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

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American Crystallographic Association
74th Annual Meeting,
Denver, Colorado
9 July 2024

Introduction: Space group settings

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

1	P1	2	P-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-4	82	I-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-42m	112	P-42c	113	$P\text{-}42_1m$	114	$P\text{-}42_1c$	115	P-4m2

116	P-4c2	117	P-4b2	118	P-4n2	119	I-4m2	120	I-4c2
121	I-42m	122	I-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-3	148	R-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-31m	163	P-31c	164	P-3m1	165	P-3c1
166	R-3m	167	R-3c	168	P6	169	$P6_1$	170	$P6_5$
171	$P6_2$	172	$P6_4$	173	$P6_3$	174	P-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-6m2	188	P-6c2	189	P-62m	190	P-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-3
201	Pn-3	202	Fm-3	203	Fd-3	204	Im-3	205	Pa-3
206	Ia-3	207	P432	208	$P4_232$	209	F432	210	$F4_132$
211	I432	212	$P4_332$	213	$P4_132$	214	$I4_132$	215	P-43m
216	F-43m	217	I-43m	218	P-43n	219	F-43c	220	I-43d
221	Pm-3m	222	Pn-3n	223	Pm-3n	224	Pn-3m	225	Fm-3m
226	Fm-3c	227	Fd-3m	228	Fd-3c	229	Im-3m	230	Ia-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 *P2/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 BSC 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?

Introduction: Group-Subgroup relationships

The BSC 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*

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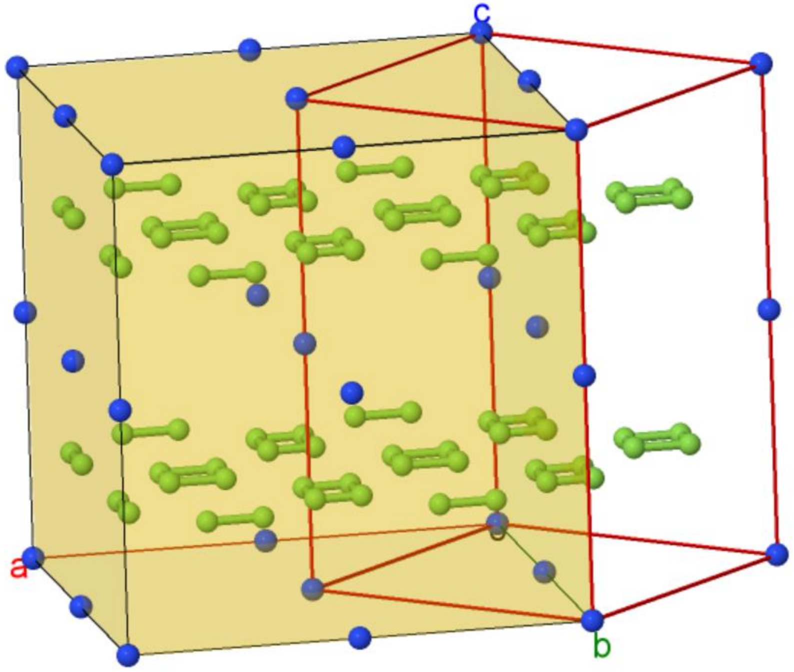
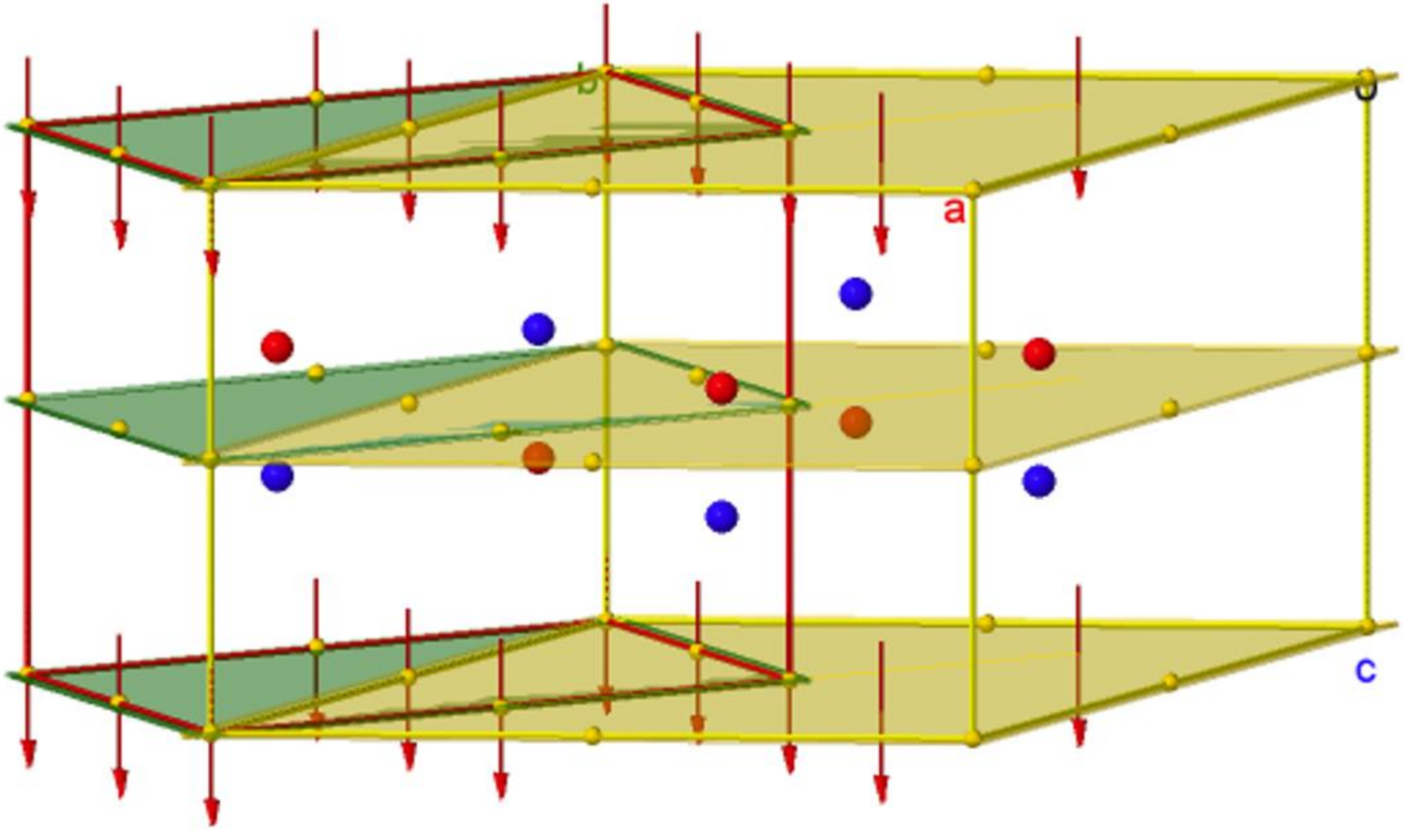
My challenge: modeling settings and subgroup relationships in Jmol





