A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

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Introduction: Space group settings

The International Tables identifies the 230 space groups that are possible for crystal structures.

1	$P1$	2	$P\text{-}1$	3	$P2$	4	$P2_1$	5	$C2$
6	Pm	7	Pc	8	Cm	9	Cc	10	$P2/m$
11	$P2_1/m$	12	$C2/m$	13	$P2/c$	14	$P2_1/c$	15	$C2/c$
16	$P222$	17	$P222_1$	18	$P2_12_12$	19	$P2_12_12_1$	20	$C222_1$
21	$C222$	22	$F222$	23	$I222$	24	$I2_12_12_1$	25	$Pmm2$
26	$Pmc2_1$	27	$Pcc2$	28	$Pma2$	29	$Pca2_1$	30	$Pnc2$
31	$Pmn2_1$	32	$Pba2$	33	$Pna2_1$	34	$Pnn2$	35	$Cmm2$
36	$Cmc2_1$	37	$Ccc2$	38	$Amm2$	39	$Aem2$	40	$Ama2$
41	$Aea2$	42	$Fmm2$	43	$Fdd2$	44	$Imm2$	45	$Iba2$
46	$Ima2$	47	$Pmmm$	48	$Pnnn$	49	$Pccm$	50	$Pban$
51	$Pmma$	52	$Pnna$	53	$Pmna$	54	$Pcca$	55	$Pbam$
56	$Pccn$	57	$Pbcm$	58	$Pnnm$	59	$Pmmn$	60	$Pbcn$
61	$Pbca$	62	$Pnma$	63	$Cmcm$	64	$Cmce$	65	$Cmmm$
66	$Cccm$	67	$Cmme$	68	$Ccce$	69	$Fmmm$	70	$Fddd$
71	$Immm$	72	$Ibam$	73	$Ibca$	74	$Imma$	75	$P4$
76	$P4_1$	77	$P4_2$	78	$P4_3$	79	$I4$	80	$I4_1$
81	$P\text{-}4$	82	$I\text{-}4$	83	$P4/m$	84	$P4_2/m$	85	$P4/n$
86	$P4_2/n$	87	$I4/m$	88	$I4_1/a$	89	$P422$	90	$P42_12$
91	$P4_122$	92	$P4_12_12$	93	$P4_222$	94	$P4_22_12$	95	$P4_322$
96	$P4_32_12$	97	$I422$	98	$I4_122$	99	$P4mm$	100	$P4bm$
101	$P4_2cm$	102	$P4_2nm$	103	$P4cc$	104	$P4nc$	105	$P4_2mc$
106	$P4_2bc$	107	$I4mm$	108	$I4cm$	109	$I4_1md$	110	$I4_1cd$
111	$P\text{-}42m$	112	$P\text{-}42c$	113	$P\text{-}42_1m$	114	$P\text{-}42_1c$	115	$P\text{-}4m2$

116	$P\text{-}4c2$	117	$P\text{-}4b2$	118	$P\text{-}4n2$	119	$I\text{-}4m2$	120	$I\text{-}4c2$
121	$I\text{-}42m$	122	$I\text{-}42d$	123	$P4/mmm$	124	$P4/mcc$	125	$P4/nbm$
126	$P4/nnc$	127	$P4/mbm$	128	$P4/mnc$	129	$P4/nmm$	130	$P4/ncc$
131	$P4_2/mmc$	132	$P4_2/mcm$	133	$P4_2/nbc$	134	$P4_2/nnm$	135	$P4_2/mbc$
136	$P4_2/mnm$	137	$P4_2/nmc$	138	$P4_2/ncm$	139	$I4/mmm$	140	$I4/mcm$
141	$I4_1/amd$	142	$I4_1/acd$	143	$P3$	144	$P3_1$	145	$P3_2$
146	$R3$	147	$P\text{-}3$	148	$R\text{-}3$	149	$P312$	150	$P321$
151	$P3_112$	152	$P3_121$	153	$P3_212$	154	$P3_221$	155	$R32$
156	$P3m1$	157	$P31m$	158	$P3c1$	159	$P31c$	160	$R3m$
161	$R3c$	162	$P\text{-}31m$	163	$P\text{-}31c$	164	$P\text{-}3m1$	165	$P\text{-}3c1$
166	$R\text{-}3m$	167	$R\text{-}3c$	168	$P6$	169	$P6_1$	170	$P6_5$
171	$P6_2$	172	$P6_4$	173	$P6_3$	174	$P\text{-}6$	175	$P6/m$
176	$P6_3/m$	177	$P622$	178	$P6_122$	179	$P6_522$	180	$P6_222$
181	$P6_422$	182	$P6_322$	183	$P6mm$	184	$P6cc$	185	$P6_3cm$
186	$P6_3mc$	187	$P\text{-}6m2$	188	$P\text{-}6c2$	189	$P\text{-}62m$	190	$P\text{-}62c$
191	$P6/mmm$	192	$P6/mcc$	193	$P6_3/mcm$	194	$P6_3/mmc$	195	$P23$
196	$F23$	197	$I23$	198	$P2_13$	199	$I2_13$	200	$Pm\text{-}3$
201	$Pn\text{-}3$	202	$Fm\text{-}3$	203	$Fd\text{-}3$	204	$Im\text{-}3$	205	$Pa\text{-}3$
206	$Ia\text{-}3$	207	$P432$	208	$P4_232$	209	$F432$	210	$F4_132$
211	$I432$	212	$P4_332$	213	$P4_132$	214	$I4_132$	215	$P\text{-}43m$
216	$F\text{-}43m$	217	$I\text{-}43m$	218	$P\text{-}43n$	219	$F\text{-}43c$	220	$I\text{-}43d$
221	$Pm\text{-}3m$	222	$Pn\text{-}3n$	223	$Pm\text{-}3n$	224	$Pn\text{-}3m$	225	$Fm\text{-}3m$
226	$Fm\text{-}3c$	227	$Fd\text{-}3m$	228	$Fd\text{-}3c$	229	$Im\text{-}3m$	230	$Ia\text{-}3d$

https://github.com/BobHanson/CLEG

Introduction: Space group settings

Each space group can be described using multiple settings.

The BCS identifies 611 “conventional” space group settings.

ITA-settings for the space group *P*2/*c* (No. 13) [unique axis b]

ITA number	Setting
13	*P* 1 2/*c* 1
13	*P* 1 2/*n* 1
13	*P* 1 2/*a* 1
13	*P* 1 1 2/*a*
13	*P* 1 1 2/*n*
13	*P* 1 1 2/*b*
13	*P* 2/*b* 1 1
13	*P* 2/*n* 1 1
13	*P* 2/*c* 1 1

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Introduction: Space group settings

One setting is the “standard” setting.

ITA-settings for the space group *P*2/*c* (No. 13) [unique axis b]

ITA number	Setting
13	*P* 1 2/*c* 1
13	*P* 1 2/*n* 1
13	*P* 1 2/*a* 1
13	*P* 1 1 2/*a*
13	*P* 1 1 2/*n*
13	*P* 1 1 2/*b*
13	*P* 2/*b* 1 1
13	*P* 2/*n* 1 1
13	*P* 2/*c* 1 1

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Introduction: Space group settings

The BCS describes settings using matrix transformations in relation to the standard setting.

The inline “(P,p)” notation describes the matrix in a convenient linear column-based format.

The general position of the group *P* 1 1 2/*n* (No. 13)

The calculations are performed applying the following transformation matrix

Transformation matrix (**P**, **p**): **a,-a-c,b** ; 0,0,0

Matrix form: (**P**, **p**) = $\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$

ITA number	Setting
13	*P* 1 2/*c* 1
13	*P* 1 2/*n* 1
13	*P* 1 2/*a* 1
13	*P* 1 1 2/*a*
13	*P* 1 1 2/*n*
13	*P* 1 1 2/*b*
13	*P* 2/*b* 1 1
13	*P* 2/*n* 1 1
13	*P* 2/*c* 1 1

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Introduction: Group-Subgroup relationships

When comparing crystal structures, we are often interested in how their symmetries differ.

How do their lattices compare?

What symmetry elements have been lost or gained?

What sort of distortions relate one structure to another?

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Introduction: Group-Subgroup relationships

The BCS also describes subgroup relationships using (P,p) matrices.

The general position of the group *P2/c* (No. 13) [unique axis b] in the basis of its supergroup *P2/m* (No. 10) [unique axis b]

Transformation matrix (**P**, **p**): **a-c,b,2c** ; 0,0,1/2

Matrix form: (**P**, **p**) = $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 2 & 1/2 \end{pmatrix}$

Click here to get the general position of the standard/default setting in text format
Click here to get the general position of the transformed setting in text format

N	Standard/Default Setting		Transformed	
	(x,y,z) form	matrix form	(x,y,z) form	matrix form
(0,0,0) + set				
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
2	-x,y,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	-x,y,-z+2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 2 \end{pmatrix}$

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Introduction: Group-Subgroup relationships

Transformation matrix

To change the basis of the group general positions is used the transformation matrix *P*:

```
[    -1     0     1 ] [      0]
[     0     1     0 ] [    1/4]
[    -1     0     0 ] [      0]
```

Inverse transformation $Q=P^{-1}$:

```
[     0     0    -1 ] [      0]
[     0     1     0 ] [   -1/4]
[     1     0    -1 ] [      0]
```

The linear part of the transformation *P*=(P,p) implies the change of basis vectors **a**, **b**, **c**: (**a'**, **b'**, **c'**) = (**a**, **b**, **c**) P

P is the transformation matrix from the basis of the supergroup to the basis of the subgroup. Because we are going to the basis of supergroup, each representative (R) is transformed with the transformation matrix *P* using: R (in new basis) = *P* * R * *Q*

