Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information for

Influence of electronic effect of ancillary ligand on MMCT and LMCT in localized cyanide-bridged complexes containing non-innocent ligands

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1. Single crystal structure

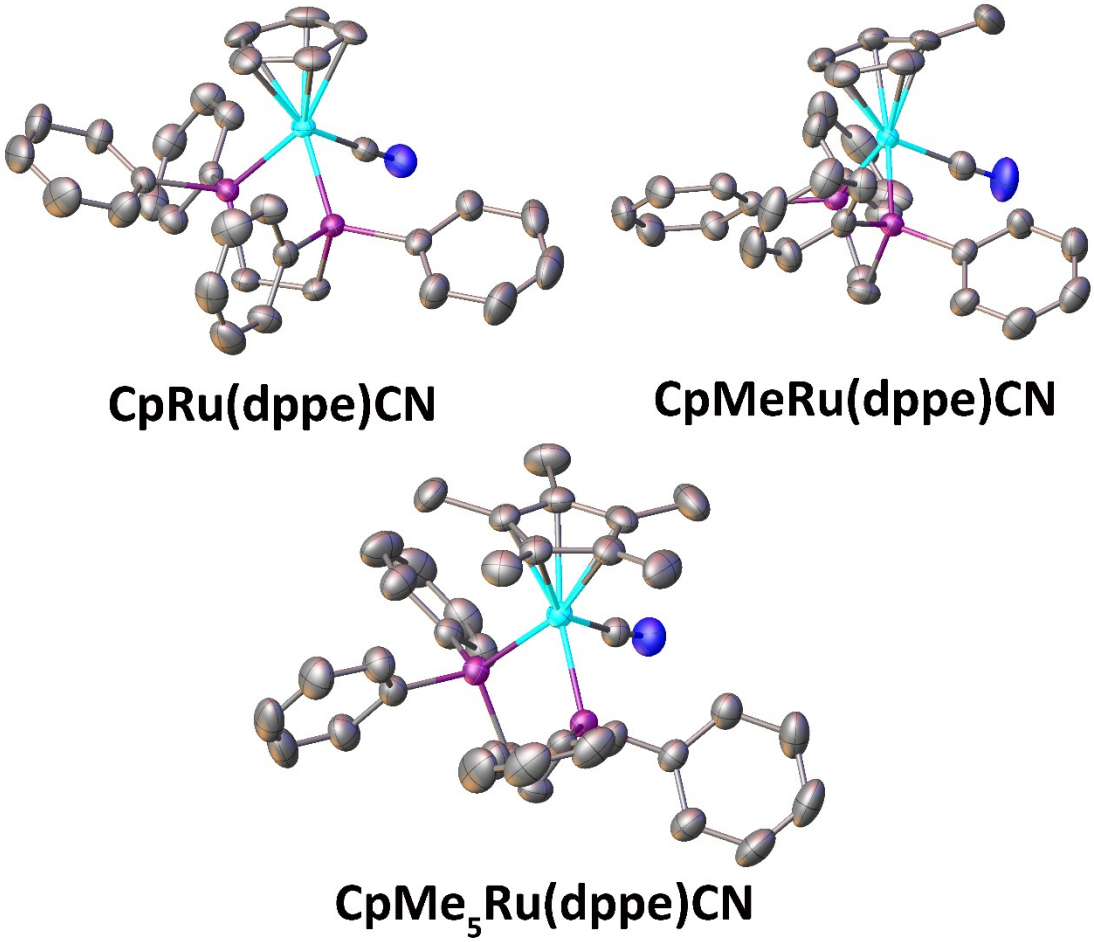

Fig. S1 Molecular structures of precursors **$CpMe_nRu(dppe)CN$** (n = 0, 1, 5)**.** Hydrogen atoms and solvents have been omitted for clarity. Ru, light blue; P, purple; C, gray; N, blue.

2. Crystallographic data

Table S1 Crystallographic data for complexes $\mathbf{1_{Me}[PF_6]}$, $\mathbf{2_{Me}[PF_6]}$ and $\mathbf{3_{Me}[I]}$.

	$\mathbf{1_{Me}[PF_6]}$	$\mathbf{2_{Me}[PF_6]}$	$\mathbf{3_{Me}[I]}$
Empirical formula	$C_{41}H_{44}F_6FeN_7P_3RuS_2$	$C_{42}H_{46}F_6FeN_7P_3RuS_2$	$C_{46}H_{54}FeIN_7P_2RuS_2$
Formula weight	1062.78	1076.81	1114.84
Temperature/K	293(2)	293(2)	293(2)
Crystal system	monoclinic	orthorhombic	monoclinic
Space group	$P2_1/c$	$P2_12_12_1$	Cc
a/Å	16.5744(4)	15.1069(4)	11.2180(3)
b/Å	19.3582(4)	15.3402(5)	19.4971(4)
c/Å	16.0088(3)	21.6504(6)	22.9165(5)
α/°	90	90	90
β/°	103.576(2)	90	99.516(2)
γ/°	90	90	90
Volume/Å^3	4992.92(19)	5017.3(3)	4943.3(2)
Z	4	4	4
ρ_{calc}g/cm^3	1.414	1.426	1.498
μ/mm^{-1}	0.831	0.828	1.412
F(000)	2160.0	2192.0	2256.0
Crystal size/mm^3	0.25 × 0.25 × 0.08	0.18 × 0.03 × 0.03	0.15 × 0.08 × 0.05
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	3.358 to 49.424	4.63 to 51.35	4.178 to 59.148
Index ranges	-19 ≤ h ≤ 19, -22 ≤ k ≤ 22, -18 ≤ l ≤ 18	-18 ≤ h ≤ 18, -18 ≤ k ≤ 18, -26 ≤ l ≤ 26	-15 ≤ h ≤ 15, -27 ≤ k ≤ 27, -31 ≤ l ≤ 31
Reflections collected	60859	49028	41037
Independent reflections	8512 [R_{int} = 0.0476, R_{sigma} = 0.0208]	9279 [R_{int} = 0.0399, R_{sigma} = 0.0257]	13810 [R_{int} = 0.0166, R_{sigma} = 0.0153]
Data/restraints/parameters	8512/0/554	9279/126/565	13810/2/539
Goodness-of-fit on F^2	1.046	1.067	1.017
Final R indexes [I>=2σ (I)]	R_1 = 0.0393, wR_2 = 0.0964	R_1 = 0.0638, wR_2 = 0.1630	R_1 = 0.0226, wR_2 = 0.0549
Final R indexes [all data]	R_1 = 0.0468, wR_2 = 0.1006	R_1 = 0.0673, wR_2 = 0.1667	R_1 = 0.0242, wR_2 = 0.0554
Largest diff. peak/hole / e Å^{-3}	0.60/-0.43	2.83/-0.82	0.66/-0.58
Flack parameter	-	0.09(4)	-0.008(10)

$R_1 = \Sigma (||F_o| - |F_c||)/\Sigma|F_o|$; $wR_2 = [\Sigma w (|F_o^2| - |F_c^2|)^2/\Sigma w|F_o^2|^2]^{1/2}$

Table S2 Crystallographic data for complexes $\mathbf{1_{Et}[PF_6]}$, $\mathbf{2_{Et}[PF_6]}$ and $\mathbf{3_{Et}[I]}$.

	$\mathbf{1_{Et}[PF_6]}$	$\mathbf{2_{Et}[PF_6]}$	$\mathbf{3_{Et}[I]}$
Empirical formula	$C_{43}H_{48}F_6FeN_7P_3RuS_2$	$C_{89}H_{102}Cl_2F_{12}Fe_2N_{14}P_6Ru_2S_4$	$C_{48}H_{58}FeIN_7P_2RuS_2$
Formula weight	1090.83	2294.64	1142.89
Temperature/K	293	293	293(2)
Crystal system	monoclinic	orthorhombic	monoclinic
Space group	$P2_1/c$	$P2_12_12_1$	$P2_1/c$
a/Å	11.5914(2)	15.3525(5)	15.5201(5)
b/Å	23.9157(5)	15.8856(7)	15.2285(4)
c/Å	18.2913(4)	21.9881(7)	22.4356(8)
α/°	90	90	90
β/°	107.362(2)	90	106.738(4)
γ/°	90	90	90
Volume/Å^3	4839.62(18)	5362.5(3)	5077.9(3)
Z	4	2	4
ρ_{calc}g/cm^3	1.497	1.421	1.495
μ/mm^{-1}	0.859	0.827	1.376
F(000)	2224.0	2340.0	2320.0
Crystal size/mm^3	0.25 × 0.23 × 0.22	0.25 × 0.05 × 0.05	0.25 × 0.05 × 0.03
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	3.682 to 59.148	3.69 to 51.362	3.83 to 54.968
Index ranges	-16 ≤ h ≤ 16, -33 ≤ k ≤ 33, -25 ≤ l ≤ 25	-17 ≤ h ≤ 18, -19 ≤ k ≤ 18, -26 ≤ l ≤ 24	-20 ≤ h ≤ 20, -19 ≤ k ≤ 19, -29 ≤ l ≤ 29
Reflections collected	83624	27482	75780
Independent reflections	13553 [R_{int} = 0.0523, R_{sigma} = 0.0337]	10065 [R_{int} = 0.0530, R_{sigma} = 0.0591]	11636 [R_{int} = 0.0401, R_{sigma} = 0.0231]
Data/restraints/parameters	13553/0/580	10065/316/598	11636/0/576
Goodness-of-fit on F^2	1.056	1.043	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0565, wR_2 = 0.1320	R_1 = 0.0688, wR_2 = 0.1789	R_1 = 0.0363, wR_2 = 0.0847
Final R indexes [all data]	R_1 = 0.0876, wR_2 = 0.1465	R_1 = 0.0855, wR_2 = 0.1922	R_1 = 0.0479, wR_2 = 0.0896
Largest diff. peak/hole / e Å^{-3}	0.79/-0.43	0.99/-1.01	0.86/-0.67
Flack parameter	-	0.03(5)	-

$R_1 = \Sigma (||F_o| - |F_c||)/\Sigma|F_o|$; $wR_2 = [\Sigma w (|F_o^2| - |F_c^2|)^2/\Sigma w|F_o^2|^2]^{1/2}$

Table S3 Crystallographic data for complexes $\mathbf{1_{Pr}[PF_6]}$, $\mathbf{2_{Pr}[PF_6]}$ and $\mathbf{3_{Pr}[I]}$.

	$\mathbf{1_{Pr}[PF_6]}$	$\mathbf{2_{Pr}[PF_6]}$	$\mathbf{3_{Pr}[I]}$
Empirical formula	$C_{45}H_{52}F_6FeN_7P_3RuS_2$	$C_{46}H_{54}F_6FeN_7P_3RuS_2$	$C_{50}H_{62}FeIN_7P_2RuS_2$
Formula weight	1118.88	1141.92	1170.94
Temperature/K	293	293	293(2)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/c$
a/Å	15.7191(3)	15.8198(3)	15.8862(4)
b/Å	17.2564(4)	17.0381(3)	15.2435(4)
c/Å	19.6213(4)	19.8147(3)	22.9894(5)
α/°	90	90	90
β/°	101.990(2)	102.958(2)	108.041(3)
γ/°	90	90	90
Volume/Å^3	5206.26(19)	5204.83(16)	5293.4(2)
Z	4	4	4
ρ_{calc}g/cm^3	1.427	1.457	1.469
μ/mm^{-1}	0.801	0.803	1.322
F(000)	2288.0	2340.0	2384.0
Crystal size/mm^3	0.22 × 0.05 × 0.05	0.25 × 0.05 × 0.04	0.15 × 0.05 × 0.05
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.244 to 51.364	4.432 to 51.362	4.582 to 51.364
Index ranges	-19 ≤ h ≤ 19, -17 ≤ k ≤ 21, -23 ≤ l ≤ 23	-19 ≤ h ≤ 19, -20 ≤ k ≤ 20, -24 ≤ l ≤ 24	-19 ≤ h ≤ 19, -18 ≤ k ≤ 18, -28 ≤ l ≤ 28
Reflections collected	45953	63025	50139
Independent reflections	9819 [R_{int} = 0.0360, R_{sigma} = 0.0191]	9659 [R_{int} = 0.0237, R_{sigma} = 0.0112]	9904 [R_{int} = 0.0277, R_{sigma} = 0.0155]
Data/restraints/parameters	9819/246/590	9659/18/600	9904/0/594
Goodness-of-fit on F^2	1.020	1.044	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0509, wR_2 = 0.1451	R_1 = 0.0494, wR_2 = 0.1367	R_1 = 0.0294, wR_2 = 0.0745
Final R indexes [all data]	R_1 = 0.0564, R_2 = 0.1510	R_1 = 0.0549, wR_2 = 0.1432	R_1 = 0.0341, wR_2 = 0.0770
Largest diff. peak/hole / e Å^{-3}	1.29/-0.67	1.71/-0.60	1.91/-1.01
Flack parameter	-	-	-

$R_1 = \Sigma\,(||F_0| - |F_C||)/\Sigma|F_0|$; $wR_2 = [\Sigma w\,(|F_0^2| - |F_C^2|)^2/\Sigma w|F_0^2|^2]^{1/2}$

Table S4 Crystallographic data for complexes $\mathbf{1_{Bu}[PF_6]}$, $\mathbf{2_{Bu}[PF_6]}$ and $\mathbf{3_{Bu}[I]}$.

