Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Theoretical study on mechanism of the photochemical ligand substitution of *fac*-$[Re^{I}(bpy)(CO)_3(PR_3)]^+$ complex: Supplementary Information

Kenichiro Saita,[*a] Yu Harabuchi[a], Tetsuya Taketsugu[a], Osamu Ishitani[b] and Satoshi Maeda[*a]

[a] *Department of Chemistry, Faculty of Science, Hokkaido University, Kita 10, Nishi 8, Kita-ku, Sapporo 060-0810, Japan*

[b] *Department of Chemistry, Graduate School of Science and Engineering, Tokyo Institute of Technology, O-okayama 2-12-1, NE-1, Meguro-ku, Tokyo 152-8551, Japan*

* Corresponding authors. Tel./Fax.: +81 11 706 4921 (KS, SM).

E-mail address: ksaita@mail.sci.hokudai.ac.jp (KS), smaeda@mail.sci.hokudai.ac.jp (SM).

The Excited States and the Relaxation Pathway

Table S1. Cartesian coordinates (in Å) of the ground state equilibrium structure (S_0-min(global)) of *fac*-[Re^{I}(bpy)$(CO)_3P(OMe)_3]^+$. The electronic energy of the S_0 state is -1600.628084 hartree.

Atom	*x*	*y*	*z*
Re	0.225854000000	-0.908492000000	-0.377207000000
N	-1.394219000000	-0.569810000000	1.104419000000
N	-1.138766000000	0.592221000000	-1.291289000000
C	-1.464024000000	-1.187507000000	2.301298000000
C	-0.949460000000	1.146234000000	-2.506543000000
C	-2.497010000000	-0.964452000000	3.205782000000
C	-1.823596000000	2.080361000000	-3.052613000000
C	-3.503996000000	-0.062893000000	2.861462000000
C	-2.942988000000	2.461065000000	-2.312895000000
C	-3.438185000000	0.580101000000	1.627837000000
C	-3.145607000000	1.892976000000	-1.057566000000
C	-2.371753000000	0.313296000000	0.761458000000
C	-2.229630000000	0.957949000000	-0.562132000000
H	-0.659739000000	-1.883729000000	2.534228000000
H	-0.064613000000	0.823974000000	-3.052808000000
H	-2.501024000000	-1.493483000000	4.158516000000

H	-1.620314000000	2.494324000000	-4.039986000000
H	-4.331872000000	0.139783000000	3.541999000000
H	-3.652218000000	3.190878000000	-2.705237000000
H	-4.215102000000	1.286862000000	1.344329000000
H	-4.014661000000	2.178686000000	-0.468782000000
C	1.525708000000	-1.011882000000	-1.823467000000
O	2.277017000000	-1.059571000000	-2.704181000000
C	1.259531000000	-2.189319000000	0.660440000000
O	1.845984000000	-2.956700000000	1.301239000000
P	1.448156000000	1.009876000000	0.603857000000
O	2.846574000000	0.797545000000	1.453090000000
C	4.015950000000	0.213909000000	0.837451000000
H	4.811103000000	0.265686000000	1.591525000000
H	4.316836000000	0.781925000000	-0.055772000000
H	3.835593000000	-0.837876000000	0.568901000000
O	0.572403000000	1.802816000000	1.731642000000
C	1.098544000000	2.691169000000	2.751448000000
H	1.991400000000	2.257194000000	3.219697000000
H	0.297210000000	2.799245000000	3.492860000000
H	1.335746000000	3.673326000000	2.318399000000
O	1.845070000000	2.065542000000	-0.592461000000
C	2.523550000000	3.324529000000	-0.360193000000
H	3.273036000000	3.231335000000	0.439028000000

H	3.021209000000	3.587234000000	-1.302350000000
H	1.787543000000	4.100237000000	-0.102413000000
C	-0.806882000000	-2.391736000000	-1.186673000000
O	-1.392239000000	-3.260445000000	-1.665820000000

Table S2. Cartesian coordinates (in Å) of the minimum-energy conical intersection for the S_3/S_2 state (S_3/S_2-MECI) of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$. The electronic energy of the MECI is -1600.508368 (S_3: -1600.508368, S_2: -1600.508368) hartree.

Atom	*x*	*y*	*z*
Re	0.162935373752	-0.838254946785	-0.416285206923
P	1.519229857932	0.999871097334	0.661242634153
N	-1.392109531488	-0.631604400280	1.095198272502
N	-1.122392168097	0.711204934543	-1.231939712399
C	-1.473114589748	-1.319878996922	2.260241577227
C	-0.937650199111	1.365691360038	-2.406729567002
C	-2.513900505724	-1.181001785764	3.158950729285
C	-1.832104268685	2.287086080667	-2.915013535886
C	-3.550191567628	-0.267923430586	2.841954264324
C	-3.005663004178	2.559473474045	-2.167581641861
C	-3.491419550111	0.442731055323	1.660907728175
C	-3.215679753058	1.908131105173	-0.969703039942

C	-2.404638606938	0.267738607982	0.763494486803
C	-2.268288947801	0.971879822725	-0.477497840921
H	-0.656388659552	-2.010294713164	2.469165426810
H	-0.023063318527	1.131053242170	-2.950195951608
H	-2.517861965192	-1.763061140083	4.079195522906
H	-1.622603442578	2.781965481402	-3.862026545437
H	-4.389333512250	-0.123811699815	3.524494375652
H	-3.739854296437	3.279189085937	-2.533350999603
H	-4.284165549308	1.146941388570	1.413872410941
H	-4.117732621282	2.112082438951	-0.395122261268
O	2.828281511679	0.652329075366	1.583352423100
C	4.057177407589	0.115171680727	1.032168289288
H	4.817614524507	0.253435233052	1.810183207902
H	4.350769942646	0.658268952589	0.122496475451
H	3.944134802735	-0.956598072270	0.813344169956
O	2.047406797859	2.000270553188	-0.518674037370
C	2.708808261768	3.266189489986	-0.249527451293
H	3.448626208385	3.162044633462	0.556989256671
H	1.957772824315	4.024638774637	0.013534310287
H	3.212964759932	3.548468442616	-1.181516117409
O	0.619751534357	1.839512936646	1.719105338691
C	1.117035497593	2.587577738095	2.864935158994
H	1.861606549636	1.998309359879	3.414488652268

H	0.238098261017	2.775270464180	3.492857422851
H	1.551498836864	3.540977976030	2.533235774313
C	-0.809699464243	-2.355639357391	-1.326439787243
O	-1.323062871763	-3.231053235261	-1.852480166528
C	1.452592102755	-0.780561188260	-1.926676917750
O	2.175522288552	-0.738539934336	-2.818841141904
C	1.201394136801	-2.149883804465	0.654213068072
O	1.775008912930	-2.907848780026	1.300631945760

Table S3. Cartesian coordinates (in Å) of the S_2 state equilibrium structure (S_2-min) of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$. The electronic energy of the S_2 state is -1600.513264 hartree.

Atom	*x*	*y*	*z*
Re	0.196588026764	-0.883577321621	-0.445462539828
P	1.444870896567	0.971721988374	0.671902604987
N	-1.330426460773	-0.652807309822	1.073213870540
N	-1.082790665892	0.676491459260	-1.225443783397
C	-1.387318696272	-1.344157990682	2.242977614109
C	-0.895539557369	1.323097049209	-2.407992092779
C	-2.394751167337	-1.185000943508	3.169352645077
C	-1.758432482924	2.281853886644	-2.890158678412
C	-3.429480890724	-0.252984304329	2.887447692929

C	-2.905386498281	2.608695544099	-2.116701296442
C	-3.391696099651	0.459294576165	1.711181277536
C	-3.117300503666	1.964184915201	-0.920006236347
C	-2.332554361888	0.272435391135	0.780805773520
C	-2.202177711575	0.982004374600	-0.449803428818
H	-0.579431931051	-2.052105063399	2.429371267725
H	-0.007304636398	1.048381804349	-2.976764907826
H	-2.380175877233	-1.768904281209	4.088533428638
H	-1.549984716115	2.764778566432	-3.843772375946
H	-4.246273912385	-0.102500863690	3.594875186331
H	-3.612616103860	3.361283845105	-2.468178893645
H	-4.178026259469	1.178093385860	1.484851517681
H	-3.994277534279	2.205202983166	-0.320676222899
O	2.739801740495	0.686734843496	1.645040829515
C	3.976200918285	0.133934682430	1.136675666397
H	4.718385140331	0.277085467560	1.931409896911
H	4.299491988569	0.660165797384	0.226524997936
H	3.864714093304	-0.941152999362	0.930142623433
O	1.996133268051	1.972720218172	-0.503260582282
C	2.632786328097	3.248866391761	-0.234315541912
H	3.343253808232	3.170049120011	0.601392014022
H	1.865778494290	4.005190531165	-0.014391444311
H	3.169144063634	3.521263002065	-1.151430855261

O	0.498311994651	1.804149761941	1.696383944083
C	0.948865346637	2.681269129451	2.764494993654
H	1.880492702885	2.307666094929	3.207344993503
H	0.145844846133	2.677598434546	3.511664042126
H	1.089419752505	3.698485249245	2.372860274314
C	-0.942756524657	-2.242187973751	-1.353288360365
O	-1.593585030747	-3.019128296868	-1.884237489786
C	1.526550120213	-0.910317750076	-1.968936177967
O	2.271536370179	-0.932851327232	-2.836229786985
C	1.242766594718	-2.341038195161	0.487065123179
O	1.818663127986	-3.182434873038	1.006189417033

Table S4. Cartesian coordinates (in Å) of the minimum-energy conical intersection for the S_2/S_1 state (S_2/S_1-MECI) of *fac*-[Re^{I}(bpy)$(CO)_3$P$(OMe)_3$]$^+$. The electronic energy of the MECI is -1600.513292 (S_3: -1600.513292, S_2: -1600.513292) hartree.

Atom	*x*	*y*	*z*
Re	0.162935373752	-0.838254946785	-0.416285206923
P	1.519229857932	0.999871097334	0.661242634153
N	-1.392109531488	-0.631604400280	1.095198272502
N	-1.122392168097	0.711204934543	-1.231939712399
C	-1.473114589748	-1.319878996922	2.260241577227

C	-0.937650199111	1.365691360038	-2.406729567002
C	-2.513900505724	-1.181001785764	3.158950729285
C	-1.832104268685	2.287086080667	-2.915013535886
C	-3.550191567628	-0.267923430586	2.841954264324
C	-3.005663004178	2.559473474045	-2.167581641861
C	-3.491419550111	0.442731055323	1.660907728175
C	-3.215679753058	1.908131105173	-0.969703039942
C	-2.404638606938	0.267738607982	0.763494486803
C	-2.268288947801	0.971879822725	-0.477497840921
H	-0.656388659552	-2.010294713164	2.469165426810
H	-0.023063318527	1.131053242170	-2.950195951608
H	-2.517861965192	-1.763061140083	4.079195522906
H	-1.622603442578	2.781965481402	-3.862026545437
H	-4.389333512250	-0.123811699815	3.524494375652
H	-3.739854296437	3.279189085937	-2.533350999603
H	-4.284165549308	1.146941388570	1.413872410941
H	-4.117732621282	2.112082438951	-0.395122261268
O	2.828281511679	0.652329075366	1.583352423100
C	4.057177407589	0.115171680727	1.032168289288
H	4.817614524507	0.253435233052	1.810183207902
H	4.350769942646	0.658268952589	0.122496475451
H	3.944134802735	-0.956598072270	0.813344169956
O	2.047406797859	2.000270553188	-0.518674037370

C	2.708808261768	3.266189489986	-0.249527451293
H	3.448626208385	3.162044633462	0.556989256671
H	1.957772824315	4.024638774637	0.013534310287
H	3.212964759932	3.548468442616	-1.181516117409
O	0.619751534357	1.839512936646	1.719105338691
C	1.117035497593	2.587577738095	2.864935158994
H	1.861606549636	1.998309359879	3.414488652268
H	0.238098261017	2.775270464180	3.492857422851
H	1.551498836864	3.540977976030	2.533235774313
C	-0.809699464243	-2.355639357391	-1.326439787243
O	-1.323062871763	-3.231053235261	-1.852480166528
C	1.452592102755	-0.780561188260	-1.926676917750
O	2.175522288552	-0.738539934336	-2.818841141904
C	1.201394136801	-2.149883804465	0.654213068072
O	1.775008912930	-2.907848780026	1.300631945760

Table S5. Cartesian coordinates (in Å) of the S_1 state equilibrium structure (S_1-min) of *fac*-[Re^{I}(bpy)$(CO)_3P(OMe)_3]^+$. The electronic energy of the S_1 state is -1600.517331 hartree.

Atom	*x*	*y*	*z*
Re	0.180826727670	-0.880662516638	-0.437846189580
P	1.442511993738	0.974628586585	0.699759715762

N	-1.326404167967	-0.662599312118	1.080850951145
N	-1.089179801519	0.676980001757	-1.226739804600
C	-1.376386229159	-1.344135344793	2.257205324050
C	-0.921675111421	1.317385454276	-2.415164833726
C	-2.384190999593	-1.187710461120	3.183198400738
C	-1.792383087613	2.272660109774	-2.890138538965
C	-3.423358642878	-0.260214173497	2.897738980149
C	-2.932330828349	2.598915960627	-2.103542758557
C	-3.392642513852	0.450742179997	1.720424748234
C	-3.131347634916	1.958728104549	-0.902964595873
C	-2.335316325433	0.264973556370	0.786719736168
C	-2.207763767520	0.979238157663	-0.438909582922
H	-0.560312785057	-2.043768098762	2.439167746704
H	-0.037677468197	1.037318187658	-2.988397956933
H	-2.368915542903	-1.767618526437	4.104918638306
H	-1.598341012237	2.754489226252	-3.847443116202
H	-4.238350091416	-0.109335239305	3.607375441467
H	-3.645543958746	3.348204759563	-2.450265149711
H	-4.182331506534	1.166762911191	1.497717768244
H	-4.003946410596	2.199480733761	-0.297334835022
O	2.722945238625	0.667529815722	1.677608672893
C	3.975669056185	0.137736441209	1.177335323746
H	4.708227026183	0.298309840480	1.977424509691

H	4.292744632569	0.668192925891	0.268066946304
H	3.883686394999	-0.938920896751	0.973543253427
O	2.000138862701	1.943986281926	-0.490427955618
C	2.661800484304	3.216902708062	-0.255007620757
H	3.342795040081	3.155333297746	0.605829686492
H	1.906007797231	3.997973501879	-0.091457028472
H	3.233472985375	3.435073052450	-1.165115618350
O	0.492415789131	1.810899693224	1.710559035782
C	0.941555386574	2.703701604500	2.768702791601
H	1.850334348441	2.313907281581	3.243745702800
H	0.119376045674	2.740185261452	3.493360098947
H	1.120335161253	3.705795148802	2.354829453237
C	-0.979818438220	-2.168916487843	-1.497532612766
O	-1.626633735339	-2.877631023188	-2.112917094224
C	1.520893533344	-0.994103371437	-1.914184555919
O	2.287166026677	-1.070284485782	-2.765292556653
C	1.296500661392	-2.274375439282	0.448596890382
O	1.932758867335	-3.084210407972	0.956653588653

Table S6. Cartesian coordinates (in Å) of the minimum-energy seam of crossing for the S_1/T_2 state (S_1/T_2-MESX) of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$. The electronic energy of the MESX is -1600.516097 (S_1: -1600.516096, S_2: -1600.516098) hartree.

Atom	*x*	*y*	*z*
Re	0.177277682851	-0.873283202011	-0.438071075756
P	1.486444710993	0.972079376988	0.681551121403
N	-1.331479244858	-0.648192010020	1.079294365724
N	-1.084299349555	0.688101299340	-1.224881670512
C	-1.386337529556	-1.330279823827	2.257421776572
C	-0.909386475187	1.340771736079	-2.409032226322
C	-2.393439187806	-1.169449632927	3.182632591029
C	-1.781707759167	2.290368533674	-2.888302245515
C	-3.433101691940	-0.245050019760	2.893212122728
C	-2.937900928807	2.599608089916	-2.116207933812
C	-3.399622015861	0.462695892879	1.710770979331
C	-3.141383178540	1.954278533787	-0.917125900596
C	-2.343146452603	0.273427027074	0.782309859698
C	-2.214952578868	0.984263509941	-0.448990673039
H	-0.570562057974	-2.028668883495	2.443533581593
H	-0.015107391285	1.075673589190	-2.972685554589
H	-2.378803584583	-1.746468750956	4.106076427720
H	-1.583145919814	2.777429279649	-3.842000882703
H	-4.248681656515	-0.090866973497	3.601205696494
H	-3.653945547850	3.343715173153	-2.467789444539
H	-4.190717991165	1.175988880566	1.484062613642

H	-4.023499778229	2.183896748639	-0.320986962829
O	2.755970040332	0.684369412513	1.676670041046
C	4.006657465962	0.119633015528	1.212708521471
H	4.724843543761	0.277680840457	2.026235245752
H	4.355869157227	0.631394236986	0.304328943709
H	3.894232050009	-0.957082810678	1.021058937107
O	2.051215544152	1.911911429998	-0.528813820625
C	2.630605394081	3.230270142404	-0.337847528701
H	3.392868278700	3.217046949753	0.454638977721
H	1.837487670371	3.951356884323	-0.094292206798
H	3.094914942931	3.493554448591	-1.295732049223
O	0.534359542929	1.841727913739	1.661985653196
C	0.959302217245	2.635810583532	2.805197541426
H	1.879065426115	2.227143246284	3.240169131001
H	0.137673875295	2.580434476650	3.529617227653
H	1.113328822208	3.675506274911	2.484896341110
C	-0.946127109885	-2.222825139227	-1.457919526881
O	-1.561996360393	-2.974839460029	-2.055908986832
C	1.511444663015	-0.896550509605	-1.920489124332
O	2.271930268697	-0.910470263355	-2.780680028906
C	1.237136162168	-2.278895317842	0.486781600850
O	1.834028331417	-3.095665729317	1.032049544621

Table S7. Cartesian coordinates (in Å) of the minimum-energy conical intersection for the T_2/T_1 state (T_2/T_1-MECI) of *fac*-[Re^{I}(bpy)$(CO)_3P(OMe)_3$]$^+$. The electronic energy of the MECI is -1600.517611 (T_2: -1600.517611, T_1: -1600.517611) hartree.

