Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information

A Streamlined Synthesis of Extended Thiophloroglucinol Ligands and their Trinuclear Ni^{II}_3 Complexes

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Figure S1 Molecular structures of a) [(bert^{Me})Ni$^{II}_3$], b) [(bert$^{t\text{-}Bu_2}$)Ni$^{II}_3$], c) [(bertdien)Ni$^{II}_3$]$^{3+}$. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity.

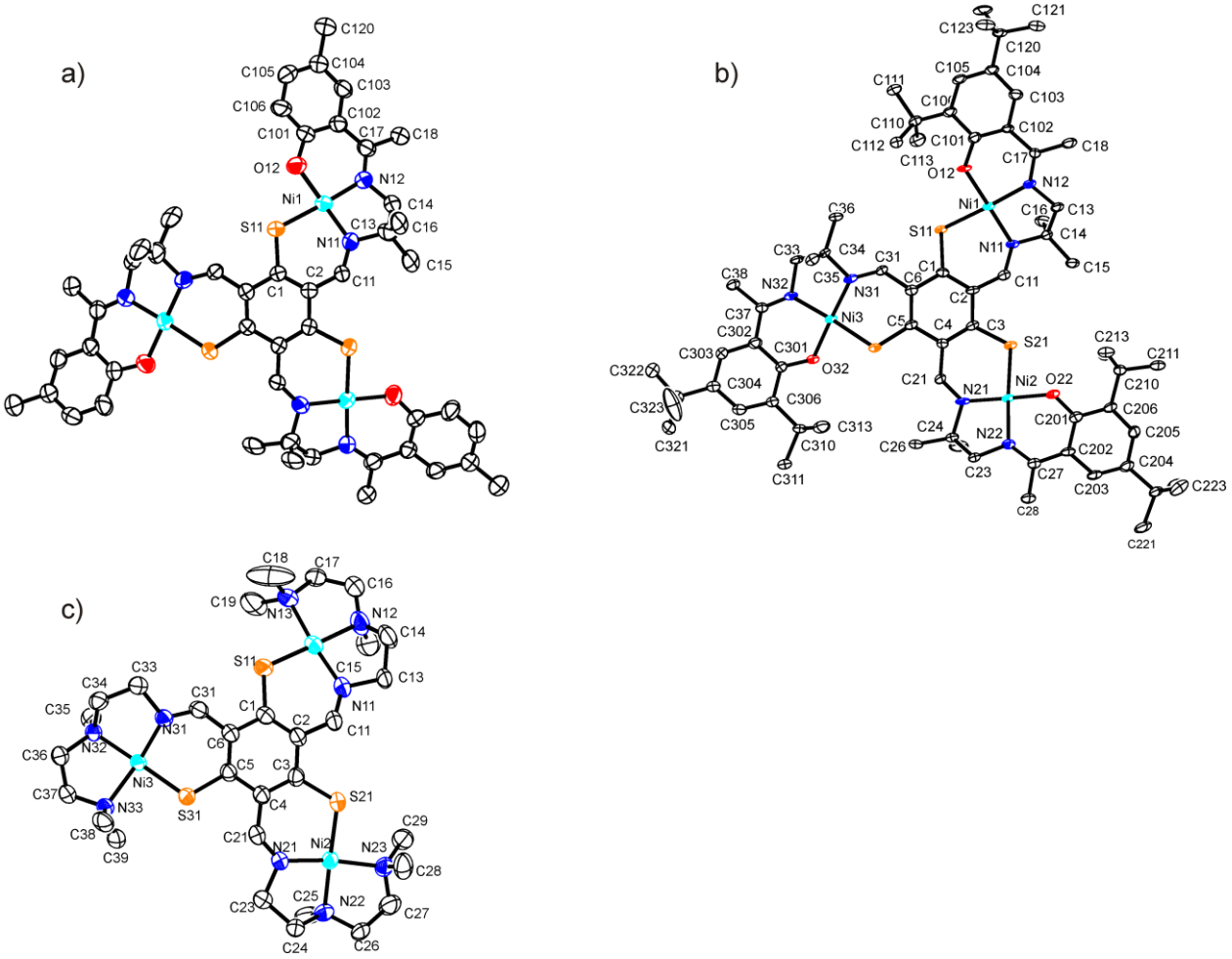

Figure S2 Molecular structures of [(habbi)Ni^{II}_3] a) molecule 1, b) molecule 2, c) molecule 3, and d) molecule 4. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity.