	$\mathbf{1_{Bu}[PF_6]}$	$\mathbf{2_{Bu}[PF_6]}$	$\mathbf{3_{Bu}[I]}$
Empirical formula	$C_{47}H_{56}F_6FeN_7P_3RuS_2$	$C_{48}H_{58}F_6FeN_7P_3RuS_2$	$C_{52}H_{66}FeIN_7P_2RuS_2$
Formula weight	1146.93	1160.96	1198.99
Temperature/K	293	293	293
Crystal system	monoclinic	monoclinic	orthorhombic
Space group	$P2_1/n$	$P2_1/n$	$P2_12_12_1$
a/Å	16.1976(4)	16.1713(6)	15.1864(3)
b/Å	17.4678(5)	17.1693(7)	15.4588(3)
c/Å	19.4441(4)	19.7929(7)	23.6654(6)
α/°	90	90	90
β/°	102.356(2)	103.023(4)	90
γ/°	90	90	90
Volume/Å^3	5374.0(2)	5354.1(4)	5555.8(2)
Z	4	4	4
ρ_{calc}g/cm^3	1.418	1.440	1.433
μ/mm^{-1}	0.777	0.781	1.261
F(000)	2352.0	2384.0	2448.0
Crystal size/mm^3	0.25 × 0.05 × 0.05	0.25 × 0.08 × 0.05	0.25 × 0.03 × 0.03
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.362 to 54.968	4.224 to 54.968	3.186 to 54.96
Index ranges	-21 ≤ h ≤ 21, -22 ≤ k ≤ 22, -25 ≤ l ≤ 25	-21 ≤ h ≤ 21, -22 ≤ k ≤ 22, -25 ≤ l ≤ 25	-19 ≤ h ≤ 19, -20 ≤ k ≤ 20, -30 ≤ l ≤ 30
Reflections collected	60158	76593	65078
Independent reflections	12248 [R_{int} = 0.0236, R_{sigma} = 0.0152]	12247 [R_{int} = 0.0309, R_{sigma} = 0.0152]	12739 [R_{int} = 0.0467, R_{sigma} = 0.0353]
Data/restraints/parameters	12248/44/596	12247/19/626	12739/302/605
Goodness-of-fit on F^2	1.022	1.025	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0458, wR_2 = 0.1319	R_1 = 0.0452, wR_2 = 0.1267	R_1 = 0.0458, wR_2 = 0.0929
Final R indexes [all data]	R_1 = 0.0553, wR_2 = 0.1396	R_1 = 0.0538, wR_2 = 0.1348	R_1 = 0.0598, wR_2 = 0.0982
Largest diff. peak/hole / e Å^{-3}	0.85/-0.60	0.97/-0.52	0.69/-0.26
Flack parameter	-	-	0.49(3)

$R_1 = \Sigma\,(||F_0| - |F_C||)/\Sigma|F_0|$; $wR_2 = [\Sigma w\,(|F_0^2| - |F_C^2|)^2/\Sigma w|F_0^2|^2]^{1/2}$

Table S5 Crystallographic data for complexes **CpRu(dppe)CN, CpMeRu(dppe)CN** and **$CpMe_5$Ru(dppe)CN**.

	CpRu(dppe)CN	**CpMeRu(dppe)CN**	**$CpMe_5$Ru(dppe)CN**
Empirical formula	$C_{33}H_{31}Cl_2NP_2Ru$	$C_{33}H_{31}NP_2Ru$	$C_{38}H_{41}Cl_2NP_2Ru$
Formula weight	675.50	604.60	745.63
Temperature/K	293.0	293.0	293.15
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1$	$P2_1/c$
a/Å	12.923(2)	9.8749(19)	14.677(5)
b/Å	9.1065(14)	15.155(3)	12.168(4)
c/Å	25.677(4)	9.9695(19)	19.926(7)
α/°	90	90	90
β/°	90.032(3)	109.836(3)	100.380(6)
γ/°	90	90	90
Volume/Å^3	3021.8(8)	1403.5(5)	3500(2)
Z	4	2	4
ρ_{calc}g/cm^3	1.485	1.431	1.415
μ/mm^{-1}	0.825	0.695	0.720
F(000)	1376.0	620.0	1536.0
Crystal size/mm^3	0.25 × 0.25 × 0.22	0.28 × 0.25 × 0.25	0.28 × 0.28 × 0.25
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.746 to 51.356	5.692 to 51.362	5.06 to 51.362
Index ranges	-15 ≤ h ≤ 15, -10 ≤ k ≤ 11, -30 ≤ l ≤ 31	-12 ≤ h ≤ 12, -18 ≤ k ≤ 18, -12 ≤ l ≤ 12	-17 ≤ h ≤ 17, -14 ≤ k ≤ 14, -24 ≤ l ≤ 24
Reflections collected	27620	18334	45256
Independent reflections	5691 [R_{int} = 0.0412, R_{sigma} = 0.0364]	5282 [R_{int} = 0.0233, R_{sigma} = 0.0211]	6638 [R_{int} = 0.0307, R_{sigma} = 0.0169]
Data/restraints/parameters	5691/0/352	5282/1/336	6638/0/402
Goodness-of-fit on F^2	1.060	1.051	1.184
Final R indexes [I>=2σ (I)]	R_1 = 0.0337, wR_2 = 0.0816	R_1 = 0.0188, wR_2 = 0.0460	R_1 = 0.0338, wR_2 = 0.0763
Final R indexes [all data]	R_1 = 0.0364, wR_2 = 0.0839	R_1 = 0.0190, wR_2 = 0.0461	R_1 = 0.0346, wR_2 = 0.0767
Largest diff. peak/hole / e Å^{-3}	1.06/-0.71	0.24/-0.25	0.31/-0.50
Flack parameter	-	0.07(2)	-

$R_1 = \Sigma\,(||F_0| - |F_C||)/\Sigma|F_0|$; $wR_2 = [\Sigma w\,(|F_0^2| - |F_C^2|)^2/\Sigma w|F_0^2|^2]^{1/2}$

3. IR spectra

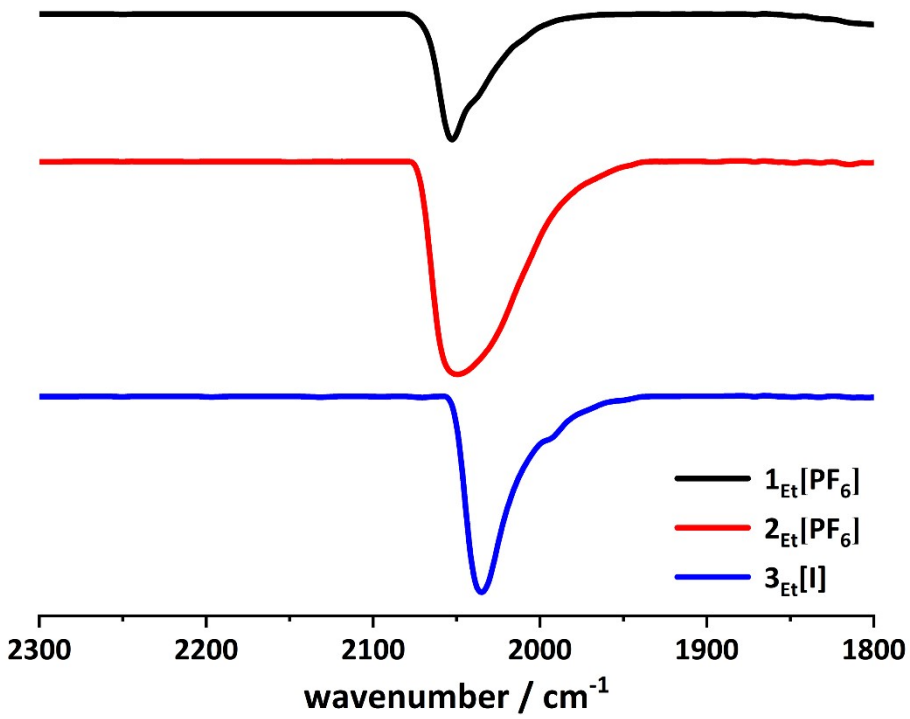

Fig. S2 Stretching frequencies of complexes $\mathbf{1_{Et}[PF_6]}$, $\mathbf{2_{Et}[PF_6]}$ and $\mathbf{3_{Et}[I]}$.

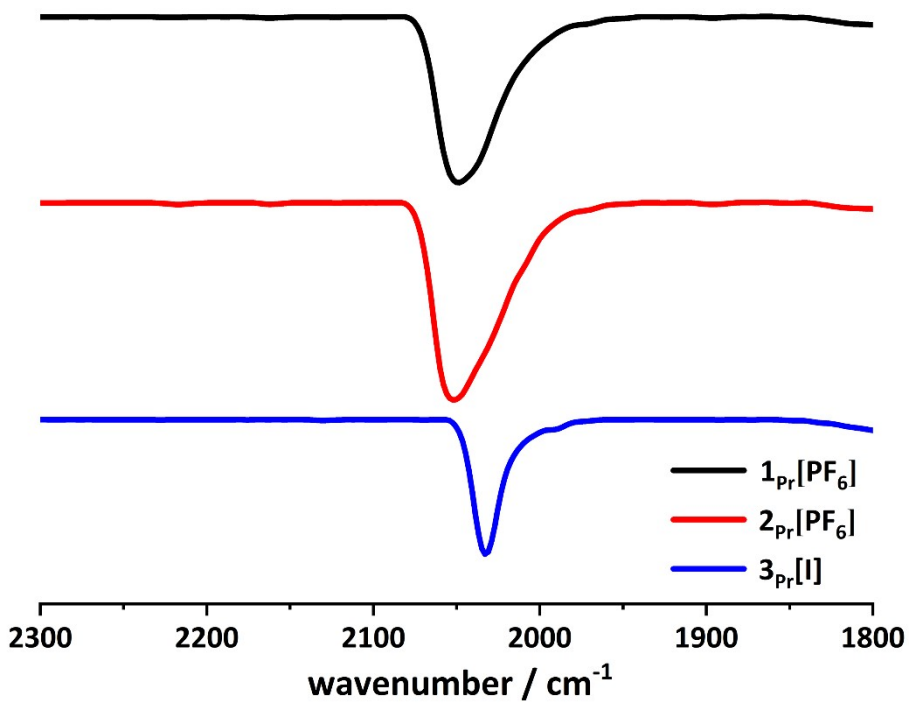

Fig. S3 Stretching frequencies of complexes $\mathbf{1_{Pr}[PF_6]}$, $\mathbf{2_{Pr}[PF_6]}$ and $\mathbf{3_{Pr}[I]}$.

