Anexo 2

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1 $[Fe(phen)_3]^{3+}$ doublet

26 -0.000100000 0.000100000 0.000300000
6 3.005900000 -1.530600000 2.728100000
6 3.180700000 -2.816700000 2.243500000
6 2.424900000 -3.247200000 1.127000000
6 1.520600000 -2.315800000 0.565400000
6 2.082400000 -0.670700000 2.108500000
6 2.518700000 -4.556300000 0.539700000
6 0.731900000 -2.671900000 -0.564700000
6 0.833100000 -3.966100000 -1.126600000
6 1.753500000 -4.901800000 -0.539700000
6 0.010500000 -4.248400000 -2.243300000
1 0.048400000 -5.227700000 -2.713500000
6 -0.838900000 -3.267000000 -2.727700000
6 -0.873700000 -2.005800000 -2.107900000
1 3.211800000 -5.272500000 0.971500000
1 3.570100000 -1.171500000 3.582800000
1 3.890600000 -3.492400000 2.713400000
1 1.930700000 0.336600000 2.478700000
1 1.832900000 -5.895300000 -0.971800000
1 -1.481200000 -3.452700000 -3.582600000
1 -1.529200000 -1.226000000 -2.478000000
7 -0.105300000 -1.707100000 -1.054200000
7 1.350000000 -1.049800000 1.055000000
6 -0.177400000 3.369600000 2.726800000
6 0.849400000 4.163500000 2.242500000
6 1.600300000 3.723800000 1.126200000
6 1.245500000 2.474900000 0.564700000
6 -0.460600000 2.139900000 2.107500000
6 2.687600000 4.459000000 0.539100000
6 1.948300000 1.969600000 -0.565200000
6 3.019000000 2.703800000 -1.126900000
6 3.369500000 3.968700000 -0.539900000
6 3.674700000 2.132200000 -2.243400000

1 4.504200000 2.654300000 -2.713400000
6 3.249200000 0.905900000 -2.727600000
6 2.174100000 0.245600000 -2.107900000
1 2.961600000 5.417300000 0.971000000
1 -0.770700000 3.679000000 3.581300000
1 1.079900000 5.116200000 2.712300000
1 -1.257400000 1.505200000 2.477500000
1 4.190600000 4.533700000 -0.971900000
1 3.731300000 0.442200000 -3.582300000
1 1.826400000 -0.712000000 -2.477800000
7 1.531000000 0.762300000 -1.054600000
7 0.234100000 1.694700000 1.054300000
6 -2.828800000 -1.836700000 2.728800000
6 -4.030000000 -1.345400000 2.244000000
6 -4.025000000 -0.476100000 1.127000000
6 -2.766200000 -0.158800000 0.565300000
6 -1.622400000 -1.467000000 2.109100000
6 -5.205500000 0.096900000 0.539500000
6 -2.680300000 0.701900000 -0.565200000
6 -3.851700000 1.261000000 -1.127300000
6 -5.122300000 0.931900000 -0.540200000
6 -3.684900000 2.114200000 -2.244200000
1 -4.552000000 2.570900000 -2.714500000
6 -2.410300000 2.359300000 -2.728500000
6 -1.300600000 1.759200000 -2.108400000
1 -6.172400000 -0.145100000 0.971500000
1 -2.799800000 -2.504400000 3.583900000
1 -4.970100000 -1.622100000 2.714100000
1 -0.674100000 -1.839000000 2.479600000
1 -6.022300000 1.359700000 -0.972400000
1 -2.250000000 3.008400000 -3.583400000
1 -0.297500000 1.937000000 -2.478500000
7 -1.426100000 0.944300000 -1.054800000
7 -1.584500000 -0.643800000 1.055100000

1 $[Fe(phen)_3]^{2+}$ Singlet

26 0.000700000 -0.000900000 -0.000400000
6 3.177300000 1.086000000 2.778300000
6 4.238900000 0.350700000 2.282600000
6 4.039300000 -0.467200000 1.146800000
6 2.743500000 -0.479100000 0.577700000
6 1.921800000 1.004700000 2.148100000
6 5.065700000 -1.277500000 0.549600000
6 2.474000000 -1.280600000 -0.575900000

6 3.498700000 -2.074200000 -1.144300000
6 4.805800000 -2.050000000 -0.546500000
6 3.163300000 -2.846500000 -2.280100000
1 3.914600000 -3.474000000 -2.752100000
6 1.873400000 -2.789900000 -2.776400000
6 0.922600000 -1.965400000 -2.146900000
1 6.058700000 -1.266100000 0.989900000
1 3.293600000 1.725000000 3.647600000
1 5.216500000 0.395800000 2.755100000
1 1.077800000 1.569400000 2.528300000
1 5.589900000 -2.659900000 -0.986200000
1 1.579900000 -3.369300000 -3.645700000
1 -0.090900000 -1.904400000 -2.527400000
7 1.203600000 -1.221700000 -1.074300000
7 1.696100000 0.242500000 1.075400000
6 -2.533600000 2.206600000 2.774300000
6 -2.426700000 3.493700000 2.279100000
6 -1.616400000 3.729900000 1.144800000
6 -0.957400000 2.613700000 0.576600000
6 -1.834400000 1.160000000 2.145200000
6 -1.426600000 5.024000000 0.548400000
6 -0.126500000 2.781200000 -0.575500000
6 0.049800000 4.065600000 -1.143100000
6 -0.625600000 5.185400000 -0.546200000
6 0.888600000 4.161700000 -2.277200000
1 1.057500000 5.126200000 -2.748400000
6 1.485000000 3.016300000 -2.773000000
6 1.244700000 1.780400000 -2.144500000
1 -1.933700000 5.878400000 0.987900000
1 -3.146700000 1.987800000 3.642600000
1 -2.955200000 4.317800000 2.750800000
1 -1.902300000 0.146700000 2.525100000
1 -0.488400000 6.169600000 -0.985300000
1 2.135100000 3.052000000 -3.641100000
1 1.698900000 0.872200000 -2.524900000
7 0.458300000 1.651700000 -1.073300000
7 -1.059700000 1.345700000 1.073900000
6 -0.650500000 -3.298200000 2.774100000
6 -1.819500000 -3.847100000 2.278600000
6 -2.427400000 -3.263000000 1.143600000
6 -1.787700000 -2.135700000 0.575100000
6 -0.091100000 -2.170800000 2.144800000
6 -3.643500000 -3.743700000 0.546600000
6 -2.346000000 -1.499700000 -0.577900000
6 -3.546800000 -1.987500000 -1.146400000
6 -4.181600000 -3.130600000 -0.549000000

6 -4.046600000 -1.309500000 -2.281800000
1 -4.966500000 -1.644200000 -2.753800000
6 -3.350200000 -0.222100000 -2.778000000
6 -2.159900000 0.186200000 -2.148500000
1 -4.132000000 -4.608700000 0.986500000
1 -0.155700000 -3.720400000 3.642800000
1 -2.270900000 -4.715600000 2.750700000
1 0.821000000 -1.724500000 2.525000000
1 -5.102800000 -3.502400000 -0.988600000
1 -3.704100000 0.322700000 -3.647100000
1 -1.598400000 1.032300000 -2.528900000
7 -1.657600000 -0.430200000 -1.076000000
7 -0.637800000 -1.592200000 1.072900000

2 $[Fe(bpy)_3]^{3+}$ Doublet

26 -0.000300000 -0.000100000 0.000100000
6 -2.280100000 -2.425100000 2.729300000
6 -3.582500000 -2.220700000 2.270600000
6 -3.790300000 -1.372900000 1.182200000
6 -2.698100000 -0.747100000 0.576100000
6 -1.232300000 -1.777700000 2.081200000
6 -2.794700000 0.164300000 -0.576300000
6 -3.993800000 0.547000000 -1.182500000
6 -3.968400000 1.419500000 -2.271000000
1 -4.894500000 1.723400000 -2.750500000
6 -2.737800000 1.892400000 -2.729600000
6 -1.577500000 1.479200000 -2.081400000
1 -2.071000000 -3.074100000 3.573600000
1 -4.424300000 -2.712100000 2.750000000
1 -0.209700000 -1.911200000 2.411100000
1 -2.669400000 2.570800000 -3.574000000
1 -0.605700000 1.824200000 -2.411300000
7 -1.596800000 0.632400000 -1.031400000
7 -1.428700000 -0.953500000 1.031300000
6 3.240700000 -0.760100000 2.729100000
6 3.715500000 -1.989900000 2.270500000
6 3.085100000 -2.594300000 1.182300000
6 1.996500000 -1.962000000 0.576400000
6 2.155500000 -0.177000000 2.081300000
6 1.255400000 -2.502100000 -0.575400000
6 1.523900000 -3.732100000 -1.181200000
6 0.755000000 -4.147600000 -2.268800000
1 0.955200000 -5.101700000 -2.747900000
6 -0.271000000 -3.319400000 -2.726900000

6 -0.493600000 -2.107700000 -2.079300000
1 3.698100000 -0.254100000 3.573300000
1 4.562400000 -2.472700000 2.749700000
1 1.759400000 0.775100000 2.411300000
1 -0.893300000 -3.600400000 -3.570500000
1 -1.279100000 -1.439400000 -2.409000000
7 0.250200000 -1.699700000 -1.030300000
7 1.540100000 -0.759600000 1.031500000
6 -0.961900000 3.188700000 2.726900000
6 -0.132900000 4.213900000 2.268500000
6 0.706000000 3.969100000 1.180900000
6 0.701800000 2.710100000 0.575300000
6 -0.925100000 1.957200000 2.079400000
6 1.540100000 2.337400000 -0.576400000
6 2.471800000 3.184000000 -1.182200000
6 3.215200000 2.725300000 -2.270100000
1 3.941900000 3.375000000 -2.749400000
6 3.009300000 1.423000000 -2.728500000
6 2.070700000 0.625200000 -2.080700000
1 -1.629200000 3.332700000 3.570600000
1 -0.137600000 5.188800000 2.747500000
1 -1.552600000 1.138800000 2.409200000
1 3.563000000 1.024200000 -3.572500000
1 1.883500000 -0.389000000 -2.410500000
7 1.346400000 1.065800000 -1.031200000
7 -0.112400000 1.714400000 1.030300000
1 -4.942200000 0.173300000 -0.813500000
1 -4.795900000 -1.206400000 0.813100000
1 3.444100000 -3.548300000 0.813300000
1 2.322500000 -4.365700000 -0.812500000
1 2.622300000 4.192200000 -0.813500000
1 1.353600000 4.756300000 0.812000000

2 $[Fe(bpy)_3]^{2+}$ Singlet

26 0.000400000 0.000300000 0.000200000
6 1.689200000 2.863900000 2.762900000
6 2.994200000 2.987400000 2.286200000
6 3.379000000 2.227300000 1.183700000
6 2.456400000 1.364000000 0.583200000
6 0.821800000 1.987800000 2.115900000
6 2.761800000 0.514400000 -0.584700000
6 4.022800000 0.436800000 -1.185600000
6 4.209900000 -0.393600000 -2.288600000
1 5.183600000 -0.463500000 -2.763900000

6 3.125100000 -1.129200000 -2.765500000
6 1.898600000 -1.006900000 -2.117900000
1 1.341400000 3.433200000 3.618800000
1 3.700200000 3.661800000 2.761200000
1 -0.198200000 1.864700000 2.459400000
1 3.219300000 -1.789000000 -3.621900000
1 1.033900000 -1.561700000 -2.461600000
7 1.706200000 -0.206900000 -1.051900000
7 1.183300000 1.247900000 1.050400000
6 -3.321700000 0.027700000 2.765800000
6 -4.083000000 1.094700000 2.289200000
6 -3.618900000 1.808500000 1.186300000
6 -2.409600000 1.443000000 0.585300000
6 -2.129100000 -0.283900000 2.118100000
6 -1.827700000 2.133700000 -0.582400000
6 -2.392400000 3.264300000 -1.182400000
6 -1.767200000 3.843600000 -2.284600000
1 -2.194500000 4.721600000 -2.759200000
6 -0.586500000 3.274200000 -2.761400000
6 -0.077900000 2.150900000 -2.114800000
1 -3.639300000 -0.558300000 3.622200000
1 -5.020200000 1.367600000 2.764600000
1 -1.510900000 -1.104600000 2.461400000
1 -0.062400000 3.687400000 -3.617000000
1 0.835700000 1.681000000 -2.458600000
7 -0.674200000 1.582400000 -1.049700000
7 -1.670900000 0.399500000 1.052100000
6 1.640200000 -2.895400000 2.759400000
6 1.094000000 -4.087000000 2.282800000
6 0.241400000 -4.039700000 1.181800000
6 -0.046200000 -2.808600000 0.582700000
6 1.314000000 -1.705800000 2.113600000
6 -0.936700000 -2.647800000 -0.583600000
6 -1.636000000 -3.700700000 -1.183300000
6 -2.450300000 -3.447200000 -2.285100000
1 -2.998900000 -4.255200000 -2.759500000
6 -2.544800000 -2.139900000 -2.762100000
6 -1.824000000 -1.139200000 -2.115500000
1 2.308500000 -2.879300000 3.614200000
1 1.326100000 -5.036000000 2.756700000
1 1.718000000 -0.761100000 2.457100000
1 -3.164200000 -1.891300000 -3.617600000
1 -1.871800000 -0.113000000 -2.459200000
7 -1.033700000 -1.373000000 -1.050600000
7 0.490800000 -1.648300000 1.049500000
1 4.854600000 1.013700000 -0.798400000