For comments, please mail to
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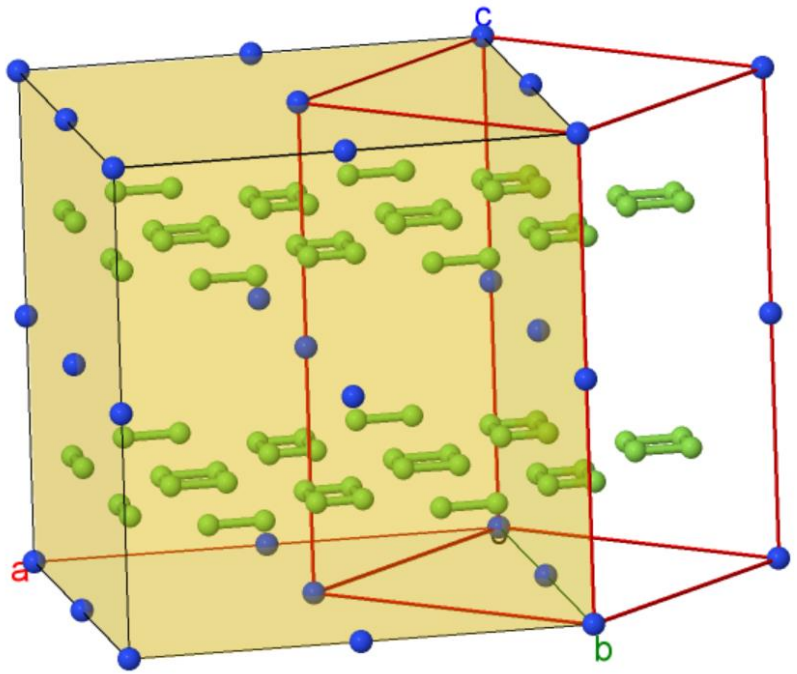
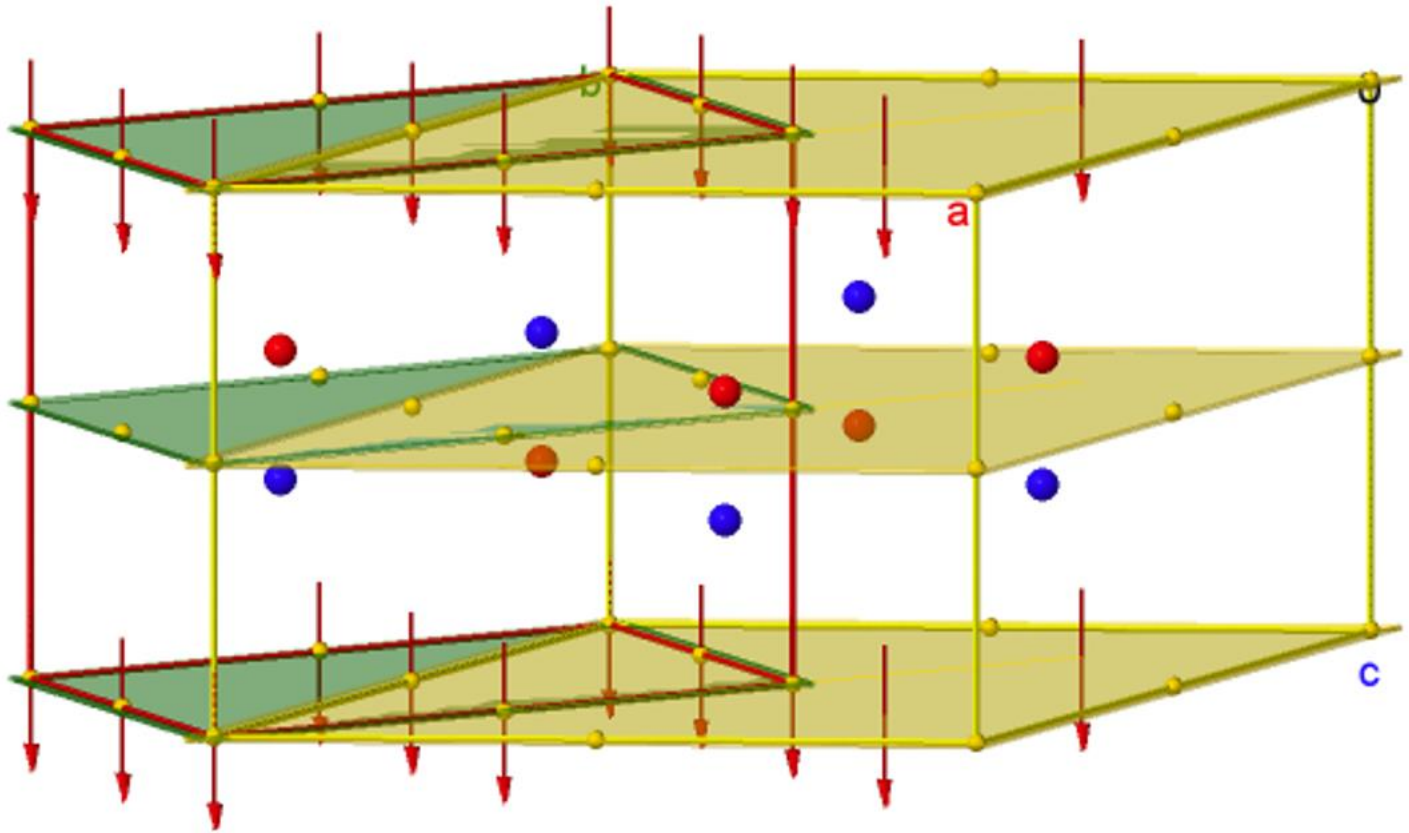
My challenge: modeling settings and subgroup relationships in Jmol





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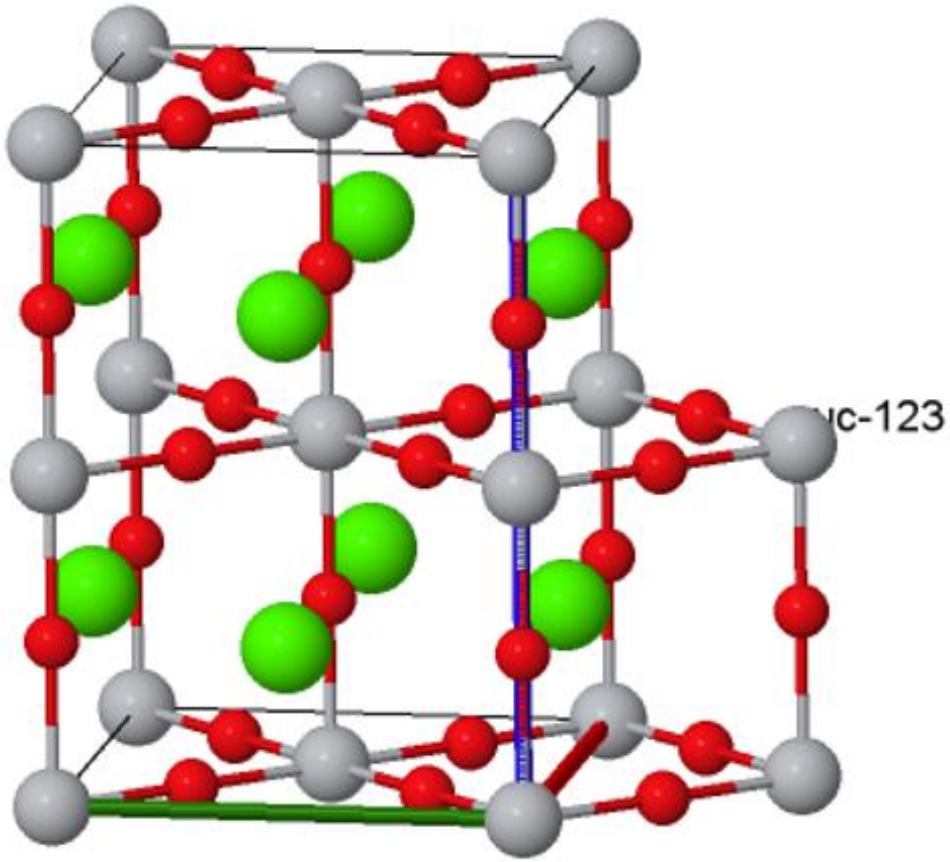
The Problem: How to express relationships concisely

