Supporting information: On the role of solvent effects on the electronic transitions in Fe(II) and Ru(II) complexes

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April 1, 2016

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S1 $[Fe(phen)_3]^{2+}$: complete active space orbitals, CAS(10,12).

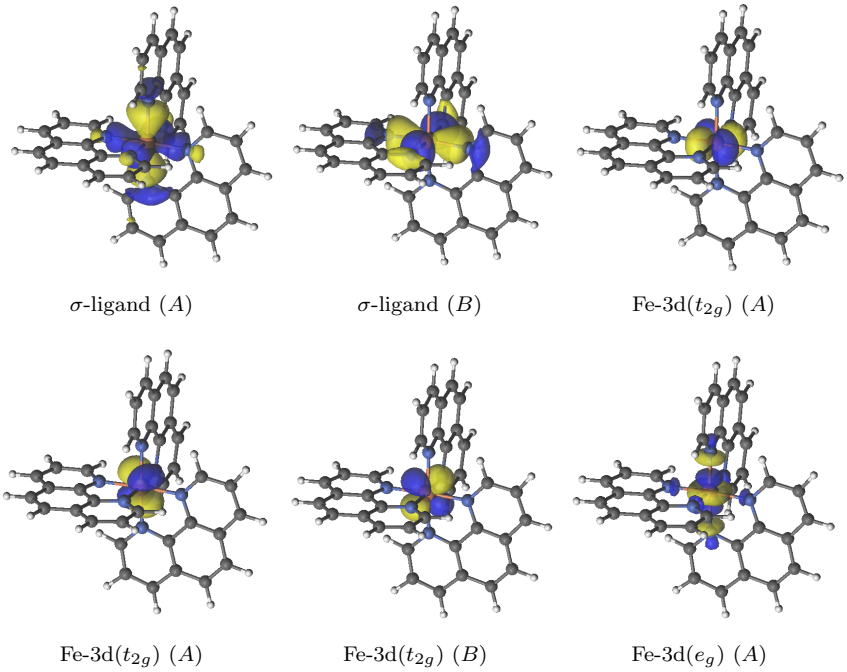


Figure S1.1: CAS(10,12) orbitals. The irreductible representation in parenthesis.

