

Space group (195) *P23*195
cP20

$\text{Cd}_8\text{As}_7\text{Cl}$	<i>cP20</i>	(195) <i>P23</i> – ge^3ba
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 $\text{Cd}_8\text{As}_7\text{Cl}$ [1]

Structural features: Cd forms a distorted Po-type framework (primitive cubic arrangement, splitting of one Cd site); As_2 dumbbells, single As and Cl in distorted cubic voids (three As_2 dumbbells for one single As). CdAs_4 and $\text{Cd}(\text{As}_3\text{Cl})$ tetrahedra share atoms to form a 3D-framework.

Shevelkov A.V. et al. (1997) [1]

$\text{As}_7\text{Cd}_8\text{Cl}$

$a = 0.7266 \text{ nm}$, $V = 0.3836 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
As1	6g	2..	0.1672	0	$\frac{1}{2}$		
Cd2	4e	.3.	0.2158	0.2158	0.2158	0.535	
Cd3	4e	.3.	0.2637	0.2637	0.2637	0.465	
Cd4	4e	.3.	0.717	0.717	0.717		tetrahedron As_4
As5	1b	23.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		square prism (cube) Cd_8
Cl6	1a	23.	0	0	0		tetrahedron Cd_4

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.026$, $T = 293 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Shevelkov A.V., Reshetova L.N., Popovkin B.A. (1997), J. Solid State Chem. 134, 282-285.

195
cP40

$\text{Ba}_4\text{Cu}_3\text{EuO}_{9.33}$	<i>cP40</i>	(195) <i>P23</i> – $\text{ihgfe}^2\text{dcba}$
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 $\text{EuBa}_4\text{Cu}_3\text{O}_{8.5+x}$ [1]

Structural features: Ignoring vacancies, ordering variant of perovskite where CuO_6 and EuO_6 octahedra share vertices to form a 3D-framework, Ba in cuboctahedral voids. Partly ordered O vacancies reduce the coordination of Cu to an O_4 square.

Zhu Y.T. et al. (1998) [1]

$\text{Ba}_4\text{Cu}_3\text{EuO}_{9.33}$

$a = 0.81668 \text{ nm}$, $V = 0.5447 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6i	2..	0.224	$\frac{1}{2}$	$\frac{1}{2}$		colinear CuEu
O2	6h	2..	0.24	$\frac{1}{2}$	0	0.58	colinear Cu_2
O3	6g	2..	0.258	0	$\frac{1}{2}$	0.53	colinear Cu_2
O4	6f	2..	0.273	0	0		colinear CuEu
Ba5	4e	.3.	0.24774	0.24774	0.24774		cuboctahedron O_{12}
Ba6	4e	.3.	0.74732	0.74732	0.74732		cuboctahedron O_{12}
Cu7	3d	222..	$\frac{1}{2}$	0	0		octahedron O_6
Cu8	3c	222..	0	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O_6
Eu9	1b	23.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O_6

Eu10 1a 23. 0 0 0 octahedron O₆

Experimental: powder, diffractometer, X-rays, $R_p = 0.077$

Remarks: Space group (200) $Pm-3$ was tested and rejected. The proposed structure deviates little from a body-centered Bravais lattice (calculated intensities zero for $h+k+l = 2n+1$, a few very weak observed intensities are reported in table 2 of [1]). In table 1 of [1] the space group number is misprinted as 200 instead of 195 and the Wyckoff positions of former O1, O2, O3 and O4 as 6e, 6h, 6f, and 6g instead of 6f, 6i, 6g, and 6h, respectively.

References: [1] Zhu Y.T., Peterson E.J., Baldonado P.S., Coulter J.Y., Peterson D.E., Mueller F.M. (1998), J. Phys. Chem. Solids 59, 1331-1336.

195
cP54

RhAl_{2.63}

cP54

(195) $P23 - j^3gfeba$

RhAl_{2.63} [1]

Structural features: Partly disordered structure (split sites), intermediate between a 3D-framework of interconnected RhAl₁₂ icosahedra and RhAl₁₂ cuboctahedra of ideal composition RhAl₃ (AuZn₃ = UH₃ type) and a 3D-framework of interconnected RhAl₁₂ icosahedra and RhAl₁₄ rhombic dodecahedra of ideal composition Rh₄Al₁₃.