Atom	*x*	*y*	*z*
Re	-0.953294590825	-0.152581969412	0.003087039528
N	-0.036952983081	1.258389135655	1.336515771143
N	-0.035674709343	1.259037836079	-1.336276461100
C	-0.089722834808	1.231442700476	2.702508867738
C	-0.088539508499	1.235653244871	-2.702646658249
C	0.535736549801	2.157351831292	3.504973812512
C	0.537555613692	2.157881818919	-3.507130742233
C	1.279732927429	3.200560289098	2.887751371932
C	1.282040973022	3.202423714980	-2.889656200921
C	1.344748042245	3.254844579731	1.508863804825
C	1.344730075428	3.257517446607	-1.511671168318
C	0.684527896335	2.286725377221	0.715566534738
C	0.685616332209	2.288854084949	-0.716953045885
H	-0.669223644279	0.422160460524	3.145617346112
H	-0.665059996038	0.423917047520	-3.142814101817
H	0.452444175352	2.077112399775	4.588343821709
H	0.455515043425	2.079697022179	-4.590325591697

H	1.792988297795	3.950917863452	3.490690288881
H	1.793948477312	3.953031767883	-3.493287324641
H	1.906314447650	4.053438276690	1.026333152672
H	1.905903909289	4.055773813533	-1.028889729748
C	-1.644787665507	-1.293295784671	-1.467391086400
O	-2.038857868467	-1.916949266638	-2.348886726263
C	-1.645389293627	-1.292216764934	1.476508988314
O	-2.039379179371	-1.920813485797	2.354298676385
P	1.165544020002	-1.579573223077	-0.000223383508
O	1.158992313053	-3.215012079868	-0.000975650502
C	0.002338743085	-4.083693298777	-0.000163819959
H	0.406265279947	-5.103451501392	-0.000189906093
H	-0.602877509899	-3.934319082073	-0.905355717184
H	-0.602918589148	-3.933401454753	0.904810818721
O	2.048539003054	-1.216808109545	1.321816342038
C	3.181104730224	-1.991737189624	1.798421055726
H	2.966747311723	-3.066983492884	1.739788265553
H	3.335520704387	-1.689265049229	2.841322956917
H	4.076683081943	-1.748710397308	1.208927456131
O	2.045401010108	-1.218028682514	-1.325224838994
C	3.181275033395	-1.990530769096	-1.798673777699
H	2.967720536088	-3.065937480429	-1.740073030174
H	3.336400570393	-1.690232388360	-2.842025803430

H	4.075238595540	-1.746882252722	-1.206742652470
C	-2.768899446594	0.695180395047	0.001985408720
O	-3.824685874436	1.135217616704	-0.002554363018

Table S8. Cartesian coordinates (in Å) of the T_1 state equilibrium structure (T_1-min(global)) of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$. The electronic energy of the T_1 state is -1600.534237 hartree. This data has been optimized by the TD-B3LYP calculation.

Atom	*x*	*y*	*z*
Re	0.238571258181	-0.895256687416	-0.440388706593
P	1.463529732095	0.963306089884	0.669213631253
N	-1.331029730382	-0.666331468610	1.076356816417
N	-1.088626589146	0.657271345253	-1.251933585145
C	-1.412850098944	-1.317061576731	2.230258522290
C	-0.929301555725	1.312026840731	-2.396020523751
C	-2.457202682978	-1.141199199532	3.163106560183
C	-1.828394048875	2.287657040458	-2.877208134746
C	-3.496011403110	-0.218208817693	2.867734228448
C	-2.982359976680	2.598755677090	-2.109925159593
C	-3.451418465289	0.476542830132	1.688374473897
C	-3.185480210087	1.948407384538	-0.921565814796
C	-2.354210612923	0.273322225817	0.755653471940

C	-2.230397763668	0.957052582040	-0.452646738822
H	-0.612262762083	-2.025562733308	2.446062458625
H	-0.043722022373	1.061535883506	-2.981124492819
H	-2.446308317964	-1.717983463804	4.086889033344
H	-1.620915770470	2.777887905095	-3.827411087748
H	-4.315864232861	-0.066313683377	3.570325005062
H	-3.695423264731	3.344324901363	-2.462870838669
H	-4.235152453418	1.188691110086	1.440117077862
H	-4.062878870793	2.168955734168	-0.317773200516
O	2.796389427474	0.703947629841	1.605487080128
C	3.996235057486	0.109307227878	1.061880784432
H	4.756346460506	0.192931167775	1.848608811507
H	4.334027878659	0.648930507414	0.164239873824
H	3.832807510407	-0.952052848628	0.822539214908
O	1.963203548004	2.026016535418	-0.480850584918
C	2.674212415007	3.254675426038	-0.189166078039
H	3.328449648996	3.138103109238	0.686645203691
H	1.952401154317	4.066669379360	-0.018691243425
H	3.282538352065	3.480581734218	-1.074380934144
O	0.528916430680	1.752179848168	1.750961337931
C	0.997241332034	2.664064374925	2.778190814316
H	1.908870063018	2.279256761331	3.253339780031
H	0.185918470982	2.726743256050	3.514007636707

H	1.181477492956	3.658379248575	2.346950936010
C	-0.826622023433	-2.302581924244	-1.348616763734
O	-1.430201885729	-3.123182666148	-1.884537377101
C	1.536965037850	-0.904814998605	-1.899177002413
O	2.290072830242	-0.899668647651	-2.778474197190
C	1.276977835532	-2.266119043460	0.483371445508
O	1.868794805148	-3.089636997184	1.043099265857

Mechanism of the Photochemical Ligand Substitution (PLS) Reaction

Table S9. Cartesian coordinates (in Å) of the T_1 state equilibrium structure (T_1-min(global)) of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$. The electronic energy of the T_1 state is -1600.525274 hartree. This data has been optimized by the UB3LYP calculation.

Atom	*x*	*y*	*z*
Re	0.230718000000	-0.970103000000	-0.150747000000
N	-1.332120000000	-0.304840000000	1.230394000000
N	-1.126412000000	0.214800000000	-1.394782000000
C	-1.407567000000	-0.572921000000	2.531539000000
C	-0.998638000000	0.460284000000	-2.696836000000
C	-2.442307000000	-0.121725000000	3.368990000000
C	-1.912021000000	1.220415000000	-3.446813000000

C	-3.483010000000	0.670891000000	2.813610000000
C	-3.050265000000	1.769771000000	-2.796559000000
C	-3.447341000000	0.971197000000	1.480726000000
C	-3.222549000000	1.543866000000	-1.459635000000
C	-2.360646000000	0.488328000000	0.644883000000
C	-2.256155000000	0.754700000000	-0.714259000000
H	-0.604681000000	-1.182276000000	2.947923000000
H	-0.123336000000	0.032924000000	-3.186681000000
H	-2.426141000000	-0.388704000000	4.424826000000
H	-1.730378000000	1.371996000000	-4.510000000000
H	-4.297255000000	1.032313000000	3.442285000000
H	-3.774533000000	2.361415000000	-3.357115000000
H	-4.233599000000	1.575697000000	1.033787000000
H	-4.086833000000	1.952999000000	-0.941261000000
C	1.516249000000	-1.427787000000	-1.552083000000
O	2.256002000000	-1.695567000000	-2.401125000000
C	1.313293000000	-1.950112000000	1.150321000000
O	1.933091000000	-2.529856000000	1.937406000000
P	1.451232000000	1.144033000000	0.339009000000
O	2.944331000000	1.109326000000	1.040020000000
C	4.055127000000	0.440761000000	0.402745000000
H	4.925599000000	0.622874000000	1.045060000000
H	4.242892000000	0.854855000000	-0.599526000000

H	3.873603000000	-0.642505000000	0.332303000000
O	0.670299000000	2.082656000000	1.421571000000
C	1.259147000000	3.155856000000	2.201650000000
H	2.242682000000	2.859406000000	2.588226000000
H	0.564995000000	3.335114000000	3.032027000000
H	1.347531000000	4.065839000000	1.591142000000
O	1.660217000000	1.993087000000	-1.051255000000
C	2.313989000000	3.285203000000	-1.114173000000
H	3.146635000000	3.344884000000	-0.398558000000
H	2.698653000000	3.389031000000	-2.136652000000
H	1.581367000000	4.080327000000	-0.912194000000
O	-0.817267000000	-2.613051000000	-0.545710000000
C	-1.410197000000	-3.571234000000	-0.775915000000

Table S10. Cartesian coordinates (in Å) of the T_1 state transition state in which the axial CO is bent (T_1-TS(bent)) of *fac*-[Re^{I}(bpy)$(CO)_3P(OMe)_3]^+$. The electronic energy of the T_1 state is -1600.510442 hartree.

Atom	*x*	*y*	*z*
Re	0.247464539744	-0.717405861911	-0.323165557290
P	1.503002239293	1.169999847978	0.603137093527
N	-1.305078842489	-0.568934178457	1.150765083155

N	-1.097790715679	0.725231642220	-1.159934697777
C	-1.323724776368	-1.212607250759	2.350457498094
C	-0.911471453636	1.393011397203	-2.332301834224
C	-2.382149807952	-1.129434251663	3.231754941092
C	-1.839199397946	2.272325376208	-2.851199757015
C	-3.502410505930	-0.347094996800	2.875363866356
C	-3.031385523835	2.505906562653	-2.131028311677
C	-3.500222276001	0.319337650571	1.664707733262
C	-3.239497162975	1.837891211440	-0.939055302302
C	-2.392369061498	0.213167116899	0.796105951502
C	-2.274592576531	0.927626759563	-0.456069662915
H	-0.445303500818	-1.813972390536	2.582957595318
H	0.025423748882	1.196052554966	-2.851725146958
H	-2.340132080181	-1.670699433769	4.176484655119
H	-1.638243926842	2.768903438754	-3.800112617574
H	-4.359465934684	-0.267632419241	3.545266415925
H	-3.779232881296	3.204787587430	-2.507779876381
H	-4.355081911412	0.929593036445	1.378673772620
H	-4.150791333416	2.014224981715	-0.370162289524
O	2.804317365409	0.920791414568	1.570437946069
C	4.011822614309	0.285169178889	1.085728986920
H	4.762321096683	0.434551106021	1.871296463875
H	4.353648373738	0.751320206162	0.150148155015

H	3.847604695793	-0.791629868469	0.934002357650
O	2.032035745432	2.100141301752	-0.631950946368
C	2.710984030986	3.371237338016	-0.437359599046
H	3.405115106326	3.322413347519	0.413596357477
H	1.967041519251	4.165316983387	-0.281314653582
H	3.270323880131	3.560993093408	-1.361517193019
O	0.572223059285	2.050843979160	1.601675041052
C	1.043955681763	2.974055024920	2.622917269894
H	1.931458601933	2.572109295170	3.127115995972
H	0.215232124428	3.075598842436	3.333949098628
H	1.267281349512	3.949400920628	2.168483769590
C	-1.089277017681	-2.273943562884	-1.210636246806
O	-1.332717930409	-3.397872535544	-1.301839781137
C	1.520251838403	-0.871935788711	-1.833080363277
O	2.252621499774	-0.976142276334	-2.717131136084
C	1.304751256059	-2.209361655653	0.452192027410
O	1.903926949378	-3.097427546220	0.875673840058

Table S11. Cartesian coordinates (in Å) of the T_1 state equilibrium structure in which the axial CO is bent (T_1-min(bent)) of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$. The electronic energy of the T_1 state is -1600.515762 hartree.

Atom	*x*	*y*	*z*
Re	0.260618000000	-0.817321000000	-0.329640000000
P	1.478658000000	1.242649000000	0.519746000000
N	-1.347645000000	-0.648845000000	1.134723000000
N	-1.117532000000	0.747446000000	-1.121804000000
C	-1.403532000000	-1.383835000000	2.269786000000
C	-0.942387000000	1.395393000000	-2.291177000000
C	-2.433322000000	-1.263454000000	3.194339000000
C	-1.842436000000	2.345223000000	-2.762850000000
C	-3.455955000000	-0.347876000000	2.941943000000
C	-2.969934000000	2.638653000000	-1.994615000000
C	-3.408342000000	0.413177000000	1.776477000000
C	-3.159267000000	1.968067000000	-0.788633000000
C	-2.344508000000	0.251459000000	0.883307000000
C	-2.219324000000	1.019549000000	-0.370342000000
H	-0.589183000000	-2.088595000000	2.429201000000
H	-0.048110000000	1.139546000000	-2.857277000000
H	-2.425061000000	-1.882079000000	4.091333000000
H	-1.653714000000	2.839755000000	-3.715439000000
H	-4.283289000000	-0.225791000000	3.642048000000
H	-3.697825000000	3.378770000000	-2.329154000000
H	-4.198750000000	1.130659000000	1.566312000000
H	-4.036064000000	2.181676000000	-0.181125000000

O	2.777222000000	1.112455000000	1.525748000000
C	3.978880000000	0.423723000000	1.110071000000
H	4.682839000000	0.517984000000	1.945889000000
H	4.406487000000	0.889738000000	0.209687000000
H	3.775231000000	-0.641147000000	0.921033000000
O	1.997605000000	2.141544000000	-0.752107000000
C	2.630160000000	3.440219000000	-0.604664000000
H	3.333274000000	3.442288000000	0.240657000000
H	1.860595000000	4.213148000000	-0.464605000000
H	3.174487000000	3.624150000000	-1.539166000000
O	0.505685000000	2.164105000000	1.453296000000
C	0.940243000000	3.088871000000	2.486806000000
H	1.653821000000	2.601470000000	3.163307000000
H	0.029995000000	3.368332000000	3.031108000000
H	1.393807000000	3.983772000000	2.037683000000
C	-0.957994000000	-2.077772000000	-1.600273000000
O	-1.491767000000	-3.107543000000	-1.361935000000
C	1.634762000000	-0.930218000000	-1.746926000000
O	2.429367000000	-1.013286000000	-2.577901000000
C	1.282307000000	-2.292985000000	0.460333000000
O	1.873713000000	-3.179894000000	0.906090000000

Table S12. Cartesian coordinates (in Å) of the T_1 state transition state for the axial CO dissociation (T_1-TS(dissociation)) of *fac*-[Re^{I}(bpy)$(CO)_3P(OMe)_3]^+$. The electronic energy of the T_1 state is -1600.509637 hartree.

Atom	*x*	*y*	*z*
Re	0.293654000000	-0.583773000000	-0.229844000000
P	1.541949000000	1.324133000000	0.624716000000
N	-1.351336000000	-0.495955000000	1.195488000000
N	-1.147601000000	0.737849000000	-1.147245000000
C	-1.375500000000	-1.130951000000	2.391626000000
C	-0.972001000000	1.358340000000	-2.342194000000
C	-2.462734000000	-1.073564000000	3.251604000000
C	-1.937280000000	2.171576000000	-2.914173000000
C	-3.585278000000	-0.331002000000	2.869798000000
C	-3.143212000000	2.369235000000	-2.231952000000
C	-3.570467000000	0.328308000000	1.646029000000
C	-3.333695000000	1.742243000000	-1.005423000000
C	-2.441588000000	0.237908000000	0.819519000000
C	-2.328579000000	0.922987000000	-0.475188000000
H	-0.482541000000	-1.698754000000	2.651604000000
H	-0.018500000000	1.185282000000	-2.837902000000
H	-2.424722000000	-1.605621000000	4.201970000000
H	-1.741368000000	2.640399000000	-3.878260000000

H	-4.459707000000	-0.266157000000	3.518294000000
H	-3.924086000000	3.005201000000	-2.650456000000
H	-4.433615000000	0.913060000000	1.334561000000
H	-4.264020000000	1.889570000000	-0.460473000000
O	2.899087000000	1.048986000000	1.513593000000
C	4.023931000000	0.322371000000	0.966597000000
H	4.783207000000	0.307234000000	1.757956000000
H	4.423517000000	0.832809000000	0.077564000000
H	3.735848000000	-0.708345000000	0.711162000000
O	2.010001000000	2.282113000000	-0.622385000000
C	2.674203000000	3.557811000000	-0.427598000000
H	3.466366000000	3.477180000000	0.330922000000
H	1.939328000000	4.321673000000	-0.134654000000
H	3.115803000000	3.821486000000	-1.396466000000
O	0.706478000000	2.239890000000	1.689591000000
C	1.281172000000	3.054864000000	2.746919000000
H	1.977848000000	2.462055000000	3.353359000000
H	0.430886000000	3.382641000000	3.357388000000
H	1.795538000000	3.930945000000	2.327617000000
C	-1.505995000000	-2.366212000000	-1.444620000000
O	-1.274168000000	-3.372712000000	-1.937856000000
C	1.536536000000	-0.723219000000	-1.721766000000
O	2.251941000000	-0.822719000000	-2.629989000000

C	1.095875000000	-2.302893000000	0.326601000000
O	1.554148000000	-3.322118000000	0.630259000000

Table S13. Cartesian coordinates (in Å) of the ground state equilibrium structure (S_0-min(global) or S_2-FC) of *fac*-[Re^{I}(bpy)$(CO)_3Cl$]. The electronic energy of the S_0 state is -1374.213754 hartree.

