	2.209423000	-4.026502000
6	3.566576000	0.402173000	-3.245750000
1	4.351155000	0.335780000	-3.993390000
6	3.503756000	-0.523996000	-2.206162000
1	4.258693000	-1.294859000	-2.145957000
6	2.492890000	-0.445105000	-1.244932000
6	2.470940000	-1.366042000	-0.007946000
6	3.696897000	-2.301068000	-0.013459000
1	4.624846000	-1.726053000	-0.010203000
1	3.702866000	-2.939903000	-0.898577000
1	3.703059000	-2.950103000	0.864203000
6	1.638985000	1.414192000	2.318597000
1	0.927726000	2.221798000	2.309109000
6	2.629618000	1.391007000	3.289735000
1	2.656180000	2.164718000	4.049557000
6	3.567610000	0.365255000	3.249314000
1	4.352310000	0.290306000	3.996018000
6	3.504088000	-0.549505000	2.199726000
1	4.258694000	-1.319965000	2.130952000
6	2.493131000	-0.459560000	1.239582000
6	-0.088306000	3.633659000	0.020733000
6	-0.147464000	5.089139000	0.026729000
1	0.849927000	5.505296000	-0.154921000
1	-0.511737000	5.445141000	0.997153000
1	-0.831852000	5.438827000	-0.754574000
7	-0.001204000	-1.485798000	-0.008549000
7	-1.507067000	0.457944000	1.364715000
7	-1.507775000	0.474438000	-1.358322000
7	1.528559000	0.503027000	-1.336861000
7	1.529174000	0.487829000	1.342234000
7	-0.038269000	2.476017000	0.014801000
27	0.001460000	0.486616000	0.003080000

$[Co^{I}(PY5Me_2)]^{+}$

27	0.000001000	0.000010000	-0.846941000
7	0.000008000	-0.000007000	1.189049000
6	-2.483357000	0.103494000	1.005564000
7	-1.638506000	-1.458883000	-0.745848000
7	1.607201000	-1.334431000	-0.981149000
7	-1.607202000	1.334448000	-0.981116000
6	3.788668000	3.216406000	-0.481937000
1	4.631362000	3.891272000	-0.365373000
6	3.692337000	2.075575000	0.312289000
1	4.469970000	1.881770000	1.037071000
6	2.606766000	1.201287000	0.160893000
6	2.483367000	-0.103508000	1.005545000
6	1.175017000	-0.061635000	1.849482000
6	-1.174990000	0.061616000	1.849504000
6	-3.691364000	0.207118000	1.961161000
1	-3.737678000	-0.653087000	2.631934000
1	-4.629850000	0.247898000	1.404628000
1	-3.628058000	1.106081000	2.578115000
6	-3.788670000	-3.216381000	-0.481928000
1	-4.631366000	-3.891244000	-0.365356000
6	-3.692322000	-2.075558000	0.312307000
1	-4.469940000	-1.881745000	1.037107000
6	-2.606750000	-1.201279000	0.160897000
6	-1.745254000	-2.558412000	-1.510622000
1	-0.946975000	-2.717904000	-2.225890000
6	-2.794200000	-3.465829000	-1.421809000
1	-2.823283000	-4.335097000	-2.070391000
6	1.712835000	-2.278573000	-1.934820000
1	1.004361000	-2.202491000	-2.753698000
6	2.661307000	-3.292924000	-1.914133000
1	2.696862000	-4.026791000	-2.712379000
6	3.547113000	-3.329017000	-0.841238000
1	4.296826000	-4.110333000	-0.760991000
6	3.476324000	-2.326746000	0.124953000
1	4.185276000	-2.343760000	0.940612000
6	2.510699000	-1.315251000	0.024936000
7	1.638508000	1.458904000	-0.745836000
6	1.745240000	2.558441000	-1.510601000
1	0.946948000	2.717938000	-2.225854000
6	2.794183000	3.465860000	-1.421799000
1	2.823252000	4.335135000	-2.070373000
6	1.199726000	-0.066045000	3.247894000
1	2.126843000	-0.118521000	3.800012000
6	0.000049000	-0.000022000	3.947730000
1	0.000064000	-0.000028000	5.033564000
6	-1.199648000	0.066009000	3.247925000
1	-2.126738000	0.118478000	3.800081000
6	-2.510698000	1.315246000	0.024969000
6	-1.712846000	2.278604000	-1.934772000

1	-1.004369000	2.202543000	-2.753650000
6	-2.661331000	3.292943000	-1.914071000
1	-2.696894000	4.026821000	-2.712307000
6	-3.547142000	3.329006000	-0.841180000
1	-4.296868000	4.110309000	-0.760924000
6	-3.476341000	2.326721000	0.124996000
1	-4.185298000	2.343709000	0.940654000
6	3.691304000	-0.207190000	1.961224000
1	3.737584000	0.652990000	2.632031000
1	4.629830000	-0.247988000	1.404762000
1	3.627919000	-1.106163000	2.578157000

