

successfully modeled isotropically as a 1:1 disorder of a CO ligand and an H₂O ligand.

After the Rh and P peaks, the next largest peak was located 5.5 Å from the Rh atom. This peak was situated in the center of three smaller peaks that formed a ca. 3-fold symmetric trigonal pyramid. Application of the crystal symmetry operations generated four symmetry-related peaks that, overall, formed a staggered ethane-like fragment that was assigned as an end-to-end disordered SO₃CF₃⁻ moiety. Upon assigning the large peak as a S atom with a site-occupation factor = 0.5, the largest peak in the subsequent difference map was located 0.96 Å from the S position and just off the vector between S and the position of its symmetry equivalent S(a). Overall, the pattern appeared to be the partially resolved superposition of the C atom (from the CF₃ group) and the S atom (of the SO₃ group). Therefore, the best approximation of the disordered SO₃CF₃⁻ resulted from a model where both the S and C(2) atoms were given site-occupation factors of 0.5 and the F(1), F(2), and F(3) atoms were assigned site-occupation factors of 1.0 each in order to approximately account for both the superposition of the F and O atoms.

Despite the disorder in the CO, H₂O, and SO₃CF₃⁻ positions, refinement of the structure to 10.57% was possible. The density of

the crystals was determined to be 1.57(2) g/cm³ by flotation in a CCl₄/hexane mixture. The calculated density for 4 molecules of *trans*-[Rh(CO)(PPh₃)₂(OH₂)] [OTf] per unit cell is 1.57 g/cm³.

Acknowledgment. The support of the National Science Foundation (Grant CHE-9215872) to J.L.H. is gratefully acknowledged. We acknowledge the NSF and the Utah State University Research Office for jointly funding the purchase of the USU X-ray diffraction (Grant CHE-9002379) and NMR (Grant CHE-9311730) facilities.

Supporting Information Available: Tables of crystallographic data, collection parameters, atomic coordinates, and equivalent isotropic displacement parameters, complete listing of bond distances and bond angles, anisotropic displacement parameters, and H-atom coordinates (5 pages). This material is contained in many libraries on microfiche, immediately follows this article in the microfilm version of the journal, and can be ordered from the ACS; see any current masthead page for ordering information.

IC951287H

Additions and Corrections

1995, Volume 34

Anthony F. Lagalante, Brian N. Hansen, Thomas J. Bruno,* and Robert E. Sievers: Solubilities of Copper(II) and Chromium(III) β -Diketonates in Supercritical Carbon Dioxide.

Page 5785. Two sponsors were accidentally omitted from the Acknowledgment. The following should be added to this section: R.E.S. and A.F.L. acknowledge NSF Grant ATM-9115295 and EG&G Rocky Flats Contract ASC222874DB for providing partial support of this research.

IC960236X