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Supporting information for 'Restricted active space simulations of the metal L-edge X-ray absorption spectra and resonant inelastic x-ray scattering: revisiting $[Co^{II/III}(bpy)_3]^{2+/3+}$ complexes'

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Geometric parameter	Exp.Co^{II}	Exp.Co^{III}	Cal.Co^{II}	Cal.Co^{III}
Co-N1	2.136	1.914	2.182	1.985
Co-N2	2.133	1.937	2.182	1.985
Co-N3	2.119	1.930	2.180	1.984
Co-N4	2.136	1.935	2.182	1.984
Co-N5	2.133	1.929	2.182	1.984
Co-N6	2.119	1.942	2.180	1.985
N1-C1	1.349	1.353	1.350	1.358
N1-C5	1.346	1.335	1.339	1.343
C1-C2	1.377	1.366	1.387	1.386
C2-C3	1.375	1.407	1.389	1.389
C3-C4	1.372	1.378	1.388	1.389
C4-C5	1.395	1.381	1.395	1.391
C5-C6	1.485	1.499	1.485	1.469
N1-C0-N2	77.1	83.1	75.7	82.1
N1-C0-N3	95.4	93.9	97.8	94.5
N2-C0-N3	171.4	175.3	171.2	175.7
N5-C2-C6	115.9	113.3	116.2	114.7

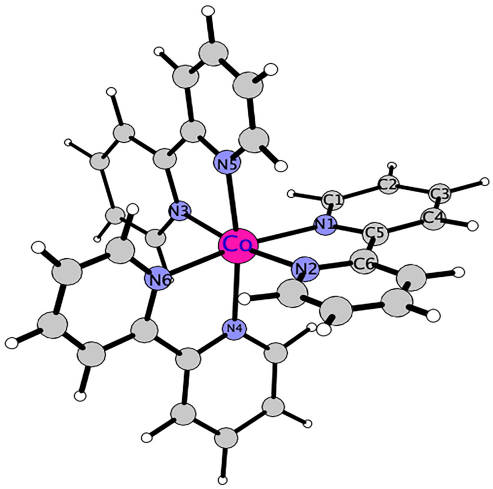

Table 1 Selected optimized and experimental geometrical parameters for $[Co^{II}(bpy)_3]^{2+}$ and $[Co^{III}(bpy)_3]^{3+}$ (bond lengths in Å and angles in degrees).

