phases mésomorphes, où les chaînes paraffiniques sont fondues et les groupes polaires ionisés, et le 'coagel', où la cristallisation des chaînes l'emporte sur l'ionisation des groupes polaires, entraînant l'insolubilité du savon dans l'eau et l'apparition d'une démixtion.

En examinant plus à fond les résultats obtenus, on s'apperçoit cependant qu'en ajoutant au stéarate de potassium de l'octadécanol, non seulement on obtient du 'gel', mais que la stabilité de ce dernier s'en trouve accrue; il suffit, pour s'en convaincre, de comparer l'étendue du domaine d'existence du 'gel' dans le stéarate de potassium pur (de +30 à +46 °C; *cf.* I) à celle dans le mélange équimoléculaire stéarate de potassium–octadécanol (de −12 à +80 °C). Une question se pose alors, c'est de savoir comment évolue l'étendue du domaine d'existence du 'gel' en fonction de la quantité d'alcool gras présent dans le système et s'il est possible de tirer profit de ce phénomène pour faire apparaître du 'gel' dans un savon qui normalement n'en fournit pas (savon de sodium ou de lithium).

Ce travail a bénéficié d'une subvention de la Société Colgate–Palmolive, France; nous tenons à exprimer nos remerciements à ses directeurs, et notamment à Monsieur J. Bergeron qui a suivi cette étude avec le plus vif intérêt.

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Parameter Interactions and the Ferroelectric Mechanism in Guanidinium Aluminum Sulfate Hexahydrate

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A detailed examination of the large correlation coefficients between parameters in the attempted full-matrix least-squares refinement of the ferroelectric guanidinium aluminum sulfate hexahydrate (GASH) shows that they arise from three factors: (1) the polar nature of the space group $P31m$, (2) the non-orthogonality of the a and b axes, and (3) the presence of a pseudo-center of symmetry at $\frac{5}{6}$, $\frac{1}{6}$, 0·54. Reversal of the direction of polarization of a crystal of GASH can be accomplished by displacement of all atoms except those of one guanidinium ion by a mean distance of about 0·15 Å and rotation of the one guanidinium ion through 60° about the carbon atom and in its own plane.

Introduction

Geller & Katz (1962) have recently reported an attempt to refine the crystal structure of the ferroelectric substance guanidinium aluminum sulfate hexahydrate (GASH), $[C(NH_2)_3]Al(SO_4)_2 . 6H_2O$, by three-dimensional least-squares methods, using intensity data obtained with the Bond–Benedict single-crystal automatic diffractometer (Bond, 1955; Benedict, 1955). The structure contains 3 formula units in a cell of dimensions $a = 11{\cdot}75$, $c = 8{\cdot}94$ Å, space group $P31m$. They encountered three primary difficulties: (*a*) severe oscillations of some parameters occurred; (*b*) many negative temperature factors appeared; and (*c*) several improbable interatomic distances were obtained. Geller & Katz attribute these difficulties to the existence of strong interactions between many of their parameters and demonstrate this by the large values of many of the correlation coefficients. Geller (1961), in an important earlier paper, has pointed out the general importance of the correlation coefficients.

Geller & Katz (1962) have given no explanation of the source of the parameter interaction other than the statement in their summary that 'the numerous high correlations of pairs of parameters, apparently linked with the nature of the structure, appear to be a primary cause of prevention of convergence'. Geller, in a footnote of his 1961 paper and in unpublished comments, has stated his belief that the interactions are caused by the fact that the structure is nearly triply primitive, as pointed out by Geller & Booth (1959).

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It is the purpose of this paper to point out that a careful examination of the pattern of occurrence of large correlation coefficients leads to a fairly detailed understanding of the source (a pseudocentering and not the triply primitive character) of the large correlation coefficients and to the suggestion of a possible mechanism of the ferroelectric reversal in GASH.

