

☆  
Weihnachts-  
Stunde mit  
kleiner  
Stern(en)kunde

☆

Cluster

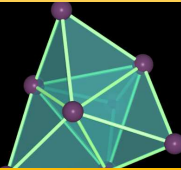
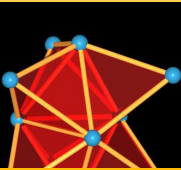
'Doppel-☆'

Oktaeder ☆

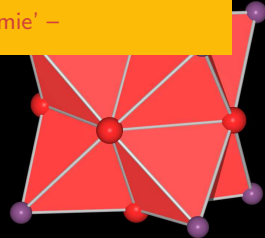
Tetraeder ☆

Ikosaeder ☆

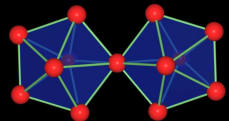
☆



☆ Weihnachts-Stunde mit kleiner Stern(en)kunde ☆  
– Vorlesung 'Anorganische Strukturchemie' –



21. Dezember 2018





Cluster

'Doppel'☆

Oktaeder☆

Tetraeder☆

Ikosaeder☆

☆

**1** Cluster

**2** 'Doppel'☆

**3** Oktaeder☆

**4** Tetraeder☆

**5** Ikosaeder☆

**6** ☆

# Zintl-Konzept (klassisch)

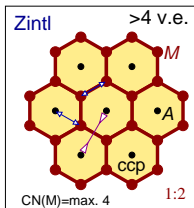


Eduard Zintl

1898 – 1941

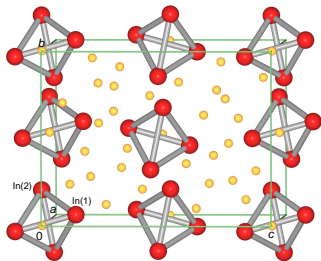
(FR: 1928 – 1933)

(DA: 1934 – 1941)

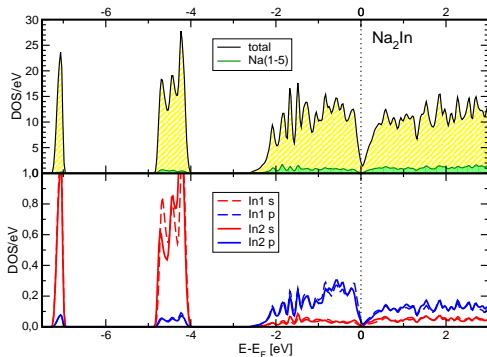
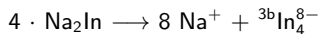


- 'ionische' Zerlegung:  $A_x M_y \longrightarrow x A^{n+} + [M_y]^{nx-}$ 
  - Coulomb-Anteile an Gitterenergie
  - KKP's (c.c.p) mit strukturbestimmend
- kovalente Bindung im  $[M_y]$ -(Poly)anion
  - isostrukturell zu isoelektronischen Elementen (Zintl)
  - Bindigkeit folgt der 8-N-Regel (Zintl-Klemm-Busmann)
  - Zahl der Bindungen bestimmt durch  $v.e./M (\leq 4)$
  - gültig für  $v.e./M \geq 4$
- physikalische Eigenschaften
  - 'Strich'-Verbindungen (keine Phasenbreiten)
  - relativ hohe Schmelzpunkte
  - Halbleiter (schmale Bandlücke)
- elektronische Strukturen
  - keine A-pDOS unterhalb  $E_F$  (A-Kationen)
  - M-s/p-Mischung abhängig vom
    - chemischen Charakter von M und
    - Dimensionalität des Polyanions
  - Valenzband: M-p-Charakter
  - bindungskritische Punkte  $[\rho_{b.c.p.}: (3,-1)]$  auf M-M-Bindungsachsen

# Na<sub>2</sub>In<sup>1</sup> (v.e./M=5)



Strukturtyp		Na <sub>2</sub> Tl
Kristallsystem		orthorhombisch
Raumgruppe		C222 <sub>1</sub>
Gitterparameter	<i>a</i>	883.3
	<i>b</i>	1385.0
	<i>c</i>	1175.8
<i>d</i> <sub>In-In</sub> [pm]		307 - 315
$\rho_{BCP}$ [e <sup>-</sup> /10 <sup>6</sup> pm <sup>3</sup> ]		1.93 - 1.74
Bader-Ldg.	Na	+0.630 ... +0.682
	In	-1.296/-1.354



tDOS (oben) und partielle In s/p-DOS (unten)<sup>2</sup>

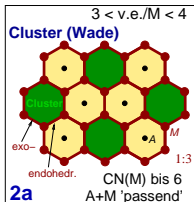
# Zintl-Konzept, erweitert durch Elektronenzählregeln für Cluster



Kenneth Wade

1932 – 2014

(Durham)



- empirische Regeln (basierend auf Beobachtungen bzw. Berechnungen molekularer Spezies)
- **Wade-Regeln** für elektronenarme Anionen/Cluster, z.B.
  - *closo*:  $N+1$  Gerüst-Elektronenpaare (s.e.p.)
  - *nido*:  $N+2$  Gerüst-Elektronenpaare
  - ...
- **Jemmis\* *mno*-Regeln**

$$\text{s.e.p.} = \underbrace{m}_{\text{Zahl der Polyeder}} + \underbrace{n}_{\text{Zahl der Ecken}} + \underbrace{o}_{\text{Zahl einfacher Eckenverknüpfungen}} + \underbrace{p}_{\text{Zahl der zu closo fehlenden Ecken}}$$

- gültig bis  $\text{v.e.}/M \geq 3$  (z.B. für B-Modifikationen)
- physikalische Eigenschaften, elektronische Strukturen:
  - vergleichbar zu klassischen Zintl-Phasen
  - endo/exo-hedrale Bindungen, jeweils mit  $\rho_{\text{bcP}}$  (3,-1)

\* E. D. Jemmis, M. M. Balakrishnarajan, P. D. Pancharatna, *Chem. Rev.* **102**, 93-144 (2002).

