

A Cationic Gold Complex Cleaves BArF₂₄

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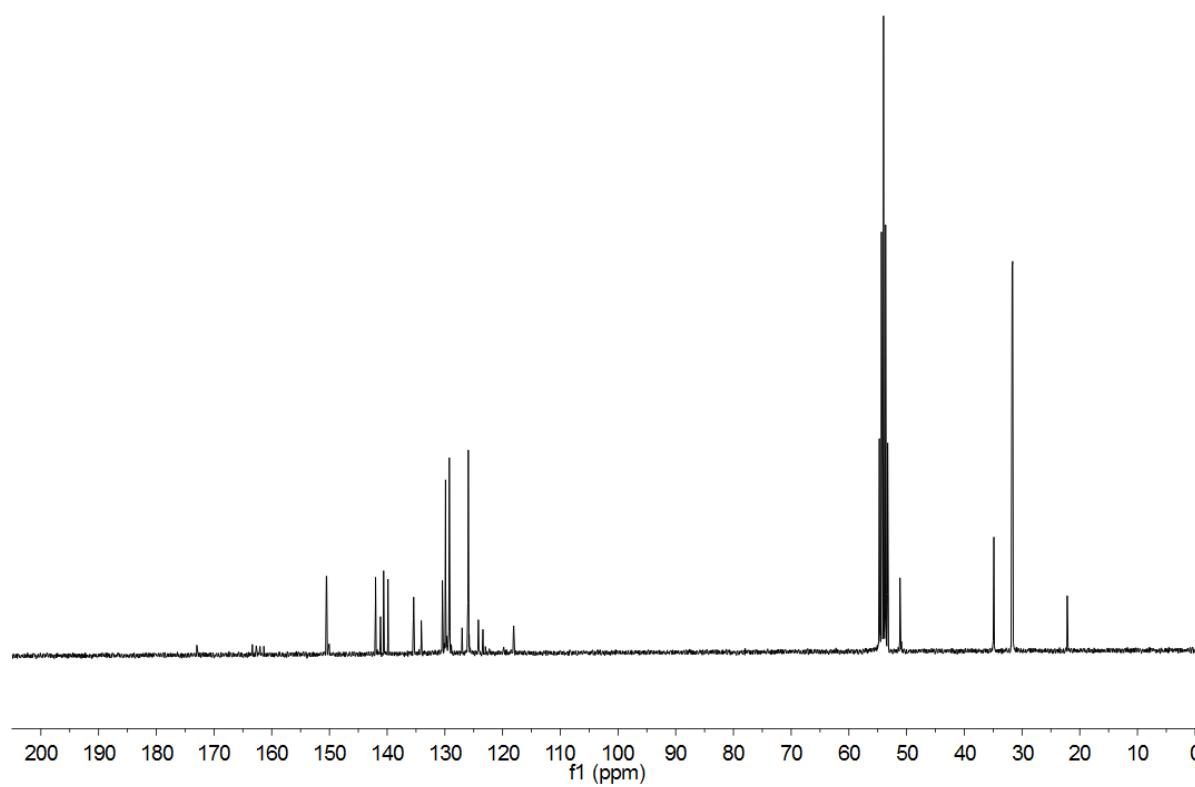
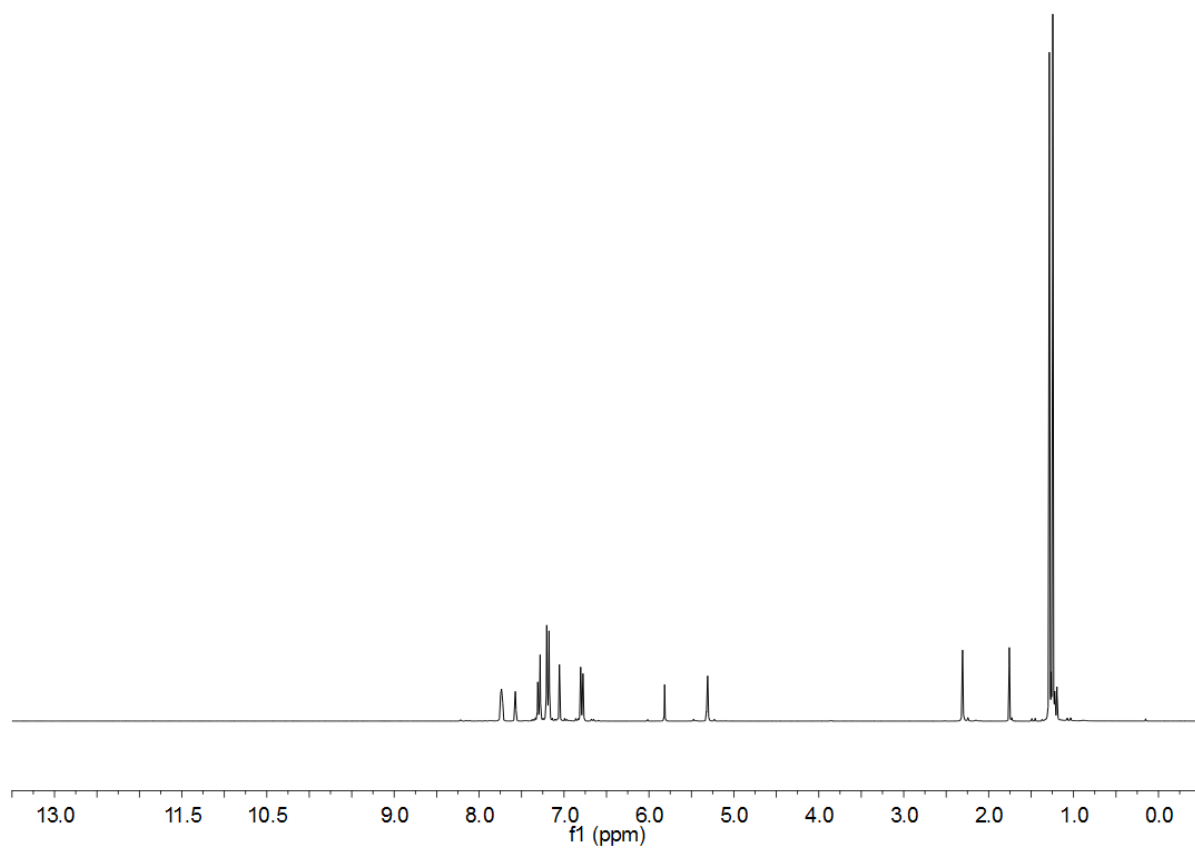
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Supporting Information