Calculations

Although Geller & Katz (1962) collected intensity data from two cylindrical crystals, one aligned along [001] and the other along (201], so that the observed structure factors were initially placed on a common scale, separate scale factors were used for the levels with $l=0$ through 6 and one additional scale factor for all levels from $l=7$ through 11. These eight scale factors were allowed to vary in the least-squares refinement along with the anisotropic thermal parameters. In their final cycle 5′*d*, twenty-one of the correlation coefficients having values above 0·4 involved these scale factors. Furthermore, Geller & Katz did not include as variables the thermal parameters, β_{11}, for atoms C(1) and Al(1). We have carried out an independent attempt to refine GASH by full-matrix least squares. We have used the observed structure factors and initial parameter values of Geller & Katz. We have fixed the scale factors at a set of values obtained from a structure factor calculation. This calculation used a set of positional and thermal parameters which were derived from a series of Fourier syntheses and were very similar to the final values of Geller & Katz. We have included the

Table 2. *Hydrogen coordinates from ΔF synthesis*

		x	*y*	*z*
H(1) on N(1)	G	0·914	0·119	0·510
	L	0·917	0·116	0·503
H(2) on N(2)	G	0·566	0·130	0·560
	L	0·583	0·158	0·550
H(3) on N(2)	G	0·744	0·209	0·560
	L	0·742	0·208	0·550
H(4) on O(8)	G	0·861	0·079	0·852
	L	0·875	0·075	0·833
H(5) on O(7)	G	0·928	0·134	0·156
	L	0·942	0·142	0·167
H(6) on O(9)	G	0·743	0·200	0·876
	L	0·720	0·180	0·889
H(7) on O(9)	G	0·600	0·126	0·889
	L	0·592	0·142	0·900
H(8) on O(10)	G	0·808	0·260	0·205
	L	0·800	0·275	0·238
H(9) on O(10)	G	0·876	0·412	0·219
	L	0·883	0·392	0·200

G = Geller & Katz.
L = Present structure.

Table 1. *Final parameters*

Atom		*x*	*y*	*z*	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
N(2)	G	5570	3415	5559	01118	01386	02108	00959	−00047	−00217
	L	5574	3422	5538	00775	01261	01628	00779	00148	00098
O(5)	G	8799	2218	7957	00300	00507	02388	00033	00217	−00045
	L	8813	2241	7988	00232	00189	01853	−00059	00284	00055
O(6)	G	7928	1143	2385	00692	00238	02399	00365	00083	00069
	L	7918	1151	2412	00344	00182	01860	00218	−00186	−00176
O(9)	G	5298	3255	9371	00357	00070	01697	00089	00017	00193
	L	5312	3268	9436	00291	00102	01105	00102	−00021	00105
O(10)	G	5374	2005	1735	00383	00274	01668	00194	00176	00225
	L	5344	1962	1770	00398	00249	01498	00089	00089	00132
N(1)	G	1172	0	5057	00600	$2\beta_{12}$	01008	00500	−00453	0
	L	1159	0	5056	00164		01599	00238	−00236	
O(8)	G	8652	0	8813	00400		01251	00300	−00487	
	L	8701	0	8835	00263		01070	00023	−00307	
O(7)	G	1333	0	1123	00459		00457	00414	−00608	
	L	1347	0	1178	00169		01082	00194	−00164	
O(4)	G	7057	0	4723	00792		00919	00788	00155	
	L	7039	0	4760	00432		00833	00451	00049	
O(3)	G	3741	0	6026	01052		01374	00862	00653	
	L	3724	0	6048	00741		01241	00971	00608	
O(2)	G	5598	0	2821	00200		00976	−00144	−00003	
	L	5576	0	2835	00108		01751	00037	00095	
O(1)	G	4581	0	8331	00283		01021	00377	00134	
	L	4565	0	8375	00245		01655	00090	−00391	
S(1)	G	3477	0	7586	00174		00684	00158	−00229	
	L	3473	0	7586	00104		00804	00054	−00074	
S(2)	G	6813	0	3156	00223		00871	00209	−00142	
	L	6816	0	3153	00141		00843	00119	−00078	
C(2)	G	3333	6667	5500	00371	β_{11}	00672	$\frac{1}{2}\beta_{11}$	0	
	L	3333	6667	5500	00222		00749			
Al(2)	G	3333	6667	0573	00089		01072			
	L	3333	6667	0573	00107		01085			
C(1)	G	0	0	5000	—		01027			
	L	0	0	5032	00228		01240			
Al(1)	G	0	0	0000	—		00630			
	L	0	0	0000	00044		00551			

G = Geller & Katz. L = Present structure.