# CsGa<sub>7</sub> (v.e./M=3.14)



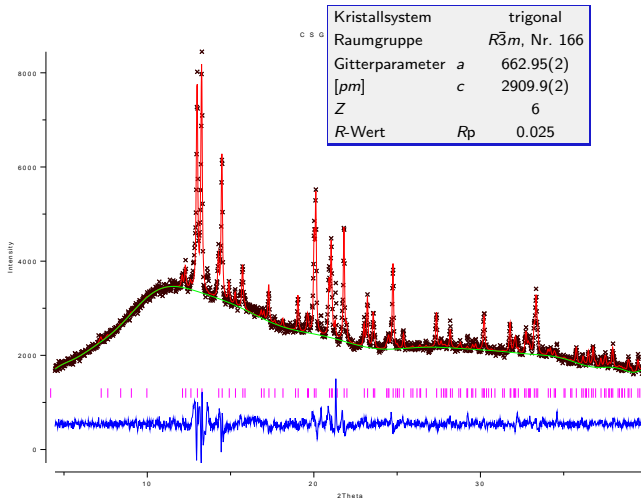
Cluster

'Doppel-'

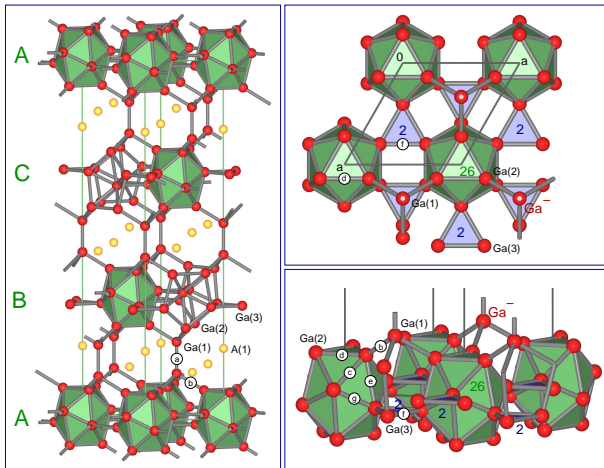
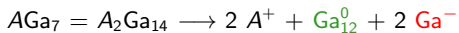
Oktaeder

Tetraeder

Ikosaeder



# $A^I Ga_7$ ( $A^I = Rb, Cs$ ; v.e./ $M=3.14$ )

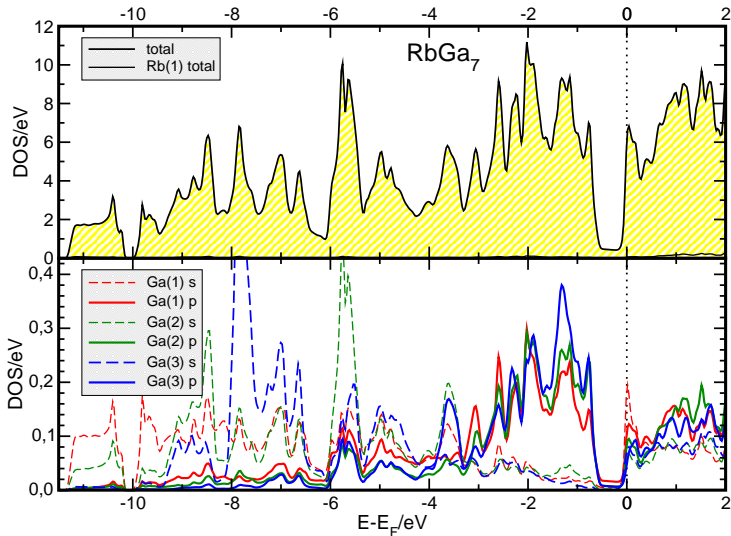


für das Ikosaeder:

$$\underbrace{26}_{N+1} + 6 \times \underbrace{\frac{2}{3}}_{\text{Dreieck}} + \underbrace{6}_{\text{exo-b.}}$$

$$= 36 \mapsto Ga_{12}^0$$

# RbGa<sub>7</sub>: Zustandsdichten





# CsGa<sub>7</sub>: Bandstruktur



Cluster

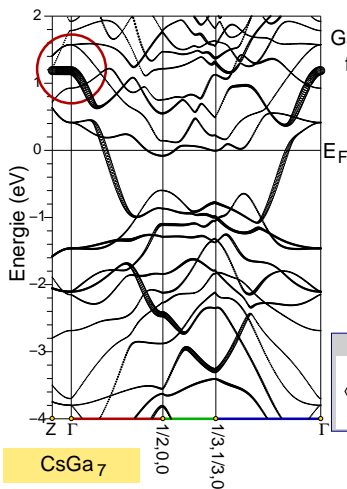
'Doppel- $\chi$ '

Oktaeder  $\chi$

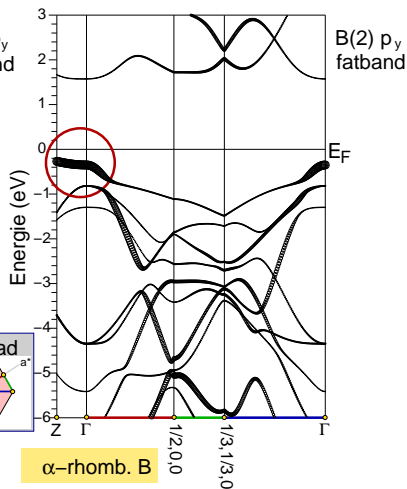
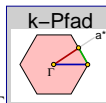
Tetraeder  $\chi$

