$4F_o^2/[\sigma^2(F_o^2) + (0{\cdot}040F_o^2)^2]$; $S = 1{\cdot}00$, $R = 0{\cdot}027$, $wR = 0{\cdot}033$; $(\Delta/\sigma)_{max} = 0{\cdot}12$; no extinction correction; largest peak in final ΔF map $\pm 0{\cdot}2$ (1) e Å^{-3}; complex neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974); programs: Enraf–Nonius *SDP* (Frenz, 1981), *ORTEP*II (Johnson, 1976), *MULTAN*80 (Main *et al.*, 1980). The structure of the title compound is shown in Fig. 1, positional parameters and equivalent values of the anisotropic temperature factors are given in Table 1,* bond distances and angles are listed in Table 2.

Table 2. *Bond distances* (Å) *and angles* (°)

As(1)–F(1)	1·781 (2)	F(24)–C(24)	1·317 (5)
As(1)–C(21)	1·915 (4)	C(11)–C(12)	1·375 (5)
As(1)–C(11)	1·915 (3)	C(11)–C(16)	1·375 (5)
F(12)–C(12)	1·336 (4)	C(12)–C(13)	1·371 (5)
F(13)–C(13)	1·330 (4)	C(13)–C(14)	1·369 (6)
F(14)–C(14)	1·332 (5)	C(14)–C(15)	1·379 (6)
F(15)–C(15)	1·327 (5)	C(15)–C(16)	1·363 (5)
F(16)–C(16)	1·341 (4)	C(21)–C(22)	1·378 (4)
F(22)–C(22)	1·334 (4)	C(22)–C(23)	1·380 (5)
F(23)–C(23)	1·339 (4)	C(23)–C(24)	1·358 (4)
F(1)–As(1)–F(i)	180·0 (2)	C(13)–C(14)–C(15)	120·6 (4)
F(1)–As(1)–C(21)	90·26 (7)	F(15)–C(15)–C(16)	121·4 (3)
F(1)–As(1)–C(11)	89·6 (1)	F(15)–C(15)–C(14)	120·0 (4)
F(1)–As(1)–C(11i)	90·1 (1)	C(16)–C(15)–C(14)	118·7 (4)
C(21)–As(1)–C(11)	120·2 (1)	F(16)–C(16)–C(15)	117·8 (3)
C(11)–As(1)–C(11i)	119·7 (2)	F(16)–C(16)–C(11)	120·0 (3)
C(16)–C(11)–C(12)	117·9 (3)	C(15)–C(16)–C(11)	122·2 (3)
C(16)–C(11)–As(1)	121·2 (3)	C(22)–C(21)–C(22i)	119·0 (4)
C(12)–C(11)–As(1)	120·9 (3)	C(22)–C(21)–As(1)	120·5 (2)
F(12)–C(12)–C(13)	118·4 (3)	F(22)–C(22)–C(21)	120·9 (3)
F(12)–C(12)–C(11)	120·4 (3)	F(22)–C(22)–C(23)	119·2 (3)
C(13)–C(12)–C(11)	121·3 (3)	C(21)–C(22)–C(23)	119·9 (3)
F(13)–C(13)–C(14)	120·2 (4)	F(23)–C(23)–C(24)	120·5 (3)
F(13)–C(13)–C(12)	120·4 (4)	F(23)–C(23)–C(22)	118·5 (3)
C(14)–C(13)–C(12)	119·4 (3)	C(24)–C(23)–C(22)	121·0 (4)
F(14)–C(14)–C(13)	119·6 (4)	F(24)–C(24)–C(23)	120·4 (2)
F(14)–C(14)–C(15)	119·8 (4)	C(23)–C(24)–C(23i)	119·3 (4)

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43204 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Room-Temperature and Low-Temperature Structure of Triphenyltin Chloride*