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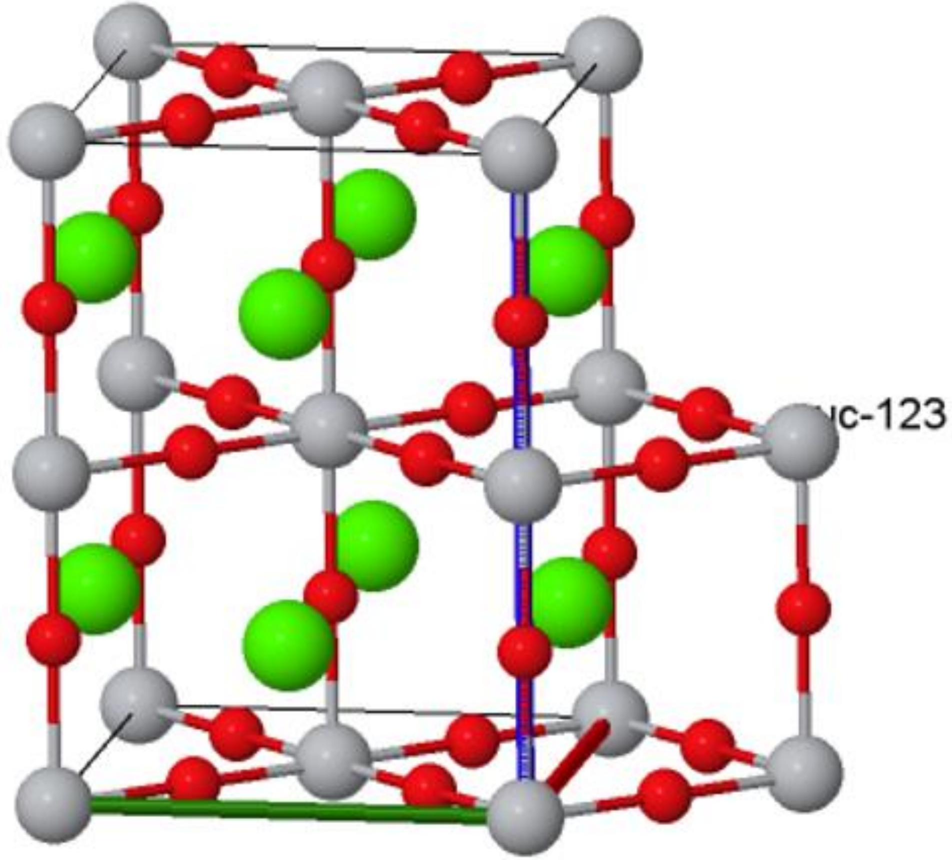
The Problem: How to express relationships concisely

- Simple, concise
- Comprehensive
- Flexible



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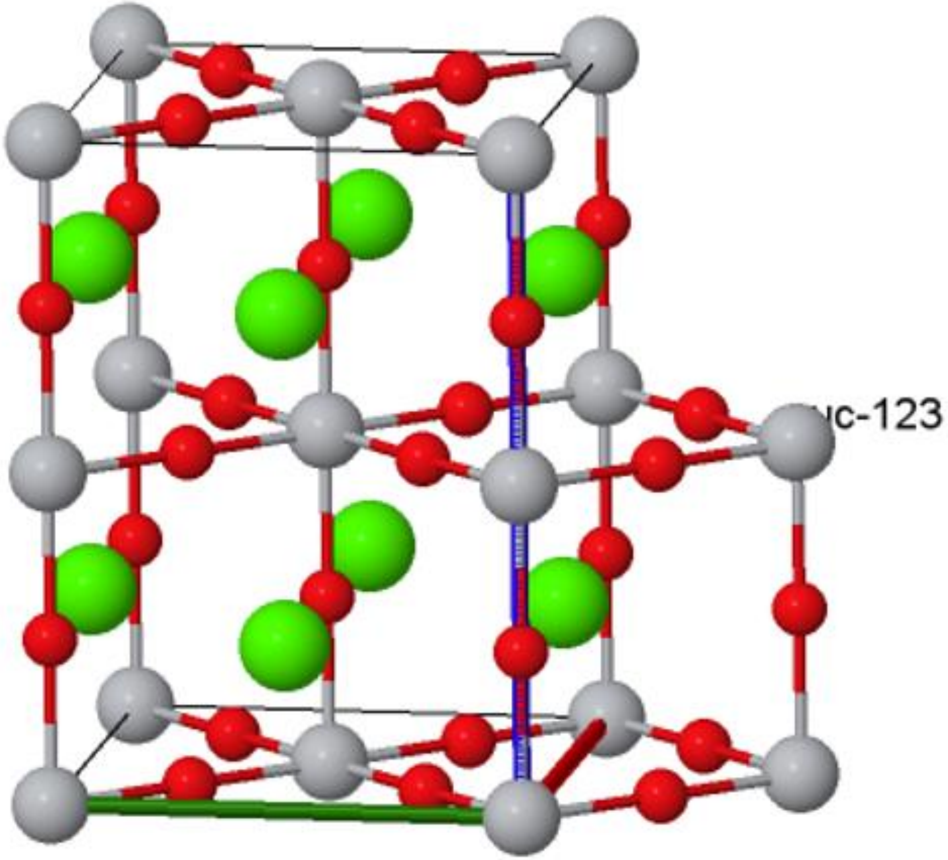
The Problem: How to express relationships concisely

- 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!

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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**) = $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 2 & 1/2 \end{pmatrix}$

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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!

https://github.com/BobHanson/CLEG

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!)

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 setting 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 setting 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!

https://github.com/BobHanson/CLEG

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	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 2 \end{pmatrix}$

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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	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 2 \end{pmatrix}$

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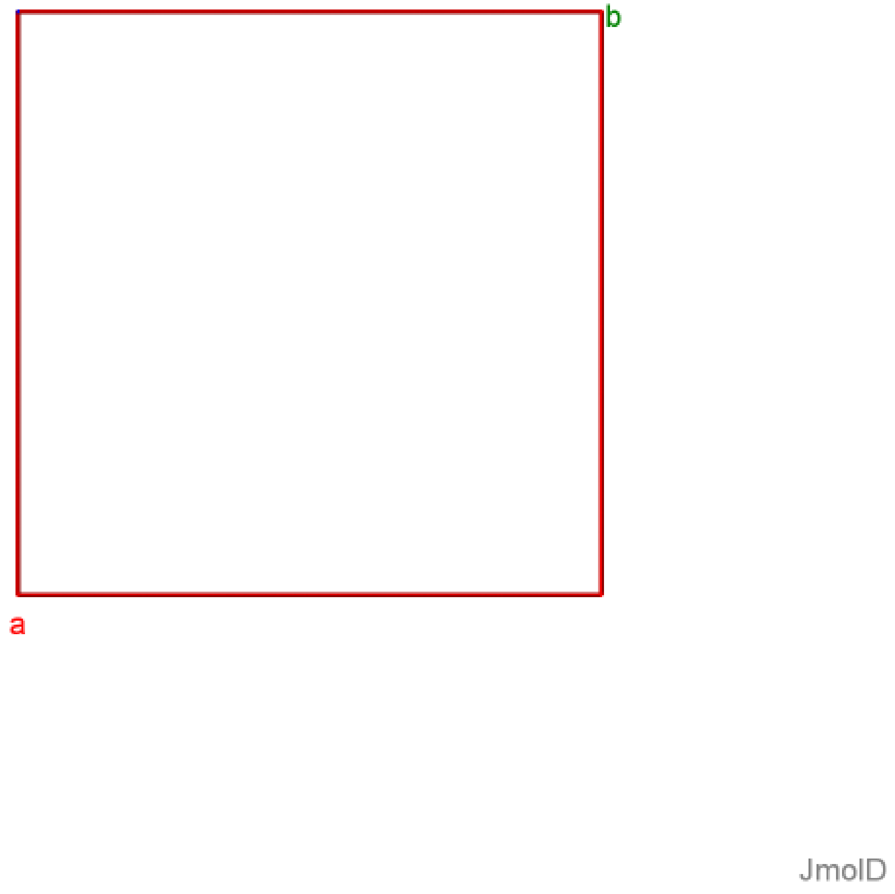
CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup 140