Ikosaeder  $\chi$

$\chi$

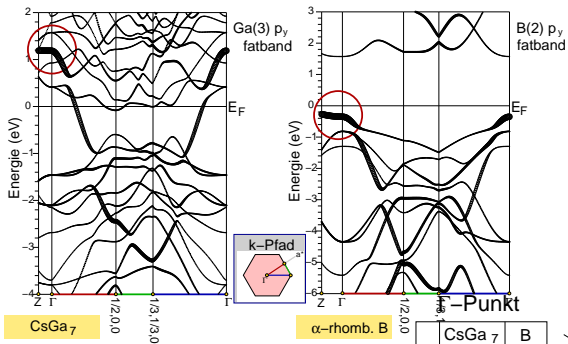


CsGa<sub>7</sub>

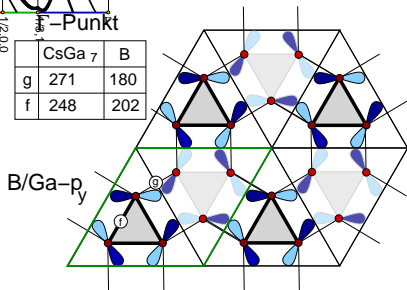


$\alpha$ -rhomb. B

# RbGa<sub>7</sub>: Bandstruktur



	CsGa <sub>7</sub>	B
g	271	180
f	248	202



# $K_3Ga_{9.6}In_{1.4}$ (v.e./ $M=3.273$ )



Cluster

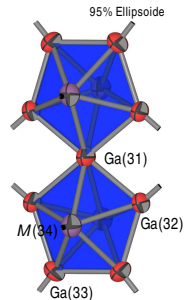
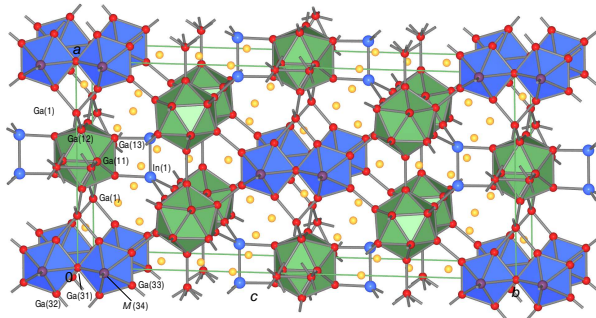
'Doppel-'

Oktaeder

Tetraeder

Ikosaeder

☆



Verbindung	$K_3Ga_{9.6}In_{1.4}$
Strukturtyp	neu, oC140
Kristallsystem	orthorhombisch
Raumgruppe	$Cmmm$ , Nr. 65
Gitterparameter $a$	1577.9(5)
[ $pm$ ]	$b$ 3355.1(8)
	$c$ 655.2(2)
$V_{EZ}$ [ $10^6 pm^3$ ]	3468.6
$Z$	10
$R$ -Werte	$R1$ 0.0471
	$wR2$ 0.1037

- $K_{15}M_{55} = 15K^+ + 4In(1)^- + 2Ga(1)^- + [Ga_{12}^I]^{2-} + 2[Ga_{12}^{II}]^{2-} + [M_{13}]^{3-}$
- $[M_{13}]^{3-} \mapsto 3 \times 13 + 3 = 42$  v.e.
- $- 12$  exo-bonds  $\mapsto 30$  s.e.
- s.e.p =  $m + n + o + p = 2 + 13$  (? + 1 ?\*) + 0
- s.e.p = 15  $\mapsto 30$  s.e.
- \*: ohne '+o' bei sog. 'intermediate' Bindungssituation

# $K_3Ga_{9.6}In_{1.4}$ (v.e./M=3.273)



Cluster

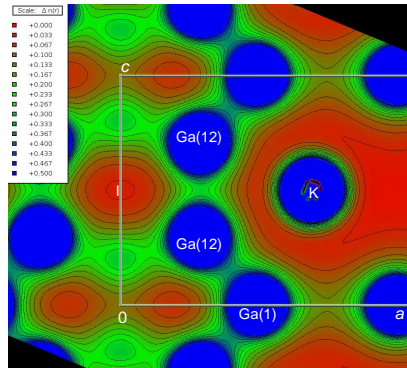
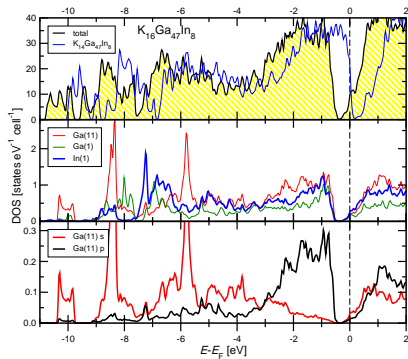
'Doppel' ✧

Oktaeder ✧

Tetraeder ✧

Ikosaeder ✧

✧





Cluster

'Doppel'☆

Oktaeder☆

Tetraeder☆

Ikosaeder☆

☆

1 Cluster

2 'Doppel'☆

3 Oktaeder☆

4 Tetraeder☆

5 Ikosaeder☆

6 ☆

# 'Tiling' bei dicht(est)en Kugelpackungen



Cluster

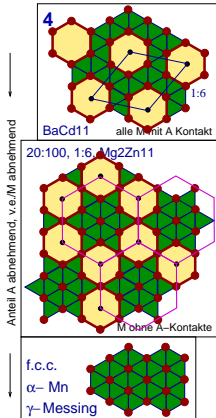
'Doppel- $\Delta$ '

Oktaeder  $\Delta$

Tetraeder  $\Delta$

Ikosaeder  $\Delta$

$\Delta$



# 'Tiling' bei dicht(est)en Kugelpackungen



Cluster

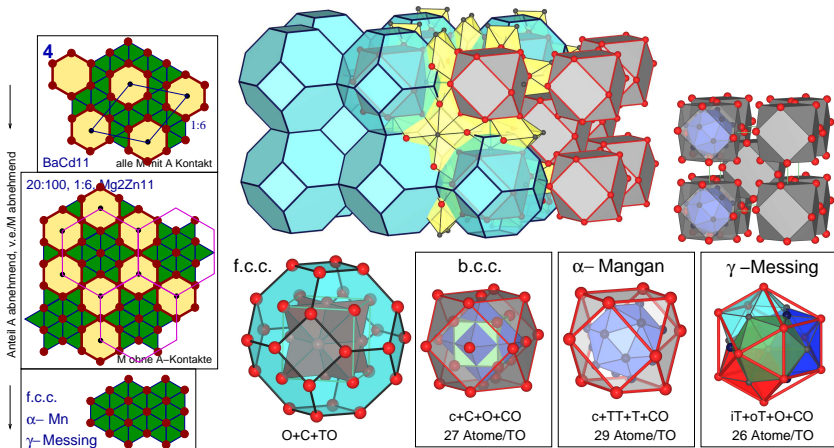
'Doppel- $\star$ '

Oktaeder  $\star$

Tetraeder  $\star$

Ikosaeder  $\star$

$\star$



'Tiling' bei einfachen Metallpackungen

# 'Tiling' bei dicht(est)en Kugelpackungen: f.c.c. und b.c.c.



Cluster

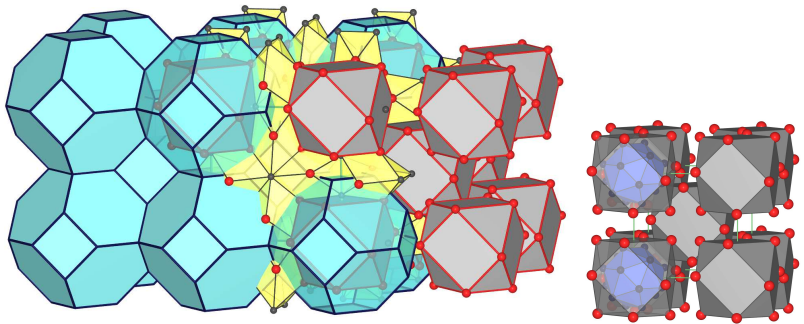
'Doppel-☆'

Oktaeder ☆

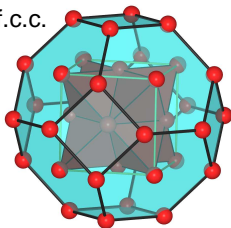
Tetraeder ☆

Ikosaeder ☆

☆

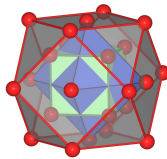


f.c.c.