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Abstract. $C_{18}H_{15}ClSn$, $M_r = 385{\cdot}5$, $P2_1/a$, $Z = 8$, $\lambda(\text{Mo } K\alpha_1) = 0{\cdot}70930$ Å, $F(000) = 1520$. At room temperature, $a = 18{\cdot}664$ (4), $b = 9{\cdot}721$ (4), $c = 18{\cdot}983$ (5) Å, $\beta = 105{\cdot}601$ (20)°, $V = 3317$ (3) Å^3, $D_x = 1{\cdot}544$ Mg m^{-3}, $\mu = 1{\cdot}70$ mm^{-1}, $R = 0{\cdot}033$ for 5060 unique reflections. At 110 K, $a = 18{\cdot}410$ (4), $b = 9{\cdot}5593$ (19), $c = 18{\cdot}704$ (5) Å, $\beta = 105{\cdot}201$ (19)°, $V = 3176$ (1) Å^3, $D_x = 1{\cdot}612$ Mg m^{-3}, $\mu = 1{\cdot}76$ mm^{-1}, $R = 0{\cdot}031$ for 5342 unique reflections. Our room-temperature results substantiate the results of an earlier report. There are eight molecules per unit cell with two crystallographically distinct molecules. Unlike its trimethyltin chloride analogue, the triphenyltin chloride molecules are loosely packed and unassociated in the crystalline state. The stereochemistry around the tin atoms is a slightly distorted tetrahedron. The average C–Sn–Cl and C–Sn–C valence angles are 105·21 (16) and 113·38 (20)° respectively. The shortest intermolecular Cl···Sn distance of 5·847 (2) Å is much longer than the sum of their van der Waals radii and precludes any reasonable intermolecular interaction. Cooling the crystal to 110 K did not lead to a phase transition as speculated earlier. The molecules remain discrete with the closest Cl···Sn distance shortened to 5·644 (2) Å. Inspection of the crystal packing diagram revealed no new or unusual feature compared with that of the room-temperature structure.

* NRCC contribution No. 25700.

Experimental. The title compound obtained from Alfa Products was recrystallized from a benzene solution. Crystal size 0·6 × 0·6 × 0·6 mm. Cell dimensions were obtained by least-squares refinement of 25 θ values measured on a Picker diffractometer. Intensity measurements were made using the θ–2θ mode up to

$2\theta = 50°$ with profile analysis. 3 standard reflections, no intensity variation. Low-temperature data were collected by cooling the crystal in a stream of cold nitrogen and the crystal was conditioned at 110 K for 2 d before the intensity collection began. There were 5882 (room temperature), 5642 (110 K) unique reflections, 5060 (room temperature), 5342 (110 K) with $I > 2{\cdot}5\sigma(I)$. Intensities were corrected for Lorentz–polarization and absorption effects. The min. and max. transmission factors are 0·453 and 0·547 respectively.

Table 1. *Atomic parameters and equivalent isotropic temperature parameters for triphenyltin chloride*

E.s.d.'s are given in parentheses.