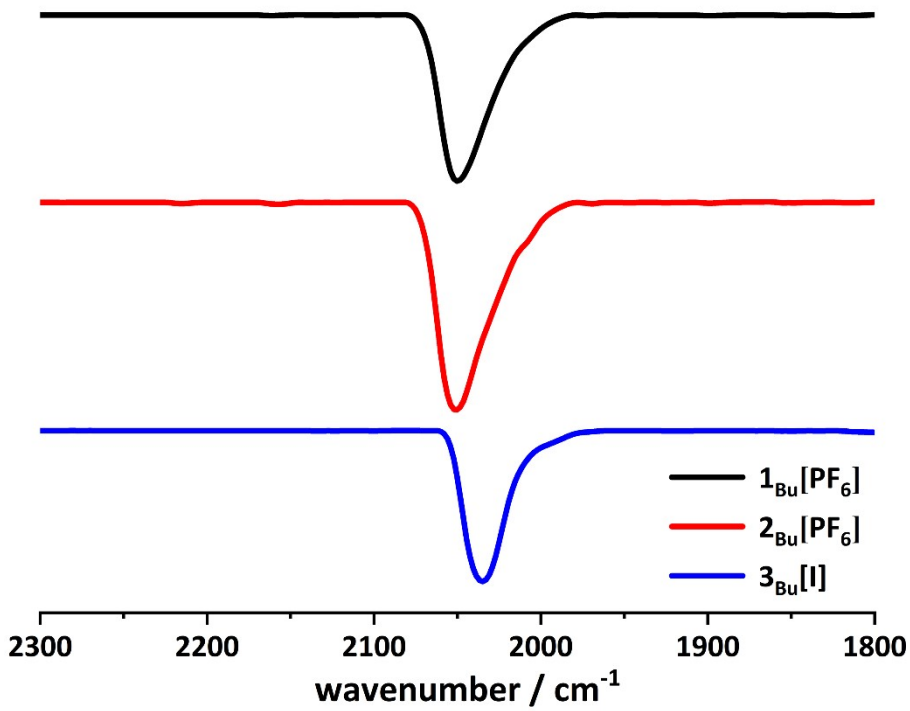

Fig. S4 Stretching frequencies of complexes $\mathbf{1_{Bu}[PF_6]}$, $\mathbf{2_{Bu}[PF_6]}$ and $\mathbf{3_{Bu}[I]}$.

4. Magnetic properties

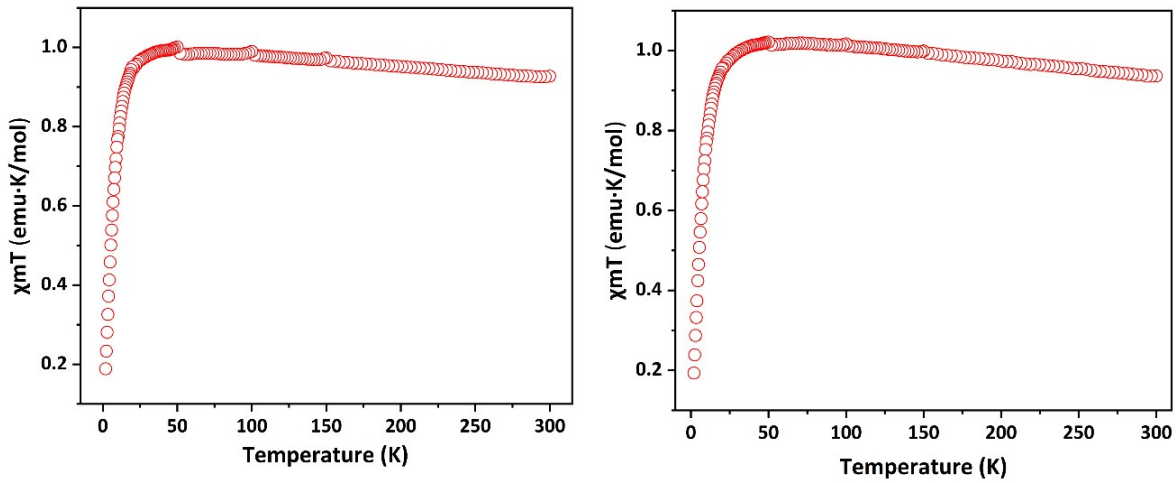

Fig. S5 The variable temperature magnetic susceptibility plots of complexes $\mathbf{1_{Me}[PF_6]}$ (left) and $\mathbf{1_{Et}[PF_6]}$ (right).

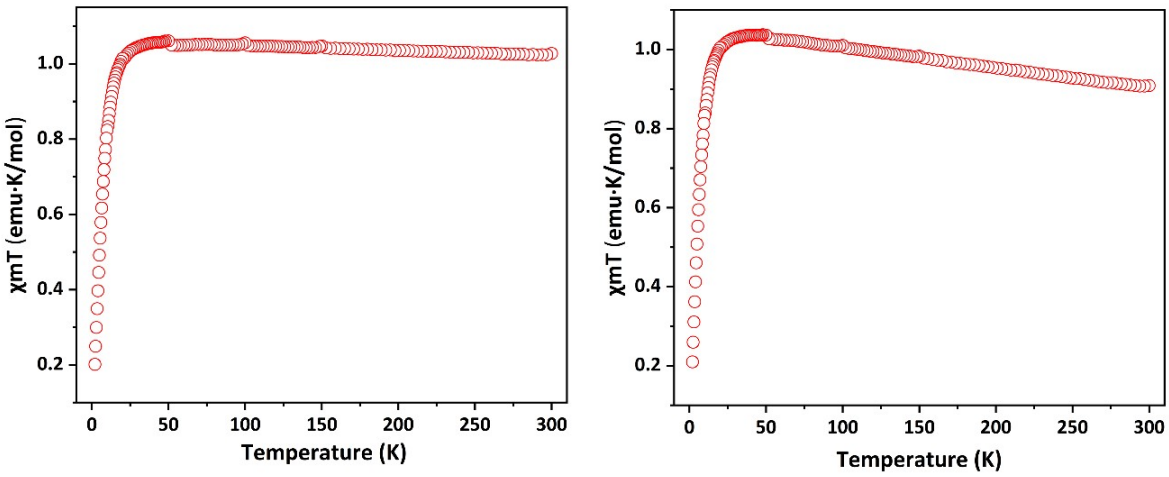

Fig. S6 The variable temperature magnetic susceptibility plots of complexes $\mathbf{1_{Pr}[PF_6]}$ (left) and $\mathbf{1_{Bu}[PF_6]}$ (right).

5. UV-vis-NIR spectroscopy

Table S6 The electronic absorption peaks of all bimetallic complexes.

complex	LMCT (cm^{-1})	ε ($M^{-1}\,cm^{-1}$)	MMCT (cm^{-1})	ε ($M^{-1}\,cm^{-1}$)
$\mathbf{1_{Me}[PF_6]}$	10217	1202	14071	1075
$\mathbf{1_{Et}[PF_6]}$	10209	1308	14124	1114
$\mathbf{1_{Pr}[PF_6]}$	10205	1282	14146	1068
$\mathbf{1_{Bu}[PF_6]}$	10202	1345	14058	1131
$\mathbf{2_{Me}[PF_6]}$	10393	1419	13791	1131
$\mathbf{2_{Et}[PF_6]}$	10383	1325	14037	1261
$\mathbf{2_{Pr}[PF_6]}$	10368	1287	14043	1219
$\mathbf{2_{Bu}[PF_6]}$	10342	1350	14032	1276
$\mathbf{3_{Me}[I]}$	10445	1190	13667	1118
$\mathbf{3_{Et}[I]}$	10416	1403	13705	1264
$\mathbf{3_{Pr}[I]}$	10408	1410	13675	1265
$\mathbf{3_{Bu}[I]}$	10402	1400	13662	1249

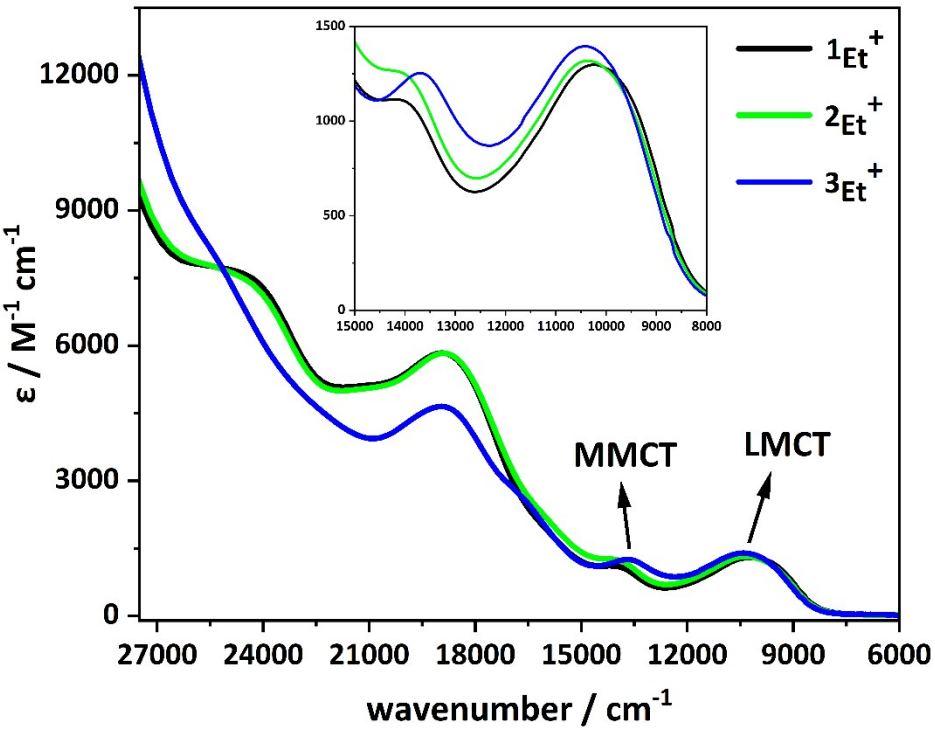

Fig. S7 The UV-vis-NIR spectra of complexes $\mathbf{1}_{Et}^{+}$, $\mathbf{2}_{Et}^{+}$ and $\mathbf{3}_{Et}^{+}$ in CH_2Cl_2 solution.

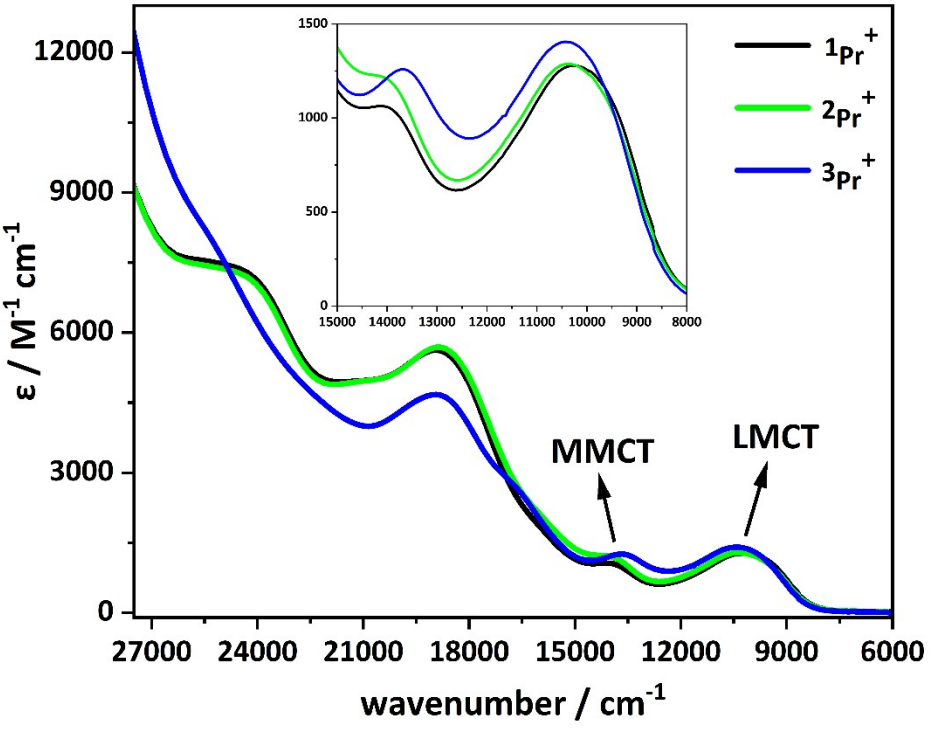

Fig. S8 The UV-vis-NIR spectra of complexes $\mathbf{1}_{Pr}^{+}$, $\mathbf{2}_{Pr}^{+}$ and $\mathbf{3}_{Pr}^{+}$ in CH_2Cl_2 solution.

