

$Mg_2Zn_{11}$ *cP39*(200) *Pm-3* – *jhgfa***Mg<sub>2</sub>Zn<sub>11</sub>** [1], Strukturbericht notation D8<sub>c</sub>Structural features: ZnZn<sub>12</sub> icosahedra and empty Zn<sub>6</sub> octahedra in a CsCl-type arrangement, separated by additional Zn and Mg atoms.

Samson S. (1949) [1]

 $Mg_2Zn_{11}$  $a = 0.8552 \text{ nm}$ ,  $V = 0.6255 \text{ nm}^3$ ,  $Z = 3$ 

| site | Wyck.       | sym.          | <i>x</i> | <i>y</i>      | <i>z</i>      | occ. | atomic environment                                  |
|------|-------------|---------------|----------|---------------|---------------|------|---|
| Zn1  | 12 <i>j</i> | <i>m</i> ..   | 0        | 0.157         | 0.257         |      | icosahedron Zn <sub>9</sub> Mg <sub>3</sub>         |
| Zn2  | 8 <i>i</i>  | .3.           | 0.278    | 0.278         | 0.278         |      | icosahedron Zn <sub>9</sub> Mg <sub>3</sub>         |
| Zn3  | 6 <i>h</i>  | <i>mm</i> 2.. | 0.265    | $\frac{1}{2}$ | $\frac{1}{2}$ |      | 10-vertex polyhedron Zn <sub>10</sub>               |
| Zn4  | 6 <i>g</i>  | <i>mm</i> 2.. | 0.340    | $\frac{1}{2}$ | 0             |      | pseudo Frank-Kasper Zn <sub>9</sub> Mg <sub>4</sub> |
| Mg5  | 6 <i>f</i>  | <i>mm</i> 2.. | 0.18     | 0             | $\frac{1}{2}$ |      | 7-capped pentagonal prism Zn <sub>16</sub> Mg       |
| Zn6  | 1 <i>a</i>  | <i>m-3</i> .  | 0        | 0             | 0             |      | icosahedron Zn <sub>12</sub>                        |

Transformation from published data: *y,x,-z*; origin shift  $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ 

Experimental: single crystal, Weissenberg photographs, X-rays

References: [1] Samson S. (1949), Acta Chem. Scand. 3, 835-843.