Atom	*x*	*y*	*z*
C	-3.275102535000	-0.044246517000	1.502075308000
C	-3.196554867000	-0.052098836000	2.892631590000
C	-2.100549080000	-0.066124547000	0.740178534000
H	-4.106717658000	-0.034368719000	3.493526714000
C	-1.939619874000	-0.083560540000	3.496676002000
N	-0.878232683000	-0.094185530000	1.337308555000
H	-1.823888852000	-0.091815265000	4.580355943000
C	-0.810559610000	-0.103191867000	2.683418959000
H	0.188924542000	-0.125931304000	3.115733939000
H	-4.248406741000	-0.020601489000	1.016325273000
C	-2.100549080000	-0.066124547000	-0.740178534000
N	-0.878232683000	-0.094185529000	-1.337308555000
C	-3.275102535000	-0.044246517000	-1.502075308000
C	-0.810559610000	-0.103191867000	-2.683418959000
C	-3.196554867000	-0.052098836000	-2.892631590000

C	-1.939619874000	-0.083560540000	-3.496676002000
H	-4.248406741000	-0.020601490000	-1.016325273000
H	0.188924542000	-0.125931304000	-3.115733938000
H	-4.106717658000	-0.034368720000	-3.493526714000
H	-1.823888852000	-0.091815265000	-4.580355943000
Re	0.894823041000	-0.052419202000	0.000000000000
C	2.265516626000	0.103478225000	1.361643884000
C	1.070050144000	-1.967896832000	0.000000000000
C	2.265516626000	0.103478225000	-1.361643884000
Cl	0.509433047000	2.478712142000	0.000000000000
O	1.176732428000	-3.127264736000	0.000000000000
O	3.066716767000	0.208111583000	2.195547625000
O	3.066716767000	0.208111583000	-2.195547625000

Table S14. Cartesian coordinates (in Å) of the T_1 state equilibrium structure (T_1-min(global)) of *fac*-[Re^{I}(bpy)$(CO)_3$Cl]. The electronic energy of the S_0 state is -1374.122477 hartree.

Atom	*x*	*y*	*z*
C	-3.261979699881	-0.193683852314	1.519241846673
C	-3.171379001672	-0.173719413924	2.889293838312
C	-2.089168922355	-0.142265004963	0.710407834126
H	-4.074010282039	-0.212806758594	3.501298090862

C	-1.885580403676	-0.100765655544	3.503596678830
N	-0.830148407328	-0.074149945120	1.333284732265
H	-1.769928948518	-0.077502051417	4.586752586548
C	-0.773314869948	-0.056636596935	2.694761760979
H	0.226767271955	0.000668784909	3.125388039455
H	-4.238498286975	-0.248352546473	1.039511489722
C	-2.091755847733	-0.139492169199	-0.710735334698
N	-0.839139104513	-0.069291758951	-1.334577809418
C	-3.267938593208	-0.191940620721	-1.515782004049
C	-0.783035549354	-0.046770969907	-2.692266356186
C	-3.179931318751	-0.166942874662	-2.886540111053
C	-1.898143238437	-0.089257916215	-3.501781830276
H	-4.243170058487	-0.251298115745	-1.034049261627
H	0.216418369120	0.013191235073	-3.124407782564
H	-4.083950642662	-0.206183458638	-3.496605206479
H	-1.783454481362	-0.061731886093	-4.584958084411
Re	0.848282846012	-0.001129366743	0.005293768255
C	2.295221044873	0.127792079655	1.355454143414
C	0.893308506152	-1.992356681475	-0.009180864065
C	2.325305015188	0.091428010644	-1.332265663507
Cl	0.644022482415	2.454574558330	-0.052003976742
O	0.912866602202	-3.139526564733	-0.022503378397
O	3.139913663189	0.207805771878	2.134905249866

O	3.186079153514	0.143371489237	-2.094366552174

Table S15. Cartesian coordinates (in Å) of the T_1 state transition state in which the axial CO is bent (T_1-TS(bent)) of *fac*-[Re^I(bpy)$(CO)_3$Cl]. The electronic energy of the T_1 state is -1374.106438 hartree.

Atom	*x*	*y*	*z*
C	-3.178537973855	0.075666504442	1.478483457086
C	-3.040000832813	0.124228253791	2.858411838810
C	-2.032413138780	0.081158863401	0.661389760044
H	-3.923281432908	0.128372567055	3.498616949123
C	-1.752017897587	0.163268000404	3.413204463040
N	-0.785056377812	0.088321559764	1.213650003136
H	-1.594076971411	0.216663584259	4.490287581813
C	-0.660955019648	0.126879703591	2.557383323016
H	0.358274807279	0.131106788164	2.944063139235
H	-4.170902913772	0.029865469655	1.033575902411
C	-2.083507060430	0.048715574697	-0.801756482303
N	-0.879460995741	-0.088990069267	-1.448009430042
C	-3.281987430918	0.128936639614	-1.530954882766
C	-0.877539016307	-0.185332961148	-2.801648687957
C	-3.262009570045	0.040286120324	-2.915751742606
C	-2.031444524770	-0.133312368023	-3.566081687386

H	-4.227900650029	0.265529365636	-1.010086368387
H	0.097809419925	-0.301510557411	-3.272336095575
H	-4.190465701636	0.105936487868	-3.484491544937
H	-1.962760322763	-0.216668923150	-4.650461270099
Re	0.923946977453	-0.053738247197	-0.235308523309
C	2.504437086629	0.151662063909	0.932206469015
C	0.905995994939	-2.005866646862	0.266045710884
C	2.238428267357	0.027567444115	-1.680067311750
Cl	0.710216497992	2.541574872040	-0.040622942210
O	1.021248551622	-3.142339327375	0.002168697100
O	3.432177631629	0.282951900990	1.605217663536
O	3.028210330062	0.049196581540	-2.530068171928

Table S16. Cartesian coordinates (in Å) of the T_1 state equilibrium structure in which the axial CO is bent (T_1-min(bent)) of *fac*-[Re^{I}(bpy)$(CO)_3$Cl]. The electronic energy of the T_1 state is -1374.110055 hartree.

Atom	*x*	*y*	*z*
C	-3.258841722941	-0.160321848548	1.497215817403
C	-3.169461131953	-0.218139516848	2.886166350055
C	-2.090705630876	-0.049410222004	0.733515794715
H	-4.073908582479	-0.303190865350	3.489927574690
C	-1.910892399510	-0.167107932831	3.486475341920

N	-0.868379693005	-0.001242184644	1.327486500862
H	-1.790136323941	-0.209236304334	4.568793880640
C	-0.788560769638	-0.060868559716	2.670640277297
H	0.213333996133	-0.019206813394	3.096670327921
H	-4.233665424198	-0.203127217306	1.015687233498
C	-2.091737711511	0.016084178236	-0.743335378711
N	-0.867935179895	0.110528278321	-1.337266012518
C	-3.262457917146	-0.017681179223	-1.509134969987
C	-0.799314096353	0.169067796472	-2.684538740648
C	-3.181688505517	0.041990656698	-2.898440667211
C	-1.925846100801	0.135763646457	-3.499070902625
H	-4.235120455412	-0.087804580358	-1.026678475055
H	0.199070223110	0.247695314863	-3.112714123412
H	-4.089962708212	0.015964880261	-3.501799839776
H	-1.809875499552	0.185734104039	-4.581492116564
Re	0.886534171995	0.212779857661	-0.018719036700
C	2.368677435062	0.310948520176	1.256309257634
C	0.979456409001	-1.898319168884	0.104015282967
C	2.310486413053	0.461812631272	-1.334934273731
Cl	0.405021796395	2.718480520502	0.279037937155
O	1.241226379965	-2.685536484006	-0.751093406043
O	3.250664415010	0.377710873417	2.002646483457
O	3.160187644213	0.613606818616	-2.106957643895

Table S17. Cartesian coordinates (in Å) of the T_1 state transition state for the axial CO dissociation (T_1-TS(dissociation)) of *fac*-[Re^{I}(bpy)$(CO)_3$Cl]. The electronic energy of the T_1 state is -1374.096167 hartree.

Atom	*x*	*y*	*z*
C	-3.221361435280	-0.398751279642	1.496117525990
C	-3.122533166260	-0.471207484015	2.881751155491
C	-2.077064340678	-0.143516464316	0.728467396650
H	-4.008572286575	-0.669924761956	3.485969460106
C	-1.872851739528	-0.282700693350	3.481022327319
N	-0.855881557728	0.028129760002	1.319006901619
H	-1.745001579862	-0.324907717780	4.562618610504
C	-0.773817437901	-0.037494143600	2.669565657844
H	0.217060925408	0.115283123250	3.095725626907
H	-4.186735509402	-0.539460649524	1.013657884500
C	-2.090899701059	-0.040746651094	-0.738834130134
N	-0.879605392158	0.206426510298	-1.323277564677
C	-3.251153037385	-0.180017022563	-1.512237031774
C	-0.822331379564	0.323251644484	-2.671944653862
C	-3.178064990138	-0.063520544164	-2.896505605795
C	-1.937453230219	0.195538937998	-3.488271202542
H	-4.209242481702	-0.376153546467	-1.034748047170

H	0.161617436487	0.527857926913	-3.092503508383
H	-4.076741922447	-0.171457656455	-3.505068150969
H	-1.829111050738	0.298664171952	-4.567902629477
Re	0.845138258559	0.400479146540	0.000198400130
C	2.320853535133	0.134358906398	1.234516337619
C	0.677650417426	-2.840886040507	-0.266673023381
C	2.287822831778	0.316565021649	-1.294757877162
Cl	0.539960914600	2.867361784396	0.179171446723
O	1.656822407175	-3.402229577476	-0.420317779388
O	3.213963487340	-0.068558349062	1.955473147146
O	3.160131256396	0.220734146573	-2.062235919334

SC-AFIR search for the T_1/S_0 MESXs

Table S18. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 2.939 eV of energy (T_1: -1374.105735, S_0: -1374.105735 hartree), of *fac*-[Re^{I}(bpy)$(CO)_3$Cl].

Atom	*x*	*y*	*z*
C	-3.293049465328	-0.061540673370	0.959855679907
C	-3.453139635077	0.318189646673	2.289646677216
C	-2.007683460094	-0.296794711697	0.456564991578
H	-4.450697247284	0.501506559300	2.691018337582
C	-2.318570849459	0.462966781619	3.090775164026

N	-0.905678802327	-0.166294624967	1.250174601134
H	-2.392400047462	0.767245116302	4.134932818474
C	-1.067201835122	0.214157953924	2.537451438408
H	-0.143393954508	0.334550626046	3.106649222546
H	-4.165118178999	-0.173754615981	0.318867538671
C	-1.746275061192	-0.690473608628	-0.938596479777
N	-0.432001125008	-0.889390050854	-1.267130350205
C	-2.757713335710	-0.859736439658	-1.891539740930
C	-0.126337950803	-1.249756601032	-2.539639760023
C	-2.432744898241	-1.237285328525	-3.191017831870
C	-1.088505032043	-1.433447618156	-3.521122011701
H	-3.799047198417	-0.700012035158	-1.619222068512
H	0.930299014182	-1.393452870606	-2.757709092535
H	-3.217733118291	-1.375972397214	-3.935307881216
H	-0.781521410771	-1.728342608127	-4.524424388708
Re	1.036380508966	-0.667934728905	0.328766158659
C	1.720654149360	-1.795930274164	1.804781685099
C	2.551195307674	-1.302742726581	-0.695085042457
C	1.729449999796	1.179869302206	0.060340543956
Cl	2.287017773507	0.985003484717	3.002674637285
O	3.438346752405	-1.695260117748	-1.336231114668
O	2.119344436114	-2.499009893679	2.636828554303
O	2.166641288802	2.221046828148	-0.182107599492

Table S19. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.049 eV of energy (T_1: -1374.101716, S_0: -1374.101716 hartree), of *fac*-[Re^{I}(bpy)$(CO)_3$Cl].

Atom	*x*	*y*	*z*
C	-3.474651667419	-0.223042440084	1.526141727362
C	-3.374431602408	-0.235200364360	2.916100547077
C	-2.314750463505	-0.159081803020	0.748655156624
H	-4.276056134856	-0.284771787725	3.527985305843
C	-2.112474475598	-0.184128168791	3.508388931303
N	-1.083240637495	-0.110346649969	1.335210772156
H	-1.985375192791	-0.191484625117	4.590429329974
C	-0.994993690615	-0.122405344979	2.683969640381
H	0.009867836707	-0.078398744486	3.101028570547
H	-4.453610985114	-0.263477971390	1.053375301111
C	-2.325709625178	-0.142005507937	-0.727527021960
N	-1.103819505725	-0.094557354806	-1.319568701459
C	-3.499808455526	-0.174334830892	-1.489168034723
C	-1.028102786928	-0.086959356579	-2.663903740975
C	-3.414681390249	-0.160200749684	-2.879370969170
C	-2.155415678786	-0.117100341172	-3.479256023038
H	-4.473984200368	-0.208135211607	-1.005451249113

H	-0.026494008881	-0.053423174653	-3.091014879366
H	-4.321876749893	-0.183432472150	-3.484389145390
H	-2.037818611854	-0.106581950708	-4.562698575478
Re	0.656239698687	0.004546458229	0.030399255627
C	2.135597388580	0.063074346533	1.306396460644
C	0.733685441891	-2.048017083635	-0.419712063145
C	2.208560095941	0.114697851311	-1.228673087098
Cl	0.401599341459	2.543495152425	-0.507798057825
O	0.525671243160	-2.857904719048	0.476911087082
O	3.030370318417	0.091648426729	2.039125209279
O	3.118877576814	0.178258962300	-1.925149998744

Table S20. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.063 eV of energy (T_1: -1374.101175, S_0: -1374.101175 hartree), of *fac*-[Re^{I}(bpy)$(CO)_3$Cl].

Atom	*x*	*y*	*z*
C	-3.278364052087	-0.281267017390	1.110554223803
C	-3.426418856079	-0.274026517025	2.496424152331
C	-1.996837000190	-0.391999830740	0.556581856077
H	-4.419544271604	-0.187227820305	2.939421890368
C	-2.292754191338	-0.380232362926	3.303261531011
N	-0.903653202033	-0.486619101660	1.348576307238

H	-2.360878310248	-0.384177918348	4.391022715433
C	-1.049288160249	-0.488077176454	2.686199899165
H	-0.133834340914	-0.577898876203	3.272327461667
H	-4.154834686868	-0.193235633578	0.471491863039
C	-1.732055209243	-0.405928730757	-0.898896840246
N	-0.423707816513	-0.419857592265	-1.267423556851
C	-2.759322131062	-0.406842644116	-1.850007677749
C	-0.129040750393	-0.416625814149	-2.580411226083
C	-2.442276382129	-0.402213597471	-3.206426375100
C	-1.099413373519	-0.402130984612	-3.579394438164
H	-3.801332096596	-0.415469136316	-1.536483726122
H	0.932353959273	-0.445367129598	-2.828233742999
H	-3.234470406361	-0.400642669827	-3.956435634029
H	-0.794720286390	-0.396897009679	-4.625990909517
Re	1.196824345640	-0.341255505507	0.364008533350
C	2.559025961411	-0.238362892532	1.747794691679
C	1.295136097122	-2.264792244671	0.806094586016
C	2.510047443126	-0.866445512439	-1.191013649712
Cl	1.042400010263	2.078818409455	0.048428451732
O	1.390732835445	-3.373758044574	1.108250400642
O	3.374833965188	-0.211981980925	2.568739287991
O	3.531907531053	-0.258080291550	-1.428265388182

Table S21. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.114 eV of energy (T_1: -1374.099318, S_0: -1374.099318 hartree), of *fac*-[Re^{I}(bpy)$(CO)_3$Cl].

Atom	*x*	*y*	*z*
C	-2.616322357484	0.220998503726	2.096579059075
C	-2.273342588270	-0.003868410416	3.429793787898
C	-1.769600457014	-0.265714549106	1.087265605933
H	-2.913394283582	0.370051216715	4.230829255013
C	-1.101521445304	-0.705358312832	3.721546767036
N	-0.628838447508	-0.915533221432	1.375993892008
H	-0.801526421136	-0.911207010544	4.749808213640
C	-0.305004763657	-1.130916188934	2.656856799287
H	0.634961518362	-1.660994234100	2.834080767067
H	-3.516499975915	0.782445500607	1.847707020474
C	-2.105215375806	-0.121896511130	-0.354753041154
N	-1.096920670333	-0.060778212020	-1.269472119869
C	-3.449330573797	-0.102111097065	-0.753824089996
C	-1.433885636828	0.003540128118	-2.578124814738
C	-3.780316413109	-0.026834699525	-2.103646606930
C	-2.746589087243	0.021825165228	-3.037109441850
H	-4.233406109398	-0.178152252373	-0.001896698896
H	-0.602486464175	0.053118628744	-3.279161518675

H	-4.825357637545	-0.022156550210	-2.417277363639
H	-2.940088305961	0.070161629241	-4.108736402673
Re	1.152580408793	-0.121965290494	-0.845954119415
C	1.325787814310	1.064970339696	0.727353221940
C	1.161490951369	-2.077873236880	-0.632211082305
C	3.082436905293	-0.238071270843	-0.764744979471
Cl	1.389690786836	1.665864377212	-2.594493653292
O	1.185747261007	-3.219106400496	-0.408868167017
O	1.512699075259	1.647518528815	1.711681935094
O	4.240178433575	-0.308363042779	-0.735034294335

Table S22. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.230 eV of energy (T_1: -1374.095056, S_0: -1374.095056 hartree), of *fac*-[Re^I(bpy)$(CO)_3$Cl].

Atom	*x*	*y*	*z*
C	-2.954674657331	-0.573093227335	1.078983130443
C	-2.953375396295	-0.697171300350	2.466899325107
C	-1.785456649781	-0.159773232730	0.424034544517
H	-3.857442090093	-1.017022691887	2.987134447711
C	-1.786094934174	-0.408767810420	3.175422499544
N	-0.660620145752	0.116947980481	1.121161594067
H	-1.739724667807	-0.492237392244	4.261327661171

C	-0.661380107842	-0.006815921890	2.458446858587
H	0.275788168063	0.230042627466	2.964882964560
H	-3.861210489143	-0.796083337833	0.519985750872
C	-1.698194744018	0.001179366016	-1.048407494279
N	-0.505054029260	0.419216009248	-1.556618372957
C	-2.785009855811	-0.264945718311	-1.891324961376
C	-0.388300702299	0.569662429007	-2.892557467062
C	-2.653952167101	-0.105552028744	-3.268206405179
C	-1.429125783217	0.318913741378	-3.780770163138
H	-3.734170956880	-0.596991901192	-1.476493961936
H	0.583335208981	0.899698732698	-3.256429487110
H	-3.498287253066	-0.311179091678	-3.927542212659
H	-1.270145702930	0.458444298556	-4.849911465187
Re	1.207659921047	0.893450102078	-0.167258853100
C	2.674655427387	1.376203894474	0.996400347190
C	1.820634101822	-0.957818435842	0.167528663899
C	2.425568373585	1.637535908948	-1.698659734119
Cl	0.123481820942	3.062697775157	0.250669275530
O	2.204013373797	-2.019524339548	0.396703618469
O	3.556969350684	1.670371468266	1.689110199211
O	2.965353402712	0.788905205459	-2.384949035532

Table S23. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.402 eV of energy (T_1: -1374.088721, S_0: -1374.088721 hartree), of *fac*-[Re^{I}(bpy)$(CO)_3$Cl].

