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Tetragonal sphere packings: minimal densities and subunits

W. Fischer

Institut für Mineralogie, Petrologie und Kristallographie der Philipps-Universität Marburg, Hans-Meerwein-Strasse, D-35032 Marburg, Germany. Correspondence e-mail: drwerner.fischer@staff.uni-marburg.de

For all 382 types of homogeneous sphere packings with tetragonal symmetry, the minimal sphere-packing densities have been calculated. The tabulated coordinates allow the graphic representation of a sample packing for each type. 1- and 2-periodic subunits of these sphere packings are listed in addition.

1. Introduction

In a systematic study (Fischer, 1970), all homogeneous sphere packings with tetragonal symmetry were derived and assigned to 394 types. At that time, only a summary of the results was published together with the symbolism for the types and the procedure used for the derivation (Fischer, 1971). In the course of the following derivation of all homogeneous sphere packings with cubic symmetry (Fischer, 1973, 1974), it became obvious that sphere packings of 12 tetragonal types are also compatible with cubic symmetry. Accordingly, these types were renamed later on, when detailed information on tetragonal sphere packings was published (Fischer, 1991*a*,*b*, 1993). Explicit values of sample coordinates are missing, however, in most cases, *i.e.* if the sphere-packing type has free parameters, and no information on the minimal densities was given. These items are presented here.

2. Results

In analogy to the cubic case (Fischer, 2004), the minimal density has been calculated for each of the 382 types of homogeneous sphere packings with tetragonal symmetry. For this, the formulae of the sphere-packing distances were derived, the respective distances set to 1, and the parameters x, y, z, a and c were varied by means of *EUREKA. THE SOLVER* (1987) such that the density ρ was minimized. The results are presented in Table 1.

In the first column, the sphere-packing type is identified by its symbol $k/m/tn$, where k is the number of contacts per sphere, m is the length of the shortest mesh, t stands for the tetragonal crystal system and n is an arbitrary numbering. In the next column, the maximal symmetry compatible with the respective type is described by a space-group symbol and a Wyckoff position. Within the tetragonal crystal system, the minimum of density is always tied to the maximal symmetry. This had to be shown explicitly because one example to prove the opposite has been found within the hexagonal crystal system (Koch *et al.*, 2005).

With respect to the minimal density, two cases have to be distinguished.

(i) If the minimal density of a sphere-packing type refers to a point inside the parameter region, the corresponding parameters and the minimal density ρ_{min} are given in columns 3 and 4, respectively.

(ii) For 80 sphere-packing types, however, the density decreases towards a point on the border of the parameter region and, therefore, no sphere packing with minimal density exists. Accordingly, only a limiting value for ρ_{min} is tabulated in column 4. The parameters in column 3 then refer to an arbitrary point inside the parameter region.

The given coordinates are always related to the first setting of the space group. For the preparation of graphic representations of sphere packings, it is helpful to know, in addition, the distance d between the centres of spheres in contact. The lattice parameters a and c given in column 3, therefore, refer to $d = 1$. Cubic sphere-packing types that had originally been found with tetragonal symmetry are not contained in Table 1.

In analogy to a table on hexagonal sphere packings (Sowa & Koch, 2005), Table 1 is supplemented by information on layer-like and/or rod-like subunits, if possible.

(i) The sphere packings of 127 out of the 382 tetragonal types contain layer-like subunits perpendicular to **c**. Most of these are either flat or corrugated but correspond to planar nets and are characterized, therefore, by the symbols of the respective Shubnikov nets 4^4, 48^2, 3^2434 or 6^3 (Shubnikov, 1916) in the fifth column. The other layers are necessarily corrugated: the quadrangles in the $4_c(8{+}2)^2$ and in the $4_c8(8{+}4)$ layers are wrenched, those in the 4_t8^2 layers are replaced by tetrahedra. Corresponding sphere layers are illustrated in Fig. 1. Three numbers and two signs (+ or −) follow each layer symbol. The first two numbers indicate how many spheres from layers above and below contact each sphere, the third one gives the number of layers per translation period (*cf.* Koch & Fischer, 1999). The first sign shows whether the layer may be flat or not. The second sign is + if there is only one possibility to split the sphere packing into the corresponding (corrugated) layers, otherwise it is −.

Table 1
Minimal densities, sample parameters and subunits of tetragonal sphere-packing types.

Type	Symmetry	*x*, *y*, *z*; *a*, *c*	$\rho_{\rm min}$	Layer description			Rod description		
3/4/*t*1	$I4_1/amd$ 16*h*	0.00000, 0.15350, 0.05538; 3.94901, 4.64911	0.11555	–			–		
3/4/*t*2	$I4_122$ 16*g*	0.04106, 0.13269, 0.07787; 3.59986, 5.67959	0.11382	–			–		
3/4/*t*3	$I4_1/amd$ 32*i*	0.08874, 0.18913, 0.05649; 5.63440, 5.31104	0.09937	–			–		
3/8/*t*1	$I4_1/amd$ 16*f*	0.12500, 0.25000, 0.12500; 4.00000, 2.82843	0.18512	–			–		
3/8/*t*2	*I*422 16*k*	0.27227, 0.11278, 0.09124; 3.98632, 2.39854	0.21980	–			–		
3/8/*t*3	*P*4/*nnc* 16*k*	0.27409, 0.11353, 0.14794; 3.16613, 2.34930	0.35573	–			–		
3/8/*t*4	$P4_2/nmc$ 16*h*	0.22312, 0.13989, 0.15188; 3.57431, 2.98648	0.21957	–			–		
3/8/*t*5	$I4_122$ 16*g*	0.11001, 0.16493, 0.20029; 2.52201, 5.99858	0.21957	–			–		
3/8/*t*6	$I\bar{4}2d$ 16*e*	0.21410, 0.03590, 0.15719; 2.30940, 2.30940	0.68017	–			–		
3/8/*t*7	$I4_1/amd$ 32*i*	0.14775, 0.13487, 0.08212; 3.70720, 6.07461	>0.20040	–			–		
3/10/*t*2	$P4_2/nbc$ 16*k*	0.28848, 0.12796, 0.17748; 3.63160, 2.54457	0.24964	–			–		
3/10/*t*3	$P4_122$ 8*d*	0.32424, 0.11832, 0.03768; 2.81980, 1.75401	0.30035	–			–		
3/10/*t*4	$I4_1/amd$ 8*e*	0.00000, 0.00000, 0.09375; 1.88562, 5.33333	0.22089	–			–		
3/10/*t*5	$I4_1/acd$ 32*g*	0.06631, 0.29339, 0.02384; 4.98685, 3.02848	0.22247	–			–		
3/10/*t*6	$I4_1/acd$ 32*g*	0.08677, 0.20489, 0.11109; 5.10549, 1.87974	0.34196	–			–		
3/10/*t*7	$I4_1/acd$ 32*g*	0.12267, 0.21585, 0.16274; 3.63271, 5.03054	0.25239	–			–		
4/4/*t*1	$I4_1/amd$ 8*c*	0.00000, 0.25000, 0.12500; 2.30940, 2.30940	0.34009	–			–		
4/4/*t*2	$I4_122$ 8*f*	0.07019, 0.25000, 0.12500; 1.92554, 3.48771	0.32392	$4_c(8+2)^2$	1,0 2	−−	–		
4/4/*t*3	$I4_1/amd$ 16*g*	0.15000, 0.15000, 0.00000; 3.33333, 2.98142	0.25289	–			–		
4/4/*t*4	$P4_2/mmc$ 8*o*	0.00000, 0.27730, 0.16959; 2.24516, 2.94823	0.28186	48^2	1,0 2	−+	$6^3(0,2)$	1,0	*p*
							$48^2(0,2)$	1,0	*p*′
4/4/*t*5	*I*4/*mmm* 8*h*	0.17431, 0.17431, 0.00000; 2.86852, 1.57840	0.32252	48^2	1,0 1	−−	$6^3(4,2)$	*c*	*c*′
4/4/*t*6	$P4_2/n$ 8*g*	0.27015, 0.09761, 0.10617; 2.00229, 2.73962	0.38137	48^2	1,0 2	−+	–		
4/4/*t*8	*I*4/*mcm* 16*l*	0.14645, 0.64645, 0.18750; 3.21895, 2.66667	0.30319	48^2	1,0 2	−+	$6^3(0,4)$	*c*	*c*
							$6^3(0,2)$	1,0	*c*′
4/4/*t*9	$P4_2/mcm$ 8*n*	0.32945, 0.06917, 0.00000; 2.71672, 1.85339	0.30622	$4_c8(8+4)$	1,0 1	−−	$6^3(4,2)$	1,0	*p*
4/4/*t*10	$P4_222$ 8*p*	0.25000, 0.03329, 0.13879; 1.98250, 3.57102	0.29844	$4_c(8+2)^2$	1,0 2	−+	$4^4(0,2)$	1,0	*p*
4/4/*t*11	$P4_22_12$ 8*g*	0.22080, 0.15460, 0.18338; 1.85499, 2.68519	0.45335	6^3	1,0 2	−+	–		
4/4/*t*12	*I*422 16*k*	0.22165, 0.08601, 0.14844; 2.97411, 2.89410	0.32726	48^2	1,0 2	−+	–		
4/4/*t*13	*I*4/*mmm* 16*l*	0.29210, 0.12099, 0.00000; 4.13248, 1.72285	0.28474	48^2	1,0 1	−−	$6^3(4,2)$	1,0	*c*′
4/4/*t*14	*I*422 16*k*	0.33172, 0.13740, 0.10944; 2.30148, 3.53907	>0.42099	$4_c8(8+4)$	1,0 2	−+	$4^4(0,2)$	1,0	*c*′
4/4/*t*15	$P\bar{4}2c$ 8*n*	0.34500, 0.14572, 0.00687; 2.35027, 1.49835	>0.50579	–			$6^3(4,2)$	*c*	*c*′
4/4/*t*16	$P\bar{4}2_1c$ 8*e*	0.25000, 0.15176, 0.15500; 1.83339, 2.10301	>0.56286	–			–		
4/4/*t*17	$P\bar{4}c2$ 8*j*	0.26313, 0.05742, 0.10938; 2.05141, 2.85305	0.34888	48^2	1,0 2	−+	$6^3(0,2)$	1,0	*p*
4/4/*t*18	$P\bar{4}n2$ 8*i*	0.27722, 0.05377, 0.09129; 2.18168, 2.68822	0.32737	48^2	1,0 2	−+	–		
4/4/*t*19	$I\bar{4}2m$ 16*j*	0.31863, 0.08015, 0.15324; 2.96514, 2.87061	0.33194	48^2	1,0 2	−+	$6^3(0,2)$	1,0	*c*′
4/4/*t*20	*P*4/*mcc* 16*n*	0.33172, 0.13740, 0.14088; 2.30148, 3.54919	>0.42099	$4_c8(8+4)$	1,0 2	−+	$6^3(0,4)$	1,0	*p*
4/4/*t*21	*P*4/*nnc* 16*k*	0.30622, 0.11608, 0.17265; 3.29628, 1.86419	>0.38913	–			$6^3(4,2)$	1,0	*c*′
4/4/*t*22	*P*4/*nnc* 16*k*	0.25000, 0.08333, 0.16667; 2.68328, 2.68328	>0.39734	48^2	1,0 2	−+	–		
4/4/*t*23	*P*4/*nnc* 16*k*	0.31247, 0.10967, 0.15944; 2.93066, 2.40236	0.40602	48^2	1,0 2	−+	$6^3(0,2)$	1,0	*c*′
4/4/*t*24	*P*4/*nnc* 16*k*	0.34665, 0.14359, 0.12506; 2.38007, 2.91831	0.50677	$4_c8(8+4)$	1,0 2	−+	–		
4/4/*t*25	$P4_2/mcm$ 16*p*	0.34392, 0.08949, 0.13387; 2.77914, 3.73503	0.29040	$4_c8(8+4)$	1,0 2	−+	$48^2(0,2)$	1,0	*p*
4/4/*t*26	$P4_2/nbc$ 16*k*	0.22544, 0.11734, 0.14316; 4.01109, 1.57982	0.32960	–			$6^3(0,2)$	1,0	*c*
4/4/*t*27	$P4_2/nbc$ 16*k*	0.20429, 0.07728, 0.07451; 2.99950, 2.52449	0.36885	48^2	1,0 2	−+	$6^3(0,2)$	1,0	*c*
4/4/*t*28	$P4_2/nbc$ 16*k*	0.24764, 0.10639, 0.12540; 1.99991, 3.63147	>0.56923	–			–		
4/4/*t*29	$P4_2/nbc$ 16*k*	0.25466, 0.20000, 0.12577; 1.99965, 3.94274	>0.52360	–			–		
	$P4_2/mbc$ 16*i*	0.25563, 0.20000, 0.12550; 1.99949, 3.98420							
	$I4_1/acd$ 32*g*	0.24539, 0.20000, 0.18775; 1.99966, 7.96623							
	$I4_1/acd$ 32*g*	0.20000, 0.24426, 0.18711; 1.99947, 7.88777							
4/4/*t*30	$P4_2/nbc$ 16*k*	0.15346, 0.14364, 0.12506; 2.37872, 2.92185	0.50673	$4_c(8+2)^2$	1,0 2	−+	–		
4/4/*t*31	$P4_2/nbc$ 16*k*	0.33088, 0.13808, 0.14056; 2.29011, 3.53907	>0.42099	$4_c(8+2)^2$	1,0 2	−+	$4^4(0,2)$	1,0	*c*′
4/4/*t*32	$P4_2/nnm$ 16*n*	0.35148, 0.09903, 0.11475; 2.80099, 3.62519	0.29455	$4_c8(8+4)$	1,0 2	−+	$4^4(0,2)$	1,0	*c*′
4/4/*t*33	*I*4/*mmm* 32*o*	0.27141, 0.11242, 0.14857; 4.44751, 3.36550	0.25169	48^2	1,0 2	−+	$48^2(0,2)$	1,0	*c*′
4/4/*t*34	*I*4/*mcm* 32*m*	0.24270, 0.10053, 0.17588; 4.51044, 2.84284	0.28971	48^2	1,0 2	−+	$6^3(0,4)$	1,0	*c*
							$48^2(0,2)$	1,0	*c*′
4/4/*t*35	$P4_122$ 8*d*	0.25939, 0.06811, 0.05248; 1.99860, 2.60904	>0.37024	–			$4^4(0,2)$	1,0	*p*
4/4/*t*36	$P4_122$ 8*d*	0.26797, 0.04286, 0.03858; 2.11995, 2.32561	>0.39861	–			$4^4(0,2)$	1,0	*p*
4/4/*t*37	$P4_122$ 8*d*	0.25000, 0.11785, 0.05893; 1.89737, 2.68328	>0.37024	–			$4^4(0,2)$	1,0	*p*
4/4/*t*38	$P4_122$ 8*d*	0.32537, 0.10010, 0.00000; 2.86327, 1.63883	0.31177	–			$6^3(4,3)$	1,0	*p*
4/4/*t*39	$I4_1/a$ 16*f*	0.25425, 0.15802, 0.07629; 1.82968, 4.14509	>0.56286	–			–		
4/4/*t*40	$I4_1/amd$ 16*h*	0.00000, 0.16487, 0.37500; 3.98977, 1.46770	0.35858	–			$6^3(4,3)$	1,0	p'_2
4/4/*t*41	$I4_1/amd$ 16*h*	0.00000, 0.22374, 0.20884; 2.23470, 5.92277	0.28324	48^2	1,0 4	−+	–		
4/4/*t*42	$I4_1/a$ 16*f*	0.21228, 0.18024, 0.19260; 1.79547, 4.41426	0.58872	48^2	1,0 4	−+	–		
4/4/*t*43	$I4_122$ 16*g*	0.13781, 0.09428, 0.21089; 2.99449, 2.33028	>0.39691	–			$4^4(0,2)$	1,0	*c*″
4/4/*t*44	$I4_122$ 16*g*	0.15198, 0.09119, 0.20813; 2.82113, 2.67010	>0.37024	–			$4^4(0,2)$	1,0	*c*″
4/4/*t*45	$I4_122$ 16*g*	0.21774, 0.02607, 0.14700; 2.27999, 2.73599	>0.37024	–			$4^4(0,2)$	1,0	*c*″
4/4/*t*46	$I4_122$ 16*g*	0.04513, 0.12846, 0.25000; 3.67224, 1.80301	0.34455	–			–		
4/4/*t*47	$I4_122$ 16*g*	0.25000, 0.09549, 0.06598; 1.86834, 6.91747	0.34694	$4_c(8+2)^2$	1,0 4	−+	–		

