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1 **Comment on "An experimental study of symmetry lowering of analcime"**

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Comment on "An experimental study of symmetry lowering of analcime"

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Abstract. In a recent article (Sugano and Kyono, 2018), analcime hydrothermally synthesized from a gel and then reheated was reported to have undergone a loss of symmetry to *Ibca*. We show that the reheated samples, reported as different, are identical to each other and actually tetragonal. The fact that the tetragonal axis was oriented along the **a** or **b** vector in the two reheated samples instead of the **c** vector as in the conventional setting seems to have been the cause of the misinterpretation of the diffraction pattern.

Introduction

The symmetry of a crystal structure is expressed through its space group, which can be described in a variety of settings. The most convenient setting is called standard: in this setting, the symmetry operations are represented by unimodular matrices and particularly simple to read off. A number of alternative settings are also in use, which are called *unconventional* or *non-standard*, depending on whether or not the metric of the alternative unit cell still corresponds to the same crystal family. These alternative settings are useful in diverse cases, like the study of the phase transitions and derivative structures, the analysis of twinned crystals, or in presence of a high degree of pseudo-symmetry (Nespolo and Aroyo, 2016). In some cases, standard and alternative settings differ just by a permutation of the axes, and one orientation is taken as standard by convention. This is typically the case of crystals with a unique axis (monoclinic, tetragonal, trigonal and hexagonal), for which the orientation of the unique axis can actually be along any of the basis vectors, but one of them has been taken as standard by convention. When experimental data of a crystal with a unique axis are expressed in a setting in which this axis is not along the standard direction, the transformation to the standard setting is just a matter of permutation of the basis vectors, and of the corresponding coordinates. Unfortunately, sometimes the unusual orientation of the unique axis may escape to the investigators, who may then be trapped in the search for a subgroup, whereas their structure is actually more symmetric. This is what happened in the experimental investigation of analcime in a recent article by Sugano and Kyono (2018).

Analcime hydrothermally synthesized from a gel at 200°C for 24 hours was reported in the usual space group $Ia\bar{3}d$. Two samples were then reheated for 24 and 48 hours respectively, and reported to have undergone a loss of symmetry to *Ibca*, following the Si/Al ordering but without changes in the extra framework site occupancy, where Na is hosted. Unfortunately, the authors have overestimated the loss of symmetry; not only the two reheated samples are practically identical to each other, but they are actually tetragonal, with space group $I4_1/acd$. Both samples have cell parameters indicative of a tetragonal lattice, although with a non-standard orientation. For the sample 24h, reported cell parameters are $a = 13.727(2) \text{ \AA}$, $b = c = 13.707(2) \text{ \AA}$, with a fourfold axis for the lattice along the **a** basis vector. For the sample 48h, reported cell parameters are $a = 13.705(2) \text{ \AA}$, $b = 13.717(2) \text{ \AA}$, $c = 13.705(6) \text{ \AA}$, with a fourfold axis for the lattice along the **b** basis vector (the difference between the a and c cell parameters, within one standard uncertainty, is not statistically significant); moreover, the cell parameters of the 48h sample actually fell within the cubic limits for three standard uncertainties: 13.699 - 13.711 Å for a , 13.711 - 13.723 Å for b , 13.700 - 13.712 Å for c . A metric specialisation (symmetry of the lattice higher than the symmetry of the structure) is far from being a rare phenomenon (Janner, 2004a,b), but should nevertheless prompt the investigators to check their model for any possible overlooked symmetry. The fact that refinement converges in *Ibca* does not exclude that the real symmetry of the structure be $I4_1/acd$; indeed, the reported structural models are actually compatible with the $I4_1/acd$ symmetry within two standard uncertainties and the structure

56 factors calculated from the published model also agree with the higher symmetry. The results shown
57 below have been obtained with the Bilbao Crystallographic Server (Aroyo et al. 2006).