β_{11} of C(1) and Al(1) as variables. We have chosen the asymmetric set differently from Geller & Katz in order to facilitate interpretation of a difference Fourier synthesis used to determine positions of hydrogen atoms. We have applied a damping factor of $\frac{1}{3}$ to all parameter shifts in order to prevent oscillation. A series of 15 cycles reduced R from 0·31 to 0·08 and gave 'final' parameters which did not differ significantly from those of Geller & Katz, thus fully corroborating their results. Tables 1 and 2 list our 'final' parameters and those of Geller & Katz (indicated by them as input for their cycle 5′, transformed to correspond to our choice of asymmetric unit). Our mean estimated standard deviations are: for x and y of C, N, O, $\sigma=0·0019$; for x of S, $\sigma=0·0006$; for z of C, N, O, $\sigma=0·0042$; for z of S, Al, $\sigma=0·0021$; for β_{ij} of C, N, O, $\sigma=0·00207$; for β_{ij} of S, Al, $\sigma=0·00076$.

Correlation coefficients

During our final cycle of least-squares calculations, we calculated the correlation coefficients, using the program patch written by D. C. Leagus and B. B. Cetlin and obtained from Geller.

All correlation coefficients having values greater than 0·40 are listed in Tables 3–5. All of these may be described in terms of three types. In Table 3 we find a large number of large correlation coefficients between z parameters of otherwise unrelated (see below) atoms. Two-thirds of these are between sulfur atoms and other atoms. The mean value of these correlation coefficients is 0·48. These, of course, arise from the polar nature of the space group (Templeton, 1960) and are due to the fact that the values of z parameters are only fixed relative to that arbitrarily chosen for Al(1). If the z parameter of all atoms [including Al(1)] were allowed to vary, all z–z correlation coefficients would become 1·0 and the calculation would be indeterminate.

Table 4 lists the set of large intra-atomic correlation coefficients between x and y and between x- and y-associated thermal parameters. All five atoms in general positions show large correlations between x and y, β_{11} and β_{12}, β_{22} and β_{12}, and β_{13} and β_{23}. In addition, four atoms show large correlations between β_{11} and β_{22}. All of these arise from the non-orthogonality of a and b, and will be found in all structures based on non-orthogonal axes (Templeton, 1959). The mean value of these correlation coefficients is 0·60.

Table 4. *Intra-atomic correlation coefficients*, 100 ϱ_{ij}

Atom	xy	$\beta_{11}\beta_{12}$	$\beta_{22}\beta_{12}$	$\beta_{13}\beta_{23}$
N(2)	55	63	70	55
O(5)	60	64	56	57
O(6)	70	74	73	69
O(9)	49	46	61	44
O(10)	63	71	73	62

Additional coefficients are $\beta_{11}\beta_{22}$ for O(10) 42; N(1) 44; O(3) 58; O(4) 53; S(1) 40; S(2) 40 and z β_{13} for O(3) 42.

Table 5 lists the most interesting set of large correlation coefficients. First, this set contains the 12 largest and 24 of the 30 having values greater than 0·7. Second, all of the correlation coefficients in this set are between parameters of atoms whose correlation is readily interpretable in terms of the special nature of the structure of the crystal.

In Table 6 are listed two sets of coordinates. The left-hand set, labelled solution A, contains all atoms in the unit cell as determined from our final cycle 15. The structure is illustrated in Fig. 1. The right-hand set, labelled solution A', has been derived from solution A by inversion through the point $\frac{5}{6}$, $\frac{1}{6}$, 0·53735. It will be noted that, except for atoms N(24)′, N(25)′ and N(26)′ the maximum difference in any fractional coordinate between an atom in solution A' and its counterpart in solution A is 0·046. Furthermore, the mean displacement between atoms in solution A' and their counterparts in solution A is 0·123 Å in x or y and 0·154 Å in z.

All correlation coefficients in Table 5 are between parameters of atoms related by this inversion.

The relationship between coordinates of atoms related by the inversion, or between thermal parameters of related atoms are directly understandable. These make up 64 of the 78 members of this set. The mean value of these 63 is 0·64. We can see no immediate