Grin Y. et al. (1997) [1]

Al_{2.63}Rh

$a = 0.76692 \text{ nm}$, $V = 0.4511 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12j	1	0.02	0.123	0.699	0.14	
Al2	12j	1	0.133	0.181	0.772	0.15	
Al3	12j	1	0.2004	0.3227	0.5		
Rh4	6g	2..	0.29314	0	$\frac{1}{2}$		
Al5	6f	2..	0.391	0	0	0.26	
Al6	4e	.3.	0.1757	0.1757	0.1757		non-coplanar triangle Al ₃
Rh7	1b	23.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron Al ₁₂
Rh8	1a	23.	0	0	0		

Transformation from published data: $y, x, -z$

Experimental: single crystal, diffractometer, X-rays, $R = 0.042$, $T = 293 \text{ K}$

Remarks: Approximate homogeneity range Al_{100-x}Rh_x, $27 < x < 29$. Short interatomic distances for partly occupied site(s). Space group (200) $Pm-3$ was tested and rejected ($R = 0.045$).

References: [1] Grin Y., Peters K., Burkhardt U., Gotzmann K., Ellner M. (1997), Z. Kristallogr. 212, 439-444.

195
cP57

K_{0.3}Na_{7.3}Ca_{0.3}Al₆[SiO₄]₆[SO₄][OH]_{0.2}

cP57

(195) $P23 - j^2hge^5a$

K_{0.24}Na_{7.2}Ca_{0.24}Al₆Si₆O₂₄(SO₄)_{0.98}(OH)_{0.24} [1], nosean, zeolite SOD-SO₄

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by SO₄ tetrahedra or OH units (ordered arrangement); Na near and (K,Ca) above the centers of 6-rings in cages centered by OH.

Hassan I., Grundy H.D. (1989) [1]

 $\text{Al}_6\text{Ca}_{0.06}\text{H}_{0.24}\text{K}_{0.06}\text{Na}_{7.20}\text{O}_{28.16}\text{S}_{0.98}\text{Si}_6$ $a = 0.9084 \text{ nm}$, $V = 0.7496 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12j	1	0.0362	0.3373	0.3479		non-colinear SiAl
O2	12j	1	0.1366	0.1471	0.5533		non-colinear SiAl
Si3	6h	2..	0.25	$\frac{1}{2}$	0		tetrahedron O ₄
Al4	6g	2..	0.25	0	$\frac{1}{2}$		tetrahedron O ₄
O5	4e	.3.	0.0977	0.0977	0.0977	0.98	single atom S
Na6	4e	.3.	0.2646	0.2646	0.2646	0.98	non-coplanar triangle O ₃
(OH)7	4e	.3.	0.53	0.53	0.53	0.06	
M8	4e	.3.	0.698	0.698	0.698	0.03	trigonal bipyramid NaO ₃ (OH)
Na9	4e	.3.	0.8317	0.8317	0.8317	0.82	single atom Ca
S10	1a	23.	0	0	0	0.98	tetrahedron O ₄

M8 = 0.5Ca + 0.5K

Transformation from published data: $-x, -y, -z$

Experimental: single crystal, diffractometer, X-rays

Remarks: Natural specimen from Laacher See, Germany. Composition $\text{K}_{0.23}\text{Ca}_{0.24}\text{Na}_{7.20}\text{Mg}_{0.04}\text{Fe}_{0.05}[\text{Al}_{5.91}\text{Si}_{6.09}\text{O}_{24}](\text{SO}_4)_{0.87}\text{S}_{0.08}\text{Cl}_{0.17} \cdot 5.1\text{H}_2\text{O}$ from chemical analysis. Model for ideal nosean assuming an ordered arrangement of OH/OH₂ and SO₄ in different cages; refined by minimizing deviations from electrostatic neutrality as calculated from bond-valence equations. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. The average structure was refined in space group (218) $P\bar{4}3n$.

References: [1] Hassan I., Grundy H.D. (1989), Can. Mineral. 27, 165-172.

195
cP60

$\text{IrAl}_{2.75}$	cP60	(195) $P23 - j^4\text{feba}$
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IrAl_{2.75} [1]

Structural features: Partly disordered structure (split sites), intermediate between a 3D-framework of interconnected IrAl₁₂ icosahedra and IrAl₁₂ cuboctahedra of ideal composition IrAl₃ (AuZn₃ = UH₃ type) and a 3D-framework of interconnected IrAl₁₂ icosahedra and IrAl₁₄ rhombic dodecahedra of ideal composition Ir₄Al₁₃.

