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Cobalt diketonate adducts with redox-active diiminosuccinonitriles

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Table S1 Total energy without (E_{total}) and with ($E_{total\ ZPE}$) the energies of the zero harmonic vibrations taken into account of the ligands, Co diketonates and the adducts **1** (R=CH_3, CF_3; R^1=H, CH_3), S^2 before and after annihilation of the structures **2-5** calculated by the DFT B3LYP*/6-311++G(d,p) method.

Structure	E_{total}, a.u.	$E_{total\ ZPE}$, a.u.	S^2 before annigilation	S^2 after annigilation
L (R^1=H)	-372.42597	-372.36613	-	-
L (R^1=CH_3)	-451.01401	-450.90013	-	-
$Co^{II}(acac)_2$	-2072.89123	-2072.66825	-	-
$Co^{II}(hfacac)_2$	-3263.63635	-3263.50515	-	-
2_{HS}	-2445.32802	-2445.04471	4.0408	3.7531
2_{LS}	-2445.34863	-2445.06191	0.7593	0.7500
3_{HS}	-2523.91814	-2523.58033	3.8571	3.7509
3_{LS}	-2523.92889	-2523.58742	0.7613	0.7501
3_{MECP}	-2523.91164	-	-	-
4_{HS}	-3636.08612	-3635.89391	3.8401	3.7508
4_{LS}	-3636.08933	-3635.89426	0.7593	0.7501
5_{HS}	-3714.68111	-3714.43462	3.7880	3.7503
5_{LS}	-3714.67200	-3714.42227	0.7621	0.7501

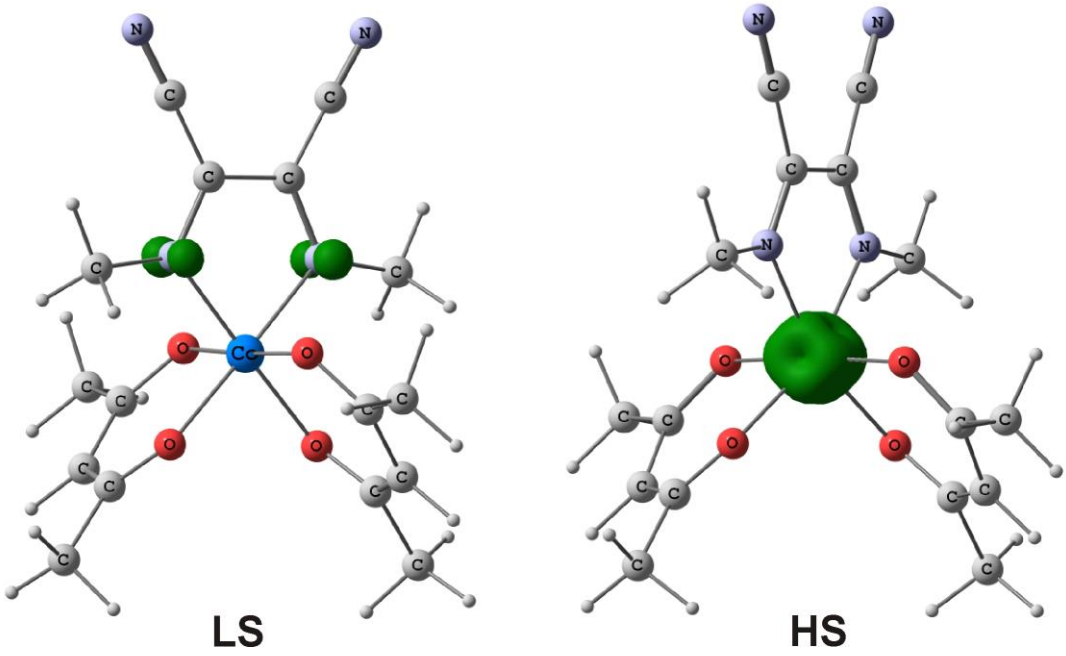

Figure S1 Typical spin density distribution of the low spin and high spin states of adducts **1**.