1 4.387800000 2.312100000 0.796800000
1 -4.198200000 2.638900000 0.799500000
1 -3.308800000 3.694400000 -0.795300000
1 -1.552300000 -4.709600000 -0.796200000
1 -0.190000000 -4.955600000 0.795000000

3 $[Fe(Pyr_2Py)_2]^{3+}$ Doublet

26 -0.001800000 -0.011100000 -0.012400000
7 -0.455500000 -1.381100000 -1.380500000
7 -1.924000000 0.061500000 0.048800000
7 -0.246100000 1.397900000 1.383500000
7 0.362600000 1.337700000 -1.432600000
7 1.924400000 -0.051000000 -0.036200000
7 0.338500000 -1.430700000 1.344300000
6 0.351100000 -2.234600000 -2.289900000
6 -0.663500000 -3.233700000 -2.896200000
6 -2.047900000 -2.582000000 -2.639700000
6 -1.729500000 -1.569700000 -1.581400000
6 -2.632500000 -0.744900000 -0.762700000
6 -4.032500000 -0.715000000 -0.740100000
6 -4.662300000 0.169200000 0.144400000
6 -3.901500000 1.000100000 0.981700000
6 -2.508100000 0.919700000 0.906600000
6 -1.489500000 1.673700000 1.662100000
6 -1.670600000 2.703400000 2.735200000
6 -0.232600000 3.259700000 2.902900000
6 0.671200000 2.193800000 2.238600000
6 -0.494300000 2.152700000 -2.332100000
6 0.471800000 3.176400000 -2.974800000
6 1.881200000 2.568100000 -2.752200000
6 1.624400000 1.561600000 -1.672400000
6 2.579300000 0.769000000 -0.879000000
6 3.978200000 0.770900000 -0.916700000
6 4.667100000 -0.098000000 -0.059500000
6 3.963200000 -0.946500000 0.806400000
6 2.564900000 -0.896800000 0.792100000
6 1.596600000 -1.681300000 1.577600000
6 1.836200000 -2.766000000 2.583100000
6 0.420200000 -2.978400000 3.179400000
6 -0.531800000 -2.327600000 2.147800000
1 1.156000000 -2.715100000 -1.726900000
1 0.812900000 -1.584000000 -3.043100000
1 -0.599700000 -4.198200000 -2.384800000
1 -0.478200000 -3.411200000 -3.957200000
1 -2.449800000 -2.070800000 -3.527200000

1 -2.814400000 -3.296200000 -2.319100000
1 -4.615900000 -1.359600000 -1.390600000
1 -5.747000000 0.213000000 0.183300000
1 -4.386300000 1.686900000 1.668900000
1 -2.049300000 2.217200000 3.646900000
1 -2.407200000 3.467500000 2.462700000
1 0.029600000 3.423700000 3.949700000
1 -0.135900000 4.217700000 2.384500000
1 1.470000000 2.619200000 1.625000000
1 1.132700000 1.512600000 2.964300000
1 -1.300000000 2.614200000 -1.754900000
1 -0.952000000 1.478000000 -3.066300000
1 0.393600000 4.142500000 -2.468500000
1 0.251700000 3.339400000 -4.031400000
1 2.270600000 2.055900000 -3.644800000
1 2.636900000 3.307600000 -2.464600000
1 4.518100000 1.425700000 -1.594200000
1 5.753200000 -0.117200000 -0.069100000
1 4.491600000 -1.626200000 1.468100000
1 2.588700000 -2.487300000 3.329200000
1 2.221700000 -3.660300000 2.070900000
1 0.337800000 -2.472200000 4.145200000
1 0.190700000 -4.033400000 3.339700000
1 -0.985600000 -3.057300000 1.465600000
1 -1.339700000 -1.748200000 2.602700000

3 $[Fe(Pyr_2Py)_2]^{2+}$ Singlet

26 0.000000000 -0.006000000 -0.006200000
7 -0.371900000 -1.409000000 -1.397900000
7 -1.922100000 -0.011400000 -0.012300000
7 -0.387600000 1.394700000 1.381900000
7 0.380900000 1.392700000 -1.399000000
7 1.922100000 -0.004200000 -0.002800000
7 0.378600000 -1.395200000 1.396700000
6 0.474100000 -2.238400000 -2.281900000
6 -0.484800000 -3.273000000 -2.917800000
6 -1.894300000 -2.664100000 -2.703300000
6 -1.627400000 -1.640800000 -1.634300000
6 -2.578800000 -0.846700000 -0.845700000
6 -3.976200000 -0.875100000 -0.875200000
6 -4.679500000 -0.019200000 -0.020000000
6 -3.985900000 0.840700000 0.839200000
6 -2.588100000 0.820200000 0.817600000
6 -1.645400000 1.619800000 1.611300000
6 -1.923200000 2.642000000 2.678700000

6 -0.518100000 3.258800000 2.899600000
6 0.449600000 2.228900000 2.269300000
6 -0.459900000 2.225700000 -2.284200000
6 0.503700000 3.259700000 -2.914100000
6 1.911000000 2.647000000 -2.695700000
6 1.637700000 1.622600000 -1.629300000
6 2.584200000 0.826400000 -0.836800000
6 3.981800000 0.846000000 -0.866100000
6 4.679500000 -0.013800000 -0.010100000
6 3.980400000 -0.867800000 0.850500000
6 2.582800000 -0.837400000 0.829600000
6 1.635100000 -1.628300000 1.626000000
6 1.906600000 -2.697500000 2.647900000
6 0.498700000 -2.916000000 3.259100000
6 -0.463500000 -2.283000000 2.225800000
1 1.281500000 -2.691300000 -1.698800000
1 0.939100000 -1.576600000 -3.024200000
1 -0.406200000 -4.232200000 -2.397300000
1 -0.262000000 -3.452100000 -3.971700000
1 -2.283300000 -2.169700000 -3.604800000
1 -2.644100000 -3.403300000 -2.401400000
1 -4.502700000 -1.546300000 -1.546200000
1 -5.765100000 -0.022200000 -0.023000000
1 -4.519900000 1.508900000 1.507300000
1 -2.313400000 2.145700000 3.578500000
1 -2.675600000 3.376900000 2.373100000
1 -0.301500000 3.439900000 3.954400000
1 -0.442200000 4.217900000 2.378400000
1 1.257000000 2.685700000 1.689500000
1 0.914200000 1.569600000 3.014100000
1 -1.268100000 2.679100000 -1.702500000
1 -0.923800000 1.566800000 -3.029700000
1 0.425400000 4.217700000 -2.391400000
1 0.285300000 3.441800000 -3.968400000
1 2.302000000 2.153300000 -3.596700000
1 2.661400000 3.384000000 -2.389800000
1 4.512600000 1.512900000 -1.538000000
1 5.765100000 -0.018200000 -0.013700000
1 4.510000000 -1.538900000 1.519100000
1 2.657000000 -2.394500000 3.386000000
1 2.296600000 -3.597700000 2.152000000
1 0.420200000 -2.395400000 4.218300000
1 0.279100000 -3.970500000 3.438700000
1 -0.925500000 -3.026300000 1.563100000
1 -1.272900000 -1.703600000 2.679700000

4 $[Fe(Pypep)_2]^{1+}$ Doublet

26 0.177000000 -0.000100000 0.000100000
6 -1.709200000 1.941300000 -0.809600000
7 -1.295600000 1.326100000 0.319500000
6 -1.914000000 1.599400000 1.481600000
6 -2.975300000 2.499500000 1.554000000
6 -3.414100000 3.129000000 0.387000000
6 -2.768700000 2.844500000 -0.816200000
7 0.102100000 0.764400000 -1.793100000
6 -0.933600000 1.602500000 -2.052800000
8 -1.234100000 2.102600000 -3.143000000
7 1.574300000 -1.319300000 -0.576700000
6 1.813700000 -2.518900000 -0.057800000
7 2.769400000 -3.147100000 -0.774400000
6 3.158300000 -2.314900000 -1.805600000
6 2.408700000 -1.173000000 -1.677700000
6 2.384400000 0.058200000 -2.524700000
6 0.964900000 0.465100000 -2.938600000
1 -1.547600000 1.080500000 2.359300000
1 -3.444900000 2.693300000 2.513000000
1 -4.243600000 3.829700000 0.416400000
1 -3.053100000 3.298100000 -1.759900000
1 3.131600000 -4.073000000 -0.585300000
1 3.913100000 -2.598600000 -2.523200000
1 1.328600000 -2.941800000 0.807900000
1 0.521400000 -0.339900000 -3.546400000
1 1.009800000 1.344700000 -3.590100000
1 2.975600000 -0.120000000 -3.429600000
1 2.866300000 0.888100000 -1.992700000
7 -1.296000000 -1.325700000 -0.319800000
7 0.101300000 -0.764600000 1.793100000
7 1.574900000 1.318600000 0.576800000
6 -1.710300000 -1.940700000 0.809200000
6 -2.770000000 -2.843600000 0.815400000
6 -3.414800000 -3.128200000 -0.388000000
6 -2.975400000 -2.498900000 -1.554900000
6 -1.914000000 -1.599000000 -1.482100000
1 -3.055000000 -3.297000000 1.759000000
1 -4.244500000 -3.828700000 -0.417700000
1 -3.444600000 -2.692800000 -2.514100000
1 -1.547000000 -1.080300000 -2.359700000
6 -0.935100000 -1.601800000 2.052700000
8 -1.236400000 -2.101300000 3.142900000
6 0.963600000 -0.465200000 2.938900000
6 2.383500000 -0.058900000 2.525400000

6 2.408500000 1.172200000 1.678400000
6 3.158300000 2.314000000 1.806500000
7 2.770300000 3.146100000 0.775000000
6 1.814800000 2.518000000 0.058000000
1 3.912800000 2.597500000 2.524600000
1 1.330200000 2.941100000 -0.807900000
1 3.132800000 4.071900000 0.586100000
1 0.520100000 0.340300000 3.546100000
1 1.007900000 -1.344600000 3.590800000
1 2.974400000 0.119100000 3.430500000
1 2.865200000 -0.889000000 1.993600000

4 $[Fe(Pypep)_2]$ Quintet

26 -0.005800000 -0.138700000 0.005100000
6 2.230200000 1.611900000 -1.037800000
7 1.488800000 1.525700000 0.082700000
6 1.679300000 2.421900000 1.061600000
6 2.617800000 3.448800000 0.967000000
6 3.391900000 3.539900000 -0.193300000
6 3.199900000 2.604300000 -1.208700000
7 0.912200000 -0.201800000 -1.902600000
6 1.995300000 0.566300000 -2.112600000
8 2.811700000 0.502600000 -3.058200000
7 -1.402600000 -1.753700000 -0.731900000
6 -2.226100000 -2.494600000 -0.014100000
7 -2.892900000 -3.375700000 -0.804700000
6 -2.464900000 -3.177700000 -2.105000000
6 -1.541700000 -2.159800000 -2.049700000
6 -0.797600000 -1.504600000 -3.176100000
6 0.692700000 -1.234600000 -2.912500000
1 1.052500000 2.303300000 1.942100000
1 2.735100000 4.154300000 1.784400000
1 4.133800000 4.327300000 -0.301600000
1 3.773500000 2.611500000 -2.129200000
1 -3.578800000 -4.050400000 -0.496000000
1 -2.848800000 -3.758200000 -2.930800000
1 -2.371600000 -2.417300000 1.053600000
1 1.168800000 -0.935000000 -3.853800000
1 1.175200000 -2.179600000 -2.607000000
1 -1.280500000 -0.549700000 -3.428800000
1 -0.887700000 -2.142300000 -4.065100000
7 -1.659900000 1.332700000 -0.250900000
7 -0.772300000 0.066200000 1.966400000
7 1.483900000 -1.602900000 0.856800000
6 -2.315800000 1.577300000 0.899600000

6 -3.413000000 2.442200000 0.954100000
6 -3.838500000 3.067800000 -0.216600000
6 -3.148700000 2.818300000 -1.406300000
6 -2.064000000 1.943000000 -1.374100000
1 -3.892900000 2.602600000 1.913300000
1 -4.689100000 3.744700000 -0.202700000
1 -3.437800000 3.291800000 -2.340100000
1 -1.486900000 1.720400000 -2.268300000
6 -1.801200000 0.911000000 2.164600000
8 -2.351200000 1.212200000 3.245300000
6 -0.216700000 -0.508600000 3.191100000
6 0.255600000 -1.964900000 3.028800000
6 1.438500000 -2.152300000 2.127400000
6 2.603800000 -2.846500000 2.353600000
7 3.354300000 -2.714900000 1.198600000
6 2.640900000 -1.955700000 0.326400000
1 2.956500000 -3.405400000 3.207700000
1 2.994000000 -1.681300000 -0.657700000
1 4.273600000 -3.100600000 1.033700000
1 0.636700000 0.097900000 3.539600000
1 -0.968800000 -0.470400000 3.988100000
1 0.509800000 -2.359500000 4.021100000
1 -0.586800000 -2.568600000 2.662100000

