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LTN-type zeolite framework as an interpenetrating net of KFI- and SOD-type parts homeomorphic to cuprite, Cu_2O

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The complex LTN-type zeolite framework is described as consisting of two interpenetrating parts in order to understand the connectivities of their underlying nets. Both parts are homeomorphic to diamond-type tetrahedral frameworks, arranged in principle in the same manner as the two interpenetrating frameworks in cuprite, Cu_2O. However, in cuprite the two frameworks are identical, while in the LTN-type framework one is made up of two kinds of truncated octahedra (*toc* units) and can be described as one half of the sodalite-type framework (SOD). The other consists of large cages, so-called truncated cubo-octahedra (*grc* units) connected by hexagonal prisms (double six-rings) and corresponds to one half of the KFI-type framework. Neither of the sub-frameworks has so far been observed in any other zeolite topology. The two sub-frameworks of SOD and KFI types in the interpenetrating LTN-type framework are models for very open interrupted frameworks, which possibly could be synthesized separately in a pure form. Their framework density would be 7.6 T atoms per 1000 $Å^3$ if they could be prepared as aluminosilicates.

1. Introduction

The LTN-type framework (Baerlocher *et al.*, 2001; Baerlocher & McCusker, 2006) of the synthetic aluminosilicate with the composition $Na_{384}\cdot Al_{384}Si_{384}O_{1536}\cdot 518.4H_2O$ was first synthesized by Acara (1968) and its crystal structure was determined by Fälth & Andersson (1982), for the compound named Linde Type N, and by Shepelev *et al.* (1983), for the compound named NaZ-21. It is one of the most complex zeolite frameworks known. Only one zeolite of cubic symmetry, CLO (Estermann *et al.*, 1991), has a unit-cell constant greater than the LTN compounds have. Fälth & Andersson (1982; see also Andersson, 1983) realised that the structure contained elements of both the frameworks of the SOD type (named after the topology displayed by the aluminosilicate framework of the mineral sodalite) and of the KFI type, named after a zeolite (ZK-5) first synthesized by Kerr (1963). For the definitions of the topology of the frameworks see Baerlocher *et al.* (2001) and Baerlocher & McCusker (2006). In fact, Fälth & Andersson (1982) used these similarities to solve the crystal structure of Linde Type A. However, they did not pursue this point any further. A promised more complete description was never published. Inasmuch as the relationships between various zeolite frameworks are of interest in understanding their properties, we have investigated in detail the similarities between LTN and the SOD and KFI frameworks.

Wells (1954*a*, 1977, 1979) introduced the concept of representing crystal structures as three-dimensional nets connecting nodes periodically in three noncollinear directions. In actual

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Table 1
Framework-type codes, chemical compositions, space groups, unit-cell constants, framework densities (highest topologically possible of the aristotype structure of a hypothetically pure SiO_2 compound, and actual for the material cited), mean T—O distances, mean T—O—T angles and references for the frameworks discussed here (T: tetrahedrally coordinated atom; X: bridging atom connecting two T atoms).

Framework	Chemical	Space group		Cell constant a (Å)		FD (T atoms per 1000 $Å^3$)		Mean T—X distance (Å)	Mean T—X—T angle (°)
code	composition	Aristotype	Actual	Aristotype	Actual	Aristotype	Actual	Actual	Actual
KFI$^{(a)}$	$Na_{30}\cdot Al_{30}Si_{66}O_{192}\cdot 98H_2O$	$Im\bar{3}m$	$Im\bar{3}m$	18.59†	18.75	14.9	14.6	1.65	145
SOD$^{(b)}$	$Ca_2Na_6\cdot Al_6Si_6O_{24}\cdot (SO_4)_2$	$Im\bar{3}\ m$	$P\bar{4}_{3n}$	8.74†	9.12	18.0	15.8	1.67	150
LTN$^{(c)}$	$Na_{384}\cdot Al_{384}Si_{384}O_{1536}\cdot 422H_2O$	$Fd\bar{3}m$	$Fd\bar{3}$	35.19‡	36.95	17.6	15.2	1.67	148
LTN–sod$^{(d)}$	$Al_{192}Si_{192}O_{864}$§	$Fd\bar{3}m$	$Fd\bar{3}$	–	36.95	–	7.6	1.68	147
LTN–kfi$^{(d)}$	$Al_{192}Si_{192}O_{864}$§	$Fd\bar{3}m$	$Fd\bar{3}$	–	36.95	–	7.6	1.67	149
–$^{(e)}$	Cu_2O	$Pn\bar{3}m$	$Pn\bar{3}m$	–	4.26	–	25.9	1.85	180
FAU$^{(f)}$	$Ca_{14}Na_{29}\cdot Al_{58}Si_{134}O_{384}\cdot 263H_2O$	$Fd\bar{3}m$	$Fd\bar{3}m$	24.55†	24.74	13.0	12.7	1.65	142
CLO$^{(g)}$	$Ga_{768}P_{768}O_{2976}(OH)_{192}$¶	$Pm\bar{3}m$	$Fm\bar{3}c$	25.86	51.71	11.1	11.1	1.66	140
[Mg-NJU]$^{(h)}$††	$P_{24}Al_{10}Mg_8O_{96}$¶	$I\bar{4}3m$	$I\bar{4}3m$	16.80	16.80	–	8.9	1.70	142

