11.2. Röntgenbeugung

11.2.1. Pulvermethode: Beispiel 1 (I_2)

JCPDS-Karte für I_2

I2 Iodine

Rad: CuKa1 Lambda: 1.54056 Filter: Mono. d-sp: Calculated
Cutoff: 15.0 Int: Calculated I/Icor: 9.3
Ref: Martin, K., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA, ICDD Grant-in-Aid, (1991)

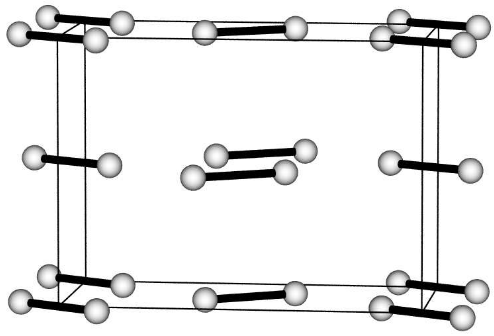
Sys: Orthorhombic S.G.: Cmca (64)
a: 7.2678 b: 4.7915 c: 9.8277 A: 0.7395 C: 0.4876
A: B: C: Z: 4 mp:
Ref: Ibid.

Dx: 4.926 Dm: SS/FOM: F(30)=370.8(.0025,32)

Peak height intensities. Calculation of diffractometer peak intensities done with MICRO-POWD v. 2.2 (D.K. Smith and K.L. Smith), using default instrument broadening function (NBS Table), diffracted beam monochromator polarization correction and atomic scattering factors corrected for anomalous dispersion. Cell parameters from 43-304. Atomic positions from Harris, P. et al., J. Am. Chem. Soc., 50 1583 (1928): I in 8f with y=0.1156, z=0.1493. Isotropic thermal parameters estimated as 1.0 for I. Intensity threshold for <1 = 0.1%. See 43-304 for experimental pattern. PSC: oC8. Mwt: 253.81. Volume[CD]: 342.24.
Strong lines: 3.10/X 3.63/6 3.71/5 1.98/2 2.04/2 2.46/2 1.96/2 2.33/1
115 reflections in pattern. Page 1 of 4. Radiation= 1.54050

2-theta	Int.	h k l	2-theta	Int.	h k l
18.036	2	0 0 2	46.945	10	0 2 3
23.998	52	1 1 1	50.167	7	4 0 0
24.474	62	2 0 0	50.539	3	3 1 3
28.755	100	1 1 2	51.777	7	1 1 5
30.568	1	2 0 2	53.365	2	0 2 4
35.378	9	1 1 3	53.642	13	2 2 3
36.540	18	0 0 4	53.741	<1	4 0 2
37.504	2	0 2 0	56.103	1	0 0 6
38.642	13	0 2 1	56.661	1	3 1 4
42.800	9	3 1 1	59.544	1	2 2 4
43.165	2	1 1 4	59.991	7	1 3 1
44.482	19	2 0 4	60.912	<1	0 2 5
45.303	2	2 2 0	61.081	9	1 1 6
45.813	24	3 1 2	62.102	1	2 0 6
46.281	15	2 2 1	62.404	1	1 3 2

usw....



Kristallstruktur von I_2

Röntgenpulverdiagramm von I_2