5 $[Fe(Prpep)_2]^{1+}$ Doublet

26 0.175500000 -0.084500000 0.000600000
6 -2.165400000 -1.422100000 0.855100000
7 -1.600300000 -0.974900000 -0.287300000
6 -2.302600000 -1.106000000 -1.427700000
7 -3.516200000 -1.638600000 -1.517300000
6 -4.081800000 -2.069300000 -0.379700000
6 -3.433900000 -1.987000000 0.853100000
7 -0.122900000 -0.708300000 1.813700000
6 -1.304300000 -1.321800000 2.086400000
8 -1.675100000 -1.826100000 3.149800000
7 1.829900000 0.936000000 0.578800000
6 2.639100000 1.634300000 -0.213000000
7 3.584100000 2.257000000 0.520200000
6 3.370600000 1.956000000 1.848300000
6 2.267400000 1.141100000 1.886100000
6 1.558200000 0.601000000 3.091000000
6 0.899800000 -0.759100000 2.858300000
1 -1.836300000 -0.748500000 -2.338400000

1 -5.078300000 -2.494900000 -0.468700000
1 -3.867900000 -2.344200000 1.780700000
1 4.322600000 2.842600000 0.151100000
1 3.995900000 2.345200000 2.637500000
1 2.553900000 1.721500000 -1.283100000
1 0.436200000 -1.105700000 3.786300000
1 1.676200000 -1.489200000 2.582400000
1 0.794200000 1.316900000 3.424100000
1 2.275700000 0.513800000 3.914900000
7 -0.880700000 1.614800000 0.161800000
7 0.346500000 0.521000000 -1.855300000
7 1.183500000 -1.777100000 -0.414800000
6 -1.000500000 2.280700000 -1.006500000
6 -1.712800000 3.471100000 -1.079500000
6 -2.280300000 3.937800000 0.105900000
7 -2.158600000 3.278200000 1.268300000
6 -1.469300000 2.143200000 1.249700000
1 -1.804600000 3.986900000 -2.029200000
1 -2.850100000 4.863300000 0.135300000
1 -1.368700000 1.592100000 2.177900000
6 -0.332500000 1.645900000 -2.196600000
8 -0.425200000 2.164600000 -3.313200000
6 1.012500000 -0.161300000 -2.970400000
6 2.258400000 -0.948500000 -2.549900000
6 1.975400000 -2.007900000 -1.534500000
6 2.392800000 -3.314000000 -1.508700000
7 1.850500000 -3.868200000 -0.368000000
6 1.127900000 -2.920800000 0.263100000
1 3.012500000 -3.879200000 -2.188300000
1 0.586600000 -3.093700000 1.179400000
1 1.966700000 -4.823400000 -0.053600000
1 0.305100000 -0.849100000 -3.460400000
1 1.285400000 0.581600000 -3.727300000
1 2.684100000 -1.420400000 -3.442300000
1 3.028400000 -0.265500000 -2.170700000

5 $[Fe(Prpep)_2]$ Singlet

26 -0.003400000 -0.136700000 0.005700000
6 2.252000000 1.594500000 -1.040000000
7 1.524100000 1.514400000 0.090000000
6 1.775800000 2.408000000 1.056100000
7 2.685100000 3.382500000 1.008100000
6 3.407300000 3.457300000 -0.121900000
6 3.233400000 2.575000000 -1.184900000
7 0.894700000 -0.177900000 -1.914300000

6 1.989700000 0.569500000 -2.127500000
8 2.799200000 0.509600000 -3.077200000
7 -1.421600000 -1.721800000 -0.729000000
6 -2.234600000 -2.475700000 -0.011500000
7 -2.922500000 -3.333200000 -0.808800000
6 -2.520800000 -3.107000000 -2.112500000
6 -1.590300000 -2.096400000 -2.053200000
6 -0.864000000 -1.422500000 -3.179900000
6 0.635800000 -1.182200000 -2.945200000
1 1.178500000 2.323600000 1.960300000
1 4.148700000 4.252900000 -0.165400000
1 3.819500000 2.620000000 -2.095900000
1 -3.607000000 -4.010400000 -0.502100000
1 -2.926000000 -3.664600000 -2.943700000
1 -2.357100000 -2.425200000 1.060600000
1 1.095200000 -0.865000000 -3.888700000
1 1.112400000 -2.140000000 -2.673900000
1 -1.338600000 -0.455500000 -3.398800000
1 -0.983400000 -2.036100000 -4.082000000
7 -1.654300000 1.361400000 -0.235400000
7 -0.748300000 0.087100000 1.973700000
7 1.468400000 -1.619300000 0.834900000
6 -2.301200000 1.590900000 0.923500000
6 -3.398200000 2.451700000 0.964200000
6 -3.782900000 3.045900000 -0.234700000
7 -3.137600000 2.826000000 -1.392100000
6 -2.099000000 1.992100000 -1.330300000
1 -3.902700000 2.633400000 1.906300000
1 -4.631400000 3.725800000 -0.280200000
1 -1.553300000 1.803600000 -2.251200000
6 -1.783500000 0.919100000 2.184100000
8 -2.342100000 1.209900000 3.261200000
6 -0.179500000 -0.492700000 3.191400000
6 0.265000000 -1.957000000 3.027000000
6 1.428800000 -2.168800000 2.106100000
6 2.580100000 -2.891200000 2.313700000
7 3.315500000 -2.777400000 1.147800000
6 2.608700000 -2.000600000 0.286800000
1 2.932000000 -3.458700000 3.162400000
1 2.953500000 -1.736200000 -0.702900000
1 4.222800000 -3.185200000 0.969200000
1 0.689400000 0.102700000 3.517700000
1 -0.916100000 -0.437700000 4.001200000
1 0.530000000 -2.351000000 4.016400000
1 -0.594200000 -2.548300000 2.679400000

6 $[Fe(PypepO)_2]^{1-}$ Sextet

26 0.000000000 0.000000000 0.520900000
7 0.000000000 2.080600000 0.196400000
7 1.535500000 0.379400000 -1.103200000
8 -1.406600000 0.545400000 1.744800000
6 -1.712900000 1.835200000 1.787300000
6 2.306800000 -0.540600000 -1.696300000
6 3.300300000 -0.198800000 -2.614400000
6 3.490900000 1.152200000 -2.917800000
6 2.689800000 2.107800000 -2.296400000
6 1.718000000 1.683000000 -1.384300000
1 2.116800000 -1.572900000 -1.416700000
1 3.905800000 -0.975900000 -3.071600000
1 4.257200000 1.454300000 -3.628500000
1 2.786500000 3.171300000 -2.485600000
6 -2.734800000 2.339300000 2.610700000
6 -3.016900000 3.708700000 2.626200000
6 -2.286500000 4.592200000 1.822400000
6 -1.263700000 4.113100000 0.992200000
6 -0.967500000 2.740700000 0.964300000
1 -3.288100000 1.638900000 3.231600000
1 -3.808800000 4.086500000 3.271300000
1 -2.506100000 5.657900000 1.840400000
1 -0.687000000 4.785200000 0.368600000
6 0.823100000 2.681100000 -0.679400000
8 0.928900000 3.890400000 -0.972500000
7 0.000000000 -2.080600000 0.196400000
7 -1.535500000 -0.379400000 -1.103200000
8 1.406600000 -0.545400000 1.744800000
6 1.712900000 -1.835200000 1.787300000
6 2.734800000 -2.339300000 2.610700000
6 3.016900000 -3.708700000 2.626200000
6 2.286500000 -4.592200000 1.822400000
6 1.263700000 -4.113100000 0.992200000
6 0.967500000 -2.740700000 0.964300000
1 3.288100000 -1.638900000 3.231600000
1 3.808800000 -4.086500000 3.271300000
1 2.506100000 -5.657900000 1.840400000
1 0.687000000 -4.785200000 0.368600000
6 -2.306800000 0.540600000 -1.696300000
6 -3.300300000 0.198800000 -2.614400000
6 -3.490900000 -1.152200000 -2.917800000
6 -2.689800000 -2.107800000 -2.296400000
6 -1.718000000 -1.683000000 -1.384300000
1 -2.116800000 1.572900000 -1.416700000

1 -3.905800000 0.975900000 -3.071600000
1 -4.257200000 -1.454300000 -3.628500000
1 -2.786500000 -3.171300000 -2.485600000
6 -0.823100000 -2.681100000 -0.679400000
8 -0.928900000 -3.890400000 -0.972500000

6 $[Fe(PypepO)_2]^{2-}$ Quintet

26 0.000000000 0.000000000 0.533200000
7 0.000000000 2.164000000 0.154400000
7 1.544600000 0.394700000 -1.065700000
8 -1.450400000 0.719900000 1.823600000
6 -1.663200000 2.005800000 1.832100000
6 2.339100000 -0.531000000 -1.621800000
6 3.323600000 -0.217900000 -2.560900000
6 3.482100000 1.120200000 -2.939000000
6 2.659700000 2.084700000 -2.358700000
6 1.700800000 1.689700000 -1.415500000
1 2.169500000 -1.553100000 -1.293200000
1 3.944400000 -1.006900000 -2.979000000
1 4.237100000 1.403900000 -3.671300000
1 2.729000000 3.140600000 -2.598800000
6 -2.621000000 2.613400000 2.684300000
6 -2.838700000 3.995100000 2.669700000
6 -2.109400000 4.821000000 1.804300000
6 -1.150600000 4.254700000 0.945900000
6 -0.912500000 2.869800000 0.942500000
1 -3.181300000 1.962700000 3.354300000
1 -3.583800000 4.428700000 3.339900000
1 -2.278000000 5.898000000 1.792300000
1 -0.571900000 4.874000000 0.270100000
6 0.813900000 2.718600000 -0.746300000
8 0.943300000 3.924700000 -1.097000000
7 0.000000000 -2.164000000 0.154400000
7 -1.544600000 -0.394700000 -1.065700000
8 1.450400000 -0.719900000 1.823600000
6 1.663200000 -2.005800000 1.832100000
6 2.621000000 -2.613400000 2.684300000
6 2.838700000 -3.995100000 2.669700000
6 2.109400000 -4.821000000 1.804300000
6 1.150600000 -4.254700000 0.945900000
6 0.912500000 -2.869800000 0.942500000
1 3.181300000 -1.962700000 3.354300000
1 3.583800000 -4.428700000 3.339900000
1 2.278000000 -5.898000000 1.792300000
1 0.571900000 -4.874000000 0.270100000

6 -2.339100000 0.531000000 -1.621800000
6 -3.323600000 0.217900000 -2.560900000
6 -3.482100000 -1.120200000 -2.939000000
6 -2.659700000 -2.084700000 -2.358700000
6 -1.700800000 -1.689700000 -1.415500000
1 -2.169500000 1.553100000 -1.293200000
1 -3.944400000 1.006900000 -2.979000000
1 -4.237100000 -1.403900000 -3.671300000
1 -2.729000000 -3.140600000 -2.598800000
6 -0.813900000 -2.718600000 -0.746300000
8 -0.943300000 -3.924700000 -1.097000000

7 $[Fe(PyIm2H_2)_2]^{1-}$ Doublet

26 0.000000000 0.000200000 0.000100000
7 -1.763100000 -2.553000000 -2.555100000
7 -0.316800000 -1.380700000 -1.382200000
7 -1.949400000 -0.000100000 -0.000200000
7 -0.317800000 1.380800000 1.382300000
7 -1.764700000 2.552600000 2.554900000
7 0.317200000 -1.382300000 1.380700000
7 1.763700000 -2.555600000 2.552300000
7 1.949400000 0.000200000 0.000200000
7 0.317400000 1.382500000 -1.380500000
7 1.764100000 2.555600000 -2.552200000
6 -1.630200000 -1.602900000 -1.604400000
6 0.386700000 -2.214600000 -2.217000000
6 -0.508000000 -2.952700000 -2.955500000
6 -2.602500000 -0.835700000 -0.836500000
6 -2.603100000 0.835300000 0.835700000
6 -4.000600000 0.860500000 0.860800000
6 -4.691200000 -0.000500000 -0.000800000
6 -4.000000000 -0.861300000 -0.862100000
6 -1.631300000 1.602700000 1.604000000
6 -0.509800000 2.952400000 2.955900000
6 0.385300000 2.214700000 2.217400000
6 1.630600000 -1.604500000 1.602500000
6 0.508700000 -2.955900000 2.952300000
6 -0.386100000 -2.217200000 2.214600000
6 2.602700000 -0.836300000 0.835400000
6 2.602900000 0.836700000 -0.834800000
6 4.000400000 0.862200000 -0.860000000
6 4.691200000 0.000300000 0.000600000
6 4.000200000 -0.861700000 0.860900000
6 1.630900000 1.604800000 -1.602200000
6 -0.385800000 2.217100000 -2.214800000

