The Synthesis, Structural Characterization and Conformational Analysis of (1,3-Bis(2-methyl-4-diethylaminophenyl)imidazolidin-2-ylidene)chloro(1,5-cyclooctadiene)rhodium(I)

Hasan Karabıyık[a], Rafet Kılınçarslan[b], Muhittin Aygün[a], Bekir Çetinkaya[b], and Orhan Büyükgüngör[c]

[a] Dokuz Eylül University, Department of Physics, Fen Edebiyat Fakultesi, Fizik Bolumu, Kaynaklar Yerleskesi, 35160-Buca, İzmir, Turkey
[b] Ege University, Department of Chemistry, 35100- Bornova, İzmir, Turkey
[c] Ondokuz Mayıs University, Department of Physics, 55139-Kurupelit, Samsun, Turkey

Reprint requests to Dr. M. Aygün. E-mail: muhittin.aygun@deu.edu.tr

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A four-coordinated Rh(I) complex with a new heterocyclic carbene ligand, functionalized by amino donor pendants, **4**, was synthesized and characterized by elemental analyses, NMR and IR spectroscopy, and the molecular structure of the title compound has been determined by X-ray crystallography. Crystallographic data: monoclinic, $P2_1/m$, $a = 7.9307(5)$, $b = 25.0061(12)$, $c = 8.0780(6)$ Å, $\beta = 101.366(6)^\circ$, $V = 1570.58(17)$ Å^3, $\rho_{\mathrm{calc}} = 1.3515(1)$ g cm^{-3}, $Z = 2$. The experimentally obtained structural parameters for compound **4** compare reasonably well with those calculated at the semi-empirical ZINDO/1 level of theory carried out to elucidate conformational flexibility and steric hindrances.

Key words: *N*-Heterocyclic Carbenes, Rhodium Complexes, Carbene Ligand, Crystal Structure, ZINDO/1