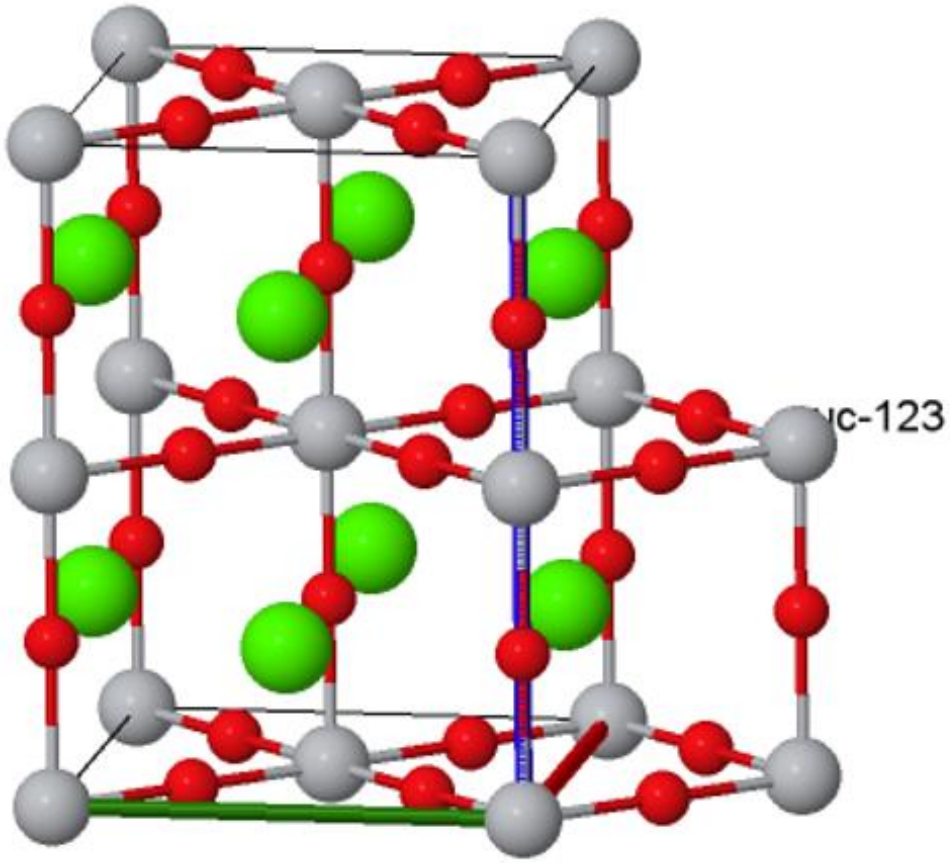
- Simple, concise
- Comprehensive
- Flexible



https://github.com/BobHanson/CLEG

The Problem: How to express relationships concisely

- Simple, concise
- Comprehensive
- Flexible
- Linear string of characters
- Scriptable



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The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Settings: Combine ITA space group number with BCS (P,p) notation:

P 1 2/m 1	**10:a,b,c;0,0,0**	P 1 2/c 1	**13:a,b,c;0,0,0**
P 1 1 2/m	**10:c,a,b;0,0,0**	P 1 1 2/n	**13:a,-a-c,b;0,0,0**
P 2/m 1 1	**10:b,c,a;0,0,0**	P 2/b 1 1	**13:b,c,a;0,0,0**

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The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Settings: Combine ITA space group number with BCS (P,p) notation:

P 1 2/m 1	**10:a,b,c;0,0,0**	P 1 2/c 1	**13:a,b,c;0,0,0**
P 1 1 2/m	**10:c,a,b;0,0,0**	P 1 1 2/n	**13:a,-a-c,b;0,0,0**
P 2/m 1 1	**10:b,c,a;0,0,0**	P 2/b 1 1	**13:b,c,a;0,0,0**

Simple!

https://github.com/BobHanson/CLEG

The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Settings: Allow for defaults “a,b,c” and “;0,0,0” :

P 1 2/m 1	**10**	P 1 2/c 1	**13**
P 1 1 2/m	**10:c,a,b**	P 1 1 2/n	**13:a,-a-c,b**
P 2/m 1 1	**10:b,c,a**	P 2/b 1 1	**13:b,c,a**

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The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Settings: Allow for defaults “a,b,c” and “;0,0,0” :

P 1 2/m 1	**10**	P 1 2/c 1	**13**
P 1 1 2/m	**10:c,a,b**	P 1 1 2/n	**13:a,-a-c,b**
P 2/m 1 1	**10:b,c,a**	P 2/b 1 1	**13:b,c,a**

Concise!

https://github.com/BobHanson/CLEG

The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Subgroups: Expand ITA “P2/m > P2/c” notation:

10 > a-c,b,2c;0,0,1/2 > 13

Transformation matrix (**P**, **p**): **a-c,b,2c** ; 0,0,1/2

Matrix form: (**P**, **p**) = $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 2 & 1/2 \end{pmatrix}$

https://github.com/BobHanson/CLEG

The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Subgroups: Add “!” meaning “not” or “inverse of”:

10:b,c,a > **!b,c,a** > 10

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The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Subgroups: Allow chaining:

10:b,c,a > **!b,c,a** > 10
10 > **a-c,b,2c;0,0,1/2** > 13
13 > **a,-a-c,b** > 13:a,-a-c,b

?

https://github.com/BobHanson/CLEG

The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Subgroups: Allow chaining by :

10:b,c,a > **!b,c,a** > 10	*$ P1 = matrix("!b,c,a")*
10 > **a-c,b,2c;0,0,1/2** > 13	*$ P2 = matrix("a-c,b,2c;0,0,1/2")*
13 > **a,-a-c,b** > 13:a,-a-c,b	*$ P3 = matrix("a,-a-c,b")*
----------	
	*$ P = $P1 * $P2 * $P3*

https://github.com/BobHanson/CLEG

The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Subgroups: Allow chaining:

10:b,c,a > **!b,c,a** > 10
10 > **a-c,b,2c;0,0,1/2** > 13
13 > **a,-a-c,b** > 13:a,-a-c,b

10:b,c,a > **-b+c,-b-c,a:0,1/2,0** > 13:a,-a-c,b

$ print matrix("!b,c,a > a-c,b,2c;0,0,1/2 > a,-a-c,b", "abc")
-b+c,-b-c,a;0,1/2,0

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The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

10:b,c,a > !b,c,a > 10	nonstandard to standard setting
10 > a-c,b,2c;0,0,1/2 > 13	group to subgroup (standard settings)
13 > a,-a-c,b > 13:a,-a-c,b	standard to nonstandard
10:b,c,a > -b+c,-b-c,a:0,1/2,0 > 13:a,-a-c,b	nonstandard group to nonstandard subgroup

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The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Examples

10:b,c,a > !b,c,a > 10	nonstandard to standard setting
10 > a-c,b,2c;0,0,1/2 > 13	group to subgroup (standard settings)
13 > a,-a-c,b > 13:a,-a-c,b	standard to nonstandard
10:b,c,a > -b+c,-b-c,a:0,1/2,0 > 13:a,-a-c,b	nonstandard group to nonstandard subgroup

Comprehensive!

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The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

Allow Hermann-Mauguin notation?

P 2/m 1 1 > !b,c,a > P 2/m	nonstandard to standard setting
P 2/m > a-c,b,2c;0,0,1/2 > P 2/c	group to subgroup (standard settings)
P 2/c > a,-a-c,b > P 1 1 2/n	standard to nonstandard
P 2/m 1 1 > -b+c,-b-c,a;0,1/2,0 > P 1 1 2/n	nonstandard group to nonstandard subgroup

(for human consumption only!)

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The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

*Q: Allow Hall notation (**for standard settings only**)*

[-P 2y]:b,c,a > !b,c,a > [-P 2y]	nonstandard to standard setting
[-P 2y] > a-c,b,2c;0,0,1/2 > [-P 2cy]	group to subgroup (standard settings)
[-P 2cy] > a,-a-c,b > [-P 2cy]:a,-a-c,b	standard to nonstandard
[-P 2y]:b,c,a > -b+c,-b-c,a:0,1/2,0 > [-P 2cy]:a,-a-c,b	nonstandard group to nonstandard subgroup

(completely machine readable; no ITA referencing)

https://github.com/BobHanson/CLEG

The Solution: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

*Q: Allow Hall notation (**for standard settings only**)*

[-P 2y]:b,c,a > !b,c,a > [-P 2y]	nonstandard to standard setting
[-P 2y] > a-c,b,2c;0,0,1/2 > [-P 2cy]	group to subgroup (standard settings)
[-P 2cy] > a,-a-c,b > [-P 2cy]:a,-a-c,b	standard to nonstandard
[-P 2y]:b,c,a > -b+c,-b-c,a:0,1/2,0 > [-P 2cy]:a,-a-c,b	nonstandard group to nonstandard subgroup

(completely machine readable; no ITA referencing) Flexible!

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CLEG applications

tabular description of BCS group/maximal subgroup relationships through index 4:

i	cleg	tr_type	tr_subtype	det	index	conj_class
1	1>2a,a+b,a+c>1	k	eu	2	2	a
2	1>2a,a+b,c>1	k	eu	2	2	b
3	1>2a,b,a+c>1	k	eu	2	2	c
191	8>a-2c,b,2c>9	k	eu	2	2	a
192	8>a,b,2c>9	k	eu	2	2	b
193	9>1/2a-1/2b,1/2a+1/2b,c>1	t		0.5	2	a
194	9>a,b,-a+c;0,1/4,0>7	k	ct	1	2	a
202	9>a,b,3c>9	k	eu	3	3	e
203	10>a,b,c>2	t		1	2	a
204	10>a,b,c>3	t		1	2	a
205	10>a,b,c>6	t		1	2	a
206	10>a-c,b,2c;0,0,1/2>10	k	eu	2	2	a
1558	69>-b,a,c>64	k	ct	1	2	c
1559	69>b,c,a>64	k	ct	1	2	d
1560	69>c,a,b>64	k	ct	1	2	e
1561	69>c,b,-a>64	k	ct	1	2	f
1562	69>a,b,c>65	k	ct	1	2	a
1563	69>c,a,b>65	k	ct	1	2	b
3764	230>a-b,b+c,-1/2a-1/2b+1/2c;1/2,0,1/2>167	t		1.5	4	a
3765	230>a,b,c>206	t		1	2	a
3766	230>a,b,c>214	t		1	2	a
3767	230>a,b,c>220	t		1	2	a

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CLEG applications

JSON description of ITA space group settings for Jmol:


```
▼ 226:
    clegId:   "47:a,b,c"
▼ 227:
    clegId:   "48:a,b,c"
▼ 228:
    clegId:   "48:a,b,c;1/4,1/4,1/4"
▼ 229:
    clegId:   "49:a,b,c"
▼ 230:
    clegId:   "49:c,a,b"
▼ 231:
    clegId:   "49:b,c,a"
```


https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for calculation:

Transformation matrix (P, p): a-c,b,2c ; 0,0,1/2

Matrix form: (**P**, **p**) = $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 2 & 1/2 \end{pmatrix}$