58 **Test for higher symmetry in direct space**

59 The structural models 24h and 48h published in Table 3 of Suygano and Kyono (2018) have been
60 checked for pseudosymmetry in the minimal *translationengleiche* supergroup $I4_1/acd$. The
61 transformations from the published settings of 24h and from 48h to $I4_1/acd$ are **abc** → **bca** and **abc**
62 → **cab** respectively. Tables S1 and S2 give, for the two structures, the original fractional atomic
63 coordinates, the idealized fractional coordinates in $I4_1/acd$ expressed in the subgroup setting, the
64 corresponding shifts u_x , u_y , u_z , and the ratio u/σ of these shifts with respect to the published standard
65 uncertainties. All ratios are smaller than 3 (in most cases even smaller than 2), showing that the
66 published structures are actually compatible with $I4_1/acd$ within three standard uncertainties. Table
67 S3 gives the structural model expressed in $I4_1/acd$. The very close result suggests that the two
68 structural models reported in the original publication are actually practically the same, just
69 expressed in a different axial setting. The larger difference in the cell parameters is between a of the
70 24h sample and the b of the 48h sample, *i.e.* the tetragonal axis that has been missed by the authors.
71 The difference is 0.0010 Å, again within three standard uncertainties, which are 0.0002 Å for both
72 models (13.721-13.733 Å vs. 13.711-13.723 Å). The fractional atomic coordinates are practically
73 identical, once expressed in the same reference. The space group of both models has affine
74 normalizer $Pm\bar{3}n$ ($1/2\mathbf{a}$, $1/2\mathbf{b}$, $1/2\mathbf{c}$)¹; if we apply to the fractional atomic coordinates of the 48h
75 model a three-fold rotation of the normalizer we obtain an alternative description of the model,
76 which is identical to the 24 model within two standard uncertainties (Table S4).
77 Even the tetragonal structural model is actually very strongly pseudosymmetric with respect to
78 $Ia\bar{3}d$. If we neglect the small difference in cell parameters of the tetragonal structure (for the 48
79 sample, the cell is actually cubic within three standard uncertainties, as shown in the previous
80 section), we can apply the same pseudosymmetry test, this time towards $Ia\bar{3}d$. The result for the 48h
81 sample is shown in Table S5, where we see that fractional atomic coordinates do fit the cubic
82 supergroup within two standard uncertainties. The reported structures are therefore tetragonal,
83 strongly pseudo-cubic.

84 **Test for higher symmetry in reciprocal space**

85 In discussing the diffraction pattern of both reheated samples, the authors state that “weak
86 reflections of type $00l$ with $l = 2n$ became observed, which correspond to the reflection conditions
87 of orthorhombic $Ibca$ ”. As we have seen, the reheated samples have the 4_1 axis along the \mathbf{a} vector
88 (24h sample) or the \mathbf{b} vector (48h sample), so that nobody could expect any influence on the $00l$
89 reflections. The statement above is therefore incorrect.
90 We have simulated the single-crystal X-ray diffraction pattern from the published cell parameters,
91 fractional atomic coordinates and atomic distribution on both samples with the software package
92 Jana2006 (Petricek et al. 2014). The computed diffraction patterns do not show any violation of
93 reflection conditions of $I4_1/acd$. We have also performed a space group test on the reflection files
94 computed in $Ibca$ and the result confirms the higher symmetry $I4_1/acd$ (see the deposited
95 supplementary material). No indication of $Ia\bar{3}d$ was however obtained.

1 The operations of a normalizer map different but equivalent descriptions of a crystal structure. In this case, because of the different orientation of the tetragonal axis in the 24h and 48h samples, we need to consider the affine normalizer, not just the Euclidean one. Details about the normalizers of space groups can be found in Koch and Fischer (2006) and a recent discussion in Nespolo (2015).

96 Discussion

97 The structure models of the analcime reheated samples as published by Sugano and Kyono (2018)
98 are actually more symmetric than what the authors stated. Both the fractional atomic coordinates
99 and the calculated diffraction pattern from the published structures perfectly fit $I4_1/acd$, a
100 translationengleiche supergroup of the $Ibca$ group reported in the article. The overlook was
101 probably originated by the orientation of the unique axis along the **a** or **b** basis vector, instead than
102 the conventional orientation along the **c** basis vector. As a consequence, the conclusions about the
103 Si/Al ordered distribution have to be reconsidered. In fact, the model proposed by Sugano and
104 Kyono (2018) shows a significant difference between the sites T11 and T12, whereas T12 and T2
105 would have almost the same Si/Al ratio. In the $I4_1/acd$ model, T11 and T2 merge into a single site
106 (32g) whereas T12 remains independent (16f) and this invalidates the Si/Al ordering scheme
107 presented.