$$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	Room temperature				110 K			
	x	y	z	B_{eq}/B_{iso}	x	y	z	B_{eq}/B_{iso}
Sn(1)	0·169792 (15)	0·05724 (3)	0·047939 (14)	3·721 (15)	0·167342 (13)	0·056187 (25)	0·045508 (12)	1·203 (10)
Sn(2)	0·187261 (15)	0·18487 (3)	0·552553 (14)	3·702 (13)	0·187603 (13)	0·185748 (25)	0·550801 (12)	1·177 (10)
Cl(1)	0·10666 (8)	0·22901 (14)	0·09499 (7)	7·15 (8)	0·10096 (6)	0·22757 (10)	0·09345 (5)	2·39 (4)
Cl(2)	0·13289 (8)	0·00280 (14)	0·60186 (7)	7·06 (8)	0·13168 (6)	0·00032 (10)	0·60092 (5)	2·34 (4)
C(11)	0·13827 (21)	−0·1316 (4)	0·08592 (21)	3·67 (19)	0·13623 (19)	−0·1361 (4)	0·08438 (18)	1·31 (14)
C(12)	0·15248 (24)	−0·1521 (5)	0·16167 (23)	4·36 (23)	0·15003 (20)	−0·1539 (4)	0·16112 (19)	1·47 (14)
C(13)	0·1376 (3)	−0·2757 (6)	0·1903 (3)	5·5 (3)	0·13490 (21)	−0·2810 (4)	0·19019 (21)	1·82 (15)
C(14)	0·1076 (3)	−0·3790 (7)	0·1435 (4)	6·1 (3)	0·10636 (22)	−0·3897 (4)	0·14335 (23)	2·01 (17)
C(15)	0·0926 (3)	−0·3627 (6)	0·0694 (4)	6·3 (3)	0·09189 (22)	−0·3734 (4)	0·06727 (22)	1·94 (16)
C(16)	0·1073 (3)	−0·2392 (6)	0·0406 (3)	5·0 (3)	0·10677 (21)	−0·2480 (4)	0·03810 (21)	1·72 (16)
C(21)	0·13919 (22)	0·0894 (4)	−0·06642 (19)	3·41 (18)	0·13818 (20)	0·0928 (3)	−0·07053 (18)	1·30 (14)
C(22)	0·0659 (3)	0·1118 (5)	−0·1064 (3)	4·40 (23)	0·06437 (21)	0·1187 (4)	−0·11021 (19)	1·42 (15)
C(23)	0·0488 (3)	0·1330 (5)	−0·1812 (3)	4·95 (24)	0·04795 (21)	0·1435 (4)	−0·18637 (19)	1·63 (14)
C(24)	0·1030 (3)	0·1318 (5)	−0·2171 (3)	5·1 (3)	0·10445 (22)	0·1391 (4)	−0·22212 (20)	1·66 (16)
C(25)	0·1750 (3)	0·1085 (5)	−0·17920 (25)	5·0 (3)	0·17720 (22)	0·1130 (4)	−0·18330 (20)	1·70 (16)
C(26)	0·19315 (25)	0·0879 (5)	−0·10437 (23)	4·20 (23)	0·19480 (20)	0·0896 (4)	−0·10732 (19)	1·42 (15)
C(31)	0·28424 (22)	0·0948 (4)	0·09717 (19)	3·79 (20)	0·28284 (19)	0·0965 (4)	0·09658 (17)	1·32 (13)
C(32)	0·3360 (3)	−0·0080 (5)	0·0983 (3)	5·3 (3)	0·33581 (22)	−0·0079 (4)	0·09889 (20)	1·68 (16)
C(33)	0·4106 (3)	0·0117 (6)	0·1291 (3)	5·9 (3)	0·41131 (22)	0·0146 (4)	0·13130 (21)	2·02 (16)
C(34)	0·4351 (3)	0·1371 (6)	0·1593 (3)	5·6 (3)	0·43495 (22)	0·1446 (4)	0·16225 (19)	1·80 (15)
C(35)	0·3865 (3)	0·2400 (6)	0·15866 (24)	5·2 (3)	0·38342 (22)	0·2491 (4)	0·16048 (18)	1·69 (15)
C(36)	0·3113 (3)	0·2193 (5)	0·12785 (24)	4·45 (24)	0·30745 (21)	0·2262 (4)	0·12799 (19)	1·50 (15)
