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Crystal Structure of $Au_7(PPh_3)_7^+$: Corrigendum

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The crystal structure of a compound of this heptanuclear cation (the anion was unidentified, but may have been OH^-) was reported[1] as triclinic, space group $P\bar{1}$, with a = 34.94 (1) Å, b = 44.25 (2) Å, c = 15.45 (1) Å, α = 99.98 (3)°, β = 102.66 (3)°, γ = 88.11 (3)°, and Z = 8. It can more appropriately be described as monoclinic, space group $C2/c$. The vectors (201), (00$\bar{1}$), ($\bar{1}$10) describe a cell with a' = 68.18 Å, b' = 15.45 Å, c' = 55.47 Å, α' = 89.99°, β' = 128.22°, γ' = 90.11°, and Z = 16. While the deviation of the angle γ' from 90° is marginally greater than would be expected on the basis of the reported uncertainties, conclusive evidence of the higher symmetry comes from the atomic positions (Table II of Ref 1), which, after the appropriate transformations ($x' = {}^1/_2(x + y)$, $y' = {}^1/_2(x + y) - z$, $z' = y$), conform in pairs to the symmetry of $C2/c$ within the reported esd's. The $C2/c$ coordinates and the shifts necessary to achieve this higher symmetry are given in Table I.

The c-glide plane of $C2/c$ requires the systematic absence of reflections $hk0$ with $(h + k)$ odd in the triclinic indexing. No such entries appear in the supplementary table of F's for 4787 reflections with $I > 3\sigma(I)$.

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Table I. Coordinates (×10⁴ for Au, ×10³ for P) for the $C2/c$ Description (Shifts Necessary To Achieve This Higher Symmetry Given in Square Brackets)

	x (±1.5)[a]	y (±6.5)[a]	z (±1.8)[a]
Au(11,22)	1412 [0]	−114 [2]	1785 [0]
Au(12,21)	1126 [2]	873 [2]	1822 [3]
Au(13,26)	1038 [0]	−972 [3]	1764 [2]
Au(14,25)	906 [0]	85 [0]	1256 [0]
Au(15,24)	1264 [2]	1529 [4]	1486 [2]
Au(16,23)	1634 [2]	1332 [5]	2162 [0]
Au(17,27)	1456 [2]	−129 [2]	2337 [1]
Au(31,42)	6439 [2]	−1409 [3]	4430 [2]
Au(32,41)	6203 [1]	−54 [0]	4402 [2]
Au(33,43)	6118 [0]	−1737 [4]	4554 [1]
Au(34,44)	5943 [3]	−1323 [5]	3939 [3]
Au(35,45)	6315 [2]	−313 [2]	3954 [1]
Au(36,46)	6714 [1]	76 [2]	4601 [1]
Au(37,47)	6605 [1]	−706 [3]	4988 [2]
	x (±0.9)[a]	y (±4.1)[a]	z (±1.2)[a]
P(11,22)	167 [1]	−101 [2]	178 [0]
P(12,21)	89 [0]	175 [1]	189 [1]
P(13,26)	85 [0]	−232 [4]	166 [1]
P(14,25)	56 [1]	−4 [0]	77 [1]
P(15,24)	132 [0]	248 [1]	124 [1]
P(16,23)	200 [0]	207 [0]	248 [2]
P(17,27)	160 [1]	−40 [2]	284 [0]
P(31,42)	662 [1]	−242 [4]	445 [0]
P(32,41)	597 [0]	109 [6]	436 [2]
P(33,43)	594 [0]	−270 [0]	470 [0]
P(34,44)	557 [1]	−150 [3]	350 [0]
P(35,45)	629 [1]	22 [0]	355 [1]
P(36,46)	703 [1]	93 [2]	476 [0]
P(37,47)	682 [1]	−58 [1]	552 [0]

[a] Esd's, estimated from the values in Table II of ref 1.

(1) van der Velden, J. W. A.; Beurskens, P. T.; Bour, J. J.; Bosman, W. P.; Noordik, J. H.; Kolenbrander, M.; Buskes, J. A. K. M. *Inorg. Chem.* **1984**, *23*, 146.

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