Electronic Supplementary Information for Dalton Transactions

Supplementary Material

A Series of Neutral Radicalar CpNi(dithiolene)• Complexes.

Marc Fourmigué* and Narcis Avarvari

Table S1. Geometry optimized coordinates of CpNi(dmit)• derived by DFT calculations.

Ni	-0.052031	-0.079674	0.005323
S	-0.033966	-0.079548	2.167573
S	2.103388	-0.114412	-0.192131
S	2.318595	-0.123925	4.133599
S	4.291274	-0.155831	1.954639
S	5.252942	-0.176784	4.808184
C	1.677310	-0.110431	2.491491
C	2.594130	-0.125320	1.478907
C	4.033643	-0.153616	3.704211
C	-2.105625	-0.012147	-0.248844
H	-2.810077	0.034950	0.571663
C	-1.541278	1.113784	-0.928156
H	-1.723031	2.153883	-0.695083
C	-0.628303	0.612001	-1.879494
H	0.010227	1.198763	-2.526454
C	-0.681867	-0.832596	-1.842356
H	-0.088125	-1.497629	-2.455180
C	-1.621341	-1.213219	-0.863382
H	-1.875967	-2.222849	-0.571810

Table S2. Selected Eigenvalues of orbitals of CpNi(dmit)$^{\bullet}$, calculated using the geometry optimized coordinates.

Label	Occupancy	Eigenvalue (Hartee)	Eigenvalue (eV)
α	1	-0.28594	-7.7808
β	1	-0.28320	-7.7062
α	1	-0.27679	-7.5318
β	1	-0.26040	-7.0858
α	1	-0.25625	-6.9729
β	1	-0.24392	-6.6374
α	1	-0.23872	-6.4959
β	1	-0.22578	-6.1438
α	1	-0.22611	-6.1527
β	1	-0.20655	-5.6205
α	1	-0.19474	-5.2991
β	0	-0.12678	-3.4498
α	0	-0.11884	-3.2338
β	0	-0.10419	-2.8351
α	0	-0.06555	-1.7837
β	0	-0.06387	-1.7380
α	0	-0.02323	-0.63212
β	0	-0.02290	-0.62314
α	0	-0.00800	-0.21769
β	0	-0.00166	-0.04517