Table 1 (continued)

Type	Symmetry	*x*, *y*, *z*; *a*, *c*	$\rho_{\min}$	Layer description			Rod description		
				6^3	1,0 4	−+			
4/4/*t*48	$I4_122$ 16*g*	0.04040, 0.25000, 0.05597; 1.97439, 7.24341	0.29670	$4_c(8+2)^2$	1,0 4	−+	–		
4/4/*t*49	$I\bar{4}2d$ 16*e*	0.21989, 0.02947, 0.14921; 2.30936, 2.30947	>0.68017	–			–		
4/4/*t*50	$I\bar{4}2d$ 16*e*	0.14998, 0.10070, 0.15492; 3.33174, 1.69384	0.44556	–			–		
4/4/*t*51	$I\bar{4}2d$ 16*e*	0.22794, 0.09864, 0.19789; 2.01314, 5.43837	0.38010	48^2	1,0 4	−+	–		
4/4/*t*52	$I4_1/amd$ 32*i*	0.23343, 0.12100, 0.14500; 4.13223, 2.59947	>0.37024	–			$4^4(0,2)$	1,0	p_2'
4/4/*t*53	$I4_1/amd$ 32*i*	0.21891, 0.11929, 0.17544; 4.19149, 2.41894	>0.38927	–			$4^4(0,2)$	1,0	p_2'
4/4/*t*54	$I4_1/amd$ 32*i*	0.19263, 0.12829, 0.18393; 3.89737, 2.68328	>0.37024	–			$4^4(0,2)$	1,0	p_2'
4/4/*t*55	$I4_1/amd$ 32*i*	0.19995, 0.08731, 0.12500; 5.72653, 1.63883	0.31177	–			$6^3(4,3)$	1,0	p_2'
4/4/*t*56	$I4_1/amd$ 32*i*	0.16865, 0.08798, 0.25000; 5.68336, 1.52261	0.34068	–			$6^3(4,3)$	1,0	p_2'
4/4/*t*57	$I4_1/amd$ 32*i*	0.13485, 0.13485, 0.08221; 3.70770, 6.08207	0.20040	–			–		
4/4/*t*58	$I4_1/amd$ 32*i*	0.16564, 0.16564, 0.19421; 3.01851, 6.21755	0.29576	48^2	1,0 4	−+	–		
4/4/*t*59	$I4_1/acd$ 32*g*	0.16630, 0.04609, 0.19776; 5.78976, 1.69136	0.29552	–			$6^3(4,2)$	1,0	p_2
4/4/*t*60	$I4_1/acd$ 32*g*	0.06468, 0.17739, 0.08615; 5.59626, 1.37966	0.38778	–			$6^3(4,2)$	1,0	p_2
4/4/*t*61	$I4_1/acd$ 32*g*	0.03690, 0.16704, 0.19505; 5.32104, 1.83937	0.32173	–			$6^3(4,2)$	1,0	p_2
4/4/*t*62	$I4_1/acd$ 32*g*	0.06878, 0.15200, 0.02228; 4.22292, 1.90529	0.49313	–			$6^3(0,2)$	1,0	p_2
4/4/*t*63	$I4_1/acd$ 32*g*	0.13082, 0.04617, 0.10017; 4.15167, 2.89579	0.33569	–			$6^3(0,2)$	1,0	p_2
4/4/*t*64	$I4_1/acd$ 32*g*	0.02696, 0.13115, 0.11057; 4.08888, 2.86193	0.35017	–			$6^3(0,2)$	1,0	p_2
4/4/*t*65	$I4_1/acd$ 32*g*	0.11770, 0.21526, 0.07252; 3.91852, 2.60904	>0.37024	–			$4^4(0,2)$	1,0	p_2'
4/4/*t*66	$I4_1/acd$ 32*g*	0.11505, 0.21708, 0.07353; 4.04585, 2.42751	>0.40274	–			$4^4(0,2)$	1,0	p_2'
4/4/*t*67	$I4_1/acd$ 32*g*	0.11716, 0.18738, 0.06607; 3.57069, 2.68328	>0.37024	–			$4^4(0,2)$	1,0	p_2'
4/4/*t*68	$I4_1/acd$ 32*g*	0.10129, 0.14113, 0.07356; 2.94452, 4.69291	0.41179	–			–		
4/4/*t*69	$I4_1/acd$ 32*g*	0.18388, 0.10458, 0.03579; 3.11111, 5.10866	0.33885	48^2	1,0 4	++	–		
4/4/*t*70	$I4_1/acd$ 32*g*	0.06541, 0.21237, 0.03672; 2.95323, 5.07014	0.37891	48^2	1,0 4	−+	–		
4/4/*t*71	$I4_1/acd$ 32*g*	0.10114, 0.24829, 0.18768; 1.99995, 7.29505	>0.56979	–			–		
4/4/*t*72	$I4_1/acd$ 32*g*	0.08679, 0.20833, 0.12500; 5.19334, 1.80301	0.34455	–			$6^3(4,3)$	1,0	p_2'
4/4/*t*73	$I4_1/acd$ 32*g*	0.09855, 0.13500, 0.16248; 2.99138, 5.64456	0.33172	6^3	1,0 4	−+	–		
4/5/*t*1	$I4_1/a$ 16*f*	0.12157, 0.13010, 0.17449; 2.80800, 2.86553	>0.37024	–			–		
4/5/*t*2	$I\bar{4}2d$ 16*e*	0.21358, 0.03572, 0.15623; 2.30898, 2.31023	>0.68017	–			–		
4/6/*t*1	$P4_122$ 4*a*	0.00000, 0.32974, 0.00000; 1.99489, 1.46770	0.35858	–			$6^3(4,3)$	1,0	p'
4/6/*t*3	$I4_1/acd$ 16*e*	0.25000, 0.08513, 0.12500; 3.98977, 1.46770	0.35858	–			$6^3(4,2)$	1,0	p_2
4/6/*t*4	$P4_2/mbc$ 8*h*	0.27748, 0.12500, 0.00000; 1.98803, 1.92336	>0.52360	–			–		
	$I4_1/acd$ 16*e*	0.25000, 0.12500, 0.12500; 2.00000, 3.74166							
4/6/*t*5	$P4_22_12$ 8*g*	0.26679, 0.14214, 0.17601; 1.83075, 2.68875	0.46482	6^3	1,0 2	−+	–		
4/6/*t*6	$P4/ncc$ 16*g*	0.24765, 0.10043, 0.00774; 3.34164, 1.48254	0.50605	–			$6^3(4,2)$	1,0	*c*
4/6/*t*7	$I\bar{4}2d$ 16*e*	0.21852, 0.03662, 0.16015; 2.31238, 2.30244	>0.68017	–			–		
4/6/*t*8	$I4_1/acd$ 32*g*	0.11993, 0.19966, 0.06277; 2.14676, 6.66479	>0.50217	–			–		
5/3/*t*1	$I4_1md$ 8*b*	0.00000, 0.22150, 0.00000; 2.25733, 2.38253	0.34503	–			–		
5/3/*t*2	$P4_2/mmc$ 8*o*	0.00000, 0.25000, 0.14645; 2.00000, 3.41421	0.30672	4_t8^2	1,0 2	−+	$3^34^2(0,2)$	1,0	*p*
							$48^2(0,2)$	*s*	p'
5/3/*t*3	$P4_2/n$ 8*g*	0.25000, 0.08515, 0.11877; 1.89320, 2.97675	0.39260	4_t8^2	1,0 2	−+	–		
				6^3	2,0 2	−+			
5/3/*t*4	$I4/mcm$ 16*l*	0.14645, 0.64645, 0.14645; 2.41421, 3.41421	0.42099	4_t8^2	1,0 2	−+	$6^3(0,4)$	2,0	*c*
							$3^34^2(0,2)$	1,0	c'
5/3/*t*5	$I422$ 16*k*	0.21874, 0.09061, 0.14661; 2.98652, 2.86773	0.32753	48^2	2,0 2	−+	–		
5/3/*t*6	$I\bar{4}2m$ 8*i*	0.15000, 0.15000, 0.23717; 2.35702, 1.49071	0.50579	–			$6^3(4,2)$	2,0	c'
5/3/*t*7	$P\bar{4}2_1c$ 8*e*	0.23526, 0.13555, 0.16167; 1.84152, 2.18687	>0.56286	6^3	2,0 2	−+	–		
5/3/*t*8	$P\bar{4}c2$ 8*j*	0.25000, 0.04626, 0.11546; 1.96661, 3.06215	0.35369	4_t8^2	1,0 2	−+	$3^34^2(0,2)$	1,0	*p*
5/3/*t*9	$I\bar{4}m2$ 8*i*	0.27252, 0.00000, 0.10727; 2.19795, 2.47715	0.35003	48^2	2,0 2	−+	–		
5/3/*t*10	$P\bar{4}n2$ 8*i*	0.25000, 0.04626, 0.11546; 1.96661, 3.06215	0.35369	4_t8^2	1,0 2	−+	–		
5/3/*t*11	$I\bar{4}2m$ 16*j*	0.34067, 0.08517, 0.13875; 2.76754, 3.17805	0.34417	4_t8^2	1,0 2	−+	$3^34^2(0,2)$	1,0	c'
				$4_c8(8+4)$	2,0 2	−+			
5/3/*t*12	$P4/nnc$ 16*k*	0.29471, 0.12207, 0.14933; 3.43012, 1.82982	0.38913	–			$6^3(4,2)$	2,0	c'
5/3/*t*13	$P4/nnc$ 16*k*	0.23298, 0.09650, 0.15679; 2.80398, 2.68164	0.39734	48^2	2,0 2	−+	–		
5/3/*t*14	$P4/nnc$ 16*k*	0.33236, 0.12646, 0.13258; 2.38113, 3.01089	0.49075	4_t8^2	1,0 2	−+	$3^34^2(0,2)$	1,0	c'
5/3/*t*15	$P4_2/nbc$ 16*k*	0.22620, 0.12613, 0.17759; 3.84526, 1.67794	0.33767	–			$6^3(4,2)$	2,0	*c*
5/3/*t*16	$P4_2/nbc$ 16*k*	0.18362, 0.10490, 0.11221; 2.36435, 3.15080	0.47564	4_t8^2	1,0 2	−+	$3^34^2(0,2)$	1,0	*c*
5/3/*t*17	$P4_2/nbc$ 16*k*	0.26586, 0.12550, 0.13094; 1.99599, 3.63454	0.57857	–			–		
5/3/*t*18	$P4_2/nmc$ 16*h*	0.28429, 0.13103, 0.15800; 3.81591, 1.77894	0.32342	–			$6^3(4,2)$	2,0	c'
5/3/*t*19	$P4_122$ 8*d*	0.26784, 0.03856, 0.03990; 2.11554, 2.34797	0.39861	–			$3^6(1,2)$	1,0	*p*
5/3/*t*20	$P4_122$ 8*d*	0.25000, 0.10503, 0.06344; 1.87083, 2.78650	>0.37024	–			$3^6(1,2)$	1,0	*p*
5/3/*t*21	$P4_12_12$ 8*b*	0.30627, 0.05223, 0.10743; 1.93769, 3.34110	0.33391	–			–		
5/3/*t*22	$I4_1/a$ 16*f*	0.11568, 0.18024, 0.03954; 3.21346, 2.90341	0.27942	–			–		
5/3/*t*23	$I4_1/a$ 16*f*	0.13585, 0.10979, 0.12972; 2.86256, 2.72550	>0.37024	–			–		
5/3/*t*24	$I4_1/a$ 16*f*	0.24068, 0.12507, 0.08072; 1.84340, 4.38006	0.56286	–			–		
5/3/*t*25	$I4_1/amd$ 16*h*	0.00000, 0.25000, 0.19822; 2.00000, 6.82843	0.30672	4_t8^2	1,0 4	−+	–		
5/3/*t*26	$I4_122$ 16*g*	0.13706, 0.09610, 0.20815; 2.98688, 2.36585	0.39691	–			$3^6(1,2)$	1,0	c''
5/3/*t*27	$I4_122$ 16*g*	0.17689, 0.07097, 0.18656; 2.62332, 2.78650	>0.37024	–			$3^6(1,2)$	1,0	c''
5/3/*t*28	$I\bar{4}2d$ 16*e*	0.21478, 0.03522, 0.15228; 2.30940, 2.30940	0.68017	–			–		