108 The presence of twin domains is extremely probable because of the pronounced cubic pseudo-
109 symmetry of tetragonal analcime. As pointed out by Mazzi and Galli (1978), if the size of these
110 domains is small enough to simulate diffraction from a single crystal, then, depending on the
111 relative proportions of the twin domain states, both the apparent symmetry and the apparent
112 ordering of the sample may be affected. In the case of the samples studied Sugano and Kyono
113 (2018) the symmetry was clearly tetragonal. No conclusions can however be drawn about the
114 possible Si/Al distribution without a careful reinvestigation of the experimental data.

115 After reading the demonstration above, the authors have performed another structure refinement on
116 an analcime sample reheated for 24 hours and again persisted with orthorhombic symmetry, $Ibca$. I
117 have analysed these new data and I show the results in Table S6. Once again, the results confirm
118 that the sample is tetragonal, $I4_1/acd$, within three standard uncertainties. The authors use reflections
119 002 , $00\bar{1}0$ and 442 as “proof” of an alleged violation of systematic absences for $I4_1/acd$. As detailed
120 in the are evidently unaware that they have collected data in an unconventional setting of the space
121 group, with the tetragonal axis along **a** instead than along **c**. When the diffraction pattern is re-
122 indexed in the standard (*c*-unique) setting, these reflections become 020 , $0\bar{1}00$ and 424 , showing no
123 violation of systematic absences for $I4_1/acd$. Their sample is therefore definitely tetragonal and the
124 discussion about Si/Al ordering is based on a misinterpretation of the diffraction pattern.

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Table S1. Fractional atomic coordinates of the sample 24h in the setting of *Ibca*, as published (in parentheses the standard uncertainty σ) and idealized to fit the *I4₁/acd* symmetry. u is the absolute value of the shift between the published and idealized coordinates, u/σ is the ratio between this shift and the standard uncertainty of the corresponding coordinate. This ratio shows that the two models are identical within three standard uncertainties.

Site	Wyckoff position	Structural model in <i>Ibca</i>			Idealized structure in <i>I4₁/acd</i>			u_x	u_y	u_z	u_x/σ_x	u_y/σ_y	u_z/σ_z
		x	y	z	x	y	z						
T11	16f	0.12507(4)	0.16228(3)	0.41224(3)	0.12500	0.16230	0.41230	0.00007	0.00002	0.00006	1.75	0.67	2.00
T12	16f	0.41228(3)	0.12497(4)	0.16222(3)	0.41230	0.12500	0.16220	0.00002	0.00003	0.00002	0.67	0.75	0.67
T2	16f	0.16222(3)	0.41225(3)	0.12500(4)	0.16230	0.41220	0.12500	0.00008	0.00005	0.00000	2.67	1.67	0.00000
Na11	8c	0.12520(19)	0	0.25	0.12500	0	0.25	0.00020	0	0	1.05	--	--
Na12	8d	0.25	0.12492(18)	0	0.25000	0.12490	0.00000	0	0.00002	0	--	0.11	--
Na2	8e	0	0.25	0.12504(19)	0	0.25	0.12510	0	0	0.00006	--	0	0.32
O11	16f	0.10456(12)	0.36608(12)	0.21960(10)	0.10450	0.36600	0.21960	0.00006	0.00008	0.00000	0.50	0.67	0.00000
O12	16f	0.38389(12)	0.14538(12)	0.46953(10)	0.38400	0.14550	0.46950	0.00011	0.00012	0.00003	0.92	1.00	0.30
O21	16f	0.21966(11)	0.10453(12)	0.36596(12)	0.21950	0.10450	0.36590	0.00016	0.00003	0.00006	1.45	0.25	0.50
O22	16f	0.14549(12)	0.46954(11)	0.38404(12)	0.14550	0.46960	0.38400	0.00001	0.00006	0.00004	0.08	0.55	0.33
O31	16f	0.36591(12)	0.21948(11)	0.10445(12)	0.36600	0.21950	0.10450	0.00009	0.00002	0.00005	0.75	0.18	0.42
O32	16f	0.46938(11)	0.38411(12)	0.14547(12)	0.46950	0.38410	0.14550	0.00012	0.00001	0.00003	1.09	0.08	0.25
W	16f	0.1252(2)	0.1249(2)	0.1251(3)	0.1250	0.1249	0.1251	0.0002	0	0	1.00	0	0