$[Co^{II}(H)\ (PY5Me_2)]^{1+}$

6	1.166466000	0.138175000	1.827016000
6	1.186704000	0.142595000	3.225732000
1	2.109449000	0.251649000	3.775065000
6	-0.001821000	0.002251000	3.927539000
1	-0.002536000	0.003055000	5.013390000
6	-1.189476000	-0.138607000	3.224424000
1	-2.113188000	-0.247126000	3.772380000
6	-1.167547000	-0.135486000	1.825892000
6	2.487162000	0.270285000	1.020439000
6	3.662956000	0.518756000	1.988356000
1	3.509768000	1.429164000	2.572703000
1	4.600329000	0.627173000	1.440259000
1	3.785897000	-0.314960000	2.682388000
6	2.744382000	-1.046513000	0.227783000
6	3.926008000	-1.786978000	0.370723000
1	4.705121000	-1.481762000	1.055194000
6	4.109426000	-2.944155000	-0.384826000
1	5.022530000	-3.522620000	-0.279805000
6	3.111206000	-3.337174000	-1.270081000
1	3.208632000	-4.226828000	-1.883391000
6	1.968785000	-2.546948000	-1.352387000
1	1.165405000	-2.810797000	-2.029863000
6	2.411438000	1.437552000	-0.000323000
6	3.338499000	2.489065000	0.004126000
1	4.092256000	2.562648000	0.774691000
6	3.306551000	3.455738000	-0.998172000
1	4.025413000	4.269552000	-0.992864000
6	2.359646000	3.340460000	-2.010759000
1	2.313837000	4.043786000	-2.835336000
6	1.460810000	2.284007000	-1.947001000
1	0.720439000	2.122384000	-2.719064000
6	-2.488062000	-0.267871000	1.018949000
6	-3.663088000	-0.512576000	1.988609000
1	-3.782181000	0.322162000	2.682141000
1	-3.511465000	-1.422740000	2.573765000
1	-4.601616000	-0.618674000	1.442146000
6	-2.744342000	1.048250000	0.224267000
6	-3.922829000	1.792971000	0.370113000
1	-4.700981000	1.491203000	1.057207000
6	-4.104540000	2.950088000	-0.386174000
1	-5.015242000	3.531880000	-0.278709000
6	-3.107830000	3.338647000	-1.274997000
1	-3.203881000	4.228018000	-1.888940000
6	-1.968414000	2.544215000	-1.359910000
1	-1.166565000	2.804194000	-2.040769000
6	-2.412470000	-1.437354000	0.000442000
6	-3.342347000	-2.486515000	0.005749000
1	-4.097090000	-2.556825000	0.775630000
6	-3.312022000	-3.455320000	-0.994489000
1	-4.033274000	-4.267011000	-0.988375000
6	-2.363640000	-3.344679000	-2.006235000
1	-2.319163000	-4.049238000	-2.829825000
6	-1.461746000	-2.290877000	-1.943027000
1	-0.720020000	-2.132754000	-2.714552000
7	0.000000000	0.000999000	1.155133000
7	1.782534000	-1.437503000	-0.625131000
7	1.455107000	1.374935000	-0.951451000
7	-1.783825000	1.435269000	-0.631709000
7	-1.454384000	-1.379934000	-0.949254000
27	0.002538000	-0.004331000	-0.876133000
1	0.004371000	-0.006986000	-2.393641000

$[Co^{III}(H)\ (PY5Me_2)]^{2+}$

27	0.000000000	-0.000015000	-0.655487000
7	0.000066000	0.000114000	1.233955000
6	-2.479450000	0.140259000	1.058980000
7	-1.429697000	-1.417279000	-0.574648000
7	1.507174000	-1.215379000	-0.908066000
7	-1.507184000	1.215315000	-0.908056000
6	3.507355000	3.275021000	-0.417915000
1	4.322392000	3.989151000	-0.346751000
6	3.529488000	2.103308000	0.342801000
1	4.366764000	1.918199000	1.001769000
6	2.487453000	1.183373000	0.248934000
6	2.479553000	-0.140131000	1.058843000
6	1.182798000	-0.129770000	1.883993000
6	-1.182625000	0.130190000	1.884032000
6	-3.711771000	0.244441000	1.976161000
1	-3.752222000	-0.583281000	2.686829000
1	-4.633818000	0.222535000	1.392594000
1	-3.698755000	1.179737000	2.541497000
6	-3.507186000	-3.275189000	-0.417118000
1	-4.322086000	-3.989441000	-0.345613000
6	-3.529242000	-2.103416000	0.343504000
1	-4.366346000	-1.918361000	1.002706000
6	-2.487348000	-1.183359000	0.249257000
6	-1.407123000	-2.557190000	-1.298761000
1	-0.547700000	-2.733413000	-1.924673000
6	-2.423680000	-3.503927000	-1.256902000
1	-2.348347000	-4.397060000	-1.868022000
6	1.616458000	-1.907176000	-2.064904000
1	0.857273000	-1.737399000	-2.822587000
6	2.665169000	-2.785722000	-2.304708000
1	2.721242000	-3.318015000	-3.248430000
6	3.616841000	-2.961987000	-1.300625000
1	4.430553000	-3.670278000	-1.426200000
6	3.544149000	-2.176156000	-0.147408000
1	4.318481000	-2.261096000	0.603375000
6	2.497648000	-1.265043000	0.005808000
7	1.429581000	1.417363000	-0.574670000
6	1.406929000	2.557224000	-1.298858000
1	0.547352000	2.733498000	-1.924541000
6	2.423612000	3.503842000	-1.257369000
1	2.348182000	4.396959000	-1.868501000
6	1.190092000	-0.157637000	3.278994000
1	2.118570000	-0.279655000	3.818634000
6	0.000168000	0.000593000	3.980877000
1	0.000210000	0.000795000	5.066996000
6	-1.189813000	0.158546000	3.279024000
1	-2.118253000	0.280727000	3.818689000
6	-2.497722000	1.264963000	0.005738000
6	-1.616548000	1.906857000	-2.065043000
1	-0.857290000	1.737098000	-2.822648000
6	-2.665432000	2.785127000	-2.305097000
1	-2.721549000	3.317230000	-3.248923000
6	-3.617219000	2.961378000	-1.301120000
1	-4.431092000	3.669446000	-1.426907000
6	-3.544425000	2.175805000	-0.147737000
1	-4.318830000	2.260726000	0.602972000
6	3.711934000	-0.244259000	1.975955000
1	3.752481000	0.583554000	2.686510000