C(41)	0·15258 (21)	0·3688 (4)	0·59234 (20)	3·57 (17)	0·15241 (19)	0·3725 (4)	0·59181 (18)	1·33 (13)
C(42)	0·17384 (24)	0·3964 (5)	0·66676 (22)	4·11 (20)	0·17668 (20)	0·4004 (4)	0·66785 (19)	1·39 (14)
C(43)	0·1546 (3)	0·5187 (6)	0·6928 (3)	5·3 (3)	0·15745 (21)	0·5249 (4)	0·69591 (20)	1·68 (15)
C(44)	0·1134 (3)	0·6135 (6)	0·6469 (3)	5·5 (3)	0·11438 (22)	0·6225 (4)	0·64891 (21)	1·89 (16)
C(45)	0·0922 (3)	0·5878 (6)	0·5740 (3)	5·9 (3)	0·09026 (23)	0·5954 (4)	0·57411 (22)	2·02 (16)
C(46)	0·11059 (25)	0·4657 (5)	0·54644 (23)	4·59 (23)	0·10837 (21)	0·4711 (4)	0·54552 (20)	1·73 (16)
C(51)	0·14518 (22)	0·1572 (4)	0·43819 (20)	3·72 (18)	0·14407 (20)	0·1558 (3)	0·43497 (18)	1·29 (14)
C(52)	0·0700 (3)	0·1344 (5)	0·40797 (24)	4·41 (22)	0·06771 (21)	0·1290 (4)	0·40608 (19)	1·45 (15)
C(53)	0·0418 (3)	0·1184 (5)	0·3334 (3)	5·3 (3)	0·03821 (21)	0·1092 (4)	0·33072 (20)	1·72 (15)
C(54)	0·0880 (4)	0·1260 (5)	0·2899 (3)	5·8 (3)	0·08434 (22)	0·1193 (4)	0·28349 (19)	1·79 (16)
C(55)	0·1620 (3)	0·1490 (6)	0·3179 (3)	5·6 (3)	0·16034 (23)	0·1470 (4)	0·31133 (20)	1·81 (16)
C(56)	0·1914 (3)	0·1653 (5)	0·39266 (23)	4·40 (22)	0·19056 (21)	0·1644 (4)	0·38713 (20)	1·54 (15)
C(61)	0·30316 (22)	0·1553 (4)	0·59556 (20)	3·81 (19)	0·30482 (19)	0·1549 (4)	0·59509 (18)	1·37 (13)
C(62)	0·3515 (3)	0·2603 (5)	0·5896 (3)	5·3 (3)	0·35565 (22)	0·2580 (4)	0·58992 (20)	1·79 (16)
C(63)	0·4274 (3)	0·2431 (7)	0·6169 (3)	6·7 (3)	0·43239 (23)	0·2390 (4)	0·61859 (21)	2·15 (16)
C(64)	0·4552 (4)	0·1224 (7)	0·6500 (3)	6·8 (3)	0·45927 (23)	0·1136 (4)	0·65243 (21)	2·17 (16)
C(65)	0·4083 (4)	0·0217 (7)	0·6564 (3)	6·5 (3)	0·40971 (24)	0·0109 (4)	0·65824 (21)	2·13 (17)
C(66)	0·3328 (3)	0·0349 (5)	0·62952 (24)	4·84 (25)	0·33290 (22)	0·0288 (4)	0·62984 (19)	1·66 (16)
H(12)	0·1767 (25)	−0·080 (4)	0·1982 (23)	7·8 (13)	0·1666 (20)	−0·080 (4)	0·1900 (19)	1·4 (8)
H(13)	0·145 (3)	−0·293 (5)	0·249 (3)	8·9 (14)	0·1451 (22)	−0·300 (4)	0·2393 (21)	2·2 (9)
H(14)	0·101 (3)	−0·448 (5)	0·163 (3)	9·0 (20)	0·0975 (22)	−0·467 (4)	0·1582 (21)	2·1 (9)
H(15)	0·0749 (24)	−0·431 (5)	0·0407 (23)	5·8 (12)	0·0736 (23)	−0·451 (4)	0·0377 (21)	2·8 (9)
H(16)	0·0964 (19)	−0·229 (4)	−0·0043 (18)	3·2 (9)	0·0963 (19)	−0·239 (4)	−0·0052 (18)	0·8 (7)
