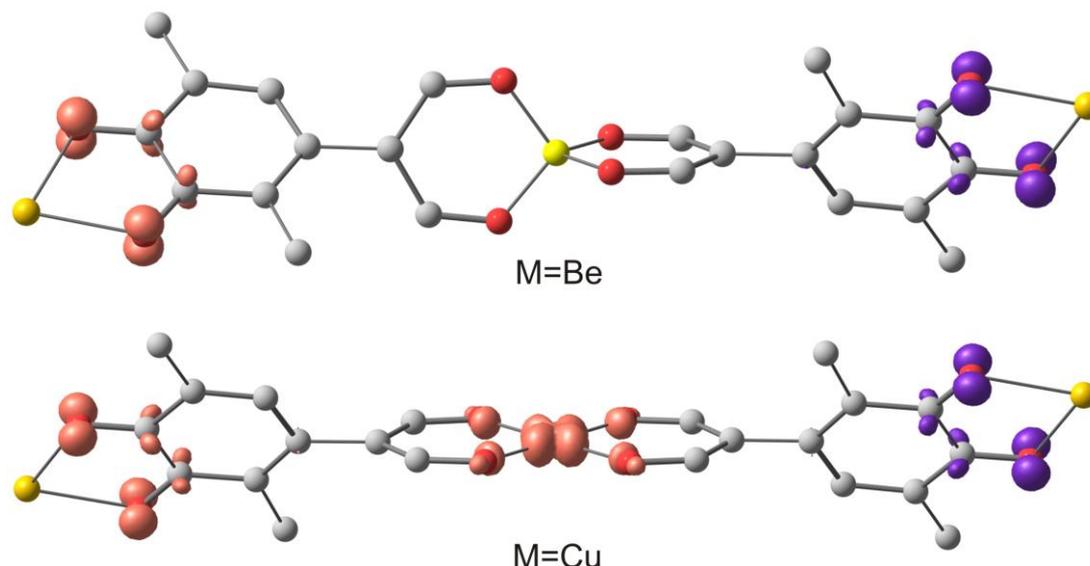


**Structure and magnetic properties of di-*o*-semiquinone complexes of alkali metals with a bischelate linker: a quantum chemical study**

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**Figure S1** Typical spin density distribution in BS1 state of complexes **3** with diamagnetic (M=Be) and paramagnetic (M=Cu) linkers. Hydrogen atoms are omitted for clarity.

**Table S1** Total energies and expectation values of the spin-squared ( $S^2$ ) operator of structures in the ground state and BS states of model complexes **3** (M=Be, Co, Ni, Cu, Zn;  $M_1$ =Na, K), calculated by DFT UB3LYP\*/6-311++G(d,p) method.

Structure	E, a. u.	$E_{BS1}^a$ , a. u.	$E_{BS2}$ , a. u.	$S^2$	$S_{BS1}^2$	$S_{BS2}^2$
M=Be, $M_1$ =Na	-1790.01916	-1790.01916	-	2.0001	1.0110	-
M=Zn, $M_1$ =Na	-3554.32796	-3554.32796	-	2.0001	1.0111	-
M= $_{LS}$ Ni, $M_1$ =Na	-3283.31126	-3283.31126	-	2.0001	1.0109	-
M= $_{HS}$ Co, $M_1$ =Na	-3157.78238	-3157.78245	-3157.78271	8.7714	4.7681	2.7651
M= $_{LS}$ Co, $M_1$ =Na	-3157.77387	-3157.77396	-3157.77407	3.7726	1.7711	1.7690
M= $_{HS}$ Ni, $M_1$ =Na	-3283.30238	-3283.30268	-3283.30276	6.0172	3.0120	2.0054
M=Cu, $M_1$ =Na	-3415.46972	-3415.46968	-3415.46963	3.7635	1.7634	1.7635
M=Be, $M_1$ =K	-2665.18154	-2665.18154	-	2.0110	1.0110	-
M=Zn, $M_1$ =K	-4429.49041	-4429.49041	-	2.0001	1.0111	-
M= $_{LS}$ Ni, $M_1$ =K	-4158.47372	-4158.47372	-	2.0113	1.0109	-
M= $_{HS}$ Co, $M_1$ =K	-4032.94487	-4032.94492	-4032.94512	8.7714	4.7685	2.7655
M= $_{LS}$ Co, $M_1$ =K	-4032.93626	-4032.93636	-4032.93647	3.7731	1.7713	1.7689
M= $_{HS}$ Ni, $M_1$ =K	-4158.46478	-4158.46505	-4158.46518	6.0172	3.0120	2.0048
M=Cu, $M_1$ =K	-4290.63211	-4290.63208	-4290.63204	3.7635	1.7634	1.7635

<sup>a</sup>BS1 corresponds to spin orientation  $\alpha\alpha\beta$ , BS2 corresponds to spin orientation  $\alpha\beta\alpha$ , where  $\alpha$  – spin up,  $\beta$  – spin down.