Click here to get the general position of the standard/default setting in text format
Click here to get the general position of the transformed setting in text format

N	Standard/Default Setting		Transformed	
	(x,y,z) form	matrix form	(x,y,z) form	matrix form
(0,0,0) + set				
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
2	-x,y,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	-x,y,-z+2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 2 \end{pmatrix}$

https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for calculation:

$ P = matrix("a-c,b,2c;0,0,1/2")
$ R = symop("-x,y,-z+1/2")
$ Q = !P
*$ print matrix(P * R * Q, "xyz")*

-x,y,-z+2

Transformation matrix (P, p): a-c,b,2c ; 0,0,1/2

Matrix form: (**P**, **p**) = $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 2 & 1/2 \end{pmatrix}$

Click here to get the general position of the standard/default setting in text format
Click here to get the general position of the transformed setting in text format

N	Standard/Default Setting		Transformed	
	(x,y,z) form	matrix form	(x,y,z) form	matrix form
(0,0,0) + set				
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
2	-x,y,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	-x,y,-z+2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 2 \end{pmatrix}$

https://github.com/BobHanson/CLEG

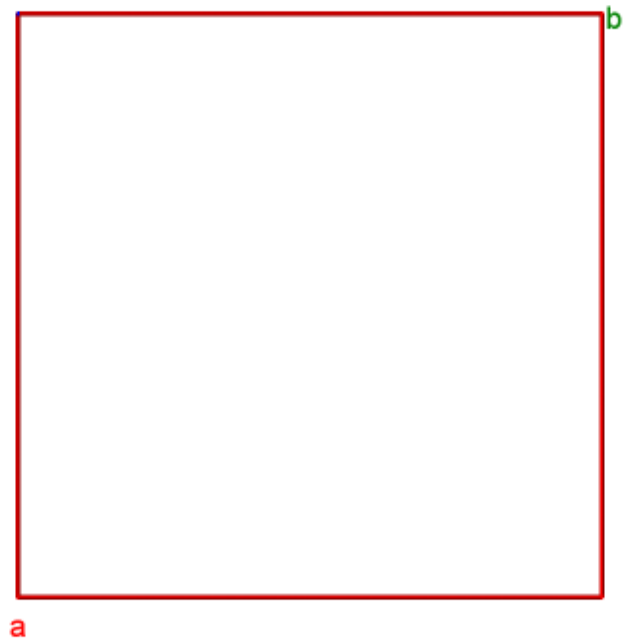
CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup 140

