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TOPOLOGY OF TECTOSILICATE FRAMEWORK

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A new concept of coordination network is introduced for classifying and deriving possible frameworks of tectosilicates. 26 topologically different networks have been derived by connecting points with the degree of freedom 3 in the 2nd distance. 39 different tectosilicate structures are examined in view of this coordination network.

Tectosilicates in which TO_4(T=Si,Al) are four-corner-linked to form three dimensional network comprise silica, feldspar,feldspathoid and zeolite groups . Among them, framework topology of zeolite groups has been investigated by Smith,Meier,Breck,Alberti and Sato. According to Meier[1] and Breck[2] zeolite groups can be classified into seven subgroups on the basis of the secondary building unit(abbr.SBU). The SBU criterion can be appreciated in a point that it is a simple and effective geometrical one for understanding the complicated framework structures, but inferior in the point that it is not able to derive them systematically. Very recently,Smith[3-5] , Alberti[6,7], Sato[8] have independently developed the method for derivation of possible framework structures by which a certain type of the framework structures has been derived systematically. A new concept of coordination network is introduced here as an alternative approach for classifying and deriving various kinds of frameworks of tectosilicates. Framework is a kind of network which consists of points(T atoms) and lines connecting adjacent points. An nth coordination number around a given point can be defined as the total number of points at a topological distance n. Then we define an nth coordination network as a set of all points from topological distances 0 to n and all thier connective lines. It is obvious that 0th coordination network comprises one point, and the 1st

coordination network a set of one centering point , 4 adjacent points and 4 connecting lines(Fig.1). In the case of topological distance 2 ,the coordination network becomes complicated .

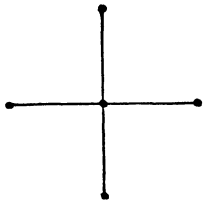
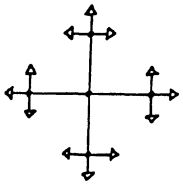
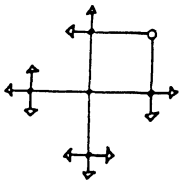


Fig.1 The 1st coordination network



(a)



(b)

Fig.2 The 2nd coordination network

The simplest form of the 2nd network is a tree (Fig.2-a) . In this tree structure, all the 2nd coordination points have a degree of freedom 3, which means each T atom coordinating 3 free oxygen atoms around it. They are represented with symbol △ in the figure. Now, if we connect any two points of them, not sharing commonly with a 1st coordiantaion point, one 4 membered ring can be formed (Fig.2-b) and this is only one topological unique network for one connection. We call it 1 connection network. In the figure, one connection point is represented with symbol O ,indicating the degree of freedom 2. Starting with this 1 connection network we can next connect two other remaining points with the degree of freedom 3 to form three kinds of 2 connection network. Likewise, 6 kinds for 3 connections, 7 kinds for 4 connections, 5 kinds for 5 connections, and 3 kinds for 6 connections can be obtained. Pattern graphs of all these networks are shown in Fig. 3, in which only the lines connecting the points with the degree of freedom 0 are represented. Numerical values added for each graph indicate modified topological indices defined by Hosoya et al [9] . They are obtained by the application of the Frame method to the adjacency matrices. Now we can classify all the tectosilicate structures on the basis of this coordination network. 39 different structures examined are shown in Table,in which alphabetical symbols a,b,c,d,e,f g and h are used instead of topological quantities. Group numbers due to Breck's classification are referred in

the right column. It is very interesting to note that (1) except natrolite, thomsonite, edingtonite, framework structures examined are concentrated on the largest 7 topological indices, and (2)this topological classification shows comparatively good correspondence to the Breck's SBU one. Natrolite, thomsonite, edingtonite have 2 different coordination networks in the 2nd distances. One of which, as already described, is formed by connection of two points with the same degrees of freedom 3, while the other by connection of two points with different degrees of freedom such as 2 and 3. All the possible networks in the latter case are now being derived.