Table 1 (continued)

Type	Symmetry	*x*, *y*, *z*; *a*, *c*	$\rho_{\min}$	Layer description			Rod description		
5/3/t29	$I\bar{4}2d$ 16*e*	0.21524, 0.02455, 0.15317; 2.30806, 2.30822	>0.68019	–			–		
5/3/t30	$I\bar{4}2d$ 16*e*	0.13388, 0.09215, 0.18849; 3.07640, 1.87570	0.47192	–			–		
5/3/t31	$I\bar{4}2d$ 16*e*	0.25000, 0.08515, 0.05939; 1.89320, 5.95351	0.39260	4_t8^2	1,0 4	−+	–		
5/3/t32	$I4_1/amd$ 32*i*	0.22181, 0.11978, 0.17828; 4.17424, 2.47028	0.38927	–			$3^6(1,2)$	1,0	p'_2
5/3/t33	$I4_1/amd$ 32*i*	0.18180, 0.12829, 0.18683; 3.89737, 2.55718	>0.37024	–			$3^6(1,2)$	1,0	p'_2
5/3/t34	$I4_1/acd$ 32*g*	0.04075, 0.17225, 0.22069; 5.34723, 1.80009	0.32553	–			$6^3(4,2)$	2,0	p_2
5/3/t35	$I4_1/acd$ 32*g*	0.06292, 0.18190, 0.10611; 5.38438, 1.47088	0.39292	–			$6^3(4,2)$	2,0	p_2
5/3/t36	$I4_1/acd$ 32*g*	0.11486, 0.23454, 0.09152; 4.26317, 2.28906	0.40274	–			$3^6(1,2)$	1,0	p'_2
5/3/t37	$I4_1/acd$ 32*g*	0.02233, 0.12510, 0.11573; 3.93449, 3.05495	0.35430	–			$3^34^2(0,2)$	1,0	p_2
5/3/t38	$I4_1/acd$ 32*g*	0.11715, 0.18737, 0.07308; 3.61986, 2.63724	>0.37024	–			$3^6(1,2)$	1,0	p'_2
5/3/t39	$I4_1/acd$ 32*g*	0.12271, 0.03551, 0.11168; 3.91406, 3.16579	0.34547	–			$3^34^2(0,2)$	1,0	p_2
5/3/t40	$I4_1/acd$ 32*g*	0.10008, 0.13838, 0.07452; 2.92772, 4.74433	0.41202	6^3	2,0 4	−+	–		
5/3/t41	$I4_1/acd$ 32*g*	0.09145, 0.19404, 0.05618; 2.33088, 6.29303	0.49006	4_t8^2	1,0 4	−+	–		
5/3/t42	$I4_1/acd$ 32*g*	0.16849, 0.12293, 0.05431; 2.39724, 6.51035	0.44784	4_t8^2	1,0 4	−+	–		
5/3/t43	$I4_1/acd$ 32*g*	0.12458, 0.23557, 0.18461; 1.99668, 7.26066	0.57884	–			–		
5/4/t1	$I4_122$ 8*d*	0.10552, 0.10552, 0.00000; 3.35071, 1.00000	0.37309	–			$4^4(1,4)$	1,0	c''
							$4^4(1,8)$	1,0	c'''
5/4/t2	$I4_1/amd$ 16*f*	0.10552, 0.25000, 0.12500; 4.73861, 1.00000	0.37309	–			$4^4(0,8)$	1,0	p_2
							$4^4(1,4)$	1,0	p'_2
5/4/t3	$I4_1cd$ 16*b*	0.13853, 0.07960, 0.00000; 3.12942, 1.73409	0.49331	–			–		
5/4/t4	$P4/mmm$ 4*l*	0.29289, 0.00000, 0.00000; 2.41421, 1.00000	0.35934	48^2	1,1 1	++	$4^4(0,4)$	1,0	*p*
5/4/t5	$P4_2/mmc$ 4*j*	0.26000, 0.00000, 0.00000; 2.08333, 1.28560	>0.37024	48^2	2,0 1	−−	$4^4(2,2)$	1,0	*p*
							$6^3(4,2)$	*d*	p'
5/4/t6	$I4/mmm$ 4*e*	0.00000, 0.00000, 0.18750; 1.33333, 2.66667	0.44179	4^4	1,0 2	−+	$6^3(0,2)$	*c*	c'
5/4/t7	$I4/m$ 8*h*	0.30561, 0.13349, 0.00000; 2.12031, 1.67367	0.55670	48^2	1,1 2	++	–		
5/4/t8	$I4/mmm$ 16*n*	0.00000, 0.26971, 0.16442; 2.62174, 3.04104	0.40079	4^4	1,0 2	−+	$6^3(0,2)$	1,1	c'
5/4/t9	$I4/m$ 16*i*	0.30019, 0.10129, 0.14590; 2.23193, 3.42709	0.49072	48^2	1,1 4	++	–		
5/4/t10	$P4/mcc$ 8*m*	0.34516, 0.14297, 0.00000; 2.37248, 1.46940	0.50646	$4_c8(8+4)$	2,0 1	−−	$4^4(4,4)$	1,0	*p*
5/4/t11	$P4/mcc$ 8*m*	0.31000, 0.15460, 0.00000; 2.04124, 1.78745	>0.54009	48^2	1,1 2	++	$4^4(0,4)$	1,0	*p*
5/4/t12	$P4/mnc$ 8*h*	0.29650, 0.07131, 0.00000; 2.31874, 1.80233	0.43227	48^2	1,1 2	++	–		
5/4/t13	$P4_2/nnm$ 8*m*	0.14775, 0.14775, 0.10486; 3.30884, 1.00000	0.38259	–			$4^4(0,4)$	1,0	*p*
							$4^4(2,8)$	*q*	p'
5/4/t14	$P4_22_12$ 8*g*	0.25000, 0.11542, 0.17281; 1.81582, 2.71510	0.46790	4^4	1,0 2	−+	–		
				$4_c(8+2)^2$	2,0 2	−+			
5/4/t15	$P4_2/mbc$ 8*h*	0.29289, 0.14645, 0.00000; 1.97120, 1.97120	0.54689	6^3	1,1 2	++	–		
5/4/t16	$I422$ 16*k*	0.25383, 0.10514, 0.07599; 4.70036, 1.00000	0.37919	–			$4^4(0,8)$	1,0	*c*
							$4^4(2,8)$	1,0	c'
5/4/t17	$I4/mcm$ 16*k*	0.22780, 0.09436, 0.00000; 3.97615, 1.32203	0.40082	48^2	1,1 1	−−	$4^4(4,4)$	1,0	*c*
							$6^3(4,2)$	2,0	c'
5/4/t18	$I4/mcm$ 16*k*	0.21524, 0.06104, 0.00000; 3.16062, 1.84513	0.45451	48^2	1,1 2	++	$4^4(0,4)$	1,0	*c*
							$6^3(4,2)$	1,1	c'
5/4/t19	$I422$ 16*k*	0.29372, 0.03416, 0.13704; 2.39130, 3.59940	0.40702	48^2	1,1 4	++	$3^34^2(0,2)$	1,0	c'
5/4/t20	$I422$ 16*k*	0.31010, 0.15505, 0.11835; 2.03951, 3.77873	>0.49958	48^2	1,1 4	++	–		
5/4/t21	$P\bar{4}2_1c$ 8*e*	0.26117, 0.13198, 0.15513; 1.83235, 2.10120	>0.56286	48^2	2,0 2	−+	–		
				6^3	2,0 2	−+			
5/4/t22	$P4/mcc$ 16*n*	0.31010, 0.15505, 0.13197; 2.03951, 3.78885	>0.49341	48^2	1,1 4	++	$4^4(0,4)$	1,0	*p*
5/4/t23	$P4/nnc$ 16*k*	0.30233, 0.11512, 0.13183; 2.18578, 3.27747	>0.52310	48^2	1,1 4	++	–		
5/4/t24	$P4/nnc$ 16*k*	0.31010, 0.15505, 0.12540; 2.03951, 3.56638	>0.54895	48^2	1,1 4	++	–		
5/4/t25	$P4/mnc$ 16*i*	0.29424, 0.04362, 0.13599; 2.37718, 3.67676	0.40321	48^2	1,1 4	++	–		
5/4/t26	$P4/ncc$ 16*g*	0.21332, 0.05627, 0.10935; 2.42038, 2.99750	0.47708	4^4	1,0 2	−+	$6^3(0,2)$	1,1	*c*
				48^2	2,0 2	−+			
5/4/t27	$P4/ncc$ 16*g*	0.19828, 0.11135, 0.11023; 2.19867, 3.44416	0.50317	48^2	1,1 4	++	–		
5/4/t28	$P4_2/nbc$ 16*k*	0.24028, 0.06971, 0.11690; 1.99849, 3.60794	0.58137	6^3	1,1 4	++	–		
5/4/t29	$P4_2/nbc$ 16*k*	0.26503, 0.08668, 0.12296; 1.99640, 3.69267	0.56923	6^3	1,1 4	++	$4^4(0,2)$	1,1	c'
5/4/t30	$P4_2/nbc$ 16*k*	0.20146, 0.15580, 0.12560; 1.96333, 3.65480	0.59466	6^3	1,1 4	++	–		
5/4/t31	$P4_2/nbc$ 16*k*	0.29842, 0.15559, 0.13044; 1.96351, 3.80176	0.57157	6^3	1,1 4	++	–		
5/4/t32	$P4_2/nnm$ 16*n*	0.25322, 0.10351, 0.10486; 4.72306, 1.00000	0.37555	–			$4^4(0,8)$	1,0	*c*
							$4^4(2,8)$	1,0	c'
5/4/t33	$P4_2/mbc$ 16*i*	0.22204, 0.11824, 0.13203; 1.98761, 3.78711	0.55995	6^3	1,1 4	++	–		
5/4/t34	$P4_2/mbc$ 16*i*	0.28367, 0.12975, 0.12690; 1.98211, 3.94020	0.54119	6^3	1,1 4	++	–		
5/4/t35	$I4/mcm$ 32*m*	0.20943, 0.06981, 0.13197; 3.20307, 3.78885	>0.42769	48^2	1,1 4	++	$4^4(0,4)$	1,0	*c*
							$48^2(0,2)$	1,1	c'
5/4/t36	$I\bar{4}c2$ 16*i*	0.20842, 0.14419, 0.12023; 1.97289, 3.79069	0.56780	6^3	1,1 4	++	–		
5/4/t37	$P4_122$ 8*d*	0.34593, 0.13795, 0.02613; 3.24086, 1.00000	0.39881	–			$4^4(3,8)$	1,0	*p*
							$4^4(1,8)$	1,0	p'
5/4/t38	$P4_122$ 8*d*	0.26920, 0.03799, 0.03237; 2.14295, 2.26680	0.40239	–			$4^4(1,4)$	1,0	*p*
5/4/t39	$P4_12_12$ 8*b*	0.26750, 0.10094, 0.32991; 1.64323, 3.23245	0.47991	–			–		
5/4/t40	$P4_12_12$ 8*b*	0.23589, 0.05982, 0.25000; 2.39125, 1.60681	0.45591	–			–		
5/4/t41	$I4_1/amd$ 16*h*	0.00000, 0.14677, 0.05194; 4.79166, 1.00000	0.36488	–			$4^4(0,4)$	1,0	p_2
							$4^4(1,8)$	*q*	p'_2
5/4/t42	$I4_1/amd$ 16*h*	0.00000, 0.14938, 0.34023; 4.48536, 1.00000	0.41641	–			$4^4(0,4)$	1,0	p_2

