Name and formula

Reference code:	98-004-8259
Mineral name:	Fluocerite (Ce)
Compound name:	Fluocerite (Ce)
Chemical name:	Cerium Fluoride
Common name:	Fluocerite (Ce)
ICSD name:	Cerium Fluoride
Chemical formula:	Ce_1F_3
Second chemical formula:	CeF_3

Crystallographic parameters

Crystal system:	Hexagonal
Space group:	P 63/m c m
Space group number:	193
a (Å):	7.1300
b (Å):	7.1300
c (Å):	7.2900
Alpha (°):	90.0000
Beta (°):	90.0000
Gamma (°):	120.0000
Calculated density (g/cm^3):	6.12
Volume of cell (10^6 pm^3):	320.95
Z:	6.00
RIR:	8.80

Subfiles and quality

Subfiles:	ICSD Pattern Inorganic Mineral
Quality:	Calculated (C)

Comments

ICSD collection code:	42470
Creation Date:	01/01/1970
Modification Date:	01/01/1970
Calculated Pattern Original Remarks:	Compound with mineral name:
Original ICSD space group:	P63/MCM
ICSD Collection Code:	42470
Original ICSD space group:	P63/MCM

Structure deduced from n.m.r. data, cf. 4

At least one temperature factor missing in the paper.

No R value given in the paper

The structure has been assigned a PDF number: 38-452

Compound with mineral name: Fluocerite (Ce)

Recording date: 7/15/2000

Mineral origin: Fluocerite (Ce) - synthetic

ANX formula: AX3

Z: 6

Calculated density: 6.12

Pearson code: hP24

Wyckoff code: k g c a

PDF code: 00-038-0452

TRANS Origin 0 0 1/2

Publ. title: The symmetry and basic structures of La F3, Ce F3, Pr F3 and Nd F3

References

Primary reference: Lundin, A.G. Habuda, S.B. Afanasiev, M.L., *Acta Crystallographica B (24,1968-38,1982)*, **28**, 2903, (1972)

Peak list

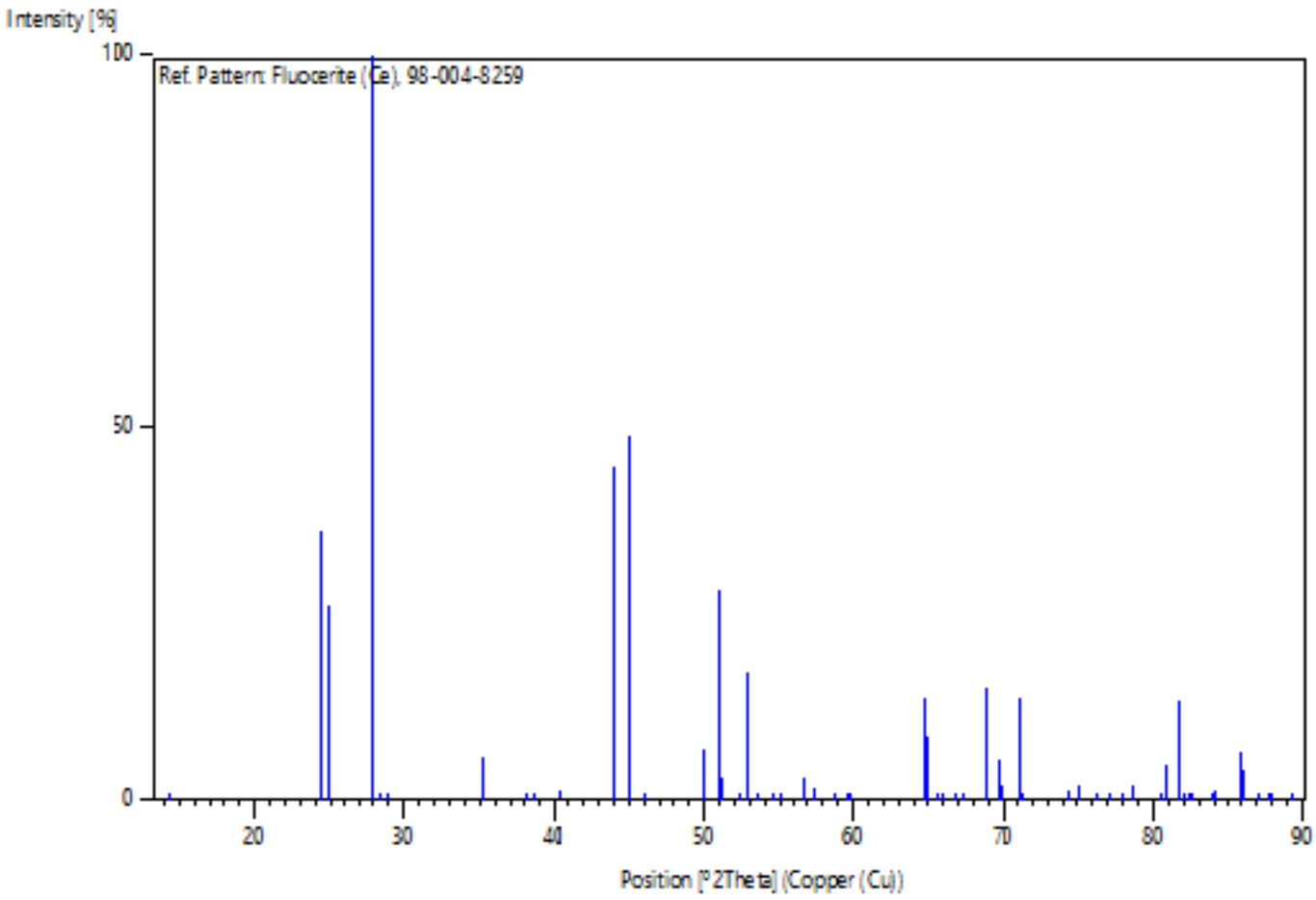
No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	0	1	0	6.17476	14.333	0.4
2	0	0	2	3.64500	24.401	36.0
3	1	1	0	3.56500	24.957	26.1
4	1	1	1	3.20257	27.835	100.0
5	0	1	2	3.13891	28.411	0.6
6	0	2	0	3.08738	28.896	0.1
7	1	1	2	2.54865	35.184	5.9
8	0	2	2	2.35586	38.170	0.8
9	1	2	0	2.33384	38.544	0.1
10	1	2	1	2.22271	40.554	1.3
11	0	3	0	2.05825	43.956	44.6
12	1	1	3	2.00791	45.118	49.1
13	1	2	2	1.96547	46.148	0.1
14	0	0	4	1.82250	50.005	6.9
15	0	3	2	1.79225	50.909	28.3
16	2	2	0	1.78250	51.208	3.2
17	0	1	4	1.74795	52.295	0.0
18	2	2	1	1.73149	52.831	17.2
19	1	3	0	1.71257	53.461	0.0
20	1	2	3	1.68324	54.468	0.1
21	1	3	1	1.66718	55.037	0.3
22	1	1	4	1.62275	56.678	3.2