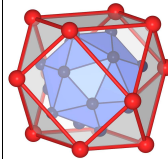
O+C+TO

b.c.c.



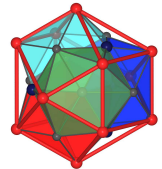
c+C+O+CO  
27 Atome/TO

$\alpha$ -Mangan



c+TT+T+CO  
29 Atome/TO

$\gamma$ -Messing



iT+oT+O+CO  
26 Atome/TO





Cluster

'Doppel'☆

Oktaeder☆

Tetraeder☆

Ikosaeder☆

☆

1 Cluster

2 'Doppel'☆

3 Oktaeder☆

**4 Tetraeder**☆

5 Ikosaeder☆

6 ☆

# 'Tiling' bei dicht(est)en Kugelpackungen: $\gamma$ -Messing



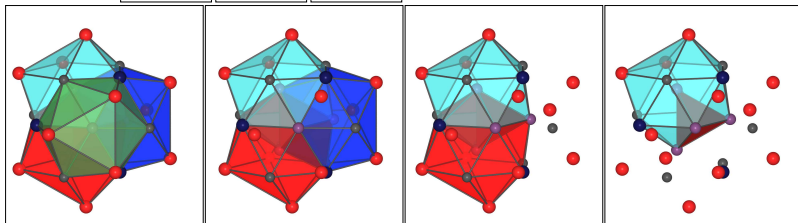
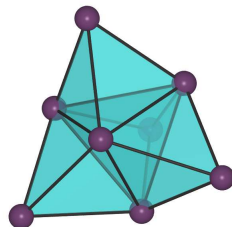
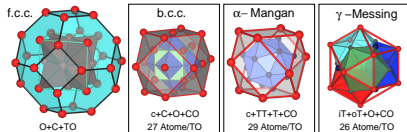
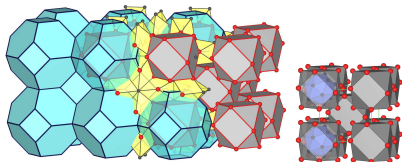
Cluster

'Doppel- $\gamma$ '

Oktaeder  $\gamma$

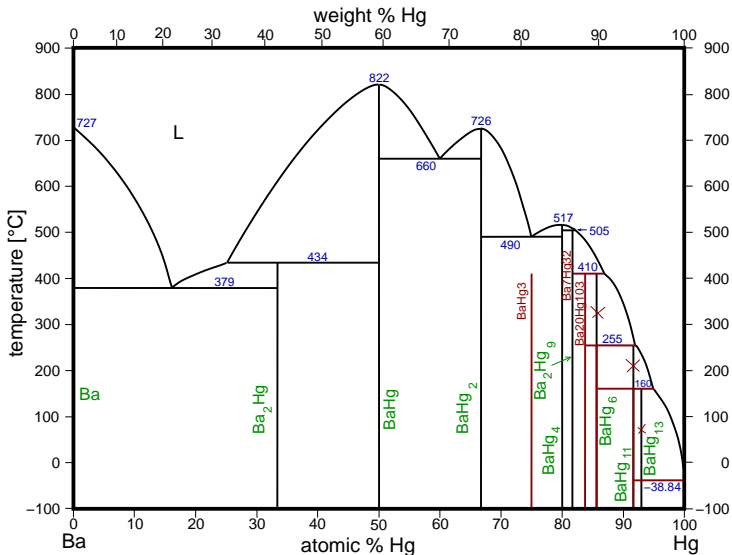
Tetraeder  $\gamma$

Ikosaeder  $\gamma$



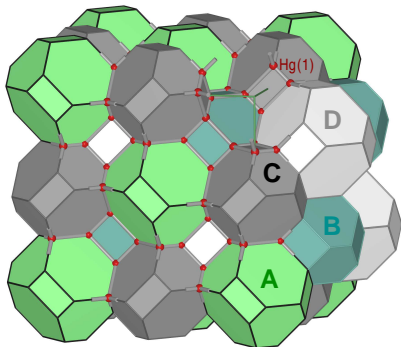
28-er Cluster in  $\gamma$ -Messing: iT + oT + O + CO = TS + O + CO

# Phasendiagramm des Systems Ba – Hg



# Ba<sub>20</sub>Hg<sub>103</sub> (v.e./M=2.388) und Varianten

Verbindung	Ba <sub>20</sub> Hg <sub>103</sub>	Ba <sub>20</sub> Cd <sub>4</sub> Hg <sub>99</sub>	Ba <sub>20</sub> Zn <sub>5</sub> Hg <sub>99</sub>	CaZn <sub>1.31</sub> Hg <sub>3.69</sub>
Kristallsystem, Z		kubisch, 4 (80)		
Pearson-Symbol		cF492	cF496	cF480
Raumgruppe		$F\bar{4}3m$ , Nr. 216		
Gitterparameter [pm] a	2333.30(10)	2331.57(14)	2332.33(7)	2145.43(9)
V <sub>EZ</sub> [10 <sup>6</sup> pm <sup>3</sup> ]	12703.2(5)	12674.9(8)	12687.3(4)	9875.1(12)
R-Werte ( $I \geq 2\sigma(I)$ )	R1	0.0651	0.0465	0.0572
	wR2	0.0873	0.1134	0.1442



- 4 A-Positionen:

- A(1,2): 16e
- A(3): 24f
- A(4): 24g

- 13 M-Positionen:

- Hg(1): 96i
- Hg(2): 48h (Ca: 24g)
- Hg(3,4): 48h
- Hg(5-9): 16e
- Hg(10): 48h
- Hg(11): 24f
- Hg(12): 4d ; Ca: 4d)
- M(13): 16e
- Zn: 4a (nur in Zn-Verb.)