Table 1 (continued)

Type	Symmetry	$x, y, z; a, c$	ρ_{min}	Layer description			Rod description		
							$4^4(3,8)$	*q*	p_2'
5/4/*t*43	$I4_1/amd$ 16*h*	0.00000, 0.13146, 0.25000; 3.97071, 1.34919	0.39383	–			$4^4(2,2)$	1,0	p_2
							$6^3(4,2)$	*d*	p_2'
5/4/*t*44	$I4_1/a$ 16*f*	0.17380, 0.06643, 0.15499; 3.20777, 1.72987	0.47065	–			–		
5/4/*t*45	$I4_1/amd$ 16*h*	0.00000, 0.22000, 0.34339; 2.31357, 2.26730	>0.68623	–			$4^4(0,2)$	*d*	p_2'
5/4/*t*46	$I4_1/a$ 16*f*	0.20366, 0.10394, 0.21615; 2.18670, 3.52241	>0.48291	48^2	1,1 4	−+	–		
5/4/*t*47	$I4_1/a$ 16*f*	0.23176, 0.09375, 0.12500; 2.00000, 3.58223	>0.56264	–			–		
5/4/*t*48	$I4_1/a$ 16*f*	0.23884, 0.13164, 0.17250; 1.83339, 4.20602	>0.56286	48^2	2,0 4	−+	–		
5/4/*t*49	$I4_1/a$ 16*f*	0.23000, 0.15202, 0.12500; 2.00000, 3.83666	>0.52360	–			–		
5/4/*t*50	$I4_1/a$ 16*f*	0.23437, 0.16300, 0.07863; 1.83690, 4.26541	>0.56286	–			–		
5/4/*t*51	$I4_1/a$ 16*f*	0.22205, 0.20372, 0.19437; 1.84192, 3.96013	>0.60433	–			–		
5/4/*t*52	$I4_1/a$ 16*f*	0.23979, 0.17929, 0.17961; 1.75148, 4.42069	>0.61030	–			–		
5/4/*t*53	$I4_1/a$ 16*f*	0.21419, 0.21419, 0.19851; 1.77010, 4.34953	>0.59935	4^4	1,0 4	−+	–		
5/4/*t*54	$I4_122$ 16*g*	0.13213, 0.09797, 0.21993; 3.03978, 2.24885	0.40316	–			$4^4(2,3)$	1,0	c''
5/4/*t*55	$I\bar{4}2d$ 16*e*	0.22080, 0.02873, 0.15142; 2.35514, 2.21509	>0.68079	–			–		
5/4/*t*56	$I\bar{4}2d$ 16*e*	0.22484, 0.03275, 0.15491; 2.27829, 2.36837	>0.68072	–			–		
5/4/*t*57	$I\bar{4}2d$ 16*e*	0.22008, 0.02084, 0.15823; 2.26180, 2.39897	>0.68085	48^2	1,1 4	−+	–		
5/4/*t*58	$I\bar{4}2d$ 16*e*	0.16196, 0.10215, 0.12500; 3.38173, 1.60681	0.45591	–			–		
5/4/*t*59	$I\bar{4}2d$ 16*e*	0.20057, 0.10219, 0.23400; 2.22121, 3.45961	0.49081	48^2	1,1 4	−+	–		
5/4/*t*60	$I4_1/amd$ 32*i*	0.07362, 0.17717, 0.05194; 6.79166, 1.00000	0.36324	–			$4^4(0,8)$	1,0	p_2
							$4^4(1,8)$	1,0	p_2'
5/4/*t*61	$I4_1/amd$ 32*i*	0.18041, 0.07710, 0.15977; 6.48536, 1.00000	0.39836	–			$4^4(0,8)$	1,0	p_2
							$4^4(3,8)$	1,0	p_2'
5/4/*t*62	$I4_1/amd$ 32*i*	0.22583, 0.11704, 0.16317; 4.27213, 2.30946	0.39751	–			$4^4(2,3)$	1,0	p_2'
5/4/*t*63	$I4_1/acd$ 32*g*	0.11997, 0.15387, 0.03645; 3.57246, 2.30677	>0.56498	–			$6^3(0,2)$	1,1	p_2
							$4^4(0,2)$	1,1	p_2'
5/4/*t*64	$I4_1/acd$ 32*g*	0.11698, 0.16790, 0.04187; 3.36808, 2.67010	>0.50819	–			$4^4(0,2)$	1,1	p_2'
5/4/*t*65	$I4_1/acd$ 32*g*	0.11627, 0.17425, 0.03561; 3.30875, 2.77935	>0.50819	48^2	1,1 4	−+	$4^4(0,2)$	1,1	p_2'
5/4/*t*66	$I4_1/acd$ 32*g*	0.06573, 0.18427, 0.12500; 5.61544, 1.34919	0.39383	–			$6^3(4,2)$	2,0	p_2
							$6^3(4,3)$	2,0	p_2'
5/4/*t*67	$I4_1/acd$ 32*g*	0.06853, 0.16544, 0.00000; 5.60095, 1.28180	0.41668	–			$4^4(4,4)$	1,0	p_2
							$6^3(4,3)$	2,0	p_2'
5/4/*t*68	$I4_1/acd$ 32*g*	0.07359, 0.14641, 0.00000; 4.31527, 1.79170	0.50219	–			$4^4(0,4)$	1,0	p_2
							$6^3(4,3)$	2,0	p_2'
5/4/*t*69	$I4_1/acd$ 32*g*	0.06067, 0.15586, 0.03502; 4.18933, 1.92066	0.49706	–			$6^3(0,2)$	2,0	p_2
5/4/*t*70	$I4_1/acd$ 32*g*	0.11429, 0.23569, 0.09852; 4.31066, 2.21987	0.40619	–			$4^4(2,3)$	1,0	p_2'
5/4/*t*71	$I4_1/acd$ 32*g*	0.09725, 0.13221, 0.10034; 3.22978, 3.29794	0.48704	–			$6^3(0,2)$	1,1	p_2
5/4/*t*72	$I4_1/acd$ 32*g*	0.06390, 0.21337, 0.00596; 3.17161, 3.71351	0.44854	48^2	1,1 4	−+	–		
5/4/*t*73	$I4_1/acd$ 32*g*	0.11408, 0.17610, 0.05712; 2.85859, 4.63601	0.44228	48^2	2,0 4	−+	–		
5/4/*t*74	$I4_1/acd$ 32*g*	0.08470, 0.23565, 0.18868; 1.99671, 7.37567	0.56979	6^3	1,1 8	++	–		
5/4/*t*75	$I4_1/acd$ 32*g*	0.06857, 0.24060, 0.05838; 1.99859, 7.21213	0.58162	6^3	1,1 8	++	–		
5/4/*t*76	$I4_1/acd$ 32*g*	0.22496, 0.11190, 0.05896; 1.99004, 7.53354	0.56160	6^3	1,1 8	++	–		
5/4/*t*77	$I4_1/acd$ 32*g*	0.21920, 0.12409, 0.18842; 1.98500, 7.82477	0.54345	6^3	1,1 8	++	–		
5/4/*t*78	$I4_1/acd$ 32*g*	0.16297, 0.19688, 0.06188; 1.95633, 7.44801	0.58779	6^3	1,1 8	++	–		
5/4/*t*79	$I4_1/acd$ 32*g*	0.16126, 0.19799, 0.18565; 1.95807, 7.72997	0.56534	6^3	1,1 8	++	–		
5/5/*t*1	$I4_1cd$ 16*b*	0.20835, 0.14430, 0.00000; 1.97282, 3.79375	0.56738	6^3	1,1 4	++	–		
5/5/*t*2	$P4_2/mbc$ 8*h*	0.21062, 0.14031, 0.00000; 1.97564, 1.81829	0.59021	6^3	1,1 2	++	–		
6/3/*t*1	$P4_122$ 4*a*	0.00000, 0.30629, 0.00000; 2.23533, 1.00000	0.41915	–			$4^4(1,4)$	2,0	*p*
							$3^34^2(4,3)$	*t*	p'
6/3/*t*4	$I4_1/acd$ 16*e*	0.25000, 0.09686, 0.12500; 4.47066, 1.00000	0.41915	–			$3^34^2(4,2)$	*t*	p_2
							$4^4(1,4)$	2,0	p_2'
6/3/*t*5	$P4_2/mmc$ 4*j*	0.25000, 0.00000, 0.00000; 2.00000, 1.41421	0.37024	4_t8^2	2,0 1	−−	$3^6(0,2)$	1,0	*p*
							$6^3(4,2)$	*d*	p'
6/3/*t*6	$P4_2/mnm$ 8*j*	0.19471, 0.19471, 0.18276; 1.81582, 2.73587	0.46435	3^2434	1,0 2	−+	$6^3(0,2)$	*d*	c'
6/3/*t*7	$I4/mmm$ 8*h*	0.15505, 0.15505, 0.00000; 3.22474, 1.00000	0.40281	48^2	2,1 1	−−	$4^4(0,4)$	2,0	*c*
							$3^34^2(4,2)$	*t*	c'
6/3/*t*8	$P4_2/ncm$ 8*i*	0.19757, 0.69757, 0.07398; 1.78954, 2.73865	0.47761	3^2434	1,0 2	−+	$6^3(0,2)$	2,1	*c*
6/3/*t*9	$I4/m$ 16*i*	0.26677, 0.07711, 0.17049; 2.54636, 2.93272	0.44056	3^2434	1,0 2	−+	$6^3(0,2)$	2,1	c'
6/3/*t*11	$I4/mmm$ 16*l*	0.26021, 0.10778, 0.00000; 4.63896, 1.00000	0.38929	48^2	2,1 1	−−	$4^4(0,8)$	2,0	*c*
							$3^34^2(4,2)$	1,0	c'
6/3/*t*12	$I422$ 16*k*	0.30421, 0.12601, 0.11562; 2.14746, 3.63637	0.49958	48^2	2,1 4	++	$4^4(0,2)$	1,1	c'
6/3/*t*13	$P\bar{4}2c$ 8*n*	0.30517, 0.13143, 0.00688; 2.12754, 1.70495	>0.54009	48^2	2,1 2	−+	$3^2434(0,2)$	1,0	*p*
6/3/*t*14	$P\bar{4}2_1c$ 8*e*	0.23207, 0.13798, 0.18101; 1.92730, 1.87035	0.60293	–			–		
6/3/*t*15	$P\bar{4}2_1c$ 8*e*	0.25000, 0.10522, 0.16144; 1.84340, 2.19003	0.56286	4_t8^2	1,1 2	−+	–		
				4^4	2,0 2	−+			
6/3/*t*16	$P\bar{4}c2$ 8*j*	0.28350, 0.03488, 0.09863; 2.28005, 1.97454	0.40807	48^2	2,1 4	++	$3^2434(0,2)$	1,0	*p*
6/3/*t*17	$I\bar{4}2m$ 16*j*	0.33411, 0.11787, 0.16331; 3.27006, 1.95007	0.40175	48^2	2,1 2	−+	$3^2434(0,2)$	1,0	c'
6/3/*t*18	$P4/mcc$ 16*n*	0.30421, 0.12601, 0.13580; 2.14746, 3.68179	0.49341	48^2	2,1 4	++	$3^34^2(0,4)$	1,0	*p*
6/3/*t*19	$P4/nnc$ 16*k*	0.32546, 0.12042, 0.16727; 3.15795, 1.94070	0.43286	48^2	2,1 2	−+	$3^2434(0,2)$	1,0	c'
6/3/*t*20	$P4/nnc$ 16*k*	0.26672, 0.07708, 0.16595; 2.54687, 2.77092	0.46610	3^2434	1,0 2	−+	$6^3(0,2)$	2,1	c'