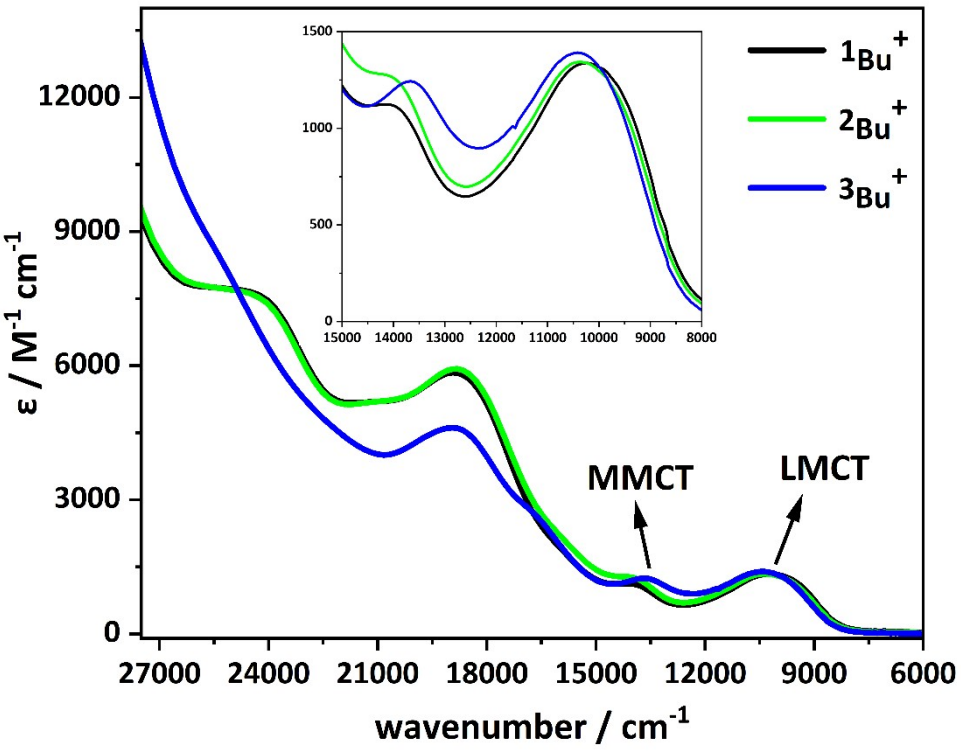

Fig. S9 The UV-vis-NIR spectra of complexes $\mathbf{1}_{Bu}^{+}$, $\mathbf{2}_{Bu}^{+}$ and $\mathbf{3}_{Bu}^{+}$ in CH_2Cl_2 solution.

6. TDDFT calculations

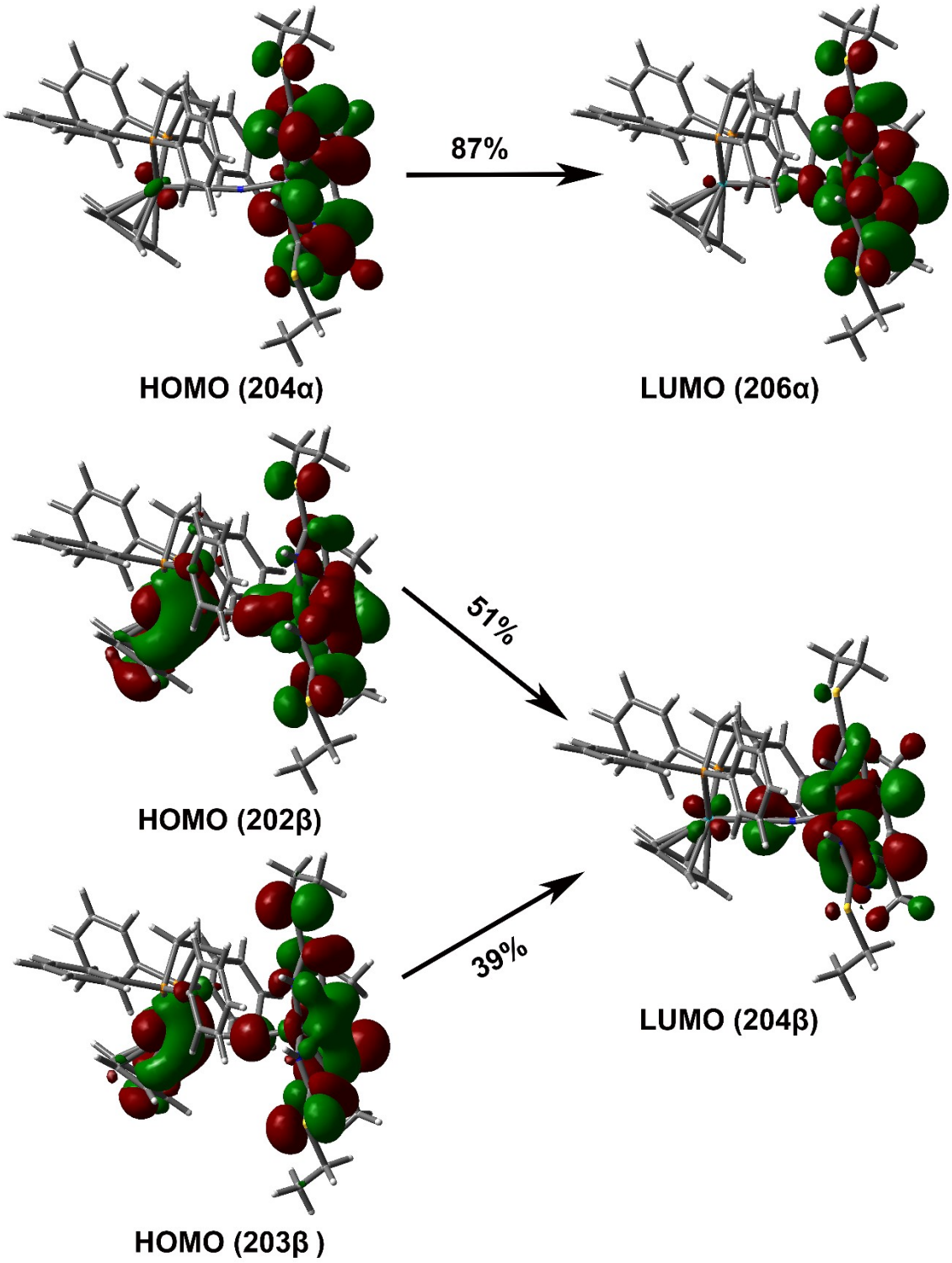

Fig. S10 Molecular orbital diagrams for the major electronic transitions corresponding to the LMCT (λ = 1003 nm, f = 0.0370) (top) and MMCT band (λ = 587 nm, f = 0.0138) (below) of complex $\mathbf{1_{Et}[PF_6]}$.

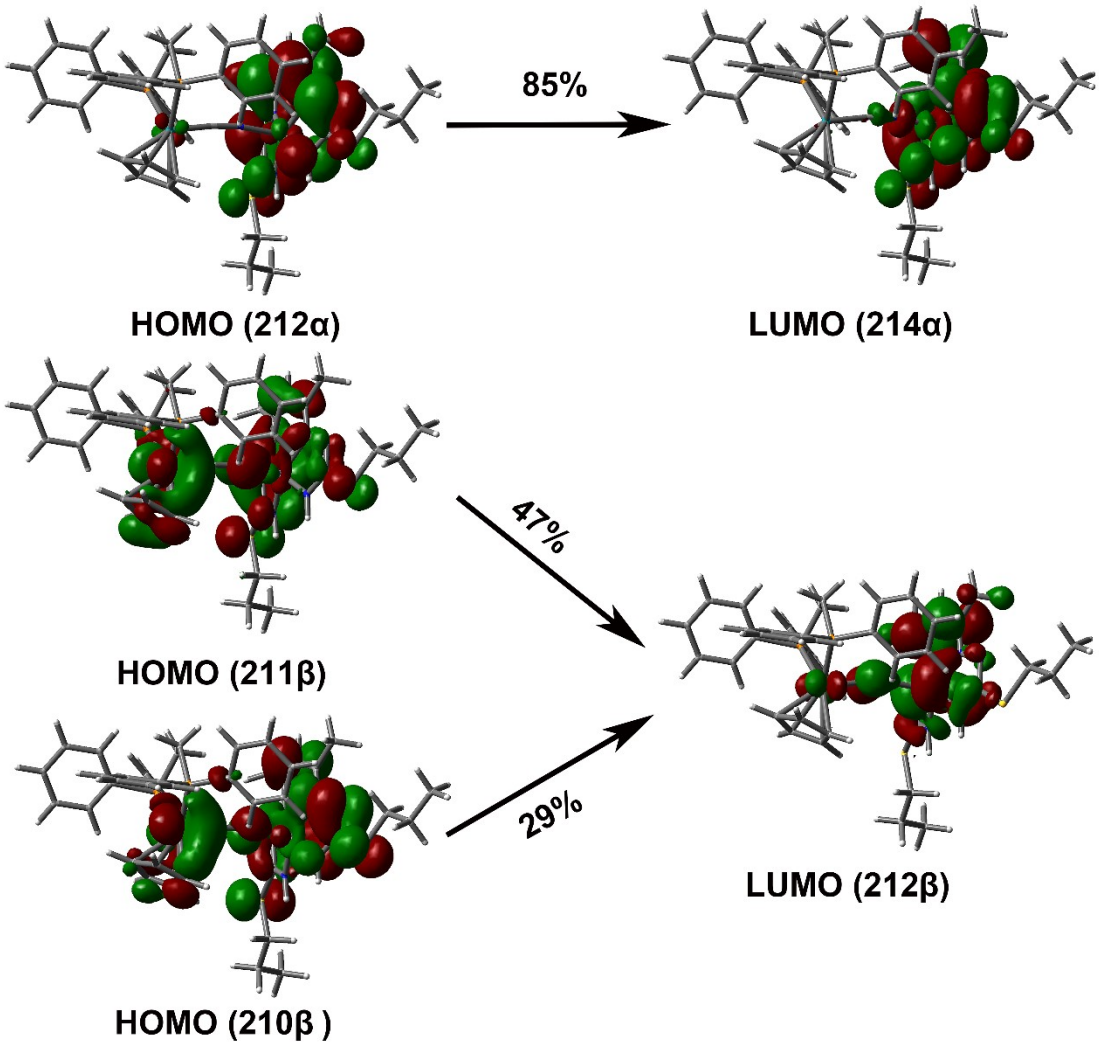

Fig. S11 Molecular orbital diagrams for the major electronic transitions corresponding to the LMCT (λ = 1021 nm, f = 0.0401) (top) and MMCT band (λ = 597 nm, f = 0.0682) (below) of complex $\mathbf{1_{Pr}[PF_6]}$.