1	4.633945000	-0.222495000	1.392326000
1	3.698896000	-1.179477000	2.541422000

$[Co^{I}(PY5Me_2)(CH_3COO)]$

6	-1.176900000	-2.250332000	-0.052747000
6	-1.194884000	-3.627437000	-0.251732000
1	-2.128485000	-4.168449000	-0.316629000
6	0.001703000	-4.336215000	-0.363068000
1	0.002059000	-5.410899000	-0.515300000
6	1.197804000	-3.626621000	-0.251772000
1	2.131783000	-4.166979000	-0.316656000
6	1.178843000	-2.249514000	-0.052844000
6	-2.503916000	-1.455056000	0.072995000
6	-3.692566000	-2.434166000	0.185806000
1	-3.803267000	-3.029625000	-0.722415000
1	-4.627102000	-1.890823000	0.346853000
1	-3.553272000	-3.126376000	1.018798000
6	-2.487650000	-0.547374000	1.336830000
6	-3.305336000	-0.802275000	2.447087000
1	-3.941915000	-1.675667000	2.487762000
6	-3.316005000	0.090146000	3.519006000
1	-3.952361000	-0.103153000	4.378814000
6	-2.525796000	1.232736000	3.454241000
1	-2.528345000	1.975306000	4.246138000
6	-1.716963000	1.410846000	2.334143000
1	-1.093888000	2.293663000	2.199752000
6	-2.693695000	-0.574891000	-1.192908000
6	-3.825920000	-0.674331000	-2.016546000
1	-4.614293000	-1.382430000	-1.801569000
6	-3.955213000	0.158888000	-3.125438000
1	-4.832264000	0.083664000	-3.762656000
6	-2.957676000	1.095747000	-3.385471000
1	-3.023894000	1.784019000	-4.222330000
6	-1.867386000	1.141273000	-2.524560000
1	-1.087499000	1.885854000	-2.629870000
6	2.505288000	-1.453240000	0.072535000
6	3.694740000	-2.431403000	0.184993000
1	3.805608000	-3.026806000	-0.723234000
1	3.556286000	-3.123674000	1.018080000
1	4.628894000	-1.887298000	0.345717000
6	2.693952000	-0.573048000	-1.193537000
6	3.826056000	-0.671590000	-2.017452000
1	4.615082000	-1.379010000	-1.802619000
6	3.954358000	0.161646000	-3.126444000
1	4.831330000	0.087132000	-3.763855000
6	2.955934000	1.097605000	-3.386325000
1	3.021370000	1.785870000	-4.223251000
6	1.865803000	1.142246000	-2.525179000
1	1.085168000	1.886044000	-2.630483000
6	2.488742000	-0.545447000	1.336239000
6	3.306887000	-0.799618000	2.446319000
1	3.944041000	-1.672612000	2.486969000
6	3.317300000	0.093043000	3.518043000
1	3.954016000	-0.099671000	4.377712000
6	2.526365000	1.235137000	3.453250000
1	2.528697000	1.977889000	4.244978000
6	1.717075000	1.412489000	2.333362000
1	1.093304000	2.294838000	2.198989000
6	-0.001730000	3.662081000	0.004586000
6	-0.005273000	4.938774000	-0.848355000
1	0.007061000	5.831096000	-0.218352000
1	-0.895925000	4.957559000	-1.488166000
1	0.867906000	4.948276000	-1.511800000
7	0.000746000	-1.549834000	0.013878000
7	-1.675563000	0.526189000	1.322165000
7	-1.724223000	0.317840000	-1.473411000
7	1.723621000	0.318809000	-1.473893000
7	1.675932000	0.527563000	1.321610000
8	-0.000957000	2.570163000	-0.663420000
8	-0.001326000	3.777466000	1.249419000
27	0.000035000	0.506173000	-0.136005000

$[Co^{II}(PY5Me_2)(CH_3COO)]^{+}$

6	1.487313000	2.119923000	-0.098952000
6	1.665993000	3.505029000	-0.189228000
1	2.649567000	3.948695000	-0.211668000
6	0.553161000	4.331053000	-0.252905000
1	0.673049000	5.407951000	-0.325553000
6	-0.714349000	3.768028000	-0.220953000
1	-1.575686000	4.416466000	-0.269311000
6	-0.847938000	2.377778000	-0.126086000
6	2.720033000	1.173758000	-0.034370000
6	4.015917000	2.012261000	-0.052410000
1	4.092490000	2.605676000	-0.965534000
1	4.893487000	1.364780000	-0.001263000
1	4.056690000	2.698627000	0.795798000
6	2.697029000	0.313776000	1.264446000
6	3.706913000	0.395515000	2.232495000
1	4.506481000	1.118363000	2.152639000
6	3.699800000	-0.479551000	3.318463000
1	4.482075000	-0.417184000	4.069145000
6	2.700071000	-1.442387000	3.407125000
1	2.675021000	-2.169809000	4.211395000
6	1.719664000	-1.450438000	2.420971000
1	0.931981000	-2.194232000	2.410047000
6	2.729113000	0.206390000	-1.255641000
6	3.775361000	0.189519000	-2.187559000
1	4.591059000	0.896218000	-2.130873000
6	3.782109000	-0.764086000	-3.205303000
1	4.591753000	-0.778174000	-3.928932000
6	2.758244000	-1.703694000	-3.260330000
1	2.739312000	-2.486549000	-4.010940000
6	1.746553000	-1.616558000	-2.310189000
1	0.942412000	-2.341056000	-2.270320000
6	-2.260648000	1.727986000	-0.079853000
6	-3.336558000	2.834195000	-0.128511000
1	-3.265317000	3.416778000	-1.049337000
1	-3.238129000	3.520659000	0.715097000
1	-4.336924000	2.400111000	-0.088076000
6	-2.462889000	0.773505000	-1.291882000
6	-3.504905000	0.949786000	-2.211693000
1	-4.183592000	1.787139000	-2.138746000
6	-3.686478000	0.027696000	-3.241066000
1	-4.495088000	0.162508000	-3.953263000
6	-2.832157000	-1.065271000	-3.327712000
1	-2.946632000	-1.823414000	-4.094757000
6	-1.816993000	-1.169505000	-2.384886000
1	-1.138579000	-2.012741000	-2.391768000
6	-2.440013000	0.905786000	1.229274000
6	-3.455021000	1.190834000	2.152025000
1	-4.123344000	2.028102000	2.011983000
6	-3.621332000	0.379012000	3.272953000
1	-4.408292000	0.597516000	3.988670000
6	-2.780999000	-0.714504000	3.445906000
1	-2.886768000	-1.391850000	4.286260000
6	-1.792289000	-0.928495000	2.493354000
1	-1.128459000	-1.779207000	2.567187000
6	-1.111902000	-3.353206000	0.135727000
6	-0.807765000	-4.847664000	0.082364000
1	-1.728053000	-5.429128000	0.161977000
1	-0.125888000	-5.123575000	0.894768000
1	-0.296510000	-5.096352000	-0.854905000
7	0.246780000	1.586508000	-0.071448000
7	1.698262000	-0.577067000	1.402869000