References: (*a*) Fischer (1990), Meier & Kokotailo (1965); (*b*) Hassan & Grundy (1991); (*c*) Shepelev *et al.* (1983); (*d*) this work; (*e*) Bragg & Bragg (1922); (*f*) Baur (1964); (*g*) Estermann *et al.* (1991); (*h*) Li *et al.* (2006). † From van Genechten & Mortier (1988). ‡ This work, calculated by DLS methods. § An actual framework of this type would need additional cations or H atoms for balancing the charge of the O atoms. ¶ Framework only. †† No framework code assigned yet.

crystal structures the nodes are occupied by atoms or atom groups, while the edges of the nets represent either bonds between the atoms or two-connected atoms located between two atoms at nodes. Wells (1954*b*) also recognized that such nets can be interpenetrating, without having connections (primary bonds) between the interpenetrating nets. As one of the few examples known then of such interpenetrating nets he mentions the structure of cuprite, Cu_2O (Bragg & Bragg, 1922), which is actually the first crystal structure of this type that was determined. In the last dozen years or so numerous examples of inorganic, organic and inorganic/organic compounds with interpenetrating networks have been described (see the reviews by Batten & Robson, 1998 and Batten, 2001). Batten is maintaining a website (Batten, 2005) listing all the structures known to him and based on interpenetrating nets. The listing is current as of 31 October 2005. Recognizing a particular crystal structure as being based on interpenetrating nets is nontrivial. As a consequence, Baburin *et al.* (2005) have used a computer code to identify such nets. The most common type of interpenetrating nets is based on the net underlying the structure of diamond. The cuprite net corresponds to the interpenetration of two diamond-type nets. The LTN-type net can be described as an interpenetration of parts of the SOD and KFI frameworks following the model of cuprite.

2. Computational details

Distance least-squares (DLS) calculations on the LTN-type structure were performed with the program DLS-76 (Meier & Villiger, 1969; Baerlocher *et al.*, 1977). For a comparison with the Na-containing sodalite structure we used the redetermi-