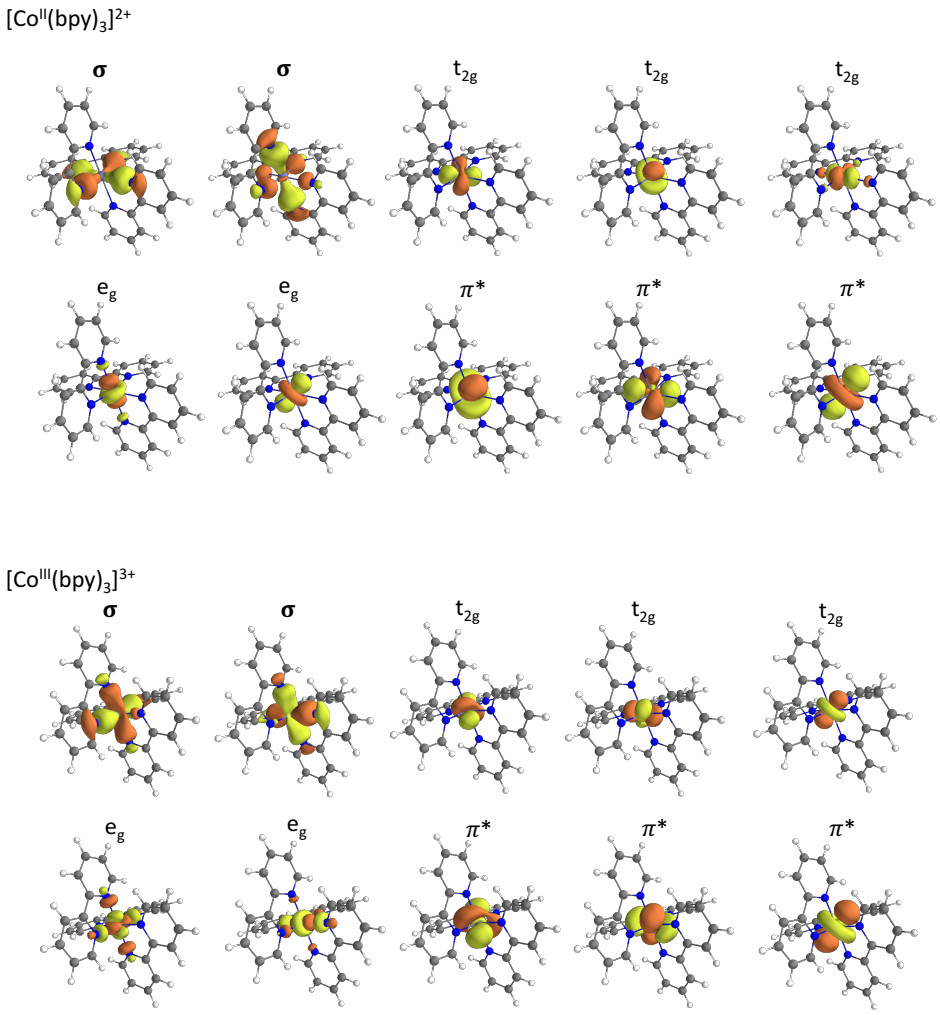

Fig. 1 The valence orbitals selected in the active space for [Co^{II}(bpy)$_3$]$^{2+}$ and [Co^{III}(bpy)$_3$]$^{3+}$ from their ground state calculations, the iso value 0.02 is used for creating the surface.

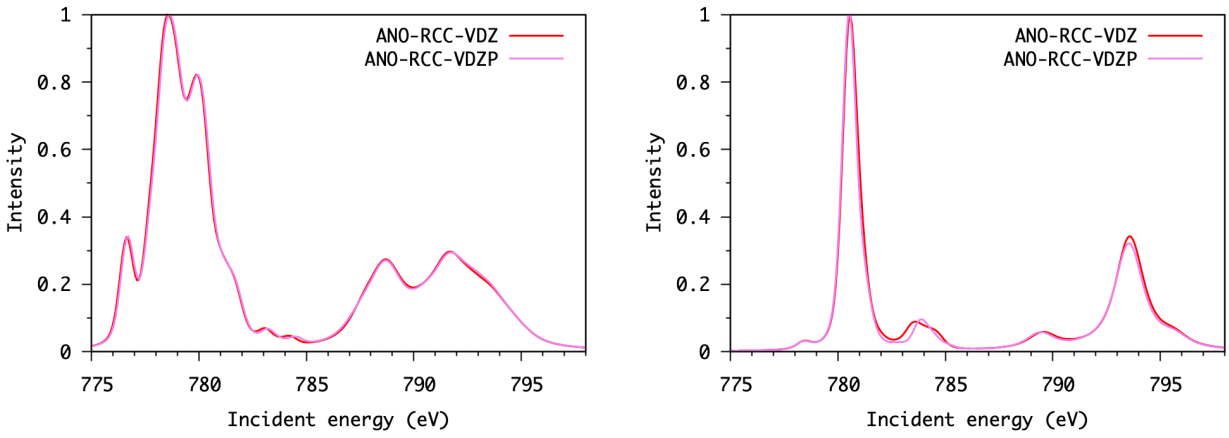

Fig. 2 The basis effects checked for [Co^{II}(bpy)$_3$]$^{2+}$ (including 40 quartet and 40 doublet core excited state) and [Co^{III}(bpy)$_3$]$^{3+}$ (including 40 singlet, 40 triplet and 40 quintet core excited state).