H(22)	0·0305 (19)	0·115 (3)	−0·0834 (18)	2·9 (8)	0·0306 (18)	0·123 (3)	−0·0840 (17)	0·1 (6)
H(23)	0·0051 (25)	0·144 (5)	−0·2119 (24)	7·0 (13)	0·0000 (18)	0·161 (3)	−0·2149 (17)	0·4 (6)
H(24)	0·0882 (20)	0·137 (4)	−0·2691 (20)	4·5 (9)	0·0935 (19)	0·149 (4)	−0·2674 (18)	0·9 (7)
H(25)	0·2100 (22)	0·107 (4)	−0·2056 (23)	5·6 (11)	0·2112 (20)	0·108 (4)	−0·2042 (19)	0·9 (7)
H(26)	0·2411 (21)	0·082 (4)	−0·0835 (18)	4·2 (10)	0·2457 (22)	0·076 (4)	−0·0827 (19)	1·6 (8)
H(32)	0·3207 (22)	−0·080 (4)	0·0825 (20)	3·9 (11)	0·3237 (19)	−0·086 (4)	0·0795 (18)	1·0 (8)
H(33)	0·4434 (25)	−0·063 (5)	0·1336 (23)	7·1 (14)	0·4477 (22)	−0·063 (4)	0·1376 (19)	2·2 (8)
H(34)	0·4848 (22)	0·154 (4)	0·1861 (19)	4·7 (10)	0·4850 (19)	0·162 (3)	0·1876 (17)	0·6 (7)
H(35)	0·406 (3)	0·332 (5)	0·184 (3)	9·5 (16)	0·3998 (21)	0·339 (4)	0·1805 (19)	1·8 (8)
H(36)	0·2811 (21)	0·287 (4)	0·1331 (21)	4·8 (11)	0·2732 (20)	0·303 (4)	0·1284 (18)	1·3 (7)
H(42)	0·2067 (17)	0·340 (3)	0·6933 (17)	2·7 (8)	0·2104 (19)	0·342 (3)	0·7009 (18)	0·8 (7)
H(43)	0·1652 (22)	0·529 (4)	0·7347 (21)	4·6 (11)	0·1735 (22)	0·544 (4)	0·7434 (21)	2·1 (9)
H(44)	0·100 (3)	0·695 (5)	0·659 (3)	8·2 (16)	0·099 (3)	0·711 (5)	0·6665 (25)	4·9 (12)
H(45)	0·0635 (24)	0·635 (5)	0·5433 (23)	5·9 (13)	0·0619 (23)	0·651 (4)	0·5452 (21)	2·1 (9)
H(46)	0·0991 (20)	0·450 (4)	0·4940 (20)	5·0 (10)	0·0926 (21)	0·456 (4)	0·4981 (21)	2·1 (9)
H(52)	0·0381 (20)	0·132 (4)	0·4417 (19)	4·1 (9)	0·0394 (19)	0·123 (4)	0·4365 (18)	0·8 (7)
H(53)	−0·0123 (24)	0·099 (4)	0·3153 (23)	6·8 (12)	−0·0142 (19)	0·087 (3)	0·3094 (17)	0·8 (7)
H(54)	0·0712 (20)	0·117 (4)	0·2505 (18)	2·9 (9)	0·0617 (20)	0·108 (4)	0·2342 (19)	1·6 (8)
H(55)	0·1943 (21)	0·163 (4)	0·2991 (21)	3·5 (11)	0·1905 (19)	0·158 (3)	0·2815 (18)	0·7 (7)
H(56)	0·2409 (18)	0·177 (3)	0·4135 (16)	2·5 (7)	0·2369 (20)	0·176 (3)	0·4062 (17)	0·5 (7)
H(62)	0·3315 (22)	0·340 (4)	0·5574 (21)	6·1 (11)	0·3415 (20)	0·340 (4)	0·5671 (18)	1·5 (8)
H(63)	0·452 (3)	0·314 (5)	0·604 (3)	8·7 (18)	0·4670 (21)	0·309 (4)	0·6166 (19)	1·9 (8)
H(64)	0·5074 (23)	0·114 (4)	0·6643 (20)	5·0 (11)	0·5115 (19)	0·102 (3)	0·6737 (17)	0·6 (6)
H(65)	0·4252 (23)	−0·053 (4)	0·6694 (21)	4·6 (11)	0·4269 (21)	−0·073 (4)	0·6772 (20)	1·9 (8)
H(66)	0·2981 (19)	−0·036 (4)	0·6337 (19)	3·9 (10)	0·2990 (19)	−0·046 (3)	0·6372 (17)	0·9 (7)