# Ba<sub>20</sub>Hg<sub>103</sub> (v.e./M=2.388) und Varianten



Cluster

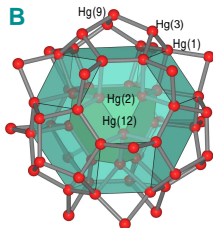
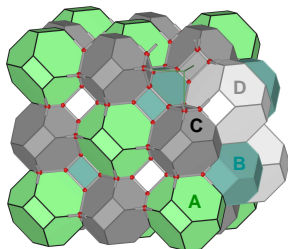
'Doppel- $\Delta$ '

Oktaeder  $\Delta$

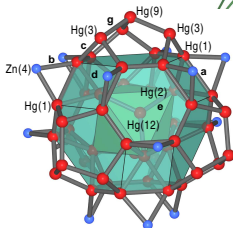
Tetraeder  $\Delta$

Ikosaeder  $\Delta$

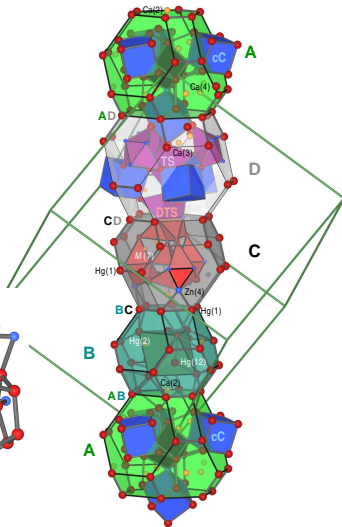
$\Delta$



Ba-Verbindungen



Ca-Verbindung



# Ba<sub>20</sub>Hg<sub>103</sub> (v.e./M=2.388) und Varianten



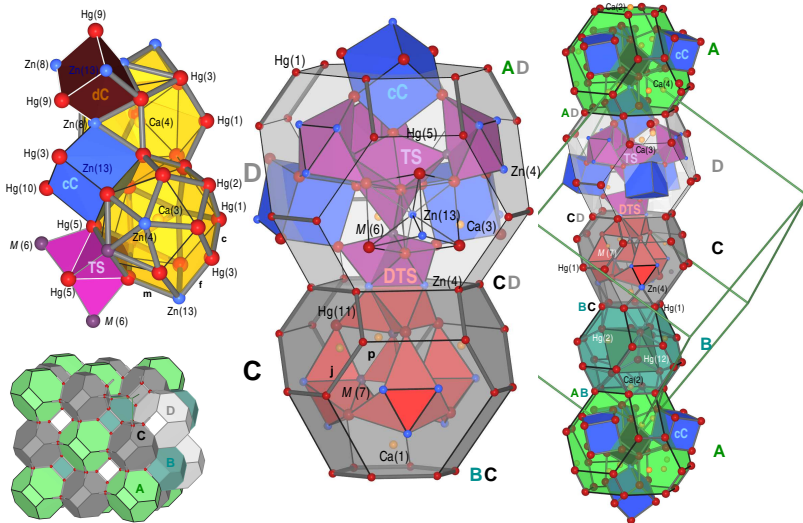
Cluster

'Doppel-'

Oktaeder

Tetraeder

Ikosaeder



# Ba<sub>20</sub>Hg<sub>103</sub> (v.e./M=2.388) und Varianten



Cluster

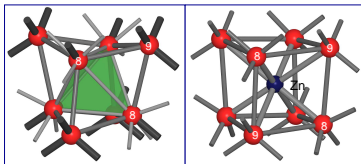
'Doppel-✧'

Oktaeder ✧

Tetraeder ✧

Ikosaeder ✧

✧



Tetraedersterne (reine Hg/Cd-Verb.)  $\mapsto$  + 1 Zn-Atom  $\mapsto$  Würfel (Zn-Verb.)

# Ba<sub>20</sub>Hg<sub>103</sub> (v.e./M=2.388) und Varianten

no.	A(1,2)	A(3,4)	M(1)	M(2)	M(3)	M(4)	M(5)	M(6)	M(7)
Wyckoff pos.	16e	24f	96i	24g	48h	48h	16e	16e	16e
point group	.3m	2.mm	1	2.mm	..m	..m	.3m	.3m	.3m
$\beta$ -cage:	<b>C,B</b>	<b>A,D</b>	TO	<b>B</b>	<b>A</b>	<b>C/D</b>	<b>D</b>	<b>D</b>	<b>C</b>
CN ( $n_I+n_{II}+n_A$ )	16	16, 17	4+3+4	6+0+3	5+2+4	8+2+2	4+6+3	9+0+3	9+0+3
Bader charge <sup>1</sup> →	+1.298	-1.353	-0.400	-0.316	-0.454	+0.136	-0.428	+0.129	-0.0124
$V_{BB}$ [ $10^6 \text{ pm}^3$ ] <sup>1</sup> →	14.67-15.51		24.03	23.23	23.84	15.50	23.58	15.95	16.75
CaZn <sub>1.31</sub> Hg <sub>3.69</sub>	Ca	Ca	Hg	Hg	Hg	Zn	Hg	75% Zn	78% Zn
Ba <sub>20</sub> Hg <sub>103</sub>	Ba	Ba	Hg	Hg (48h)	Hg	Hg	Hg	Hg	Hg
Ba <sub>20</sub> Zn <sub>5</sub> Hg <sub>99</sub>	Ba	Ba	Hg	Hg (48h)	Hg	Hg	Hg	Hg	Hg
Ba <sub>20</sub> Cd <sub>4</sub> Hg <sub>99</sub>	Ba	Ba	Hg	Hg (48h)	Hg	Hg	Hg	Hg	Hg