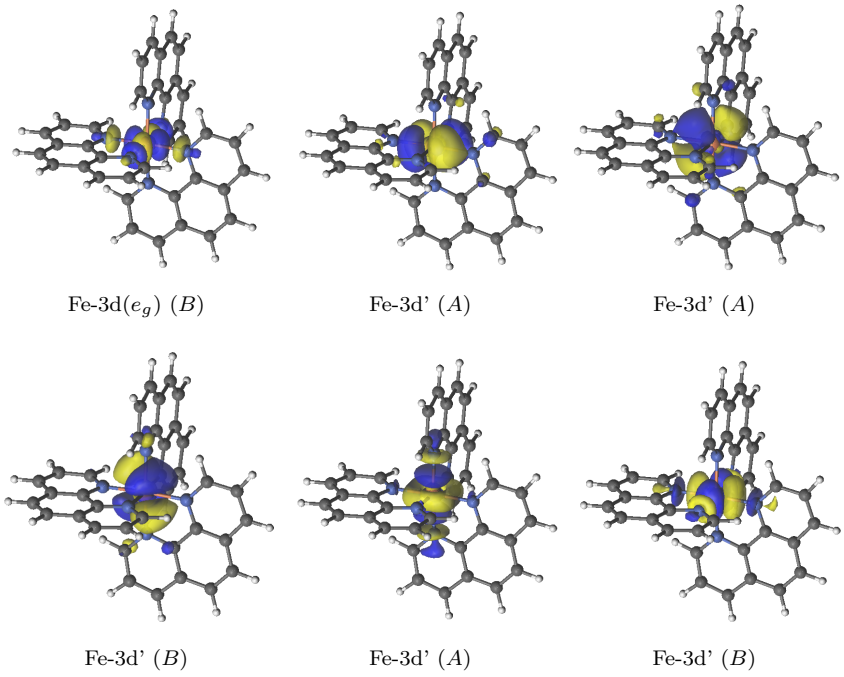
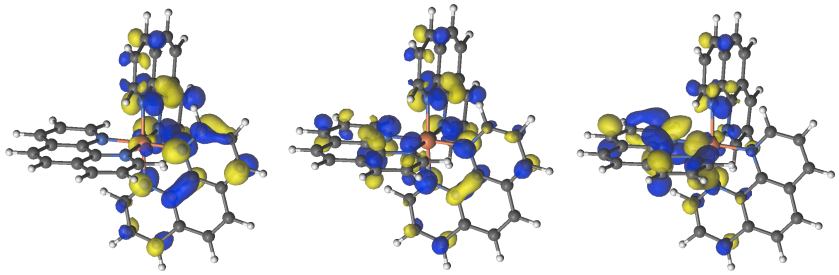
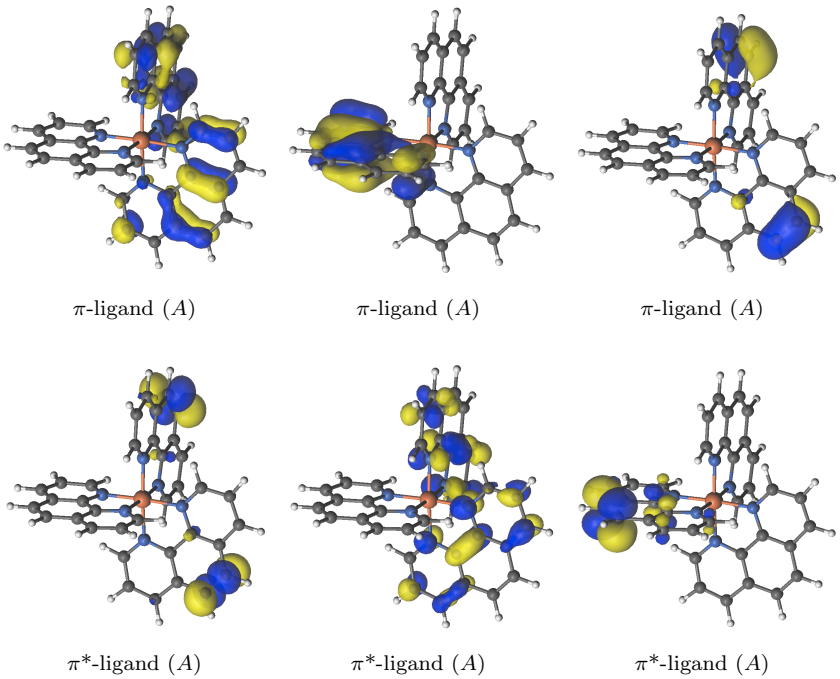


Figure S1.1: (*Continued*) CAS(10,12) orbitals. The irreductible representation in parenthesis.



π*-ligand (A) π*-ligand (B) π*-ligand (B)

Figure S1.2: Orbitals added in the CAS(10,15) calculation. The irreductible representation in parenthesis.



π-ligand (A) π-ligand (A) π-ligand (A)

π*-ligand (A) π*-ligand (A) π*-ligand (A)

Figure S1.3: CAS(12,12) orbitals. The irreductible representation in parenthesis.