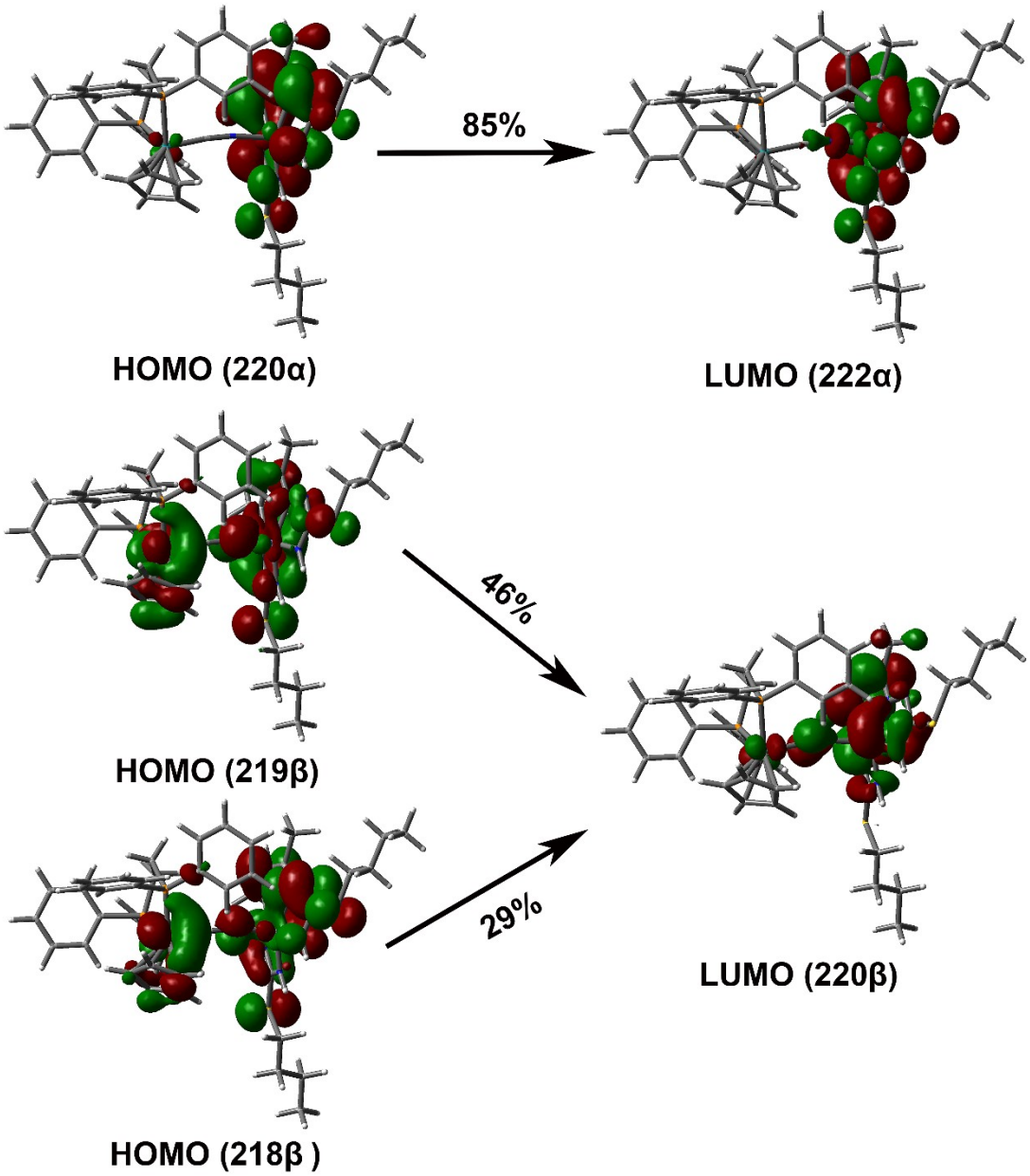

Fig. S12 Molecular orbital diagrams for the major electronic transitions corresponding to the LMCT (λ = 1022 nm, f = 0.0408) (top) and MMCT band (λ = 597 nm, f = 0.0674) (below) of complex $\mathbf{1_{Bu}[PF_6]}$.

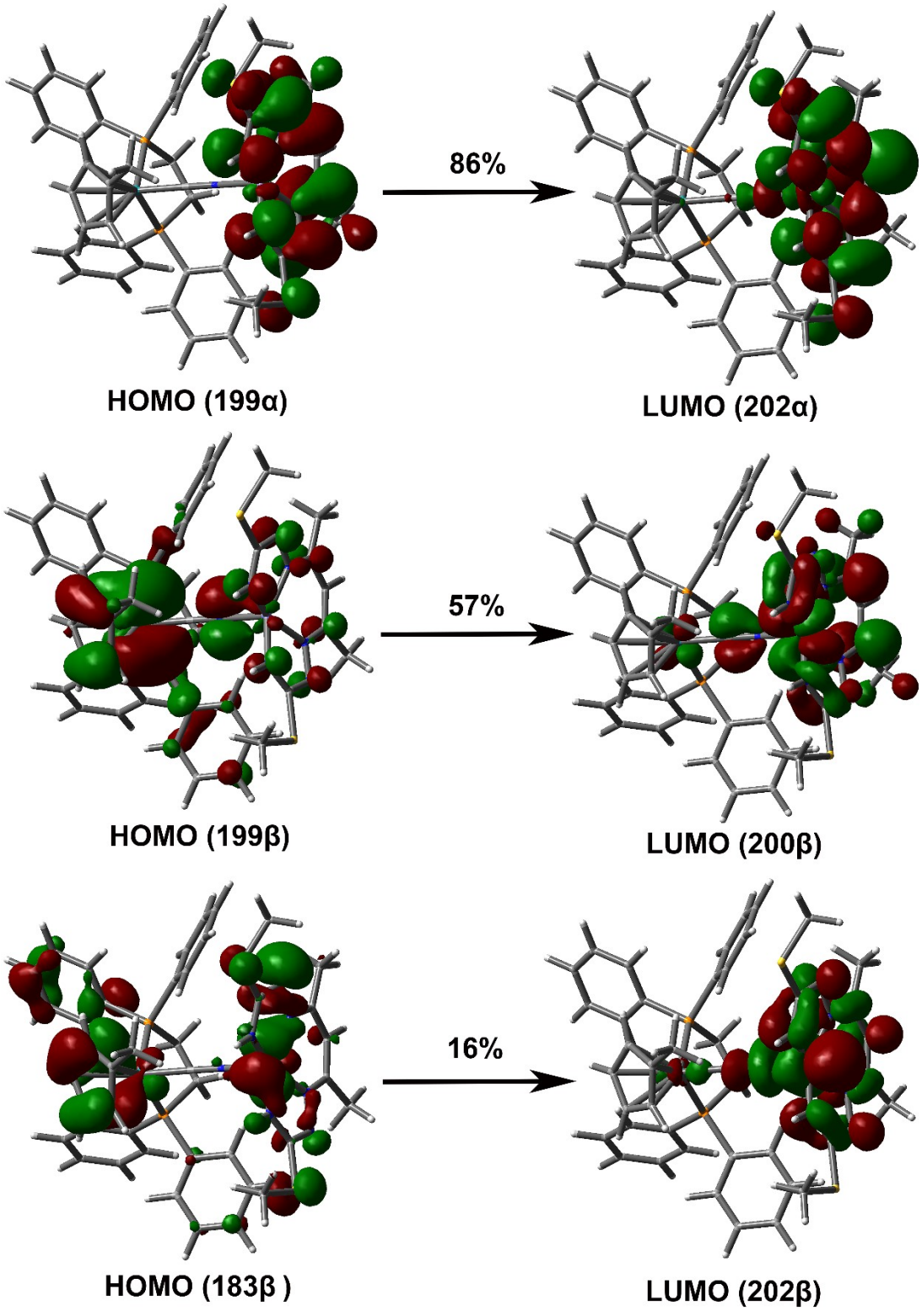

Fig. S13 Molecular orbital diagrams for the major electronic transitions corresponding to the LMCT (λ = 1015 nm, f = 0.0361) (top) and MMCT band (λ = 626 nm, f = 0.0439) (middle and below) of complex $\mathbf{2_{Me}[PF_6]}$.

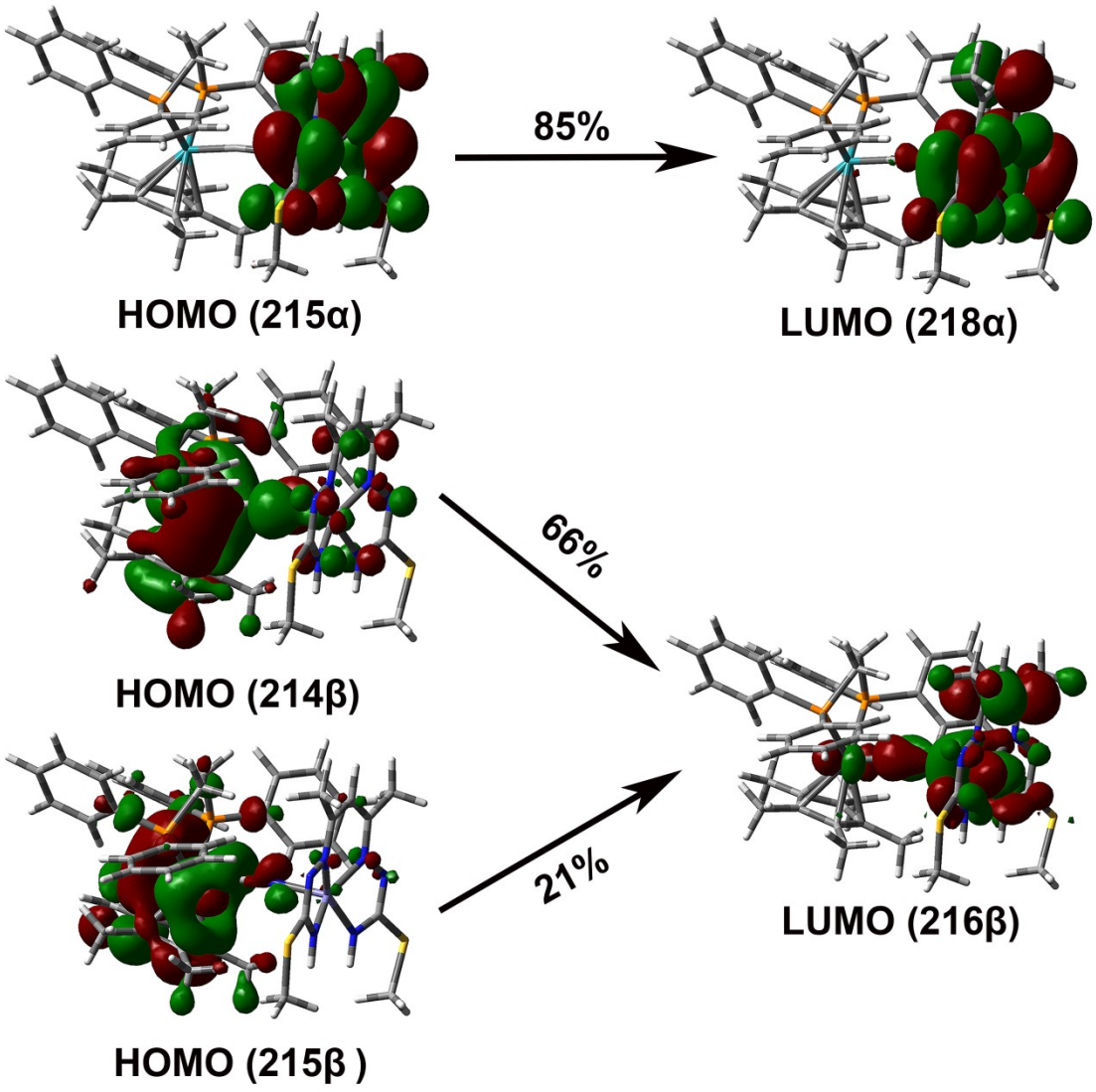

Fig. S14 Molecular orbital diagrams for the major electronic transitions corresponding to the LMCT (λ = 1010 nm, f = 0.0372) (top) and MMCT band (λ = 667 nm, f = 0.0473) (below) of complex $\mathbf{3_{Me}[I]}$.