6 0.509100000 2.955700000 -2.952500000
1 -4.545500000 1.524100000 1.524800000
1 -5.777400000 -0.000700000 -0.001000000
1 -4.544400000 -1.525100000 -1.526400000
1 1.464400000 2.242200000 2.245200000
1 -0.361100000 3.709000000 3.713500000
1 1.465800000 -2.241800000 -2.244500000
1 -0.358900000 -3.709500000 -3.712800000
1 4.545100000 1.526700000 -1.523200000
1 5.777400000 0.000300000 0.000700000
1 4.544800000 -1.526100000 1.524300000
1 -1.464900000 2.244500000 -2.242500000
1 0.360200000 3.713100000 -3.709400000
1 -1.465200000 -2.244600000 2.242200000
1 0.359800000 -3.713500000 3.708900000
1 -2.633200000 -2.923700000 -2.925900000
1 -2.635100000 2.923000000 2.925500000
1 2.634000000 -2.926400000 2.922700000
1 2.634300000 2.926500000 -2.922500000

7 $[Fe(PyIm2H_2)_2]^{2-}$ Quintet

26 0.000000000 0.001700000 0.000500000
7 2.236100000 2.589800000 -2.556700000
7 0.608600000 1.548600000 -1.488400000
7 2.179100000 0.000300000 0.002400000
7 0.604300000 -1.545300000 1.491300000
7 2.228800000 -2.588700000 2.562000000
7 -0.610300000 1.556600000 1.481000000
7 -2.239600000 2.601800000 2.542600000
7 -2.178700000 -0.001300000 -0.002600000
7 -0.602200000 -1.554600000 -1.482500000
7 -2.226000000 -2.604300000 -2.548300000
6 1.935100000 1.656400000 -1.614600000
6 0.055800000 2.437000000 -2.376200000
6 1.056600000 3.095500000 -3.052100000
6 2.844900000 0.837900000 -0.813700000
6 2.842600000 -0.838100000 0.819500000
6 4.241600000 -0.870300000 0.847500000
6 4.938500000 -0.001400000 0.004500000
6 4.244100000 0.868300000 -0.839500000
6 1.930500000 -1.655200000 1.619300000
6 1.047800000 -3.092500000 3.056000000
6 0.049000000 -2.432600000 2.378600000
6 -1.937000000 1.663900000 1.605600000
6 -1.060900000 3.111200000 3.036300000

6 -0.059100000 2.450100000 2.364500000
6 -2.845700000 0.840300000 0.808500000
6 -2.841200000 -0.844600000 -0.815600000
6 -4.240200000 -0.877800000 -0.844200000
6 -4.938200000 -0.004800000 -0.006500000
6 -4.244800000 0.870000000 0.833300000
6 -1.928300000 -1.665600000 -1.610400000
6 -0.046400000 -2.446700000 -2.364700000
6 -1.044700000 -3.110500000 -3.039000000
1 4.782500000 -1.547200000 1.501100000
1 6.024300000 -0.002100000 0.005300000
1 4.786800000 1.544600000 -1.492300000
1 -1.020100000 -2.549300000 2.480600000
1 1.022100000 -3.853600000 3.821800000
1 -1.013000000 2.555300000 -2.479700000
1 1.033000000 3.856800000 -3.817700000
1 -4.780200000 -1.558600000 -1.494500000
1 -6.024000000 -0.006200000 -0.008000000
1 -4.788400000 1.549500000 1.481900000
1 1.022800000 -2.563600000 -2.465700000
1 -1.018400000 -3.875700000 -3.800600000
1 1.009600000 2.570000000 2.468100000
1 -1.038600000 3.876600000 3.797900000
1 3.161000000 2.873800000 -2.856400000
1 3.152900000 -2.873900000 2.863200000
1 -3.165000000 2.886400000 2.840300000
1 -3.149900000 -2.891400000 -2.848300000

8 $[Fe(sar)]^{3+}$ Doublet

26 0.000000000 0.000000000 0.000000000
7 1.162400000 1.515600000 0.755600000
7 1.162400000 -1.411900000 0.934500000
7 -1.162300000 -0.103600000 1.689800000
7 -1.162400000 1.515600000 -0.755700000
7 -1.162400000 -1.412000000 -0.934300000
7 1.162300000 -0.103700000 -1.689800000
6 0.755000000 2.790100000 0.066000000
6 2.665700000 1.287200000 0.728200000
6 3.076600000 0.000400000 0.000000000
6 2.665700000 -1.273700000 0.750300000
6 0.754800000 -1.452800000 2.382900000
6 -0.755300000 -1.338200000 2.448700000
6 -2.665600000 -0.012500000 1.478400000
6 -3.076600000 0.000400000 0.000000000
6 -2.665700000 1.287200000 -0.728300000

6 -2.665700000 -1.273800000 -0.750300000
6 -0.755000000 2.790100000 -0.066200000
6 2.665600000 -0.012700000 -1.478400000
6 0.755300000 -1.338400000 -2.448600000
6 -0.754800000 -1.453000000 -2.382800000
1 -4.175800000 0.000400000 0.000000000
1 4.175800000 0.000400000 0.000000000
1 3.026900000 1.264600000 1.760600000
1 3.132800000 2.152500000 0.248800000
1 3.027000000 -2.156400000 0.214500000
1 3.132800000 -1.291200000 1.739500000
1 3.026500000 0.892800000 -1.975300000
1 3.132900000 -0.860500000 -1.988000000
1 -3.026900000 1.264400000 -1.760700000
1 -3.132800000 2.152500000 -0.249000000
1 -3.026500000 0.892900000 1.975200000
1 -3.132900000 -0.860300000 1.988100000
1 -3.132800000 -1.291400000 -1.739400000
1 -3.027000000 -2.156400000 -0.214300000
1 -1.109600000 -2.375400000 -2.856300000
1 -1.239100000 -0.616800000 -2.898100000
1 1.110500000 -1.288200000 -3.484100000
1 1.239600000 -2.202200000 -1.980900000
1 -1.110100000 3.661700000 -0.627600000
1 -1.239300000 2.817300000 0.915700000
1 1.110100000 3.661800000 0.627300000
1 1.239300000 2.817200000 -0.915900000
1 -1.110500000 -1.287900000 3.484200000
1 -1.239600000 -2.202100000 1.981100000
1 1.109600000 -2.375200000 2.856500000
1 1.239100000 -0.616600000 2.898200000
1 -0.920200000 1.645400000 -1.740500000
1 0.919600000 0.684000000 -2.294800000
1 0.920200000 1.645600000 1.740300000
1 -0.919600000 0.684200000 2.294700000
1 0.920200000 -2.329500000 0.554200000
1 -0.920200000 -2.329600000 -0.554100000

8 $[Fe(sar)]^{2+}$ Singlet

26 0.000200000 0.000100000 0.000000000
7 1.184000000 1.693700000 0.172300000
7 1.184300000 -0.996200000 1.380400000
7 -1.183700000 0.479900000 1.632900000
7 -1.183900000 1.174300000 -1.232100000
7 -1.184000000 -1.654400000 -0.400700000

7 1.184100000 -0.697700000 -1.553000000
6 0.757400000 2.629500000 -0.913100000
6 2.674600000 1.468000000 0.200600000
6 3.080700000 0.000200000 -0.000200000
6 2.674900000 -0.907600000 1.170800000
6 0.757800000 -0.523900000 2.733400000
6 -0.758200000 -0.416600000 2.751200000
6 -2.674300000 0.467800000 1.405800000
6 -3.080800000 0.000100000 0.000100000
6 -2.674600000 0.983400000 -1.108000000
6 -2.674700000 -1.451300000 -0.297700000
6 -0.758500000 2.591100000 -1.014800000
6 2.674800000 -0.560200000 -1.371700000
6 0.757600000 -2.105700000 -1.820000000
6 -0.758400000 -2.174700000 -1.736200000
1 -4.180600000 0.000200000 0.000300000
1 4.180500000 0.000300000 -0.000200000
1 3.065700000 1.824700000 1.159200000
1 3.142400000 2.086300000 -0.573100000
1 3.066100000 -1.916100000 1.000400000
1 3.142700000 -0.546600000 2.093100000
1 3.065700000 0.091600000 -2.160000000
1 3.142800000 -1.539400000 -1.520200000
1 -3.064300000 0.629200000 -2.068100000
1 -3.143400000 1.956200000 -0.924400000
1 -3.064200000 1.476300000 1.579400000
1 -3.143100000 -0.177900000 2.156200000
1 -3.143600000 -1.778300000 -1.232000000
1 -3.064800000 -2.105800000 0.489000000
1 -1.117400000 -3.197500000 -1.904100000
1 -1.213300000 -1.542400000 -2.507000000
1 1.116000000 -2.458200000 -2.795000000
1 1.212600000 -2.748100000 -1.057700000
1 -1.117700000 3.247800000 -1.816800000
1 -1.213700000 2.942300000 -0.082000000
1 1.115500000 3.650100000 -0.730000000
1 1.212500000 2.291300000 -1.850800000
1 -1.117100000 -0.050500000 3.721000000
1 -1.213200000 -1.400200000 2.589100000
1 1.116100000 -1.192400000 3.525900000
1 1.212800000 0.457400000 2.908800000
1 -0.952300000 0.966400000 -2.205200000
1 0.953600000 -0.177600000 -2.401600000
1 0.953300000 2.168000000 1.047300000
1 -0.952200000 1.426500000 1.939500000
1 0.953600000 -1.991000000 1.353600000

1 -0.952600000 -2.393200000 0.266000000

9 $[Fe(diammac)]^{3+}$ Doublet

26 0.000000000 0.000000000 0.054000000
6 -1.607300000 -3.915800000 -0.071300000
6 -0.711800000 -2.673700000 -0.058700000
6 0.235700000 -2.666000000 1.168600000
7 0.614900000 -1.243700000 1.529800000
6 0.000000000 -0.759700000 2.823400000
6 0.000000000 0.759700000 2.823400000
7 -0.614900000 1.243700000 1.529800000
6 -0.235700000 2.666000000 1.168600000
6 0.711800000 2.673700000 -0.058700000
6 1.607300000 3.915800000 -0.071300000
7 1.497200000 1.377000000 0.052500000
7 0.737300000 -1.171200000 -1.422300000
6 0.635400000 -0.419800000 -2.730000000
6 -0.635400000 0.419800000 -2.730000000
7 -0.737300000 1.171200000 -1.422300000
6 -0.040300000 2.511700000 -1.391000000
7 -1.497200000 -1.377000000 0.052500000
6 0.040300000 -2.511700000 -1.391000000
1 1.733400000 -1.346000000 -1.263600000
1 1.631000000 -1.210300000 1.652700000
1 -1.631000000 1.210300000 1.652700000
1 -1.733400000 1.346000000 -1.263600000
1 -2.089700000 -1.403200000 0.888900000
1 -2.166000000 -1.327500000 -0.723500000
1 2.089700000 1.403200000 0.888900000
1 2.166000000 1.327500000 -0.723500000
1 -0.671000000 -2.552000000 -2.222100000
1 0.763000000 -3.318200000 -1.546000000
1 -0.250600000 -3.131400000 2.031200000
1 1.139900000 -3.246300000 0.964300000
1 -1.019800000 -1.151600000 2.883400000
1 0.547900000 -1.159500000 3.683900000
1 1.019800000 1.151600000 2.883400000
1 -0.547900000 1.159500000 3.683900000
1 -1.139900000 3.246300000 0.964300000
1 0.250600000 3.131400000 2.031200000
1 0.671000000 2.552000000 -2.222100000
1 -0.763000000 3.318200000 -1.546000000
1 -0.650300000 1.113500000 -3.577700000
1 -1.527000000 -0.208900000 -2.820200000
1 0.650300000 -1.113500000 -3.577700000

1 1.527000000 0.208900000 -2.820200000
1 -2.218800000 -3.976400000 0.835800000
1 -0.998900000 -4.826300000 -0.116500000
1 -2.275000000 -3.924200000 -0.939800000
1 0.998900000 4.826300000 -0.116500000
1 2.218800000 3.976400000 0.835800000
1 2.275000000 3.924200000 -0.939800000

9 $[Fe(diammac)]^{2+}$ Singlet

26 0.000000000 0.000000000 0.055600000
6 0.495200000 4.208300000 -0.068600000
6 0.000000000 2.758200000 -0.055200000
6 -0.923600000 2.504000000 1.168700000
7 -0.939800000 1.047000000 1.541300000
6 -0.198800000 0.735700000 2.808300000
6 0.198800000 -0.735700000 2.808300000
7 0.939800000 -1.047000000 1.541300000
6 0.923600000 -2.504000000 1.168700000
6 0.000000000 -2.758200000 -0.055200000
6 -0.495200000 -4.208300000 -0.068600000
7 -1.108400000 -1.747700000 0.059600000
7 -1.028900000 0.948600000 -1.434400000
6 -0.721600000 0.250800000 -2.724900000
6 0.721600000 -0.250800000 -2.724900000
7 1.028900000 -0.948600000 -1.434400000
6 0.681600000 -2.406600000 -1.393300000
7 1.108400000 1.747700000 0.059600000
6 -0.681600000 2.406600000 -1.393300000
1 -2.035700000 0.870100000 -1.290500000
1 -1.912000000 0.770600000 1.685200000
1 1.912000000 -0.770600000 1.685200000
1 2.035700000 -0.870100000 -1.290500000
1 1.664500000 1.942600000 0.896600000
1 1.765200000 1.891000000 -0.712500000
1 -1.664500000 -1.942600000 0.896600000
1 -1.765200000 -1.891000000 -0.712500000
1 0.010300000 2.627800000 -2.213900000
1 -1.571300000 3.024200000 -1.554200000
1 -0.584800000 3.099400000 2.023700000
1 -1.941800000 2.834900000 0.942800000
1 0.694700000 1.367300000 2.845400000
1 -0.796800000 0.979600000 3.694700000
1 -0.694700000 -1.367300000 2.845400000
1 0.796800000 -0.979600000 3.694700000
1 1.941800000 -2.834900000 0.942800000