Table 1 (continued)

Type	Symmetry	*x*, *y*, *z*; *a*, *c*	ρ_{min}	Layer description			Rod description		
6/3/*t*21	*P*4/*nnc* 16*k*	0.30421, 0.12601, 0.12705; 2.14746, 3.30930	0.54895	48^2	2,1 4	++	–		
6/3/*t*22	*P*4/*ncc* 16*g*	0.25385, 0.10196, 0.01264; 3.37402, 1.45138	0.50704	–			6^3(4,2)	3,0	*c*
							4^4(4,4)	2,0	c'
6/3/*t*23	*P*4/*ncc* 16*g*	0.22785, 0.08055, 0.02500; 2.91448, 1.76582	>0.54009	48^2	2,1 2	−+	3^2434(0,2)	1,0	*c*
6/3/*t*24	*P*4/*ncc* 16*g*	0.22065, 0.08532, 0.09957; 2.42087, 2.94544	0.48532	3^2434	1,0 2	−+	6^3(0,2)	2,1	*c*
6/3/*t*25	*P*4/*ncc* 16*g*	0.20538, 0.04933, 0.11333; 2.36713, 3.11962	0.47926	48^2	2,1 4	++	3^34^2(0,2)	1,1	*c*
6/3/*t*26	$P4_2/nbc$ 16*k*	0.24291, 0.10784, 0.14514; 4.53359, 1.00000	0.40760	–			3^34^2(4,2)	1,0	*c*
							4^4(2,8)	2,0	c'
6/3/*t*27	$P4_2/nbc$ 16*k*	0.17866, 0.11101, 0.06779; 3.24824, 1.90098	0.41768	48^2	2,1 2	−+	3^2434(0,2)	1,0	*c*
6/3/*t*28	$P4_2/nbc$ 16*k*	0.21770, 0.12709, 0.12760; 1.98351, 3.52770	0.60361	6^3	2,1 4	++	–		
6/3/*t*29	$P4_2/nbc$ 16*k*	0.28230, 0.12709, 0.13207; 1.98351, 3.66154	0.58155	6^3	2,1 4	++	4^4(0,2)	2,1	c'
6/3/*t*30	$P4_2/ncm$ 16*j*	0.20898, 0.06925, 0.03361; 3.18845, 1.79441	0.45924	48^2	2,1 2	−+	3^2434(0,2)	1,0	*c*
							6^3(4,2)	2,1	c'
6/3/*t*31	*I*4/*mcm* 32*m*	0.20027, 0.08296, 0.13580; 3.26197, 3.68179	0.42769	48^2	2,1 4	++	3^34^2(0,4)	1,0	*c*
							48^2(0,2)	2,1	c'
6/3/*t*32	$I\bar{4}2d$ 8*d*	0.12500, 0.25000, 0.12500; 2.30940, 1.63299	0.48096	–			–		
6/3/*t*33	$I\bar{4}c2$ 16*i*	0.20728, 0.07297, 0.02559; 3.20459, 1.76779	0.46147	48^2	2,1 2	−+	3^2434(0,2)	1,0	*c*
							6^3(4,2)	2,1	c'
6/3/*t*34	$P4_122$ 8*d*	0.34546, 0.13384, 0.00000; 3.23533, 1.00000	0.40018	–			3^34^2(4,3)	1,0	*p*
							4^4(1,8)	2,0	p'
6/3/*t*35	$P4_12_12$ 8*b*	0.24354, 0.10331, 0.34293; 1.69276, 2.99846	0.48753	–			–		
6/3/*t*36	$I4_1/a$ 16*f*	0.25348, 0.13954, 0.08276; 1.89295, 3.82093	>0.58803	–			–		
6/3/*t*37	$I4_1/amd$ 16*h*	0.00000, 0.15314, 0.37500; 4.47066, 1.00000	0.41915	–			4^4(0,4)	2,0	p_2
							3^34^2(4,3)	*t*	p'_2
6/3/*t*38	$I4_1/a$ 16*f*	0.18750, 0.06250, 0.12500; 3.26599, 1.63299	0.48096	–			–		
6/3/*t*39	$I4_1/amd$ 16*h*	0.00000, 0.12917, 0.25000; 3.87083, 1.41421	0.39536	–			3^6(0,2)	1,0	p_2
							6^3(4,3)	*d*	p'_2
6/3/*t*40	$I4_1/a$ 16*f*	0.12500, 0.12500, 0.12500; 2.82843, 2.82843	0.37024	–			–		
6/3/*t*41	$I4_1/a$ 16*f*	0.15387, 0.06546, 0.18600; 2.99011, 1.90083	0.49295	–			–		
6/3/*t*42	$I4_1/amd$ 16*h*	0.00000, 0.21785, 0.34000; 2.29513, 2.30012	>0.69103	–			4^4(0,2)	*d*	p'_2
6/3/*t*43	$I4_1/a$ 16*f*	0.20096, 0.09339, 0.24597; 2.25625, 3.40779	0.48291	48^2	2,1 4	−+	–		
6/3/*t*44	$I4_1/a$ 16*f*	0.25000, 0.10522, 0.08072; 1.84340, 4.38006	0.56286	4_t8^2	2,0 4	−+	–		
				4^4	2,0 4	−+			
6/3/*t*45	$I4_1/a$ 16*f*	0.21651, 0.12500, 0.12500; 2.00000, 3.72242	0.56264	–			–		
6/3/*t*46	$I4_1/a$ 16*f*	0.22786, 0.14714, 0.08072; 1.84340, 4.38006	0.56286	–			–		
6/3/*t*47	$I4_1/a$ 16*f*	0.23496, 0.16461, 0.17927; 1.74286, 4.51911	0.61030	48^2	3,0 4	−+	–		
6/3/*t*48	$I4_1/a$ 16*f*	0.20145, 0.20145, 0.20061; 1.75500, 4.53821	0.59935	3^2434	1,0 4	−+	–		
6/3/*t*49	$I\bar{4}2d$ 16*e*	0.21974, 0.03535, 0.16398; 2.29011, 2.34657	0.68072	–			–		
6/3/*t*50	$I\bar{4}2d$ 16*e*	0.21927, 0.03911, 0.15151; 2.35446, 2.21373	>0.68079	–			–		
6/3/*t*51	$I\bar{4}2d$ 16*e*	0.21362, 0.03531, 0.15308; 2.30929, 2.30957	0.68019	–			–		
6/3/*t*52	$I\bar{4}2d$ 16*e*	0.21247, 0.02742, 0.15675; 2.33397, 2.25552	>0.68079	–			–		
6/3/*t*53	$I\bar{4}2d$ 16*e*	0.21707, 0.03102, 0.16612; 2.28020, 2.36660	0.68085	48^2	2,1 4	−+	–		
6/3/*t*54	$I\bar{4}2d$ 16*e*	0.19608, 0.19608, 0.21467; 1.80309, 5.46982	0.47110	3^2434	1,0 4	−+	–		
6/3/*t*55	$I4_1/amd$ 32*i*	0.18308, 0.07727, 0.12500; 6.47066, 1.00000	0.40018	–			4^4(0,8)	2,0	p_2
							3^34^2(4,3)	1,0	p'_2
6/3/*t*56	$I4_1/amd$ 32*i*	0.17419, 0.07830, 0.25000; 6.38598, 1.00000	0.41086	–			3^34^2(4,2)	1,0	p_2
							3^34^2(4,3)	1,0	p'_2
6/3/*t*57	$I4_1/acd$ 32*g*	0.17418, 0.06638, 0.19806; 6.52371, 1.00000	0.39369	–			3^34^2(4,2)	1,0	p_2
							4^4(1,8)	2,0	p'_2
6/3/*t*58	$I4_1/acd$ 32*g*	0.06965, 0.17741, 0.09023; 6.21741, 1.00000	0.43344	–			3^34^2(4,2)	1,0	p_2
							4^4(3,8)	2,0	p'_2
6/3/*t*59	$I4_1/acd$ 32*g*	0.05462, 0.15207, 0.02277; 4.36212, 1.75838	0.50077	–			3^2434(0,2)	1,0	p_2
6/3/*t*60	$I4_1/acd$ 32*g*	0.14189, 0.02046, 0.09331; 4.58901, 1.96441	0.40502	–			3^2434(0,2)	1,0	p_2
6/3/*t*61	$I4_1/acd$ 32*g*	0.01542, 0.14151, 0.10202; 4.54392, 1.98026	0.40979	–			3^2434(0,2)	1,0	p_2
6/3/*t*62	$I4_1/acd$ 32*g*	0.12177, 0.15247, 0.03823; 3.56563, 2.33261	0.56498	–			6^3(0,2)	2,1	p_2
							3^6(1,2)	1,1	p'_2
6/3/*t*63	$I4_1/acd$ 32*g*	0.10908, 0.16699, 0.05389; 3.41954, 2.44762	>0.58138	–			6^3(0,2)	2,1	p_2
							4^4(0,2)	2,1	p'_2
6/3/*t*64	$I4_1/acd$ 32*g*	0.11043, 0.17624, 0.03778; 3.32972, 2.67558	>0.56200	–			4^4(0,2)	2,1	p'_2
6/3/*t*65	$I4_1/acd$ 32*g*	0.11337, 0.17373, 0.04590; 3.29967, 2.73289	>0.56057	–			4^4(0,2)	2,1	p'_2
6/3/*t*66	$I4_1/acd$ 32*g*	0.12102, 0.17017, 0.03338; 3.32653, 2.80221	>0.50819	48^2	2,1 4	−+	3^6(1,2)	1,1	p'_2
6/3/*t*67	$I4_1/acd$ 32*g*	0.11250, 0.17742, 0.03909; 3.28628, 2.76508	>0.56057	48^2	2,1 4	−+	4^4(0,2)	2,1	p'_2
6/3/*t*68	$I4_1/acd$ 32*g*	0.06459, 0.18541, 0.12500; 5.47418, 1.41421	0.39536				6^3(4,2)	3,0	p_2
							6^3(4,3)	3,0	p'_2
6/3/*t*69	$I4_1/acd$ 32*g*	0.09424, 0.12599, 0.10418; 3.17790, 3.39375	0.48886	6^3	2,1 4	−+	3^34^2(0,2)	1,1	p_2
6/3/*t*70	$I4_1/acd$ 32*g*	0.11408, 0.17610, 0.06017; 2.38298, 5.87567	0.50217	4_t8^2	2,0 4	−+	–		
				6^3	3,0 4	−+			
6/3/*t*71	$I4_1/acd$ 32*g*	0.12316, 0.21966, 0.06369; 1.98544, 7.04498	0.60333	6^3	2,1 8	++	–		
6/3/*t*72	$I4_1/acd$ 32*g*	0.12316, 0.21966, 0.18412; 1.98544, 7.30594	0.58178	6^3	2,1 8	++	–		
6/4/*t*2	$I4_1/amd$ 4*a*	0.00000, 0.00000. 0.00000; 1.93649, 1.00000	0.55851	–			4^4(1,4)	*q*	p'_2
6/4/*t*3	$I4_1/amd$ 8*c*	0.00000, 0.25000, 0.12500; 2.73861, 1.00000	0.55851	–			4^4(0,4)	*c*	p_2