Atom	*x*	*y*	*z*
C	-3.380224598257	-0.357331739903	1.584467946686
C	-3.293365210984	-0.406050337244	2.973706188462
C	-2.229378003738	-0.129679124541	0.822691714339
H	-4.186911445891	-0.584054535716	3.573207683476
C	-2.048069312324	-0.224351269891	3.578795055974
N	-1.012319246990	0.047995588627	1.420644326809
H	-1.928010302835	-0.251816379336	4.661632923113
C	-0.939421198969	-0.001978100781	2.772104924650
H	0.048219495202	0.146426999682	3.205403897956
H	-4.342326998599	-0.500349072773	1.096572030953
C	-2.237812762909	-0.063948182122	-0.652521975066
N	-1.022090498481	0.102317339093	-1.239167133851
C	-3.404267191268	-0.153696668661	-1.421977136867
C	-0.948155267387	0.189669883748	-2.582374226657
C	-3.319409330623	-0.074020644149	-2.809894652684
C	-2.068064363073	0.101642634811	-3.402917146531
H	-4.373605287799	-0.280024295812	-0.943985394779
H	0.047814007342	0.334756549471	-2.999544492650
H	-4.221814578325	-0.144296125244	-3.418569866569

H	-1.951838145969	0.172991281069	-4.484190244446
Re	0.721270948815	0.273845707394	0.112759051413
C	2.053162591331	0.629473368479	1.469390674624
C	1.251055752617	-1.662004690088	-0.022862809352
C	2.114500852246	-0.565839459147	-1.101115663242
Cl	0.795862354693	2.640229995180	-0.671784155535
O	1.316190344514	-2.840564958999	0.134083160887
O	2.827787474828	0.874562327890	2.300135171216
O	2.953688265042	-0.767453394714	-1.920144168653

Table S24. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.735 eV of energy (T_1: -1374.076475, S_0: -1374.076475 hartree), of *fac*-[Re^{I}(bpy)$(CO)_3$Cl].

Atom	*x*	*y*	*z*
C	-3.189203696215	-0.234191407928	1.565729188240
C	-3.180461126583	-0.042463653951	2.933588971894
C	-1.995884776582	-0.062709515403	0.815531489569
H	-4.097331391454	-0.183669179105	3.509091480904
C	-1.980811441347	0.316963941762	3.580399488922
N	-0.830955185314	0.281131586632	1.467123624801
H	-1.932198137199	0.473461116400	4.657412994374
C	-0.841140653201	0.460539225152	2.806846256707

H	0.112899345415	0.737862040492	3.256389173113
H	-4.103734168556	-0.539996153699	1.059235184968
C	-1.920760339707	-0.209943727131	-0.609430912709
N	-0.594926778552	-0.321380733067	-1.183678320151
C	-3.025556461438	-0.130203294241	-1.476449647398
C	-0.482354775682	-0.288208020905	-2.597909356757
C	-2.890208962394	-0.131962998733	-2.852357049665
C	-1.564709977139	-0.205055336360	-3.408907565835
H	-4.015440378812	-0.017763655063	-1.031594487372
H	0.534347511443	-0.369991748610	-2.979591898226
H	-3.762401948051	-0.051129895044	-3.499932741501
H	-1.410203764625	-0.199189565421	-4.488962782812
Re	0.953444478774	0.448808153222	0.168353569822
C	2.284814780511	-0.280508667378	1.430601319247
C	0.538819079388	-1.427795323791	-0.389768258275
C	2.368601091464	0.715807598946	-1.149511716787
Cl	1.227323399027	2.733328020949	1.037582725920
O	0.459761178562	-2.589449223926	-0.542236743966
O	3.033662471639	-0.781274913937	2.141378841238
O	3.197517246343	0.887755610926	-1.935161829791

Table S25. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.779 eV of energy (T_1: -1374.074867, S_0: -1374.074867 hartree), of *fac*-[Re^{I}(bpy)$(CO)_3$Cl].

Atom	*x*	*y*	*z*
C	-3.157170096025	-0.147284245067	1.599162082908
C	-3.156874531486	0.044170648568	2.965954663071
C	-1.952503009619	-0.009137294111	0.856398688544
H	-4.084916890603	-0.064072596649	3.530475327023
C	-1.954808426830	0.373652376733	3.624866093642
N	-0.783405149268	0.289264567688	1.523896174113
H	-1.913829670993	0.537133776078	4.701099328469
C	-0.803680593820	0.476207166289	2.862622050014
H	0.155115045759	0.720478643451	3.322992635892
H	-4.080827426630	-0.409737714151	1.085807694443
C	-1.872164742792	-0.155602868733	-0.565997607856
N	-0.546936074076	-0.120419001060	-1.147496732316
C	-2.975624172789	-0.304901554584	-1.429670980852
C	-0.447354569266	0.000328036068	-2.559397756752
C	-2.840682386239	-0.309248587205	-2.803689147386
C	-1.530149715569	-0.111128545873	-3.365108031999
H	-3.969827236766	-0.379724576042	-0.988290281891
H	0.560884209458	0.148107565673	-2.942073756502
H	-3.710713290895	-0.419220908385	-3.449835640668
H	-1.390424612440	-0.030769561951	-4.444156434759
Re	1.026371002343	0.405333644522	0.267888515485

C	2.224484520521	-0.648257492011	1.450796488036
C	0.503240052562	-1.347157746673	-0.491570741606
C	2.484567598784	0.658821935649	-1.008213701643
Cl	0.503747993141	2.797883409434	0.137604894722
O	0.396658808309	-2.489154478284	-0.758688134491
O	2.883033213028	-1.342132231697	2.087458420082
O	3.326696771889	0.825337913119	-1.779063109228

Table S26. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.896 eV of energy (T_1: -1374.070564, S_0: -1374.070564 hartree), of *fac*-[Re^I(bpy)$(CO)_3$Cl].

Atom	*x*	*y*	*z*
C	-3.231470059707	-0.355116097621	1.091706316038
C	-3.292113142068	0.285852675481	2.320723174358
C	-1.977307098155	-0.544809828944	0.468939858518
H	-4.255175636461	0.459714545756	2.803807999570
C	-2.101983184857	0.701281710595	2.934195258932
N	-0.808781796376	-0.160226948123	1.095324254400
H	-2.101707055592	1.194558345826	3.906003273651
C	-0.891188106529	0.448846117539	2.288935436613
H	0.054681713459	0.735560003616	2.749939664925
H	-4.134699447985	-0.707812027860	0.593153763040

C	-1.768436763974	-1.271424690850	-0.747659454153
N	-0.526470458641	-0.831827435450	-1.433508337173
C	-2.839249365298	-1.765534005098	-1.652050678699
C	-0.863149728493	0.022022199970	-2.354318796766
C	-3.218322545668	-0.810120392209	-2.580041292799
C	-2.244043476546	0.181075723254	-2.838775739439
H	-3.133492069520	-2.816435866122	-1.715230912315
H	-0.073844190619	0.621219383464	-2.816902838717
H	-4.072148414928	-0.923590682575	-3.253687118393
H	-2.415104626399	0.949778472549	-3.594377806371
Re	1.115585333102	-0.728720219320	0.022000186402
C	2.326953751983	-0.417062162393	1.504295418487
C	0.940363303950	-2.579673163587	0.518712994109
C	2.614548892458	-1.139286692565	-1.129107377492
Cl	1.241830426348	1.758678956933	-0.574649462862
O	0.852831311451	-3.697578629088	0.833348933537
O	3.044019625943	-0.215013194906	2.394280298495
O	3.498929250510	-1.371214009024	-1.844568390215

Table S27. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 4.209 eV of energy (T_1: -1374.059056, S_0: -1374.059056 hartree), of *fac*-[Re^I(bpy)$(CO)_3$Cl].

Atom	*x*	*y*	*z*
C	-2.502876834091	0.253535286519	2.042104531577
C	-2.164926365443	0.009518995653	3.361607481331
C	-1.645066613899	-0.097887473159	0.977952726939
H	-2.840255936138	0.290752322469	4.169515152912
C	-0.928117049545	-0.671117413687	3.644231164653
N	-0.299527402710	-0.503242834955	1.304687611715
H	-0.699312138945	-1.017318922510	4.653782187398
C	-0.050950232259	-0.918623943469	2.642743414635
H	0.910462385486	-1.411577900880	2.796680238707
H	-3.472075392140	0.699718279453	1.814924376205
C	-2.054318391132	-0.092928391763	-0.406417913097
N	-1.107831592651	-0.171297790135	-1.404929480173
C	-3.426999472952	-0.003380532218	-0.765972635734
C	-1.510140064316	-0.154888307255	-2.698808692216
C	-3.813839794522	0.015286249200	-2.092078254007
C	-2.833356278089	-0.063619786441	-3.095523882353
H	-4.183338524080	0.013545457262	0.016137068247
H	-0.718182798668	-0.221302460947	-3.446793214180
H	-4.872862880663	0.070461299510	-2.351222808642
H	-3.085716165311	-0.063902519026	-4.155335656151
Re	1.086292438530	-0.215506515704	-0.993421022812
C	0.793955250347	0.512523616337	0.845647727916

C	1.196533709135	-2.162227777236	-0.562972255281
C	3.000970110055	-0.188949838657	-0.588944636683
Cl	1.167773817946	1.978815084662	-2.057201920260
O	1.308752686233	-3.280009565102	-0.323482520275
O	1.170246961778	1.395655990138	1.564607976502
O	4.120632708990	-0.172437081089	-0.307328836723

Table S28. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 4.327 eV of energy (T_1: -1374.054738, S_0: -1374.054738 hartree), of *fac*-[Re^I(bpy)$(CO)_3$Cl].

Atom	*x*	*y*	*z*
C	-3.096468846171	-1.005964292586	1.614816218852
C	-3.071874842610	-0.805588878696	2.986318392519
C	-1.944665977089	-0.480467568945	0.866327849710
H	-3.823476374572	-1.192149927752	3.672263821405
C	-1.996406207344	-0.000418116757	3.370560177468
N	-0.632456073898	-0.642522561805	1.396086819780
H	-1.872301679021	0.425943292388	4.368116993036
C	-1.016852814277	0.307482355038	2.340361056240
H	-0.427958955871	1.232401145728	2.382200922939
H	-3.902948626844	-1.521500330796	1.090592010347
C	-2.019941510747	-0.049397882242	-0.521962436397

N	-0.829389377065	0.006246742735	-1.195912279382
C	-3.235060084221	0.258107750427	-1.158082614501
C	-0.842267090362	0.374216416970	-2.490406054378
C	-3.231335005356	0.629705833328	-2.498497086718
C	-2.012025520354	0.690840990996	-3.178641781913
H	-4.166763043132	0.217612552126	-0.594402192126
H	0.124935967425	0.409244982799	-2.991204046286
H	-4.166307528479	0.874389342000	-3.004679673249
H	-1.956675205072	0.978830640004	-4.228348300008
Re	1.000955247208	-0.536446237572	-0.025665450360
C	2.420767581060	-0.918019299335	1.238218051831
C	0.823987376745	-2.404347510503	-0.447247120596
C	2.312067929728	-0.307551223057	-1.448978309591
Cl	1.142852382053	1.982554090204	0.469454213034
O	0.721743922507	-3.534071690279	-0.710237073746
O	3.248905548712	-1.135180097990	2.021959449848
O	3.078139095487	-0.148383798013	-2.306190828558

Table S29. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.304 eV of energy (T_1: -1600.506621, S_0: -1600.506622 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*

Re	-0.200629395287	-1.385017374091	-1.118220097061
P	1.856959130269	0.934274487478	2.143459219662
N	-1.331339948963	-0.790055551289	0.597620085748
N	-1.229944892009	0.426204135112	-1.764976835306
C	-1.341584990334	-1.474885596457	1.777420963183
C	-1.116777860794	0.969634032140	-3.004578495315
C	-2.087948915722	-1.050834786640	2.869601699513
C	-1.783998916300	2.139041749438	-3.357699954523
C	-2.853062151374	0.114821664861	2.757400543830
C	-2.592742579424	2.770356585985	-2.407189216851
C	-2.849172700814	0.818646902137	1.552015344204
C	-2.711462105067	2.212734004308	-1.133170781145
C	-2.082388983042	0.360657287968	0.476847848481
C	-2.021352970091	1.034451711614	-0.825959937000
H	-0.740930968664	-2.369963836319	1.825403495684
H	-0.482462081902	0.448387687833	-3.708097378585
H	-2.064834799007	-1.625645860757	3.785855491677
H	-1.668561220342	2.540541402256	-4.355825908526
H	-3.443410333975	0.470961036623	3.592185416547
H	-3.124566577678	3.681312653215	-2.652463175472
H	-3.440310589032	1.718251824864	1.454847777547
H	-3.335614511422	2.693172950525	-0.392804467179
O	3.364305717957	1.650899240536	2.102466041684

C	4.450891294353	1.070856451702	1.300159604032
H	5.352362811636	1.624902607002	1.558557963086
H	4.241311994722	1.181786878158	0.232827462684
H	4.587790275302	0.011722583077	1.540727742939
O	1.174374832764	1.532993199875	0.752694717296
C	1.268781286904	2.912233863955	0.230404947406
H	2.242857355729	3.344265975789	0.467755821620
H	0.467959204459	3.517942467280	0.660607129335
H	1.141367646631	2.844914956388	-0.849439831924
O	1.240810299154	1.835132439968	3.367140498334
C	1.546975253474	3.232118660812	3.735512548718
H	2.624015897094	3.399167479685	3.708515471308
H	1.164953919318	3.366246074493	4.746795334830
H	1.039847092775	3.918822681002	3.053798302132
C	-1.134737276645	-2.568453905801	-2.394639635558
O	-1.595576200607	-3.269479267152	-3.223200176851
C	1.588948269337	-0.655067375074	-1.530819947583
O	2.647556211246	-0.266735542910	-1.876788481479
C	0.628694896112	-2.933380323751	-0.288737826056
O	1.119860222975	-3.864178106617	0.247543711096

Table S30. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.339 eV of energy (T_1:

-1600.505334, S_0: -1600.505334 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.960294677454	-0.586352461496	0.180588684317
P	1.963197831015	1.334256767488	1.304364295139
N	-0.981350505788	-0.285277243156	1.140725338797
N	-0.119109340327	0.690401686358	-1.177833177160
C	-1.336108325879	-0.826256789874	2.336100950824
C	0.390308702203	1.149303514383	-2.358368297694
C	-2.589002068481	-0.610806740935	2.901147976578
C	-0.339197699784	1.970681021232	-3.207864444096
C	-3.512795604822	0.187817646198	2.216874130846
C	-1.637313885220	2.346417105382	-2.841157080222
C	-3.151966554535	0.748555103063	0.991867021917
C	-2.164993758514	1.882114031314	-1.636143114505
C	-1.877262526203	0.504636381010	0.464985569813
C	-1.400468610860	1.049028822049	-0.811856454512
H	-0.590559912605	-1.434670437893	2.828944446441
H	1.397102523164	0.843054534450	-2.599698986932
H	-2.831744395394	-1.062254684876	3.854307708408
H	0.104460938142	2.307883294965	-4.135563653214
H	-4.497152515399	0.370872745076	2.629620486670
H	-2.228296454718	2.988879941672	-3.481994237749

H	-3.857908207441	1.367052870674	0.455214772800
H	-3.165908377551	2.167684551848	-1.343863069617
O	2.975185544985	1.013269444080	2.537089168970
C	4.195314991919	0.178262112038	2.456247160985
H	4.596496946683	0.156295602181	3.466923531856
H	4.911406758911	0.635434791907	1.770962147196
H	3.937027284795	-0.830001994104	2.127099848350
O	2.797203472261	2.249128020313	0.257732360184
C	3.443407948503	3.560180190712	0.535956068511
H	4.036698253739	3.501876005537	1.449963013829
H	2.672215340476	4.327552969945	0.617590058769
H	4.084001532586	3.754873639883	-0.320897986717
O	0.901049430486	2.279767975177	2.062765401148
C	1.094953333256	3.162281550603	3.244283699961
H	1.746265967075	2.670610757682	3.965783977809
H	0.099708118840	3.313504608896	3.656013224842
H	1.521541546245	4.111391077398	2.917633957934
C	1.148850684630	-2.478060801311	0.691384306871
O	1.274975694705	-3.614186021112	1.014607067607
C	-1.100378819927	-2.959596586690	-1.883745927383
O	-1.994412608474	-2.276378784753	-2.152902776215
C	2.537928089281	-0.799073884542	-0.892518469151
O	3.489696376716	-0.927778433953	-1.597553013745

Table S31. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.453 eV of energy (T_1: -1600.501163, S_0: -1600.501163 hartree), of *fac*-$[Re^I(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.202041568366	-0.941901417993	-0.285824262826
P	1.576003688130	1.353804814053	0.387160744503
N	-1.427243837593	-0.795354039186	1.135190755509
N	-1.131683605921	0.712886613385	-1.033929300568
C	-1.492684463021	-1.569181696237	2.244191002169
C	-0.961234000110	1.370304492718	-2.197255480988
C	-2.463290775935	-1.395819016490	3.223192794769
C	-1.857504184329	2.331871595491	-2.653205531303
C	-3.410530132384	-0.387291355652	3.049979586455
C	-2.985606271808	2.616013031409	-1.882557987300
C	-3.360013123242	0.406090272121	1.904695600815
C	-3.176630140233	1.928079538268	-0.686516490579
C	-2.359213038584	0.188095597417	0.955727914328
C	-2.230492762691	0.980063906636	-0.281527158614
H	-0.737027578708	-2.347354082939	2.337068660549
H	-0.075757152396	1.109112051608	-2.775420976220
H	-2.466780469296	-2.044136508723	4.098674405495