23	2	2	2	1.60128	57.508	1.8
24	0	2	4	1.56945	58.787	0.0
25	1	3	2	1.55001	59.599	0.5
26	0	4	0	1.54369	59.868	0.1
27	2	2	3	1.43728	64.816	13.7
28	1	2	4	1.43642	64.859	8.4
29	0	4	2	1.42147	65.627	0.6
30	2	3	0	1.41659	65.882	0.0
31	1	3	3	1.39985	66.771	0.0
32	2	3	1	1.39058	67.276	0.3
33	0	3	4	1.36447	68.741	15.2
34	1	1	5	1.34950	69.613	5.6
35	1	4	0	1.34744	69.734	2.1
36	1	4	1	1.32500	71.092	13.6
37	2	3	2	1.32038	71.379	0.5
38	2	2	4	1.27432	74.382	1.5
39	1	4	2	1.26385	75.105	2.2
40	1	3	4	1.24802	76.226	0.1
41	1	2	5	1.23654	77.064	0.3
42	0	5	0	1.23495	77.181	0.0
43	2	3	3	1.22382	78.015	0.0
44	0	0	6	1.21500	78.690	2.0
45	0	1	6	1.19214	80.504	0.0
46	3	3	0	1.18833	80.815	4.9
47	1	4	3	1.17840	81.639	13.3
48	0	4	4	1.17793	81.679	8.6
49	3	3	1	1.17285	82.109	0.0
50	0	5	2	1.16964	82.383	0.2
51	2	4	0	1.16692	82.617	0.0
52	2	4	1	1.15225	83.905	0.3
53	1	1	6	1.15004	84.103	1.4
54	0	2	6	1.13060	85.894	1.9
55	3	3	2	1.12981	85.969	6.6
56	2	2	5	1.12856	86.087	4.0
57	2	3	4	1.11846	87.057	0.1
58	2	4	2	1.11136	87.755	0.0
59	1	3	5	1.11017	87.873	0.1
60	1	5	0	1.10902	87.987	0.0
61	1	5	1	1.09641	89.267	0.3

Structure

No.	Name	Elem.	X	Y	Z	Biso	sof	Wyck.
1	F1	F	0.29000	0.00000	0.56000	0.5000	1.0000	12k
2	F2	F	0.33330	0.66670	0.25000	0.5000	1.0000	4c
3	F3	F	0.00000	0.00000	0.25000	0.5000	1.0000	2a
4	CE1	Ce	0.34000	0.00000	0.25000	0.5000	1.0000	6g

Stick Pattern


Intensity [%]
100
50
0
Ref. Pattern: Fluocerite (Ce), 98-004-8259
20
30
40
50
60
70
80
90
Position [°2Theta] (Copper (Cu))