Table 3. *z–z correlation coefficients*, 100 ϱ_{ij}

O(1)S(2)	O(1)S(2)	O(2)S(1)	O(2)S(2)	O(3)S(1)	O(3)S(2)
43	43	44	42	41	40
O(4)S(1)	O(4)S(2)	O(5)S(1)	O(5)S(2)	O(6)S(1)	O(6)S(2)
49	48	59	57	59	58
O(7)S(1)	O(7)S(2)	O(8)S(1)	O(8)S(2)	O(9)S(1)	O(9)S(2)
53	51	49	49	62	60
O(10)S(1)	O(10)S(2)	N(2)S(1)	N(2)S(2)	C(1)S(1)	C(1)S(2)
58	57	46	45	41	41
C(2)S(1)	C(2)S(2)	O(3)O(7)	O(3)O(9)	O(4)O(7)	O(4)O(9)
40	42	43	45	43	46
O(5)O(8)	O(5)O(9)	O(5)O(10)	O(6)O(9)	O(6)O(10)	O(8)O(9)
40	43	46	47	45	47
O(7)O(10)	O(5)N(2)	O(8)N(2)	O(9)N(2)	O(10)N(2)	
41	40	40	44	48	

specific explanation for the other 14, which are correlations between coordinate and thermal parameters. The mean value of these 14 is 0·51.

It will be noted that there are a number of differences between the correlation coefficients listed in Tables 3, 4, and 5 and those in Table X of Geller & Katz. There are several reasons for these differences:

1. Although the order of magnitude of any particular correlation coefficient is determined by the structural model, as pointed out by Geller, small changes in the parameters can cause changes of several tenths in the correlation coefficients. For example, in a related refinement which we have carried out using different data, the *z–z* correlation coefficient between atoms

Table 5. *Correlation coefficients* (100 ϱ_{ij}) *between parameters of inversion-related atoms*

Atoms										
O(3)–O(4)	xx	zz	$\beta_{13}\beta_{13}$	$\beta_{33}\beta_{33}$	$x\beta_{22}$	$\beta_{22}x$	$\beta_{11}x$	$\beta_{33}x$	$z\beta_{13}$	$\beta_{13}z$
	57	82	53	64	57	58	41	64	42	47
O(1)–(O6)	xx	xy	zz	$\beta_{11}\beta_{11}$	$\beta_{11}\beta_{22}$	$\beta_{11}\beta_{12}$	$\beta_{33}\beta_{33}$	$\beta_{13}\beta_{13}$	$\beta_{13}\beta_{23}$	
	73	74	82	57	54	69	76	63	59	
O(2)–O(5)	xx	xy	zz	$\beta_{11}\beta_{11}$	$\beta_{11}\beta_{22}$	$\beta_{11}\beta_{12}$	$\beta_{33}\beta_{33}$	$\beta_{13}\beta_{13}$	$\beta_{13}\beta_{23}$	
	69	75	81	48	56	72	73	63	69	
O(5)–O(6)	xx	yy	zz	$\beta_{11}\beta_{11}$	$\beta_{22}\beta_{22}$	$\beta_{11}\beta_{12}$	$\beta_{12}\beta_{12}$	$z\beta_{33}$	$\beta_{33}z$	
	56	60	49	57	51	40	51	41	41	
O(8)–O(10)	xx	xy	zz	$\beta_{11}\beta_{11}$	$\beta_{11}\beta_{22}$	$\beta_{11}\beta_{12}$	$\beta_{33}\beta_{33}$	$\beta_{13}\beta_{13}$	$\beta_{12}\beta_{23}$	
	70	70	87	63	59	74	76	62	64	
S(1)–S(2)	xx	zz	$\beta_{11}\beta_{22}$	$\beta_{22}\beta_{11}$	$\beta_{13}\beta_{13}$	$\beta_{33}\beta_{33}$	$x\beta_{11}$	$x\beta_{22}$	$\beta_{22}x$	
	68	97	56	42	70	83	45	47	52	
O(7)–O(9)	xx	zz	$\beta_{11}\beta_{11}$	$\beta_{22}\beta_{22}$	$\beta_{33}\beta_{33}$	$\beta_{13}\beta_{13}$				
	71	86	62	61	75	69				
N(1)–N(2)	xx	zz	$\beta_{11}\beta_{11}$	$\beta_{22}\beta_{22}$	$\beta_{33}\beta_{33}$	$\beta_{13}\beta_{13}$				
	57	78	44	53	63	53				
Al(1)–Al(2)			$\beta_{33}\beta_{33}$	$\beta_{11}\beta_{11}$	$\beta_{33}z$					
			68	73	52					
C(1)–C(2)	zz		$\beta_{11}\beta_{11}$	$\beta_{33}\beta_{33}$	$\beta_{33}z$					
	73		68	58	58					
O(9)–O(10)	xy	zz	$\beta_{11}\beta_{22}$							
	48	58	45							
Al(2)–Al(2)			$\beta_{33}z$							
			70							