draw ID uc1 unitcell color red

draw ID ax1 axes



JmolD

https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup 140

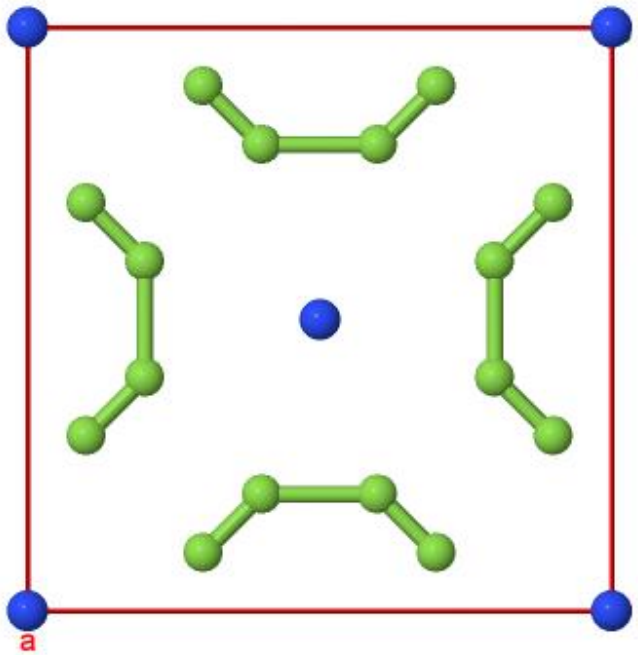
draw ID uc1 unitcell color red

draw ID ax1 axes

modelkit add F {0.60 0.20 0.25/1}

modelkit add N wyckoff c packed

connect 1.0 2.1



JmolD

https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup 140

draw ID uc1 unitcell color red

draw ID ax1 axes

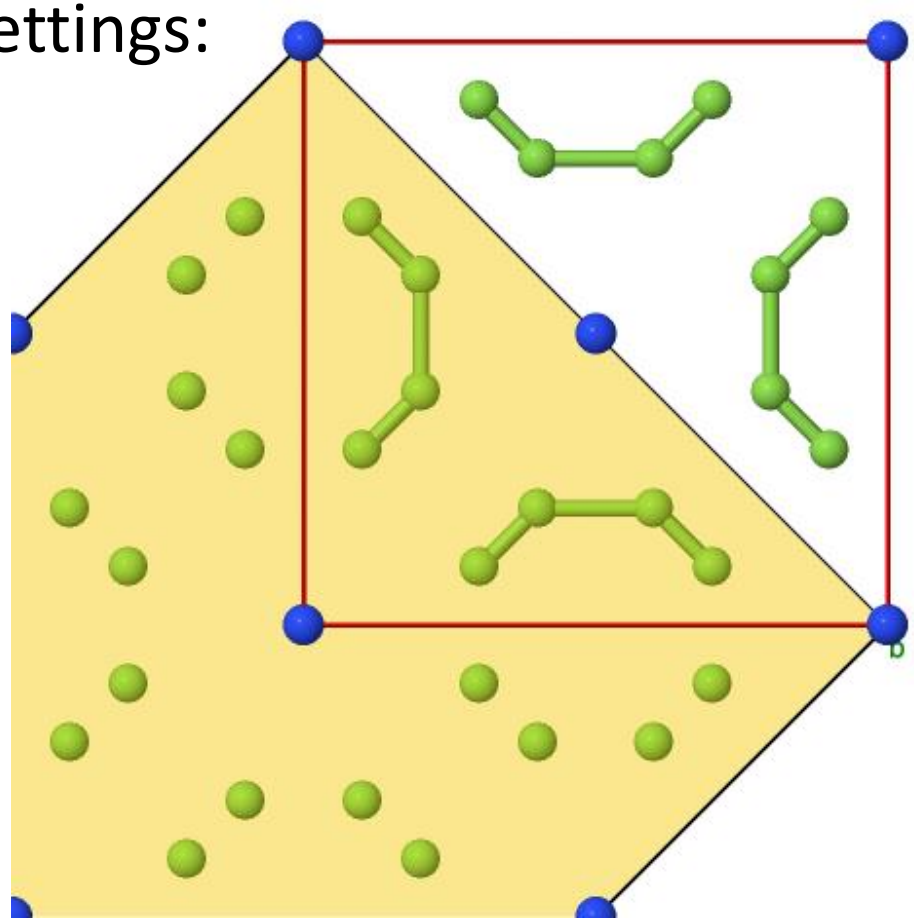
modelkit add F {0.60 0.20 0.25/1}

modelkit add N wyckoff c packed

connect 1.0 2.1

modelkit spacegroup "140:a-b,a+b,c" packed

draw ID uc2 unitcell fill nomesh color translucent 0.8



https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup 140

draw ID uc1 unitcell color red

draw ID ax1 axes

modelkit add F {0.60 0.20 0.25/1}

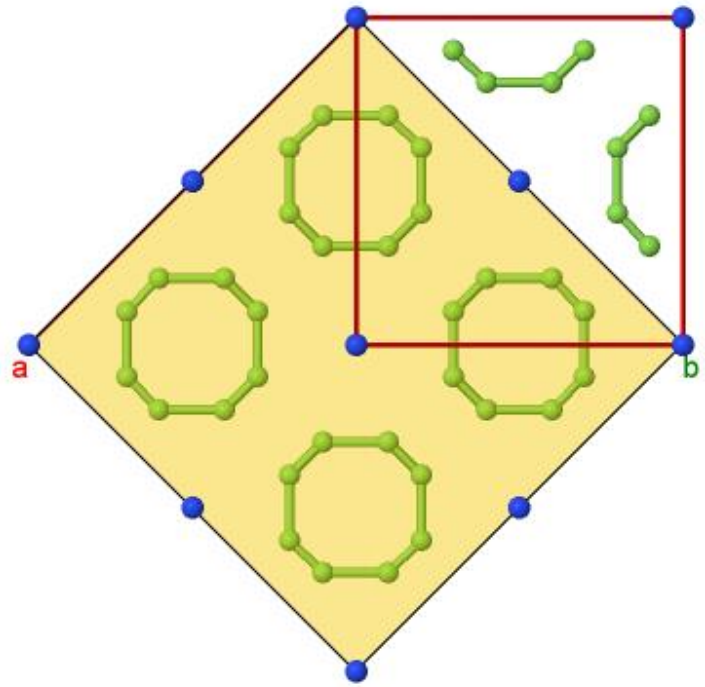
modelkit add N wyckoff c packed

connect 1.0 2.1

modelkit spacegroup "140:a-b,a+b,c" packed

draw ID uc2 unitcell fill nomesh color translucent 0.8

connect 1.0 2.1; center unitcell; zoom 100



JmolD

https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup 140

draw ID uc1 unitcell color red

draw ID ax1 axes

modelkit add F {0.60 0.20 0.25/1}

modelkit add N wyckoff c packed

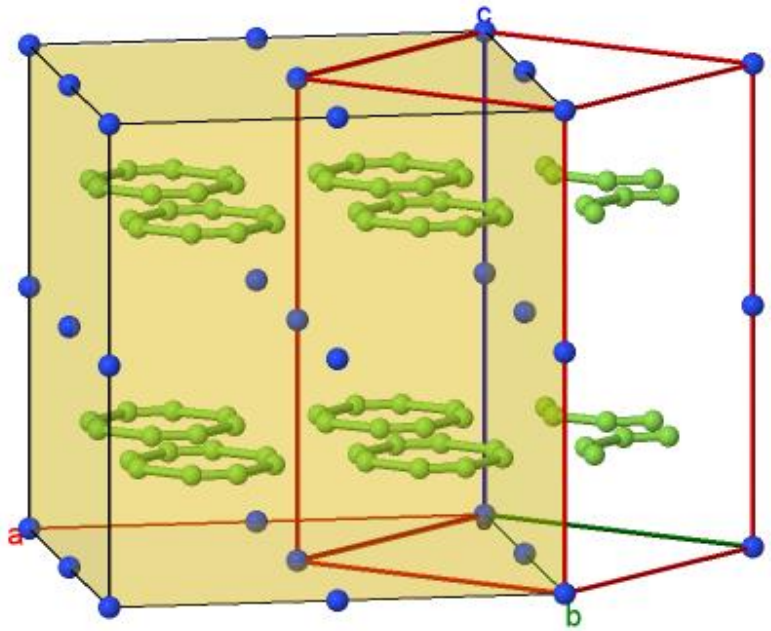
connect 1.0 2.1

modelkit spacegroup "140:a-b,a+b,c" packed

draw ID uc2 unitcell fill nomesh color translucent 0.8

connect 1.0 2.1; center unitcell; zoom 100

rotate z -35; rotate x -80



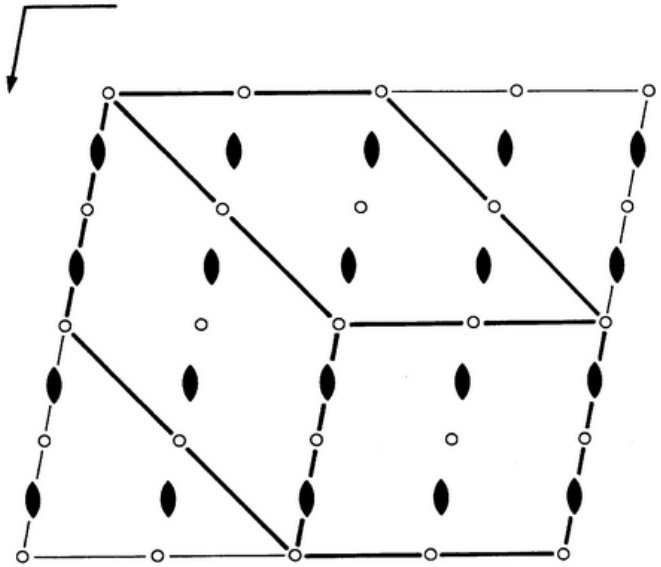
JmolD

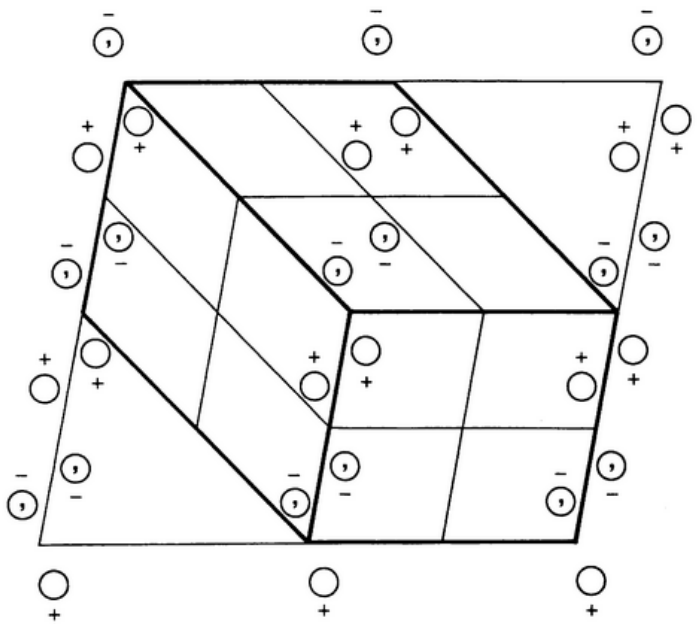
https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

Can someone
explain this to me?





https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup "13:a,b,c"

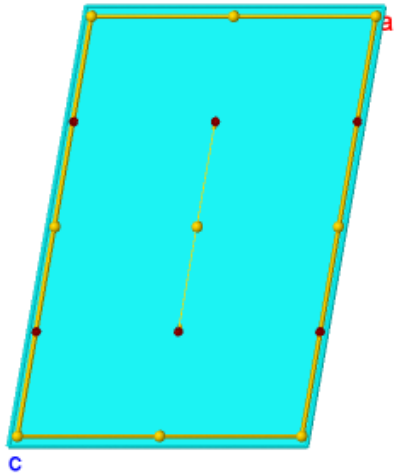
moveto axis b1

draw uc1 unitcell

draw sg1 spacegroup all

show symops

1	**x,y,z**	**identity**
2	**-x,y,-z+1/2**	**2 axis**
3	**-x,-y,-z**	**Ci: 0 0 0**
4	**x,-y,z+1/2**	**c-glide plane|translation: 0 0 1/2**



JmolD

https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup "13:a,b,c"

moveto axis b1

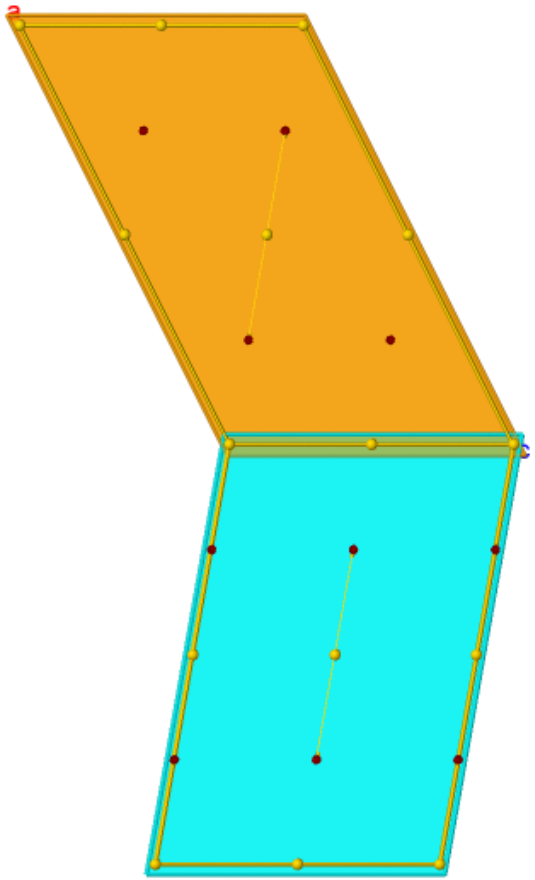
draw uc1 unitcell

draw sg1 spacegroup all

modelkit spacegroup "13:-a-c,b,a"

draw uc2 unitcell

draw sg2 spacegroup all



JmolD

https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup "13:a,b,c"

moveto axis b1

draw uc1 unitcell

draw sg1 spacegroup all

modelkit spacegroup "13:-a-c,b,a"

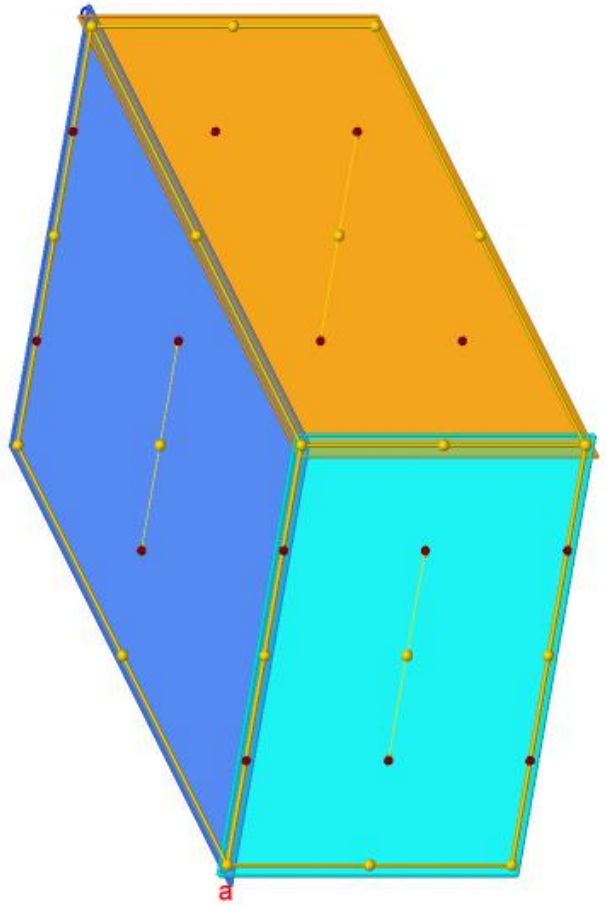
draw uc2 unitcell

draw sg2 spacegroup all

modelkit spacegroup "13:c,b,-a-c"

draw uc3 unitcell

draw sg3 spacegroup all



https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup "13:a,b,c"

moveto axis b1

draw uc1 unitcell

draw sg1 spacegroup all

modelkit spacegroup “13:-a-c,b,a"