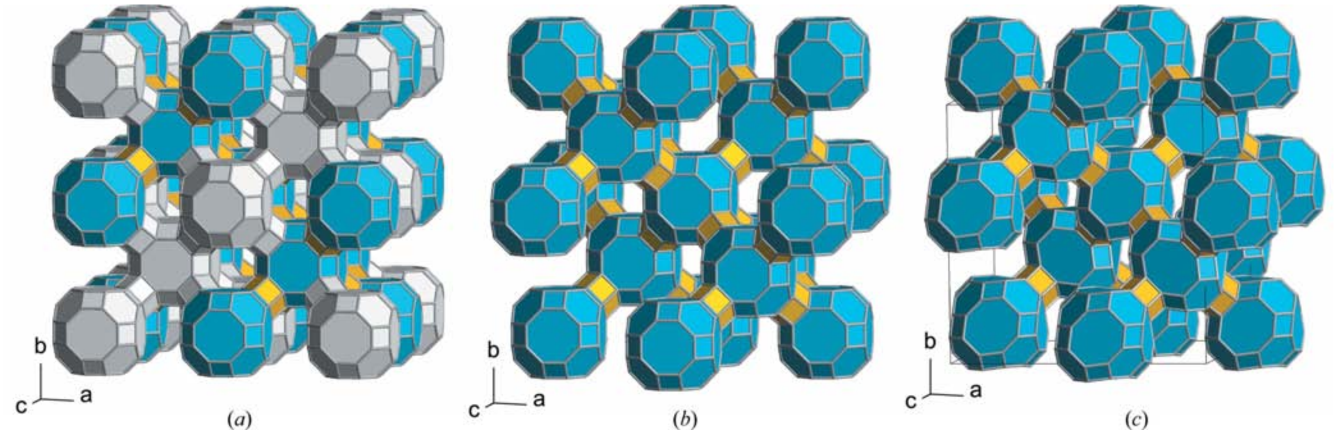

Figure 1
The KFI-type part (LTN–kfi) in the LTN structure. View parallel to [001] rotated by 5° about [100] and 10° about [010]. (*a*) View of the KFI-type framework of zeolite ZK-5 (Meier & Kokotailo, 1965) based on the coordinates of Fischer (1990). Each *grc* unit is surrounded by eight other *grc* units in a body-centered arrangement. The large *grc* units are connected by double six rings of tetrahedra. The diagram shows eight unit cells of the **KFI**-type framework and their surroundings. Polyhedral units belonging to the **LTN**–kfi part are blue (*grc*) and yellow (double six-rings), respectively. (*b*) View of the **LTN**–kfi part in the KFI-type framework. One half of the *grc* cages are systematically omitted leaving them in a diamond-type structural arrangement. (*c*) View of LTN–kfi part in the LTN-type framework of zeolite NaZ-21 based on the coordinates of Shepelev *et al.* (1983). The content of one unit cell is shown. This can also be viewed as being analogous to the cristobalite-type structure, with the *grc* units corresponding to the Si atoms and the double six rings replacing the O atoms.

nation of the KFI-type structure by Fischer (1990) based on the structure factors published in Meier & Kokotailo (1965). Crystal structure drawings were performed with the program *STRUPLO* (Fischer & Messner, 2006) as part of the *BRASS* program package (Birkenstock *et al.*, 2006). Bond distances and angles were calculated using *SADIAN*90 (Baur & Kassner, 1991).

3. Discussion

The most prominent feature of the KFI-type framework is a large polyhedral unit outlined by 12 four-rings, eight six-rings and six eight-rings of oxygen coordination tetrahedra around Si or Al atoms (*grc* unit, face symbol $4^{12}6^8 8^6$; Smith, 2000). It is called an α-cage or the truncated cubo-octahedron in the older literature. These *grc* units are connected in a body-centered arrangement (space group $Im\overline{3}m$) *via* double six-rings joining the six-rings of the *grc* units. This leaves much open space forming *pau* ($4^8 4^4 8^4 8^2$) units around the large units, as shown by the relatively low framework density (FD) of the KFI-type structures (Table 1, Fig. 1*a*). The largest unit in the SOD-type framework is a truncated octahedron, see Fig. 2(*a*) (*toc*, face symbol $4^6 6^8$; Smith, 2000; named ß-cage in the older literature). The *toc* units are connected to each other directly *via* both the four-rings and the six-rings in a close-packed arrangement in the space group $Im\overline{3}m$ (highest topologically possible symmetry).

