Trigonal Planar Chromium(II) N-Heterocyclic Carbene Complexes as Potential Mononuclear Single Molecule Magnets

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During the last 30 years, a large number of multinuclear metal complexes have been shown to exhibit slow magnetisation relaxation and are referred to as single molecule magnets (SMMs). However, due to their small magnetic anisotropy, recent research efforts have been focused to mono- and bi-nuclear 3*d*- or lanthanide- based SMMs [1]. Among the 3*d*-systems, only a handful of high-spin ($S = 2$) Cr(II) complexes have been identified to date as mononuclear SMMs [2].

The [Cr{N(SiMe$_3$)$_2$}(Bn)(IPr)] complex (**1**), IPr = 1,3-bis(2,6- iPr$_2$C$_6$H$_3$)imidazol-2-ylidene, Bn = CH$_2$C$_6$H$_5$ (Figure 1), was obtained by the thermolysis of [Cr(IPr)Bn$_2$] in HN(SiMe$_3$)$_2$. A combined study by high-frequency and -field EPR spectroscopy, AC magnetometry and ab initio quantum chemical methods revealed that complex 1 is the first trigonal planar Cr(II) mononuclear SMM, which, interestingly, also contains a Cr–C_{NHC} bond. Along these lines, the structural and magnetic properties of additional trigonal planar and T-shaped Cr(II) complexes will be presented and discussed.

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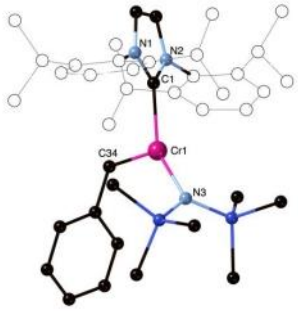
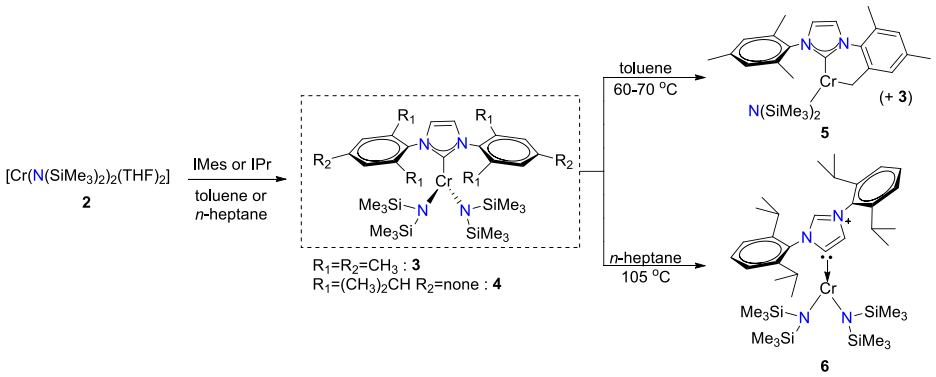


Figure 1. The molecular structure of **1**



Scheme 1: The synthesis of 3-coordinate Cr(II) complexes of this work

References:

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[2] Q.-C. Luo, N. Ge, Y.-Q. Zhai, T.-B. Wang, L. Sun, Q. Sun, F. Li, Z. Ouyang , Z.-X. Wang and Y.-Z. Zheng Dalton Trans., 2022, **51**, 9218-9222