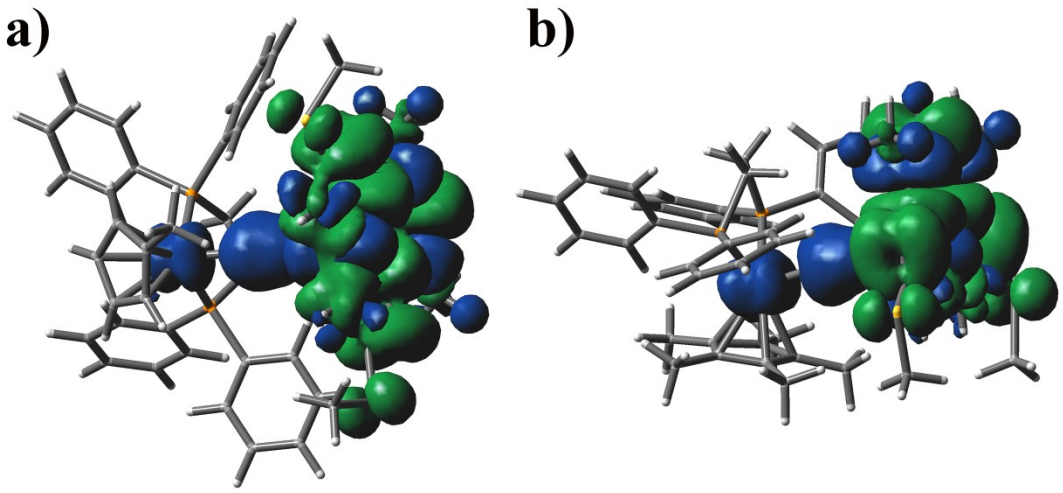

Fig. S15 The computed spin density distribution of $\mathbf{2_{Me}[PF_6]}$ (Ru^{II}, 0.1467; Fe^{III}, 2.5405; $(L^{\bullet}_{Me})^{2-}$, -0.6872) (left) and $\mathbf{3_{Me}[I]}$ (Ru^{II}, 0.1570; Fe^{III}, 2.5338; $(L^{\bullet}_{Me})^{2-}$, -0.6907) (right).

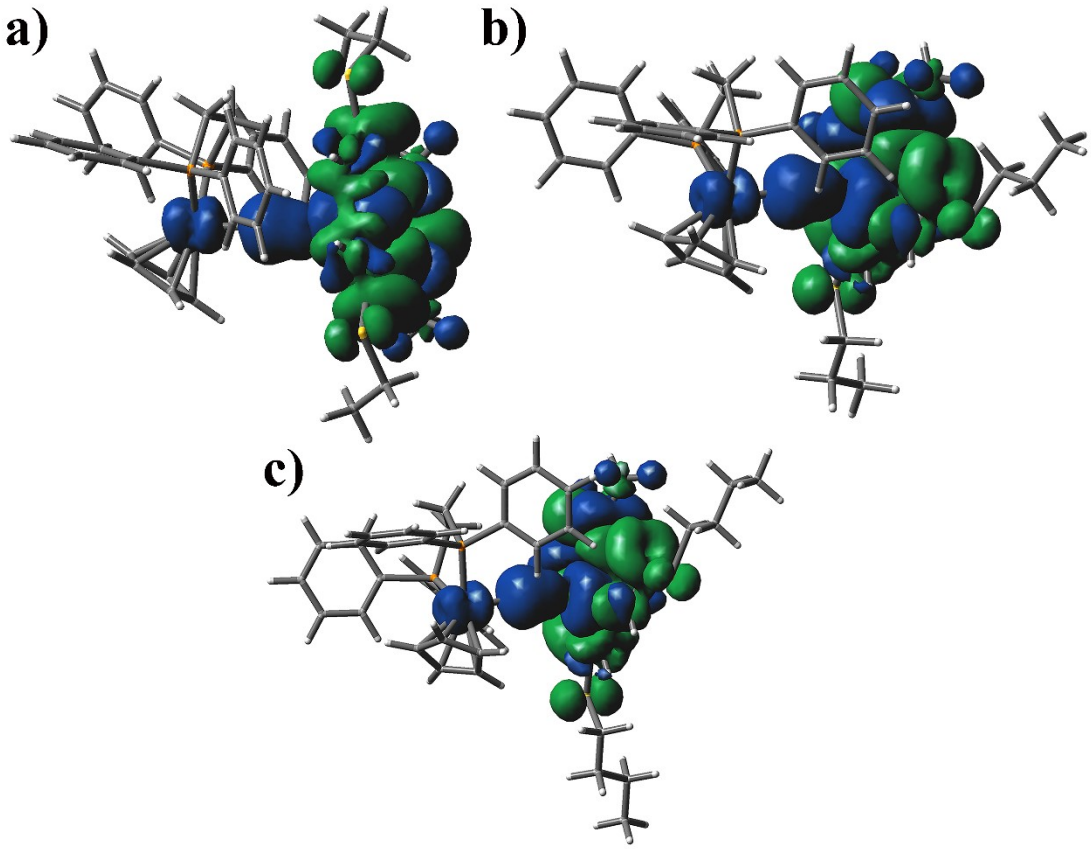

Fig. S16 The computed spin density distribution of $\mathbf{1_{Et}[PF_6]}$ (**a**, Ru^{II}, 0.1381; Fe^{III}, 2.5379; $(L^{\bullet}_{Et})^{2-}$, -0.6760), $\mathbf{1_{Pr}[PF_6]}$ (**b**, Ru^{II}, 0.1393; Fe^{III}, 2.5459; $(L^{\bullet}_{Pr})^{2-}$, -0.6852**)** and $\mathbf{1_{Bu}[PF_6]}$ (**c**, Ru^{II}, 0.1390; Fe^{III}, 2.5456; $(L^{\bullet}_{Bu})^{2-}$, -0.6846**)**

Optimized Cartesian Coordinates of complex $\mathbf{1}_{Me}^{+}$

Atom	X	Y	Z	Atom	X	Y	Z
Ru	-1.488125	0.000979	1.375916	C	2.921188	0.437353	-2.880926
Fe	3.351863	-0.073686	-0.227317	C	0.060792	-5.534478	-1.126953
P	-2.288307	-1.547844	-0.286787	H	0.589178	-6.467436	-1.306764
P	-1.81547	1.63047	-0.358774	C	-0.843646	0.240067	3.591859
S	5.360682	1.574954	3.479615	H	0.188216	0.390338	3.878289
S	2.463679	1.181804	-4.481002	C	-5.098588	4.022337	0.560838
N	4.341904	-1.239645	0.962826	H	-5.383415	4.666032	1.389021
N	4.095843	1.236766	0.962565	C	3.369299	-3.598655	-2.738598
H	3.999543	2.247168	0.908145	H	2.33564	-3.500299	-3.090424
N	4.859368	-0.65525	2.104083	H	3.569526	-4.644272	-2.490319
N	1.498615	-0.298326	0.418233	H	4.008794	-3.295834	-3.57598
N	3.410155	-1.370515	-1.667232	C	-5.111767	-1.232528	-0.02103
N	3.115167	1.103253	-1.723719	H	-4.925033	-0.18034	-0.223616
H	2.98769	2.111907	-1.699455	C	-5.95589	3.878118	-0.548647
N	3.064242	-0.904001	-2.924491	H	-6.904789	4.406979	-0.578351
C	4.696789	0.683612	2.036508	C	-6.42932	-1.652359	0.233824
C	0.348983	-0.202882	0.741396	H	-7.239643	-0.928347	0.206371
C	-3.48081	2.504396	-0.474116	C	0.437468	3.229347	0.396339
C	-1.623572	0.677775	-1.997351	H	0.561915	2.502219	1.193204
H	-1.918505	1.304182	-2.847055	C	5.051883	-3.363499	2.014591
H	-0.549539	0.484298	-2.089733	H	5.051145	-4.436761	1.80588
C	-4.047878	-2.162993	0.004021	H	4.495893	-3.168743	2.939154
C	3.608132	-2.708245	-1.543126	H	6.080442	-3.034794	2.205694
C	-1.32971	-3.122555	-0.649687	C	-3.067129	0.634182	2.987696
C	-3.872219	3.337227	0.598725	H	-3.997205	1.137342	2.765799
H	-3.216732	3.466365	1.456983	C	-4.319481	-3.513279	0.308208
C	-2.414146	-0.645785	-1.983831	H	-3.516758	-4.243987	0.338483
H	-2.034127	-1.317384	-2.760053	C	-1.794471	1.272815	3.29156
H	-3.478444	-0.478492	-2.177178	H	-1.615571	2.336975	3.359406
C	-0.323554	-3.548713	0.239251	C	-6.697781	-3.003448	0.530477

H	-0.077911	-2.94181	1.105365	H	-7.715859	-3.32744	0.729775
C	-2.880379	-0.77949	3.09334	C	-5.573187	3.050876	-1.619753
H	-3.641246	-1.529739	2.928133	H	-6.225079	2.938922	-2.482348
C	0.366777	-4.753166	0.002452	C	1.315764	4.326186	0.290893
H	1.13483	-5.077988	0.699867	H	2.106383	4.45908	1.026644
C	-0.615283	3.07534	-0.52767	C	-0.781807	4.027578	-1.557962
C	-1.636557	-3.91027	-1.782606	H	-1.60937	3.941575	-2.258403
H	-2.426537	-3.611309	-2.468225	C	0.101674	5.116998	-1.667783
C	4.457173	-2.590965	0.86119	H	-0.041422	5.851866	-2.455818
C	-4.340603	2.368339	-1.58418	C	-5.639586	-3.929678	0.570474
H	-4.06726	1.746491	-2.431888	H	-5.836731	-4.973109	0.802439
C	4.067131	-3.257394	-0.322331	C	2.646993	3.017931	-4.09477
H	4.195414	-4.334647	-0.315242	H	3.66635	3.236946	-3.766972
C	-0.940783	-5.108236	-2.022663	H	1.909605	3.344784	-3.357503
H	-1.186114	-5.70959	-2.89412	H	2.458306	3.528131	-5.04232
C	-1.500629	-1.040181	3.44622	C	5.101339	3.364871	2.954347
H	-1.069832	-2.006885	3.663886	H	5.647847	3.580521	2.032401
C	1.152615	5.270527	-0.740562	H	5.520088	3.964537	3.765759
H	1.82112	6.124911	-0.812283	H	4.036711	3.594454	2.855051

Optimized Cartesian Coordinates of complex $\mathbf{1}_{Et}^{+}$

Atom	X	Y	Z	Atom	X	Y	Z
Ru	1.480552	0.731492	-1.432398	C	-4.183673	-2.942118	-0.885825
Fe	-3.070434	-0.241712	0.561482	H	-4.450852	-3.836672	-1.438717
P	2.316332	-1.329019	-0.528738	C	-1.442026	4.00416	1.436639
P	1.886241	1.58413	0.78243	H	-2.136121	4.558041	0.808671
S	-1.258748	-1.32413	4.516513	C	1.975992	-1.251992	1.344456
S	-5.394463	3.286901	-0.924779	H	0.904477	-1.454158	1.444232
N	-4.427781	-0.548121	-0.792155	H	2.51136	-2.058053	1.859806
N	-1.420208	-0.081315	-0.507934	C	2.005746	0.470375	-3.674019
N	-3.039208	-2.117934	1.066564	H	2.093933	-0.484671	-4.172908
N	-2.398005	-2.418307	2.263018	C	0.405614	2.62033	3.045249
N	-2.394063	-0.079549	2.337413	H	1.126034	2.119046	3.686353