The unit-cell constant *a* of the LTN-type compound is approximately double that of the KFI-type and four times that of the SOD-type compound (Table 1). Inasmuch as the Si/Al ratios of these compounds are similar, their mean $T—\text{O}$ distances are similar as well. In addition, their mean $T—\text{O}—T$ angles have similar values. This means that they are commensurate in terms of their unit cells and their $T—T$ distances. When we double the *a* value of the KFI-type compound we obtain a unit cell with eight times its original volume and the same size as the unit cell of the LTN type. We can remove in a gedankenexperiment from this enlarged unit cell in a systematic fashion half of the *grc* units, namely the cage at the center of the larger unit cell, those in the middle of the three basis vectors of the unit cell and four of those eight surrounding the center, in such a way that the center is surrounded tetrahedrally by the four remaining cages, as shown in Fig. 1. Thus, we obtain an arrangement with the topology of the net of the diamond crystal structure (two F-centered lattices offset by $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from each other). Instead of being occupied by C atoms the nodes are occupied here by *grc* cages which are joined by double six-rings, as they were in the original KFI-type arrangement, but now each unit has four tetrahedral neighbors (Fig. 1*b*), instead of the eight neighboring units in the KFI-type structure. The space group is now $Fd\overline{3}$ rather than $Im\overline{3}m$, as it was for the KFI-type compound. Actually this framework is very similar to the framework of FAU-type structures (Baur, 1964), as present in the mineral faujasite and in the commercially important synthetic zeolites Y and X. In the FAU-type structure the *toc* units are located on the diamond nodes, while in this diluted KFI-type structure the much larger *grc* cages occupy the same places. This results in a unit cell which is *ca* 50% larger and has a framework density which is much lower than for the FAU-type compounds (Table 1). As expected, the space groups of maximal topological symmetry for FAU and LTN–kfi are identical. The diamond-type net topology goes by various names as it is shared by numerous compounds: sphalerite or zinc blende arrangement (for one of the polymorphs of ZnS), or cristobalite (for one of the polymorphs of SiO_2). For more examples see the review by Schindler *et al.* (1999), where these complex inorganic structures which are homeomorphic to simple three-dimensional nets are called their metastructures.

The void space between the *grc* units of the LTN–kfi framework is filled by a second framework entirely composed of parts of the SOD-type framework (Fig. 2*b*). There are two

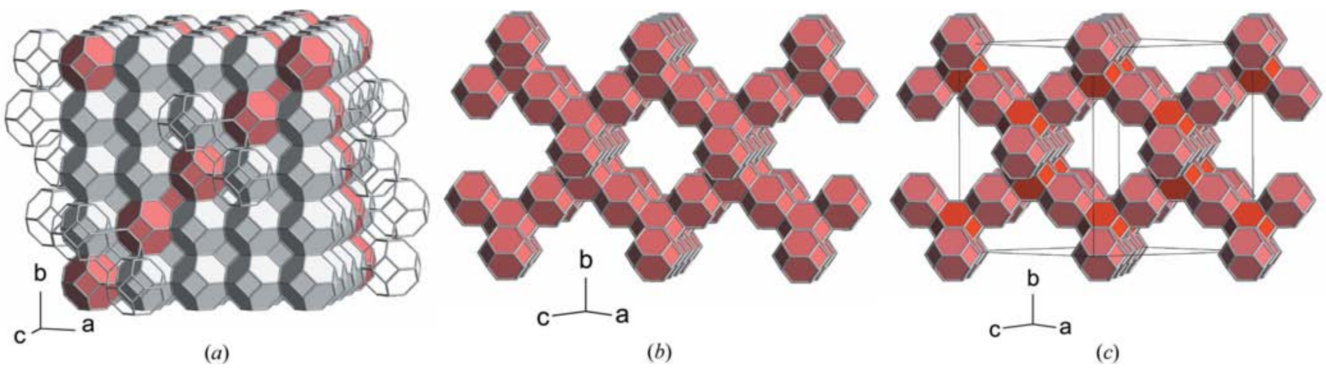

Figure 2
The SOD-type part (LTN–sod) in the LTN structure. (*a*) View of 64 unit cells and their surroundings of the SOD-type framework of the mineral nosean based on the coordinates of Jaeger (1929). The framework can be thought of as a body-centered close packing of truncated octahedra (*toc* units). These *toc* units share all their six square faces with neighboring units in the directions of the cube faces and all their hexagonal faces with neighboring units in the direction of the octahedral faces. The *toc* units belonging to the LTN–sod part of the SOD structure are red. Additional units used for the representation shown in (*b*) are drawn transparently. View parallel to [001] rotated by 5° about [100] and 10° about [010]. (*b*) View of the LTN–sod part of the SOD structure shown in (*a*). View parallel to [101] rotated by 2° about [$10\overline{1}$] and 5° about [010]. (*c*) View of LTN–sod part in the LTN-type framework of zeolite NaZ-21 based on the coordinates of Shepelev *et al.* (1983). One unit cell and some of its surroundings are shown. One half of the *toc* units present in sodalite are left out in a systematic fashion. What remains is a cristobalite-type arrangement, where the dark red *toc* units represent the tetrahedrally coordinated Si atoms and the light red polyhedra represent the O atoms. View parallel to [101] rotated by 2° about [$10\overline{1}$] and 5° about [010].

