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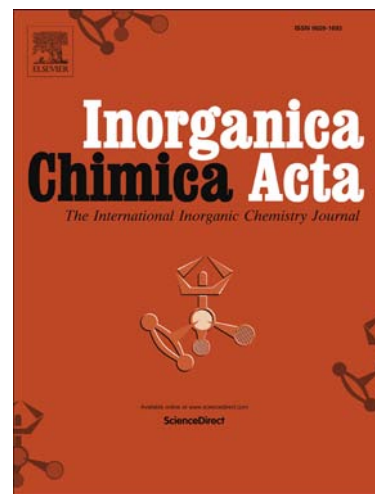
The BIAN ligand 1,2-bis[(2,6-diisopropylphenyl)imino]acenaphthene: An electron sponge or a “normal” α -diimine ligand ?

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The BIAN ligand 1,2-bis[(2,6-diisopropylphenyl)imino]acenaphthene:

An electron sponge or a „normal“ α -diimine ligand ?

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ABSTRACT

The compounds $[fac-Re(CO)_3Cl(L)]$ and $[M(CO)_4(L)]$, $M = Cr, Mo, W$ and $L = 1,2-bis[(2,6-diisopropylphenyl)imino]acenaphthene$, have been studied electrochemically and spectroelectrochemically (IR, UV-vis-NIR, EPR). The neutral rhenium complex contains an isopropyl-shielded chloride ligand; its reversible oxidation was shown to involve a largely metal-based HOMO. One electron could be added reversibly to the diimine-based LUMO of all complexes, as evident from EPR spectroscopy. However, there was no evidence for the reversible acquisition of more than one electron by L in these complexes, ruling out an electron reservoir functionality with multielectron reactivity. DFT and TD-DFT calculations were performed for the $[Re(CO)_3Cl(L)]^n$ redox series ($n = +, 0, -$).

Keywords:

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