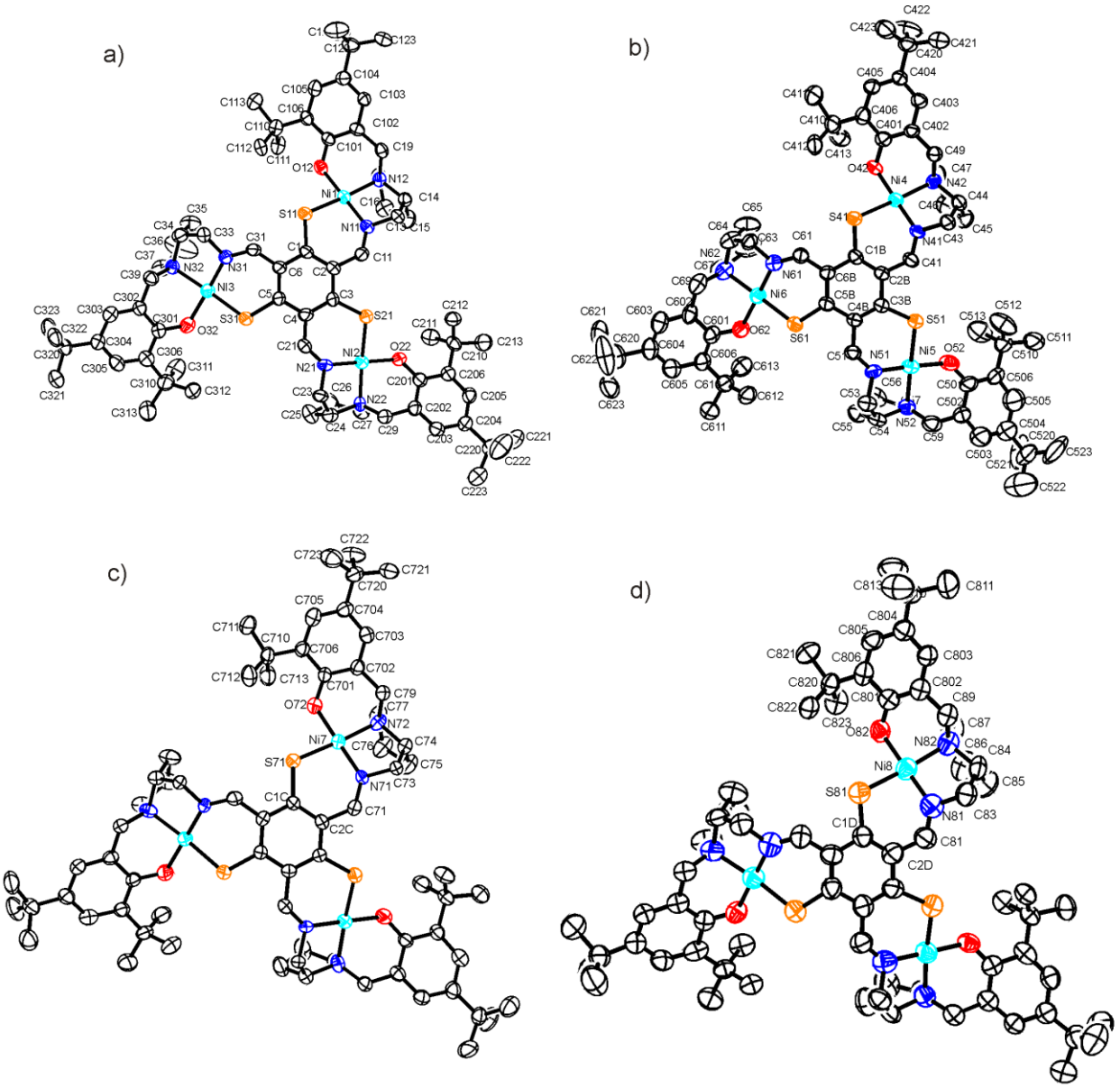

Figure S3 The structure of $[(bertdien)Ni_3]^{3+}$ exhibits the same disorder phenomenon of one ethylene bridge which has already been observed in $[(felddien)Ni^{II}_3]^{3+}$.[79] The coordinated ethylene diamine units of the chelating arms are not planar but exhibit a *gauche* conformation, which leads to two enantiomeric conformations of the five-membered chelat rings, labeled by λ and δ (Figure 3). The two chelate rings around Ni3 in $[(bertdien)Ni^{II}_3]^{3+}$ are in the $\lambda\delta$ conformation, where the first designation (λ) refers to the chelate ring involving N31 and N32, while the second designation (δ) refers to the chelate ring involving N32 and N33. The chelate rings around Ni1 and Ni2 show a disorder of $\lambda\delta$ and $\delta\lambda$ orientations in the ratio 50:50 around Ni1 and of 70:30 around Ni2. The orientation of the methyl group (C25 for the pendant arm around Ni2) defines the conformation of both chelate rings, *i. e.* C25 pointing downwards forces conformation $\lambda\delta$ and C25 pointing upwards forces conformation $\delta\lambda$.