Grin Y. et al. (1997) [1]

 $\text{Al}_{2.75}\text{Ir}$ $a = 0.7674 \text{ nm}$, $V = 0.4519 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ir1	12j	1	0.006	0.5198	0.2862	0.5	
Al2	12j	1	0.01	0.116	0.31	0.26	
Al3	12j	1	0.139	0.195	0.764	0.22	
Al4	12j	1	0.2028	0.324	0.492		
Al5	6f	2..	0.354	0	0	0.36	
Al6	4e	.3.	0.185	0.185	0.185	0.52	non-coplanar triangle Al ₃
Ir7	1b	23.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron Al ₁₂

Ir8 1a 23. 0 0 0

Transformation from published data: $y, x, -z$

Experimental: single crystal, diffractometer, X-rays, $R = 0.053$, $T = 293$ K

Remarks: Homogeneity range $\text{Al}_{100-x}\text{Ir}_x$, $26 < x < 27$. Short interatomic distances for partly occupied site(s). Space group (200) $Pm-3$ was tested and rejected ($R = 0.058$).

References: [1] Grin Y., Peters K., Burkhardt U., Gotzmann K., Ellner M. (1997), Z. Kristallogr. 212, 439-444.

195
cP61

$\text{Na}_{7.8}\text{Al}_6[\text{SiO}_4]_6[\text{CO}_3]_{0.9}$

cP61

(195) $P23 - j^3hge^3a$

$\text{Na}_{7.88}\text{Al}_6\text{Si}_6\text{O}_{24}(\text{CO}_3)_{0.93}$ [1], zeolite SOD- CO_3

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra), approximately every second of which (partial order) is centered by a CO_3 trigonal unit (orientational disorder); Na near and above the centers of 6-rings (disorder).

Fechtelkord M. (1999) [1]

$\text{Al}_6\text{C}_{0.93}\text{Na}_{7.88}\text{O}_{26.80}\text{Si}_6$

$a = 0.90223$ nm, $V = 0.7344$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12j	1	0.045	0.361	0.346		non-colinear SiAl
O2	12j	1	0.06	0.067	0.11	0.233	
O3	12j	1	0.148	0.149	0.55		non-colinear SiAl
Al4	6h	2..	0.253	$\frac{1}{2}$	0		tetrahedron O ₄
Si5	6g	2..	0.243	0	$\frac{1}{2}$		tetrahedron O ₄
Na6	4e	.3.	0.231	0.231	0.231	0.59	
Na7	4e	.3.	0.321	0.321	0.321	0.47	
Na8	4e	.3.	0.803	0.803	0.803	0.91	non-coplanar triangle O ₃
C9	1a	23.	0	0	0	0.93	

Transformation from published data: $-x, -y, -z$

Experimental: powder, diffractometer, X-rays, $R_p = 0.025$, $T = 298$ K

Remarks: Short interatomic distances for partly occupied site(s); impossibly short distances occur for the refined occupancies.

References: [1] Fechtelkord M. (1999), Microporous Mesoporous Mater. 28, 335-351.

195
cP63

$\text{Na}_8\text{Al}_6[\text{SiO}_4]_6[\text{CO}_3]$

cP63

(195) $P23 - j^3hgfe^2a$

$\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}\text{CO}_3$ [1], zeolite SOD- CO_3

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra), every second of which is centered by a CO_3 trigonal unit (orientational disorder); Na above the centers of 6-rings.

Gesing T.M., Buhl J.C. (1998) [1]

$\text{Al}_6\text{CNa}_8\text{O}_{27.01}\text{Si}_6$

$a = 0.9001$ nm, $V = 0.7292$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12j	1	0.051	0.352	0.356		non-colinear SiAl
O2	12j	1	0.065	0.099	0.087	0.167	
O3	12j	1	0.135	0.154	0.55		non-colinear SiAl
Si4	6h	2..	0.259	1/2	0		tetrahedron O ₄
Al5	6g	2..	0.241	0	1/2		tetrahedron O ₄
O6	6f	2..	0.133	0	0	0.167	
Na7	4e	.3.	0.271	0.271	0.271		non-coplanar triangle O ₃
Na8	4e	.3.	0.815	0.815	0.815		
C9	1a	23.	0	0	0		

Transformation from published data: $y, x, -z$

Experimental: powder, diffractometer, X-rays, $R_p = 0.046$

Remarks: Short interatomic distances for partly occupied site(s). Space group (218) $P-43n$ was tested and rejected ($R_p = 0.077$).