7	1.714484000	-0.670827000	-1.359349000
7	-1.621437000	-0.269432000	-1.409644000
7	-1.608085000	-0.131477000	1.430816000
8	-0.042428000	-2.592664000	0.054165000
8	-2.264232000	-2.938005000	0.247517000
27	-0.007966000	-0.611989000	0.017803000

$[Co^{III}(PY5Me_2)(CH3COO)]^{2+}$

6	-0.903296000	2.348484000	-0.046160000
6	-0.806049000	3.740226000	-0.074324000
1	-1.692125000	4.357395000	-0.085595000
6	0.445873000	4.341027000	-0.088315000
1	0.538082000	5.422460000	-0.110241000
6	1.576977000	3.536577000	-0.073931000
1	2.556186000	3.991914000	-0.084949000
6	1.430206000	2.149127000	-0.045111000
6	-2.266581000	1.639557000	-0.031981000
6	-3.412934000	2.668959000	-0.053024000
1	-3.368712000	3.326351000	0.817698000
1	-4.383482000	2.169747000	-0.044124000
1	-3.367062000	3.291765000	-0.948701000
6	-2.348351000	0.718057000	-1.262588000
6	-3.362540000	0.844181000	-2.215098000
1	-4.115200000	1.612920000	-2.118256000
6	-3.421017000	-0.026053000	-3.300332000
1	-4.210310000	0.072006000	-4.038986000
6	-2.458524000	-1.022321000	-3.403280000
1	-2.460689000	-1.743191000	-4.213190000
6	-1.481940000	-1.096086000	-2.421471000
1	-0.746114000	-1.878949000	-2.458711000
6	-2.350011000	0.767174000	1.233833000
6	-3.367255000	0.928808000	2.177672000
1	-4.120632000	1.691962000	2.048535000
6	-3.427783000	0.101243000	3.295682000
1	-4.219666000	0.226538000	4.027413000
6	-2.464324000	-0.888862000	3.439955000
1	-2.468211000	-1.578187000	4.276868000
6	-1.484826000	-0.999341000	2.464572000
1	-0.749315000	-1.780175000	2.533310000
6	2.636463000	1.209537000	-0.026222000
6	3.952209000	2.010243000	-0.044613000
1	4.023747000	2.670790000	0.821914000
1	4.023111000	2.631254000	-0.939980000
1	4.815080000	1.341633000	-0.029933000
6	2.578391000	0.305128000	1.231050000
6	3.588219000	0.303726000	2.195589000
1	4.380069000	1.038757000	2.165285000
6	3.604377000	-0.673372000	3.191576000
1	4.387593000	-0.673113000	3.943276000
6	2.638739000	-1.673037000	3.161081000
1	2.649363000	-2.502844000	3.859221000
6	1.643825000	-1.597158000	2.194171000
1	0.911477000	-2.381552000	2.078099000
6	2.577308000	0.250443000	-1.242585000
6	3.586913000	0.205893000	-2.206401000
1	4.378588000	0.941611000	-2.209113000
6	3.602966000	-0.815087000	-3.157339000
1	4.386083000	-0.848522000	-3.908400000
6	2.637736000	-1.812727000	-3.081367000
1	2.648792000	-2.673350000	-3.741139000
6	1.643073000	-1.693628000	-2.118660000
1	0.911314000	-2.472400000	-1.966234000
6	-1.266580000	-3.011677000	0.061918000
6	-1.011494000	-4.512086000	0.068419000
1	-0.309384000	-4.791197000	0.860250000
1	-0.562531000	-4.822603000	-0.882117000
1	-1.956969000	-5.038730000	0.205012000
7	0.207912000	1.575792000	-0.031526000
7	-1.405300000	-0.241500000	-1.384534000
7	-1.406122000	-0.185504000	1.395578000
7	1.566850000	-0.591401000	1.303298000
7	1.565915000	-0.648508000	-1.274291000
8	-0.122801000	-2.314438000	0.051163000
8	-2.384503000	-2.527369000	0.056629000
27	0.022813000	-0.433767000	0.010537000