H	-1.668006550480	2.839624608259	-3.598672792550
H	-4.184882073291	-0.215278213233	3.798650004842
H	-3.714629150358	3.358509235057	-2.209786846990
H	-4.091324258646	1.198235481180	1.760206926952
H	-4.061575254231	2.119814632816	-0.083162520812
O	2.785178510690	1.287967790579	1.512924049053
C	3.961648581598	0.474040661033	1.304677663743
H	4.583096970985	0.610668267943	2.198624943180
H	4.518447434196	0.805256461377	0.414850116637
H	3.694474753166	-0.589353208028	1.206624939312
O	2.185645870134	2.221501812898	-0.868989530670
C	2.819914614673	3.518462009710	-0.710712467508
H	3.510969289274	3.514959192590	0.144874127840
H	2.052544036581	4.295245172345	-0.579096493296
H	3.377669248785	3.702656857439	-1.637494035831
O	0.513101237309	2.294260282498	1.205803780568
C	0.836984392993	3.254782782517	2.244962836500
H	1.625488013302	2.864174281745	2.900357040641
H	-0.090819944697	3.402736359259	2.812376841190
H	1.152771406880	4.206883150372	1.794092064216
C	-0.810886466869	-1.884521270332	-1.878470102578
O	-1.617455656889	-2.777773243692	-1.704530549019
C	1.714158507070	-1.012980925197	-1.614825395643

O	2.570591043873	-1.096440912292	-2.372584875203
C	1.118579761248	-2.564734273018	0.330942192320
O	1.649775085287	-3.540801772212	0.639999777679

Table S32. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.504 eV of energy (T_1: -1600.499292, S_0: -1600.499292 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.648634173975	-0.982250847801	-0.002564219008
P	1.912451458815	0.933755868601	0.920303096901
N	-1.363504538372	-0.366786223550	1.311721954346
N	-0.753151074798	0.777531214308	-1.020386438013
C	-1.624117644330	-0.999586234698	2.477551540152
C	-0.380323180422	1.326277669932	-2.199617655705
C	-2.744976164895	-0.712684903665	3.254860172863
C	-1.103929970519	2.344125267737	-2.817467513247
C	-3.634272191712	0.268939375194	2.810761967479
C	-2.260192441630	2.818512778854	-2.192863792838
C	-3.370071364736	0.923805926809	1.608244460029
C	-2.648721837125	2.256341648791	-0.977258673090
C	-2.224223386878	0.588781004099	0.871020461660
C	-1.878660579216	1.231760664745	-0.406523726483

H	-0.913241493599	-1.750734560444	2.790893011238
H	0.520905204239	0.940559605025	-2.651602737481
H	-2.909116648023	-1.249187979027	4.180600429579
H	-0.762764200126	2.748789755768	-3.761736379579
H	-4.516896221904	0.520161157575	3.386384954340
H	-2.848512292093	3.610215077882	-2.640650844290
H	-4.052682794300	1.683009980493	1.253034592515
H	-3.539655801185	2.615550239209	-0.482287402140
O	3.252606044948	0.659741922528	1.806838271877
C	4.446518231206	-0.078127775522	1.335539597408
H	5.159193902601	-0.028810906291	2.155644359492
H	4.856444970026	0.402935109552	0.445447053368
H	4.187039776496	-1.117618986969	1.124232243039
O	2.391576586649	1.918103766308	-0.276356752817
C	3.100820898097	3.216045950725	-0.130860175209
H	3.855074865958	3.150597075256	0.655155247603
H	2.369818314968	3.994189385808	0.092981426895
H	3.571488425949	3.402495120064	-1.093552448165
O	1.056556909796	1.787501072135	1.979763469838
C	1.531164385680	2.669103433550	3.078616474067
H	2.385392973717	2.209523768443	3.574336162518
H	0.687004089373	2.759047974792	3.758320152350
H	1.796643587149	3.644241003237	2.668283588861

C	-0.491801539577	-2.411658585057	-0.716681426714
O	-1.203747152833	-3.245809301251	-1.139961404182
C	1.624694896787	-0.872419616091	-1.724461449368
O	2.440354757462	-1.085807301943	-2.557692166613
C	1.050457622585	-2.045309676475	1.628866108677
O	1.679415839332	-2.816047814128	2.283870914286

Table S33. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.508 eV of energy (T_1: -1600.499121, S_0: -1600.499121 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.172286867964	-0.543241374570	-0.759104190801
P	1.351408027816	1.330894480100	0.352152806642
N	-1.381661520131	-0.392296143203	0.809993920645
N	-1.320808408296	0.926856211923	-1.467079305603
C	-1.316830639238	-1.131313844358	1.944743561148
C	-1.201125105350	1.552125756510	-2.664848480503
C	-2.289872599292	-1.036924162353	2.936526979979
C	-2.136761046087	2.487106390177	-3.101058688532
C	-3.361397611471	-0.157175542215	2.750043601954
C	-3.229808862619	2.786516435938	-2.281240312943
C	-3.428340227267	0.600092149937	1.579200638364

C	-3.354204171286	2.140541156325	-1.050394851219
C	-2.423128671379	0.470226628625	0.613872637464
C	-2.387252038195	1.209176077281	-0.655659282606
H	-0.471238388017	-1.799757584840	2.035358656291
H	-0.341416553292	1.287175266910	-3.265053049842
H	-2.205907400945	-1.642657590091	3.829425248710
H	-2.006152997528	2.965051003686	-4.063157075807
H	-4.134629912597	-0.063190557985	3.502557014952
H	-3.973736917781	3.508816751180	-2.593889456076
H	-4.254928560477	1.279612603284	1.423402678271
H	-4.194405108798	2.361429713203	-0.406436367116
O	2.393029285844	1.061774849629	1.584912290473
C	3.560832675490	0.158599469358	1.516975658172
H	4.053441156192	0.244859921854	2.483146682889
H	4.236181416369	0.475532071851	0.719299773882
H	3.230453628107	-0.869152114332	1.353326129932
O	2.214755646078	2.179462981846	-0.735688929943
C	3.003639189189	3.410884916871	-0.477699277116
H	3.570566695108	3.310592447590	0.449521940398
H	2.326024014400	4.264790077367	-0.427536020980
H	3.677592818021	3.512729065313	-1.325498220741
O	0.339157602613	2.348664962412	1.091570623358
C	0.595929401821	3.293453925957	2.206211987118

H	1.306123545931	2.855097913313	2.906584880833
H	-0.369828057813	3.452448171132	2.681423975999
H	0.978472310698	4.231175195684	1.800425864849
C	-0.764922965849	-2.000728422086	-1.618730836484
O	-1.339105325137	-2.889368173621	-2.158538343120
C	1.847634427939	-1.190348299417	-1.561353083422
O	2.855489407563	-1.604646855917	-2.037613626099
C	1.638210966695	-3.957409462138	0.667697046069
O	1.160468156585	-3.806271095310	1.710074381588

Table S34. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.524 eV of energy (T_1: -1600.498537, S_0: -1600.498537 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	-0.025686482829	-1.297036800831	-0.624654528829
P	1.340758819182	0.635546777766	0.029226597591
N	-1.017486377194	0.074398178357	1.746284229748
N	-1.856423969191	-0.046001115687	-0.975007600719
C	-0.652219205667	-0.100481658523	3.035302487512
C	-2.185860627803	0.229561184332	-2.273004624658
C	-1.585271592006	-0.146987977137	4.073098219535
C	-3.288737068065	0.992714475467	-2.636940334044

C	-2.942942257814	-0.025526355294	3.758476499506
C	-4.107409640561	1.514867352307	-1.633995780322
C	-3.321864968435	0.160911682843	2.426500135243
C	-3.782294771813	1.248641286502	-0.305316054452
C	-2.329755515182	0.219748917989	1.434067565992
C	-2.662372090074	0.467332135859	0.014667096858
H	0.408515035524	-0.195403660382	3.223534211246
H	-1.538930782216	-0.177937101255	-3.033398777434
H	-1.254230696491	-0.281205706292	5.095355553280
H	-3.489569238484	1.170187794156	-3.685444129310
H	-3.696657952946	-0.079859706442	4.534997904980
H	-4.970127542343	2.122974812937	-1.876922149514
H	-4.369403105162	0.235953022843	2.164992842320
H	-4.379497832704	1.669092945094	0.492146277500
O	2.071191176892	0.722271324573	1.477039676251
C	3.092699073417	-0.218737586461	1.993751565282
H	3.447956784012	0.224800826100	2.921087689468
H	3.911053352787	-0.312523901097	1.278116851884
H	2.636598127049	-1.190746135438	2.189655123240
O	2.524467393195	0.725866541065	-1.075772269962
C	3.427772905935	1.893001688364	-1.276209434509
H	4.014957296195	2.064537631439	-0.372672917415
H	2.831013917235	2.771726077100	-1.522749537627

H	4.072444061787	1.616387885857	-2.106704694457
O	0.620633601930	2.066941078857	-0.036462626668
C	0.446215438402	3.102932659932	1.009669255392
H	1.328863951999	3.139562149977	1.646605851061
H	-0.442179333615	2.862474067620	1.592667401581
H	0.313726461085	4.037823573295	0.469159851091
C	0.127145964539	-1.854000972315	-2.524101371882
O	0.278225709751	-2.341972903985	-3.588331650661
C	1.600043946724	-2.347984025900	-0.406283658774
O	2.576810057998	-3.000177498236	-0.293571151435
C	-0.789494765902	-2.526245704415	0.705285839578
O	-1.280888176193	-3.353242394151	1.393349891029

Table S35. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.577 eV of energy (T_1: -1600.496615, S_0: -1600.496616 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.278199610749	-0.513788443966	-1.672971510159
P	0.539679173687	1.520952739923	3.435505099035
N	-0.694129667481	0.002335468436	0.227086389978
N	-1.470511748009	0.651798236263	-2.255424581542
C	-0.225342039066	-0.331788160239	1.417712954211

C	-1.798910551396	0.941456885502	-3.540959479916
C	-0.786911345648	0.158753048445	2.675769917744
C	-2.905617075001	1.717119512253	-3.869562660200
C	-2.113065880456	0.783575130616	2.529669305192
C	-3.708523516827	2.221176825848	-2.836041309730
C	-2.586588240937	1.116076372056	1.289115561336
C	-3.382332761357	1.931425233418	-1.516134832081
C	-1.854623546977	0.782838666283	0.114958329920
C	-2.255192439439	1.135219102838	-1.224919948304
H	0.653385974081	-0.960487917091	1.451826922542
H	-1.155356886437	0.536931635079	-4.308635695725
H	-0.713000054000	-0.587872433857	3.474563602632
H	-3.126786919429	1.922305053997	-4.908646010547
H	-2.690110301473	1.010468683933	3.418093532473
H	-4.574225104151	2.832501799478	-3.059748755331
H	-3.545190877598	1.608925907490	1.197207620077
H	-3.990505608834	2.323746489107	-0.713211306244
O	1.713200408036	0.363476731313	3.564502849499
C	3.143374997234	0.697882027375	3.750077444854
H	3.339700779874	0.881478008131	4.807909012344
H	3.414096815054	1.575375281877	3.156740465326
H	3.701761438953	-0.171661465751	3.408269621618
O	1.201117453035	1.245478012541	-1.319871992425

C	2.418711292349	1.800783908921	-1.870935037922
H	2.967652786657	2.299350314957	-1.066571073915
H	2.143634505702	2.551615005522	-2.622575712913
H	3.046385167571	1.034602396011	-2.336896642540
O	-0.061323947900	1.687778112187	4.944422787637
C	-0.206963636002	0.661192273282	6.001760392990
H	0.594226874579	-0.075259113779	5.925364759269
H	-1.183218900233	0.182479233770	5.902212515305
H	-0.146547914230	1.193017883992	6.949695500646
C	-0.818701232230	-2.166047080748	-1.823539558993
O	-1.467211634066	-3.140749305102	-1.908038813878
C	1.026400725048	-0.782298749316	-3.453511249418
O	1.462600139889	-0.939767449131	-4.537719497509
C	1.785334871394	-1.576448263797	-0.976642342091
O	2.676716856365	-2.217551877107	-0.557021970341

Table S36. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.606 eV of energy (T_1: -1600.495515, S_0: -1600.495515 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.121070227692	0.816042850829	0.084345082359
P	1.799973865842	1.360244173462	1.842581371022

N	-1.800065886780	1.396353577496	1.158923058358
N	-1.486109621442	0.419838840287	-1.325208905997
C	-1.882578393988	1.894019140493	2.417724578005
C	-1.234865201051	-0.064960597705	-2.569758377610
C	-3.105412777448	2.219861961095	3.003272302262
C	-2.261415336127	-0.320279991559	-3.473913189443
C	-4.280151019211	2.027486706879	2.273693359726
C	-3.581696017786	-0.070457056343	-3.088804617521
C	-4.196922233306	1.516903402039	0.977263570201
C	-3.835584097132	0.428840961756	-1.811061252860
C	-2.946458573167	1.206208050988	0.430194622778
C	-2.773457366113	0.672736037913	-0.931800690650
H	-0.947594056643	2.022320474749	2.945263673690
H	-0.194472860989	-0.238384466937	-2.813880620692
H	-3.125406195581	2.613916500091	4.011267752724
H	-2.022440232055	-0.705996032067	-4.456303617596
H	-5.245304657468	2.269169869865	2.701500181177
H	-4.401844425833	-0.259125093487	-3.770416592203
H	-5.100020759219	1.364823988032	0.403069960565
H	-4.853136227814	0.626369135303	-1.505537937208
O	2.768506511271	0.197783358754	2.410569395689
C	3.819896367276	-0.586155939655	1.724061128325
H	4.464379538579	-0.957938207261	2.518450811467

H	4.377503214722	0.048233423251	1.035152270946
H	3.355163768488	-1.412095040824	1.186532447317
O	2.773678350535	2.534446313443	1.315813253146
C	3.967233971546	3.107152389842	1.994326072098
H	4.481350904418	2.341643853703	2.577381632908
H	3.640532959154	3.928855408258	2.632340226711
H	4.609993023375	3.474081129892	1.197288697204
O	1.103761343189	1.828224495797	3.214786938962
C	1.662370760147	1.843990052760	4.593132075246
H	2.141926760150	0.888391796599	4.800506867222
H	0.806309353788	2.002889513813	5.244705000276
H	2.371733865723	2.667084539214	4.684434246678
C	-0.017264160459	-1.046271172414	0.774575027865
O	-0.090061753472	-2.145515265355	1.177316702157
C	0.323774424163	2.665198518693	-0.638715300534
O	0.456790318982	3.747436343812	-1.067140418679
C	1.994025938891	0.280382587118	-0.864170466652
O	1.898691287068	-0.124065402965	-2.030556470028

Table S37. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.891 eV of energy (T_1: -1600.485074, S_0: -1600.485074 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.361879674283	-0.966675435531	-0.158962411938
P	1.840246147133	0.634299686892	1.036723696257
N	-1.384205045660	-0.266229333361	1.002315200237
N	-0.473058757182	0.653118514599	-1.347213053745
C	-1.863114225604	-0.924814233352	2.093444521139
C	-0.238634725212	0.877038185641	-2.645513882864
C	-3.010328642848	-0.511751370338	2.760766685300
C	-0.933455765272	1.827295278476	-3.412693357737
C	-3.692513154588	0.615564543679	2.293163475762
C	-2.007699807367	2.542567230850	-2.824719692148
C	-3.201840160869	1.293366247118	1.174778398631
C	-2.282650304738	2.385224349129	-1.492662718243
C	-2.045367879597	0.835494047737	0.538533852517
C	-1.390455089258	1.560580860986	-0.621512675747
H	-1.306788455319	-1.792259186410	2.416559283216
H	0.502829770383	0.245584537177	-3.119060046115
H	-3.356422726468	-1.065156331807	3.623934649841
H	-0.683320804262	1.947344399294	-4.458438317934
H	-4.590777130929	0.963633017150	2.788566524852
H	-2.620724160507	3.194941065392	-3.435482715066
H	-3.717728026378	2.169654405754	0.808840889975
H	-3.093827136747	2.931877494630	-1.029200149334

O	3.424955026200	0.392479645229	0.936895346314
C	4.435242605753	1.004020266206	0.039239104961
H	5.396888855106	0.761695430314	0.485443400360
H	4.283257832466	2.081715127710	-0.000525177460
H	4.349957617271	0.559026355341	-0.952794504023
O	1.805287179041	2.239142320002	0.567911626389
C	0.782760348779	3.162477413267	0.794452625951
H	0.316519779639	3.165315043039	1.774675378008
H	-0.680164256657	2.315040386797	-0.104708794366
H	0.891146060876	4.065290930918	0.209857468154
O	1.562103443985	0.638413857025	2.619390586257
C	2.414160840150	1.266885510062	3.670116705093
H	3.388775555941	0.779831118309	3.673971249650
H	1.884928537088	1.094015188931	4.603539093819
H	2.514205169506	2.335069686086	3.473382115129
C	-0.797491918277	-2.255856642099	-1.089112286945
O	-1.478138378864	-3.039693150740	-1.640282055818
C	1.833826108821	-1.409400187024	-1.345796443243
O	2.717655261803	-1.666813409845	-2.088076519137
C	0.938905763393	-2.345974306756	1.091522322600
O	1.271466029680	-3.176272284578	1.863995873257