Table 2
Atomic coordinates of the framework atoms of $Na_{384}\cdot Al_{384}Si_{384}O_{1536}\cdot 422\,H_2O$ (Shepelev *et al.*, 1983) identified as belonging either to the SOD-part (LTN–sod) or the KFI-part (LTN–kfi) of the framework.

Coordinates are standardized according to Fischer & Baur (2006). Origin choice 2 (*International Tables for Crystallography*, Vol. A, 2002), at the center of symmetry.

	x	*y*	*z*	Part of
Si11	0.2481 (1)	0.0633 (1)	0.1252 (1)	SOD
Al12	0.0641 (1)	0.2484 (1)	0.1251 (1)	SOD
Si21	0.3103 (1)	0.1213 (1)	0.2456 (1)	SOD
Al22	0.1221 (1)	0.3066 (1)	0.2484 (1)	SOD
O4	0.0029 (2)	0.3444 (2)	0.1556 (2)	SOD
O6	0.4651 (2)	0.4635 (2)	0.8645 (2)	SOD
O7	0.4113 (2)	0.4083 (2)	0.9857 (2)	SOD
O8	0.0308 (2)	0.0360 (2)	0.8857 (2)	SOD
O9	0.0866 (2)	0.0894 (2)	0.2580 (2)	SOD
O1_1	0.1135 (2)	0.0417 (2)	0.9616 (2)	SOD
O1_2	0.0417 (2)	0.1126 (2)	0.9654 (2)	SOD
O21	0.3261 (2)	0.0877 (2)	0.0060 (2)	SOD and KFI
O22	0.0844 (2)	0.3233 (2)	0.0046 (2)	SOD and KFI
Si31	0.1717 (1)	0.0154 (1)	0.4540 (1)	KFI
Al32	0.0164 (1)	0.1706 (1)	0.4535 (1)	KFI
Si41	0.2230 (1)	0.0852 (1)	0.7858 (1)	KFI
Al42	0.0853 (1)	0.2273 (1)	0.7850 (1)	KFI
O31	0.2160 (2)	0.1228 (2)	0.4583 (2)	KFI
O32	0.1193 (2)	0.2197 (2)	0.4564 (2)	KFI
O5	0.0037 (2)	0.0709 (2)	0.4302 (2)	KFI
O10	0.4482 (2)	0.4505 (2)	0.2083 (2)	KFI
O11	0.2639 (2)	0.2652 (2)	0.6814 (2)	KFI
O12	0.0018 (2)	0.0067 (2)	0.5777 (2)	KFI
O13	0.0653 (2)	0.0648 (2)	0.4661 (2)	KFI

types of *toc* units in that framework. One type is located at the nodes of a diamond-type net. These are joined *via* one half of their six rings by additional intervening *toc* units halfway between those at the nodes. They form a second sub-framework within the LTN topology. This LTN–sod framework interpenetrates the LTN–kfi framework (Fig. 3*a*). Both, LTN–kfi and LTN–sod are based on the diamond-type net. Thus, the topology of LTN is homeomorphic (topologically equivalent) to the cuprite net (Fig. 3*c*), which is based on two interpenetrating nets of the diamond type offset by $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ (Schindler *et al.*, 1999) and where the O atom is tetrahedrally coordinated by the Cu atoms. In cuprite the two nets are both of the same type and have no primary bonds connecting them to each other. In LTN the polyhedra located on the two sub-nets have the same chemical composition, but have different topologies and are connected to each other by two O atoms which belong to both the LTN–kfi and to the LTN–sod framework (O21 and O22, see Table 2). The value of the framework density of the LTN-type compound expressed as the number of tetrahedrally coordinated atoms per 1000 Å^3 is between those of the SOD and the KFI frameworks (Table 1). The densities of LTN–kfi and LTN–sod, the two component parts of the LTN-type framework, are half as large as for the LTN compound itself (Table 1), as follows from the fact that one half of each of its tetrahedrally coordinated atoms belong to its two parts.