draw ID uc1 unitcell color red

draw ID ax1 axes



https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup 140

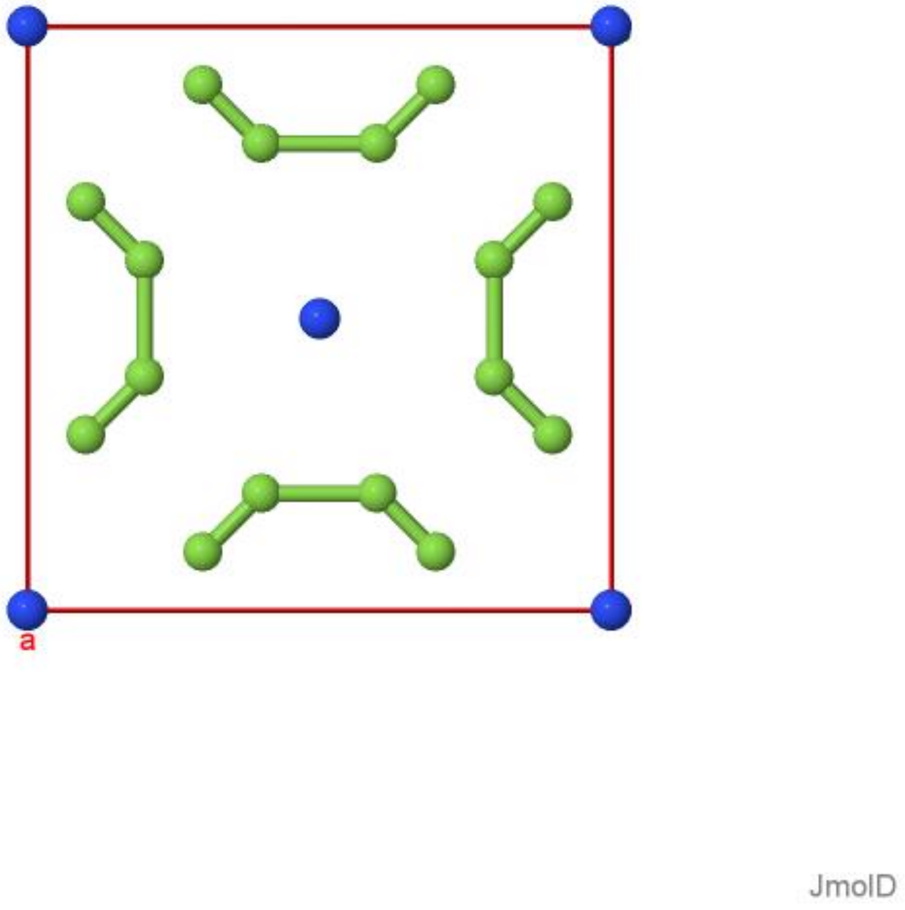
draw ID uc1 unitcell color red

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



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CLEG applications

Jmol scripting for visualization of settings:

modelkit zap spacegroup 140

draw ID uc1 unitcell color red

draw ID ax1 axes

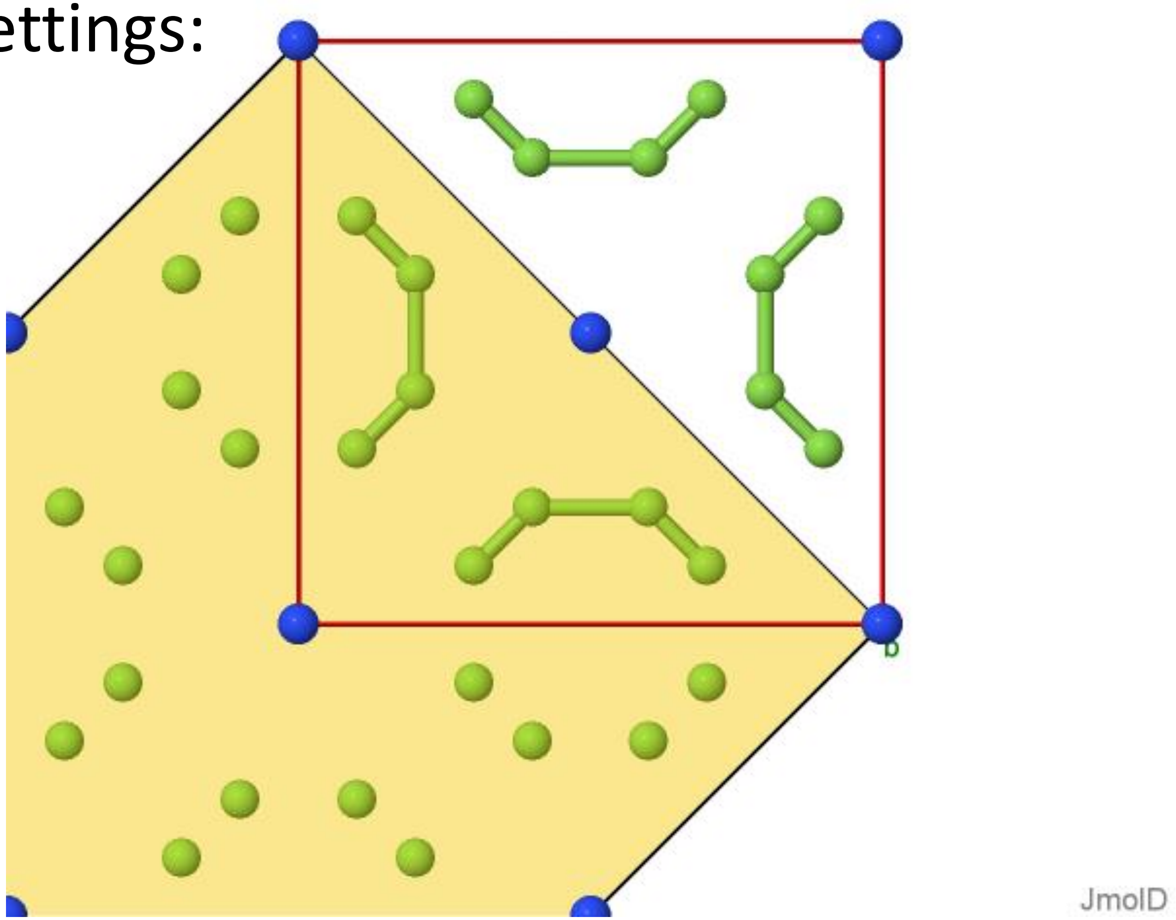
modelkit add F {0.60 0.20 0.25/1}

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



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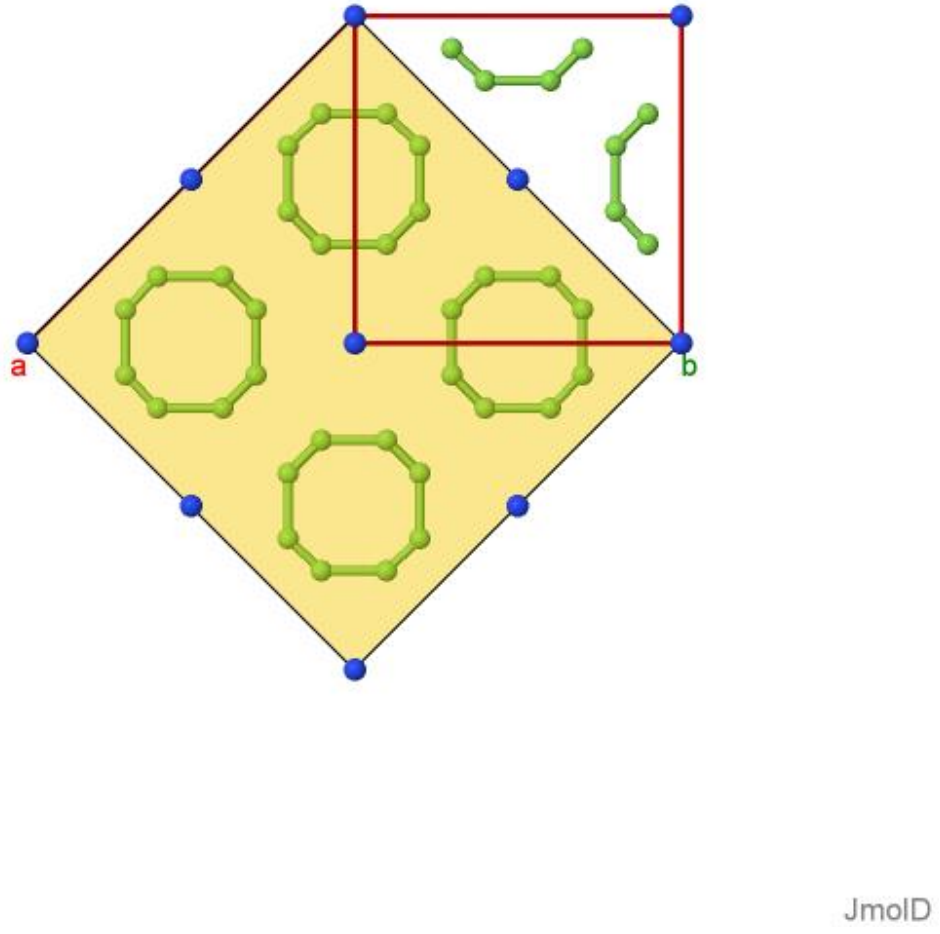
CLEG applications