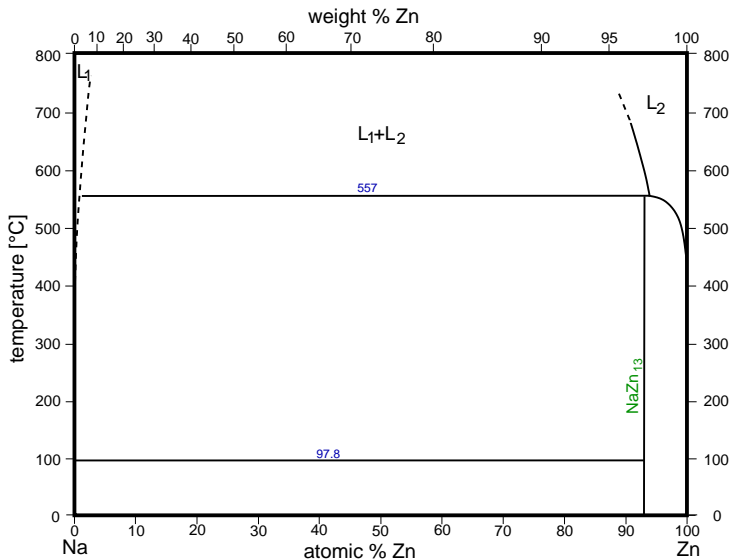
no.	M(8)	M(9)	M(10)	M(11)	M(12)	M(13)
Wyckoff pos.	16e	16e	48h	24f	16e	16e
point group	.3m	.3m	..m	2.mm	.3m	.3m
$\beta$ -cage:	<b>A</b>	<b>A</b>	<b>D</b>	<b>C</b>	<b>B</b>	<b>A/D</b>
CN ( $n_I+n_{II}+n_A$ )	7+0+3	6+0+4	4+5+3	2+8+2	3+3+4	8+0+0
Bader charge <sup>1</sup> →	+0.164	-0.651	-0.488	-0.444	-0.232	+0.422
$V_{BB}$ [ $10^6 \text{ pm}^3$ ] <sup>1</sup> →	15.60	24.78	23.96	25.16	26.75	12.03
CaZn <sub>1.31</sub> Hg <sub>3.69</sub>	Zn	Hg	Hg	Hg	Hg	Zn
Ba <sub>20</sub> Hg <sub>103</sub>	Hg	Hg	Hg	Hg	Hg (4d)	-
Ba <sub>20</sub> Zn <sub>5</sub> Hg <sub>99</sub>	Hg	Hg	Hg	Hg	Hg/Zn (4d)	Zn
Ba <sub>20</sub> Cd <sub>4</sub> Hg <sub>99</sub>	Hg	Hg	Hg	Hg	Hg/Cd (4d)	-

• Verbindungen mit verwandten EZ-Inhalten

- Ce<sub>20</sub>Mg<sub>19</sub>Zn<sub>81</sub> (cF480): 96i, 48h4, 24g, 24f2, 16e7, 4c, 4a
- Ce<sub>20</sub>Pd<sub>36</sub>In<sub>67</sub> (cF492): 96i(2/2), 48h4, 24g2, 24f, 16e8, 4a



# Charakteristisches Phasendiagramm $A^1$ -Zn/Cd: Das System Na – Zn



# NaZn<sub>13</sub>-Strukturtyp (v.e./ $M=2.077-2.154$ )



Cluster

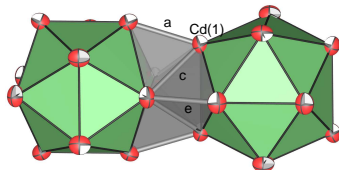
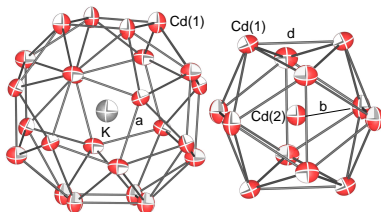
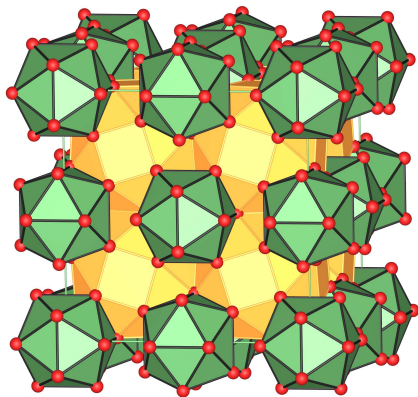
'Doppel-'

Oktaeder

Tetraeder

Ikosaeder

☆



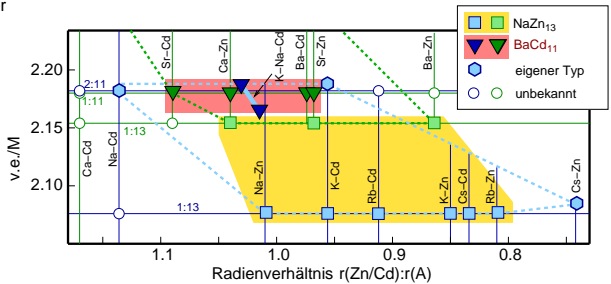
- kubisch,  $cF112$ , Raumgruppe  $Fm\bar{3}c$ ,  $a \approx 1200$  pm
- $CN_A = 24$  (Snub-cube)
- $CN_{M(2)} = 12$ ;  $CN_{M(1)} = 10 + 2$  (jeweils Ikosaeder)
- Tetraederstern (TS) zwischen Ikosaedern (kürzeste Bindung: **a**)

# NaZn<sub>13</sub>-Typ: bekannte A<sup>I/II</sup>-Zn/Cd-Verbindungen

	Zn	Cd	Hg
Ca			
Sr			
Ba			
Na			
K		mod.	
Rb			
Cs	mod.		2:27

- Strukturtyp
- NaZn<sub>13</sub>
  - BaCd<sub>11</sub>
  - BaHg<sub>11</sub>
  - eigener

- A<sup>I/II</sup>-Zinkide (ohne Cs/Zn); A<sup>I</sup>-Cadmide (ohne Na/Cd)
- keine binären Mercuride, keine A<sup>II</sup>-Cadmide



- $0.81 < r_M:r_A < 1.03$
- Substitutionen ausgehend von A<sup>II</sup>Zn<sub>13</sub><sup>2</sup>
  - + Cd: maximal in BaZn<sub>5.5</sub>Cd<sub>5.5</sub>
  - + Hg: nur kleine Hg-Gehalte (CaZn<sub>12.1</sub>Hg<sub>0.5</sub>, SrZn<sub>9.6</sub>Hg<sub>2.9</sub>, BaZn<sub>8.1</sub>Hg<sub>4.6</sub>)
- keine ternären In/Ga-Varianten  $\mapsto$  v.e./M-Grenze  $\downarrow$

<sup>1</sup>M. Wendorff, C.R., *J. Alloys Comp.* **421**, 24 (2006); <sup>2</sup>M. Schwarz, Diplomarbeit, Univ. FR (2011).