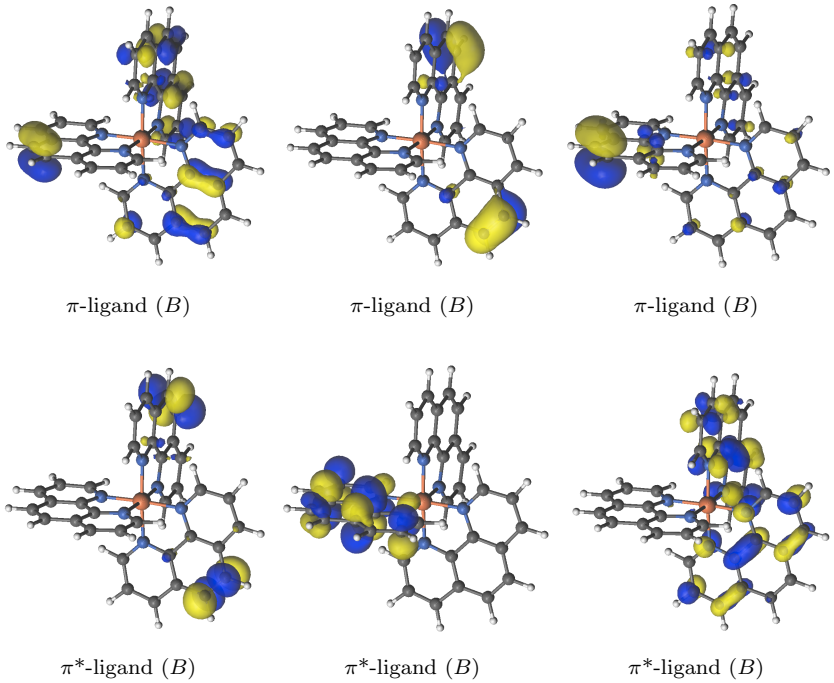


Figure S1.3: (*Continued*) CAS(12,12) orbitals. The irreductible representation in parenthesis.

S2 trans(Cl)-Fe(bpy)$Cl_2(CO)_2$: complete active space orbitals, CAS(10,14).

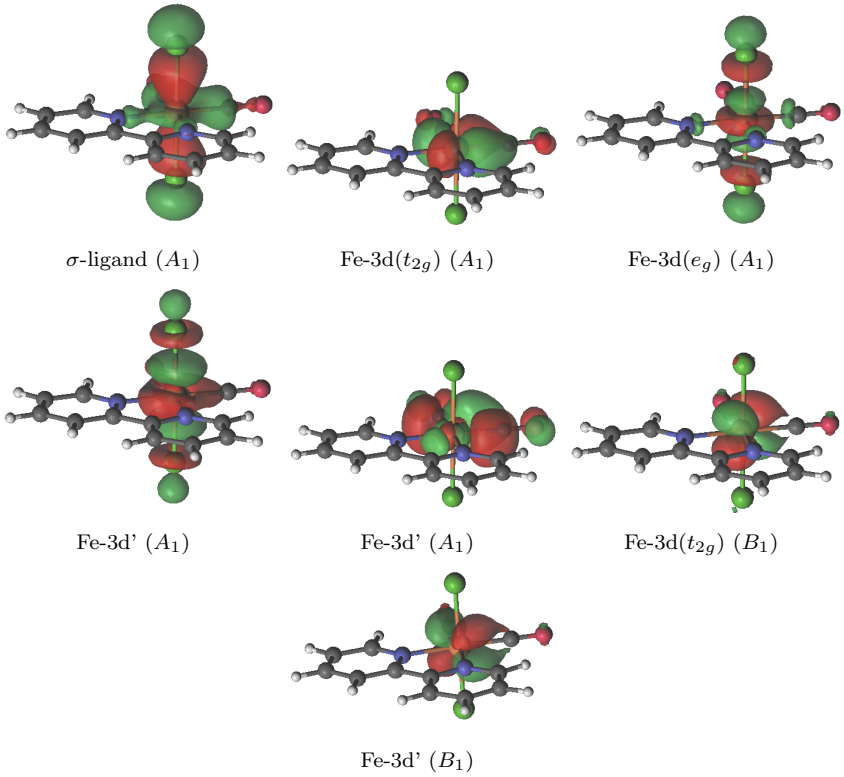


Figure S2.1: CAS(10,14) orbitals. The irreductible representation in parenthesis.