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



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

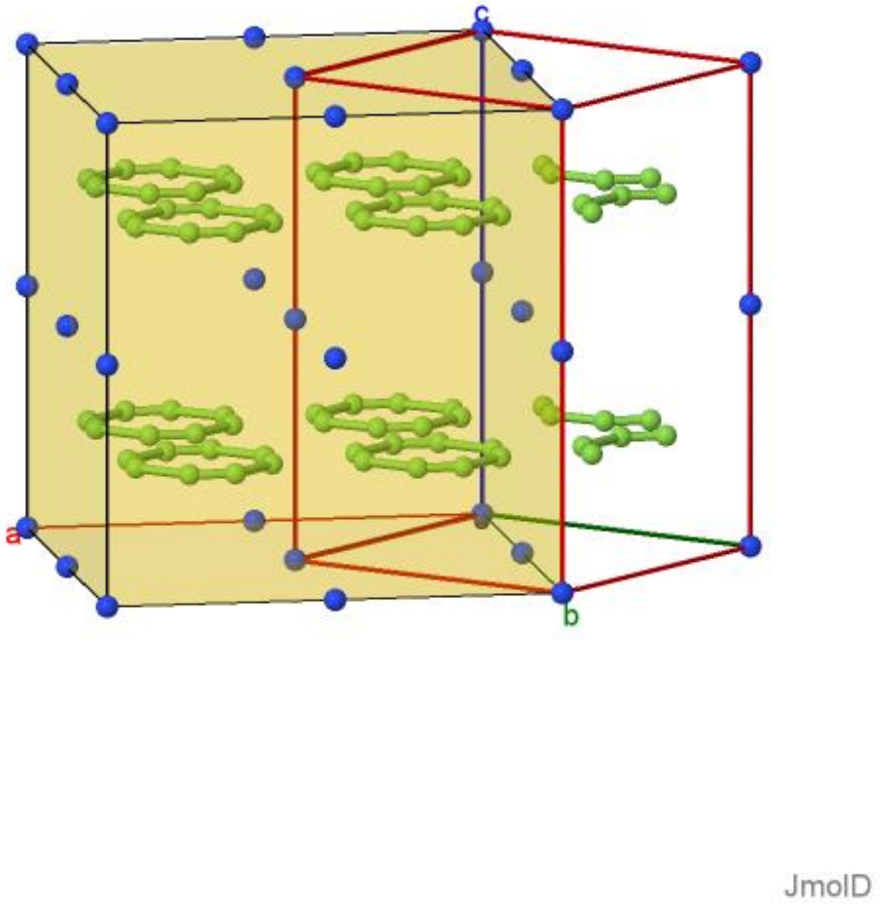
connect 1.0 2.1

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

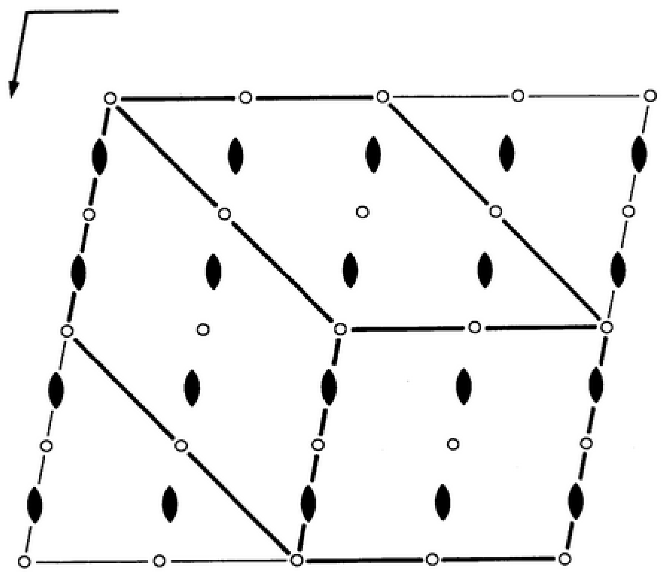


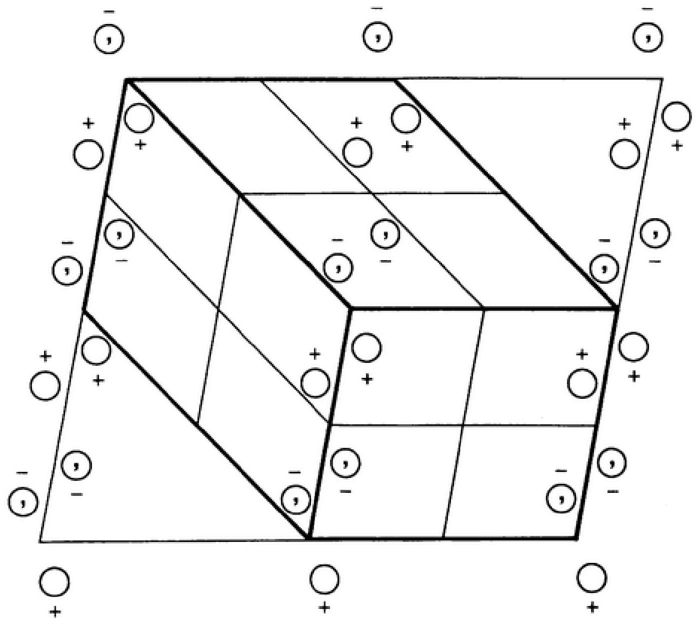
https://github.com/BobHanson/CLEG

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"

