



Table 2 Atomic parameters of the tetragonal structure (space-group: $P4/mmm$ (No. 123))

Atom	Ox.	Wyck.	Site symmetry	x/a	y/b	z/c
Pb	+2	1a	4/mmm	0	0	0
Tm/Yb	+3	1d	4/mmm	1/2	1/2	1/2
F	-1	4i	2/mm	0	1/2	1/4
F interstitial	-1	1b	4/mm	0	0	1/2

data_20597-ICSD

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_chemical_formula_sum 'F2 Pb1'
_publ_section_title

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The neutron diffraction pattern investigation of cubic modificaton of
Pb F2

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_citation_journal_id_ASTM
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2 'Golden Book of Phase Transitions, Wroclaw' 2002 1 1 123 GBOPT5
_publ_author_name

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Yamzin, I.I.;Nozik, Yu.Z.;Belov, N.V.

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_cell_length_b 5.940(1)
_cell_length_c 5.940(1)
_cell_angle_alpha 90.
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_cell_angle_gamma 90.
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6 'x, y, -z'
7 'z, -y, x'
8 'y, -x, z'
9 'x, -z, y'
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11 'y, -z, x'
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14 '-y, x, z'
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17 '-y, z, x'
18 '-x, y, z'
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32 '-y, x, -z'
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34 '-z, x, -y'
35 '-y, z, -x'
36 '-x, y, -z'
37 'z, -y, -x'
38 'y, -x, -z'
39 'x, -z, -y'
40 'z, -x, -y'
41 'y, -z, -x'
42 'x, -y, -z'
43 'z, y, x'
44 'y, x, z'
45 'x, z, y'
46 'z, x, y'

47 'y, z, x'
48 'x, y, z'
49 'z, y+.5, -x+.5'
50 'z+.5, y, -x+.5'
51 'z+.5, y+.5, -x'
52 'y, x+.5, -z+.5'
53 'y+.5, x, -z+.5'
54 'y+.5, x+.5, -z'
55 'x, z+.5, -y+.5'
56 'x+.5, z, -y+.5'
57 'x+.5, z+.5, -y'
58 'z, x+.5, -y+.5'
59 'z+.5, x, -y+.5'
60 'z+.5, x+.5, -y'
61 'y, z+.5, -x+.5'
62 'y+.5, z, -x+.5'
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83 'x+.5, -y, z+.5'
84 'x+.5, -y+.5, z'
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86 '-z+.5, y, x+.5'
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88 '-y, x+.5, z+.5'
89 '-y+.5, x, z+.5'
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Reason for no structure factor data deposited:

ICSD #20597

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Coll Code 20597

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