Table 6. *Atoms related by inversion through* ($\frac{5}{6}$, $\frac{1}{6}$, 0·5 3735)

Solution *A*				Solution *A′*				Solution *A*				Solution *A′*			
Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
N(21)	5574	3422	5538	N(11)′	5507	3333	5691	O(53)	3428	1187		O(63)′	3434	1252	
N(22)	6578	2152		N(12)′	6667	2174		O(54)	2241	8813		O(23)′	2242	8909	7912
N(23)	7848	4426		N(13)′	7826	4493		O(55)	6572	7759		O(22)′	6667	7758	
N(24)	3422	5574		N(25)′	4514	6755	5209	O(56)	1187	3428		O(21)′	1091	3333	
N(25)	2152	6578		N(26)′	2241	5486		O(61)	7918	1151	2412	O(51)′	7853	1093	2758
N(26)	4426	7848		N(24)′	3245	7759		O(62)	8849	6767		O(52)′	8907	6760	
N(11)	1159	0000	5056	N(21)′	1093	−0089		O(63)	3233	2082		O(53)′	3240	2147	
N(12)	0000	1159		N(22)′	0089	1181		O(64)	1151	7918		O(13)′	1232	7899	2372
N(13)	8841	8841		N(23)′	8819	8907		O(65)	6767	8849		O(12)′	6667	8768	
C(11)	0000	0000	5032	C(22)′	0000	0000	5247	O(66)	2082	3233		O(11′)	2101	3333	
C(21)	3333	6667	5500	C(21)′	3333	6667		O(71)	1347	0000	1178	O(91)′	1355	0066	1311
C(22)	6667	3333		C(11)′	6667	3333	5715	O(72)	0000	1347		O(92)′	−0066	1289	
Al(11)	0000	0000	0000	Al(22)′	0000	0000	0174	O(73)	8653	8653		O(93)′	8711	8645	
Al(21)	3333	6667	0573	Al(21)′	3333	6667		O(101)	5344	1962	1770	O(83)′	5368	2034	1912
Al(22)	6667	3333		Al(11)′	6667	3333	0747	O(102)	8038	3382		O(81)′	7966	3333	
S(11)	3473	0000	7586	S(23)′	3483	0149	7593	O(103)	6618	4656		O(82)′	6667	4632	
S(12)	0000	3473		S(21)′	−0149	3333		O(104)	1962	5344		O(96)′	1979	5378	1311
S(13)	6527	6527		S(22)′	6667	6517		O(105)	3382	8038		O(94)′	3399	8021	
S(21)	6816	0000	3153	S(12)′	6667	−0140	3161	O(106)	4656	6618		O(95)′	4622	6601	
S(22)	0000	6816		S(13)′	0140	6807		O(91)	5312	3268	9436	O(71)′	5319	3333	9568
S(23)	3184	3184		S(11)′	3193	3333		O(92)	6732	2044		O(72)′	6667	1986	
O(31)	3724	0000	6048	O(43)′	3706	0373	5987	O(93)	7956	4688		O(73)′	8014	4681	
O(32)	0000	3724		O(41)′	−0373	3333		O(94)	3268	5312		O(105)′	3284	5295	8977
O(33)	6276	6276		O(42)′	6667	6294		O(95)	2044	6732		O(106)′	2011	6716	
O(41)	7039	0000	4760	O(32)′	6667	−0391	4699	O(96)	4688	7956		O(104)′	4705	7989	
O(42)	0000	7039		O(33)′	0391	7058		O(21)	5576	0000	2835	O(56)′	5480	−0094	2759
O(43)	2961	2961		O(31)′	2942	3333		O(22)	0000	5576		O(55)′	0094	5574	
O(11)	4565	0000	8376	O(66)′	4585	0101	8335	O(23)	4424	4424		O(54)′	4426	4519	
O(12)	0000	4565		O(65)′	−0101	4484		O(81)	8701	0000	8835	O(102)′	8629	−0049	8977
O(13)	5435	5435		O(64)′	5516	5415		O(82)	0000	8701		O(103)′	0049	8678	
O(51)	8813	2241	7988	O(61)′	8748	2182		O(83)	1299	1299		O(101)′	1322	1371	
O(52)	7759	6572		O(62)′	7818	6566									

O(2) and O(5) changed from 0·60 to 0·77 in successive cycles.