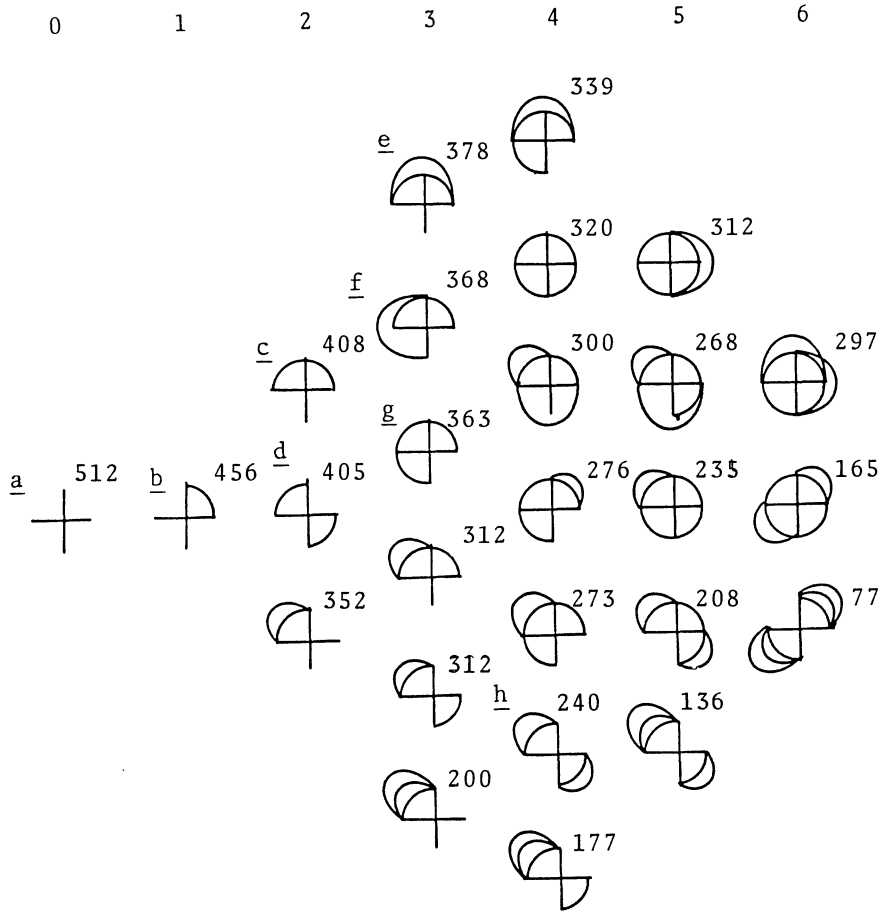


Fig.3 Pattern graphs of 26 possible coordination networks. The numbers in the first row are connection numbers , and the other numerical values added are modified topological indices (Hosoya et al[9]).

Table The distribution of 39 different tectosilicate frameworks examined on the possible coordination networks

	a	b	c	d	e	f	g	h	R
CR	+								
TR	+								
NE	+								
QU	+								
FE	+								6
DA	+	+							6
EP	+	+							6
MO	+	+							6
HE	+	+	+						7
ST	+	+	+		+				7
SC		+							
BR		+	+						7
CD		+		+					
YU		+		+					1
AL			+						
CA			+						
CO			+						
LO			+	+					2
ER			+				+		2
ZL			+				+		4

	a	b	c	d	e	f	g	h	R
OF			+				+		2
OM			+				+		2
SO				+					2
LA				+					1
AA				+					1
LE				+			+		2
ZA					+				3
CY						+			
HA							+		1
PA							+		1
PH							+		1
GI							+		1
GM							+		4
CH							+		4
FA							+		4
ZK							+		4
ED								+	5
NA								+	5
TH								+	5

AA	Analcime	FA	Faujasite	OF	Offretite
AL	Albite	FE	Ferrierite	OM	Omega
BR	Brewsterite	GI	Gismondite	PA	Paulingite
CA	Cancrinite	GM	Gmelinite	PH	Philipsite
CH	Chabazite	HA	Harmotome	QU	Quartz
CD	Cordierite	HE	Heulandite	SC	Scapolite
CR	Cristobalite	LA	Laumontite	SO	Sodalite
CY	Cymrite	ZL	Zeolite L	ST	Stilbite
CO	Coesite	LE	Levynite	TH	Thomsonite
DA	Dachiardite	LO	Losod	TR	Tridymite
ED	Edingtonite	NE	Nepheline	YU	Yugawaralite
EP	Epistilbite	MO	Mordenite	ZK	ZK-5
ER	Erionite	NA	Natrolite	ZA	Zeolite A

Alphabetical symbols a,b,c,d,e,f,g and h correspond to those in Fig.3,and R means Breck's grouping number of zeolite groups.

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