$[Co^{II}(PY5Me_2)]^{2+}$

27	0.000028000	0.000112000	-0.809811000
7	0.000001000	0.000045000	1.282287000
6	-2.439206000	0.027174000	1.058069000
7	-1.481741000	-1.370878000	-0.783677000
7	1.541867000	-1.269446000	-0.905878000
7	-1.541934000	1.269532000	-0.905868000
6	3.483638000	3.304709000	-0.582191000
1	4.261036000	4.055692000	-0.481758000
6	3.438936000	2.220488000	0.292891000
1	4.195166000	2.139775000	1.060463000
6	2.443986000	1.246846000	0.168337000
6	2.439206000	-0.027190000	1.058088000
6	1.170298000	-0.029978000	1.937252000
6	-1.170308000	0.030011000	1.937236000
6	-3.690836000	0.054537000	1.957518000
1	-3.711387000	-0.807494000	2.627030000
1	-4.607790000	0.044226000	1.364711000
1	-3.701455000	0.950718000	2.581573000
6	-3.483380000	-3.304848000	-0.582145000
1	-4.260692000	-4.055915000	-0.481667000
6	-3.438756000	-2.220614000	0.292926000
1	-4.194952000	-2.139985000	1.060540000
6	-2.443924000	-1.246860000	0.168308000
6	-1.555752000	-2.401194000	-1.648952000
1	-0.807510000	-2.436170000	-2.426133000
6	-2.532508000	-3.386413000	-1.592140000
1	-2.536730000	-4.186937000	-2.323635000
6	1.691054000	-2.154552000	-1.911234000
1	1.002384000	-2.062978000	-2.741673000
6	2.685487000	-3.122715000	-1.934962000
1	2.759485000	-3.805835000	-2.773910000
6	3.565867000	-3.177544000	-0.859124000
1	4.344670000	-3.932363000	-0.812449000
6	3.463327000	-2.214619000	0.144178000
1	4.180689000	-2.223482000	0.952489000
6	2.463758000	-1.238309000	0.087753000
7	1.481772000	1.370955000	-0.783605000
6	1.555864000	2.401251000	-1.648898000
1	0.807598000	2.436298000	-2.426050000
6	2.532730000	3.386364000	-1.592143000
1	2.537007000	4.186878000	-2.323649000
6	1.203603000	-0.038242000	3.333868000
1	2.135366000	-0.070246000	3.880760000
6	-0.000022000	-0.000044000	4.032178000
1	-0.000032000	-0.000084000	5.117862000
6	-1.203637000	0.038186000	3.333851000
1	-2.135410000	0.070124000	3.880728000
6	-2.463833000	1.238305000	0.087754000
6	-1.691203000	2.154627000	-1.911224000
1	-1.002528000	2.063115000	-2.741664000
6	-2.685722000	3.122702000	-1.934951000
1	-2.759784000	3.805813000	-2.773900000
6	-3.566106000	3.177451000	-0.859113000
1	-4.344977000	3.932200000	-0.812438000
6	-3.463485000	2.214530000	0.144182000
1	-4.180850000	2.223322000	0.952492000
6	3.690843000	-0.054624000	1.957527000

1	3.711615000	0.807575000	2.626815000
1	4.607789000	-0.044681000	1.364701000
1	3.701261000	-0.950645000	2.581814000

Cartesian coordinates of Transition States (TS)

$TS1_{AP}$

7	-0.872021000	-1.562020000	0.035940000
6	1.531211000	-2.212303000	0.123295000
7	1.271516000	-0.170029000	1.527040000
7	-1.921057000	0.709401000	1.490117000
7	1.120961000	-0.357786000	-1.499433000
6	-3.427029000	1.368083000	-3.479124000
1	-4.095089000	1.464262000	-4.329846000
6	-3.689958000	0.420367000	-2.491077000
1	-4.570914000	-0.197945000	-2.587750000
6	-2.831222000	0.294526000	-1.390051000
6	-3.180186000	-0.623551000	-0.180496000
6	-2.193696000	-1.816957000	-0.036919000
6	0.021386000	-2.566508000	0.154842000
6	2.364247000	-3.510735000	0.165743000
1	2.178442000	-4.071458000	1.084177000
1	3.429086000	-3.276208000	0.124575000
1	2.125753000	-4.160670000	-0.678605000
6	3.179211000	-0.957924000	3.378793000
1	3.921228000	-1.286680000	4.100245000
6	2.851947000	-1.770044000	2.300399000
1	3.365922000	-2.712694000	2.189679000
6	1.903699000	-1.344334000	1.359074000
6	1.625489000	0.633856000	2.543639000
1	1.147096000	1.604875000	2.564616000
6	2.565209000	0.285661000	3.500416000
1	2.808740000	0.970420000	4.305599000
6	-1.830911000	1.440914000	2.610253000
1	-0.846227000	1.815808000	2.855443000
6	-2.916681000	1.733392000	3.428833000
1	-2.780653000	2.327193000	4.326369000
6	-4.162927000	1.248528000	3.050146000
1	-5.047702000	1.452522000	3.645839000
6	-4.265714000	0.490830000	1.884762000
1	-5.236092000	0.117906000	1.589670000
6	-3.121996000	0.226914000	1.119627000
7	-1.714218000	1.045700000	-1.317068000
6	-1.493325000	1.993194000	-2.242477000
1	-0.617905000	2.611592000	-2.078328000
6	-2.321953000	2.200246000	-3.339548000
1	-2.097324000	2.981888000	-4.057340000
6	-2.671428000	-3.129751000	0.044219000
1	-3.725854000	-3.353477000	-0.014200000
6	-1.768542000	-4.171729000	0.210437000
1	-2.122627000	-5.195377000	0.288912000
6	-0.410375000	-3.893459000	0.262546000
1	0.292223000	-4.705314000	0.377767000
6	1.818128000	-1.474570000	-1.220054000
6	1.341632000	0.278550000	-2.660705000
1	0.788527000	1.193975000	-2.816382000
6	2.222318000	-0.174935000	-3.630061000
1	2.352949000	0.379719000	-4.553015000
6	2.925308000	-1.346965000	-3.367719000
1	3.632490000	-1.748356000	-4.087427000
6	2.720819000	-1.996464000	-2.157632000
1	3.292119000	-2.887519000	-1.947139000
6	-4.614546000	-1.164864000	-0.368715000
1	-4.678244000	-1.823939000	-1.237170000
1	-5.322675000	-0.346896000	-0.515494000
1	-4.939672000	-1.732386000	0.505031000
6	0.862918000	3.551685000	0.350912000
7	0.044007000	2.733101000	0.441188000
6	1.823689000	4.641441000	0.261170000
1	2.297754000	4.615646000	-0.722410000
1	1.328065000	5.605015000	0.419631000
1	2.604285000	4.496450000	1.012214000
27	-0.080491000	0.519215000	0.079822000
6	4.869259000	2.220270000	-0.366634000
1	4.761097000	2.855496000	-1.253840000
1	4.914924000	2.887066000	0.504358000
1	5.807059000	1.663404000	-0.429857000
6	3.671078000	1.262589000	-0.236984000
8	2.512460000	1.810694000	-0.279124000
8	3.902517000	0.043380000	-0.092182000