Table 1 (continued)

Type	Symmetry	*x*, *y*, *z*; *a*, *c*	ρ_{min}	Layer description			Rod description		
							4^4(1,4)	*c*	p'_2
6/4/*t*4	$I4_1/amd$ 16*g*	0.12702, 0.12702, 0.00000; 3.93649, 1.00000	0.54063	–			4^4(0,4)	1,1	p_2
							4^4(1,4)	1,1	p'_2
6/4/*t*5	$I4_1/acd$ 16*f*	0.10799, 0.10799, 0.25000; 3.29666, 1.40438	0.54889	–			4^4(2,2)	1,1	p_2
6/4/*t*6	$I4/mcm$ 8*i*	0.14645, 0.64645, 0.00000; 2.78769, 1.15470	0.46680	48^2	3,0 1	−−	4^4(4,4)	2,0	*c*
6/4/*t*7	$I4/mmm$ 8*i*	0.28000, 0.00000, 0.00000; 2.52538, 1.23718	>0.50819	4^4	2,0 1	−−	4^4(2,2)	1,1	*c*′
6/4/*t*8	$I\bar{4}2m$ 8*i*	0.21000, 0.21000, 0.15000; 1.76666, 2.23467	>0.58768	4^4	1,1 2	−+	6^3(0,2)	*p*	*c*′
6/4/*t*9	$P4/ncc$ 16*g*	0.26360, 0.07880, 0.06250; 2.83766, 1.78885	>0.55913	48^2	2,1 2	−+	6^3(4,2)	2,1	*c*
				48^2	2,1 2	−+	4^4(0,4)	2,0	*c*′
6/4/*t*10	$I4_1/amd$ 8*e*	0.00000, 0.00000, 0.20505; 1.27500, 4.81239	0.53543	4^4	2,0 4	−+	–		
6/4/*t*11	$I4_1/amd$ 16*h*	0.00000, 0.23000, 0.36000; 2.21178, 2.48061	>0.68017	–			4^4(0,2)	*p*	p'_2
6/4/*t*12	$I4_1/a$ 16*f*	0.20535, 0.16612, 0.19516; 1.89303, 3.86839	0.60433	48^2	2,1 4	−+	–		
6/4/*t*13	$I\bar{4}2d$ 16*e*	0.13452, 0.11841, 0.13514; 3.79889, 1.00000	0.58050	–			4^4(0,4)	1,1	p_2
6/4/*t*14	$I\bar{4}2d$ 16*e*	0.21952, 0.03139, 0.15973; 2.25474, 2.41498	>0.68099	48^2	2,1 4	−+	–		
6/4/*t*15	$I4_1/acd$ 32*g*	0.12192, 0.15093, 0.03026; 3.61042, 2.25033	0.57120	–			6^3(0,2)	2,1	p_2
							4^4(2,3)	1,1	p'_2
7/3/*t*1	$I4_1md$ 8*b*	0.00000, 0.18809, 0.00000; 2.65831, 1.00000	0.59276	–			4^4(1,4)	*c*	p'_2
7/3/*t*2	$I4_1/acd$ 16*f*	0.10763, 0.10763, 0.25000; 3.28504, 1.41421	0.54894	–			3^6(0,2)	1,1	p_2
7/3/*t*3	$I4_1/acd$ 16*f*	0.18301, 0.18301, 0.25000; 1.93185, 3.86370	0.58099	3^2434	1,1 4	++	–		
7/3/*t*4	$P4_2/mmc$ 4*j*	0.27526, 0.00000, 0.00000; 2.22474, 1.00000	0.42315	48^2	3,1 1	−−	3^6(2,4)	1,0	*p*
							3^34^2(4,2)	*q*	*p*′
7/3/*t*5	$P4/mbm$ 4*g*	0.18301, 0.68301, 0.00000; 1.93185, 1.00000	0.56119	3^2434	1,1 1	++	4^4(0,4)	*c*	*c*
7/3/*t*6	$I4/mcm$ 8*i*	0.14645, 0.64645, 0.00000; 2.41421, 1.41421	0.50819	$4,8^2$	3,0 1	−−	4^4(4,4)	*c*	*c*
							3^6(0,2)	2,0	*c*′
7/3/*t*7	$I4/mmm$ 8*i*	0.29289, 0.00000, 0.00000; 2.41421, 1.41421	0.50819	48^2	2,2 2	++	3^6(0,2)	1,1	*c*′
7/3/*t*8	$I4/mcm$ 8*i*	0.18301, 0.68301, 0.00000; 1.93185, 1.86121	0.60304	3^2434	1,1 2	++	4^4(0,4)	*c*	*c*
7/3/*t*9	$P4_2/n$ 8*g*	0.28162, 0.06583, 0.07537; 2.40000, 1.26600	>0.55951	–			4^4(2,2)	2,1	*c*′
7/3/*t*10	$I4/m$ 16*i*	0.30000, 0.10000, 0.14645; 2.23607, 3.41421	0.49075	48^2	3,1 4	++	3^34^2(0,2)	2,1	*c*′
7/3/*t*11	$I4/mcm$ 16*l*	0.18301, 0.68301, 0.12949; 1.93185, 3.86121	0.58136	3^2434	1,1 4	++	4^4(0,4)	*c*	*c*
7/3/*t*12	$P4/mcc$ 8*m*	0.30421, 0.12601, 0.00000; 2.14746, 1.68179	0.54009	48^2	2,2 2	++	3^6(0,4)	1,0	*p*
7/3/*t*13	$I4/mcm$ 16*k*	0.23916, 0.09906, 0.00000; 4.37101, 1.00000	0.43849	48^2	3,1 1	−−	3^6(4,8)	1,0	*c*
							3^34^2(4,2)	2,0	*c*′
7/3/*t*14	$I4/mcm$ 16*k*	0.20027, 0.08296, 0.00000; 3.26197, 1.68179	0.46815	48^2	2,2 2	++	3^6(0,4)	1,0	*c*
							6^3(4,2)	3,1	*c*′
7/3/*t*15	$I\bar{4}2m$ 8*i*	0.19894, 0.19894, 0.15666; 1.77715, 2.25683	0.58768	3^2434	2,0 2	−+	–		
7/3/*t*16	$P\bar{4}2_1c$ 8*e*	0.26028, 0.10139, 0.17569; 1.92101, 1.85339	0.61244	6^3	3,1 2	−+	–		
				48^2	3,1 2	−+			
7/3/*t*17	$P\bar{4}2_1c$ 8*e*	0.22060, 0.13252, 0.19321; 1.94294, 1.82988	0.60639	6^3	3,1 2	−+	–		
7/3/*t*18	$P4/nnc$ 16*k*	0.30000, 0.10000, 0.13962; 2.23607, 3.20307	0.52310	48^2	3,1 4	++	3^34^2(0,2)	2,1	*c*′
7/3/*t*19	$P4/ncc$ 16*g*	0.23976, 0.03023, 0.09788; 2.69897, 1.97319	0.58284	4^4	2,1 2	−+	3^2434(0,2)	1,1	*c*
				48^2	3,1 2	−+	4^4(0,4)	2,1	*c*′
7/3/*t*20	$P4/ncc$ 16*g*	0.20000, 0.10000, 0.10676; 2.23607, 3.31158	0.50596	48^2	3,1 4	++	3^34^2(0,2)	2,1	*c*
7/3/*t*21	$I\bar{4}$ 8*g*	0.30376, 0.13008, 0.03694; 2.12375, 1.65938	0.55968	48^2	3,1 2	−+	–		
7/3/*t*22	$I4_1/amd$ 8*e*	0.00000, 0.00000, 0.06699; 1.00000, 7.46410	0.56119	4^4	2,1 8	++	–		
7/3/*t*23	$P4_12_12$ 8*b*	0.32793, 0.00000, 0.35147; 1.39185, 3.76359	0.57451	4^4	2,1 4	−+	–		
7/3/*t*24	$P4_12_12$ 8*b*	0.24567, 0.01764, 0.25000; 2.68550, 1.00000	0.58081	–			4^4(1,4)	2,1	*c*′
7/3/*t*25	$I4_1/amd$ 16*h*	0.00000, 0.13962, 0.25000; 4.38598, 1.00000	0.43550	–			3^6(2,4)	1,0	p_2
							3^34^2(4,3)	*q*	p'_2
7/3/*t*26	$I4_1/a$ 16*f*	0.09352, 0.16049, 0.03403; 3.79791, 1.00000	0.58080	–			4^4(0,4)	2,1	p_2
							4^4(1,4)	2,1	p'_2
7/3/*t*27	$I4_1/a$ 16*f*	0.13953, 0.08585, 0.25000; 3.40000, 1.23207	>0.56966	–			4^4(2,2)	2,1	p_2
7/3/*t*28	$I4_1/amd$ 16*h*	0.00000, 0.23157, 0.35163; 2.35678, 2.19792	0.68623	–			3^6(1,2)	*d*	p'_2
7/3/*t*29	$I4_1/amd$ 16*h*	0.00000, 0.22150, 0.35161; 2.25733, 2.38253	0.69006	–			4^4(0,2)	*p*	p'_2
7/3/*t*30	$I4_1/amd$ 16*h*	0.00000, 0.22150, 0.34607; 2.25733, 2.38253	0.69006	–			–		
7/3/*t*31	$I4_1/a$ 16*f*	0.24327, 0.07000, 0.10228; 1.97517, 3.45680	>0.58803	–			–		
7/3/*t*32	$I4_1/a$ 16*f*	0.23885, 0.10140, 0.16165; 1.92688, 3.65538	0.61727	48^2	3,1 4	−+	–		
7/3/*t*33	$I4_1/a$ 16*f*	0.23244, 0.15797, 0.08467; 1.90000, 3.87117	>0.58803	–			–		
7/3/*t*34	$I4_1/a$ 16*f*	0.23156, 0.15578, 0.17444; 1.84759, 3.87210	0.63382	–			–		
7/3/*t*35	$I4_1/a$ 16*f*	0.19608, 0.19608, 0.20896; 1.85111, 3.91949	0.62377	4^4	2,1 4	−+	–		
7/3/*t*36	$I\bar{4}2d$ 16*e*	0.13599, 0.11835, 0.12500; 3.79788, 1.00000	0.58081	–			4^4(0,4)	2,1	p_2
7/3/*t*37	$I\bar{4}2d$ 16*e*	0.21050, 0.03827, 0.15691; 2.33695, 2.25323	0.68079	–			–		
7/3/*t*38	$I\bar{4}2d$ 16*e*	0.21684, 0.03474, 0.16673; 2.27680, 2.37317	0.68099	–			–		
7/3/*t*39	$I4_1/acd$ 32*g*	0.06981, 0.18019, 0.12500; 6.20271, 1.00000	0.43550	–			3^34^2(4,2)	2,0	p_2
							3^34^2(4,3)	2,0	p'_2
7/3/*t*40	$I4_1/acd$ 32*g*	0.07078, 0.17087, 0.00000; 6.11803, 1.00000	0.44764	–			3^6(4,8)	1,0	p_2
							3^34^2(4,3)	2,0	p'_2
7/3/*t*41	$I4_1/acd$ 32*g*	0.06111, 0.14754, 0.00000; 4.42776, 1.68179	0.50817	–			3^6(0,4)	1,0	p_2
							6^3(4,3)	3,1	p'_2
7/3/*t*42	$I4_1/acd$ 32*g*	0.05191, 0.15409, 0.03150; 4.32106, 1.78742	0.50204	–			3^2434(0,2)	2,0	p_2
7/3/*t*43	$I4_1/acd$ 32*g*	0.10706, 0.16792, 0.04867; 3.45489, 2.37115	0.59200	–			6^3(0,2)	3,1	p_2
							4^4(2,3)	2,1	p'_2