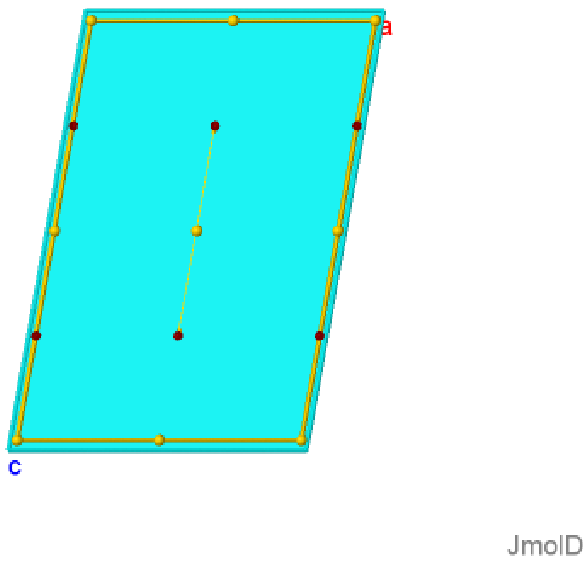
moveto axis b1

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**



https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

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

moveto axis b1

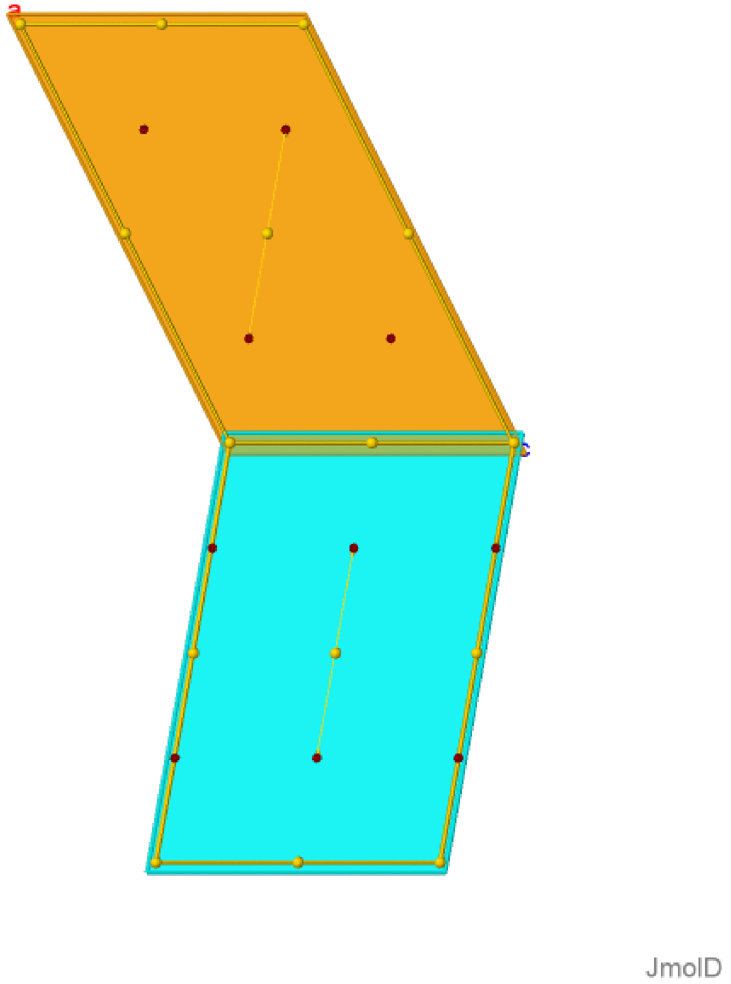
draw uc1 unitcell

draw sg1 spacegroup all

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

draw uc2 unitcell

draw sg2 spacegroup all



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"