1 0.584800000 -3.099400000 2.023700000
1 -0.010300000 -2.627800000 -2.213900000
1 1.571300000 -3.024200000 -1.554200000
1 0.899800000 -0.899800000 -3.590900000
1 1.417800000 0.590000000 -2.812100000
1 -0.899800000 0.899800000 -3.590900000
1 -1.417800000 -0.590000000 -2.812100000
1 1.067000000 4.438700000 0.837400000
1 -0.345300000 4.910000000 -0.114300000
1 1.136400000 4.404500000 -0.935400000
1 0.345300000 -4.910000000 -0.114300000
1 -1.067000000 -4.438700000 0.837400000
1 -1.136400000 -4.404500000 -0.935400000

10 $[Fe(tacn)_2]^{3+}$ Doublet

26 0.000000000 0.076800000 0.000000000
7 1.354600000 0.042300000 1.534000000
7 1.337000000 -1.290700000 -0.746700000
7 1.251000000 1.434700000 -0.845600000
7 -1.337000000 -1.290600000 0.746900000
7 -1.354600000 0.042000000 -1.534000000
7 -1.251000000 1.434900000 0.845300000
6 1.847600000 -1.374400000 1.725900000
6 1.826800000 -2.159700000 0.388000000
6 2.473000000 -0.620200000 -1.496100000
6 2.042600000 0.768500000 -1.940300000
6 2.062100000 2.070100000 0.257000000
6 2.489800000 1.020100000 1.273900000
6 -1.847600000 -1.374700000 -1.725700000
6 -1.826800000 -2.159700000 -0.387600000
6 -2.473000000 -0.619900000 1.496200000
6 -2.042600000 0.768900000 1.940200000
6 -2.062100000 2.070100000 -0.257300000
6 -2.489800000 1.019800000 -1.274000000
1 1.392100000 0.714900000 -2.819600000
1 2.907100000 1.380800000 -2.221300000
1 2.933400000 2.590200000 -0.157100000
1 1.430400000 2.834400000 0.721400000
1 3.352200000 0.453600000 0.923900000
1 2.788700000 1.493300000 2.214600000
1 2.848000000 -1.349300000 2.167800000
1 1.201600000 -1.858200000 2.463600000
1 2.813800000 -2.560300000 0.139100000
1 1.158100000 -3.020700000 0.466100000
1 3.341400000 -0.580000000 -0.838900000

1 2.762600000 -1.231600000 -2.356700000
1 -2.813900000 -2.560200000 -0.138700000
1 -1.158200000 -3.020800000 -0.465500000
1 -3.341500000 -0.579700000 0.839000000
1 -2.762600000 -1.231100000 2.356900000
1 -2.907000000 1.381200000 2.221100000
1 -1.392000000 0.715400000 2.819500000
1 -2.933400000 2.590200000 0.156700000
1 -1.430400000 2.834300000 -0.721900000
1 -3.352200000 0.453400000 -0.923800000
1 -2.788800000 1.492900000 -2.214800000
1 -2.847900000 -1.349700000 -2.167700000
1 -1.201500000 -1.858600000 -2.463300000
1 0.922000000 0.318900000 2.417900000
1 0.745900000 2.203200000 -1.294300000
1 0.882500000 -1.918200000 -1.412700000
1 -0.745900000 2.203400000 1.293900000
1 -0.882500000 -1.918000000 1.413000000
1 -0.922000000 0.318500000 -2.417900000

10 $[Fe(tacn)_2]^{2+}$ Singlet

26 0.000000000 0.000000000 0.000000000
7 0.786900000 1.375300000 1.341800000
7 -1.584400000 -0.006200000 1.341800000
7 0.797600000 -1.369100000 1.341800000
7 -0.786900000 1.375300000 -1.341800000
7 -0.797600000 -1.369100000 -1.341800000
7 1.584400000 -0.006200000 -1.341800000
6 -0.231300000 1.779800000 2.376900000
6 -1.635500000 1.361000000 1.942600000
6 -1.425700000 -1.090200000 2.376900000
6 -0.360900000 -2.096900000 1.942600000
6 1.657000000 -0.689600000 2.376900000
6 1.996500000 0.735900000 1.942600000
6 -1.657000000 -0.689600000 -2.376900000
6 -1.996500000 0.735900000 -1.942600000
6 0.231300000 1.779800000 -2.376900000
6 1.635500000 1.361000000 -1.942600000
6 1.425700000 -1.090200000 -2.376900000
6 0.360900000 -2.096900000 -1.942600000
1 -0.753400000 -2.774400000 1.177600000
1 -0.054500000 -2.718200000 2.794000000
1 1.117800000 -0.682400000 3.327300000
1 2.574400000 -1.260600000 2.550700000
1 2.381300000 1.311900000 2.794000000

1 2.779400000 0.734700000 1.177600000
1 0.032000000 1.309200000 3.327300000
1 -0.195400000 2.859800000 2.550700000
1 -2.326800000 1.406300000 2.794000000
1 -2.026000000 2.039600000 1.177600000
1 -1.149900000 -0.626900000 3.327300000
1 -2.378900000 -1.599200000 2.550700000
1 -2.381300000 1.311900000 -2.794000000
1 -2.779400000 0.734700000 -1.177600000
1 -0.032000000 1.309200000 -3.327300000
1 0.195400000 2.859800000 -2.550700000
1 2.326800000 1.406300000 -2.794000000
1 2.026000000 2.039600000 -1.177600000
1 1.149900000 -0.626900000 -3.327300000
1 2.378900000 -1.599200000 -2.550700000
1 0.054500000 -2.718200000 -2.794000000
1 0.753400000 -2.774400000 -1.177600000
1 -1.117800000 -0.682400000 -3.327300000
1 -2.574400000 -1.260600000 -2.550700000
1 1.102600000 2.228500000 0.880500000
1 1.378600000 -2.069200000 0.880500000
1 -2.481300000 -0.159300000 0.880500000
1 2.481300000 -0.159300000 -0.880500000
1 -1.102600000 2.228500000 -0.880500000
1 -1.378600000 -2.069200000 -0.880500000

11 $[Fe(EDTA)(H_2O)]^{1-}$ Sextet

7 -1.472900000 -0.143200000 1.102300000
6 -0.727700000 0.140200000 2.340300000
1 -0.642300000 1.225800000 2.443300000
1 -1.272200000 -0.228900000 3.226500000
6 0.668000000 -0.487500000 2.306100000
1 1.191000000 -0.257600000 3.250800000
1 0.592500000 -1.575800000 2.235800000
7 1.428200000 -0.002900000 1.144400000
6 -2.532100000 0.836700000 0.802800000
1 -3.453000000 0.640600000 1.369900000
1 -2.172400000 1.836500000 1.063000000
6 -2.844700000 0.854300000 -0.706900000
6 -1.967200000 -1.533400000 1.037400000
1 -2.873000000 -1.554000000 0.422600000
1 -2.237900000 -1.911600000 2.032900000
6 -0.972600000 -2.504600000 0.372600000
6 1.860200000 1.403800000 1.285600000
1 2.846100000 1.521700000 0.824400000

1 1.967000000 1.683500000 2.342300000
6 0.933900000 2.420000000 0.588300000
6 2.537600000 -0.882600000 0.736200000
1 3.421200000 -0.766100000 1.379600000
1 2.199500000 -1.922000000 0.788000000
6 2.918500000 -0.596100000 -0.730600000
8 0.135100000 1.925200000 -0.305500000
8 1.022700000 3.606600000 0.900800000
8 1.949100000 -0.107400000 -1.441900000
8 4.056200000 -0.845700000 -1.124800000
8 -0.124800000 -1.946400000 -0.438000000
8 -1.052400000 -3.706300000 0.618700000
8 -1.891600000 0.399600000 -1.460400000
8 -3.926600000 1.294800000 -1.091500000
26 0.001700000 -0.006000000 -0.768400000
8 -0.006400000 -0.138400000 -3.013000000
1 -0.703000000 0.500500000 -3.245100000
1 0.871800000 0.222600000 -3.227500000

11 $[Fe(EDTA)(H_2O)]^{2-}$ Quintet

7 -1.484700000 0.028100000 1.129200000
6 -0.678500000 0.361200000 2.311300000
1 -0.511900000 1.441700000 2.318400000
1 -1.211400000 0.102200000 3.247100000
6 0.680100000 -0.370500000 2.309500000
1 1.213600000 -0.115200000 3.245900000
1 0.513500000 -1.451000000 2.312400000
7 1.485600000 -0.032800000 1.128200000
6 -2.440900000 1.060900000 0.693700000
1 -3.391300000 1.014900000 1.248900000
1 -1.986400000 2.044100000 0.852500000
6 -2.734200000 0.958000000 -0.831300000
6 -2.099700000 -1.312100000 1.207300000
1 -3.007400000 -1.305900000 0.593600000
1 -2.405600000 -1.545600000 2.239600000
6 -1.219200000 -2.469200000 0.656100000
6 2.100600000 1.307200000 1.211100000
1 3.007900000 1.303400000 0.597000000
1 2.406900000 1.536600000 2.244200000
6 1.219700000 2.466400000 0.665000000
6 2.441500000 -1.063800000 0.688000000
1 3.392200000 -1.020000000 1.242800000
1 1.987000000 -2.047600000 0.843000000
6 2.734000000 -0.954800000 -0.836700000
8 0.378100000 2.145000000 -0.233700000

8 1.446900000 3.602800000 1.133800000
8 1.786900000 -0.439200000 -1.541200000
8 3.820500000 -1.387200000 -1.249700000
8 -0.378300000 -2.144100000 -0.242000000
8 -1.445900000 -3.607400000 1.120500000
8 -1.787500000 0.445100000 -1.538100000
8 -3.820800000 1.392200000 -1.242000000
26 0.000000000 0.000800000 -0.617300000
8 -0.003400000 0.010300000 -4.004400000
1 -0.745400000 0.210800000 -3.402000000
1 0.740200000 -0.193800000 -3.405200000

12 $[Fe(PaPy_2O)(Cl)]$ Sextet

26 -0.231000000 0.114100000 -0.558900000
17 -1.437000000 0.720200000 -2.510600000
8 1.786300000 -1.581300000 2.753400000
8 1.422700000 -0.335800000 -1.281300000
7 -1.513300000 -1.684400000 -0.500200000
7 -2.040500000 0.764800000 0.734500000
7 0.404700000 -0.489700000 1.282900000
7 0.055200000 2.267700000 -0.165000000
6 -1.100800000 -2.899600000 -0.889600000
1 -0.104800000 -2.947500000 -1.320400000
6 -1.895500000 -4.034500000 -0.751300000
1 -1.526400000 -4.999700000 -1.082900000
6 -3.157700000 -3.895100000 -0.171200000
1 -3.802900000 -4.758800000 -0.035800000
6 -3.578300000 -2.631000000 0.241100000
1 -4.551900000 -2.488800000 0.702000000
6 -2.728400000 -1.538200000 0.053500000
6 -3.164600000 -0.120800000 0.374100000
1 -3.619700000 0.281900000 -0.537500000
1 -3.934400000 -0.131300000 1.161400000
6 -1.587900000 0.611500000 2.145200000
1 -2.458800000 0.512200000 2.813000000
1 -1.067100000 1.534200000 2.416200000
6 -0.617700000 -0.552800000 2.322100000
1 -0.164500000 -0.494900000 3.318200000
1 -1.149800000 -1.517400000 2.291900000
6 1.593900000 -1.070800000 1.633500000
6 2.714300000 -1.078600000 0.627700000
6 3.975700000 -1.493800000 1.087600000
1 4.053100000 -1.771000000 2.134200000
6 5.083600000 -1.555200000 0.246200000
1 6.047000000 -1.874800000 0.634500000

6 4.941300000 -1.207500000 -1.104700000
1 5.795400000 -1.256500000 -1.776800000
6 3.704000000 -0.803200000 -1.592300000
1 3.564000000 -0.538600000 -2.637000000
6 2.579000000 -0.728600000 -0.741000000
6 -2.306600000 2.179200000 0.406800000
1 -2.962100000 2.654200000 1.153800000
1 -2.811100000 2.210500000 -0.564600000
6 -1.012600000 2.958000000 0.273200000
6 -0.936000000 4.327300000 0.532900000
1 -1.809700000 4.860400000 0.897400000
6 0.271400000 4.991900000 0.314600000
1 0.352500000 6.058300000 0.507200000
6 1.371100000 4.267600000 -0.147100000
1 2.329600000 4.743600000 -0.327300000
6 1.219400000 2.900900000 -0.370400000
1 2.038600000 2.283000000 -0.725200000