Table S2. Fractional atomic coordinates of the sample 48h in the setting of $Ibca$, as published and idealized to fit the $I4_1/acd$ symmetry. Same conventions and in Table 1. The two models are identical within two standard uncertainties.

Site	Wyckoff position	Structural model in $Ibca$			Idealized structure in $I4_1/acd$			u_x	u_y/σ_y	u_z	u_z/σ_z	
		x	y	z	x	y	z					
T11	16f	0.12498(3)	0.16223(3)	0.41224(3)	0.12500	0.16220	0.41220	0.00002	0.00003	1.00	0.00004	1.33
T12	16f	0.41224(3)	0.12505(3)	0.16226(3)	0.41230	0.12500	0.16220	0.00006	0.00005	1.67	0.00006	2.00
T2	16f	0.16225(3)	0.41224(3)	0.12501(3)	0.16220	0.41220	0.12500	0.00005	0.00004	1.33	0.00001	0.33
Na11	8c	0.12486(17)	0	0.25	0.12490	0	0.25	0.00004	0		0	0.00
Na12	8d	0.25	0.12516(17)	0	0.25	0.12500	0	0	0.00016	0.94	0	
Na2	8e	0	0.25	0.12512(17)	0	0.25	0.1251	0	0	0.00	0.00002	0.12
O11	16f	0.10450(11)	0.36577(12)	0.21947(10)	0.10450	0.36590	0.21950	0.00000	0.00013	1.08	0.00003	0.30
O12	16f	0.38419(12)	0.14557(11)	0.46950(10)	0.38420	0.14550	0.46950	0.00001	0.00007	0.64	0.00000	0.00
O21	16f	0.21946(10)	0.10455(12)	0.36571(12)	0.21950	0.10450	0.36580	0.00004	0.00005	0.42	0.00009	0.75
O22	16f	0.14539(12)	0.46948(10)	0.38407(12)	0.14540	0.46950	0.38410	0.00001	0.00002	0.20	0.00003	0.25
O31	16f	0.36590(12)	0.21952(10)	0.10453(11)	0.36590	0.21950	0.10460	0.00000	0.00002	0.20	0.00007	0.64
O32	16f	0.46952(10)	0.38396(12)	0.14549(11)	0.46950	0.38410	0.14550	0.00002	0.00014	1.17	0.00001	0.09
W	16f	0.1250(2)	0.1254(2)	0.1251(2)	0.1250	0.1250	0.1250	0	0.0004	2.00	0.0001	0.50

Table S3. Fractional atomic coordinates of the two reheated samples expressed in the $I4_1/acd$ translationengleiche supergroup of $Ibca$. Cell parameters are $a = 13.707(2)$, $c = 13.727(2)$, and $a = 13.705(2)$, $c = 13.717(2)$ respectively.

Site	Wyckoff position	Structural model 24h			Structural model 48h		
		x	y	z	x	y	z
T1	16f	0.16226	0.41226	0.125	0.16225	0.412250	0.125
T2	32g	0.12499	0.16224	0.41225	0.12502	0.16224	0.41223
Na1	8b	0.	0.25	0.125	0	0.25	0.125
Na2	16e	0.12494	0	0.25	0.12512	0	0.25
O1	32g	0.36602	0.21957	0.10454	0.36576	0.21948	0.10449
O2	32g	0.14547	0.46951	0.38399	0.14549	0.46949	0.38410
O3	32g	0.10453	0.36593	0.21952	0.10457	0.36591	0.21950
W	16f	0.1249	0.1251	0.125	0.1251	0.1250	0.125

Table S4. Fractional atomic coordinates of the two reheated samples in the setting of the sample 24h. Same conventions as in Table 1. The values u/σ are reported with respect to both samples when the σ differs. The two models are identical within two standard uncertainties.

