

MAGNETISM AND MAGNETIC MATERIALS

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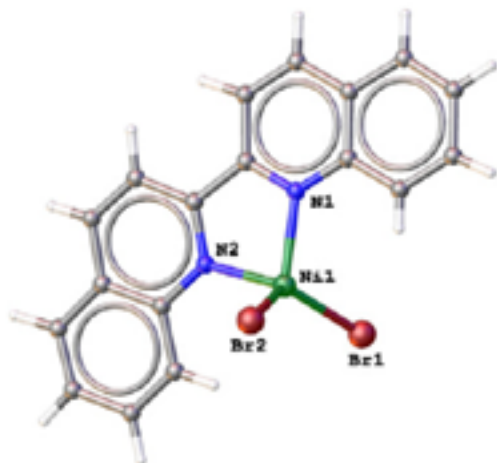
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DIFFERENT MAGNETIC PROPERTIES OF NI(II) COMPLEXES WITH (PSEUDO)HALIDE LIGANDS DEPENDING ON THEIR GEOMETRY

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Four tetracoordinate Ni(II) complexes have been prepared, structurally characterized, and subjected to magnetometric studies. The complexes $[\text{Ni}(\text{PPh}_3)_2(\text{NCS})_2]$, $[\text{Ni}(\text{dppp})(\text{NCS})_2]$, and $[\text{Ni}(\text{dppm})\text{Br}_2]$ are planar and thus diamagnetic. The complex $[\text{Ni}(\text{biqu})\text{Br}_2]$ is quasi-tetrahedral, with the geometry close to C_{2v} symmetry, and paramagnetic. While on one side it resembles a prolate bisphenoid (the angle N-Ni-N=83 deg), on the second side it mimics an oblate bisphenoid (Br-Ni-Br=126 deg). It exhibits a zero-field splitting of the ground term 3A_2 into three crystal-field multiplets that can be described by D and E parameters within the spin Hamiltonian formalism. The ab initio calculations confirm this interpretation; however, the evaluation of the spin-Hamiltonian parameters meets difficulties owing to the quasi-degeneracy of the electronic terms.



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