Table 1 (continued)

Type	Symmetry	$x, y, z; a, c$	$\rho_{\min}$	Layer description			Rod description		
7/3/*t*44	$I4_1/acd$ 32*g*	0.11091, 0.16608, 0.05817; 3.38588, 2.51387	0.58138	–			$6^3(0,2)$	2,2	p_2
							$3^6(1,2)$	2,1	p_2'
7/3/*t*45	$I4_1/acd$ 32*g*	0.11123, 0.17847, 0.03576; 3.29709, 2.74250	0.56200	48^2	2,2 4	−+	$3^6(1,2)$	2,1	p_2'
7/3/*t*46	$I4_1/acd$ 32*g*	0.11408, 0.17610, 0.04311; 3.27082, 2.79386	0.56057	48^2	3,1 4	−+	$3^6(1,2)$	2,1	p_2'
7/3/*t*47	$I4_1/acd$ 32*g*	0.18301, 0.18301, 0.06134; 1.93185, 7.58612	0.59181	3^2434	1,1 8	++	–		
7/3/*t*48	$I4_1/acd$ 32*g*	0.18301, 0.18301, 0.18642; 1.93185, 7.86370	0.57092	3^2434	1,1 8	++	–		
7/4/*t*1	$I4_1/a$ 16*f*	0.15728, 0.08685, 0.18750; 3.64846, 1.00000	>0.62056	–			$4^4(0,4)$	2,1	p_2
							$4^4(1,4)$	2,1	p_2'
7/4/*t*2	$I4_1/amd$ 16*h*	0.00000, 0.23215, 0.35514; 2.37238, 2.16477	0.68760	–			$4^4(2,3)$	*d*	p_2'
8/3/*t*1	$I4_1/amd$ 4*a*	0.00000, 0.00000, 0.00000; 1.00000, 3.46410	0.60460	4^4	2,2 4	++	–		
8/3/*t*2	$P4_12_12$ 4*a*	0.16667, 0.16667, 0.00000; 1.83712, 1.00000	0.62056	–			$4^4(1,4)$	*c*	*c*
8/3/*t*3	$I4_1/acd$ 16*f*	0.11803, 0.11803, 0.25000; 3.66854, 1.00000	0.62249	–			$3^6(2,4)$	1,1	p_2
							$4^4(1,4)$	2,2	p_2'
8/3/*t*4	$I4/mcm$ 8*i*	0.14645, 0.64645, 0.00000; 2.95680, 1.00000	0.47912	48^2	4,1 1	−−	$3^6(4,8)$	*t*	*c*
							$3^6(2,4)$	2,0	*c*′
8/3/*t*5	$I4/mmm$ 8*i*	0.26795, 0.00000, 0.00000; 2.63896, 1.00000	0.60148	4^4	3,1 1	−−	$4^4(0,4)$	2,2	*c*
							$3^6(2,4)$	1,1	*c*′
8/3/*t*6	$I4/m$ 8*h*	0.29380, 0.09543, 0.00000; 2.28904, 1.35500	0.58998	3^2434	3,0 1	−−	$4^4(2,2)$	3,1	*c*′
8/3/*t*7	$P4_2/n$ 8*g*	0.29260, 0.06490, 0.07823; 2.30081, 1.41421	0.55951	48^2	3,2 2	−+	$3^6(0,2)$	2,1	*c*′
8/3/*t*8	$I\bar{4}2m$ 8*i*	0.19823, 0.19823, 0.17410; 1.87313, 1.92330	0.62073	4^4	3,1 2	−+	$3^2434(0,2)$	*c*	*c*′
8/3/*t*9	$P4/ncc$ 16*g*	0.28113, 0.09066, 0.07322; 2.98481, 1.68179	0.55913	48^2	3,2 2	−+	$6^3(4,2)$	4,1	*c*
				48^2	3,2 2	−+	$3^6(0,4)$	2,0	*c*′
8/3/*t*10	$P4/ncc$ 16*g*	0.24731, 0.06855, 0.05335; 2.70066, 1.85784	0.61826	3^2434	2,1 2	−+	$3^2434(0,2)$	2,1	*c*
				48^2	4,1 2	−+	$4^4(0,4)$	3,1	*c*′
8/3/*t*11	$I\bar{4}2d$ 8*d*	0.08333, 0.25000, 0.12500; 2.59808, 1.00000	0.62056	–			$4^4(0,4)$	*c*	p_2
8/3/*t*12	$P4_12_12$ 8*b*	0.37039, 0.12961, 0.21277; 1.35815, 3.74389	0.60655	4^4	3,1 2	−+	–		
8/3/*t*13	$I4_1/a$ 16*f*	0.16667, 0.08333, 0.12500; 3.67423, 1.00000	0.62056	–			$4^4(0,4)$	3,1	p_2
							$4^4(1,4)$	3,1	p_2'
8/3/*t*14	$I4_1/a$ 16*f*	0.08293, 0.13101, 0.25000; 3.22474, 1.41421	0.56966	–			$3^6(0,2)$	2,1	p_2
8/3/*t*15	$I4_1/amd$ 16*h*	0.00000, 0.21619, 0.34354; 2.31278, 2.25974	0.69309	–			$3^6(0,2)$	2,1	p_2
							$4^4(2,3)$	*d*	p_2'
8/3/*t*16	$I4_1/amd$ 16*h*	0.00000, 0.21842, 0.33885; 2.28917, 2.31348	0.69103	48^2	3,2 4	−+	$3^6(1,2)$	*d*	p_2'
8/3/*t*17	$I4_1/a$ 16*f*	0.22059, 0.13235, 0.09375; 1.94365, 3.77124	0.58803	–			–		
8/3/*t*18	$I4_1/a$ 16*f*	0.22707, 0.14541, 0.17380; 1.85431, 3.83909	0.63464	48^2	3,2 4	−+	–		
8/3/*t*19	$I4_1/a$ 16*f*	0.19068, 0.19068, 0.21111; 1.85419, 3.90201	0.62449	3^2434	2,1 4	−+	–		
9/3/*t*1	$P4_2/mnm$ 4*f*	0.22150, 0.22150, 0.00000; 1.59618, 1.19126	0.69006	3^2434	4,0 1	−−	$4^4(2,2)$	*p*	*c*′
9/3/*t*2	$I4/mmm$ 4*e*	0.00000, 0.00000, 0.14645; 1.00000, 3.41421	0.61343	4^4	4,1 4	++	$3^34^2(0,2)$	*c*	*c*′
9/3/*t*3	$I4/m$ 8*h*	0.30000, 0.10000, 0.00000; 2.23607, 1.41421	0.59238	48^2	3,3 4	++	$3^6(0,2)$	3,1	*c*′
9/3/*t*4	$P4_2/n$ 8*g*	0.26784, 0.06662, 0.07174; 2.53543, 1.00000	0.65161	–			$4^4(0,4)$	3,2	*c*
							$3^6(2,4)$	2,1	*c*′
9/3/*t*6	$I4_1/a$ 16*f*	0.08824, 0.14706, 0.25000; 3.57071, 1.00000	0.65707	–			$3^6(2,4)$	2,1	p_2
							$4^4(1,4)$	3,2	p_2'
10/3/*t*1	$I4/mmm$ 2*a*	0.00000, 0.00000, 0.00000; 1.22474, 1.00000	0.69813	4^4	5,1 1	−−	$3^6(2,4)$	*t*	*c*′
10/3/*t*2	$I4/m$ 8*h*	0.26975, 0.07901, 0.00000; 2.51564, 1.00000	0.66190	3^2434	4,1 1	−−	$4^4(0,4)$	4,2	*c*
							$3^6(2,4)$	3,1	*c*′
10/3/*t*3	$I4_1/amd$ 8*e*	0.00000, 0.00000, 0.19381; 1.00000, 6.29253	0.66568	4^4	4,2 8	++	–		
11/3/*t*1	$P4_2/mnm$ 4*f*	0.20711, 0.20711, 0.00000; 1.70711, 1.00000	0.71868	3^2434	5,1 1	−−	$3^6(2,4)$	*c*	*c*′

(ii) The sphere packings of 215 tetragonal types contain rod-like subunits (other than chains) around the fourfold (rotation, screw or roto-inversion) axes. Such subunits may be considered as plane nets that are rolled up. They may be characterized by the symbol of the net (3^6, 4^4, 48^2, 3^2434, 3^34^2 or 6^3) together with the shortest vector between two vertices that fall onto each other when the net is rolled up (Koch & Fischer, 1978). Corresponding symbols are given in the sixth column. In most cases, they are followed by the number of contacts of a sphere to spheres from one or two neighbouring subunits. In some cases, the subunits share spheres. Then the pattern of such common spheres is described by a lower-case letter: *r* stands for one or two rows of spheres without mutual contact, *c* for a chain, *d* for a row of dumb-bells, *s* for a row of squares, *t* for a triangular ribbon and *q* for a quadrangular ribbon of spheres. The last item in this column describes the position of the rod axes within the unit cell: *p* stands for $00z$; p' for $\frac{1}{2}\frac{1}{2}z$; p_2 for $00z$, $\frac{1}{2}0z$, $0\frac{1}{2}z$, $\frac{1}{2}\frac{1}{2}z$; p_2' for $\frac{1}{4}\frac{1}{4}z$, $\frac{3}{4}\frac{1}{4}z$, $\frac{1}{4}\frac{3}{4}z$, $\frac{3}{4}\frac{3}{4}z$; *c* for $00z$, $\frac{1}{2}\frac{1}{2}z$; c' for $\frac{1}{2}0z$, $0\frac{1}{2}z$; c'' for $\frac{1}{4}\frac{1}{4}z$, $\frac{3}{4}\frac{3}{4}z$; c''' for $\frac{1}{4}\frac{3}{4}z$, $\frac{3}{4}\frac{1}{4}z$.