Site	Structural model 24h			Structural model 48h in the setting of 24h			u_x	u_y/σ_x	u_y	u_y/σ_y	u_z	u_z/σ_z	
	x	y	z	Site	x	y							z
T11	0.12507(4)	0.16228(3)	0.41224(3)	T2	0.12501(3)	0.16225(3)	0.41224(3)	0.00006	1.50/2.00	0.00003	1.00	0	0.00
T12	0.41228(3)	0.12497(4)	0.16222(3)	T11	0.41224(3)	0.12498(3)	0.16223(3)	0.00004	1.33	0.00001	0.25/0.33	0.00001	0.33
T2	0.16222(3)	0.41225(3)	0.12500(4)	T12	0.16226(3)	0.41224(3)	0.12505(3)	0.00004	1.33	0.00001	0.33	0.00005	1.25/1.67
Na11	0.12520(19)	0	0.25	Na2	0.12512(17)	0	0.25	0.00008	0.42/0.47	0	--	0	--
Na12	0.25	0.12492(18)	0	Na11	0.25	0.12486(17)	0	0	--	0.00006	0.33/0.35	0	--
Na2	0	0.25	0.12504(19)	Na12	0	0.25	0.12516(17)	0	--	0	--	0.00012	0.63/0.71
O11	0.10456(12)	0.36608(12)	0.21960(10)	O31	0.10453(11)	0.36590(12)	0.21952(10)	0.00003	0.25/0.27	0.00018	1.50	0.00008	0.80
O12	0.38389(12)	0.14538(12)	0.46953(10)	O22	0.38407(12)	0.14539(12)	0.46948(10)	0.00018	1.50	0.00001	0.08	0.00005	0.50
O21	0.21966(11)	0.10453(12)	0.36596(12)	O11	0.21947(10)	0.10450(11)	0.36577(12)	0.00019	1.73/1.90	0.00003	0.25/0.27	0.00019	1.58
O22	0.14549(12)	0.46954(11)	0.38404(12)	O32	0.14549(11)	0.46952(10)	0.38396(12)	0	0.00	0.00002	0.18/0.20	0.00008	0.67
O31	0.36591(12)	0.21948(11)	0.10445(12)	O21	0.36571(12)	0.21946(10)	0.10455(12)	0.00020	1.67	0.00002	0.18/0.20	0.00010	0.83
O32	0.46938(11)	0.38411(12)	0.14547(12)	O12	0.46950(10)	0.38419(12)	0.14557(11)	0.00012	1.09/1.20	0.00008	0.67	0.00010	0.83/0.91
W	0.1252(2)	0.1249(2)	0.1251(3)	W	0.1251(2)	0.1250(2)	0.1254(2)	0.0001	0.50	0.0001	0.50	0.0003	1.00/1.50

Table S5. Fractional atomic coordinates of the sample 48h in the setting of $Ibca$, as published and idealized to fit the $Ia\bar{3}d$ symmetry. Same conventions and in Table 1. The two models are identical within two standard uncertainties.