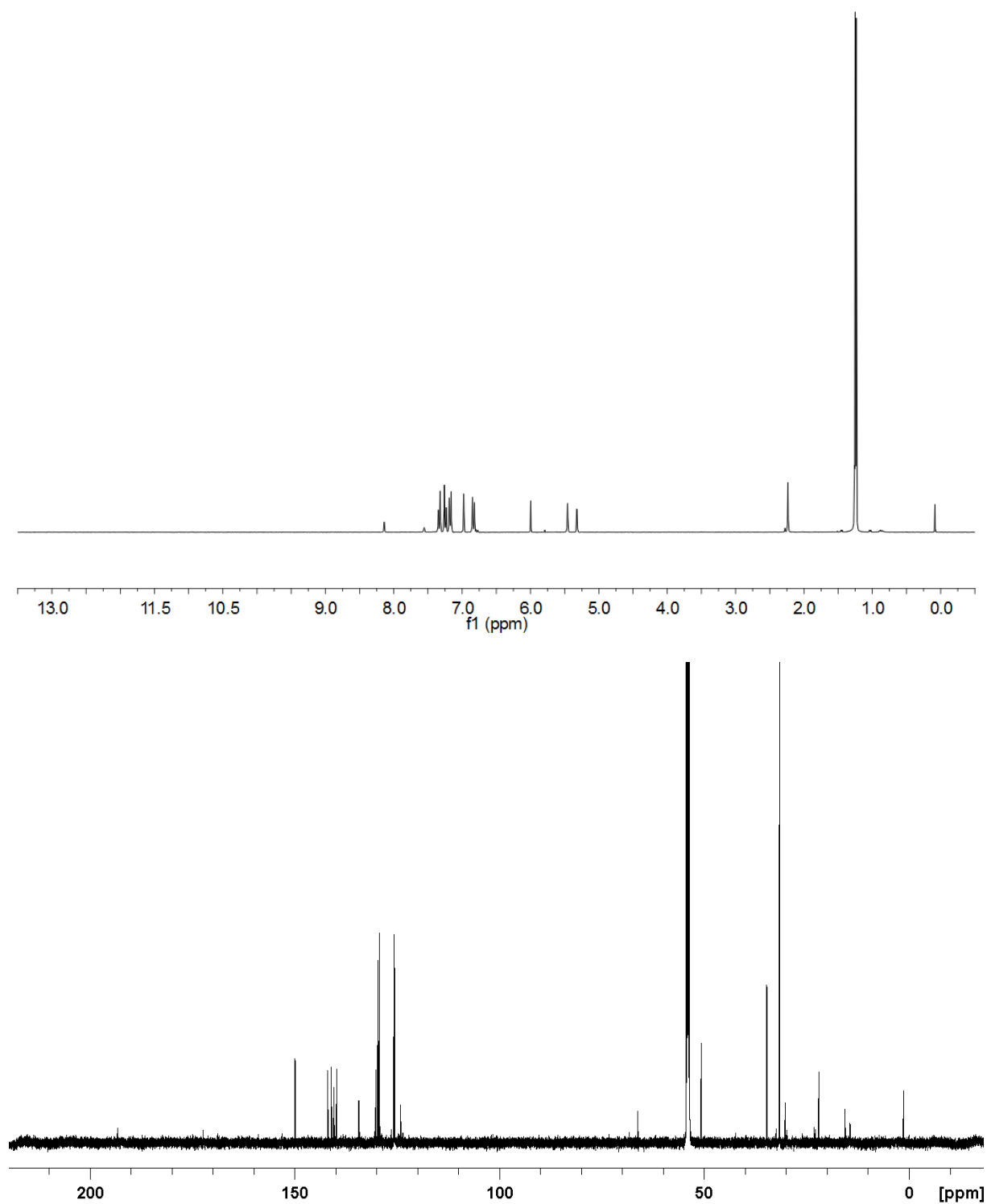
General Experimental Methodology

Chemicals and solvents used in this work were supplied by the Department of Organic Chemistry at the Ruprecht-Karls-University Heidelberg or bought directly from Acros Organics, Sigma Aldrich, Strem, and TCI. Reactions involving air-sensitive reagents were carried out in an atmosphere of nitrogen or argon using standard Schlenk techniques or an MBraun LABmaster 130 glovebox operated with nitrogen.^[1] Absolute solvents were taken from an MBraun MB SCS-800 solvent purification system containing appropriate drying agents. Deuterated solvents for the use of NMR spectroscopy were supplied by Deutero GmbH and Euriso-top. All reported yields are isolated yields. ¹H NMR spectra were recorded at room temperature using hardware by Bruker. The following instruments were employed: Bruker Avance 300 (300 MHz) and Bruker Avance 500 (500 MHz). Chemical shifts δ are reported in ppm relative to TMS and were determined by reference to the residual ¹H solvent peaks (dichloromethane – 5.32 ppm; chloroform – 7.26 ppm)^[2], coupling constants J in Hz. The following abbreviations were used for describing the signals' multiplicities: s – singlet, d – doublet, m – multiplet. ¹³C{¹H} NMR spectra were recorded at room temperature with the following spectrometers: Bruker Avance 300 (75 MHz) and Bruker Avance 500 (126 MHz). The spectra were calibrated with respect to the solvent (chloroform – 77.0 ppm; dichloromethane – 54.00 ppm)^[3]. The assignment of signals in the ¹³C{¹H} NMR spectra was achieved by interpretation of two-dimensional NMR spectra (HMBC, HSQC). Mass spectra were recorded by the Mass Spectrometry Service Facility of the Chemical Department at the Ruprecht-Karls-University Heidelberg. The following machines were employed: Bruker ICR Apex-Qe, Finnigan