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Corrigendum

Corrigendum to "New cerium nitride chlorides: $Ce_6Cl_{12}N_2$ and CeNCl" [J. Alloys Comp. 206 (1994) 95][1]

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In the above paper, the space group of the compound $Ce_6Cl_{12}N_2$ was reported to be $P2_1/c$, with unit cell $a = 11.233(4)$, $b = 16.527(8)$, $c = 10.708(3)$ Å, $\beta = 90.15°$. Work by H. Mattausch of the Max-Planck Institut, Stuttgart, has indicated the correct space group to be *Pbca*. Refinement on F^2 with SHELXTL [1] in *Pbca* using the original data with $\beta = 90.0°$ converged routinely to $R = 2.59$ ($wR2 = 9.68$) for 2109 reflections (>4s (F_0)) and 92 parameters. The program MISSYM [2] was run on the original data but failed to detect the missing symmetry elements until the chlorine atoms were removed. Apparently, the additional parameters in the monoclinic refinement allowed the chlorine atoms to refine to positions slightly off symmetry. Nonetheless, the overall structural description remains unchanged.

Table 1
Crystal data and structure refinement for Ce_3Cl_6N refined in *Pbca*

Identification code	r273
Empirical formula	Ce_3Cl_6N
Formula weight	647.07
Temperature	293(2) K
Wavelength	0.71069 Å
Crystal system	Orthorhombic
Space group	*Pbca*
Unit cell dimensions	$a = 10.708(2)$ Å, $\alpha = 90°$
	$b = 11.233(2)$ Å, $\beta = 90°$
	$c = 16.527(3)$ Å, $\gamma = 90°$
Volume	1987.9(6) Å^3
Z	8
Density (calculated)	4.324 Mg m^{-3}
Absorption coefficient	15.046 mm^{-1}
$F(000)$	2264
Crystal size	0.26 × 0.22 × 0.09 mm
θ range for data collection	2.46 to 27.59°
Index ranges	$-13 \leq h \leq 13, 0 \leq k \leq 14, -21 \leq l \leq 0$
Reflections collected	4501
Independent reflections	2300 ($R_{int} = 0.0755$)
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	2300/0/92
Goodness-of-fit on F^2	0.842
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0273$, $wR2 = 0.0969$
R indices (all data)	$R1 = 0.0421$, $wR2 = 0.1042$
Extinction coefficient	0.0044(2)
Largest diff. peak and hole	2.556 and −2.827 eÅ^{-3}

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Table 2
Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for Ce_3Cl_6N; U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	U_{eq}
Ce(1)	1409(1)	219(1)	4367(1)	14(1)
Ce(2)	3394(1)	−352(1)	1773(1)	16(1)
Ce(3)	132(1)	2105(1)	484(1)	16(1)
Cl(1)	2519(1)	−2166(1)	4544(1)	22(1)
Cl(2)	3711(1)	608(1)	3399(1)	24(1)
Cl(3)	1034(1)	−805(1)	2722(1)	23(1)
Cl(4)	6418(1)	−309(1)	4471(1)	18(1)
Cl(5)	1691(1)	2105(1)	1878(1)	24(1)
Cl(6)	5311(1)	−3118(1)	3758(1)	23(1)
N(1)	4481(4)	−929(4)	612(2)	14(1)

Table 3
Anisotropic displacement parameters ($Å^2 \times 10^3$) for Ce_3Cl_6N; the anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + \cdots + 2hk\ a^*b^*U_{12})$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ce(1)	10(1)	18(1)	13(1)	−1(1)	1(1)	0(1)
Ce(2)	13(1)	23(1)	12(1)	−2(1)	1(1)	−1(1)
Ce(3)	12(1)	17(1)	18(1)	1(1)	0(1)	−1(1)
Cl(1)	16(1)	20(1)	30(1)	0(1)	−5(1)	1(1)
Cl(2)	18(1)	39(1)	16(1)	−7(1)	3(1)	−7(1)
Cl(3)	17(1)	33(1)	18(1)	−4(1)	3(1)	−1(1)
Cl(4)	13(1)	21(1)	19(1)	0(1)	−1(1)	1(1)
Cl(5)	23(1)	26(1)	24(1)	3(1)	−5(1)	0(1)
Cl(6)	23(1)	24(1)	24(1)	2(1)	5(1)	−4(1)
N(1)	11(2)	18(2)	13(2)	−1(2)	3(2)	−2(2)

References

[1] SHELXTL version 5, G.M. Sheldrick, Siemens Analytical X-ray Instruments, Inc.
[2] Y.J. LePage, *J. Appl. Cryst.*, *20* (1987) 264.