$TS2_{AP}$

6	-0.877496000	-2.355263000	0.157300000
6	-0.760359000	-3.746165000	0.044395000
1	-1.630296000	-4.385270000	0.030280000
6	0.498955000	-4.319478000	-0.052493000
1	0.607161000	-5.395841000	-0.147521000
6	1.618892000	-3.501173000	-0.013718000
1	2.600459000	-3.947065000	-0.073115000
6	1.449152000	-2.117621000	0.101884000
6	-2.277184000	-1.694992000	0.261487000
6	-3.341184000	-2.788257000	0.510257000
1	-3.425411000	-3.462730000	-0.343545000
1	-4.323323000	-2.341483000	0.676161000
1	-3.093004000	-3.390032000	1.387236000
6	-2.334722000	-0.665374000	1.428505000
6	-3.110662000	-0.901761000	2.570590000
1	-3.626171000	-1.840641000	2.714033000
6	-3.243531000	0.090270000	3.541867000
1	-3.847000000	-0.093701000	4.426022000
6	-2.619490000	1.314457000	3.339967000
1	-2.725235000	2.135370000	4.041311000
6	-1.835212000	1.470458000	2.200161000
1	-1.333770000	2.407939000	1.980620000
6	-2.596322000	-0.969411000	-1.075225000
6	-3.769040000	-1.231063000	-1.796125000
1	-4.493076000	-1.953565000	-1.447392000
6	-4.022122000	-0.546793000	-2.983631000
1	-4.928601000	-0.750978000	-3.545835000
6	-3.106190000	0.402516000	-3.420932000
1	-3.262493000	0.973153000	-4.330182000
6	-1.974537000	0.622645000	-2.642752000
1	-1.267925000	1.400274000	-2.898420000
6	2.679818000	-1.174718000	0.156442000
6	3.966243000	-2.014317000	0.324695000
1	4.142909000	-2.648888000	-0.545441000
1	3.902787000	-2.660781000	1.202420000
1	4.838524000	-1.368683000	0.445288000
6	2.765291000	-0.388134000	-1.185060000
6	3.924113000	-0.387161000	-1.972927000
1	4.813837000	-0.915168000	-1.661114000
6	3.944716000	0.305895000	-3.182310000
1	4.842341000	0.302091000	-3.793494000
6	2.810116000	1.003329000	-3.583930000
1	2.781168000	1.565385000	-4.511118000
6	1.705847000	0.982956000	-2.741573000
1	0.820421000	1.566246000	-2.962054000
6	2.551878000	-0.203505000	1.367227000
6	3.431010000	-0.267426000	2.456398000
1	4.206770000	-1.017509000	2.506543000
6	3.320154000	0.652577000	3.498443000
1	4.001530000	0.598565000	4.342459000
6	2.350900000	1.646155000	3.422530000
1	2.251390000	2.409800000	4.186422000

6	1.504901000	1.651684000	2.319633000
1	0.775256000	2.438225000	2.157671000
7	0.218511000	-1.567807000	0.162312000
7	-1.665350000	0.497025000	1.286615000
7	-1.711898000	-0.053157000	-1.512593000
7	1.676984000	0.298721000	-1.585083000
7	1.579368000	0.730017000	1.340382000
27	0.023040000	0.678792000	-0.209243000
1	1.591035000	2.354410000	-0.309229000
6	-0.625910000	3.600018000	-0.331485000
6	-1.181214000	4.748372000	-1.162703000
1	-1.194578000	5.671118000	-0.580727000
1	-0.573110000	4.888743000	-2.063084000
1	-2.198741000	4.509891000	-1.493172000
8	-0.521445000	2.472282000	-0.969848000
8	-0.308444000	3.774947000	0.854298000

$TS1_{SBP}$

27	-0.032901000	-0.037289000	-0.857608000
7	0.027971000	0.034072000	1.261373000
6	2.466916000	-0.115542000	1.025953000
7	1.549357000	1.388883000	-0.747534000
7	-1.513273000	1.263388000	-0.947121000
7	1.472113000	-1.323903000	-0.917512000
6	-3.629616000	-3.232734000	-0.375775000
1	-4.434416000	-3.945511000	-0.224994000
6	-3.534536000	-2.102043000	0.434871000
1	-4.277044000	-1.948951000	1.204451000
6	-2.504853000	-1.176736000	0.243839000
6	-2.424238000	0.135576000	1.075511000
6	-1.135345000	0.106753000	1.929493000
6	1.200122000	-0.064822000	1.908200000
6	3.717395000	-0.219209000	1.922353000
1	3.776056000	0.624328000	2.612283000
1	4.633076000	-0.229514000	1.327735000
1	3.692040000	-1.131357000	2.522699000
6	3.586204000	3.273793000	-0.438048000
1	4.384790000	3.996845000	-0.304219000
6	3.544861000	2.122137000	0.345789000
1	4.320590000	1.965552000	1.081178000
6	2.520242000	1.184935000	0.175927000
6	1.606825000	2.497302000	-1.509924000
1	0.832437000	2.613453000	-2.253827000
6	2.596056000	3.465153000	-1.393772000
1	2.583706000	4.333165000	-2.043806000
6	-1.630613000	2.118312000	-1.983433000
1	-0.942731000	1.968095000	-2.807146000
6	-2.586762000	3.122817000	-2.033214000
1	-2.641001000	3.779244000	-2.894687000
6	-3.453691000	3.250582000	-0.952226000
1	-4.201410000	4.037213000	-0.926469000
6	-3.378174000	2.323735000	0.087051000
1	-4.083713000	2.393368000	0.902575000
6	-2.419692000	1.305620000	0.058443000
7	-1.564239000	-1.390323000	-0.712188000
6	-1.678876000	-2.470655000	-1.508806000
1	-0.935750000	-2.584425000	-2.283857000
6	-2.690352000	-3.413865000	-1.383695000
1	-2.729533000	-4.259154000	-2.061848000
6	-1.154221000	0.109229000	3.326568000
1	-2.078034000	0.180651000	3.882704000
6	0.051310000	0.009082000	4.014497000
1	0.060653000	0.003089000	5.100120000
6	1.243923000	-0.088047000	3.304600000
1	2.177155000	-0.174641000	3.842601000
6	2.430830000	-1.311380000	0.040118000
6	1.563629000	-2.209503000	-1.930864000
1	0.842514000	-2.099445000	-2.731442000
6	2.537993000	-3.194094000	-1.999816000
1	2.563615000	-3.876336000	-2.842309000
6	3.463334000	-3.264483000	-0.963071000
1	4.231959000	-4.030994000	-0.951123000
6	3.417001000	-2.304645000	0.046595000
1	4.166691000	-2.329663000	0.824068000
6	-3.654984000	0.256648000	1.996664000
1	-3.707477000	-0.579522000	2.695979000
1	-4.581996000	0.270194000	1.419775000
1	-3.608955000	1.173839000	2.587933000
1	0.617476000	0.368968000	-2.865060000