Site	Wyckoff position	Structural model in $Ibca$			Idealized structure in $Ia\bar{3}d$			u_x	u_x/σ_x	u_y	u_y/σ_y	u_z	u_z/σ_z
		x	y	z	x	y	z						
T11	16f	0.12498(3)	0.16223(3)	0.41224(3)	0.12500	0.16224	0.41224	0.00002	0.67	0.00001	0.33	0	0
T12	16f	0.41224(3)	0.12505(3)	0.16226(3)	0.41224	0.125	0.16224	0	0	0.00005	1.67	0.00002	0.67
T2	16f	0.16225(3)	0.41224(3)	0.12501(3)	0.16224	0.41224	0.125	0.00001	0.33	0	0	0.00001	0.33
Na11	8c	0.12486(17)	0	0.25	0.12500	0	0.25	0.00014	0.82	0	0	0	0
Na12	8d	0.25	0.12516(17)	0	0.25	0.125	0	0	0	0.00016	0.94	0	0
Na2	8e	0	0.25	0.12512(17)	0	0.25	0.125	0	0	0	0	0.00012	0.71
O11	16f	0.10450(11)	0.36577(12)	0.21947(10)	0.10452	0.36586	0.21949	0.00002	0.18	0.00009	0.75	0.00002	0.20
O12	16f	0.38419(12)	0.14557(11)	0.46950(10)	0.38414	0.14548	0.46949	0.00005	0.42	0.00009	0.81	0.00001	0.10
O21	16f	0.21946(10)	0.10455(12)	0.36571(12)	0.21949	0.10452	0.36586	0.00003	0.30	0.00003	0.25	0.00015	1.25
O22	16f	0.14539(12)	0.46948(10)	0.38407(12)	0.14548	0.46949	0.38414	0.00009	0.75	0.00001	0.10	0.00007	0.58
O31	16f	0.36590(12)	0.21952(10)	0.10453(11)	0.36586	0.21949	0.10452	0.00004	0.33	0.00003	0.30	0.00001	0.09
O32	16f	0.46952(10)	0.38396(12)	0.14549(11)	0.46949	0.38414	0.14548	0.00003	0.30	0.00018	1.5	0.00001	0.09
W	16f	0.1250(2)	0.1254(2)	0.1251(2)	0.125	0.125	0.125	0	0	0.0004	2.0	0.0001	0.50

Table S6. Fractional atomic coordinates of the sample reheated for 24h given in the authors' reply, expressed in the setting of *Ibca*, as published (in parentheses the standard uncertainty σ) and idealized to fit the *I4₁/acd* symmetry. u is the absolute value of the shift between the published and idealized coordinates, u/σ is the ratio between this shift and the standard uncertainty of the corresponding coordinate. This ratio shows that the two models are identical within three standard uncertainties.

Site	Wyckoff position	Structural model in <i>Ibca</i>			Idealized structure in <i>I4₁/acd</i>			u_x	u_x/σ_x	u_y	u_y/σ_y	u_z	u_z/σ_z
		x	y	z	x	y	z						
T11	16f	0.12499	0.16226	0.41226	0.12500	0.16230	0.41230	0.00001	0.50	0.00004	2.00	0.00004	2.00
T12	16f	0.41225	0.12501	0.16226	0.41230	0.12500	0.16220	0.00005	2.50	0.00001	0.50	0.00006	3.00
T2	16f	0.16226	0.41224	0.12500	0.16230	0.41220	0.12500	0.00004	2.00	0.00004	2.00	0.00000	0.00
Na11	8c	0.12498	0	0.25	0.125	0	0.25	0.00002	0.15	---	---	---	---
Na12	8d	0.25	0.12497	0	0.25	0.12490	0	---	---	0.00007	0.54	---	---
Na2	8e	0	0.25	0.12495	0	0.25	0.12510	0.00000	---	0.00000	---	0.00015	---
O11	16f	0.10449	0.36575	0.21943	0.10450	0.3660	0.21960	0.00001	0.12	0.00025	2.78	0.00017	2.43
O12	16f	0.38422	0.14552	0.46942	0.38400	0.1455	0.46950	0.00022	2.44	0.00002	0.25	0.00008	1.14
O21	16f	0.21946	0.10452	0.3657	0.21950	0.1045	0.36590	0.00004	0.57	0.00002	0.25	0.00020	2.50
O22	16f	0.14555	0.46941	0.38408	0.14550	0.4696	0.38400	0.00005	0.62	0.00019	2.71	0.00008	1.00
O31	16f	0.36586	0.21945	0.10445	0.36600	0.2195	0.10450	0.00014	1.56	0.00005	0.71	0.00005	0.62
O32	16f	0.46942	0.38416	0.14572	0.46950	0.3841	0.14550	0.00008	1.14	0.00006	0.67	0.00022	2.75
W	16f	0.12487	0.12483	0.12486	0.12500	0.1249	0.12510	0.00013	0.76	0.00007	0.41	0.00024	1.50