

# Additions and Corrections

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**Douglas B. Grotjahn,\* Xi Zeng, Andrew L. Cooksy, W. Scott Kassel, Antonio G. DiPasquale, Lev N. Zakharov, and Arnold L. Rheingold:** Experimental and Computational Study of the Transformation of Terminal Alkynes to Vinylidene Ligands on *trans*-(Chloro)bis(phosphine)Rh Fragments and Effects of Phosphine Substituents

Pages 3385–3402. The artwork given for the original Figure 1 was inadvertently included in the paper instead of the correct figure for **6b**, which appears below as the correct Figure 1. The CIF file listed as being for **8** was in fact the CIF for the complex inadvertently shown in the previous Figure 1; the correct CIF for **8** is now available in the Supporting Information. To the

single entry in Table 1 for the Rh–P bond distance for **6b** should be added the value 2.3431(14) Å, because in this particular structure, the two Rh–P bond distances are slightly different. In addition, Table 6 in the original paper had incorrect entries for compound **8**. The correct version of Table 6 appears below.

**Supporting Information Available:** A CIF file giving the crystal data for compound **8**. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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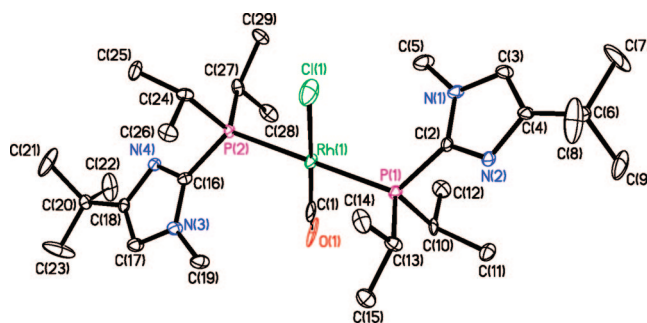


Figure 1

Table 6. Collection Data for Crystal Structures of the Complexes

|   | <b>6b</b>   | <b>6c</b>  | <b>6d</b>  | <b>8</b>   |
|---|---|--|--|--|
| formula   | C <sub>29</sub> H <sub>54</sub> ClN <sub>4</sub> OP <sub>2</sub> Rh | C <sub>25</sub> H <sub>38</sub> ClOP <sub>2</sub> Rh | C <sub>27</sub> H <sub>42</sub> ClOP <sub>2</sub> Rh | C <sub>28</sub> H <sub>54</sub> ClN <sub>4</sub> P <sub>2</sub> Rh · CH <sub>2</sub> Cl <sub>2</sub> |
| mw  | 675.06  | 554.85   | 582.91   | 731.98   |
| cryst syst  | monoclinic  | monoclinic   | monoclinic   | monoclinic   |
| space group   | P2 <sub>1</sub> /n  | P2 <sub>1</sub> /n                                   | P2 <sub>1</sub> /c                                   | P2 <sub>1</sub> /c   |
| color, habit  | yellow, block   | yellow, blade  | yellow, blade  | orange, plate  |
| <i>a</i> (Å)  | 7.9000(4)   | 8.5410(8)  | 10.232(11)   | 14.1238(9)   |
| <i>b</i> (Å)  | 24.4193(12)   | 7.7860(7)  | 15.409(17)   | 13.6555(9)   |
| <i>c</i> (Å)  | 8.9974(4)   | 19.8080(17)  | 9.569(10)  | 18.8057(12)  |
| $\beta$ (deg)   | 96.793(1)   | 96.300(2)  | 113.509(15)  | 97.2960(10)  |
| <i>V</i> (Å <sup>3</sup> )  | 1723.53(14)   | 1309.3(2)  | 1383(3)  | 3597.6(4)  |
| <i>Z</i>  | 2   | 2  | 2  | 4  |
| <i>D</i> <sub>calcd</sub> (g cm <sup>−3</sup> )   | 1.301   | 1.407  | 1.399  | 1.351  |
| <i>T</i> (K)  | 100   | 208  | 208  | 213  |
| 2 $\theta$ <sub>max</sub> (deg)   | 55.0  | 50.0   | 52.0   | 56.2   |
| no. of meas rflns   | 10 730  | 7073   | 8269   | 8413   |
| no. of indep rflns  | 3928  | 2314   | 2714   | 7796   |
| no. of params   | 195   | 146  | 151  | 386  |
| <i>R</i> ( <i>F</i> ) [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )], % <sup>a</sup>               | 3.62  | 4.96   | 4.75   | 3.47   |
| <i>R</i> ( <i>wF</i> <sup>2</sup> ) [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )], % <sup>b</sup> | 8.72  | 5.31   | 11.19  | 9.37   |
| GOF   | 1.137   | 1.210  | 1.089  | 1.045  |
| resid electron density  | 0.488   | 0.928  | 0.712  | 0.963  |

<sup>a</sup>  $R = \sum ||F_o| - |F_c|| / \sum |F_o|$ . <sup>b</sup>  $R(wF^2) = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$ ;  $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ ,  $P = [2F_c^2 + \max(F_o, 0)]/3$ .