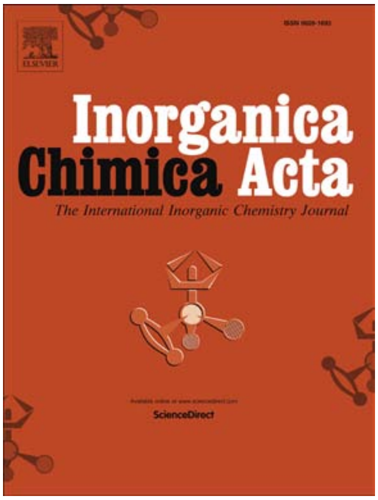

Research paper

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

Isabell Löw, Martina Bubrin, Alexa Paretzki, Jan Fiedler, Stanislav Záliš, Wolfgang Kaim

PII: S0020-1693(16)30309-7
DOI: http://dx.doi.org/10.1016/j.ica.2016.05.054
Reference: ICA 17090

To appear in: *Inorganica Chimica Acta*

Received Date: 26 February 2016
Accepted Date: 29 May 2016

Please cite this article as: I. Löw, M. Bubrin, A. Paretzki, J. Fiedler, S. Záliš, W. Kaim, The BIAN ligand 1,2-bis[(2,6-diisopropylphenyl)imino]acenaphthene: An electron sponge or a “normal“ α-diimine ligand ?, *Inorganica Chimica Acta* (2016), doi: http://dx.doi.org/10.1016/j.ica.2016.05.054

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

Isabell Löw,[a] Martina Bubrin,[a] Alexa Paretzki,[a] Jan Fiedler,[b] Stanislav Záliš,[b] Wolfgang Kaim[a,*]

[a] *Institut für Anorganische Chemie, Universität Stuttgart, Pfaffenwaldring 55, D-70550 Stuttgart, Germany*

[b] *J. Heyrovský Institute of Physical Chemistry, v.v.i., Academy of Sciences of the Czech Republic, Dolejškova 3, CZ-18223 Prague, Czech Republic*

ABSTRACT

The compounds [*fac*-Re(CO)$_3$Cl(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)$_3$Cl(L)]^n redox series (n = +, 0, -).

Keywords:

---

[*] Corresponding author.
E-mail: kaim@iac.uni-stuttgart.de.