draw uc2 unitcell

draw sg2 spacegroup all

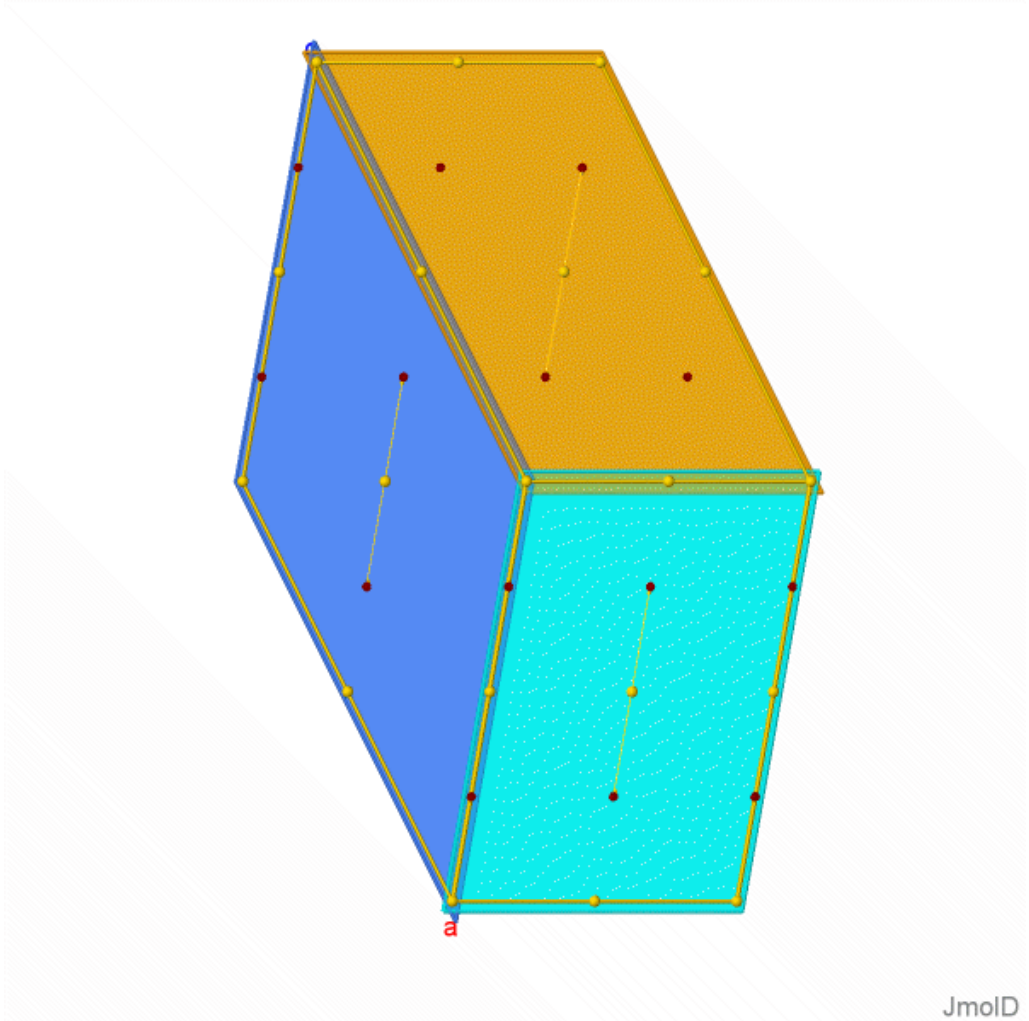
modelkit spacegroup "13:c,b,-a-c"

draw uc3 unitcell

draw sg3 spacegroup all

center {0 1/2 0}; zoom 50; rotate z 15; rotate y 75; rotate z 90;

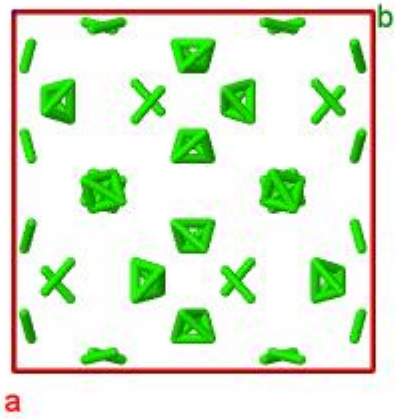
spin on



https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of subgroups:



modelkit zap spacegroup 230

zoom 60

draw ID uc1 unitcell color red

draw ID ax1 axes

modelkit add N Wyckoff G

connect 0.5 1.5

spacefill off

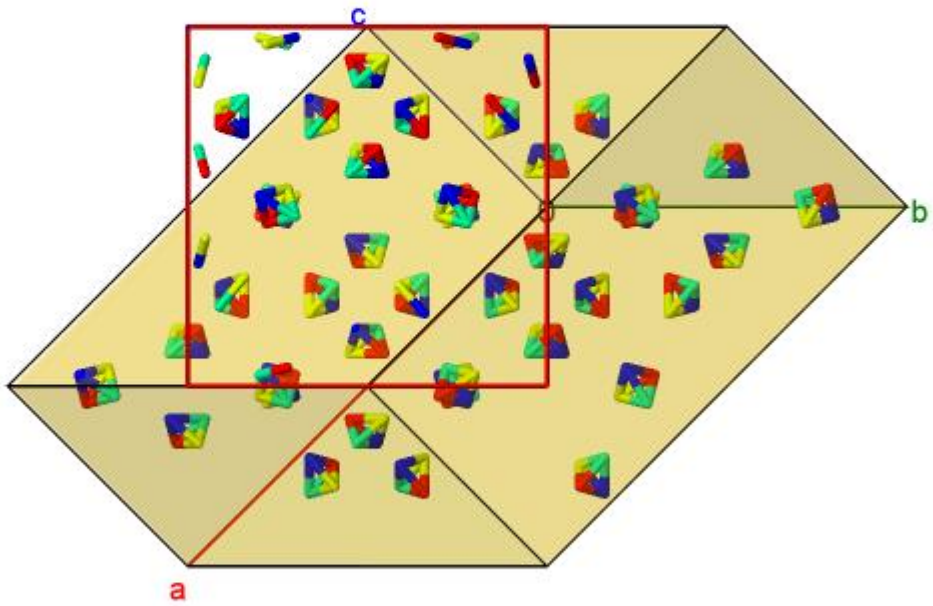
color property site

JmolD

https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of subgroups:



modelkit zap spacegroup 230

draw ID uc1 unitcell color red

draw ID ax1 axes

modelkit add N Wyckoff G

modelkit spacegroup "230>a-b,b+c,-1/2a-1/2b+1/2c;1/2,1,-1/2>167" packed

draw ID uc2 unitcell fill nomesh color translucent 0.8

connect 0.5 1.5

spacefill off

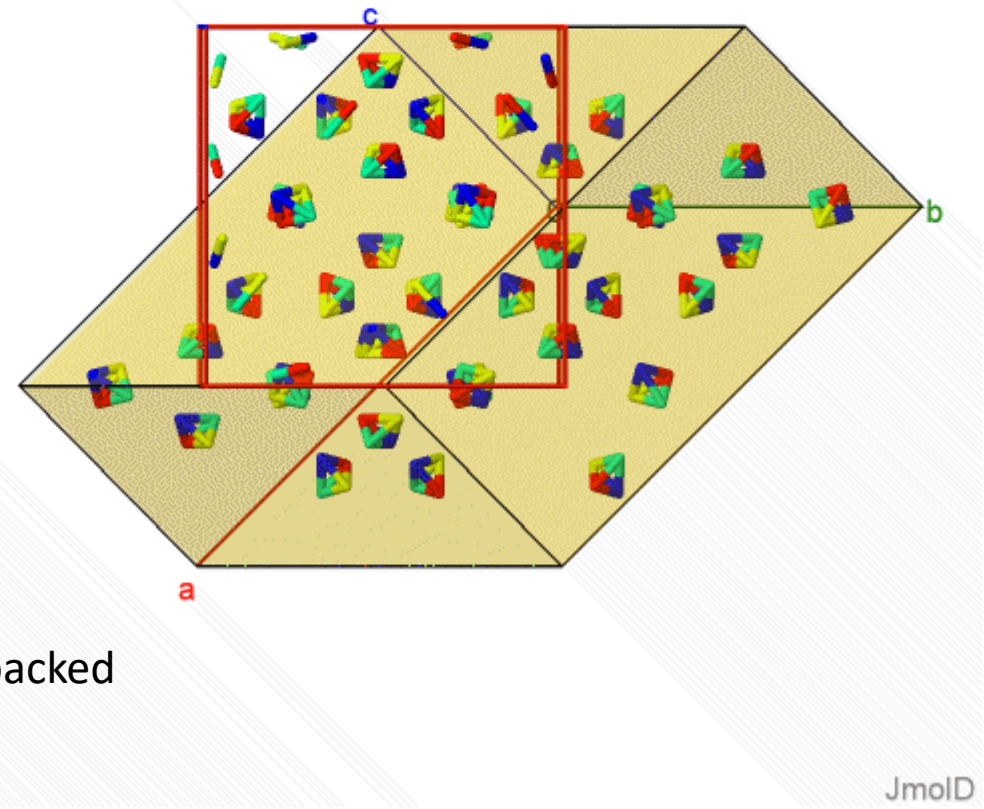
color property site

spin on

https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of subgroups:



modelkit zap spacegroup 230

draw ID uc1 unitcell color red

draw ID ax1 axes

modelkit add N Wyckoff G

modelkit spacegroup "230>a-b,b+c,-1/2a-1/2b+1/2c;1/2,1,-1/2>167" packed

draw ID uc2 unitcell fill nomesh color translucent 0.8

connect 0.5 1.5

spacefill off

color property site

spin on

https://github.com/BobHanson/CLEG

CLEG applications

ISODISTORT/Jmol scripting for visualization of subgroups:

