

La<sub>6</sub>Rh<sub>32</sub>P<sub>17</sub>

hP168

(176)  $P6_3/m - h^{27}fb$ **La<sub>6</sub>Rh<sub>32</sub>P<sub>17</sub>** [1]; Ce<sub>6</sub>Rh<sub>32</sub>P<sub>17</sub> [1]

Structural features: Infinite columns of base-linked P(La<sub>2</sub>Rh<sub>4</sub>)Rh<sub>3</sub> tricapped trigonal prisms share atoms to form a 3D-framework with double and partial propeller-like columns; additional P in channels of hexagonal cross-section parallel to [001] (partial disorder).

Pivan J.Y. et al. (1988) [1]

La<sub>6</sub>P<sub>17</sub>Rh<sub>32</sub> $a = 2.7054$ ,  $c = 0.3944$  nm,  $c/a = 0.146$ ,  $V = 2.4999$  nm<sup>3</sup>,  $Z = 3$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Rh1	6h	m..	0.0016	0.4659	$\frac{1}{4}$		13-vertex polyhedron P <sub>4</sub> Rh <sub>6</sub> La <sub>3</sub>
Rh2	6h	m..	0.027	0.2243	$\frac{1}{4}$		cuboctahedron P <sub>4</sub> Rh <sub>5</sub> La <sub>3</sub>
Rh3	6h	m..	0.056	0.0946	$\frac{1}{4}$		square pyramid P <sub>5</sub>
P4	6h	m..	0.0611	0.3827	$\frac{1}{4}$		square pyramid Rh <sub>5</sub>
Rh5	6h	m..	0.1092	0.4885	$\frac{1}{4}$		11-vertex polyhedron P <sub>4</sub> Rh <sub>5</sub> La <sub>2</sub>
Rh6	6h	m..	0.1157	0.335	$\frac{1}{4}$		11-vertex polyhedron P <sub>4</sub> Rh <sub>5</sub> La <sub>2</sub>
P7	6h	m..	0.1346	0.0125	$\frac{1}{4}$		tricapped trigonal prism Rh <sub>7</sub> La <sub>2</sub>
La8	6h	m..	0.15741	0.23345	$\frac{1}{4}$		23-vertex polyhedron P <sub>9</sub> Rh <sub>12</sub> La <sub>2</sub>
Rh9	6h	m..	0.1668	0.1143	$\frac{1}{4}$		cuboctahedron P <sub>4</sub> Rh <sub>5</sub> La <sub>3</sub>
P10	6h	m..	0.2081	0.5427	$\frac{1}{4}$		monocapped trigonal prism Rh <sub>7</sub>
P11	6h	m..	0.216	0.3981	$\frac{1}{4}$		tricapped trigonal prism Rh <sub>7</sub> La <sub>2</sub>
Rh12	6h	m..	0.239	0.6373	$\frac{1}{4}$		
Rh13	6h	m..	0.2651	0.4993	$\frac{1}{4}$		11-vertex polyhedron P <sub>4</sub> Rh <sub>5</sub> La <sub>2</sub>
P14	6h	m..	0.2675	0.1773	$\frac{1}{4}$		tricapped trigonal prism Rh <sub>7</sub> La <sub>2</sub>
Rh15	6h	m..	0.2692	0.3564	$\frac{1}{4}$		cuboctahedron P <sub>3</sub> Rh <sub>7</sub> La <sub>2</sub>
P16	6h	m..	0.2995	0.0417	$\frac{1}{4}$		bicapped square prism Rh <sub>7</sub> La <sub>2</sub> P
Rh17	6h	m..	0.3026	0.2728	$\frac{1}{4}$		11-vertex polyhedron P <sub>5</sub> Rh <sub>6</sub>
Rh18	6h	m..	0.3337	0.1458	$\frac{1}{4}$		cuboctahedron P <sub>4</sub> Rh <sub>5</sub> La <sub>3</sub>
Rh19	6h	m..	0.3806	0.0339	$\frac{1}{4}$		cuboctahedron P <sub>2</sub> Rh <sub>8</sub> La <sub>2</sub>
La20	6h	m..	0.3855	0.48094	$\frac{1}{4}$		22-vertex polyhedron Rh <sub>14</sub> P <sub>6</sub> La <sub>2</sub>
Rh21	6h	m..	0.4145	0.3775	$\frac{1}{4}$		cuboctahedron P <sub>3</sub> Rh <sub>7</sub> La <sub>2</sub>
Rh22	6h	m..	0.4394	0.1572	$\frac{1}{4}$		13-vertex polyhedron P <sub>4</sub> Rh <sub>6</sub> La <sub>3</sub>
La23	6h	m..	0.44072	0.2787	$\frac{1}{4}$		23-vertex polyhedron P <sub>9</sub> Rh <sub>12</sub> La <sub>2</sub>
P24	6h	m..	0.5379	0.205	$\frac{1}{4}$		monocapped trigonal prism Rh <sub>7</sub>
P25	6h	m..	0.5566	0.0661	$\frac{1}{4}$		monocapped trigonal prism Rh <sub>7</sub>
Rh26	6h	m..	0.5789	0.3048	$\frac{1}{4}$		square pyramid P <sub>5</sub>
Rh27	6h	m..	0.5961	0.165	$\frac{1}{4}$		cuboctahedron P <sub>4</sub> Rh <sub>5</sub> La <sub>3</sub>
P28	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.13	0.5	
P29	2b	-3..	0	0	0	0.5	square prism (cube) P <sub>2</sub> Rh <sub>6</sub>

Transformation from published data: origin shift 0 0  $\frac{1}{2}$ 

Experimental: single crystal, diffractometer, X-rays, R = 0.050

Remarks: Short interatomic distances for partly occupied site(s). In table II of [1] the y-coordinate of former Rh(6) is misprinted as 0.6592 instead of 0.6952 (checked on interatomic distances).

References: [1] Pivan J.Y., Guérin R., Peña O., Padiou J., Sergent M. (1988), Mater. Res. Bull. 23, 513-520.