$h = -22$–21, $k = 0$–11, $l = 1$–21 (room temperature), $h = -21$–21, $k = 0$–11, $l = 1$–21 (110 K). The structure was solved by *MULTAN* (Germain, Main & Woolfson, 1971) and refined with full-matrix least squares on F. All H atoms were located in difference Fourier maps. Refinement using anisotropic and isotropic temperature factors for non-H and H atoms respectively yielded $R = 0.033$ (room temperature) and $R = 0.031$ (110 K), number of variables 482, max. $\Delta/\sigma = 0.031$. Highest peak in final difference synthesis 0·69 e Å^{-3} (room temperature), 1·97 e Å^{-3} (110 K) near the Sn atoms. Details of the computer programs used and experimental procedure have been presented previously (Grant & Gabe, 1978; Gabe, Lee & Le Page, 1985). The molecules are depicted in Fig. 1. The atomic coordinates and isotropic thermal parameters are given in Table 1, selected bond distances and bond angles are listed in Table 2.*

Table 2. *Selected bond distances* (Å) *and bond angles* (°) *for* Ph_3ClSn

	Room temperature	110 K
Sn(1)–Cl(1)	2·3538 (14)	2·3620 (10)
Sn(2)–Cl(2)	2·3557 (14)	2·3692 (10)
Sn(1)–C(11)	2·113 (4)	2·117 (3)
Sn(1)–C(21)	2·114 (4)	2·124 (3)
Sn(1)–C(31)	2·120 (4)	2·126 (3)
Sn(2)–C(41)	2·109 (4)	2·117 (3)
Sn(2)–C(51)	2·118 (4)	2·123 (3)
Sn(2)–C(61)	2·116 (4)	2·120 (3)
Cl(1)–Sn(1)–C(11)	105·28 (10)	105·85 (12)
Cl(1)–Sn(1)–C(21)	104·81 (10)	105·08 (11)
Cl(1)–Sn(1)–C(31)	105·01 (10)	104·98 (12)
C(11)–Sn(1)–C(21)	118·45 (13)	117·11 (14)
C(11)–Sn(1)–C(31)	109·46 (13)	109·83 (14)
C(21)–Sn(1)–C(31)	112·59 (13)	112·90 (15)
Cl(2)–Sn(2)–C(41)	106·66 (10)	106·74 (12)
Cl(2)–Sn(2)–C(51)	102·41 (10)	103·38 (12)
Cl(2)–Sn(2)–C(61)	104·12 (10)	104·45 (12)
C(41)–Sn(2)–C(51)	114·52 (13)	114·18 (14)
C(41)–Sn(2)–C(61)	110·70 (13)	110·94 (14)
C(51)–Sn(2)–C(61)	116·94 (13)	115·91 (15)

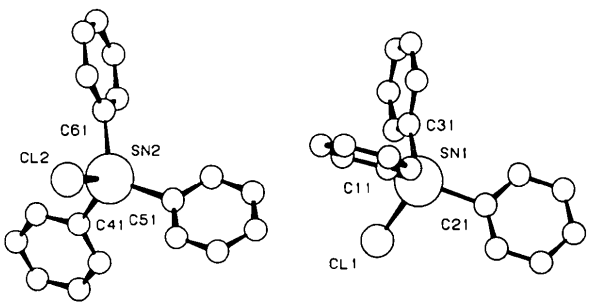

Fig. 1. Numbering scheme and perspective drawing of the two independent molecules of Ph_3SnCl.

Related literature. Bancroft, Bulter & Sham (1975); Bokii, Zalkharova & Struchkov (1970); Bokii, Struchkov & Prokofiev (1972); Bondi (1964); Srivistawa (1967).

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43162 (86 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Bis(η^5-methylcyclopentadienyl)divanadium Pentaselenide

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Abstract. μ-Diseleno-*Se,Se'*-μ-(η-diseleno-μ-*Se,Se'*)-μ-seleno-bis(methylcyclopentadienylvanadium)(*V—V*), $[V_2(C_6H_7)_2Se_5]$, $M_r = 654.9$, triclinic, $P\bar{1}$, $a = 7.121$ (3), $b = 10.473$ (4), $c = 11.694$ (4) Å, $\alpha = 96.66$ (3), $\beta = 93.80$ (3), $\gamma = 109.12$ (3)°, $V = 813.4$ (5) Å^3, $Z = 2$, $D_x = 2.674$ g cm^{-3}, Mo $K\alpha$ (λ

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