Table S38. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.913 eV of energy (T_1: -1600.484242, S_0: -1600.484242 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.076929859103	0.215659965253	0.715893426836
P	2.068924747888	1.551169886519	0.630020749529
N	-1.989751043484	-0.367627436332	1.221725617446
N	-1.244899712282	1.743379440549	-0.219019194660
C	-2.297576626399	-1.449658970942	1.986159897525
C	-0.792847298332	2.763863088314	-1.000008752494
C	-3.596307583339	-1.724305312411	2.403056832849
C	-1.652401995606	3.702379901819	-1.561098266691
C	-4.626258413058	-0.857847467417	2.027187958575
C	-3.026503793518	3.587646636093	-1.329551182515
C	-4.320316563895	0.252991814315	1.240254157927
C	-3.496905939454	2.535380065797	-0.543608705429
C	-2.998436763984	0.483438520191	0.842082475958
C	-2.592979065770	1.620940886634	0.009920554110
H	-1.479207049188	-2.098510610847	2.257291707787
H	0.272452786961	2.804157762012	-1.175171009782
H	-3.787484120527	-2.598985514818	3.011091049932
H	-1.247512448074	4.499359057722	-2.170991555778
H	-5.646765421587	-1.039464452236	2.340828203146

H	-3.721837316005	4.298527741770	-1.758553873942
H	-5.106777639291	0.932412697250	0.943731733328
H	-4.558536546845	2.428819477376	-0.371144985926
O	3.460645648348	0.955652740727	1.212410763926
C	4.073869169839	-0.349985768227	0.872768096504
H	4.869324128237	-0.491790123945	1.600688540914
H	4.482629506590	-0.305096073059	-0.137830361466
H	3.337178681639	-1.151326740277	0.953043043893
O	2.384026728049	2.123416008319	-0.845884392888
C	3.461779660141	3.098617955136	-1.173983719214
H	4.413332744996	2.738553880466	-0.781337820438
H	3.206198318140	4.067515385191	-0.745833994921
H	3.483130842698	3.142383672186	-2.260016770456
O	1.986509495302	2.928293847282	1.473006680516
C	2.011648122694	3.062465108996	2.947463520898
H	2.921727704298	2.606717273942	3.339394408100
H	1.123991157627	2.595015152720	3.378485069880
H	2.004415867205	4.132999201286	3.138830595322
C	0.305851992376	-2.077290997073	0.629394976290
O	1.213448522125	-2.843954553682	0.538689714804
C	0.624227422579	-0.244777887512	-1.130379714408
O	1.041293629280	-0.509737877487	-2.201848348645
C	0.902841991987	-0.378155656991	2.394563494142

O	1.395173596659	-0.803283728081	3.391242844380

Table S39. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 3.970 eV of energy (T_1: -1600.482172, S_0: -1600.482173 hartree), of *fac*-$[Re^I(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	-0.072680840640	-0.952527304785	-0.299000413062
P	1.734071326272	0.706457773711	0.126726537941
N	-1.132764085438	-0.110071619615	1.351999239055
N	-1.268304485335	0.722381719295	-1.124138082946
C	-0.905131815382	-0.368205701441	2.764390563267
C	-1.242899679345	1.116553235070	-2.420938688934
C	-2.150167544977	-0.580906084158	3.565506929170
C	-2.019302196596	2.177006286572	-2.886180145019
C	-3.115418673234	0.357125591831	3.314460679177
C	-2.850230434832	2.855870158228	-1.990988331458
C	-2.970581386370	1.204067175160	2.162161672185
C	-2.886314145376	2.449804734876	-0.654939419001
C	-2.033647687313	0.866738430507	1.136983333924
C	-2.089931984048	1.379196665403	-0.238519401063
H	-0.243382032653	0.405081578659	3.178842660296
H	-0.586375681566	0.570802418131	-3.082257950722

H	-2.244431666590	-1.365260442360	4.306633806004
H	-1.965534429052	2.459492608234	-3.929478329741
H	-4.034057789924	0.408021853226	3.888362249736
H	-3.460558795479	3.686109923277	-2.324024111201
H	-3.714619532629	1.966258813312	1.972820889895
H	-3.521861889092	2.965899929107	0.051853427140
O	3.215659766603	0.206020910396	0.584234987420
C	4.095280195723	-0.703905116838	-0.182549118476
H	5.035874820013	-0.725577772410	0.363182161591
H	4.249635736312	-0.317343076115	-1.191728238603
H	3.657608367442	-1.703141466748	-0.216933040479
O	1.980954905257	1.583987778062	-1.214280498116
C	2.931878417520	2.711101849479	-1.399308204642
H	3.876137080566	2.498991825786	-0.895045565418
H	2.477262970035	3.622729591169	-1.009221078925
H	3.084890781088	2.792442794206	-2.473116467044
O	1.397842804358	1.697262567044	1.351191084452
C	2.324349470004	2.531498379116	2.161665989770
H	3.212594579517	1.953020475289	2.413027071934
H	1.764027869203	2.794574591717	3.055849863417
H	2.588311593859	3.427664149435	1.599113541831
C	-1.532223209595	-2.224313393695	-0.670558561722
O	-2.392210399915	-2.990938538641	-0.902513944812

C	0.824489691690	-1.477653736121	-1.953755241727
O	1.341312383536	-1.775856460902	-2.973417900710
C	0.870089097024	-2.309860949028	0.721152369436
O	1.418422259603	-3.126381134514	1.376345832201

Table S40. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 4.051 eV of energy (T_1: -1600.479176, S_0: -1600.479176 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.321822223058	-1.143147518353	-0.789798749036
P	1.855864896941	0.432257362452	0.394166644195
N	-1.283802982286	-0.606865175496	0.621808950636
N	-0.745138164751	0.553078773311	-1.731971231755
C	-1.357032970808	-0.948420635040	1.942202662988
C	-0.412574881549	1.139475121171	-2.904877373462
C	-2.160234649132	-0.208535608047	2.890949334089
C	-1.185971514606	2.153331360763	-3.477252151096
C	-3.107941134445	0.655572978438	2.430036945112
C	-2.356713953413	2.572255098337	-2.830489575811
C	-3.413926449187	0.445653394261	0.981829595331
C	-2.722540274255	1.964784930543	-1.631533166885
C	-2.189442195638	0.305141087481	0.149456726520

C	-1.898569028406	0.963749691804	-1.082373323167
H	-0.634287018601	-1.672222087043	2.288726935787
H	0.489196047087	0.787820316388	-3.385290204144
H	-1.902794960220	-0.291033151804	3.940941968693
H	-0.873189263347	2.594347095873	-4.414611580367
H	-3.629163971727	1.373673815015	3.052150532859
H	-2.974681797354	3.351172564336	-3.259469772912
H	-4.125864857000	-0.376265663724	0.813445457176
H	-3.629973191091	2.243963200926	-1.110768543643
O	3.453887898147	0.222492072612	0.193189403685
C	4.189678480056	-1.050612939412	0.345277806704
H	4.046994626715	-1.453300479575	1.349728693872
H	5.235080745649	-0.794407274246	0.189052988534
H	3.865832177553	-1.769750988922	-0.408182214788
O	1.887592764920	2.006186617365	-0.005829603995
C	0.850082340390	3.013204062149	0.309843581962
H	0.332561266673	2.760909325316	1.237396054587
H	0.145755812197	3.073133685432	-0.519387730260
H	1.380044106273	3.957271320902	0.420504230001
O	1.576390423442	0.375888526985	1.990856889076
C	2.376740074314	1.058316247615	3.045595564440
H	3.248241917293	0.445410885455	3.277211717511
H	1.718108314743	1.131936892625	3.907939684621

H	2.682749177072	2.049792829363	2.708713498918
C	-0.890725600875	-2.383254996539	-1.722512931685
O	-1.596886787623	-3.138625601207	-2.281318135044
C	1.656081055159	-1.389989307580	-2.179632357741
O	2.449508620087	-1.525727328567	-3.045863456041
C	1.038293724400	-2.621160017706	0.244469367381
O	1.432351510531	-3.526950968249	0.894232525024

Table S41. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 4.326 eV of energy (T_1: -1600.469061, S_0: -1600.469061 hartree), of *fac*-$[Re^I(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	-0.385357549400	-1.129488937592	-0.799487586889
P	2.012067061644	1.183947465992	0.221142426975
N	-1.416392941831	-0.579913573542	0.988094185571
N	-1.911214112979	0.265166650752	-1.470557173173
C	-1.119693161481	-1.068716224370	2.235515651254
C	-2.078994062311	0.648685395732	-2.766947144111
C	-1.819556649826	-0.685718346713	3.367753811364
C	-3.052070527624	1.565242470878	-3.143953667445
C	-2.871514950403	0.236112523027	3.245581393466
C	-3.887891613465	2.113220825283	-2.160183470837

C	-3.184342532047	0.739377193132	1.984994221883
C	-3.719388980025	1.727316104080	-0.832304875815
C	-2.457170264541	0.327822782404	0.860108622031
C	-2.722986065598	0.798378046357	-0.497130940010
H	-0.304953693139	-1.774686626532	2.291519543237
H	-1.410255372040	0.202767934536	-3.490054668856
H	-1.546512867962	-1.102666141801	4.328612871169
H	-3.153087223198	1.841685440693	-4.185530357879
H	-3.434295347112	0.552044331346	4.115083818574
H	-4.656039898060	2.829158610443	-2.425475701620
H	-3.994160617440	1.447724342613	1.875482992743
H	-4.355714498907	2.146578132907	-0.065113091607
O	2.575370694976	0.255216922981	1.381541531211
C	3.837212698915	-0.545408246770	1.431308789175
H	4.131307430301	-0.544727609324	2.477516758787
H	4.599246545424	-0.074358125728	0.810781201909
H	3.605088332830	-1.551091547066	1.086632870835
O	3.164847064756	2.035199994641	-0.438497497830
C	3.936714269147	3.240849766048	-0.003598828812
H	4.404769355566	3.045868155567	0.960528979654
H	3.251544241856	4.086089558442	0.047131712964
H	4.683107989554	3.386659741963	-0.779286558071
O	0.908383682290	2.061314968975	0.926428955869

C	0.784746207593	2.539570889509	2.339127735925
H	1.251646753649	1.815292679443	3.004640356069
H	-0.283966231631	2.613022532906	2.519583340419
H	1.264703488919	3.514380727145	2.406818246112
C	-0.665115602375	-2.446624521340	-2.232266487767
O	-0.783628766056	-3.200552217485	-3.146586622550
C	1.098467212387	0.251075171737	-1.191415044362
O	1.475907940753	0.540391058536	-2.348318906821
C	0.846006623166	-2.360615485630	0.020287880132
O	1.586348715437	-3.126525687241	0.556699745369

Table S42. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 4.433 eV of energy (T_1: -1600.465142, S_0: -1600.465143 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.207119292253	-0.681820552554	-0.740731735664
P	1.455613177688	1.048757787086	0.533479854657
N	-1.388412701543	-0.513797228393	0.793376225203
N	-1.091837794488	0.957350093655	-1.443176452184
C	-1.682216406214	-1.392634571068	1.777505836303
C	-1.069821564142	1.564790335511	-2.639308666355
C	-2.783128983248	-1.233186029339	2.656199429462

C	-1.981330737374	2.588646638151	-2.972018550230
C	-3.508769436742	-0.068012708583	2.630326909093
C	-2.902841176957	3.040714988610	-2.021707752975
C	-3.167485371601	0.989556182918	1.666012736372
C	-3.083384618298	2.309142644648	-0.828582052873
C	-2.180439592025	0.587190806098	0.648836117850
C	-2.102022124721	1.330829571444	-0.556375014618
H	-1.041057254657	-2.260123532680	1.857221803933
H	-0.300574629231	1.262453359917	-3.336792673615
H	-2.988849288343	-2.015607586071	3.374245011146
H	-1.940131133326	3.017018429176	-3.967296617304
H	-4.285167943228	0.123627925673	3.362213578036
H	-3.522344459738	3.904054651251	-2.246359922318
H	-2.835510236051	1.881725193255	2.227098410553
H	-3.990307419937	1.476077845685	1.053375167485
O	2.753076579041	0.668293356449	1.443253532891
C	4.019918559015	0.088136283565	0.941124889254
H	4.730491256100	0.193517348706	1.757959131635
H	4.366833336514	0.636054093511	0.062909838506
H	3.872126666775	-0.966211230646	0.703211899706
O	1.984070173046	2.195839871060	-0.484202553673
C	2.731515366253	3.435922355953	-0.147524647390
H	3.449698691573	3.244093398304	0.651397988484

H	2.018397925468	4.206685538676	0.147596035542
H	3.247659162454	3.724758514192	-1.060390884772
O	0.524958089332	1.726939454932	1.660047101822
C	0.914841167413	2.545874900511	2.836973674781
H	1.816379166225	2.133212914130	3.288701225138
H	0.073053959802	2.484646170410	3.523012863798
H	1.073102304452	3.576698876792	2.517796541593
C	-0.855607642807	-1.987091540086	-1.758926772565
O	-1.478241130837	-2.771720572816	-2.375211102315
C	1.515152408817	-0.586147878265	-2.170118216685
O	2.297060661428	-0.511610700943	-3.052859267545
C	1.190133182523	-2.120603221272	0.115746128541
O	1.768639139443	-2.998781530479	0.657680509463

Table S43. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 4.508 eV of energy (T_1: -1600.462396, S_0: -1600.462396 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.498792166340	-0.806435381617	-0.328380485271
P	1.907407215661	0.965928225162	0.556296302342
N	-1.022490432720	-0.412440805050	1.213347725568
N	-0.802304165403	0.817729451674	-1.151410973481

C	-1.213269036063	-0.312234555745	2.515029105903
C	-0.513496287076	1.817127921603	-2.020367079099
C	-2.508508395112	-0.383185582560	3.091796285551
C	-1.486182942019	2.739241630711	-2.407238253997
C	-3.631409124277	-0.669378841378	2.271245155405
C	-2.779206861632	2.637106053182	-1.882979990860
C	-3.507357424239	-0.758036446950	0.904881520688
C	-3.078293040987	1.606099325540	-0.983138871138
C	-2.187774789143	-0.503337323861	0.267637869470
C	-2.070433651206	0.712861836137	-0.641944229936
H	-0.329576272660	-0.218573753696	3.135184779520
H	0.504200392698	1.871644211438	-2.378463450706
H	-2.613764380556	-0.287222896561	4.164178858495
H	-1.226784618898	3.524404640576	-3.105584486401
H	-4.597021638863	-0.832480729095	2.736014769879
H	-3.545183441967	3.348042448337	-2.168088249464
H	-4.350957671183	-0.999750005048	0.268568413918
H	-4.068288778722	1.500435391745	-0.558976838071
O	3.298244554577	0.549873401816	1.287670762586
C	4.470486469928	-0.105511146623	0.662973654020
H	5.283093944018	0.018384814286	1.375222905529
H	4.714763576335	0.378794880304	-0.284164868149
H	4.257597830979	-1.164416079898	0.510471206383

O	2.334678850831	1.990730095378	-0.623207458245
C	3.130545669925	3.242439425515	-0.497843970613
H	3.972419802693	3.090019900938	0.179164099552
H	2.477922634801	4.039244739287	-0.139225346617
H	3.485270303823	3.462603212224	-1.501924146655
O	1.201484340932	1.787195920757	1.741251365853
C	1.824044583671	2.595456943837	2.824799763342
H	2.686707843366	2.065192388992	3.226175182085
H	1.047510136245	2.706456177820	3.577784698045
H	2.113060526984	3.568381102397	2.426208158675
C	-1.458505737420	-1.616792496729	-0.608541279313
O	-1.935397599721	-2.597314205564	-1.161770224969
C	1.484504188620	-1.080208535216	-1.980750996397
O	2.045029078099	-1.227483979546	-3.011443704809
C	1.360376365663	-2.242495255472	0.658206965204
O	1.838473593228	-3.115936528753	1.293856895170

Table S44. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 4.558 eV of energy (T_1: -1600.460548, S_0: -1600.460548 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.852890378783	-0.509611720460	-0.119478404167

P	1.710567139489	1.761531840467	0.435857818940
N	-0.481423992910	-0.264210533958	1.547268626068
N	-0.914990929864	0.547283120174	-0.962432873468
C	-1.380907989826	-1.191747511034	2.112911819089
C	-1.076106435021	0.854747486827	-2.272074586934
C	-2.049766352138	-0.897833963945	3.374151832019
C	-2.193537587412	1.543772964312	-2.743621571248
C	-2.437114549293	0.431782966765	3.600487475115
C	-3.189468304532	1.929882129041	-1.837785351275
C	-2.275904249164	1.228413540079	2.479129943667
C	-3.041618129203	1.611394598151	-0.489315174723
C	-1.637251901752	0.583662140389	1.318398246962
C	-1.897317140139	0.915068567266	-0.061357938826
H	-1.423492554099	-2.195057940978	1.698815192833
H	-0.287612185097	0.544451988137	-2.942386270889
H	-2.236785790495	-1.706379123855	4.072147797027
H	-2.273863851059	1.770257806973	-3.798814900591
H	-2.842715263548	0.785688583451	4.537140018975
H	-4.068608943956	2.462814575522	-2.178843969425
H	-2.570009457514	2.270556308551	2.430920224098
H	-3.803172437529	1.883259353836	0.230326095611
O	3.097236459194	1.961734143841	1.269685697517
C	4.445909377517	1.550763994845	0.818706511282

H	5.140952222856	2.043364291123	1.495206711186
H	4.618078869011	1.879100244945	-0.208191302718
H	4.547417961782	0.467295500458	0.896983595331
O	1.928503517664	2.591440878871	-0.943234859409
C	2.327886038732	4.015912890521	-1.078682246571
H	3.117339627727	4.260499472804	-0.365813017664
H	1.451763409401	4.646156444678	-0.919158210478
H	2.691787899071	4.123013195585	-2.098121698811
O	0.709266635298	2.598201854012	1.380159463662
C	0.996268117030	3.743142831226	2.281510666185
H	1.949493022737	3.584308139848	2.784328842094
H	0.176401460204	3.760386071885	2.996214582619
H	1.012680565007	4.664117764271	1.697331123311
C	0.114813889632	-2.253458486977	-0.639236543544
O	-0.299896458543	-3.299630624761	-0.988145105305
C	1.961132099747	-0.509184432130	-1.726095604758
O	2.616504841316	-0.506757546363	-2.710087427338
C	2.244409282101	-1.385413513739	0.911619261194
O	3.058637422514	-1.925609972044	1.577633180916