$TS1_{UMHP}$

6	1.287665000	2.176042000	-0.000542000
6	1.382341000	3.569489000	-0.000840000
1	2.341511000	4.065897000	-0.001042000
6	0.219876000	4.330140000	-0.000858000
1	0.272648000	5.414483000	-0.001081000
6	-1.009877000	3.685070000	-0.000590000
1	-1.918820000	4.268831000	-0.000625000
6	-1.047726000	2.288971000	-0.000304000
6	2.531031000	1.274915000	-0.000478000
6	3.809339000	2.136568000	-0.000944000
1	3.848793000	2.781067000	-0.881124000
1	4.704148000	1.510980000	-0.001011000
1	3.849189000	2.781455000	0.878932000
6	2.505599000	0.362654000	1.249023000
6	3.508465000	0.427560000	2.221439000
1	4.289401000	1.171436000	2.159471000
6	3.527958000	-0.480746000	3.277625000
1	4.306804000	-0.426265000	4.031831000
6	2.553564000	-1.470295000	3.318603000
1	2.542232000	-2.234864000	4.087602000
6	1.575829000	-1.466783000	2.332958000
1	0.829907000	-2.243540000	2.314188000
6	2.505321000	0.361830000	-1.249377000
6	3.507751000	0.426318000	-2.222272000
1	4.288336000	1.170645000	-2.161322000
6	3.527295000	-0.483060000	-3.277542000
1	4.305788000	-0.428919000	-4.032136000
6	2.553523000	-1.473295000	-3.317001000
1	2.542435000	-2.238788000	-4.085085000
6	1.576120000	-1.469236000	-2.331032000
1	0.830768000	-2.246517000	-2.310910000
6	-2.371385000	1.509732000	-0.000063000
6	-3.564781000	2.484998000	-0.000082000
1	-3.546423000	3.129940000	-0.880703000
1	-3.546251000	3.130173000	0.880368000
1	-4.511740000	1.941492000	0.000089000
6	-2.423486000	0.604308000	-1.250643000
6	-3.412339000	0.757180000	-2.228950000
1	-4.130829000	1.561074000	-2.165106000
6	-3.490438000	-0.132548000	-3.296124000
1	-4.255054000	-0.008167000	-4.056537000
6	-2.593847000	-1.193850000	-3.344603000
1	-2.638974000	-1.949565000	-4.120748000
6	-1.642737000	-1.291387000	-2.341178000
1	-0.975308000	-2.135476000	-2.311256000
6	-2.423410000	0.604551000	1.250659000
6	-3.412104000	0.757581000	2.229108000
1	-4.130325000	1.561732000	2.165488000
6	-3.490394000	-0.132378000	3.296075000
1	-4.254852000	-0.007878000	4.056628000
6	-2.594311000	-1.194140000	3.344108000
1	-2.639804000	-1.950142000	4.119953000
6	-1.643284000	-1.291748000	2.340613000
1	-0.976257000	-2.136176000	2.310222000

7	0.087248000	1.565189000	-0.000265000
7	1.512820000	-0.554044000	1.344591000
7	1.512880000	-0.555339000	-1.343752000
7	-1.516239000	-0.391744000	-1.346270000
7	-1.516387000	-0.391683000	1.346111000
27	-0.035884000	-0.512136000	0.000218000
1	-2.657848000	-2.358157000	-0.000231000
6	-0.185281000	-3.939298000	0.000666000
6	-0.706218000	-5.298023000	0.000671000
1	-0.371401000	-5.840912000	-0.888685000
1	-0.372530000	-5.840460000	0.890727000
1	-1.802538000	-5.235931000	-0.000032000
7	0.117607000	-2.819021000	0.000656000