ISODISTORT: subgroup tree
Subgroup 1
221 Pm-3m, basis={(0,-1,0),(-1,0,0),(0,0,-1)}, origin=(0,0,0), s=1, i=1
Maximal subgroups: 2
a=4.20000,b=4.20000,c=4.20000,alpha=90.00000,beta=90.00000,gamma=90.00000
Order parameters: GM1+ (a)
Active k vectors: (0,0,0)
This subgroup does not produce any selected distortions

Subgroup 2
123 P4/mmm, basis={(1,0,0),(0,1,0),(0,0,1)}, origin=(0,0,0), s=1, i=3
Maximal subgroups: 3
a=4.20000,b=4.20000,c=4.20000,alpha=90.00000,beta=90.00000,gamma=90.00000
Order parameters: GM1+ (a) GM3+ (a,0)
Active k vectors: (0,0,0)

Subgroup 3
140 I4/mcm, basis={(-1,1,0),(-1,-1,0),(0,0,2)}, origin=(0,0,0), s=2, i=6
Maximal subgroups:
a=5.93970,b=5.93970,c=8.40000,alpha=90.00000,beta=90.00000,gamma=90.00000
Order parameters: R4+ (a,0,0) GM1+ (a) GM3+ (a,0)
Active k vectors: (1/2,1/2,1/2), (0,0,0)

https://github.com/BobHanson/CLEG

CLEG applications

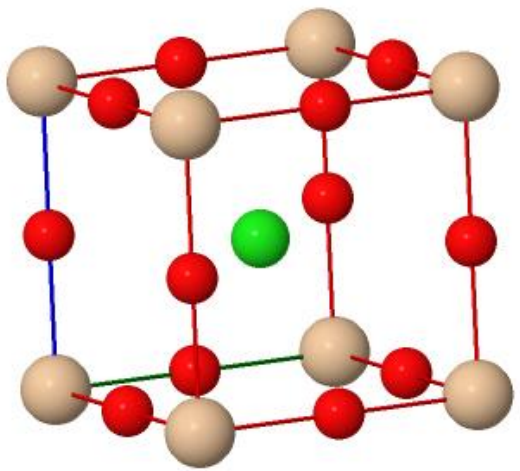
ISODISTORT/Jmol scripting for visualization of subgroups:

modelkit zap spacegroup "221:-b,-a,-c" unitcell [4.2 4.2 4.2 90 90 90]

modelkit add Si Wyckoff a packed

modelkit add Cl Wyckoff b packed

modelkit add O Wyckoff d packed



https://github.com/BobHanson/CLEG

JmolD

CLEG applications

ISODISTORT/Jmol scripting for visualization

modelkit zap spacegroup "221:-b,-a,-c" unitcell [4.2 4.2 4.2 90 90 9

modelkit add Si Wyckoff a packed

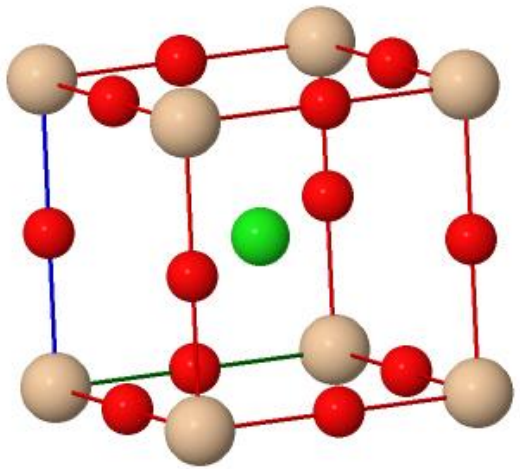
modelkit add Cl Wyckoff b packed

modelkit add O Wyckoff d packed

modelkit spacegroup “221:-b,-a,-c > a,b,c > 123” packed

draw ID uc1 unitcell color red

draw ID ax1 axes



https://github.com/BobHanson/CLEG

JmolD

CLEG applications

ISODISTORT/Jmol scripting for visualization of subgroups:

modelkit zap spacegroup "221:-b,-a,-c" unitcell [4.2 4.2 4.2 90 90 90]

modelkit add Si Wyckoff a packed

modelkit add Cl Wyckoff b packed

modelkit add O Wyckoff d packed

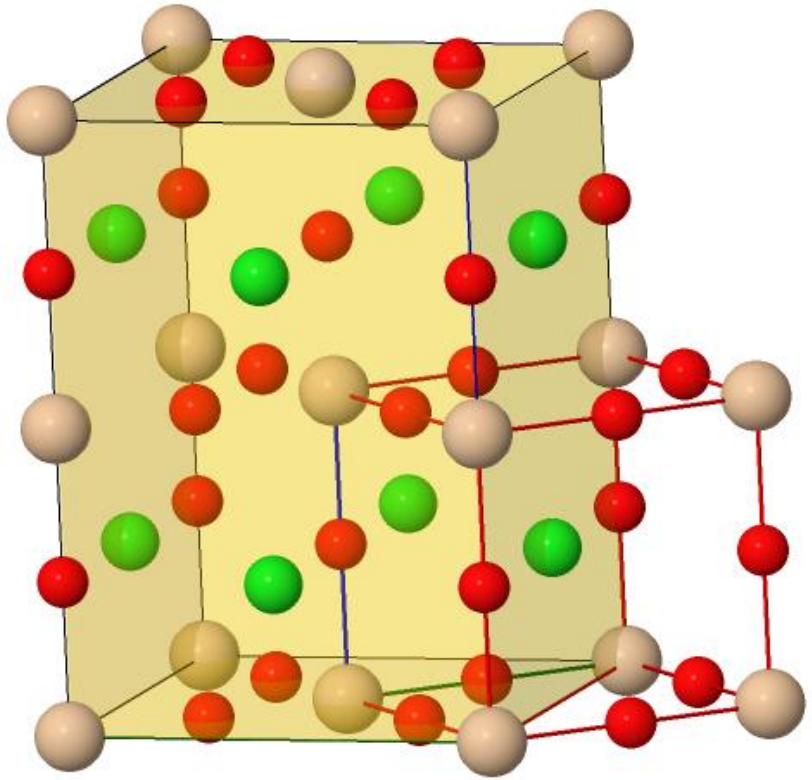
modelkit spacegroup "221:-b,-a,-c > a,b,c > 123” packed

draw ID uc1 unitcell color red

draw ID ax1 axes

modelkit spacegroup “123 > -a+b,-a-b,2c;1,0,0 > 140" packed

draw ID uc2 unitcell fill nomesh translucent 0.8



https://github.com/BobHanson/CLEG

CLEG applications

ISODISTORT/Jmol scripting for visualization of subgroups:

modelkit zap spacegroup “221:-b,-a,-c” unitcell [4.2 4.2 4.2 90 90 90]

modelkit add Si Wyckoff a packed

modelkit add Cl Wyckoff b packed

modelkit add O Wyckoff d packed

modelkit spacegroup “221:-b,-a,-c > a,b,c > 123” packed

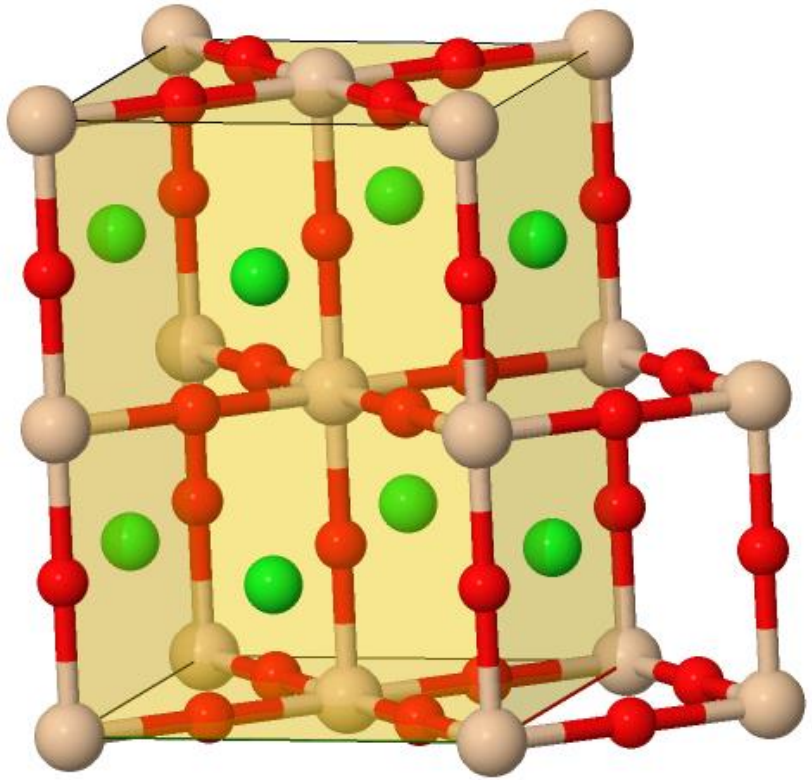
draw ID uc1 unitcell color red

draw ID ax1 axes

modelkit spacegroup “123 > -a+b,-a-b,2c;1,0,0 > 140” packed

draw ID uc2 unitcell fill nomesh translucent 0.8

connect 2.0 2.2



https://github.com/BobHanson/CLEG

Summary: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

- **Simple**

P 1 2/m 1	**10:a,b,c;0,0,0**	P 1 2/c 1	**13:a,b,c;0,0,0**
P 1 1 2/m	**10:c,a,b;0,0,0**	P 1 1 2/n	**13:a,-a-c,b;0,0,0**
P 2/m 1 1	**10:b,c,a;0,0,0**	P 2/b 1 1	**13:b,c,a;0,0,0**

https://github.com/BobHanson/CLEG

Summary: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

- Simple
- **Concise**

P 1 2/m 1	**10**	P 1 2/c 1	**13:a,b,c**
P 1 1 2/m	**10:c,a,b**	P 1 1 2/n	**13:a,-a-c,b**
P 2/m 1 1	**10:b,c,a**	P 2/b 1 1	**13:b,c,a**