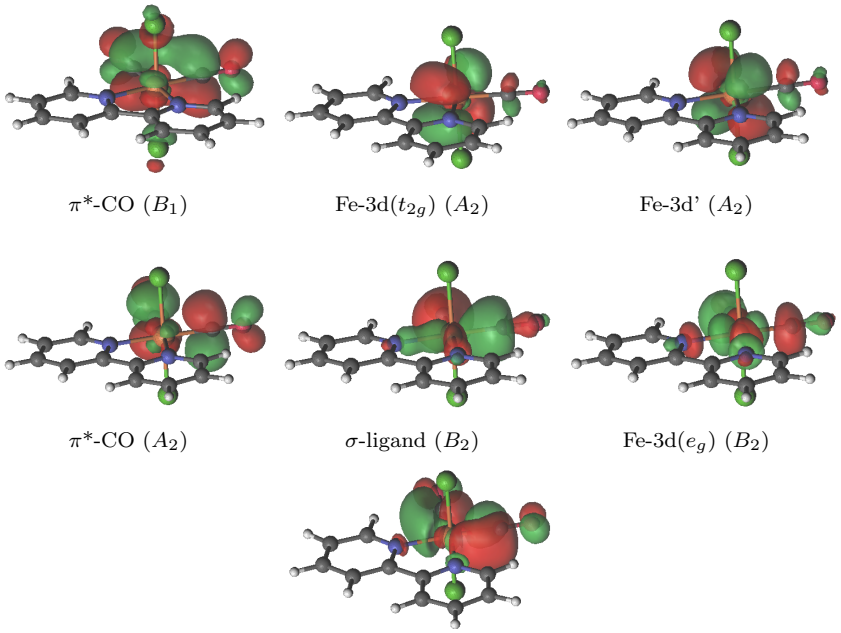


Figure S2.1: (*Continued*) CAS(10,14) orbitals. The irreductible representation in parenthesis.

S3 trans(Cl)-Ru(bpy)$Cl_2(CO)_2$: complete active space orbitals, CAS(10,14).

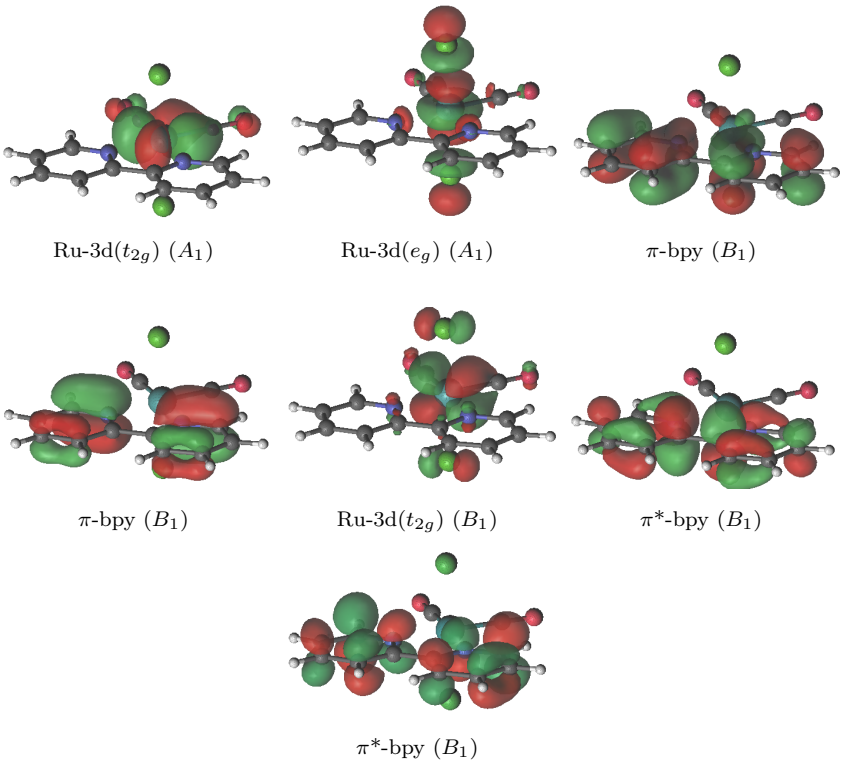


Figure S3.1: CAS(10,14) orbitals. The irreductible representation in parenthesis.

