2,3-Dimethyl-2,3-butanediol (pinacol)

G. A. Jeffrey and A. Robbins
Hydrogen atomic coordinates ($x \times 10^3$) in the crystal structure of pinacol

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Anisotropic (x 10^4) and isotropic thermal parameters in the crystal structure of pinacol.

The anisotropic temperature factor expression used was
\[ \exp[-(h^2\alpha_{11} + k^2\alpha_{22} + l^2\alpha_{33} + 2hk\alpha_{12} + 2hl\alpha_{13} + 2kl\alpha_{23})]. \]
The isotropic temperature factor expression was \[ \exp[-\frac{1}{3}(h^2\alpha + k^2\alpha + l^2\alpha)]. \]

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Isotropic B's of hydrogen atoms were obtained by conversion from the anisotropic $\delta$'s of the non-hydrogen atoms to which they are bonded.
Additional valence angles (°) for pinacol, not shown in Fig. 1. E.s.d.'s are 0.3°

Molecule 2

C(5)-C(4)-C(6)  110.4
C(6)-C(4)-C(7)  113.3
C(6)-C(4)-O(2)  108.2
C(5)-C(4)-C(7)  111.3
C(4)-C(7)-C(9)  112.7
C(8)-C(7)-C(9)  109.9
C(4)-C(7)-O(3)  109.0
C(4)-C(7)-C(8)  111.4

Molecule 3

C(10')-C(10)-C(11)  112.8
C(12)-C(10)-O(4)  105.2
Torsion angles (°) in pinacol. E.s.d.'s are 0.5°. Because of high e.s.d.'s in positional parameters of the low occupancy unit of molecule 3, values for only the low occupancy form are given.

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(°) related by two-fold axes at 1/2, 1/4.
(°) related by center of symmetry at 1/2, 1/4, 1/2.
Observed and calculated structure factors for pinacol.

Asterisks denote unobserved reflections.

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