https://github.com/BobHanson/CLEG

Summary: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

- Simple
- Concise
- **Comprehensive**

10:b,c,a > !b,c,a > 10	nonstandard to standard setting
10 > a-c,b,2c;0,0,1/2 > 13	group to subgroup (standard settings)
13 > a,-a-c,b > 13:a,-a-c,b	standard to nonstandard
10:b,c,a > -b+c,-b-c,a:0,1/2,0 > 13:a,-a-c,b	nonstandard group to nonstandard subgroup

https://github.com/BobHanson/CLEG

Summary: CLEG

A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

- Simple
- Concise
- Comprehensive
- **Flexible**

10 > -b+c,-b-c,a:0,1/2,0 > 13 **(for human or machine consumption)**

P 2/m 1 1 > -b+c,-b-c,a:0,1/2,0 > P 1 1 2/n **(for human consumption)**

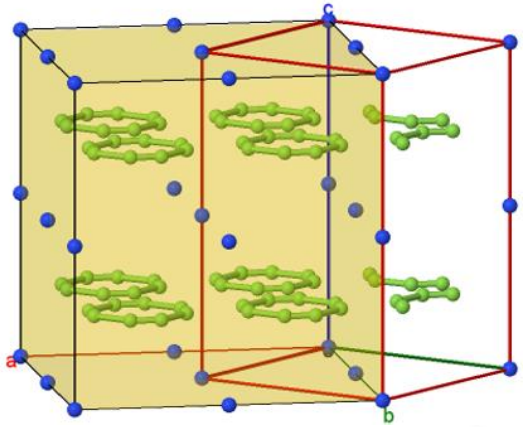
[-P 2y]:b,c,a > -b+c,-b-c,a:0,1/2,0 > [-P 2cy]:a,-a-c,b **(for machine consumption)**

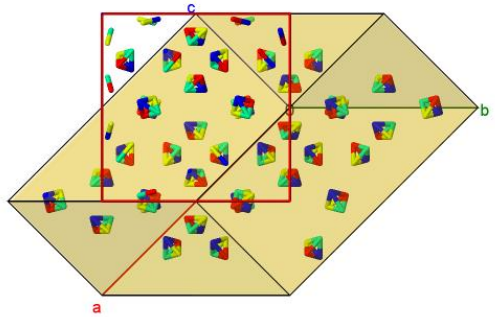
https://github.com/BobHanson/CLEG

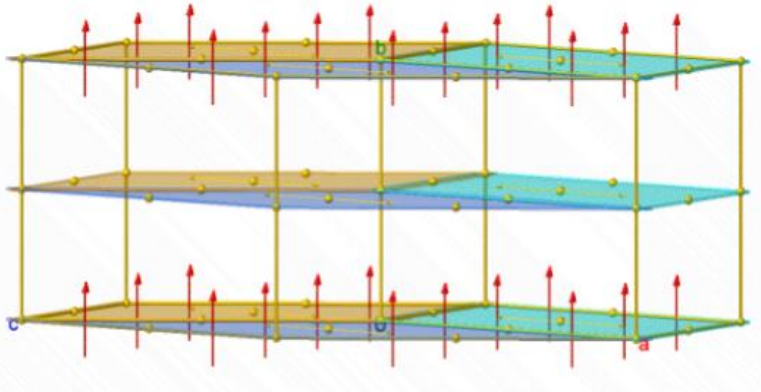
Summary: CLEG

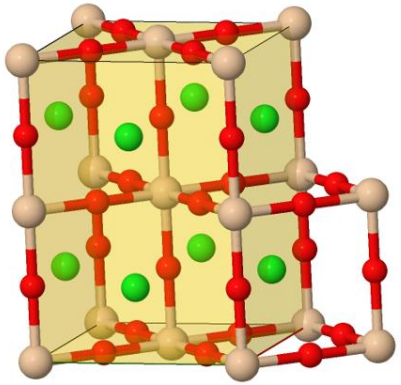
A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

- Simple
- Concise
- Comprehensive
- Flexible
- **And it works!**









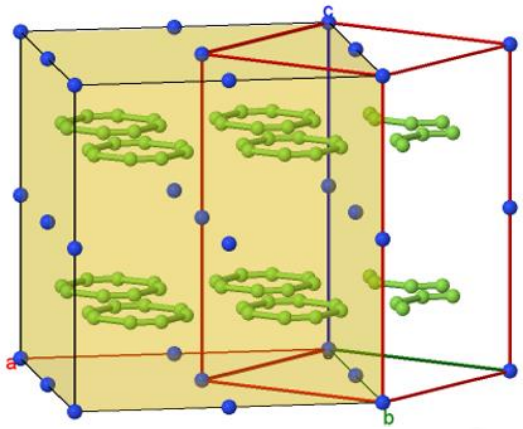
https://github.com/BobHanson/CLEG

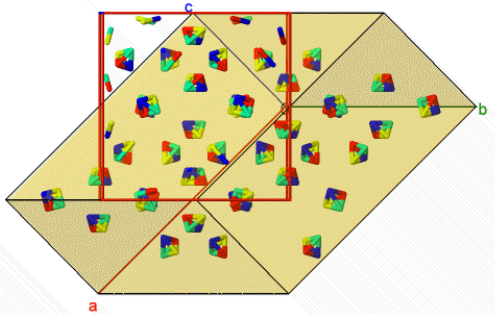
Summary: CLEG

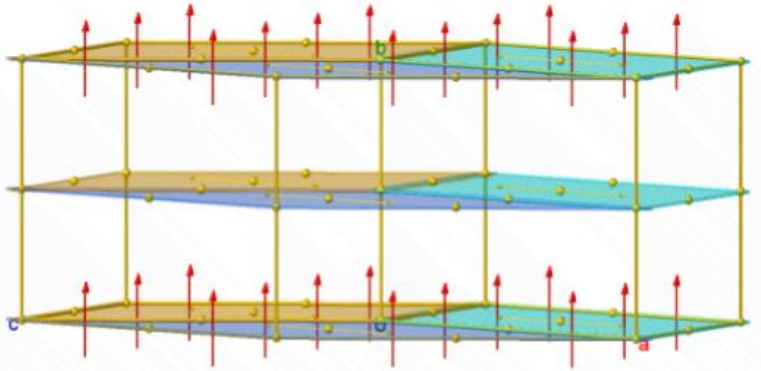
A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

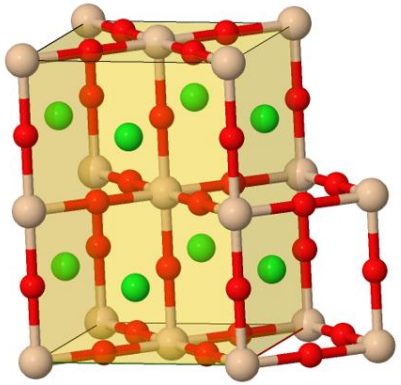
Many thanks to Branton Campbell, Harold Stokes, Mois Aroyo, and Gotzon Madariaga for their patience, support, and many great conversations.

Thank you!









https://github.com/BobHanson/CLEG

More Jmol implementations this afternoon!

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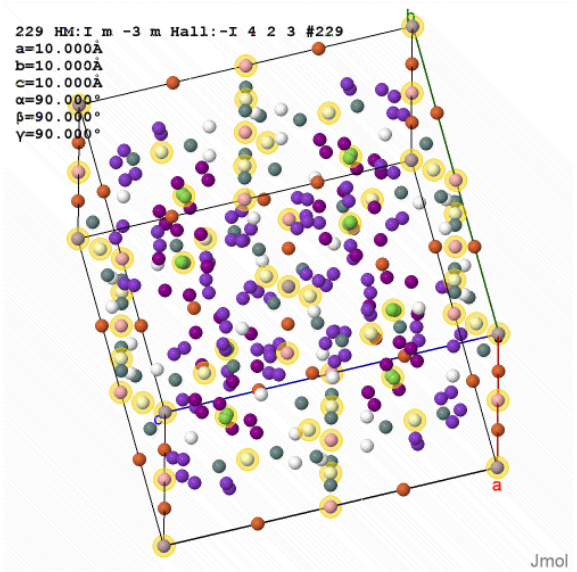
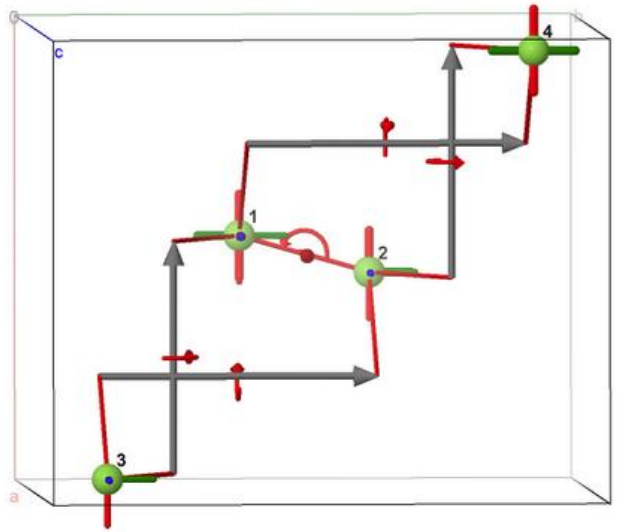
Using Jmol to engage students and teach crystallography and crystallographic symmetry

Dean Johnston[1], Robert Hanson[2]

[1] Otterbein University, Westerville, OH, USA. [2] St. Olaf College, Northfield, MN, USA





https://github.com/BobHanson/CLEG