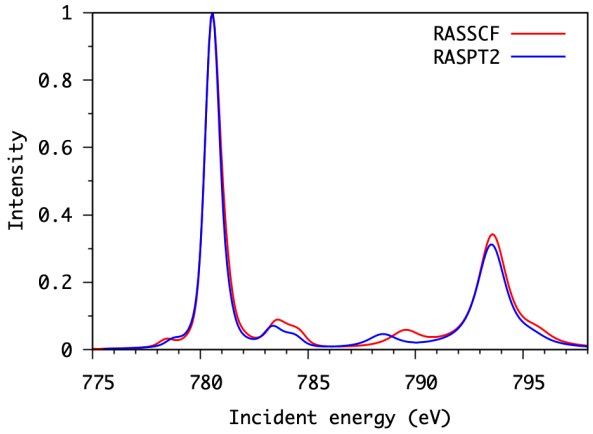

Fig. 3 The dynamic correction effect calculation (RASPT2) for $[Co^{III}(bpy)_3]^{3+}$ (including 40 singlet, 40 triplet and 40 quintet core excited state).

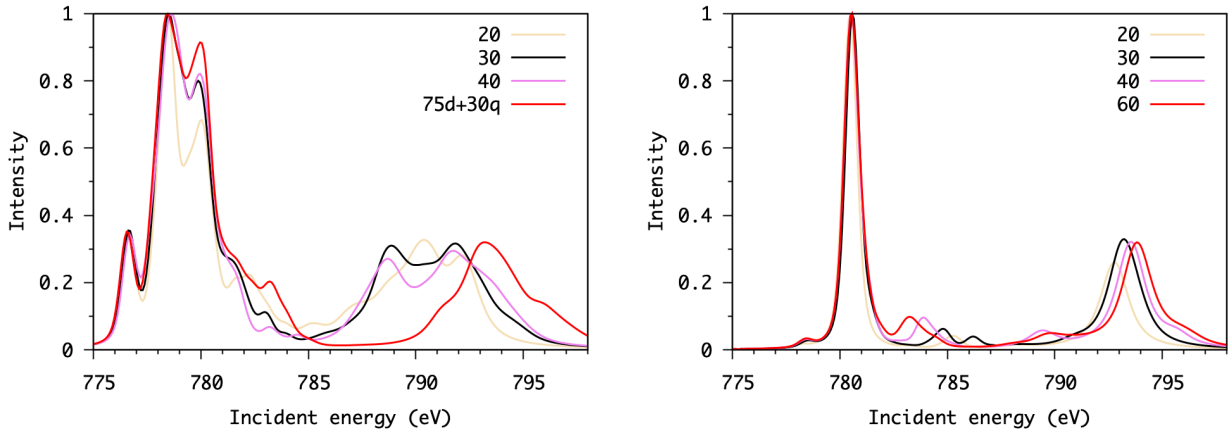

Fig. 4 The dependence on the number of final states checked for $[Co^{II}(bpy)_3]^{2+}$ and $[Co^{III}(bpy)_3]^{3+}$.