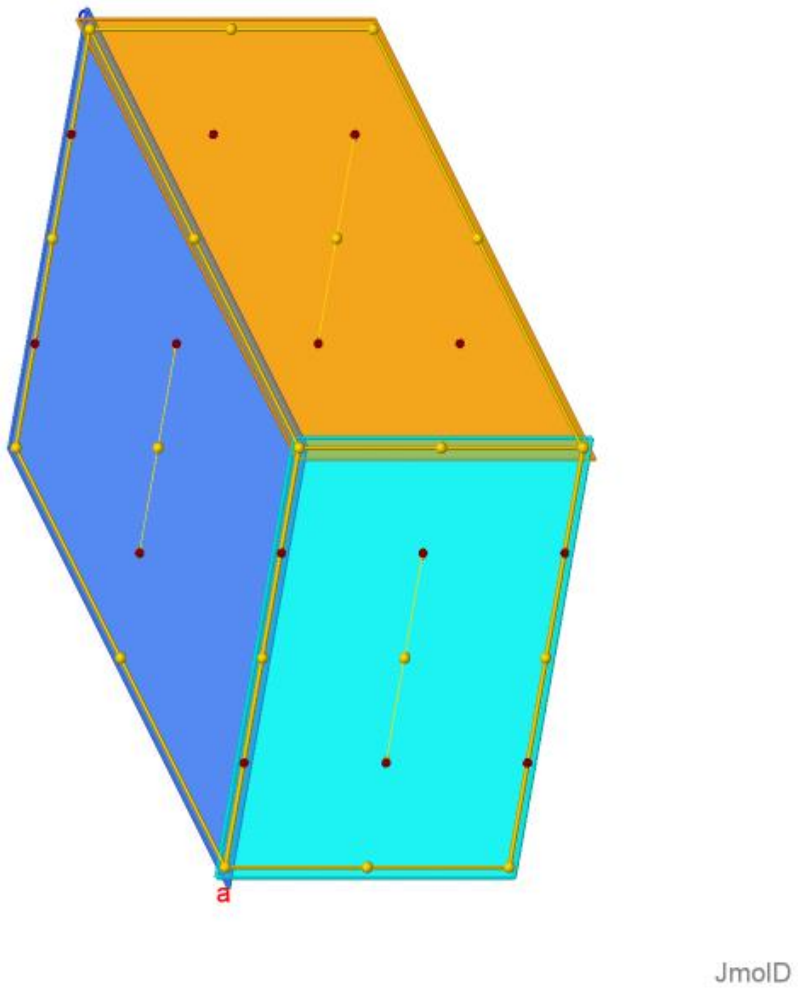
draw uc2 unitcell

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 13.1

moveto axis b1

draw uc1 unitcell

draw sg1 spacegroup all

modelkit spacegroup 13.2

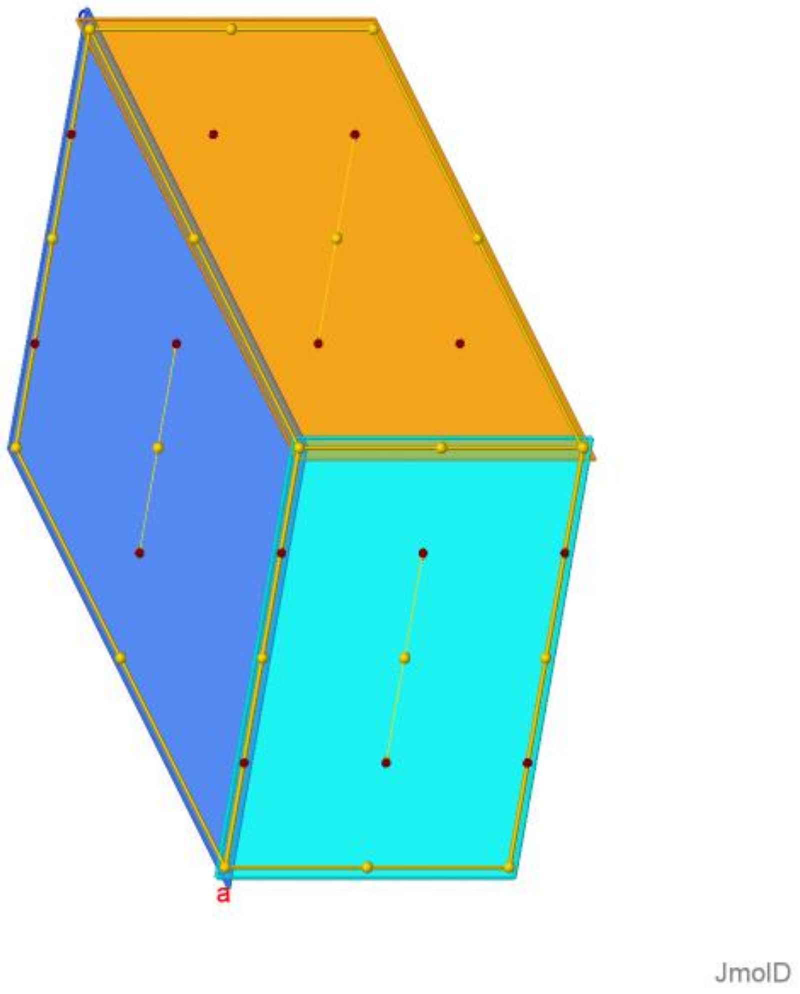
draw uc2 unitcell

draw sg2 spacegroup all

modelkit spacegroup 13.3

draw uc3 unitcell

draw sg3 spacegroup all

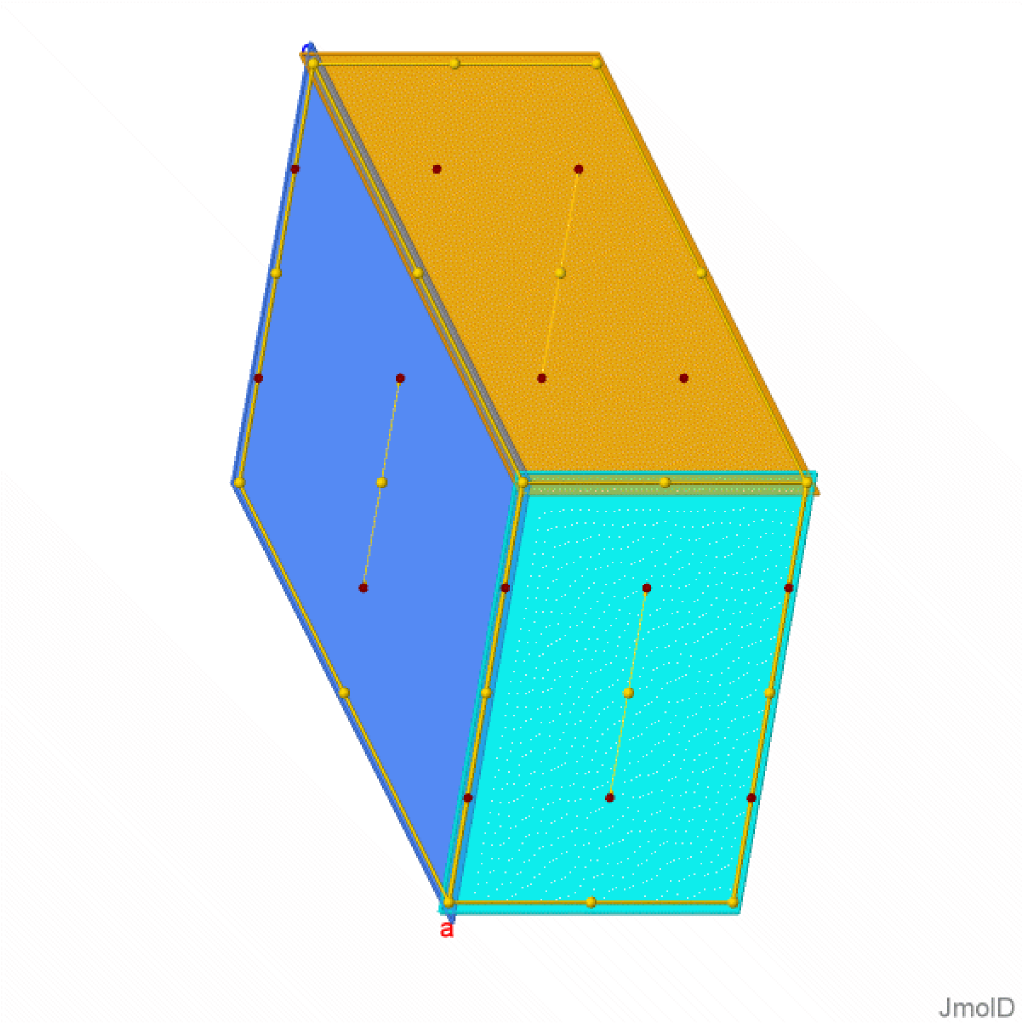


https://github.com/BobHanson/CLEG

CLEG applications

Jmol scripting for visualization of settings:

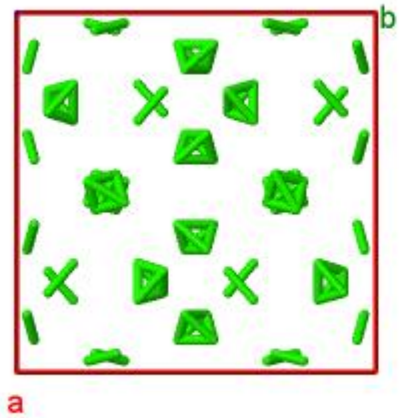
```
modelkit zap spacegroup "13:a,b,c"
moveto axis b1
draw uc1 unitcell
draw sg1 spacegroup all
modelkit spacegroup "13:-a-c,b,a"
draw uc2 unitcell
draw sg2 spacegroup all
modelkit spacegroup "13:c,b,-a-c"
draw uc3 unitcell
draw sg3 spacegroup all
```



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

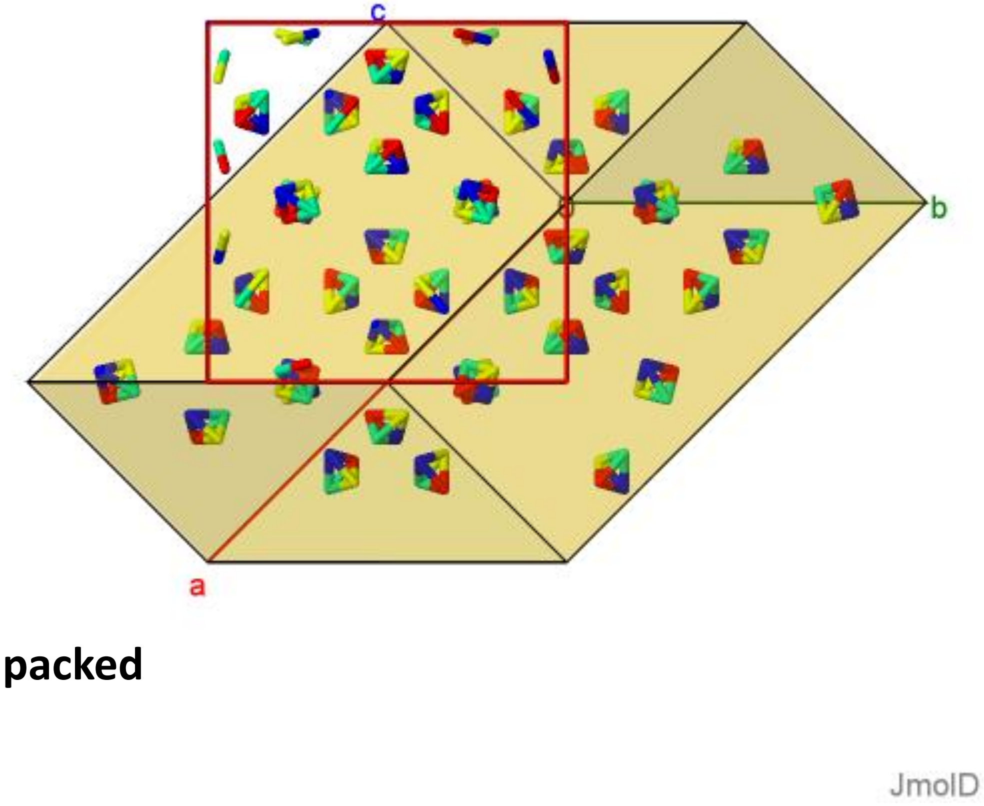
color property site

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

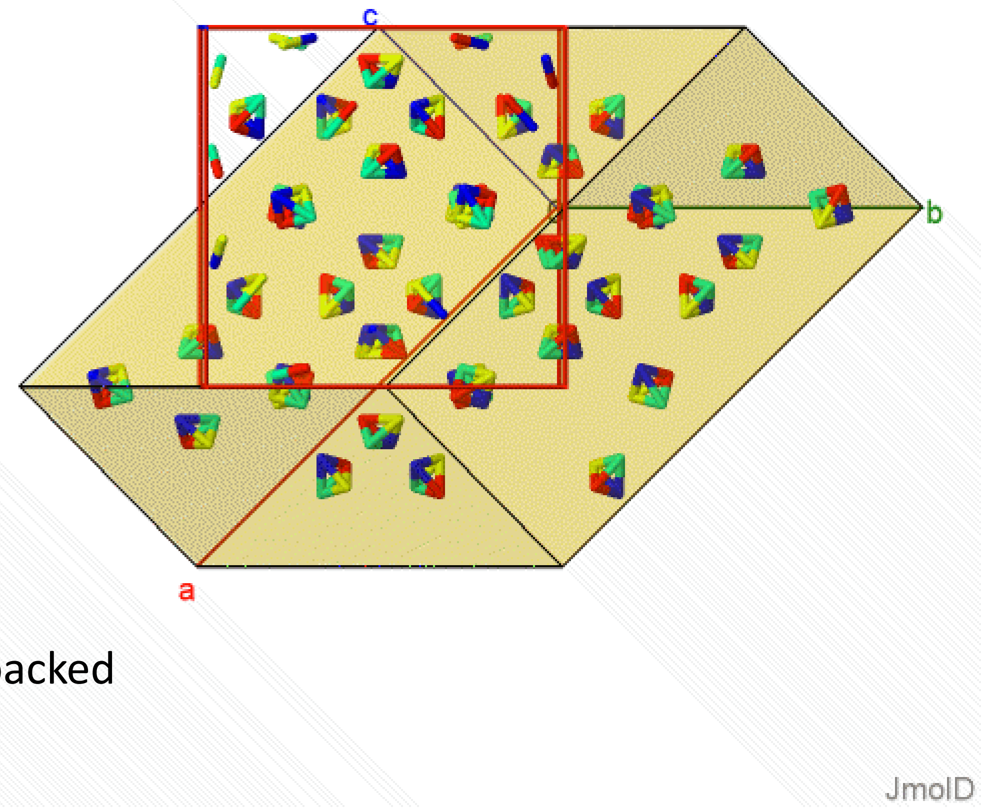
spin on

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

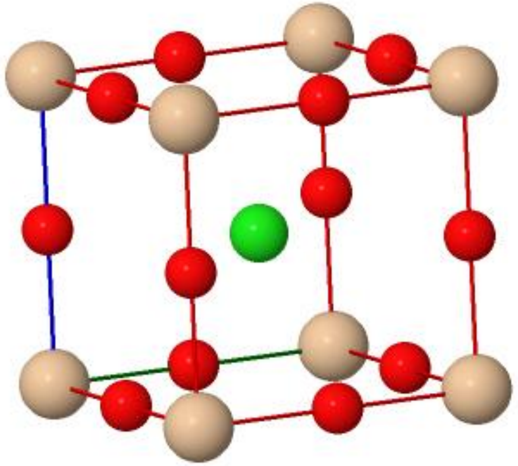
ISODISTORT/Jmol scripting for visualization of subgroups:

