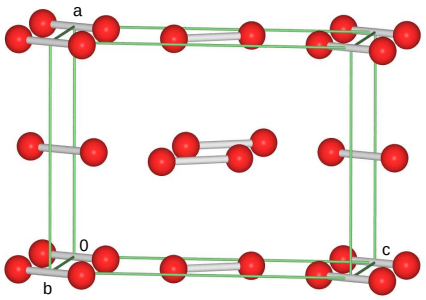
## 4.2. Beispiel 1 ($I_2$)

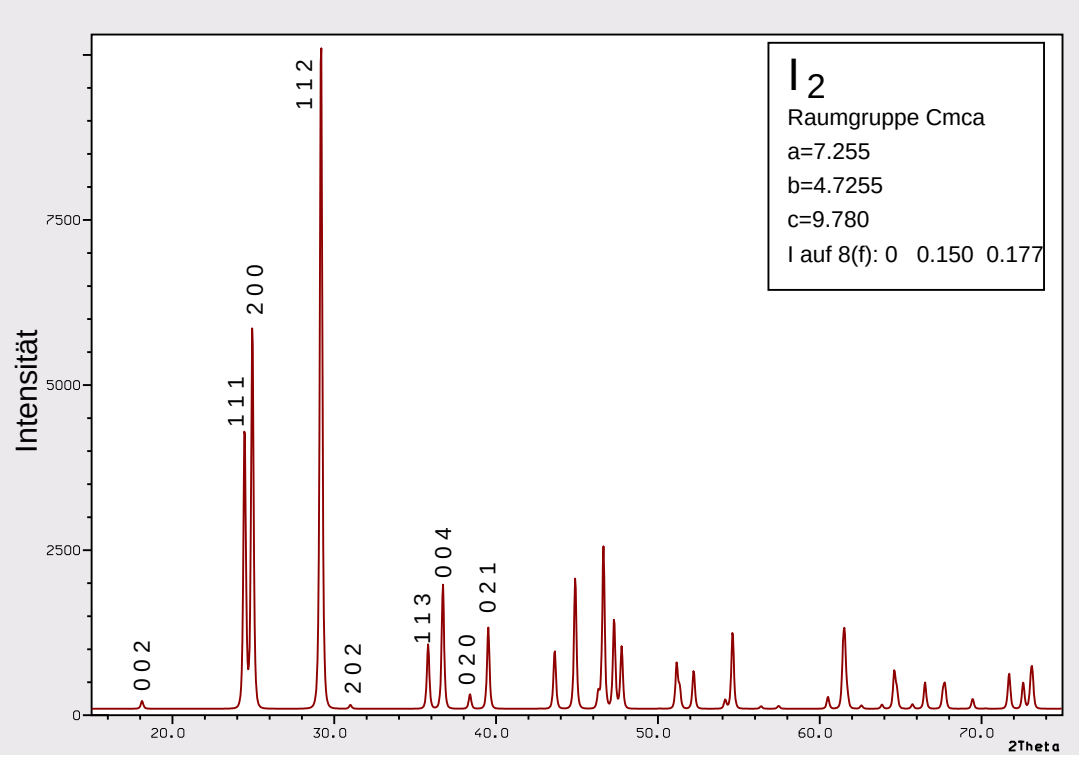



**Kristallstruktur von $I_2$**

### 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....
```

### Röntgenpulverdiagramm von $I_2$