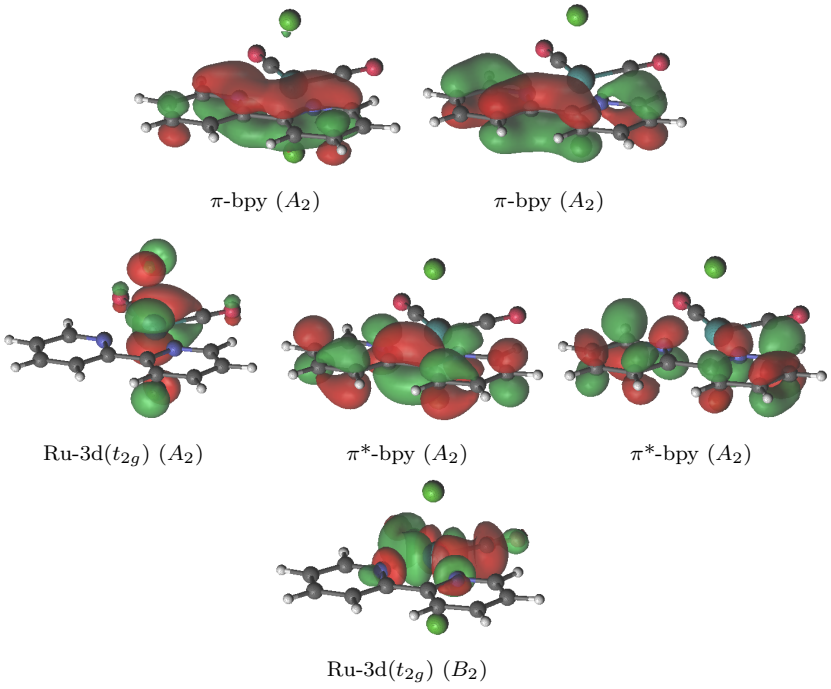


Figure S3.1: (*Continued*) CAS(14,13) orbitals. The irreductible representation in parenthesis.

S4 trans(Cl)-Ru(bpy)$Cl_2(CO)_2$: Selected PBE0 bond distances and angles

Table S4.1: Selected distances, angles and dihedral angles for trans(Cl)-Ru(bpy)$Cl_2(CO)_2$. The experimental structure is compared to the LS optimized geometry. Atom labels are defined in Figure S4.1.

	Exp. [1]	PBE0/def2-TZVP
bond distances [Å]		
Ru–N1	2.112	2.128
Ru–N2	2.102	2.128
Ru–C11	1.835	1.853
Ru–C12	1.817	1.853
Ru–Cl1	2.391	2.384
Ru–Cl2	2.390	2.385
C11–O	1.133	1.139
C12–O	1.159	1.139
bond angles [degrees]		
N1–Ru–N2	77.2	76.7
Cl1–Ru–Cl2	176.3	172.7
Cl1–Ru–N1	89.4	87.3
Cl1–Ru–N2	87.3	87.4
N1–Ru–C11	174.8	174.4
N2–Ru–C12	179.6	174.4
Ru–C11–O	178.6	179.1
Ru–C12–O	177.0	179.1

[1] M. Haukka, J. Kiviaho, M. Ahlgren, and T. A. Pakkanen, Organometallics 14, 825 (1995).