(iii) The sphere packings of 75 tetragonal types cannot be subdivided into either layer-like or rod-like subunits. This is necessarily the case for all sphere packings with 3 contacts per sphere.

The 12 cubic sphere-packing types that also occur with tetragonal symmetry are described in Table 2. The maximal tetragonal symmetry together with the parameters corre-

Table 2
Tetragonal occurrence of cubic sphere-packing types.

Type		Symmetry	$x, y, z; a, c$	$\rho_{\min}$
3/10/c1	(*t*1)	$I4_122$ 8*d*	0.12500, 0.12500, 0.00000; 2.82843, 2.82843	0.18512
4/3/c6	(*t*1)	$I4_1/amd$ 16*h*	0.00000, 0.13763, 0.06881; 3.63299, 5.13783	0.12354
4/4/c2	(*t*7)	$I4/mmm$ 16*m*	0.15849, 0.15849, 0.15849; 3.15470, 3.15470	0.26684
4/6/c1	(*t*2)	$I4_1/amd$ 4*a*	0.00000, 0.00000, 0.00000; 1.63299, 2.30941	0.34009
5/5/c1	(*t*3)	$I\bar{4}2d$ 16*e*	0.21339, 0.03661, 0.16161; 2.30940, 2.30940	0.68017
6/3/c1	(*t*2)	$P4_12_12$ 4*a*	0.12500, 0.12500, 0.00000; 1.63299, 1.63299	0.48096
6/3/c2	(*t*3)	$I4_1/amd$ 8*c*	0.00000, 0.25000, 0.12500; 2.00000, 2.82843	0.37024
6/3/c4	(*t*10)	$I4/mmm$ 16*n*	0.00000, 0.29289, 0.14645; 2.41421, 3.41421	0.42099
6/4/c1	(*t*1)	$P4/mmm$ 1*a*	0.00000, 0.00000, 0.00000; 1.00000, 1.00000	0.52360
8/4/c1	(*t*1)	$I4/mmm$ 2*a*	0.00000, 0.00000, 0.00000; 1.15470, 1.15470	0.68017
9/3/c2	(*t*5)	$I\bar{4}2m$ 8*i*	0.18750, 0.18750, 0.18750; 1.88562, 1.88562	0.62478
12/3/c1	(*t*1)	$I4/mmm$ 2*a*	0.00000, 0.00000, 0.00000; 1.00000, 1.41421	0.74048

sponding to the minimal density are listed for each of these types.

For all types of sphere packings with the same number k of contacts, the lowest minimal density $\rho_{\text{absmin}}(k)$ is given in Table 3. Calculating the corresponding linear regression results in

$$\rho_{\text{absmin}}(k) = c_1 k - c_2$$
$$\text{with} \quad c_1 = 0.077 \pm 0.002, \quad c_2 = 0.111 \pm 0.016$$

and a correlation coefficient of $R = 0.997$.

3. Sphere-packing types with special properties

Some of the tetragonal sphere-packing types are of particular interest because they show special properties.

Normally each sphere-packing type is connected with a maximal symmetry compatible with one of its sphere packings. There exist, however, two tetragonal exceptions, *i.e.* 4/6/*t*4 (Fischer, 1991*a*,*b*) and 4/4/*t*29 (Fischer, 1993). The first of these cases refers to an example described by O'Keeffe & Hyde (1996). They discussed a graph with symmetry $P4_2/mmc$ – *mmm.* that can only be embedded as a sphere packing if the symmetry is reduced to $I4_1/acd$ – .2. (*cf.* also Delgado-Friedrichs *et al.*, 2003). Sphere packings of type 4/6/*t*4 have also been derived in space group $P4_2/mbc$ – *m..* (*cf.* also Koch & Sowa, 2004). If the symmetry of the sphere-packing graph (with vertices corresponding to the midpoints of the spheres and with edges corresponding to the sphere contacts) is maximized, additional shortest distances between the vertices are enforced. Consequently, the spheres get additional contacts, resulting in the sphere packing of the cubic primitive lattice. The same is true for the more complicated second example. Here, the maximal symmetry of the graph is $P4_2/mmc$ – 2*mm.* and four different kinds of distortion within the general positions of space groups $P4_2/nbc$, $P4_2/mbc$ and $I4_1/acd$ (twice) occur. They are illustrated in Fig. 2.

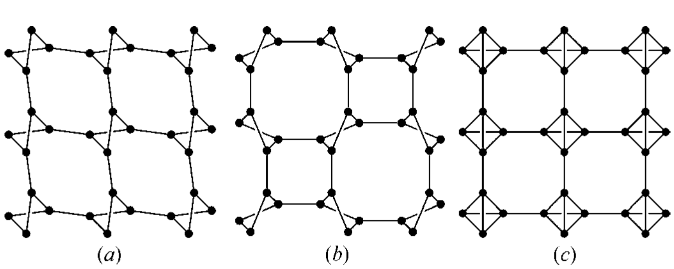

Figure 1
Sphere layers corresponding to non-planar graphs: (*a*) $4_c(8{+}2)^2$ layer; (*b*) $4_c8(8{+}4)$ layer; (*c*) 4_t8^2 layer.

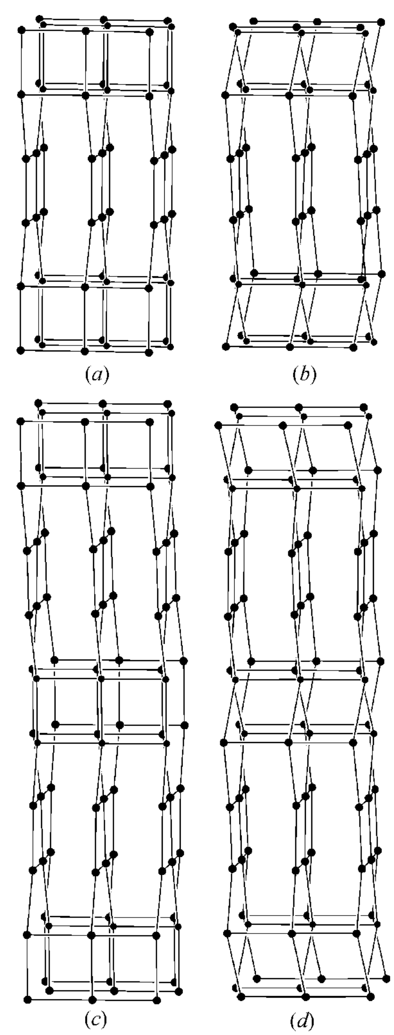

Figure 2
Sphere packings of type 4/4/*t*29 with different symmetry: (*a*) $P4_2/nbc$ 16*k*; (*b*) $P4_2/mbc$ 16*i*; (*c*), (*d*) $I4_1/acd$ 32*g*.

Table 3
Absolute minimal sphere-packing densities for each value of *k*.

k	ρ_{absmin}	Type
3	0.09937	3/4/*t*3
4	0.20040	4/4/*t*57
5	0.27942	5/3/*t*22
6	0.37024	6/3/*t*5, 6/3/*t*40
7	0.42315	7/3/*t*4
8	0.47912	8/3/*t*4
9	0.59238	9/3/*t*3
10	0.66190	10/3/*t*2
11	0.71868	11/3/*t*1

If there exists a minimum of density, it is tied to a set of fixed parameters in almost all cases. Only two exceptions have been found so far, namely for the tetragonal sphere-packing types 3/8/*t*6 and 5/3/*t*24. Both times the minimal density refers not only to a single point of the parameter range of the sphere-packing type but even to a one-dimensional parameter field. The situation for 3/8/*t*6 has been described in a paper on sphere packings with 3 contacts per sphere (Koch & Fischer, 1995). The special property of 5/3/*t*24 with space-group symmetry $I4_1/a$ was only found in the course of the preparation of the current paper. It is illustrated and described in detail by Koch *et al.* (2005).

In many cases, the minimal density is related to other special properties but this need not be the case. (i) It was assumed for a long time that the minimum is bound to the maximal compatible symmetry. This assumption is true for the cubic and the tetragonal crystal system but was disproved by an example recently found in the hexagonal crystal system (Koch *et al.*, 2005). (ii) In the sphere packings of type 3/10/*t*4 with symmetry $I4_1/amd$ 8*e* 00*z* (corresponding to the position of the Si atoms in the crystal structure of α-$ThSi_2$), the three spheres in contact with a central one in general form an isosceles triangle. For the parameters $z = \frac{1}{12}$ and $c/a = 2\surd 3$, this triangle becomes equilateral, *i.e.* it shows higher local symmetry, and the density amounts to 0.23271. The minimal density $\rho_{min} = 0.22089$ occurs, however, at $z = \frac{3}{32}$ and $c/a = 2\surd 2$ with 'bonding' angles of 141.06, 109.47 and 109.47° instead of 120° (Koch, 1985). (iii) 5/4/*t*74 with symmetry $I4_1/acd$ 32*g xyz* (Fischer, 1993) demonstrates that the minimal density need not be related to an extremum of the axial ratio. The maximal value $c/a = 3.69987$ gives rise to $\rho = 0.57119$, whereas the minimal density $\rho_{min} = 0.56979$ is reached at $c/a = 3.69390$.

Recently, it turned out that for a few hexagonal and cubic sphere-packing types the topological characterization solely by means of the graph-theoretical approach is insufficient because rings of spheres generated by the same set of symmetry operations may be either separate or interwoven (Koch & Sowa, 2004; Fischer, 2004). Such a phenomenon does not exist for tetragonal sphere-packing types.

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References

Delgado-Friedrichs, O., O'Keeffe, M. & Yaghi, O. M. (2003). *Solid State Sci.* **5**, 73–78.
EUREKA. THE SOLVER (1987). Borland International, Inc., Scotts Valley, USA.
Fischer, W. (1970). Habilitationsschrift, Marburg, Germany.
Fischer, W. (1971). *Z. Kristallogr.* **133**, 18–42.
Fischer, W. (1973). *Z. Kristallogr.* **138**, 129–146.
Fischer, W. (1974). *Z. Kristallogr.* **140**, 50–74.
Fischer, W. (1991*a*). *Z. Kristallogr.* **194**, 67–85.
Fischer, W. (1991*b*). *Z. Kristallogr.* **194**, 87–110.
Fischer, W. (1993). *Z. Kristallogr.* **205**, 9–26.
Fischer, W. (2004). *Acta Cryst.* A**60**, 246–249.
Koch, E. (1985). *Z. Kristallogr.* **173**, 205–224.
Koch, E. & Fischer, W. (1978). *Z. Kristallogr.* **148**, 107–152.
Koch, E. & Fischer, W. (1995). *Z. Kristallogr.* **210**, 407–414.
Koch, E. & Fischer, W. (1999). *International Tables for Crystallography*, Vol. C, 2nd ed., edited by A. J. C. Wilson & E. Prince, Section 9.1. Dordrecht/Boston/London: Kluwer Academic Publishers.
Koch, E. & Sowa, H. (2004). *Acta Cryst.* A**60**, 239–245.
Koch, E., Sowa, H. & Fischer, W. (2005). *Acta Cryst.* A**61**, 426–434.
O'Keeffe, M. & Hyde, B. G. (1996). *Crystal Structures I: Patterns and Symmetry*. Washington, DC: Mineralogical Society of America.
Shubnikov, A. V. (1916). *Izv. Akad. Nauk SSSR Ser. 6*, **10**, 755–799.
Sowa, H. & Koch, E. (2005). *Acta Cryst.* A**61**, 331–342.