# NaZn<sub>13</sub> und CaZn<sub>13</sub>: Elektronische Struktur



Cluster

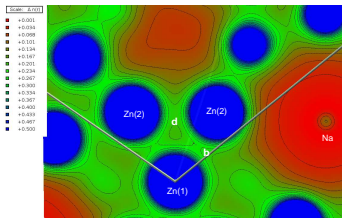
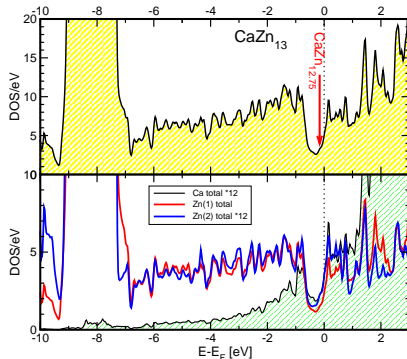
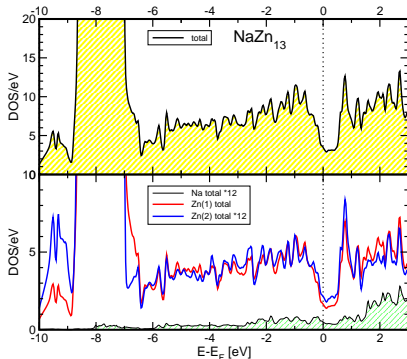
'Doppel' ⚡

Oktaeder ⚡

Tetraeder ⚡

Ikosaeder ⚡

⚡



Zn(2)-Besetzung:

- CaZn<sub>13</sub>: 74 %
- SrZn<sub>13</sub>: 78 %
- BaZn<sub>13</sub>: 89 %



Cluster

'Doppel'☆

Oktaeder☆

Tetraeder☆

Ikosaeder☆

☆

1 Cluster

2 'Doppel'☆

3 Oktaeder☆

4 Tetraeder☆

5 Ikosaeder☆

6 ☆

# vollständige Ikosaedersterne



- Zentrales Ikosaeder mit 20 Tetraeder-'Zacken'
- Punktgruppe

$$\bar{5}3\frac{2}{m}$$

Cluster

'Doppel-☆'

Oktaeder-☆

Tetraeder-☆

Ikosaeder-☆

☆

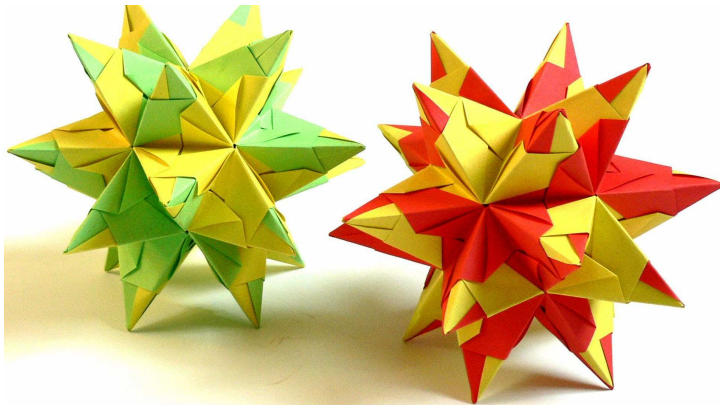
# vollständige Ikosaedersterne



- Zentrales Ikosaeder mit 20 Tetraeder-'Zacken'
- Punktgruppe

$$\bar{5}3\frac{2}{m}$$

- 'Bascetta'-Sterne: [www.mathematische-basteleien.de](http://www.mathematische-basteleien.de)
- z.B. Video bei [www.besserbasteln.de](http://www.besserbasteln.de) ↓



Cluster

'Doppel-☆'

Oktaeder ☆

Tetraeder ☆

Ikosaeder ☆

☆

# unvollständige Ikosaedersterne



Cluster

'Doppel-☆'

Oktaeder ☆

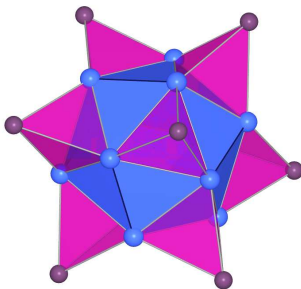
Tetraeder ☆

Ikosaeder ☆

☆

- Zentrales Ikosaeder mit 8 Tetraeder-'Zacken'
- Punktgruppe = Untergruppe

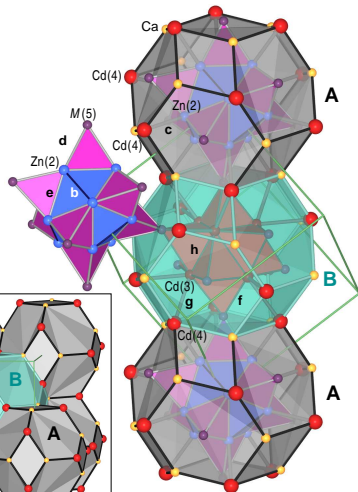
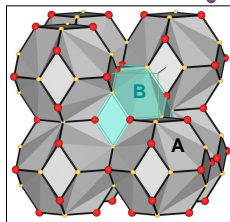
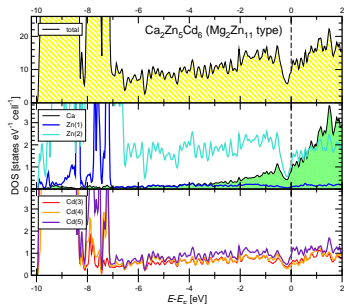
$$\frac{2}{m}\bar{3}$$





# Ca<sub>2</sub>Zn<sub>5.1</sub>Cd<sub>5.8</sub> (v.e./M=2.364)

Verbindung	Ca <sub>2</sub> Zn <sub>5.1</sub> Cd <sub>5.8</sub>	
Strukturtyp	Mg <sub>2</sub> Zn <sub>11</sub>	
Pearson-Symbol	cP39-δ	
Kristallsystem	kubisch	
Raumgruppe	Pm $\bar{3}$ , Nr. 200	
Gitterparameter [pm] a	918.1(1)	
V <sub>EZ</sub> [10 <sup>6</sup> pm <sup>3</sup> ]	773.9(4)	
Z	3	
R-Werte	R1	0.0349
	wR2	0.0662



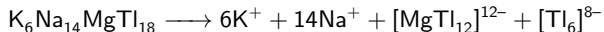
# Mg<sub>2</sub>Zn<sub>11</sub>-Typ: Übersicht, mit 'Coloring'