12 $[Fe(PaPy_2O)(Cl)]^{1-}$ Quintet

26 -0.255800000 0.110200000 -0.596300000
17 -1.918100000 0.495300000 -2.554500000
8 2.180500000 -1.363700000 2.683500000
8 1.532600000 0.062800000 -1.332400000
7 -1.135300000 -1.936300000 -0.573200000
7 -2.135500000 0.292700000 0.816100000
7 0.597200000 -0.425300000 1.297700000
7 -0.494600000 2.258300000 -0.205200000
6 -0.477000000 -3.020800000 -1.002900000
1 0.465700000 -2.827500000 -1.508400000
6 -0.957000000 -4.316200000 -0.814800000
1 -0.388100000 -5.166000000 -1.180700000
6 -2.167800000 -4.484000000 -0.139900000
1 -2.572100000 -5.477900000 0.037500000
6 -2.846100000 -3.353700000 0.316700000
1 -3.784400000 -3.445200000 0.858700000
6 -2.299200000 -2.089200000 0.078200000
6 -3.032200000 -0.816000000 0.465400000
1 -3.596500000 -0.506300000 -0.421600000
1 -3.750400000 -1.031900000 1.276800000
6 -1.580600000 0.217500000 2.190200000
1 -2.380800000 -0.056500000 2.903900000
1 -1.239700000 1.225200000 2.448400000
6 -0.384600000 -0.728500000 2.321300000
1 0.037200000 -0.613000000 3.330300000
1 -0.720600000 -1.780500000 2.267300000

6 1.852200000 -0.808400000 1.598000000
6 2.934300000 -0.534600000 0.574700000
6 4.257800000 -0.723100000 1.011300000
1 4.380900000 -1.048400000 2.040600000
6 5.364800000 -0.516000000 0.189800000
1 6.372500000 -0.667500000 0.572600000
6 5.152500000 -0.115300000 -1.138300000
1 5.998200000 0.049100000 -1.806500000
6 3.858500000 0.068200000 -1.608900000
1 3.670900000 0.367500000 -2.638100000
6 2.716000000 -0.129900000 -0.782000000
6 -2.719400000 1.611700000 0.528500000
1 -3.440300000 1.925900000 1.305000000
1 -3.242500000 1.536800000 -0.431200000
6 -1.643100000 2.668900000 0.363000000
6 -1.844500000 4.002000000 0.728200000
1 -2.779600000 4.299300000 1.197000000
6 -0.833900000 4.934500000 0.485400000
1 -0.969200000 5.977900000 0.760600000
6 0.353900000 4.500000000 -0.106700000
1 1.171000000 5.186400000 -0.309700000
6 0.481400000 3.149900000 -0.430600000
1 1.382100000 2.747100000 -0.886100000

13 $[Fe(NTA)(H_2O)_2]$ Sextet

7 0.859200000 -1.076500000 0.035500000
6 1.003100000 -1.365500000 1.478200000
1 1.190500000 -2.428500000 1.667900000
1 1.860800000 -0.804800000 1.866300000
6 0.132400000 -2.115500000 -0.721500000
1 0.810900000 -2.851800000 -1.167500000
1 -0.532200000 -2.654000000 -0.036000000
6 -0.230900000 -0.902200000 2.271300000
6 -0.757600000 -1.493300000 -1.814300000
8 -0.921900000 0.061000000 1.676300000
8 -0.501500000 -1.375300000 3.356200000
8 -1.153800000 -2.152400000 -2.753700000
8 -1.079200000 -0.226900000 -1.589400000
6 2.116900000 -0.643200000 -0.606500000
1 2.977100000 -1.229400000 -0.262900000
1 2.027600000 -0.784900000 -1.689600000
6 2.366000000 0.855500000 -0.363800000
8 3.482700000 1.330300000 -0.423900000
8 1.260300000 1.544600000 -0.137500000
26 -0.501600000 0.749000000 -0.061300000

8 -2.828700000 1.106600000 0.161700000
1 -3.230300000 0.620600000 -0.579200000
1 -2.983500000 0.578000000 0.965700000
8 -0.898400000 2.837000000 -0.380700000
1 -1.660400000 3.252000000 0.055100000
1 -0.089700000 3.351200000 -0.207000000

13 $[Fe(NTA)]$ Quintet

7 1.091300000 -0.066700000 0.883000000
6 0.250100000 -0.160700000 2.089300000
1 0.755900000 -0.691200000 2.907600000
1 0.040800000 0.855600000 2.444300000
6 1.893400000 -1.274800000 0.612600000
1 2.912600000 -1.192700000 1.014600000
1 1.415500000 -2.124900000 1.114400000
6 -1.131800000 -0.814800000 1.838900000
6 1.967000000 -1.650800000 -0.892900000
8 -1.565600000 -0.751000000 0.612700000
8 -1.742500000 -1.289900000 2.796000000
8 2.889600000 -2.375100000 -1.264800000
8 0.996900000 -1.205300000 -1.636600000
6 1.838400000 1.199000000 0.776100000
1 2.291900000 1.498100000 1.732000000
1 2.654400000 1.054200000 0.057600000
6 0.969200000 2.368900000 0.232900000
8 1.314100000 3.521500000 0.498500000
8 -0.039800000 2.016400000 -0.503800000
26 -0.305500000 0.032600000 -0.840300000
8 -3.926800000 -0.394200000 -0.558800000
1 -4.281800000 -1.242200000 -0.863400000
1 -3.188000000 -0.627500000 0.071400000
8 -1.965600000 0.727100000 -2.090700000
1 -2.802400000 0.411800000 -1.658200000
1 -1.896400000 1.682100000 -1.916500000

14 $[Fe(Py_3tacn)]^{3+}$ Doublet

26 -0.009400000 -0.009100000 0.308800000
7 1.240700000 -1.172600000 -0.777100000
7 1.574500000 0.020500000 1.577100000
7 -1.646000000 -0.441300000 -0.793300000
7 0.454000000 1.666900000 -0.732300000

7 -0.756400000 -1.438300000 1.532900000
7 -0.883700000 1.325700000 1.558200000
6 0.920600000 -1.942400000 -1.844500000
6 1.854100000 -2.743900000 -2.493100000
6 3.170900000 -2.762500000 -2.027600000
6 3.510300000 -1.962000000 -0.932800000
6 2.530000000 -1.174600000 -0.336200000
6 2.819300000 -0.195500000 0.770400000
6 1.553300000 1.382500000 2.217500000
6 1.410100000 -1.072800000 2.627100000
6 0.123700000 1.719600000 2.634200000
6 0.414800000 -2.131000000 2.165800000
6 -2.161200000 0.257900000 -1.833100000
6 -2.280300000 -1.580500000 -0.392500000
6 1.345800000 1.806200000 -1.742200000
6 -0.240300000 2.766700000 -0.321200000
6 -1.564900000 -2.368100000 0.675500000
6 -1.637400000 -0.780200000 2.588300000
6 -1.285800000 2.511400000 0.736100000
6 -2.064500000 0.622500000 2.164000000
6 -3.323100000 -0.131600000 -2.489300000
6 -3.452600000 -2.019800000 -1.000800000
6 1.583800000 3.025500000 -2.366400000
6 -0.039500000 4.019400000 -0.893900000
6 -3.987100000 -1.285500000 -2.063600000
6 0.885800000 4.155700000 -1.932900000
1 -0.107900000 -1.904500000 -2.182100000
1 1.547200000 -3.341600000 -3.345700000
1 3.921100000 -3.384800000 -2.507700000
1 4.527200000 -1.944400000 -0.551100000
1 3.112200000 0.765900000 0.334600000
1 3.648100000 -0.521500000 1.407500000
1 1.925800000 2.099500000 1.484800000
1 2.224800000 1.414300000 3.084300000
1 1.083900000 -0.602700000 3.555900000
1 2.380600000 -1.530300000 2.839000000
1 -0.149800000 1.202700000 3.554700000
1 0.036700000 2.789500000 2.844800000
1 0.859500000 -2.785800000 1.414800000
1 0.094700000 -2.757800000 3.007300000
1 -1.619500000 1.145000000 -2.138400000
1 1.867500000 0.910800000 -2.056900000
1 -0.875200000 -3.074900000 0.200900000
1 -2.256100000 -2.959000000 1.285800000
1 -1.076800000 -0.753500000 3.523400000
1 -2.517700000 -1.402000000 2.776000000

1 -2.242200000 2.280200000 0.254300000
1 -1.452400000 3.389300000 1.369400000
1 -2.850900000 0.583000000 1.409100000
1 -2.454900000 1.183200000 3.022200000
1 -3.697500000 0.462900000 -3.316800000
1 -3.937300000 -2.928100000 -0.653800000
1 2.305500000 3.082800000 -3.175300000
1 -0.601900000 4.876900000 -0.535100000
1 -4.901700000 -1.611100000 -2.551500000
1 1.056900000 5.124700000 -2.393400000

14 $[Fe(Py_3tacn)]^{2+}$ Singlet

26 -0.000600000 0.000000000 0.286300000
7 -1.724800000 0.142300000 -0.777900000
7 -1.189600000 -1.083300000 1.555900000
7 0.987300000 1.422100000 -0.776200000
7 0.739600000 -1.565900000 -0.775400000
7 -0.346300000 1.571400000 1.555000000
7 1.531400000 -0.486700000 1.557800000
6 -2.015900000 0.966300000 -1.807400000
6 -3.257700000 0.985500000 -2.436300000
6 -4.255300000 0.121400000 -1.983000000
6 -3.963300000 -0.740600000 -0.924000000
6 -2.691800000 -0.713600000 -0.353600000
6 -2.265000000 -1.685200000 0.722800000
6 -0.300300000 -2.107900000 2.175800000
6 -1.765700000 -0.154300000 2.600300000
6 1.013700000 -1.448100000 2.603500000
6 -1.679400000 1.313600000 2.172700000
6 1.848700000 1.262400000 -1.803700000
6 0.728500000 2.687400000 -0.352500000
6 0.172900000 -2.230900000 -1.805000000
6 1.964000000 -1.974600000 -0.349700000
6 -0.328300000 2.803800000 0.722000000
6 0.744300000 1.605700000 2.601400000
6 2.591000000 -1.118500000 0.726800000
6 1.973200000 0.797000000 2.176100000
6 2.487600000 2.328200000 -2.431300000
6 1.341800000 3.802200000 -0.921700000
6 0.778100000 -3.316000000 -2.432700000
6 2.624300000 -3.062200000 -0.919000000
6 2.236700000 3.624300000 -1.978600000
6 2.025200000 -3.747000000 -1.978100000
1 -1.217200000 1.622800000 -2.134200000
1 -3.433100000 1.668200000 -3.261600000

1 -5.238800000 0.116100000 -2.443500000
1 -4.711500000 -1.431800000 -0.547100000
1 -1.854600000 -2.581300000 0.244200000
1 -3.118400000 -2.010600000 1.331100000
1 -0.113700000 -2.878500000 1.426000000
1 -0.776100000 -2.593200000 3.039200000
1 -1.221900000 -0.312600000 3.533700000
1 -2.808300000 -0.418200000 2.808400000
1 0.878000000 -0.896200000 3.535600000
1 1.763300000 -2.218800000 2.813800000
1 -2.438700000 1.537200000 1.421600000
1 -1.863300000 1.968400000 3.035800000
1 2.019000000 0.242500000 -2.130100000
1 -0.795000000 -1.868300000 -2.132900000
1 -1.308700000 2.896800000 0.241700000
1 -0.184200000 3.705400000 1.330600000
1 0.333300000 1.213700000 3.533900000
1 1.036700000 2.640600000 2.810200000
1 3.163300000 -0.316100000 0.248100000
1 3.298200000 -1.694900000 1.336500000
1 2.547900000 1.342700000 1.426100000
1 2.630600000 0.629000000 3.040500000
1 3.168400000 2.138900000 -3.254900000
1 1.116300000 4.795800000 -0.545300000
1 0.275600000 -3.810000000 -3.258100000
1 3.596800000 -3.363900000 -0.541000000
1 2.724700000 4.478700000 -2.438200000
1 2.522300000 -4.596000000 -2.437700000

15 $[Fe(bpy)CN_4]^{1-}$ Doublet

26 -0.001300000 -1.134300000 0.000000000
7 -1.303400000 0.431900000 0.000000000
7 1.304600000 0.429500000 0.000000000
7 -0.001400000 -0.892700000 3.130200000
7 -2.302800000 -3.191600000 0.000000000
7 2.297900000 -3.194400000 0.000000000
7 -0.001400000 -0.892700000 -3.130200000
6 -1.380200000 -2.470100000 0.000000000
6 1.376100000 -2.472000000 0.000000000
6 -0.001400000 -1.066100000 -1.971500000
6 -0.001400000 -1.066100000 1.971500000
6 -0.736000000 1.660200000 0.000000000
6 -1.519000000 2.819700000 0.000000000
6 -2.906100000 2.705400000 0.000000000
6 -3.476700000 1.433400000 0.000000000