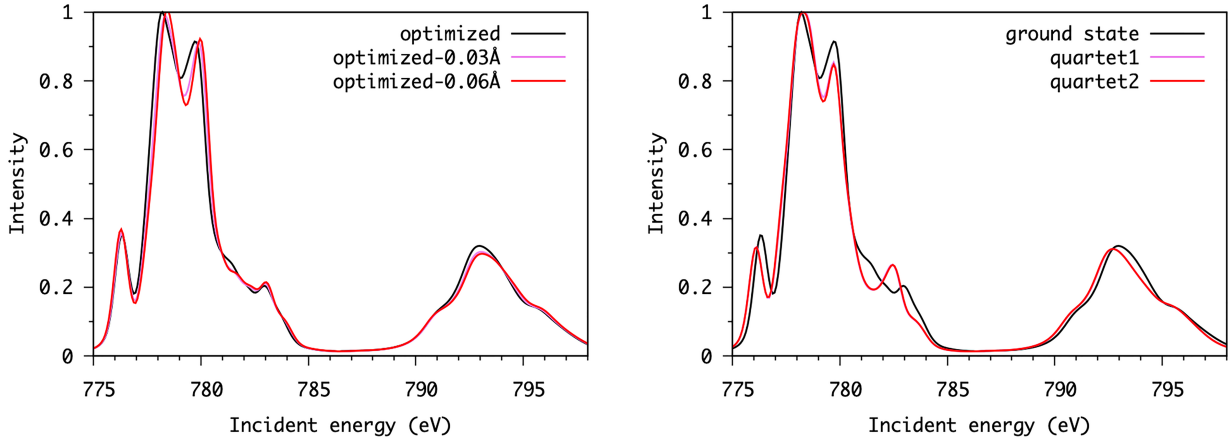

Fig. 5 The $[Co^{II}(bpy)_3]^{2+}$ spectrum with different Co-N bond lengths, and the spectrum calculated with low-lying quartet states having different electron configuration.Ground state: $d^2_{xz}d^2_{yz}d^1_{xy}d^1_{x^2-y^2}d^1_{z^2}$, quartet1:$d^1_{xz}d^2_{yz}d^2_{xy}d^1_{x^2-y^2}d^1_{z^2}$, quartet2:$d^2_{xz}d^1_{yz}d^2_{xy}d^1_{x^2-y^2}d^1_{z^2}$.

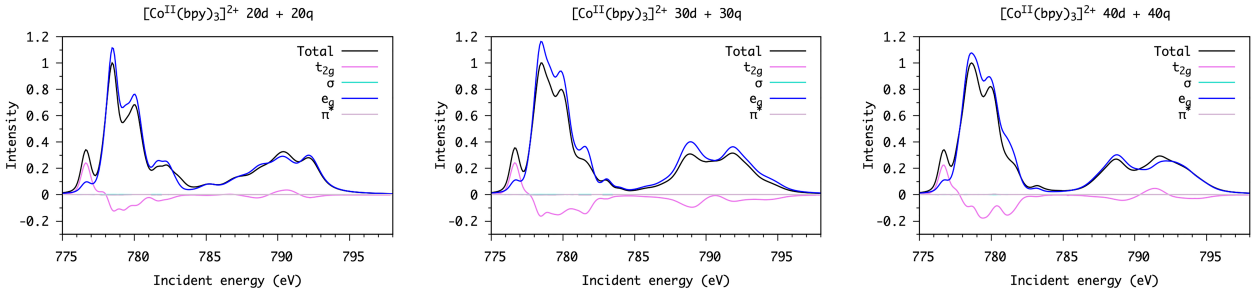

Fig. 6 The orbital contribution analysis to the XAS of $[Co^{II}(bpy)_3]^{2+}$ with different number of final states.

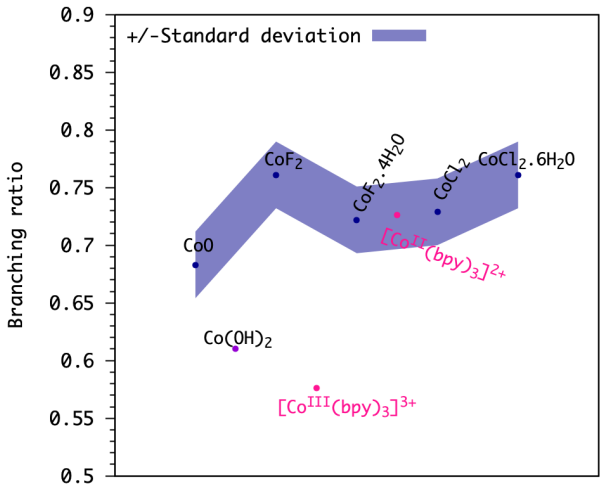

Fig. 7 The branching ratio plotting with numbers from Table 1 in the main text, the standard deviations are included for the high-spin cobalt complexes.