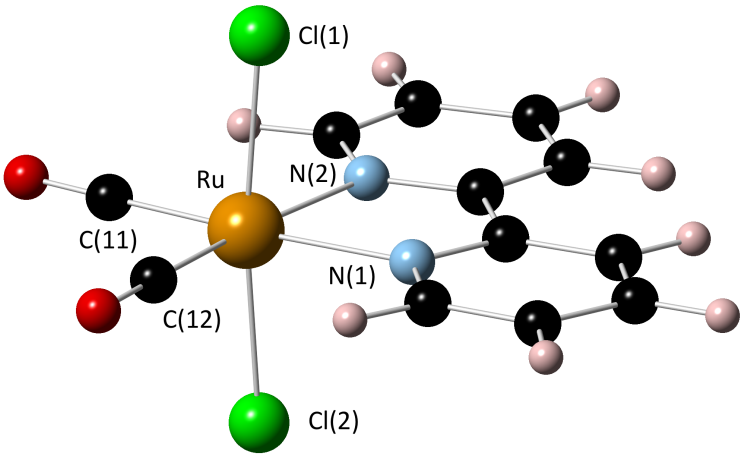


Figure S4.1: Ball and stick representation of trans(Cl)-Ru(bpy)$Cl_2(CO)_2$ with atom labels as used in Table S4.1.

S5 $[Fe(phen)_3]^{2+}$: QGROT localized orbitals.

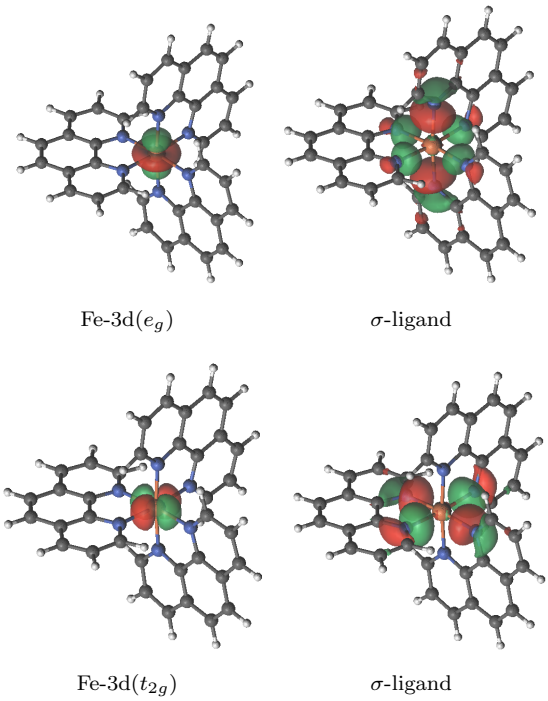


Figure S5.1: Localized active orbitals of $[Fe(phen)_3]^{2+}$.

S6 trans(Cl)-Fe(bpy)$Cl_2(CO)_2$: QGROT localized orbitals.

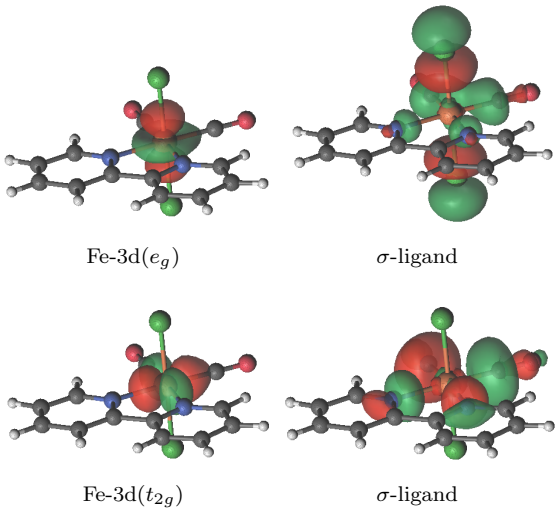


Figure S6.1: Localized active orbitals of trans(Cl)-Fe(bpy)$Cl_2(CO)_2$. The orbitals of trans(Cl)-Ru(bpy)$Cl_2(CO)_2$ are similar.