Accessory Publication

Mono- and Di-nuclear Gold(I) Complexes Containing 1,12-Dicarba-closo-dodecaborane(12)

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School of Chemistry
The University of Sydney
Sydney, NSW 2006, Australia.
Table 1. Crystal data and structure refinement for C26H30B10P2.

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<tr>
<td>Wavelength</td>
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<tr>
<td></td>
<td>b = 13.763(5) ≈ β= 105.490(7)°</td>
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<tr>
<td></td>
<td>c = 10.891(4) ≈ γ= 90°</td>
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<td>R indices (all data)</td>
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Table 2. Atomic coordinates ($x \times 10^4$) and equivalent isotropic displacement parameters ($\approx 2 \times 10^3$) for C26H30B10P2. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

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B(15)-B(16) 1.772(3)
B(15)-H(15) 1.089(19)
B(16)-B(14)#1 1.761(3)
B(16)-B(18)#1 1.768(3)
B(16)-B(17) 1.782(3)
B(16)-H(16) 1.07(2)
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B(17)-B(14)#1 1.765(3)
B(17)-B(18) 1.776(3)
B(17)-H(17) 1.05(2)
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B(18)-H(18) 1.07(2)

C(1)-P(1)-C(7) 104.31(8)
C(1)-P(1)-C(13) 105.87(7)
C(7)-P(1)-C(13) 102.57(7)
C(2)-C(1)-C(6) 118.39(15)
C(2)-C(1)-P(1) 127.59(13)
C(6)-C(1)-P(1) 113.99(12)
C(3)-C(2)-C(1) 120.52(16)
C(3)-C(2)-H(2) 119.7
C(1)-C(2)-H(2) 119.7
C(4)-C(3)-C(2) 120.37(16)
C(4)-C(3)-H(3) 119.8
C(2)-C(3)-H(3) 119.8
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C(4)-C(5)-H(5) 120.0
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C(5)-C(6)-H(6) 119.6
C(1)-C(6)-H(6) 119.6
C(8)-C(7)-C(12) 118.45(16)
C(8)-C(7)-P(1) 126.03(13)
C(12)-C(7)-P(1) 115.36(13)
C(9)-C(8)-C(7) 120.44(17)
C(9)-C(8)-H(8) 119.8
C(7)-C(8)-H(8) 119.8
C(10)-C(9)-C(8) 120.06(18)
C(10)-C(9)-H(9) 120.0
C(8)-C(9)-H(9) 120.0
C(11)-C(10)-C(9) 120.19(17)
C(11)-C(10)-H(10) 119.9
C(9)-C(10)-H(10) 119.9
C(10)-C(11)-C(12) 119.93(17)
C(10)-C(11)-H(11) 120.0
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C(11)-C(12)-C(7) 120.90(17)
C(11)-C(12)-H(12) 119.6
C(7)-C(12)-H(12) 119.6
B(14)-C(13)-B(15) 62.38(11)
B(14)-C(13)-B(18) 62.30(11)
B(15)-C(13)-B(18) 113.59(12)
B(14)-C(13)-B(17) 112.89(12)
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C(13)-B(14)-B(16)#1 105.29(13)
C(13)-B(14)-B(17)#1 105.08(13)
B(16)#1-B(14)-B(17)#1 60.73(11)
C(13)-B(14)-B(18) 58.99(10)
B(16)#1-B(14)-B(18) 59.89(11)
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Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1
Table 4. Anisotropic displacement parameters ($=2 \times 10^3$) for C26H30B10P2. The anisotropic displacement factor exponent takes the form: $-2\pi^2 \left[ h^2 a^* a^* U_{11} + \ldots + 2 h k a^* b^* U_{12} \right]$

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Table 5. Hydrogen coordinates ($x \times 10^4$) and isotropic displacement parameters ($\AA^2 \times 10^3$) for C26H30B10P2.

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