Schindler *et al.* (1999) discuss several instances of compounds based on nets homeomorphic to cuprite. The most interesting in our context is the structure of K_2PdSe_{10} (Kim & Kanatzidis, 1992), which is also based on two interpenetrating diamond-type nets, which are compositionally different from each other: one has the composition $[Pd(Se_4)_2]^{2-}$, the other $[Pd(Se_6)_2]^{2-}$. In each case the Pd atom is tetrahedrally coordinated by Se chains. Since the Se_6 chain is more folded than the Se_4 chain the dimensions of the two diamond-type nets fit each other. These cases, the LTN type and the K_2PdSe_{10} structure, show that the two nets intertwined as in the cuprite type do not have to be identical.

The interpenetrating framework of the LTN-type is different in character from the hypothetical hybrid frame-

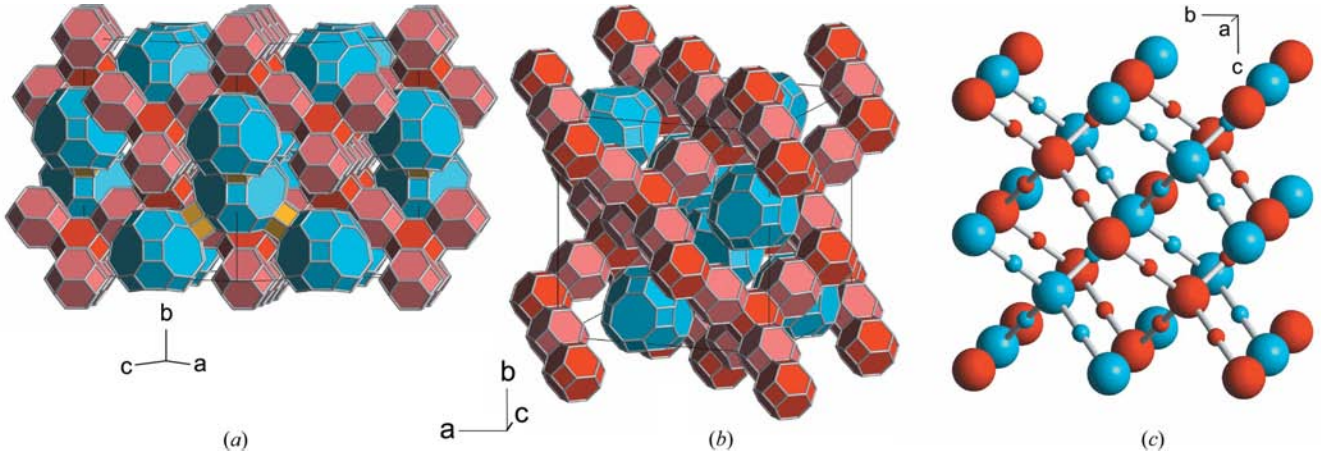

Figure 3
The LTN-type structure of zeolite NaZ-21 as an interpenetrating net of Cu_2O frameworks. (*a*) View of the complete LTN framework based on the coordinates of Shepelev *et al.* (1983). The blue *grc* units shown in Fig. 1(*c*) are filling the pores in the framework of the red *toc* units shown in Fig. 2(*c*) and *vice versa*. View parallel to [101] rotated by 2° about [$10\bar{1}$] and 5° about [010]. (*b*) View of the structure shown in (*a*) with a different range parallel to [$00\bar{1}$] rotated by 11° about [100] and 22° about [010]. (*c*) View of the framework of cuprite, Cu_2O, based on the coordinates of Bragg & Bragg (1922). Eight unit cells are shown. In order to emphasize the two interpenetrating Cu_2O frameworks, one of them is drawn with blue atoms, the other with red atoms, but of course they are symmetrically equivalent. The diagrams of Figs. 1 and 2, as well as 3(*a*), are all drawn to scale, while the Cu_2O-type framework is presented with a magnification (Schindler *et al.*, 1999) of 8.7 (= 36.95/4.26, see Table 1), where the magnification is the ratio of the unit-cell constants of the compared homeomorphic crystal structures. View parallel to [100] rotated by 10° about [010] and [001].

works described by Treacy *et al.* (2004), where the SOD-type parts of the structure are separated by LTA-type parts by a simple transformation of a single four-ring into a double four-ring of silicate coordination tetrahedra (framework 225-6-22585).