MAT LCQ und JEOL JMS-700. Apart from the method of ionization and the peak of the molecular ion, the basis peak and characteristic fragmentation peaks with their relative intensities are reported. Elemental analyses were carried out by the Laboratory of Microanalysis in the Department of Chemistry at the Ruprecht-Karls-University Heidelberg. Infrared spectra were recorded on an infrared spectrometer Vector 22 FTIR by Bruker. Measurements were carried out with KBr-pellets. The following abbreviations were used to describe both the intensity and profile of the signals: w (weak), m (medium), s (strong), br (broad). Determination of melting points was carried out in open capillaries using a Gallenkamp hot-stage microscope. X-ray analyses were carried out in the Department of Organic Chemistry at the Ruprecht-Karls-University Heidelberg by Dr. Rominger and co-workers using the following hardware: Bruker Smart Apex Diffractometer, Bruker Smart Apex II Quazar Diffractometer and Bruker Smart 1000 Diffractometer. For analysis and graphic representation, the programs ORTEP^[4] and POV-Ray^[5] were used.

NMR Spectra of [IPr**Au]BArF₂₄ (2)



NMR Spectra of IPr**AuC₆H₃(CF₃)₂ (3)



References

- [1] D. F. Shriver, M. A. Drezdon, *The Manipulation of Air-Sensitive Compounds, Vol. 2*, John Wiley & Sons, **1986**.
- [2] G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw, K. I. Goldberg, *Organometallics* **2010**, *29*, 2176-2179.
- [3] a) M. Hesse, H. Meier, B. Zeeh, *Spektroskopische Methoden in der organischen Chemie : 114 Tabellen*, 8., überarb. und erw. Aufl. ed., Thieme, Stuttgart [u.a.], **2012**;
b) *The Merck Index : an encyclopedia of chemicals, drugs and biologicals*, 11.ed. ed., Merck & Co., Rahway, N.J., **1989**.
- [4] L. J. Farrugia, *J. Appl. Crystallogr.* **1997**, *30*, 565-565.
- [5] www.povray.org.