Table S45. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 4.574 eV of energy (T_1: -1600.459946, S_0: -1600.459946 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.298823389819	-1.686277733647	-0.210091074709
P	0.433721546815	1.382185190567	0.900481351436
N	-1.429885682983	-1.239867003560	1.075684034528
N	-0.608211893835	0.013501475011	-1.096477062729
C	-1.989828336968	-2.112228715769	1.961118753998
C	-0.746879598020	0.359749000594	-2.380272304828
C	-3.142591490443	-1.798027893129	2.669766129167
C	-1.482280129581	1.479647564762	-2.805569824915
C	-3.750274700924	-0.552478678241	2.464360473637
C	-2.099866065885	2.359836746696	-1.859748453189
C	-3.173019316255	0.350287156102	1.570281490043
C	-1.980669479629	2.104362830019	-0.531864942734
C	-2.010865336398	-0.012715137906	0.884827018514
C	-1.230398271437	0.894274330331	-0.025136328944
H	-1.494001604383	-3.065441340151	2.077847867384
H	-0.275174911606	-0.287631390586	-3.109793863746
H	-3.557523901368	-2.518590658763	3.362540374946
H	-1.570331263751	1.667779923748	-3.868219670188
H	-4.659625661172	-0.289911761383	2.991192457595
H	-2.630310267407	3.235925394384	-2.211579529803
H	-3.622378801774	1.319505131455	1.405574385492

H	-2.393516346841	2.769854295223	0.216221940387
O	1.843068658402	1.198927910322	1.776137528277
C	3.075930325764	0.477074983260	1.421460529754
H	3.763896528471	0.680019908528	2.240633212161
H	3.487415655154	0.842822769787	0.479382442728
H	2.874358784631	-0.593376973843	1.355977024987
O	0.828078267967	2.467227417725	-0.227191068205
C	2.065590649093	3.271114012540	-0.360995827775
H	2.515546133597	3.454021943163	0.614378151798
H	1.753711909828	4.206199944394	-0.822351882881
H	2.755140027576	2.736154434104	-1.014671520322
O	-0.398246337321	2.047007914610	2.111908574406
C	0.099350402406	2.582328326106	3.400054059060
H	0.617803053017	1.796939019096	3.947678219817
H	-0.794030368906	2.906075654479	3.929961390884
H	0.767374346582	3.424427222787	3.216445037808
C	-0.552122223367	-3.095497660984	-1.161552296046
O	-1.103793136533	-3.947658920806	-1.776882622038
C	1.826979699518	-1.751067710308	-1.406722637669
O	2.747209326891	-1.761955433090	-2.151599721835
C	1.133741553037	-2.987815124979	0.977869821883
O	1.626443485653	-3.758683843720	1.729926003166

Table S46. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 4.842 eV of energy (T_1: -1600.450103, S_0: -1600.450103 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.034619935693	-1.022889486536	-0.505598678869
P	1.543423942225	0.664695848745	0.532018693993
N	-1.416563789850	-0.616060948189	1.017042190073
N	-1.129131476691	0.723189299158	-1.237224400240
C	-1.605485150254	-1.282261483102	2.272386134857
C	-0.925578393531	1.348369635009	-2.424509506696
C	-1.580563679425	-0.526368064099	3.505757987491
C	-1.687179695478	2.445321001748	-2.821453132816
C	-2.950764142420	-0.320168483016	2.987580007321
C	-2.691200875040	2.921841764117	-1.971140819043
C	-3.206903440627	0.560731315482	1.869822023485
C	-2.906293903135	2.285020171369	-0.748492482966
C	-2.265676879512	0.425630066808	0.833504354373
C	-2.118861048756	1.182592439140	-0.399486481497
H	-1.528685452873	-2.364378926441	2.254954104749
H	-0.138780223381	0.956145049928	-3.052253578933
H	-1.368196747052	-0.941609677115	4.482086786659
H	-1.490296861509	2.913484660666	-3.777105651695

H	-3.782621722035	-0.669359749585	3.592606488017
H	-3.294466756415	3.775529929522	-2.254595998539
H	-4.078553170938	1.200176657207	1.833045626178
H	-3.671309031555	2.639518695457	-0.069981012148
O	2.770216158775	0.221425188287	1.508204126161
C	3.949678688296	-0.581027094425	1.110378961302
H	4.666867361065	-0.462887991059	1.919767448549
H	4.366310572725	-0.203786482894	0.174497106538
H	3.664172144241	-1.628801583502	1.008695381751
O	2.237698634457	1.537900990450	-0.647538504945
C	3.115752420003	2.725755681104	-0.487038299315
H	3.852625945110	2.550685367709	0.298592310089
H	2.498624794346	3.594848962331	-0.254449253084
H	3.608882792830	2.856329719593	-1.447624259493
O	0.757113265606	1.662450338066	1.518605095353
C	1.284006936326	2.523015638024	2.609529334932
H	2.109658816417	2.018598246599	3.110222496445
H	0.448544656941	2.671815405545	3.289897886559
H	1.606707179302	3.474505271333	2.185422240430
C	-1.198874621106	-2.283434470279	-1.384836148260
O	-1.921997550974	-3.038559758507	-1.921845182763
C	1.264813114629	-1.152561876278	-2.017648700486
O	1.993095428108	-1.218815556432	-2.944492323021

C	0.918352197727	-2.494442052985	0.399268304455
O	1.433338099663	-3.390747619795	0.973832283044

Table S47. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 4.886 eV of energy (T_1: -1600.448476, S_0: -1600.448476 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.708271713857	-0.093222153184	-1.296518938973
P	2.198069926780	1.621323505596	-0.232942410954
N	-1.042212403246	0.459335711044	2.378686588455
N	-0.942941748628	1.293611144334	-0.970505050421
C	-1.366344270991	-0.277947714628	3.426665071221
C	-1.199184309060	2.323450678784	-1.822715205979
C	-2.141838231440	-1.471297545148	3.375627670669
C	-2.250246920740	3.205562461448	-1.598866484677
C	-2.718341432825	-1.852260703776	2.143614418616
C	-3.057564918968	3.025319466308	-0.469006539934
C	-2.418153695228	-1.146155759385	1.001811523000
C	-2.788140234339	1.964689684361	0.399110437343
C	-1.383327023358	-0.057744349752	1.043420382201
C	-1.721591926135	1.106582621101	0.129136736668
H	-1.040224185196	0.101162483750	4.391109361800

H	-0.542155889816	2.420918849477	-2.677583550381
H	-2.345784575177	-2.020657845408	4.285962464644
H	-2.427010516745	4.015753528332	-2.294183252974
H	-3.421472745050	-2.677080402891	2.104364028114
H	-3.881541294427	3.699299520880	-0.268011102613
H	-2.871689699528	-1.388829880817	0.047079464758
H	-3.392223353732	1.798972563330	1.282006449597
O	3.110973892985	1.219997041436	1.047703989730
C	3.845666935418	-0.046836611094	1.264084030463
H	4.352292422579	0.075585490793	2.218923839457
H	4.577115672253	-0.197159872014	0.468031989596
H	3.139403023828	-0.876727604314	1.316699910520
O	3.177662861006	2.191546233172	-1.380574500112
C	4.134034476944	3.321747522462	-1.217764029865
H	4.875598331601	3.062326615024	-0.461095807579
H	3.584922120130	4.219186578924	-0.932112700224
H	4.601903305111	3.444675215547	-2.191256356092
O	1.503686245337	2.958254448174	0.343047226160
C	1.134011285734	3.259022187454	1.751901609407
H	2.035588923438	3.263337485019	2.363839536339
H	0.418854286717	2.516654353981	2.112817783127
H	0.684252239843	4.249057153432	1.717944932816
C	-0.480289689923	-1.361716331822	-2.219330541774

O	-1.173803080288	-2.132628326185	-2.774629980346
C	2.184593520979	-1.434261189644	-1.439721792111
O	3.018541701141	-2.254981231588	-1.510577442123
C	0.009134963555	-0.732271522430	0.492829922968
O	0.593230339601	-1.573991933964	1.193169604684

Table S48. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 5.185 eV of energy (T_1: -1600.437522, S_0: -1600.437522 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.458277211590	-0.511142832849	-0.114507611181
P	1.440929752756	1.742781028323	0.312868458743
N	-0.463518561520	-0.317010876615	1.706175221587
N	-1.289946651551	0.579471258580	-1.028838577107
C	-0.726497931328	-0.298894522584	2.951514283188
C	-1.104006629469	1.363011110649	-2.118607150942
C	-2.047971550250	-0.338684981851	3.590223490860
C	-2.100787250546	2.165078010101	-2.676579762651
C	-3.214068051644	-0.694394177821	2.999268363064
C	-3.371016427829	2.194293756260	-2.077230781868
C	-3.411390397086	-0.981102481934	1.571134264220
C	-3.606124349890	1.398499152346	-0.970608657790

C	-2.868585496761	-0.288581582071	0.592171260315
C	-2.571136959196	0.550012405075	-0.452382856679
H	0.124315254827	-0.293678442824	3.646552916025
H	-0.109370521187	1.370706371810	-2.539075614762
H	-2.034200165605	-0.169813205435	4.661587562800
H	-1.873574394109	2.760845334532	-3.550959382863
H	-4.087173714554	-0.841104671908	3.630968613378
H	-4.157232620778	2.823877804464	-2.475979264264
H	-4.061473202926	-1.829373175253	1.337443126291
H	-4.573410028735	1.378093282879	-0.485432473173
O	2.788330420035	1.912797913061	1.210762392654
C	4.144612879553	1.435605972942	0.854321564522
H	4.828628689200	2.013983353542	1.471797518732
H	4.344480015700	1.614003777290	-0.203970753678
H	4.229812667158	0.374071649681	1.088137164716
O	1.789842813382	2.450713516621	-1.105595094599
C	2.259523016815	3.843168255868	-1.328220118974
H	3.015735500079	4.112656975488	-0.589066608485
H	1.403691570243	4.517222234902	-1.273590083353
H	2.687011089261	3.851003197945	-2.328265909536
O	0.442511438940	2.691809065147	1.140997764239
C	0.746695129974	3.880121262166	1.980510347159
H	1.677580574682	3.718722688079	2.522624938044

H	-0.093039241078	3.970807389275	2.665776114593
H	0.815253212497	4.760437141536	1.340490864682
C	-0.413734614697	-2.248120232576	-0.453668765586
O	-0.916752257712	-3.287859406987	-0.664015383806
C	1.404537160599	-0.618153631602	-1.835842752473
O	2.001701692966	-0.689841139736	-2.848799446024
C	1.946833781698	-1.436149946749	0.742531489305
O	2.825836933868	-2.015926285720	1.271673196197

Table S49. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 5.241 eV of energy (T_1: -1600.435433, S_0: -1600.435433 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.052946691558	-0.550914189851	-1.047976289165
P	0.898237712305	1.171960357543	0.517673304221
N	-1.251271301750	-1.345810555514	0.502637303509
N	-1.765946339432	0.630273801797	-1.223324245298
C	-0.933610551687	-2.392908740296	1.327385582582
C	-1.978213529913	1.611485968343	-2.153418545665
C	-1.792205565032	-2.889398689386	2.296678208609
C	-3.152686376931	2.333233324268	-2.230570668789
C	-3.044890452631	-2.250653771284	2.377199698417

C	-4.192006686051	2.048004572577	-1.303942347965
C	-3.439926048293	-1.213764242406	1.589777361027
C	-4.004705175263	1.059732372804	-0.360786666878
C	-2.513472175731	-0.729268900448	0.608577707983
C	-2.784593607998	0.328515261015	-0.307579640884
H	0.047559717250	-2.829339026466	1.190456894145
H	-1.163873563172	1.800529680026	-2.839964776050
H	-1.496835967353	-3.715291974879	2.930108913695
H	-3.267297745288	3.098800372629	-2.987379699908
H	-0.695522808237	1.429355504981	2.446313913788
H	-5.123828492003	2.600664137259	-1.339930732528
H	-4.419347810286	-0.760330740516	1.683152337098
H	-4.791644619887	0.832760493104	0.347490029279
O	0.218486619596	1.105762847185	2.295883298938
C	0.768412919363	0.286627912168	3.438254614896
H	0.825704876054	0.948121259648	4.299571912535
H	1.753327254126	-0.039099718853	3.116893418291
H	0.098901253671	-0.555798903351	3.596436565961
O	2.421053064818	1.057099261492	0.931263998906
C	3.457215720977	1.975536988522	1.492711114871
H	3.054228041319	2.518934073063	2.346521661953
H	3.775353136176	2.649569564871	0.699064854277
H	4.270235949125	1.322940614931	1.798208615856

O	0.462353832779	2.663875982282	0.232332686428
C	0.721429331815	4.002097010425	0.842196176874
H	0.713984342554	3.918053740276	1.928530141845
H	-0.095506292575	4.629412101506	0.496642647048
H	1.677829424371	4.366838100216	0.470789864585
C	-0.619854422311	-1.874863981320	-2.315353896933
O	-1.025989063712	-2.672832601832	-3.077381311951
C	1.035369327875	0.341391426306	-2.477317575280
O	1.607065420746	0.888529047609	-3.358360674695
C	1.597578445993	-1.674227126012	-0.657433760419
O	2.523460876628	-2.368612982840	-0.407178151635

Table S50. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 5.365 eV of energy (T_1: -1600.430888, S_0: -1600.430888 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.244918599300	0.690411833410	-0.273759307520
P	1.895514594958	1.405613955437	1.372395268970
N	-1.323821438778	0.614971217145	1.319571586950
N	-1.167048391910	2.338612353588	-0.644398256834
C	-1.230955082570	-0.067828646956	2.491372861963
C	-0.790058871742	2.223344460706	-1.941905834847

C	-2.266811252363	-0.083044253237	3.419805579277
C	-1.525348169056	1.156227093582	-2.708902381771
C	-3.442723995416	0.631890837467	3.149246811354
C	-3.013624016758	1.373830295843	-2.517575533623
C	-3.550370455123	1.341968237592	1.954806591531
C	-3.444225925644	1.745359838259	-1.278797263474
C	-2.478280644917	1.330770584164	1.054592880501
C	-2.445148448292	1.950912303682	-0.254122299430
H	-0.313516544712	-0.609638875746	2.671114625663
H	-0.069073668842	2.910167257040	-2.364171881007
H	-2.153096607781	-0.648442696200	4.335604931323
H	-1.230263740345	1.065381861028	-3.755517859454
H	-4.257653454656	0.637947732005	3.862890182392
H	-3.690441713798	1.186453110231	-3.341839482689
H	-4.439038881618	1.914362803574	1.720942046166
H	-4.498346990673	1.815522291960	-1.035794054108
O	2.921340404885	0.356836242585	2.062998182078
C	4.002111019758	-0.406814671541	1.397740656806
H	4.572786896203	-0.858663898276	2.205578242606
H	4.632032201170	0.265857217652	0.813456281829
H	3.570302395556	-1.180879765480	0.761624022668
O	2.823739038946	2.542956641304	0.691917597964
C	3.845094030208	3.387841208697	1.372414756563

H	4.431296493342	2.786670380697	2.069252915493
H	3.337598068269	4.203372972275	1.888590603980
H	4.476748757389	3.773462549746	0.575831781352
O	1.190721661396	2.015617175243	2.676375318008
C	1.705853837454	2.154690323381	4.066855391823
H	2.372620705326	1.324248019317	4.294763508753
H	0.823709696969	2.135207419994	4.702593365632
H	2.222596147661	3.110819996236	4.152564439332
C	-0.998941160032	-0.182402156751	-1.946508861416
O	-1.269995671266	-1.304047437192	-2.332019210335
C	1.667630671037	0.880961505505	-1.593622556269
O	2.541788913054	1.000936844322	-2.374884853417
C	0.690548370826	-1.166020553278	0.044762763744
O	0.837685881043	-2.326221188816	0.185051348843

Table S51. Cartesian coordinates (in Å) of the T_1/S_0-MESX at 5.978 eV of energy (T_1: -1600.408369, S_0: -1600.408369 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	1.282623898210	-0.788452011195	-0.661530489109
P	2.072874631164	1.251208763183	0.555282135259
N	-2.116442826304	-0.965378288600	0.410746594752

N	-1.726102027341	0.381519849970	-2.018988539247
C	-2.377476276210	-1.706486146909	1.504738284271
C	-2.551705902021	-0.179754779301	-2.863303604934
C	-3.356761546039	-1.372989906650	2.449365580067
C	-3.974648469968	0.186974201105	-2.925486992170
C	-4.086233650536	-0.189605229393	2.255283501491
C	-4.406505612901	1.413614043975	-2.325092560273
C	-3.824905390837	0.600503073283	1.140087993712
C	-3.536556363525	1.996687016810	-1.430978120658
C	-2.841306740372	0.187736841214	0.196985108072
C	-2.501688822599	1.015629061489	-0.932348153421
H	-1.772636913621	-2.598938120102	1.627916233247
H	-2.149336775554	-0.815927963593	-3.647522119610
H	-3.525929728704	-2.007368295915	3.311007012765
H	-4.599894742926	-0.316203892950	-3.654531566397
H	-4.842732061969	0.113247058483	2.971239820876
H	-5.281396918812	1.923352745443	-2.716773910397
H	-4.359092860386	1.530921712167	0.989172345975
H	-3.554282604748	3.048213345082	-1.166053778765
O	3.309388962956	1.194571482094	1.603252501242
C	4.716660511698	0.844956710935	1.297297708360
H	5.289469920307	1.169644640311	2.162959725040
H	5.050999679611	1.371128846542	0.401335170888

H	4.805918179727	-0.234713627147	1.168857321149
O	2.467284703501	2.366003250804	-0.546352412753
C	2.873818695652	3.780282043429	-0.324224696173
H	3.582968076932	3.843548309092	0.502554901055
H	1.981984771534	4.374583305229	-0.121650676045
H	3.341531114227	4.098202613962	-1.252949589662
O	0.917657964080	1.817224561851	1.516410830223
C	1.035130467445	2.675310995117	2.726174636251
H	1.831532860092	2.295418889807	3.364705741301
H	0.069109151795	2.604414719948	3.219860078687
H	1.236369948396	3.703212063918	2.422363256898
C	0.482261917464	-2.301892758271	-1.668861569984
O	0.012199241323	-3.201957975321	-2.251133233284
C	3.023700189396	-1.277675617481	-1.232183077666
O	4.105113397620	-1.581956759298	-1.603209392326
C	1.528244366728	-1.911230539652	0.845217665519
O	1.665364950415	-2.603196144336	1.794036998809

Selectivity of CO position on the PLS reaction

Table S52. Cartesian coordinates (in Å) of the T_1 state transition state in which the equatorial CO is bent (T_1-TS(bent)) of *fac*-[Re^{I}(bpy)$(CO)_3P(OMe)_3]^+$. The electronic energy of the T_1

state is -1600.516284 hartree.