The crystal structure of the sodalite type was determined by Jaeger (1929). When Pauling (1930) refined it, using sodalite, $Na_4Al_3Si_3O_{12}Cl$, as an example, he remarked that its aluminosilicate framework was not rigid but instead was collapsible. A rotation of the TO_4 tetrahedra (T = Al or Si) allowed it to have a unit-cell constant smaller than theoretically possible. The framework collapses 'until the oxygen ions come into contact with the sodium ions' (Pauling, 1930). The mechanics of the stability of noncollapsible frameworks have been first described for the case of the synthetic LTA-type (Linde Type A) zeolite (Baur, 1992*a*,*b*, 1995; Fischer & Baur, 2006). In noncollapsible frameworks the tetrahedra rotate in opposite directions so that when one $T—O—T$ angle increases by necessity another $T—O—T$ angle must decrease. This keeps the volume of the unit cell of such a framework relatively constant. The $T—O—T$ angles act as hinges between the coordination tetrahedra. Thus, the principle of noncollapsibility is the self-limiting distortion by antirotating hinges (Baur, 1992*a*,*b*). Since then the same mechanism has been described for the feldspar framework (Baur *et al.*, 1996) and in the zeolitic FAU- and KFI-type frameworks (Baur & Fischer, 2002). The question whether or not structures with the LTN framework are noncollapsible cannot be decided empirically by looking at how different compounds based on this framework respond when the pores are filled with various cations, as it could be in the cases of the LTA, FAU and KFI frameworks, where numerous crystal structure determinations of chemically different compounds are available. The two structure determinations by Fälth & Andersson (1982) and by Shepelev *et al.* (1983) were both performed on the hydrated Na-exchanged form. Therefore, we simulated the crystal structure of LTN at various values of the unit cell constant by DLS modelling. Two of the 16 crystallographically independent $T—O—T$ angles behave in an antirotating manner upon a reduction of the size of the unit cell. This may indicate that the LTN-type framework is noncollapsible. It would agree with the observation that one of its components, KFI, is clearly noncollapsible (Baur & Fischer, 2002).

The observation of the two sub-frameworks of SOD and KFI types in the interpenetrating LTN-type framework leaves open the question whether either of these two sub-frameworks could be synthesized separately in a pure form. At a framework density of 7.6 T atoms per 1000 $Å^3$ in its hypothetical aluminosilicate form it would be a very interesting material. Inasmuch as the ratio of O atoms to tetrahedral atoms in LTN–sod and LTN–kfi is 2.25 (compared with 2 for noninterrupted frameworks), it is obvious that some of the O atoms are not bridging between two tetrahedral atoms. They are not fully connected and the framework is interrupted at atoms O21 and O22 (Table 2). Numerous interrupted frameworks are known. We mention two of them here, because they are among the most open frameworks described so far. One is the CLO framework (Estermann *et al.*, 1991) and the other is Mg-NJU (Li *et al.*, 2006). Further details are given in Table 1. Both are more open than the FAU-type framework. Especially the framework density of Mg-NJU at 8.9 T atoms per 1000 $Å^3$ is not all that different from the density of the hypothetical frameworks postulated here. It is extremely likely that the LTN–sod and LTN–kfi topologies are completely new. So far the main effort in generating new hypothetical topologies of potential zeolites has been limited to four-connected tetrahedrally coordinated nets (Treacy *et al.*, 2004; Foster & Treacy, 2006) and not to interrupted frameworks. However, six zeolites with interrupted frameworks have been identified so far and have been included by the Structure Commission of the International Zeolite Association in its compilation of 174 zeolite topologies (Baerlocher & McCusker, 2006).

One can also look at our result from a different angle and say that likely hypothetical interrupted frameworks can be generated by judicious 'pruning' of already known fully tetrahedral and four-connected nets of existing or proposed zeolites.

4. Conclusion

The present analysis is very much *ad hoc* and applies only to the case of the LTN-type framework. This does not exclude the possibility that one will encounter in the future other frameworks which can be shown to be interpenetrating in an analogous manner. We show that the topology of the net of the LTN-type zeolite can be described as consisting of two different interpenetrating parts, each of which by itself is of a diamond-type topology. Our finding of these two diamontoid interpenetrating components (LTN–kfi and LTN–sod) in the framework of the LTN-type identifies two potential frameworks as candidates for very open interrupted frameworks.

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