N	-5.066126	0.576896	-1.285766	C	6.415473	-1.934375	0.215654
N	-3.827268	1.503743	0.46522	H	7.083477	-1.936215	1.073218
C	-0.309053	0.21398	-0.845062	C	-5.606193	-1.746433	-2.611106
C	-2.087901	-1.268442	2.897303	H	-5.221505	-1.077847	-3.389985
C	1.560557	-2.96975	-1.056493	H	-6.603158	-1.372298	-2.348465
C	-3.433667	-3.161196	0.29711	H	-5.700471	-2.758017	-3.014898
C	-4.701699	-1.732892	-1.401126	C	3.375627	2.727706	0.966095
C	4.160056	-1.673795	-0.698261	C	-1.54284	4.078236	2.839993
C	4.67254	-1.940799	-1.98846	H	-2.320624	4.680615	3.302622
H	4.004721	-1.964611	-2.846647	C	-0.619194	3.378882	3.643316
C	-4.696773	1.653378	-0.553743	H	-0.682548	3.439595	4.726548
C	0.813917	1.266222	-3.588556	C	4.63976	2.255904	0.543284
H	-0.159493	0.992611	-3.97171	H	4.744474	1.258457	0.122181
C	0.46001	-2.991749	-1.936042	C	0.431252	-5.431377	-1.853133
H	0.045491	-2.059047	-2.30595	H	0.003115	-6.380138	-2.167112
C	1.135975	2.49645	-2.900344	C	1.531959	-5.411905	-0.972808
H	0.468237	3.330852	-2.740316	H	1.953456	-6.344274	-0.606
C	-0.101216	-4.220658	-2.333841	C	3.262309	4.036112	1.47876
H	-0.944157	-4.229736	-3.02048	H	2.300566	4.420992	1.803761
C	5.04273	-1.674658	0.401886	C	-1.235343	-3.194098	4.907134
H	4.682089	-1.488532	1.409435	H	-1.188214	-3.218028	6.000311
C	-0.429911	3.226935	0.84061	H	-2.199386	-3.584644	4.575927
H	-0.369425	3.152487	-0.2412	C	5.775771	3.077295	0.648833
C	2.097613	-4.186292	-0.578908	H	6.74326	2.702735	0.324361
H	2.964419	-4.185678	0.078098	C	-6.471522	2.939708	-2.463842
C	-3.098531	-4.568678	0.730725	H	-6.985805	1.997064	-2.268158
H	-3.481354	-5.298389	0.012352	H	-7.194709	3.761014	-2.448699
H	-3.525979	-4.778675	1.718253	C	4.401564	4.859802	1.575996
H	-2.013336	-4.692221	0.827038	H	4.302877	5.867168	1.972118
C	6.040487	-2.203097	-2.173999	C	-5.662416	2.898035	-3.763581
H	6.419044	-2.415355	-3.170499	H	-4.939448	2.075781	-3.744968
C	2.551731	2.464016	-2.597425	H	-5.125314	3.837822	-3.934396
H	3.107903	3.245304	-2.097799	H	-6.342505	2.736759	-4.61152
C	3.090807	1.223959	-3.062452	C	5.659791	4.383397	1.165563
H	4.125761	0.918392	-3.006797	H	6.537246	5.019963	1.243537

C	2.328325	0.120074	1.953298	C	-0.062486	-3.933147	4.256178
H	3.400716	0.206046	2.154746	H	-0.08514	-4.989843	4.557006
H	1.800652	0.247061	2.903472	H	0.900857	-3.513942	4.569616
C	6.918452	-2.196954	-1.071186	H	-0.135349	-3.887369	3.1648
H	7.976387	-2.400624	-1.213782	H	-2.168366	0.774977	2.844125
C	0.503216	2.53349	1.638874	H	-3.55593	2.321971	1.007262

Optimized Cartesian Coordinates of complex $\mathbf{1}_{Pr}^{+}$

Atom	X	Y	Z	Atom	X	Y	Z
Ru	1.846021	-0.055128	-1.160161	H	5.080244	-0.257712	2.525392
Fe	-3.057547	-0.524691	0.159967	C	2.075482	-4.698764	2.9282
P	2.337125	1.952047	0.080895	H	2.555545	-5.227079	3.747974
P	2.717661	-1.163387	0.793405	C	0.924559	-5.236462	2.317225
S	-3.461034	-4.903719	-0.926609	H	0.513751	-6.180549	2.666194
S	-4.913306	3.281306	-1.328182	C	5.088497	-2.431032	-0.124079
N	-3.014608	-1.897239	1.532632	H	4.426046	-2.906474	-0.843319
N	-3.516533	0.845595	1.458421	C	2.613187	-3.482742	2.47119
N	-4.023988	2.034694	0.949201	H	3.51655	-3.092106	2.933635
N	-1.119553	-0.244872	-0.112651	C	0.313134	-4.552882	1.250124
N	-3.068705	-3.205577	1.096375	H	-0.576916	-4.959493	0.778825
N	-3.907633	0.735076	-0.992272	C	-2.496522	-2.890943	3.740993
H	-4.10731	0.649391	-1.986839	H	-2.299169	-2.575373	4.769155
N	-3.464609	-2.06999	-0.908318	H	-1.637541	-3.454768	3.359348
H	-3.687962	-2.096598	-1.899623	H	-3.346711	-3.58364	3.734119
C	0.030942	-0.15122	-0.436953	C	-3.412498	2.067661	3.605389
C	1.043592	3.299066	0.291313	H	-2.820454	2.885906	3.179206
C	3.844079	2.897898	-0.549922	H	-3.110242	1.898846	4.642471
C	1.251966	4.355377	1.207829	H	-4.457245	2.400903	3.586917
H	2.160584	4.400217	1.804546	C	-3.884997	-4.528894	-2.747343
C	-2.780925	-1.698513	2.859464	H	-4.812325	-3.944734	-2.763916
C	-0.125106	3.283534	-0.494403	H	-3.05911	-3.944669	-3.168594
H	-0.293789	2.470601	-1.19376	C	7.32914	-2.161774	0.802284
C	1.998706	-2.792561	1.401778	H	8.387462	-2.408698	0.79481

C	3.719419	4.170289	-1.146285	C	2.831193	0.684693	-3.154385
H	2.749886	4.654978	-1.212571	H	3.324338	1.643465	-3.236167
C	2.835645	1.482261	1.88071	C	6.819223	-1.260158	1.753542
H	3.919169	1.615722	1.95755	H	7.481933	-0.808657	2.487475
H	2.361984	2.194484	2.563644	C	6.45685	-2.75079	-0.135128
C	-3.326011	-3.227864	-0.232991	H	6.840009	-3.457725	-0.866473
C	4.855049	4.82975	-1.656296	C	1.199543	-0.978901	-3.186459
H	4.746204	5.810629	-2.111892	H	0.256461	-1.492952	-3.30874
C	4.568402	-1.523278	0.826358	C	1.426422	0.437197	-3.387671
C	6.123308	4.226093	-1.574823	H	0.701766	1.1578	-3.738678
H	6.998867	4.738055	-1.965391	C	3.460735	-0.547156	-2.784554
C	-3.245329	0.810147	2.785163	H	4.51177	-0.687381	-2.577767
C	-1.078002	4.313289	-0.368942	C	2.441379	-1.584708	-2.800962
H	-1.97643	4.291312	-0.980142	H	2.598393	-2.638867	-2.619494
C	0.298343	5.3801	1.336659	C	-4.063079	-5.850362	-3.519026
H	0.469487	6.191382	2.039573	H	-4.160031	-5.587982	-4.582556
C	-4.221112	1.89787	-0.376542	H	-3.149953	-6.455136	-3.431347
C	-2.849932	-0.400211	3.409386	C	-5.292709	-6.675085	-3.084253
H	-2.644876	-0.331256	4.47264	H	-5.38718	-7.574681	-3.703781
C	2.41803	0.042347	2.237545	H	-6.217085	-6.092735	-3.194744
H	1.340428	-0.012332	2.428206	H	-5.219761	-6.994316	-2.03787
H	2.929993	-0.308208	3.141381	C	-5.434763	4.493355	0.055718
C	0.84927	-3.333306	0.792198	H	-6.144255	3.95902	0.692268
H	0.375315	-2.80806	-0.031124	H	-4.538109	4.723258	0.635977
C	6.250762	2.952247	-0.986446	C	-6.058223	5.74221	-0.585467
H	7.225445	2.475063	-0.923801	H	-5.33246	6.222959	-1.255975
C	5.117668	2.288357	-0.483504	H	-6.922807	5.455519	-1.199126
H	5.237482	1.295819	-0.055564	C	-6.507515	6.749016	0.497939
C	-0.868131	5.361595	0.545366	H	-5.660576	7.077053	1.115185
H	-1.600083	6.160083	0.639234	H	-7.261315	6.307929	1.162929
C	5.445746	-0.944198	1.767172	H	-6.94952	7.639002	0.034342

Optimized Cartesian Coordinates of complex $\mathbf{1}_{Bu}^{+}$

Atom	X	Y	Z	Atom	X	Y	Z
Ru	2.009182	0.051834	-1.164517	H	4.83522	-2.531673	-0.770873
Fe	-2.79755	-0.747948	0.351506	C	2.868235	0.759408	-3.227244
P	2.354529	2.161	-0.051114	H	3.266595	1.75303	-3.379471
P	3.015546	-0.864497	0.822724	C	-3.377519	-4.986482	-2.270681
S	-2.86841	-5.206704	-0.446177	H	-4.360064	-4.500901	-2.289373
S	-5.021217	2.787602	-1.291142	H	-2.62766	-4.346592	-2.749388
N	-3.326158	0.660437	1.581047	C	-3.252217	2.022583	3.643208
N	-2.591332	-2.021114	1.803075	H	-2.747999	2.857993	3.143725
N	-3.108359	-2.387433	-0.602908	H	-2.900085	1.946811	4.675537
H	-3.36334	-2.496463	-1.580884	H	-4.321667	2.265863	3.646971
N	-0.900926	-0.324418	-0.015279	C	-5.587856	4.043539	0.034723
N	-3.949934	1.768285	1.020583	H	-6.217218	3.493943	0.738893
N	-2.550266	-3.354805	1.450819	H	-4.690071	4.388108	0.553243
N	-3.791533	0.360077	-0.840491	C	3.620841	-0.384838	-2.808038
H	-4.017273	0.19434	-1.819239	H	4.685636	-0.414754	-2.628019
C	1.087683	4.523645	0.968311	C	1.487835	0.369278	-3.40222
H	1.999983	4.679355	1.540253	H	0.689425	0.997447	-3.770462
C	-2.849713	-3.484005	0.136343	C	7.69572	-1.459796	0.765161
C	3.760769	3.193293	-0.772774	H	8.771171	-1.614704	0.743173
C	0.954301	3.403223	0.116338	C	6.859032	-2.167546	-0.121192
C	0.227527	-0.153904	-0.382537	H	7.28729	-2.874188	-0.827367
C	0.051591	5.469011	1.062865	C	-6.347747	5.186298	-0.653606
H	0.164927	6.330478	1.716004	H	-5.699374	5.682883	-1.39012
C	-2.329833	-1.718832	3.105033	H	-7.211415	4.786215	-1.203327
C	3.514025	4.415054	-1.433594	C	2.703811	-1.511313	-2.73398
H	2.505173	4.811443	-1.499798	H	2.964132	-2.53367	-2.497553
C	5.083172	2.698305	-0.707911	C	7.128832	-0.559146	1.684587
H	5.297483	1.745164	-0.230296	H	7.764664	-0.016102	2.379218
C	4.890961	-1.061022	0.827322	C	1.40063	-1.047395	-3.113697
C	-0.223023	3.243496	-0.639885	H	0.507546	-1.653101	-3.177748
H	-0.333444	2.380353	-1.288981	C	-3.436537	-6.361776	-2.960884
C	4.577112	5.138441	-2.00907	H	-3.59438	-6.176296	-4.034299
H	4.374239	6.079375	-2.514072	H	-2.461952	-6.863564	-2.873817
C	-3.007277	0.732945	2.895598	C	-4.556926	-7.292577	-2.443932