6 -2.640000000 0.319700000 0.000000000
6 0.739300000 1.658900000 0.000000000
6 2.641000000 0.315100000 0.000000000
6 3.479600000 1.427300000 0.000000000
6 2.911300000 2.700300000 0.000000000
6 1.524300000 2.817000000 0.000000000
1 1.059100000 3.796300000 0.000000000
1 3.535400000 3.590000000 0.000000000
1 4.555400000 1.284100000 0.000000000
1 3.025100000 -0.698800000 0.000000000
1 -1.052100000 3.798200000 0.000000000
1 -3.528700000 3.596200000 0.000000000
1 -4.552800000 1.292100000 0.000000000
1 -3.025800000 -0.693500000 0.000000000

15 $[Fe(bpy)CN_4]^{2-}$ Singlet

26 -0.000700000 -1.097600000 0.000000000
7 -1.280900000 0.414500000 0.000000000
7 1.281500000 0.412700000 0.000000000
7 -0.000700000 -0.966100000 3.156500000
7 -2.356100000 -3.157400000 0.000000000
7 2.351900000 -3.160500000 0.000000000
7 -0.000700000 -0.966100000 -3.156500000
6 -1.423700000 -2.438700000 0.000000000
6 1.420400000 -2.440600000 0.000000000
6 -0.000700000 -1.093500000 -1.986500000
6 -0.000700000 -1.093500000 1.986500000
6 -0.730500000 1.661800000 0.000000000
6 -1.522900000 2.820000000 0.000000000
6 -2.908100000 2.706300000 0.000000000
6 -3.467200000 1.421000000 0.000000000
6 -2.627300000 0.313900000 0.000000000
6 0.732800000 1.660800000 0.000000000
6 2.627800000 0.310400000 0.000000000
6 3.469100000 1.416300000 0.000000000
6 2.911800000 2.702400000 0.000000000
6 1.526800000 2.817900000 0.000000000
1 1.059600000 3.798300000 0.000000000
1 3.541800000 3.589800000 0.000000000
1 4.545800000 1.265200000 0.000000000
1 3.007000000 -0.706500000 0.000000000
1 -1.054400000 3.799700000 0.000000000
1 -3.536900000 3.594700000 0.000000000
1 -4.544000000 1.271300000 0.000000000
1 -3.007900000 -0.702400000 0.000000000

16 $[Fe(DITim)_2]^{1+}$ Doublet

26 0.000000000 0.006200000 0.000000000
16 0.894900000 1.460000000 -1.416800000
16 -0.895000000 1.459900000 1.416700000
7 -1.760000000 0.152700000 -1.015400000
7 1.760000000 0.152900000 1.015300000
7 0.691700000 -1.555600000 -1.222800000
7 -0.691500000 -1.555600000 1.222900000
6 -0.114000000 -2.336100000 -2.031500000
6 0.678400000 -3.173500000 -2.777000000
7 1.977200000 -2.889300000 -2.405900000
6 1.942300000 -1.906300000 -1.476800000
6 -1.593900000 -2.146200000 -2.062400000
6 -2.009600000 -0.674900000 -2.216300000
6 -2.583000000 1.121200000 -0.757900000
6 -2.351800000 2.042500000 0.429800000
6 -3.789500000 1.422800000 -1.627100000
6 -2.078000000 3.481500000 -0.076300000
6 -3.588800000 2.044300000 1.359800000
6 0.114300000 -2.336000000 2.031600000
6 -0.678100000 -3.173400000 2.777200000
7 -1.976900000 -2.889200000 2.406100000
6 -1.942100000 -1.906300000 1.476800000
6 1.594200000 -2.146000000 2.062400000
6 2.009800000 -0.674700000 2.216200000
6 2.582900000 1.121600000 0.757900000
6 3.789300000 1.423300000 1.627100000
6 2.351600000 2.042800000 -0.429900000
6 2.077500000 3.481800000 0.076200000
6 3.588600000 2.044800000 -1.359800000
1 2.812400000 -3.318300000 -2.782500000
1 2.824300000 -1.458200000 -1.047500000
1 0.440300000 -3.918400000 -3.521300000
1 -2.062300000 -2.570100000 -1.165900000
1 -2.003100000 -2.697000000 -2.916700000
1 -1.457000000 -0.224200000 -3.051300000
1 -3.069400000 -0.660300000 -2.478000000
1 -4.301300000 2.325400000 -1.296400000
1 -3.495900000 1.568700000 -2.672500000
1 -4.520400000 0.604900000 -1.599600000
1 -1.894200000 4.129900000 0.785900000
1 -1.196800000 3.505800000 -0.722200000
1 -2.933600000 3.892900000 -0.626000000
1 -3.369300000 2.650800000 2.244000000

1 -4.471300000 2.476500000 0.873600000
1 -3.835500000 1.034600000 1.704900000
1 -2.812100000 -3.318300000 2.782800000
1 -0.439900000 -3.918100000 3.521600000
1 -2.824100000 -1.458300000 1.047500000
1 2.003400000 -2.696800000 2.916600000
1 2.062500000 -2.569900000 1.165900000
1 3.069700000 -0.660100000 2.477700000
1 1.457400000 -0.224100000 3.051400000
1 4.300800000 2.326100000 1.296600000
1 3.495700000 1.569000000 2.672500000
1 4.520400000 0.605600000 1.599400000
1 1.893600000 4.130100000 -0.786100000
1 1.196300000 3.506000000 0.722100000
1 2.933000000 3.893300000 0.625900000
1 3.369000000 2.651300000 -2.244000000
1 4.471000000 2.477100000 -0.873500000
1 3.835500000 1.035100000 -1.704900000

16 $[Fe(DITim)_2]^{2-}$ Singlet

26 0.000000000 0.063200000 0.000000000
16 0.959000000 1.476600000 -1.692500000
16 -0.959800000 1.476000000 1.692600000
7 -2.306100000 0.045600000 -0.550700000
7 2.306100000 0.046500000 0.550600000
7 0.105300000 -1.662300000 -1.523600000
7 -0.104500000 -1.662300000 1.523600000
6 -0.943400000 -2.438500000 -1.977900000
6 -0.519500000 -3.193100000 -3.046600000
7 0.811300000 -2.861200000 -3.232300000
6 1.137800000 -1.927500000 -2.299600000
6 -2.312100000 -2.317100000 -1.388500000
6 -2.905600000 -0.899000000 -1.502200000
6 -2.948200000 1.128700000 -0.276600000
6 -2.418200000 2.131600000 0.756700000
6 -4.259400000 1.479200000 -0.965100000
6 -2.029400000 3.441500000 0.025900000
6 -3.536700000 2.430800000 1.786500000
6 0.944600000 -2.438100000 1.977800000
6 0.521100000 -3.193000000 3.046500000
7 -0.809800000 -2.861600000 3.232400000
6 -1.136700000 -1.927900000 2.299800000

6 2.313100000 -2.316200000 1.388200000
6 2.906100000 -0.898000000 1.501900000
6 2.947700000 1.129900000 0.276500000
6 4.258800000 1.481000000 0.964900000
6 2.417200000 2.132800000 -0.756600000
6 2.027800000 3.442400000 -0.025600000
6 3.535400000 2.432700000 -1.786500000
1 1.419800000 -3.212200000 -3.958500000
1 2.097300000 -1.435600000 -2.246800000
1 -1.029200000 -3.906000000 -3.677800000
1 -2.302200000 -2.612100000 -0.331900000
1 -2.983400000 -3.010800000 -1.909900000
1 -2.764900000 -0.530300000 -2.529100000
1 -3.988100000 -0.979800000 -1.333900000
1 -4.555100000 2.511900000 -0.781600000
1 -4.183600000 1.336500000 -2.049000000
1 -5.074000000 0.834500000 -0.606900000
1 -1.677700000 4.167000000 0.766700000
1 -1.220400000 3.259100000 -0.687300000
1 -2.880900000 3.889500000 -0.507500000
1 -3.138500000 3.106700000 2.549400000
1 -4.414000000 2.913500000 1.334400000
1 -3.861000000 1.514700000 2.293300000
1 -1.418000000 -3.212900000 3.958700000
1 1.031200000 -3.905800000 3.677600000
1 -2.096400000 -1.436400000 2.247200000
1 2.984800000 -3.009700000 1.909500000
1 2.303300000 -2.611300000 0.331600000
1 3.988600000 -0.978300000 1.333500000
1 2.765400000 -0.529400000 2.528800000
1 4.554100000 2.513800000 0.781600000
1 4.183100000 1.338100000 2.048800000
1 5.073700000 0.836700000 0.606700000
1 1.675700000 4.167800000 -0.766200000
1 1.218900000 3.259500000 0.687600000
1 2.879100000 3.890600000 0.507800000
1 3.136800000 3.108400000 -2.549200000
1 4.412500000 2.915700000 -1.334400000
1 3.860100000 1.516700000 -2.293400000

17 $[Fe(H_2O)_6]^{3+}$ Sextet

26 0.000000000 0.000100000 0.000000000
8 -1.606400000 0.254200000 -1.246500000
1 -1.795100000 1.041400000 -1.805300000
8 0.701700000 1.851900000 -0.526500000

1 1.311800000 2.056800000 -1.270400000
8 1.606500000 -0.254300000 1.246600000
1 1.794600000 -1.041100000 1.806000000
8 1.061500000 -0.839500000 -1.538500000
1 0.745200000 -0.980800000 -2.459100000
8 -0.701800000 -1.852000000 0.526200000
1 -1.311400000 -2.057100000 1.270400000
8 -1.061400000 0.839600000 1.538600000
1 -1.984400000 1.177300000 1.497200000
1 -2.335500000 -0.388100000 -1.399600000
1 0.492200000 2.704800000 -0.083500000
1 -0.492800000 -2.704700000 0.082700000
1 2.336200000 0.387500000 1.399000000
1 1.984200000 -1.177900000 -1.496700000
1 -0.744900000 0.981000000 2.459200000

17 $[Fe(H_2O)_6]^{2+}$ Quintet

26 0.000000000 0.000000000 0.000000000
8 -1.853500000 -0.006000000 -1.113800000
1 -1.941900000 -0.004900000 -2.083900000
8 1.151300000 0.008100000 -1.792800000
1 1.482900000 -0.773700000 -2.270800000
8 1.853500000 0.006100000 1.113800000
1 1.941900000 0.005100000 2.083900000
8 0.009500000 -2.170200000 -0.003600000
1 -0.556700000 -2.753100000 -0.540600000
8 -1.151300000 -0.008100000 1.792800000
1 -1.482900000 0.773800000 2.270800000
8 -0.009400000 2.170200000 0.003500000
1 -0.581000000 2.749800000 -0.531400000
1 -2.755600000 -0.010700000 -0.746300000
1 1.476100000 0.794500000 -2.267900000
1 -1.476200000 -0.794400000 2.268000000
1 2.755600000 0.010400000 0.746300000
1 0.580900000 -2.749800000 0.531500000
1 0.556900000 2.753100000 0.540400000

18^{2+} $[Fe(Ohishis)(H_2O)_3]^{2+}$ Quintet

6 4.320700000 0.220200000 0.142000000
6 3.094600000 -1.586200000 -0.178200000
6 2.995600000 0.539600000 0.313300000
6 -4.281300000 -0.096700000 0.205200000
6 -2.905600000 -1.780700000 -0.169500000
6 -2.986400000 0.345600000 0.325100000

7 4.360900000 -1.120000000 -0.168400000
7 2.232600000 -0.613900000 0.108600000
7 -4.208400000 -1.434800000 -0.109300000
7 -2.126500000 -0.732000000 0.085600000
6 2.458600000 1.883700000 0.726700000
6 1.709100000 2.724200000 -0.347500000
6 0.286800000 2.265400000 -0.536800000
6 -2.547100000 1.736300000 0.693400000
7 -0.725400000 3.114800000 -0.387400000
8 0.028500000 1.060700000 -0.817700000
6 -2.122400000 2.664400000 -0.490600000
1 5.215100000 0.818900000 0.224500000
1 2.842800000 -2.615700000 -0.381900000
1 -5.223900000 0.415600000 0.324900000
1 -2.566500000 -2.783300000 -0.380800000
1 1.817800000 1.777800000 1.610800000
1 3.314900000 2.480200000 1.053200000
1 -3.378500000 2.210800000 1.222400000
1 -1.726300000 1.687100000 1.416300000
1 2.222500000 2.644000000 -1.312400000
1 1.731600000 3.777700000 -0.054000000
1 -0.532400000 4.089600000 -0.192500000
1 -2.248200000 2.153400000 -1.447900000
1 -2.737500000 3.564700000 -0.509500000
1 -4.994500000 -2.055500000 -0.257000000
1 5.195400000 -1.665200000 -0.345700000
26 0.059500000 -0.754900000 0.019900000
8 0.044600000 -0.647500000 2.226600000
1 -0.740200000 -0.723700000 2.788600000
1 0.823400000 -0.688600000 2.800400000
8 0.081100000 -1.604700000 -2.096900000
1 0.836900000 -1.359200000 -2.651400000
1 -0.704900000 -1.431900000 -2.636700000
8 0.111900000 -3.000100000 0.291000000
1 0.157800000 -3.569900000 -0.490300000
1 0.151900000 -3.560300000 1.078700000