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

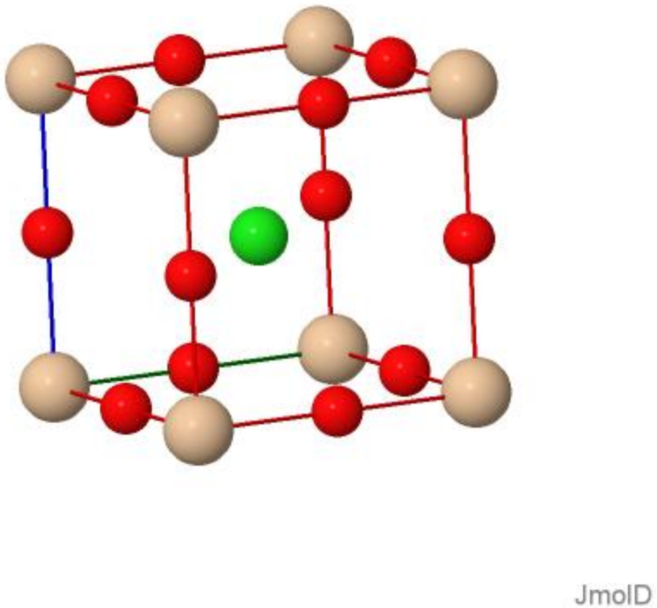
modelkit add Cl Wyckoff b packed

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

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

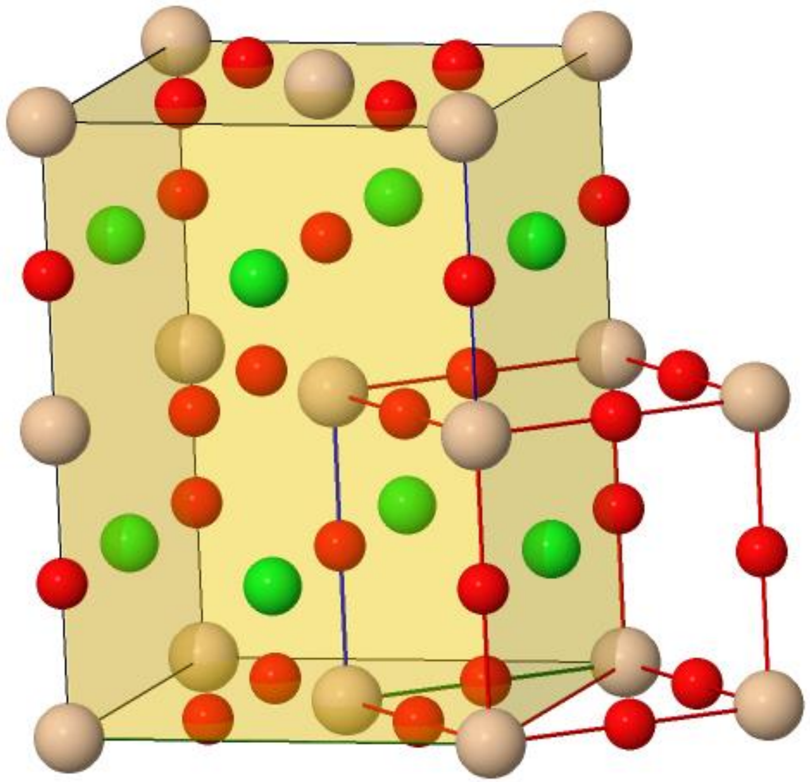
modelkit spacegroup "221:-b,-a,-c > a,b,c > 123” packed

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

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

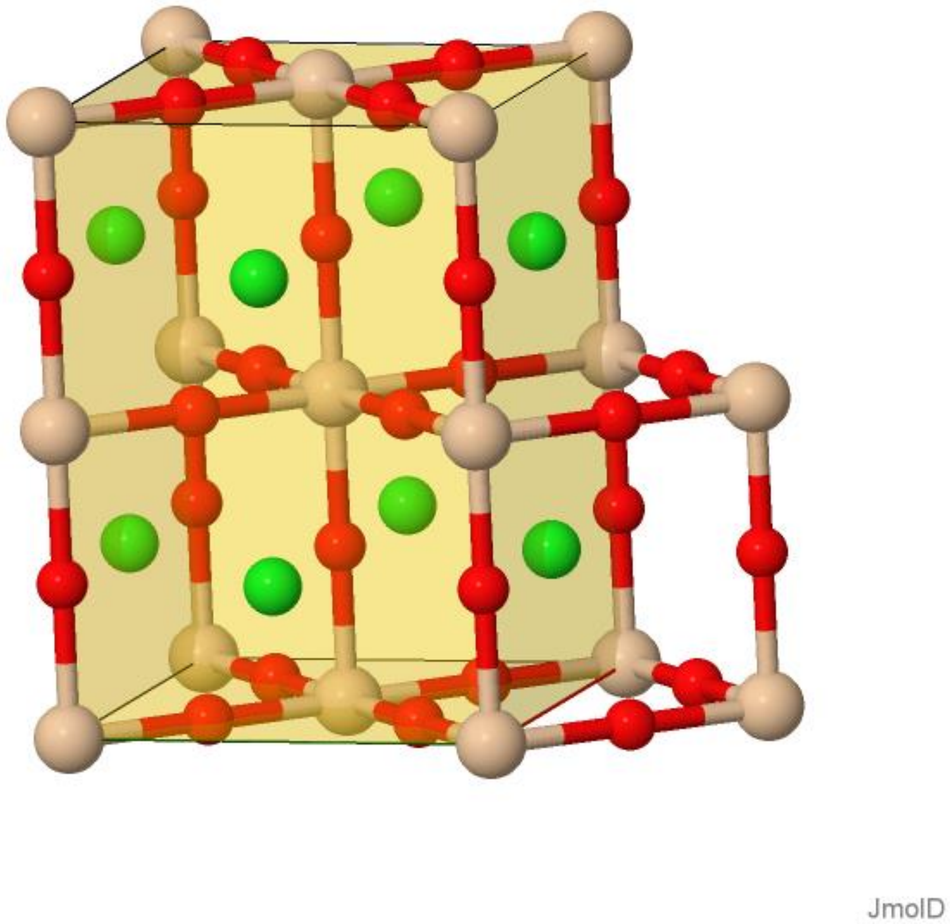
draw ID uc1 unitcell color red

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

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)**

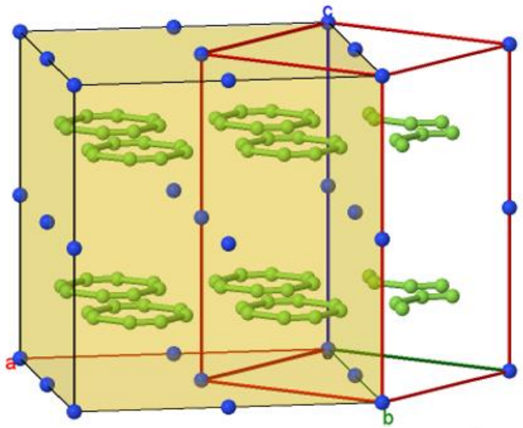
(-P 2y):b,c,a > -b+c,-b-c,a:0,1/2,0 > (-P 2cy):a,-a-c,b **(for machine consumption)**