C	-1.258836	4.193694	-0.549034	H	-5.524123	-6.773798	-2.527101
H	-2.163469	4.06043	-1.136473	H	-4.406798	-7.50233	-1.375812
C	2.929109	1.838998	1.758377	C	-4.61399	-8.620736	-3.226092
H	3.998904	2.06626	1.799321	H	-5.415111	-9.266721	-2.846883
H	2.41157	2.547269	2.413001	H	-3.668878	-9.173348	-3.137717
C	-2.489432	-0.397991	3.576685	H	-4.802309	-8.445368	-4.293976
H	-2.254587	-0.244036	4.624771	C	-6.841784	6.231133	0.376911
C	-4.180876	1.530568	-0.285388	H	-7.492795	5.737423	1.113749
C	-1.915974	-2.824976	4.045862	H	-5.981423	6.631295	0.934807
H	-1.706043	-2.428315	5.042994	C	-7.608153	7.392039	-0.290686
H	-1.029494	-3.343659	3.663223	H	-6.972512	7.923955	-1.011261
H	-2.706886	-3.581245	4.118844	H	-7.950435	8.119375	0.455874
C	2.642753	0.39195	2.205383	H	-8.491277	7.023991	-0.829523
H	1.57771	0.257978	2.425292	C	2.72486	-4.317616	3.159379
H	3.200664	0.138425	3.114422	H	3.263724	-4.756068	3.99544
C	5.894036	4.649718	-1.929282	C	3.145341	-3.086507	2.626192
H	6.71345	5.211077	-2.370521	H	4.01874	-2.593752	3.046824
C	-1.123381	5.306243	0.301209	C	2.45388	-2.512804	1.53519
H	-1.91982	6.043362	0.36823	C	1.34639	-3.184525	0.980822
C	6.143525	3.426344	-1.276437	H	0.814282	-2.748461	0.141087
H	7.156754	3.03757	-1.214398	C	0.9278	-4.418954	1.515038
C	5.733586	-0.362395	1.717291	H	0.069085	-4.927119	1.085993
H	5.325159	0.327301	2.450273	C	1.615431	-4.986474	2.603554
C	5.468563	-1.966525	-0.091465	H	1.295432	-5.941898	3.011713

Optimized Cartesian Coordinates of complex 2_{Me}^{+}

Atom	X	Y	Z	Atom	X	Y	Z
Ru	1.545588	0.009434	-1.172124	C	0.632703	4.817216	2.584472
Fe	-3.428431	-0.14094	-0.096318	H	0.892245	5.418371	3.452075
P	2.125705	-1.67869	0.451883	C	-0.826346	4.362452	0.686073
P	2.238206	1.521543	0.572816	H	-1.701038	4.60058	0.087588
S	-4.438421	-4.489846	-0.87865	C	1.811829	-0.846158	2.140185
S	-4.583712	3.733257	-2.04162	H	0.728535	-0.729375	2.246932

N	-4.083003	2.586037	0.40384	H	2.169378	-1.497776	2.944992
N	-3.701827	-1.381623	1.3732	C	2.517756	0.52297	2.192571
N	-3.801297	1.386226	1.050771	H	3.596257	0.394876	2.329076
N	-1.461415	-0.111632	-0.231235	H	2.14252	1.116066	3.032624
N	-4.010077	1.112161	-1.411508	C	4.298961	-3.07897	1.690147
H	-4.159259	0.963463	-2.407413	H	3.557785	-3.426455	2.406277
C	3.918741	-2.241689	0.615295	C	6.606571	-3.079469	0.897098
N	-3.915332	-2.701626	1.033135	H	7.638223	-3.404473	1.004016
N	-3.966573	-1.704555	-1.08003	C	-3.664325	1.42969	2.396101
H	-4.105236	-1.78647	-2.083913	C	-0.305551	-5.706856	0.518876
C	3.882129	3.733682	-0.21414	H	-0.872125	-6.634317	0.525503
H	2.947519	4.268175	-0.360621	C	1.748323	-4.485877	0.024906
C	5.097061	4.384305	-0.499323	H	2.768653	-4.489873	-0.348394
H	5.085002	5.406022	-0.870131	C	-0.50271	5.139865	1.812999
C	1.441805	3.726105	2.223309	H	-1.120455	5.991951	2.08618
H	2.33289	3.509486	2.80875	C	-0.162019	-3.315932	0.984588
C	-4.194984	2.357279	-0.91709	H	-0.643511	-2.404987	1.328343
C	4.894883	-1.83048	-0.313082	C	1.014183	-5.686198	0.03018
H	4.616321	-1.180505	-1.135347	H	1.473299	-6.597984	-0.343305
C	-0.295394	-0.063312	-0.51375	C	5.635259	-3.491432	1.832265
C	1.119055	2.943316	1.091019	H	5.915857	-4.135409	2.661605
C	0.855758	0.62444	-3.327676	C	-0.892298	-4.518413	0.993147
C	6.321778	3.719934	-0.299136	H	-1.917094	-4.5176	1.352742
H	7.259919	4.22536	-0.512772	C	-5.144689	5.072344	-0.832985
C	3.877851	2.40814	0.27331	H	-5.305115	5.963249	-1.444543
C	1.168574	-3.293945	0.512516	H	-4.366634	5.241869	-0.08934
C	-3.500597	0.234382	3.14477	H	-6.0719	4.761221	-0.350923
H	-3.38966	0.367779	4.215762	C	2.6016	-0.911765	-3.035441
C	-3.566741	-1.10196	2.701191	H	3.15239	-1.841991	-3.003108
C	5.108621	1.741618	0.459662	C	-4.068474	-2.802307	-0.310429
H	5.14136	0.715465	0.814697	C	3.140101	0.403393	-2.825494
C	-3.553327	-2.240435	3.694269	H	4.173204	0.662305	-2.642984
H	-3.408123	-1.866166	4.711173	C	-3.735938	2.760725	3.106044
H	-2.761054	-2.959784	3.455866	H	-3.589606	2.635538	4.182201
H	-4.496024	-2.798813	3.648471	H	-4.707675	3.237188	2.929327

C	2.051963	1.34866	-2.998664	H	-2.975617	3.444948	2.712588
H	2.140247	2.425709	-2.954871	C	-0.472314	1.218574	-3.713833
C	6.322654	2.396906	0.182161	H	-1.307065	0.630595	-3.316854
H	7.262711	1.874974	0.342286	H	-0.567772	1.245238	-4.808424
C	1.192274	-0.789664	-3.314564	H	-0.57565	2.246286	-3.348082
H	0.520716	-1.600687	-3.56017	C	-4.557471	-4.232332	-2.74058
C	6.233102	-2.250306	-0.176068	H	-3.60559	-3.877615	-3.144187
H	6.975567	-1.931584	-0.903341	H	-5.379219	-3.554545	-2.98648
C	-0.01868	3.265368	0.327215	H	-4.775852	-5.219981	-3.152824
H	-0.273939	2.663538	-0.539405				

Optimized Cartesian Coordinates of complex 3_{Me}^{+}

Atom	X	Y	Z	Atom	X	Y	Z
Ru	-1.399828	0.054579	0.997567	C	-5.063411	3.822769	-2.330754
Fe	3.56303	-0.14735	-0.134417	H	-5.223833	4.525037	-3.14468
P	-1.81401	1.757712	-0.682059	C	-1.422367	-3.712433	-2.37214
P	-2.146638	-1.432449	-0.786847	H	-2.263348	-3.439255	-3.006043
S	4.406845	-4.300072	1.470042	C	-2.016102	-1.178201	2.884356
S	4.989097	4.065737	0.74129	C	-0.706048	-0.615629	3.088115
N	3.898771	1.108878	-1.576606	C	-4.471834	-0.256559	2.784657
N	3.922958	-2.897485	-0.747388	H	-4.992692	0.697432	2.651109
N	4.094785	-1.50215	1.121165	H	-4.795477	-0.661417	3.754824
N	4.247288	2.39569	-1.203706	H	-4.825008	-0.948026	2.011066
N	4.268431	1.328288	0.876026	C	-0.832642	0.839516	3.070376
N	3.733672	-1.661109	-1.338658	C	3.534295	-1.647701	-2.682255
C	0.438068	-0.007691	0.338348	C	-2.213107	-0.430775	-2.43179
C	-3.767879	3.345988	-2.065162	H	-1.809308	-1.06074	-3.230759
H	-2.936398	3.699543	-2.670509	H	-3.264275	-0.231916	-2.662757
C	4.118747	-2.736205	0.577307	C	-2.382906	-2.635236	2.985665
C	3.690335	0.888813	-2.901912	H	-2.587654	-2.899372	4.03417
C	-0.762126	3.315263	-0.675389	H	-1.57827	-3.290252	2.634342
C	-0.490318	5.682189	-0.117175	H	-3.283558	-2.866998	2.40972
H	-0.912071	6.609039	0.263582	C	5.145862	3.735394	2.588683

C	-3.545739	2.43274	-1.008553	H	5.466304	4.685178	3.022831
C	0.712937	-4.48905	-0.713099	H	5.911094	2.979346	2.783902
H	1.541962	-4.781463	-0.075043	H	4.180234	3.453558	3.016596
C	-4.635779	2.007433	-0.226767	C	-0.674832	-4.861947	-2.681606
H	-4.471981	1.296239	0.575166	H	-0.93	-5.452452	-3.557928
C	3.434465	-2.958583	-3.424423	C	0.26452	1.819538	3.396432
H	3.247553	-2.789116	-4.488312	H	0.352366	1.96217	4.484357
H	2.63221	-3.576191	-3.005208	H	0.076873	2.800723	2.947572
H	4.360101	-3.535232	-3.308881	H	1.234122	1.469192	3.024806
C	4.448436	2.436958	0.132118	C	1.381694	4.433555	-1.044824
C	-0.03393	-3.334318	-0.406302	H	2.416426	4.383098	-1.370727
H	0.21962	-2.73701	0.464096	C	-2.972693	-0.08394	2.764713
C	-1.290561	4.52643	-0.174481	C	0.393203	-5.254934	-1.848884
H	-2.325037	4.581063	0.153659	H	0.96659	-6.148514	-2.082517
N	1.610301	-0.032103	0.072397	C	4.72086	-3.675288	3.219395
C	-5.933917	2.489577	-0.487536	H	5.601854	-3.028684	3.24503
H	-6.767411	2.157423	0.126703	H	4.91972	-4.57128	3.811806
C	0.584322	3.275259	-1.098111	H	3.838183	-3.16996	3.620415
H	1.025768	2.349058	-1.45365	C	-5.026894	-1.456322	-0.981939
C	3.469556	-0.421441	-3.384869	H	-4.951604	-0.428862	-1.324189
H	3.305787	-0.50443	-4.454193	C	-6.306007	-2.02977	-0.855808
C	3.758303	2.053771	-3.861683	H	-7.184277	-1.442437	-1.111917
H	3.051648	2.841142	-3.574388	C	-6.448793	-3.355636	-0.405222
H	3.54237	1.728273	-4.882794	H	-7.436547	-3.799084	-0.310675
H	4.753757	2.513099	-3.834157	C	-5.300841	-4.104379	-0.083756
C	0.846527	5.640267	-0.556198	H	-5.397569	-5.130634	0.261447
H	1.464406	6.533537	-0.516126	C	-4.021168	-3.534124	-0.216176
C	-1.10589	-2.941427	-1.229862	H	-3.147775	-4.135973	0.017562
C	-2.824528	2.537339	3.006156	C	-3.870141	-2.205023	-0.672258
H	-2.137667	3.299935	2.624127	C	-2.237748	1.153557	2.901729
H	-3.025017	2.777274	4.060828	C	0.54676	-1.378743	3.43057
H	-3.769768	2.633229	2.464385	H	0.482987	-2.424289	3.10991
C	-6.150683	3.397312	-1.540066	H	0.706127	-1.376657	4.519328
H	-7.150927	3.771334	-1.742839	H	1.4312	-0.935596	2.96004
C	-1.423853	0.890082	-2.335737	H	4.448207	1.368988	1.875681

H	-1.67918	1.554784	-3.16863	H	4.273261	-1.395372	2.116216
H	-0.346138	0.701124	-2.360051				