18^{3+} $[Fe(Ohishis)(H_2O)_3]^{3+}$ Sextet

6 4.264900000 0.189800000 0.139600000
6 3.029400000 -1.606400000 -0.203800000
6 2.948600000 0.542900000 0.293700000
6 -4.205000000 -0.216900000 0.206800000
6 -2.783500000 -1.876500000 -0.089100000
6 -2.933900000 0.293100000 0.295000000
7 4.286200000 -1.152200000 -0.175100000

7 2.167400000 -0.608200000 0.070200000
7 -4.082700000 -1.566800000 -0.039900000
7 -2.031800000 -0.774400000 0.101300000
6 2.457900000 1.895600000 0.745000000
6 1.666000000 2.768200000 -0.267000000
6 0.238800000 2.326700000 -0.395100000
6 -2.601200000 1.723100000 0.640500000
7 -0.784900000 3.146500000 -0.419700000
8 -0.022600000 1.067900000 -0.474200000
6 -2.184300000 2.673100000 -0.528100000
1 5.171200000 0.769900000 0.240400000
1 2.770300000 -2.632400000 -0.414700000
1 -5.168400000 0.261800000 0.311300000
1 -2.413900000 -2.877100000 -0.250800000
1 1.878800000 1.800600000 1.671900000
1 3.346700000 2.469200000 1.021100000
1 -3.504400000 2.141700000 1.093100000
1 -1.845000000 1.762600000 1.431000000
1 2.125800000 2.717600000 -1.262900000
1 1.704300000 3.815800000 0.046000000
1 -0.611700000 4.147900000 -0.373500000
1 -2.308700000 2.191700000 -1.502000000
1 -2.802300000 3.570900000 -0.523700000
1 -4.851700000 -2.222500000 -0.150000000
1 5.120000000 -1.708600000 -0.344600000
26 0.071000000 -0.736900000 -0.032100000
8 0.090300000 -0.761900000 2.106000000
1 -0.692500000 -0.775800000 2.681000000
1 0.880100000 -0.734400000 2.670700000
8 0.082600000 -1.359600000 -2.098400000
1 0.838500000 -1.171300000 -2.680100000
1 -0.713200000 -1.300800000 -2.653800000
8 0.166800000 -2.909800000 0.167800000
1 0.211100000 -3.542500000 -0.567500000
1 0.218200000 -3.409100000 0.999300000

19^{2+} $[Fe(Ohishis)(Im)(H_O)_2]^{2+}$ Quintet

6 -3.818300000 -2.094000000 0.082300000
6 -3.211900000 -0.035500000 -0.397500000
6 -2.476400000 -1.950700000 0.313400000
6 4.216800000 0.913700000 0.136100000
6 2.404300000 2.024500000 -0.426000000
6 3.123200000 0.105900000 0.294700000
7 -4.264300000 -0.875800000 -0.369100000
7 -2.109200000 -0.645500000 0.006600000

7 3.743700000 2.119100000 -0.322700000
7 1.985100000 0.821400000 -0.064500000
6 -1.560300000 -3.001900000 0.856600000
6 -0.573800000 -3.649800000 -0.135400000
6 0.621600000 -2.780000000 -0.375900000
6 3.121300000 -1.305600000 0.786000000
7 1.845200000 -3.252700000 -0.142000000
8 0.489600000 -1.601200000 -0.774700000
6 3.016100000 -2.394200000 -0.309400000
1 -4.478500000 -2.940900000 0.210200000
1 -3.282600000 1.000700000 -0.705100000
1 5.268100000 0.734700000 0.315900000
1 1.771500000 2.842600000 -0.748700000
1 -0.999100000 -2.612700000 1.718700000
1 -2.193300000 -3.802000000 1.256600000
1 4.046100000 -1.458100000 1.354100000
1 2.304800000 -1.452000000 1.505400000
1 -1.069300000 -3.818600000 -1.100600000
1 -0.265400000 -4.630300000 0.244700000
1 1.963700000 -4.214500000 0.152500000
1 2.963400000 -1.934800000 -1.303000000
1 3.893000000 -3.045300000 -0.297600000
1 4.301300000 2.937100000 -0.534600000
1 -5.217800000 -0.645700000 -0.619900000
1 -1.150100000 2.872400000 -1.873800000
6 -1.189000000 3.089400000 -0.813700000
7 -0.849200000 2.249600000 0.155800000
7 -1.591800000 4.267500000 -0.295400000
6 -1.046300000 2.933000000 1.339800000
6 -1.508100000 4.189700000 1.074000000
1 -1.901300000 5.072200000 -0.827100000
1 -1.777800000 5.012400000 1.720000000
1 -0.847300000 2.482800000 2.302200000
26 -0.119300000 0.237900000 -0.080400000
8 0.036000000 -0.073200000 2.114500000
1 0.760600000 0.254300000 2.662900000
1 -0.710200000 -0.258700000 2.699100000
8 -0.280100000 0.647000000 -2.319900000
1 0.574100000 0.581200000 -2.767400000
1 -0.849200000 0.003900000 -2.763200000

19^3+ $[Fe(Ohishis)(Im)(H_2O)_2]^{3+}$ Sextet

6 -2.984600000 -3.119100000 0.180900000
6 -3.051900000 -0.947400000 -0.202800000

6 -1.714900000 -2.619300000 0.318400000
6 3.655400000 2.199800000 0.251500000
6 1.548400000 2.723800000 -0.134600000
6 2.907500000 1.052200000 0.331900000
7 -3.798200000 -2.057200000 -0.149500000
7 -1.767400000 -1.234800000 0.068700000
7 2.786300000 3.225700000 -0.047300000
7 1.563700000 1.397200000 0.080400000
6 -0.516300000 -3.414800000 0.765700000
6 0.628500000 -3.642600000 -0.256500000
6 1.513500000 -2.436800000 -0.384600000
6 3.446400000 -0.303400000 0.709300000
7 2.827100000 -2.514700000 -0.358200000
8 0.991000000 -1.274600000 -0.510100000
6 3.694300000 -1.322000000 -0.447900000
1 -3.368800000 -4.121700000 0.301400000
1 -3.448000000 0.029700000 -0.428800000
1 4.713600000 2.366400000 0.392300000
1 0.674600000 3.321100000 -0.340700000
1 -0.098300000 -2.992600000 1.687700000
1 -0.889100000 -4.403500000 1.046100000
1 4.406000000 -0.123500000 1.201800000
1 2.815900000 -0.770100000 1.472500000
1 0.217900000 -3.871700000 -1.248100000
1 1.220900000 -4.509800000 0.048800000
1 3.262600000 -3.429000000 -0.276700000
1 3.546400000 -0.858200000 -1.426900000
1 4.718900000 -1.692600000 -0.412600000
1 3.039300000 4.202100000 -0.165900000
1 -4.799600000 -2.105700000 -0.312100000
1 -1.875300000 2.331400000 -2.064400000
6 -2.042000000 2.512100000 -1.013900000
7 -1.502600000 1.817200000 0.003700000
7 -2.833500000 3.484400000 -0.532800000
6 -1.994100000 2.398700000 1.172700000
6 -2.821800000 3.435700000 0.846300000
1 -3.356300000 4.148700000 -1.096700000
1 -3.386700000 4.123500000 1.458400000
1 -1.725100000 2.041700000 2.152900000
26 -0.178100000 0.175100000 -0.085600000
8 -0.056400000 0.023700000 2.059600000
1 0.575000000 0.499200000 2.622500000
1 -0.667300000 -0.467900000 2.631000000
8 -0.335400000 0.426900000 -2.268300000
1 0.467800000 0.679900000 -2.753300000
1 -0.747700000 -0.284600000 -2.786000000

20^{2+} $[Fe(Nhishis)(Ph)(H_2O)]$ Quintet

6 -1.690000000 4.009300000 -0.431500000
6 -2.461600000 1.931700000 -0.531400000
6 -0.641100000 3.130200000 -0.547200000
6 3.996100000 -2.328800000 -0.535000000
6 2.430900000 -1.581400000 -1.907100000
6 3.007800000 -1.707400000 0.190800000
7 -2.836800000 3.232200000 -0.425100000
7 -1.145000000 1.840500000 -0.611100000
7 3.612200000 -2.242600000 -1.860000000
7 2.036500000 -1.244600000 -0.687400000
6 0.838500000 3.356700000 -0.567200000
6 1.566200000 2.787300000 0.665100000
6 2.928500000 -1.569300000 1.690300000
6 1.809400000 -0.650700000 2.203600000
1 -1.723500000 5.084600000 -0.352200000
1 -3.153300000 1.101900000 -0.524500000
1 4.910700000 -2.813300000 -0.230700000
1 1.896900000 -1.353600000 -2.817200000
1 1.257700000 2.903500000 -1.477100000
1 1.043100000 4.431100000 -0.629400000
1 2.786200000 -2.567400000 2.125200000
1 3.887800000 -1.198200000 2.069400000
1 1.228600000 3.324000000 1.563500000
1 2.637900000 3.008700000 0.571400000
1 0.841800000 -1.003300000 1.826800000
1 1.779000000 -0.732100000 3.294100000
1 4.122400000 -2.597400000 -2.654800000
1 -3.784900000 3.567300000 -0.339400000
7 1.359500000 1.346800000 0.838400000
6 2.047700000 0.831600000 1.886900000
8 2.840000000 1.471200000 2.603000000
26 0.293000000 0.140900000 -0.385100000
8 -0.073100000 -0.172800000 -2.829200000
1 -0.724800000 -0.751200000 -2.362700000
1 -0.572400000 0.599500000 -3.123900000
8 -1.119300000 -1.195200000 -0.665200000
6 -2.217200000 -1.610500000 -0.032100000
6 -2.471700000 -1.282300000 1.318900000
6 -3.172500000 -2.400400000 -0.711000000
6 -3.632000000 -1.726300000 1.956200000
1 -1.745900000 -0.679000000 1.858400000
6 -4.329200000 -2.836800000 -0.064700000

1 -2.980300000 -2.668800000 -1.746500000
6 -4.572600000 -2.504800000 1.273400000
1 -3.798900000 -1.462300000 2.997700000
1 -5.045400000 -3.446300000 -0.610600000
1 -5.472000000 -2.850400000 1.774000000

20^{3+} $[Fe(Nhishis)(Ph)(H_2O)]^{1+}$ Sextet

6 -1.438000000 4.134500000 -0.543800000
6 -1.223000000 2.472800000 -1.990100000
6 -0.672100000 3.145500000 0.021100000
6 3.253800000 -2.915300000 -0.794400000
6 1.088900000 -2.715000000 -1.227100000
6 2.854300000 -1.633500000 -0.509300000
7 -1.768900000 3.693400000 -1.810900000
7 -0.544100000 2.112800000 -0.904500000
7 2.125900000 -3.577500000 -1.245200000
7 1.499600000 -1.527800000 -0.792900000
6 -0.079500000 3.060800000 1.396500000
6 -0.070600000 1.621200000 1.943000000
6 3.624900000 -0.497000000 0.086900000
6 3.289900000 -0.197700000 1.568700000
1 -1.771700000 5.085800000 -0.160200000
1 -1.350000000 1.880200000 -2.883700000
1 4.211600000 -3.403900000 -0.706400000
1 0.079600000 -2.963300000 -1.518400000
1 0.946800000 3.445400000 1.410800000
1 -0.661800000 3.700000000 2.068800000
1 4.688500000 -0.747500000 0.028800000
1 3.495000000 0.410100000 -0.517200000
1 -1.056600000 1.165100000 1.795900000
1 0.134000000 1.648300000 3.014900000
1 3.079400000 -1.140200000 2.090500000
1 4.176400000 0.223900000 2.046900000
1 2.079000000 -4.546500000 -1.530100000
1 -2.343200000 4.186300000 -2.481100000
7 0.949200000 0.767600000 1.284900000
6 2.169500000 0.778200000 1.946800000
8 2.376000000 1.519400000 2.908500000
26 0.310800000 0.183800000 -0.449000000
8 1.368400000 0.760000000 -2.391700000
1 1.569000000 1.686300000 -2.586300000
1 2.062900000 0.212400000 -2.783500000
8 -1.262900000 -0.745300000 -0.616600000
6 -2.285000000 -1.336500000 0.017900000
6 -2.202900000 -1.670300000 1.386200000

6 -3.457000000 -1.640600000 -0.704800000
6 -3.280100000 -2.293000000 2.013200000
1 -1.293500000 -1.442500000 1.934500000
6 -4.525900000 -2.262500000 -0.063800000
1 -3.506300000 -1.378700000 -1.757200000
6 -4.444900000 -2.590800000 1.295200000
1 -3.211500000 -2.548600000 3.066400000
1 -5.426900000 -2.492700000 -0.624600000
1 -5.280500000 -3.075500000 1.789600000