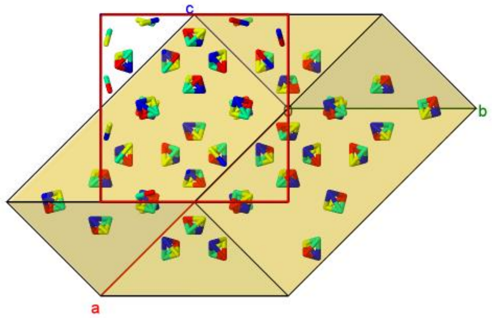
https://github.com/BobHanson/CLEG

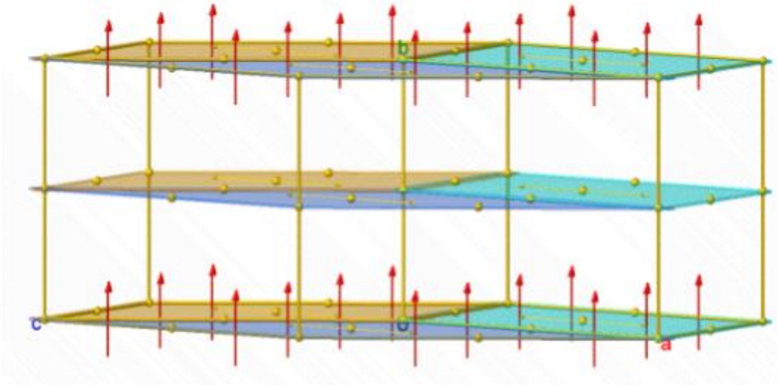
Summary: CLEG

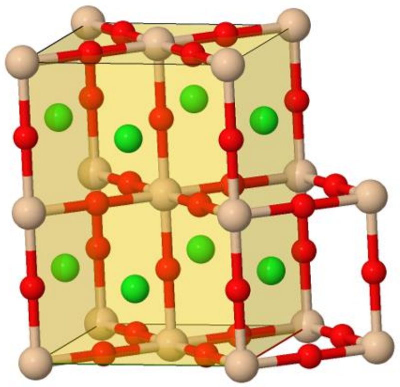
A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

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









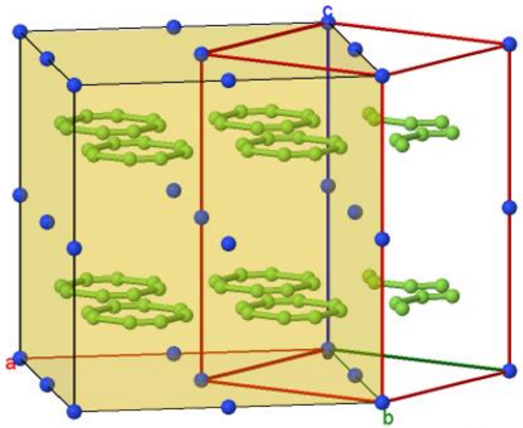
https://github.com/BobHanson/CLEG

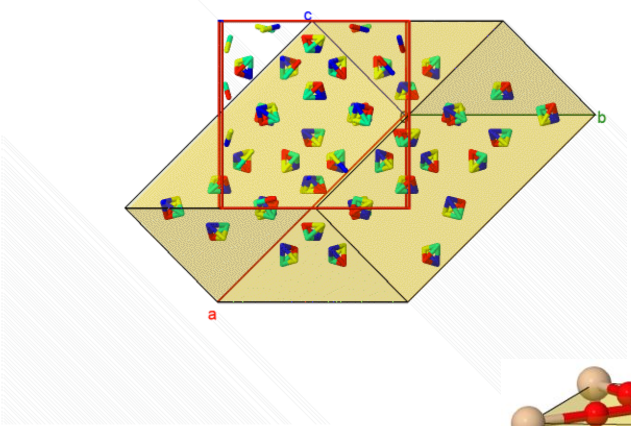
Summary: CLEG

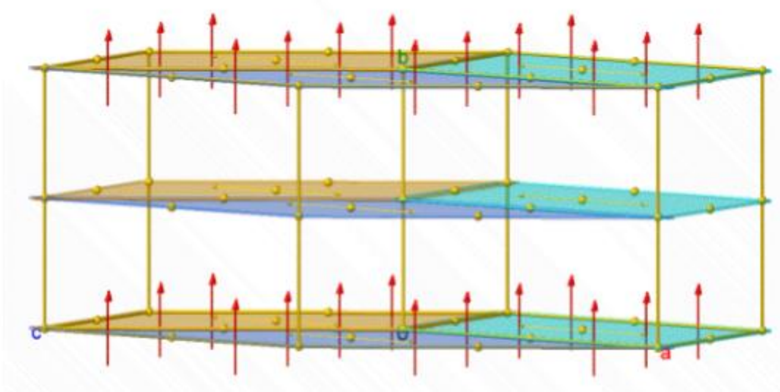
A Concise Linear Encoding of Crystallographic Space Group Settings and Group-Subgroup Relationships (CLEG)

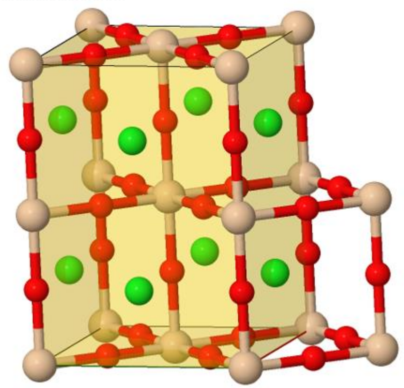
Many thanks to Branton Campbell, Harold Stokes, Mois Aroyo, and Gotzon Madariaga for their patience, support, and many great conversations.

Thank you!









https://github.com/BobHanson/CLEG

More Jmol implementations this afternoon!

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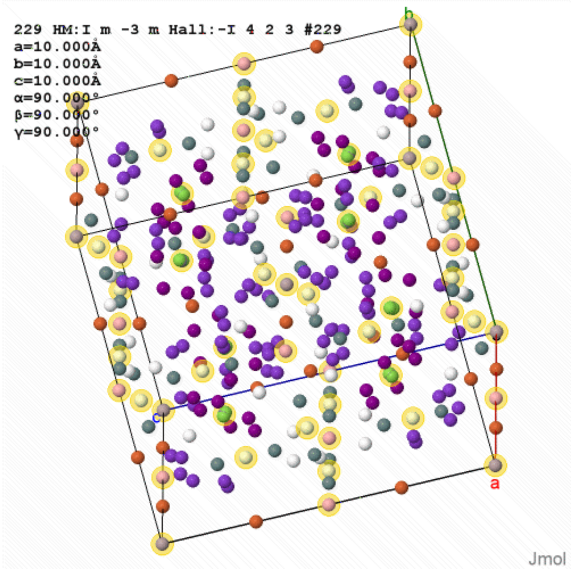
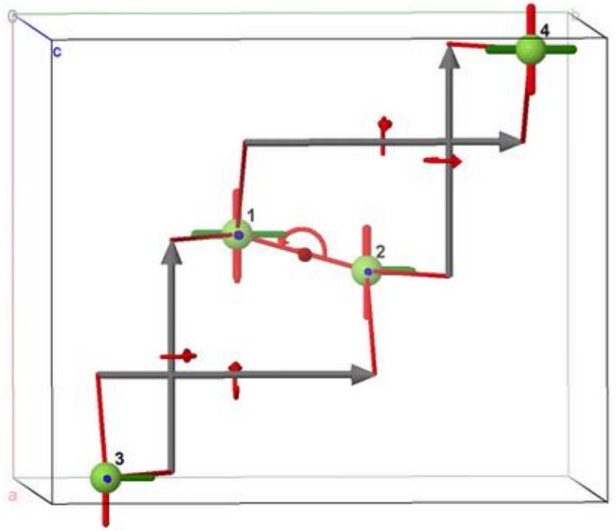
Using Jmol to engage students and teach crystallography and crystallographic symmetry

Dean Johnston[1], Robert Hanson[2]

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





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