$TS1_{FHEP}$

6	-0.113892000	-2.013893000	-1.426838000
6	0.340905000	-3.024101000	-2.276647000
1	-0.344206000	-3.756758000	-2.677005000
6	1.683219000	-3.073895000	-2.627726000
1	2.046194000	-3.841614000	-3.304062000
6	2.557137000	-2.129838000	-2.102500000
1	3.602206000	-2.161361000	-2.373455000
6	2.077091000	-1.165420000	-1.216209000
6	-1.605256000	-1.824512000	-1.114728000
6	-2.442986000	-2.908512000	-1.818119000
1	-2.305355000	-2.874272000	-2.900509000
1	-3.505735000	-2.768997000	-1.615142000
1	-2.164990000	-3.906254000	-1.469659000
6	-1.886452000	-1.834308000	0.397862000
6	-2.812662000	-2.698348000	0.986711000
1	-3.258897000	-3.499866000	0.415707000
6	-3.196336000	-2.511591000	2.312964000
1	-3.919784000	-3.178338000	2.771552000
6	-2.673794000	-1.429325000	3.012457000
1	-2.989686000	-1.191477000	4.022129000
6	-1.732322000	-0.630208000	2.381315000
1	-1.338467000	0.243782000	2.878474000
6	-1.978705000	-0.414249000	-1.630622000
6	-3.004272000	-0.226114000	-2.556537000
1	-3.589338000	-1.063903000	-2.906971000
6	-3.286595000	1.049290000	-3.038274000
1	-4.091051000	1.200081000	-3.751138000
6	-2.511866000	2.109939000	-2.591268000
1	-2.672449000	3.125034000	-2.936769000
6	-1.519064000	1.858548000	-1.654436000
1	-0.933440000	2.675058000	-1.276840000
6	3.020563000	-0.184537000	-0.498952000
6	4.476331000	-0.404842000	-0.949692000
1	4.583905000	-0.222622000	-2.021526000
1	4.806971000	-1.424915000	-0.745425000
1	5.151854000	0.274903000	-0.427205000
6	2.610956000	1.282381000	-0.734561000
6	3.479369000	2.246073000	-1.252070000
1	4.447744000	1.966245000	-1.642687000
6	3.108160000	3.590950000	-1.242880000
1	3.780947000	4.343092000	-1.643260000
6	1.889236000	3.951294000	-0.675751000
1	1.581902000	4.987733000	-0.588714000
6	1.051869000	2.945567000	-0.210070000
1	0.097789000	3.169730000	0.258634000
6	2.864744000	-0.465077000	1.016885000
6	3.949345000	-0.836233000	1.814214000
1	4.940713000	-0.914170000	1.390983000
6	3.764871000	-1.111338000	3.168265000
1	4.609024000	-1.397186000	3.788056000
6	2.484257000	-1.013228000	3.699392000
1	2.277477000	-1.218655000	4.743891000
6	1.449414000	-0.628620000	2.857439000
1	0.448954000	-0.531830000	3.246703000
6	-3.025926000	2.166626000	1.265146000
6	-3.636430000	3.172763000	2.222568000
1	-3.586144000	4.175995000	1.783605000
1	-3.074839000	3.209609000	3.162485000
1	-4.680812000	2.923820000	2.420288000
7	0.760014000	-1.120786000	-0.910034000
7	-1.296010000	-0.864791000	1.125473000
7	-1.253826000	0.631640000	-1.171321000
7	1.388484000	1.639462000	-0.292439000
7	1.623072000	-0.355875000	1.549331000
8	-1.727436000	2.260947000	1.069153000
8	-3.701240000	1.317280000	0.680142000
27	0.107139000	0.266422000	0.313121000
1	0.242400000	1.452976000	1.934230000
1	-0.463818000	1.805952000	1.803895000

$TS1_{SHEP}$

6	-0.068547000	-2.402475000	-0.922808000
6	0.440500000	-3.585661000	-1.459871000
1	-0.217575000	-4.406465000	-1.703926000
6	1.803464000	-3.703021000	-1.693073000
1	2.213784000	-4.613256000	-2.119273000
6	2.634432000	-2.637549000	-1.373640000
1	3.696192000	-2.716937000	-1.553751000
6	2.092387000	-1.480327000	-0.813151000
6	-1.569503000	-2.191344000	-0.716001000
6	-2.363661000	-3.428693000	-1.173894000
1	-2.183106000	-3.647763000	-2.228049000
1	-3.435503000	-3.269040000	-1.044174000
1	-2.084901000	-4.311227000	-0.593889000
6	-1.871228000	-1.881635000	0.764031000
6	-2.755106000	-2.643597000	1.529344000
1	-3.168353000	-3.564235000	1.142582000
6	-3.139233000	-2.202078000	2.795704000
1	-3.825180000	-2.793369000	3.394273000
6	-2.672032000	-0.973133000	3.245867000
1	-2.996394000	-0.545231000	4.187893000
6	-1.780912000	-0.271807000	2.444450000
1	-1.463153000	0.722849000	2.714242000
6	-1.978402000	-0.943329000	-1.532906000
6	-2.939083000	-1.006746000	-2.542436000
1	-3.395845000	-1.949026000	-2.808361000
6	-3.330645000	0.152821000	-3.210655000
1	-4.075238000	0.103862000	-3.999099000
6	-2.771891000	1.362759000	-2.823246000
1	-3.066822000	2.303799000	-3.274001000
6	-1.822254000	1.362936000	-1.808639000
1	-1.433426000	2.296171000	-1.439383000
6	2.977431000	-0.305896000	-0.381600000
6	4.456267000	-0.593721000	-0.703489000
1	4.600959000	-0.750346000	-1.774539000
1	4.810507000	-1.485138000	-0.182244000
1	5.088036000	0.243793000	-0.402161000
6	2.523628000	0.990728000	-1.079003000
6	3.371605000	1.739379000	-1.895589000
1	4.350206000	1.367745000	-2.164067000
6	2.971616000	2.996404000	-2.350940000
1	3.628364000	3.579205000	-2.989471000
6	1.748581000	3.499316000	-1.926389000
1	1.416441000	4.499320000	-2.182824000
6	0.932990000	2.694737000	-1.137965000
1	0.005371000	3.089634000	-0.729214000
6	2.779010000	-0.117956000	1.141699000
6	3.852130000	-0.179069000	2.033754000
1	4.855465000	-0.354631000	1.673849000
6	3.643874000	-0.008405000	3.401021000

1	4.480117000	-0.053462000	4.091714000
6	2.350286000	0.223640000	3.851506000
1	2.123352000	0.370494000	4.901633000
6	1.327640000	0.278420000	2.914604000
1	0.320308000	0.476530000	3.239051000
6	-2.504922000	3.068443000	0.845526000
6	-3.687177000	3.865227000	1.350709000
1	-3.923365000	4.667933000	0.644876000
1	-3.424802000	4.343348000	2.301895000
1	-4.561697000	3.227687000	1.499623000
7	0.759010000	-1.381892000	-0.603285000
7	-1.330359000	-0.751429000	1.267773000
7	-1.397570000	0.236143000	-1.207845000
7	1.285328000	1.442033000	-0.777658000
7	1.520553000	0.109008000	1.591222000
8	-1.487800000	3.700791000	0.406970000
8	-2.527935000	1.801545000	0.885378000
27	0.006124000	0.254836000	0.217129000
1	0.158389000	2.032842000	1.469804000
1	-0.297780000	2.588403000	1.196742000