Supporting Information

First Cr(III)-SNS Complexes and their use as Highly Efficient Catalysts for the Trimerization of Ethylene to 1-Hexene

David S. McGuinness,* Peter Wasserscheid,* Wilhelm Keim, David Morgan, John T. Dixon, Annette Bollmann, Hulisani Maumela, Fiona Hess and Ulli Englert
Institut für Technische Chemie und Makromolekulare Chemie der RWTH Aachen, Worringerweg 1, 52074 Aachen, Germany, Sasol Technology (Pty) Ltd, R & D Division, 1 Klasie Havenga Rd, Sasolburg, 9570 South Africa, and Institut für Anorganische Chemie der RWTH Aachen, Professor Pirlet Strasse 1, 52074 Aachen, Germany

Preparation of 1-4: The synthesis of complexes **1-4** is illustrated by the procedure followed for **1**: A solution of ligand **II** (0.0842g, 0.509 mmol) in 5mL of THF was added to a solution/suspension of $CrCl_3(THF)_3$ (0.175g, 0.467 mmol) in 8mL of THF. The solvent was removed in vacuo until ca. 3mL remained and 5mL of ether added to complete precipitation. The product was washed with ether and dried in vacuo. Yield: 0.145g (96%). Complexes **2-4** were prepared in an identical fashion with yields of over 80% in each case. MS for **2** (+FAB): *m/z* 352 $[M]^+$, 315 $[M\text{-}HCl]^+$. Elemental analysis:
1 Calcd. for $C_6H_{15}S_2NCl_3Cr$ (found): C 22.27 (21.79), H 4.67 (5.12), N 4.33 (4.10).
2 Calcd. for $C_8H_{19}S_2NCl_3Cr$ (found): C 27.32 (26.97), H 5.45 (5.99), N 3.98 (3.64).
3 Calcd. for $C_{12}H_{27}S_2NCl_3Cr$ (found): C 35.34 (35.18), H 6.67 (6.57), N 3.43 (3.46).
4 Calcd. for $C_{24}H_{51}S_2NCl_3Cr$ (found): C 50.04 (50.23), H 8.86 (9.19), N 2.43. (2.16).

Crystallographic study: intensity data for 2 were collected at 213 K on a Nonius CAD4 diffractometer using Mo-K radiation (= 0.71073Å). A numerical absorption based on Gaussian integration was applied[1]. The structure was solved by direct methods[2] and refined by full-matrix, least-squares on $|F|^2$ [3]. All non-hydrogen atoms were refined anisotropically; hydrogen atoms were placed in calculated positions and refined according to a riding model. Crystal data: monoclinic space group $P2_1/c$, a = 7.6255(12), b = 13.059(5), c = 14.3703(10) Å, = 90.790(11)º, V = 1430.9(6) Å^3, Z = 4, D_c = 1.633 g cm^{-3}, μ = 1.622 mm^{-1}, $F(000)$ = 724, 2 $_{max}$ = 54º, 4013 reflections, 3126 independent data. Convergence for 138 parameters at $wR2$ = 0.0857, $R1$ = 0.0351, GOF = 1.074 for all data and $R1$ = 0.0309 for 2846 reflections with $I > 2(I)$. Residual electron density was 0.439 and -0.549 e Å^{-3}.

(1) Coppens, P.; Leiserowitz, L.; Rabinovich, D. *Acta Crystallogr.* **1965**, *18*, 1035.
(2) Sheldrick, G. M. "SHELXS97, Program for Crystal Structure Solution," University of Göttingen, **1997**.
(3) Sheldrick, G. M. "SHELXL97, Program for Crystal Structure Refinement," University of Göttingen, **1997**.