References: [1] Gesing T.M., Buhl J.C. (1998), Eur. J. Mineral. 10, 71-77.

195
cP65

$\text{Na}_{7.8}\text{Al}_6[\text{SiO}_4]_6[\text{CO}_3]_{0.9}[\text{H}_2\text{O}]_{2.9}$	cP65	(195) $P23 - j^3hge^4a$
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$\text{Na}_{7.86}\text{Al}_6\text{Si}_6\text{O}_{24}(\text{CO}_3)_{0.93} \cdot 2.92\text{H}_2\text{O}$ [1], zeolite SOD- CO_3

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra), approximately every second of which is centered by a CO_3 trigonal unit (orientational disorder); Na near and above the centers of 6-rings, H_2O in the carbonate-free cages.

Fechtelkord M. (1999) [1]

$\text{Al}_6\text{C}_{0.93}\text{H}_{5.84}\text{Na}_{7.60}\text{O}_{29.72}\text{Si}_6$

$a = 0.89963 \text{ nm}$, $V = 0.7281 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12j	1	0.035	0.118	0.086	0.233	
O2	12j	1	0.054	0.346	0.358		non-colinear SiAl
O3	12j	1	0.144	0.149	0.549		non-colinear SiAl
Si4	6h	2..	0.244	1/2	0		tetrahedron O ₄
Al5	6g	2..	0.258	0	1/2		tetrahedron O ₄
Na6	4e	.3.	0.225	0.225	0.225	0.42	
Na7	4e	.3.	0.321	0.321	0.321	0.53	
(OH ₂) ₈	4e	.3.	0.602	0.602	0.602	0.73	6-vertex polyhedron (OH ₂) ₃ Na ₃
Na9	4e	.3.	0.813	0.813	0.813	0.95	
C10	1a	23.	0	0	0	0.93	

Transformation from published data: $y, x, -z$

Experimental: powder, diffractometer, X-rays, $R_p = 0.026$, $T = 298 \text{ K}$

Remarks: We adjusted the charge balance in the published chemical formula by changing the Na index from 7.6 to 7.86. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Fechtelkord M. (1999), Microporous Mesoporous Mater. 28, 335-351.

195
cP88

Na[N ₂ H ₆][Co(NO ₂) ₆]							cP88	(195) P23 – j ⁴ ihgfe ² dcba
NaN₂H₆[Co(NO₂)₆] [1]								
Structural features: Co(NO ₂) ₆ octahedral units in a Cu-type (c.c.p.) arrangement; Na atoms in "octahedral", H ₃ N-NH ₃ hydrazine units in "tetrahedral" voids.								
Ferrari A., Nardelli M. (1947) [1]								
CoH ₆ N ₈ NaO ₁₂								
$a = 1.035 \text{ nm}$, $V = 1.1087 \text{ nm}^3$, $Z = 4$								
site	Wyck.	sym.	x	y	z	occ.	atomic environment	
O1	12j	1	0.0	0.1	0.25		single atom N	
O2	12j	1	0.0	0.4	0.25		single atom N	
O3	12j	1	0.1	0.25	0.5		single atom N	
O4	12j	1	0.25	0.5	0.4		single atom N	
N5	6i	2..	0.2	$\frac{1}{2}$	$\frac{1}{2}$		non-colinear O ₂	
N6	6h	2..	0.3	$\frac{1}{2}$	0		non-colinear O ₂	
N7	6g	2..	0.3	0	$\frac{1}{2}$		non-colinear O ₂	
N8	6f	2..	0.2	0	0		non-colinear O ₂	
(NH ₃)9	4e	.3.	0.15	0.15	0.15		non-coplanar triangle O ₃	
(NH ₃)10	4e	.3.	0.35	0.35	0.35		non-coplanar triangle O ₃	
Na11	3d	222..	$\frac{1}{2}$	0	0		icosahedron O ₁₂	
Co12	3c	222..	0	$\frac{1}{2}$	$\frac{1}{2}$		octahedron N ₆	
Na13	1b	23.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		16-vertex Frank-Kasper (NH ₃) ₄ O ₁₂	
Co14	1a	23.	0	0	0		octahedron N ₆	

Experimental: powder, film, X-rays

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Ferrari A., Nardelli M. (1947), Gazz. Chim. Ital. 77, 422-426.