Wyckoff Position	A	M(1)	M(2)	M(3)	M(4)	M(5)
Punktgruppe	6f	1a	12j	6h	6g	8i
Cluster	<i>mm</i> 2	<i>m</i> $\bar{3}$	<i>m</i>	<i>mm</i> 2	<i>mm</i> 2	3
'Doppel' $\star$	TO	<b>A</b>	<b>A</b>	<b>B</b>	TO	<b>A+B</b>
Oktaeder $\star$		cl		OS (f.c.c.)		OS (f.c.c.), C
Tetraeder $\star$						
Ikosaeder $\star$						
CN ( $n_I + n_{II} + n_A$ ) $\rightarrow$	16+1	12+0+0	9+0+3	6+4+2	4+4+4	6+3+3
Bader Ldg. $\rightarrow$	+1.285	-0.045	-0.269	-0.143	-0.323	-0.205
$V_{BB}$ [ $10^6 \text{pm}^3$ ] <sup>1</sup> $\rightarrow$	14.91	13.06	17.64	21.96	24.28	22.68
Ca <sub>2</sub> Zn <sub>5.07</sub> Cd <sub>5.83</sub> <sup>1</sup>	Ca	71 % Zn	Zn	Cd	Cd	69 % Cd
Na <sub>2</sub> Cd <sub>11</sub> <sup>2</sup>	Na	Cd	Cd	Cd	Cd	Cd
Ca <sub>2</sub> Cu <sub>2</sub> Cd <sub>9</sub> <sup>3</sup>	Ca	Cu	42 % Cu	Cd	Cd	Cd
Mg <sub>2</sub> Cu <sub>6</sub> (Al/Ga) <sub>5</sub> <sup>4</sup>	Mg	Al/Ga	Cu	Cu	Al/Ga	Al/Ga
Mg <sub>2</sub> Zn <sub>11</sub> <sup>5</sup>	Mg	70 % Zn	Zn	Zn	Zn	Zn
Na <sub>2</sub> Au <sub>6</sub> In <sub>5</sub> <sup>6</sup>	Na	In	Au	Au	In	In
K <sub>6</sub> Na <sub>14</sub> MgTl <sub>18</sub> <sup>7</sup>	K	Mg (Zn)	Tl	Tl	Na	Na

<sup>1</sup>M. Schwarz, M. Wendorff, C.R., *Z. Kristallogr.* **232**, 515 (2017); <sup>2</sup>V. Mihajlov, C.R., *Z. Anorg. Allg. Chem.* **636**, 1792 (2010); <sup>3</sup>N. A. Harris, A. B. Hadler, D. C. Fredrickson, *Z. Anorg. Allg. Chem.* **637** (2011); <sup>4</sup>Q. Lin, J. D. Corbett, *Inorg. Chem.* **42** 8762 (2003); <sup>5</sup>H. Euchner, M. Mihalkovič, G. Gähler, M. R. Johnson, H. Schober, S. Rols, E. Suard, A. Bosak, S. Ohhashi, A.-P. Tsai, S. Lidin, C. P. Gómez, J. Clusters, S. Paschen, M. Boissieu *Phys. Rev. B* **83**, 144202 (2011); <sup>6</sup>U. Zachwieja *J. Alloys Compd.* **235**, 7 (1996); <sup>7</sup>Z.-C. Dong, J. D. Corbett *Angew. Chem.* **35**, 1006 (1996).

# Mg<sub>2</sub>Zn<sub>11</sub>-Typ: Übersicht, mit 'Coloring'

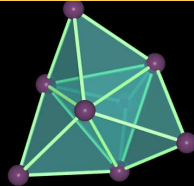
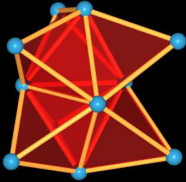
Wyckoff Position	A	M(1)	M(2)	M(3)	M(4)	M(5)
Punktgruppe	6f	1a	12j	6h	6g	8i
Cluster	mm2	m $\bar{3}$	m	mm2	mm2	3
'Doppel' $\star$	TO	<b>A</b>	<b>A</b>	<b>B</b>	TO	<b>A+B</b>
Struktur- element $\Rightarrow$		cl		OS (f.c.c.)		OS (f.c.c.), C
CN ( $n_I + n_{II} + n_A$ ) $\rightarrow$	16+1	12+0+0	9+0+3	6+4+2	4+4+4	6+3+3
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Na <sub>2</sub> Cd <sub>11</sub> <sup>2</sup>	Na	Cd	Cd	Cd	Cd	Cd
Ca <sub>2</sub> Cu <sub>2</sub> Cd <sub>9</sub> <sup>3</sup>	Ca	Cu	42 % Cu	Cd	Cd	Cd
Mg <sub>2</sub> Cu <sub>6</sub> (Al/Ga) <sub>5</sub> <sup>4</sup>	Mg	Al/Ga	Cu	Cu	Al/Ga	Al/Ga
Mg <sub>2</sub> Zn <sub>11</sub> <sup>5</sup>	Mg	70 % Zn	Zn	Zn	Zn	Zn
Na <sub>2</sub> Au <sub>6</sub> In <sub>5</sub> <sup>6</sup>	Na	In	Au	Au	In	In
K <sub>6</sub> Na <sub>14</sub> MgTl <sub>18</sub> <sup>7</sup>	K	Mg (Zn)	Tl	Tl	Na	Na



<sup>1</sup>M. Schwarz, M. Wendorff, C.R., *Z. Kristallogr.* **232**, 515 (2017); <sup>2</sup>V. Mihajlov, C.R., *Z. Anorg. Allg. Chem.* **636**, 1792 (2010); <sup>3</sup>N. A. Harris, A. B. Hadler, D. C. Fredrickson, *Z. Anorg. Allg. Chem.* **637** (2011); <sup>4</sup>Q. Lin, J. D. Corbett, *Inorg. Chem.* **42** 8762 (2003); <sup>5</sup>H. Euchner, M. Mihalkovič, G. Gähler, M. R. Johnson, H. Schober, S. Rols, E. Suard, A. Bosak, S. Ohhashi, A.-P. Tsai, S. Lidin, C. P. Gómez, J. Clusters, S. Paschen, M. Boissieu *Phys. Rev. B* **83**, 144202 (2011); <sup>6</sup>U. Zachwieja *J. Alloys Compd.* **235**, 7 (1996); <sup>7</sup>Z.-C. Dong, J. D. Corbett *Angew. Chem.* **35**, 1006 (1996).



- Cluster
- 'Doppel-'
- Oktaeder
- Tetraeder
- Ikosaeder
- 



# DANKE

und schöne Weihnachtsfeiertage