2. The transformation from one choice of asymmetric unit to another changes the particular parameters which interact, *e.g.* our x of N(2) corresponds to the $x-y$ of N(2) of Geller & Katz.

3. Because of the interaction between group scale factors and anisotropic thermal parameters, we did not allow the scale factors to vary during our least-squares cycles. Geller & Katz reduced the interaction by forcing the scale factors from $l=7$ through $l=11$ to remain equal to one another, but allowed all others to vary. Thus in cycle $5'd$ they found 12 interactions between scale factors and 9 interactions between scale factors and thermal parameters, with values above 0·4.

The structural source of the difficulties in the refinement of GASH now seems clear. Solutions A and A' represent two equally satisfactory solutions to the structure determination problem, since they give exactly the same calculated intensities, their structure factors differing only in phase. For all atoms in the unit cell except three nitrogen atoms, the difference in position between the two solutions is small compared with the radii of the atoms. This leads to difficulty in distinguishing between the solutions and exhibits itself in the large values of the correlation coefficients.

The ferroelectric structure of GASH

Solutions A and A' correspond to polarization of GASH in opposite directions. The small shifts in atomic positions required to transform one structure into the other suggest the reason for the appearance of ferroelectric behavior. Thus to reverse the direction of polarization in a crystal of GASH it is only necessary to displace all atoms except those of one guanidinium ion by a mean distance of about 0·15 Å, and to rotate the one guanidinium ion through an angle of 60° about the carbon atom and in its own plane, since this set of displacements is exactly equivalent to an inversion of the structure through the point $\frac{5}{6}$, $\frac{1}{6}$, 0·54.

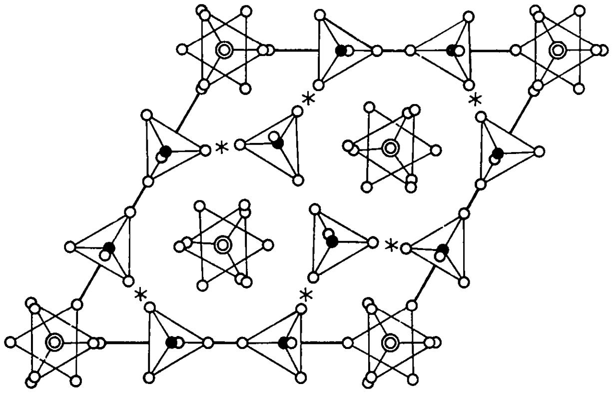
Fig. 1. Projection of the structure on (001). The inversion points relating the two solutions are indicated by*.

It should be further noted that there exists another point (at $\frac{1}{2}$, 0, 0·54) which is nearly a center of symmetry. Inversion through this point, to give another possible solution, is equivalent to another set of small atomic displacements with mean displacement about double that for the point $\frac{5}{6}$, $\frac{1}{6}$, 0·54 and involving rotation of all three of the guanidinium ions. Combination of these two inversions produces the translational effect pointed out by Geller & Booth (1959), *i.e.* the cell tends to be triply primitive.

The fact that it is the pseudo-center at $\frac{5}{6}$, $\frac{1}{6}$, 0·54 which is most important in causing the large correlation coefficients, rather than that at $\frac{1}{2}$, 0, 0·54 or the pseudo-triply primitive character of the structure is emphasized by the following observations. The pseudo-center at $\frac{5}{6}$, $\frac{1}{6}$, 0·54 predicts direct one-to-one correlation between 72 pairs of parameters and the corresponding 72 correlation coefficients have a mean value of 0·55. The pseudo-center at $\frac{1}{2}$, 0, 0·54 predicts 38 and the mean value is 0·28. The pseudo-triply primitive character predicts 46 and the mean value is 0·31. Or, if we consider only the direct one-to-one interactions predicted by one mechanism and not by the other two, we find 33 with an average value of 0·62 for the pseudo-center at $\frac{5}{6}$, $\frac{1}{6}$, 0·54, 10 with an average value of 0·09 for the pseudo-center at $\frac{1}{2}$, 0, 0·54, and 33 with an average value of 0·21 for the pseudo-triply primitive character.

We plan to study polarized crystals of an isomorph of GASH, such as the chromium compound, making use of the anomalous dispersion effect to investigate the relation between the direction of polarization and the details of the structure.

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