195
cP296

Ru _{15.4} Pd _{25.6} Al ₈₇							cP296	(195) P23 – j ¹⁹ ihg ² f ² e ⁶ dcba
Ru₁₂Pd₂₀Al₆₈ form c [1]								
Structural features: Commensurate approximant of icosahedral quasicrystals.								
Mahne S., Steurer W. (1996) [1]								
Al _{86.63} Pd _{37.94}								
$a = 1.554 \text{ nm}$, $V = 3.7528 \text{ nm}^3$, $Z = 2$								
site	Wyck.	sym.	x	y	z	occ.	atomic environment	
Pd1	12j	1	0.0006	0.2517	0.3513			
Pd2	12j	1	0.0026	0.26	0.1508			
Al3	12j	1	0.0114	0.3666	0.43	0.4		
Al4	12j	1	0.0272	0.0752	0.6364	0.42		
Al5	12j	1	0.0599	0.5226	0.1483	0.4		
Al6	12j	1	0.0854	0.3863	0.4299	0.4		
Al7	12j	1	0.0881	0.6025	0.0924			
Al8	12j	1	0.0937	0.404	0.0976		non-colinear Al ₂	

Al9	12j	1	0.0955	0.6562	0.249		
Al10	12j	1	0.0961	0.3463	0.2589		
Al11	12j	1	0.0982	0.1572	0.7541		
Al12	12j	1	0.1036	0.1616	0.2487		
Al13	12j	1	0.144	0.5071	0.4289	0.5	non-colinear Al ₂
Pd14	12j	1	0.15	0.5009	0.263		
Al15	12j	1	0.1617	0.2388	0.4013		
Al16	12j	1	0.1634	0.2486	0.604		bicapped square prism Pd ₄ Al ₆
Pd17	12j	1	0.2452	0.3549	0.4996		pseudo Frank-Kasper Al ₁₀ Pd ₃
Al18	12j	1	0.2462	0.3983	0.3365		14-vertex Frank-Kasper Pd ₅ Al ₉
Al19	12j	1	0.2561	0.5987	0.3358		pseudo Frank-Kasper Pd ₅ Al ₈
Al20	6i	2..	0.3057	$\frac{1}{2}$	$\frac{1}{2}$		pseudo Frank-Kasper Pd ₆ Al ₇
Al21	6h	2..	0.1833	$\frac{1}{2}$	0		
Al22	6g	2..	0.1932	0	$\frac{1}{2}$	0.24	
Al23	6g	2..	0.3071	0	$\frac{1}{2}$	0.76	
Al24	6f	2..	0.186	0	0	0.79	single atom Al
Al25	6f	2..	0.3128	0	0	0.21	
Pd26	4e	.3.	0.0955	0.0955	0.0955		pseudo Frank-Kasper Al ₉ Pd ₄
Pd27	4e	.3.	0.2494	0.2494	0.2494		icosahedron Al ₁₂
Pd28	4e	.3.	0.4034	0.4034	0.4034		pseudo Frank-Kasper Al ₇ Pd ₆
Pd29	4e	.3.	0.5962	0.5962	0.5962		pseudo Frank-Kasper Al ₇ Pd ₆
Pd30	4e	.3.	0.7508	0.7508	0.7508		icosahedron Al ₁₂
M31	4e	.3.	0.9048	0.9048	0.9048		pseudo Frank-Kasper Al ₆ Pd ₇
Pd32	3d	222..	$\frac{1}{2}$	0	0		
Pd33	3c	222..	0	$\frac{1}{2}$	$\frac{1}{2}$		
Al34	1b	23.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.71	rhombic dodecahedron Pd ₈ Al ₆
M35	1a	23.	0	0	0		rhombic dodecahedron Al ₁₀ Pd ₄

M31 = 0.68Al + 0.32Pd; M35 = 0.61Pd + 0.39Al

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.052

Remarks: Composition from electron microprobe analysis. No effort was made to distinguish Ru and Pd in the refinement. Short interatomic distances for partly occupied site(s).

References: [1] Mahne S., Steurer W. (1996), Z. Kristallogr. 211, 17-24.