Atom	*x*	*y*	*z*
Re	0.328186000000	-0.451447000000	1.059688000000
P	1.592258000000	0.849569000000	-0.625236000000
N	-1.404447000000	1.157191000000	0.722146000000
N	-1.191261000000	-1.121309000000	-0.648909000000
C	-1.463975000000	2.278355000000	1.462610000000
C	-1.037595000000	-2.288785000000	-1.297766000000
C	-2.448998000000	3.246640000000	1.291666000000
C	-1.889115000000	-2.710061000000	-2.315220000000
C	-3.417116000000	3.042740000000	0.308458000000
C	-2.950354000000	-1.881781000000	-2.678940000000
C	-3.363255000000	1.881343000000	-0.458015000000
C	-3.117286000000	-0.672653000000	-2.008794000000
C	-2.342539000000	0.948473000000	-0.230159000000
C	-2.221963000000	-0.314156000000	-0.992457000000
H	-0.690271000000	2.399687000000	2.220992000000
H	-0.194706000000	-2.905975000000	-0.985022000000
H	-2.447667000000	4.136188000000	1.921526000000
H	-1.713899000000	-3.668274000000	-2.804352000000
H	-4.207422000000	3.775432000000	0.139376000000
H	-3.641803000000	-2.170246000000	-3.471790000000

H	-4.113864000000	1.705761000000	-1.225787000000
H	-3.940924000000	-0.014910000000	-2.278143000000
O	3.156416000000	0.515287000000	-1.024650000000
C	3.529610000000	-0.727669000000	-1.662134000000
H	4.521487000000	-0.558071000000	-2.100052000000
H	2.818908000000	-0.997813000000	-2.457674000000
H	3.588518000000	-1.536082000000	-0.919706000000
O	0.790538000000	0.864685000000	-2.057436000000
C	1.230385000000	1.608671000000	-3.221255000000
H	2.327557000000	1.638498000000	-3.284882000000
H	0.824047000000	2.629727000000	-3.179783000000
H	0.824880000000	1.085091000000	-4.096294000000
O	1.781999000000	2.387717000000	-0.104067000000
C	2.707112000000	3.362250000000	-0.652847000000
H	3.665877000000	2.890546000000	-0.903958000000
H	2.851574000000	4.112448000000	0.134714000000
H	2.270624000000	3.840097000000	-1.541557000000
C	-0.815794000000	-1.377281000000	2.381213000000
O	-1.498357000000	-1.905036000000	3.143368000000
C	1.343886000000	-2.133572000000	0.760290000000
O	2.138899000000	-2.974314000000	0.914517000000
C	1.115675000000	0.666261000000	2.490040000000
O	1.747104000000	1.128570000000	3.347462000000

Table S53. Cartesian coordinates (in Å) of the T_1 state equilibrium structure in which the equatorial CO is bent (T_1-min(bent)) of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$. The electronic energy of the T_1 state is -1600.517437 hartree.

Atom	*x*	*y*	*z*
Re	0.354529000000	-0.671018000000	-0.757763000000
P	1.477396000000	0.668993000000	0.983676000000
N	-1.479115000000	-0.999599000000	0.741880000000
N	-1.246425000000	1.096502000000	-0.890548000000
C	-1.540260000000	-2.079859000000	1.539634000000
C	-1.073482000000	2.122881000000	-1.742360000000
C	-2.584312000000	-2.306919000000	2.431860000000
C	-1.982029000000	3.170513000000	-1.860781000000
C	-3.614054000000	-1.369245000000	2.502358000000
C	-3.123426000000	3.154107000000	-1.059431000000
C	-3.558238000000	-0.249041000000	1.677171000000
C	-3.308693000000	2.093857000000	-0.176077000000
C	-2.476716000000	-0.087358000000	0.800838000000
C	-2.351364000000	1.072514000000	-0.109495000000
H	-0.715464000000	-2.788194000000	1.456874000000
H	-0.170408000000	2.099158000000	-2.352171000000

H	-2.578933000000	-3.202511000000	3.053106000000
H	-1.788940000000	3.975659000000	-2.569592000000
H	-4.451218000000	-1.505299000000	3.188372000000
H	-3.862525000000	3.954154000000	-1.119755000000
H	-4.353412000000	0.492338000000	1.718174000000
H	-4.194309000000	2.064915000000	0.455142000000
O	2.899197000000	0.167155000000	1.651034000000
C	4.061432000000	-0.076313000000	0.826784000000
H	4.883976000000	-0.288431000000	1.520949000000
H	4.308966000000	0.808944000000	0.221573000000
H	3.901184000000	-0.946841000000	0.172488000000
O	1.794612000000	2.175847000000	0.409229000000
C	2.409870000000	3.218891000000	1.205759000000
H	3.188579000000	2.807698000000	1.864301000000
H	1.641345000000	3.735056000000	1.799803000000
H	2.861581000000	3.923459000000	0.496072000000
O	0.577681000000	0.808007000000	2.337957000000
C	1.078037000000	1.124928000000	3.663124000000
H	1.978464000000	0.538677000000	3.887110000000
H	0.270134000000	0.857438000000	4.355287000000
H	1.294106000000	2.199627000000	3.745290000000
C	-0.665264000000	-1.686769000000	-2.117691000000
O	-1.273629000000	-2.267576000000	-2.903389000000

C	1.432939000000	0.203227000000	-2.169355000000
O	2.226097000000	0.495104000000	-2.966547000000
C	1.161822000000	-2.342687000000	-0.048721000000
O	1.890726000000	-3.239671000000	0.102094000000

Table S54. Cartesian coordinates (in Å) of the T_1 state transition state for the equatorial CO dissociation (T_1-TS(dissociation)) of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$. The electronic energy of the T_1 state is -1600.496104 hartree.

Atom	*x*	*y*	*z*
Re	0.146700000000	-0.681635000000	-0.622636000000
P	1.378384000000	1.182113000000	0.448498000000
N	-1.487028000000	-0.459991000000	0.881067000000
N	-1.238789000000	0.886677000000	-1.383777000000
C	-1.526970000000	-1.164544000000	2.030180000000
C	-1.041540000000	1.512243000000	-2.562678000000
C	-2.545326000000	-1.014067000000	2.966014000000
C	-1.956561000000	2.419042000000	-3.087230000000
C	-3.565911000000	-0.099634000000	2.704410000000
C	-3.114431000000	2.699910000000	-2.359710000000
C	-3.530697000000	0.629040000000	1.517851000000
C	-3.314963000000	2.064606000000	-1.136374000000

C	-2.479071000000	0.432797000000	0.616153000000
C	-2.360009000000	1.157330000000	-0.664415000000
H	-0.711746000000	-1.868505000000	2.193335000000
H	-0.120159000000	1.269894000000	-3.092327000000
H	-2.527849000000	-1.609319000000	3.878655000000
H	-1.753226000000	2.894351000000	-4.046633000000
H	-4.381428000000	0.046654000000	3.413744000000
H	-3.853817000000	3.407043000000	-2.737397000000
H	-4.316566000000	1.349193000000	1.298688000000
H	-4.212614000000	2.271164000000	-0.556821000000
O	2.557906000000	0.921875000000	1.576045000000
C	3.753260000000	0.187131000000	1.235447000000
H	4.310690000000	0.062763000000	2.172177000000
H	4.364633000000	0.748862000000	0.512686000000
H	3.506056000000	-0.803036000000	0.822295000000
O	2.105641000000	2.112082000000	-0.698606000000
C	2.856982000000	3.313696000000	-0.396423000000
H	3.397938000000	3.217374000000	0.556073000000
H	2.175556000000	4.176399000000	-0.359712000000
H	3.575202000000	3.446404000000	-1.215678000000
O	0.376719000000	2.126200000000	1.331643000000
C	0.773595000000	3.066854000000	2.362024000000
H	1.579561000000	2.650011000000	2.979672000000

H	-0.121350000000	3.235804000000	2.973977000000
H	1.093389000000	4.015406000000	1.907103000000
C	-0.823169000000	-2.256225000000	-1.290115000000
O	-1.398345000000	-3.191059000000	-1.656072000000
C	1.714885000000	-0.898482000000	-1.807360000000
O	2.633703000000	-1.019909000000	-2.496752000000
C	1.571721000000	-2.790426000000	0.582086000000
O	1.210295000000	-3.138139000000	1.618993000000

Table S55. Cartesian coordinates (in Å) of the T_1 state transition state in which the equatorial CO is bent (T_1-TS(bent)) of *fac*-[Re^{I}(bpy)$(CO)_3$Cl]. This TS are obtained as the T_2/T_1-MECI by the TD-B3LYP calculation. The electronic energy of the MECI is -1374.101169 (T_2: -1374.101166, T_1: -1374.101171) hartree.

Atom	*x*	*y*	*z*
C	-3.365791373446	0.092553288055	1.481859635549
C	-3.281466307421	0.007373213743	2.864116218932
C	-2.200453726174	-0.011635011562	0.698519942797
H	-4.180904965846	0.091187931248	3.475889526661
C	-2.023433205626	-0.184193692594	3.455928031366
N	-0.976023263716	-0.179869756072	1.286610703521
H	-1.904674402279	-0.270463091446	4.535955729592
C	-0.909565846122	-0.262216891755	2.631481547796

H	0.090342134842	-0.402033247414	3.046169032617
H	-4.332375005210	0.250250445528	1.006391513853
C	-2.208081520130	0.063223488601	-0.760198196576
N	-0.979834864562	0.086420571287	-1.371766189749
C	-3.385680869997	0.112493165666	-1.529806534949
C	-0.919974028442	0.175640891002	-2.721224366296
C	-3.310280792112	0.215964297357	-2.910860644102
C	-2.045526080785	0.260404906151	-3.524281125992
H	-4.358083199004	0.062675511880	-1.042881396529
H	0.079621194392	0.180548897717	-3.155946822005
H	-4.221755283943	0.254116091106	-3.509100426862
H	-1.934413832109	0.347842793267	-4.604800814096
Re	0.841792114064	-0.119242573025	-0.077529742294
C	2.049034500201	-0.557565139385	1.506259098663
C	0.888843834816	-2.024982843324	-0.509900898174
C	2.202527178895	0.075095550940	-1.449354769311
Cl	0.934063300648	2.300287157003	0.423685200284
O	0.942646550073	-3.147712381415	-0.781454135912
O	3.061652555907	-0.658974552151	2.082980689460
O	3.027883293911	0.187518241807	-2.256600728734

Table S56. Cartesian coordinates (in Å) of the T_1 state equilibrium structure in which the equatorial CO is bent (T_1-min(bent)) of *fac*-[Re^{I}(bpy)$(CO)_3$Cl]. The electronic energy of the T_1 state is -1374.108645 hartree.

Atom	*x*	*y*	*z*
C	-3.174849743450	-0.217030661916	1.102379077955
C	-3.277876675818	-0.241954553705	2.491587371715
C	-1.922815477445	-0.390836650935	0.499237784558
H	-4.248342213160	-0.106231642379	2.970930643613
C	-2.126692413604	-0.446502751334	3.253715445383
N	-0.808044986549	-0.573212153957	1.249380723779
H	-2.158114931416	-0.482153811533	4.342604857900
C	-0.913573302897	-0.609542325427	2.591733879967
H	0.011921916549	-0.773945414414	3.144065785273
H	-4.064875737773	-0.059193196869	0.496486858823
C	-1.718952322414	-0.397884130166	-0.966433029497
N	-0.432886282625	-0.513015255217	-1.389973480273
C	-2.778589779456	-0.303252989683	-1.876976415252
C	-0.187843651359	-0.527181129217	-2.712673845129
C	-2.514808463375	-0.316741821795	-3.244784015495
C	-1.192348036544	-0.428002992759	-3.671853351203
H	-3.804934360366	-0.224581449906	-1.524081871273
H	0.861730239236	-0.632040650979	-2.993543569699
H	-3.332963540851	-0.243702483452	-3.962710867973

H	-0.931062846960	-0.442263031438	-4.730135231358
Re	1.220028876240	-0.589054582213	0.197141358598
C	2.491247882920	-0.569978852397	1.662191854452
C	1.269212770293	-2.524094673654	0.430406484414
C	2.594812159817	-0.835067587234	-1.360496466267
Cl	1.181798535894	1.889134462997	0.019310136486
O	1.321858768900	-3.668936867067	0.601616420610
O	3.251171439036	-0.576967725372	2.538823661985
O	3.745015766536	-0.585065210970	-1.518957948742

Table S57. Cartesian coordinates (in Å) of the T_1 state transition state for the equatorial CO dissociation (T_1-TS(dissociation)) of *fac*-[Re^{I}(bpy)$(CO)_3$Cl]. The electronic energy of the T_1 state is -1374.091014 hartree.

Atom	*x*	*y*	*z*
C	-3.467707961875	-0.271048144754	1.617554173415
C	-3.401012197013	-0.268479572241	3.009030366409
C	-2.289623115635	-0.216254829432	0.864079493806
H	-4.315816823701	-0.311517629417	3.601505432121
C	-2.149964305815	-0.210700512443	3.626226819217
N	-1.069866833774	-0.170032265640	1.476151882609
H	-2.046128429189	-0.201524265678	4.711147320319
C	-1.014168991157	-0.164066875163	2.826331932397

H	-0.017682519398	-0.116016993027	3.262929235442
H	-4.435882210556	-0.320277285677	1.123084578423
C	-2.279252344983	-0.210354555634	-0.615676854269
N	-1.051072703733	-0.246221701970	-1.199921124337
C	-3.445883835962	-0.166812577795	-1.389424438091
C	-0.965505671874	-0.235096547999	-2.544867232241
C	-3.349640260413	-0.162536675423	-2.779068205456
C	-2.085449557947	-0.197181978195	-3.369888339996
H	-4.424326529564	-0.129317676816	-0.914627798005
H	0.043517732445	-0.252090233821	-2.956755699381
H	-4.252251826026	-0.128563117281	-3.390653146474
H	-1.959269025866	-0.192544160834	-4.452520447188
Re	0.696685335031	-0.257810585289	0.170476851604
C	2.060777380264	-0.204626720863	1.504214758292
C	1.538715191967	-1.867153244523	-0.544972579470
C	2.431778032011	0.601059261332	-1.822949335346
Cl	0.533658795084	2.263056397641	0.130080704571
O	2.023758476082	-2.848112405306	-0.946801915256
O	2.873617309086	-0.158308719708	2.345702808739
O	3.540421782406	0.839153513307	-1.654364442210

Table S58. Cartesian coordinates (in Å) of the T_3/S_1-MESX at 3.100 eV of energy (T_3: -1600.514121, S_1: -1600.514151 hartree), of *fac*-$[Re^{I}(bpy)(CO)_3P(OMe)_3]^+$.

Atom	*x*	*y*	*z*
Re	0.201405147664	-0.876262268358	-0.448237119662
P	1.454243717252	0.984709584166	0.657501779054
N	-1.323561680456	-0.649968397673	1.070597646149
N	-1.074768503537	0.693529720202	-1.219517834252
C	-1.378846400135	-1.344270200812	2.240321685288
C	-0.893465372879	1.342312256831	-2.403807342371
C	-2.384847381955	-1.185670135391	3.167452353972
C	-1.770977399360	2.285550228410	-2.888962034803
C	-3.418971081042	-0.250948792488	2.892560907107
C	-2.924037506871	2.601156416962	-2.118232059986
C	-3.382673047504	0.461994582038	1.717014346423
C	-3.124529053487	1.960154542216	-0.918409371858
C	-2.325816897603	0.276708037215	0.782904511711
C	-2.198226559530	0.988758948418	-0.445549127943
H	-0.572581109277	-2.054218231443	2.424661647148
H	-0.000025187699	1.080354444317	-2.970805614480
H	-2.371928228188	-1.774277783016	4.083859951929
H	-1.567168305927	2.772057030491	-3.842083238238
H	-4.234879564913	-0.100614746407	3.600942568663

H	-3.639758929989	3.345015980298	-2.470764959217
H	-4.166586207644	1.184220143348	1.493753264851
H	-4.005096233229	2.190340979609	-0.320289538454
O	2.736021846826	0.718043715391	1.652278567550
C	3.973597754675	0.131954475292	1.189559013051
H	4.694745541238	0.277360353850	2.003283628249
H	4.332784844530	0.634304349261	0.279497545628
H	3.847248901848	-0.944734439592	1.001274945281
O	2.014954401549	1.953234972234	-0.541726637637
C	2.626381952256	3.245674539919	-0.301491526513
H	3.374245423011	3.186105475010	0.502324286996
H	1.850432445722	3.982492415186	-0.048401467972
H	3.114167798981	3.530652800559	-1.241593048087
O	0.511146743977	1.861456990017	1.650345146934
C	0.950822358672	2.661065733737	2.782454851283
H	1.868204723353	2.247207222077	3.218480917853
H	0.133619138493	2.624072024595	3.513701254158
H	1.116353667522	3.697932850240	2.457014366027
C	-0.939698357722	-2.230980820027	-1.365340853683
O	-1.591854835124	-3.002684071381	-1.901832049120
C	1.546301054970	-0.895157958226	-1.955861595532
O	2.305842642292	-0.914252692011	-2.810899703217
C	1.219876118891	-2.351784924162	0.479978951228

O	1.775213620756	-3.211046351183	0.992691986576