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Minimal densities of cubic sphere-packing types

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The minimal sphere-packing densities have been calculated for all 199 types of homogeneous sphere packings with cubic symmetry. The tabulated coordinates allow the graphic representation of each type.

1. Introduction

In the past, all homogeneous sphere packings with cubic symmetry were derived and assigned to sphere-packing types as follows [for the procedure, *cf.* Fischer (1973, 1974); for definitions of the terms used *cf.* also Fischer & Koch (2002), Sowa *et al.* (2003)]. First, the symmetry regions ('*Symmetriebereiche*': Niggli, 1927, 1928) were determined inside a prismatic domain containing the asymmetric unit of the Euclidean normalizer ('Cheshire group': Hirshfeld, 1968) of the regarded space group. To this end, the symmetry operation(s) giving rise to the shortest distance(s) was (were) calculated for each point on a sufficiently fine grid by means of a Fortran program. Then the borders of these symmetry regions were inspected because they yield necessary conditions for the existence of sphere packings. It had to be proved whether the corresponding symmetry operations generate the space group under consideration. Otherwise, the sphere pattern disintegrates into parts without mutual contacts. For the remaining borders, the equations were established and solved (mostly by refinement procedures) for common intersection points. For the characterization and identification of the sphere packings, two criteria were used: (i) For each pair of neighbouring spheres, the shortest contact circuits containing these spheres were determined. The length and the number of these circuits were combined to form a symbol, the mesh symbol (*Maschen\forcelb]symbol*). (ii) The numbers of spheres up to the tenth contact shell were calculated and gathered into a coordination sequence (*Kaskadenfolge*) K_{10}. In most cases, the combination of both criteria resulted in a unique characterization. Only for very few examples was graphical examination necessary (in addition to the use of group–subgroup relations) to distinguish between pairs of sphere-packing types. In order to get convenient symbols for sphere-packing types, only the number k of contacts per sphere and the length m of the shortest mesh were included in a symbol $k/m/cn$, where c stands for the cubic crystal system and n is an arbitrary number. All these calculations could be confined to the characteristic Wyckoff position of each lattice complex.

For each lattice complex, the conditions for the existence of sphere-packing types are tabulated in the corresponding papers by Fischer (1973, 1974). Each entry for a type shows the generating symmetry operations whereas information on the respective parameter region, *i.e.* on the range of the coordinates, is given only implicitly. Explicit values of sample coordinates are missing in most cases, namely if the sphere-packing type has free parameters. Such values are needed if one wants to visualize examples of cubic sphere packings by means of graphic programs.

In addition, it turned out in the meantime that the minimal density of a sphere-packing type is a useful property (*cf. e.g.* O'Keeffe, 1991; Fischer & Koch, 2002; Sowa *et al.*, 2003; Sowa & Koch, 2004). As a sphere packing with minimal density is maximally extended within its type, it seemed to be reasonable to use the corresponding coordinates as an example for a graphic representation.

2. Results

Using the program *EUREKA. THE SOLVER* (1987), the minimal density has been calculated for each of the 199 types of homogeneous sphere packings with cubic symmetry. For this, the formulae of the sphere-packing distances were derived, the respective distances set to 1, and the parameters x, y, z and a varied such that the density ρ became a minimum. The results are presented in Table 1.

In the first column, the sphere-packing type is identified by its symbol $k/m/cn$. In the next column, the maximal symmetry compatible with this type is described by a space-group symbol and a Wyckoff position. Within the cubic crystal system, the minimum of density is always tied to that maximal symmetry. (The network of contacts may allow a higher symmetry if the edges need not be of equal length. According to a private communication from one of the referees, this is the case for 3/12/*c*1, 4/3/*c*31, 5/3/*c*13, 5/3/*c*39, 5/4/*c*6, 5/5/*c*1 and 6/3/*c*31.) The remaining columns need a closer description because two cases have to be distinguished:

(I) Normally, the minimal density refers to sphere-packing parameters somewhere inside the parameter region. In such a case, the density increases towards all borders of that region as might be expected when additional contacts between spheres are formed. Then, the corresponding coordinates and the

Table 1
Minimal densities and sample parameters of cubic sphere-packing types.

Type	Symmetry	*x*, *y*, *z*; *a*	$\rho_{\min}$
3/3/c1	$I4_132$ 24*h*	0.12500, 0.05801, 0.19199; 6.09441	0.05552
3/4/c1	$Im\bar{3}m$ 24*g*	0.14645, 0.00000, 0.50000; 4.82843	0.11163
3/4/c2	$Im\bar{3}m$ 48*j*	0.00000, 0.40825, 0.29588; 6.29253	0.10087
3/4/c3	$I432$ 48*j*	0.35000, 0.15222, 0.06150; 4.30702	>0.26145
3/4/c4	$I432$ 48*j*	0.48274, 0.18393, 0.07618; 6.40083	0.09584
3/4/c5	$I4_132$ 48*i*	0.18099, 0.20915, −0.05000; 5.86735	>0.07894
3/4/c6	$I4_132$ 48*i*	0.16667, 0.16667, 0.00000; 6.92820	0.07557
3/4/c7	$I4_132$ 48*i*	0.18750, 0.18750, 0.02589; 7.39104	0.06225
3/4/c8	$Pn\bar{3}m$ 48*l*	0.42919, 0.32081, 0.02933; 6.52395	0.09051
3/4/c9	$Im\bar{3}m$ 96*l*	0.37008, 0.28481, 0.06030; 8.29253	0.08815
3/4/c10	$Ia\bar{3}d$ 96*h*	0.04401, 0.17515, −0.14701; 7.66584	0.11158
3/6/c1	$I4_132$ 24*f*	0.00000, 0.00000, 0.25000; 4.00000	0.19635
3/6/c2	$Pn\bar{3}m$ 24*j*	0.25000, 0.08333, 0.41667; 4.24264	0.16455
3/6/c3	$Fd\bar{3}m$ 96*g*	0.19822, 0.19822, 0.05178; 6.82843	0.15787
3/6/c4	$Im\bar{3}m$ 48*k*	0.30283, 0.30283, 0.09151; 5.46410	0.15406
3/6/c5	$Ia\bar{3}$ 48*e*	0.26987, 0.31929, 0.09155; 5.33730	0.16530
3/6/c6	$Ia\bar{3}d$ 96*h*	0.05931, 0.07666, −0.11041; 6.70588	0.16669
3/8/c1	$I432$ 24*i*	0.25000, 0.10355, 0.39645; 3.41421	0.31575
3/8/c2	$I4_132$ 48*i*	0.08611, 0.20324, −0.08044; 5.10244	0.18919
3/8/c3	$Im\bar{3}m$ 96*l*	0.35000, 0.18976, 0.07860; 6.36129	>0.15787
3/10/c1	$I4_132$ 8*a*	0.12500, 0.12500, 0.12500; 2.82843	0.18512
3/12/c1	$I23$ 24*f*	0.31400, 0.18200, 0.01130; 2.74200	>0.58006
4/3/c1	$I4_132$ 12*c*	0.12500, 0.00000, 0.25000; 3.26599	0.18036
4/3/c2	$F4_132$ 48*g*	0.12500, 0.02145, 0.22855; 3.94239	0.41017
4/3/c3	$I432$ 24*i*	0.25000, 0.12500, 0.37500; 3.26600	0.36072
4/3/c4	$I4_132$ 24*h*	0.12500, 0.22855, 0.02145; 3.94239	0.20508
4/3/c5	$Pm\bar{3}n$ 24*j*	0.25000, 0.13763, 0.63763; 3.63299	0.26207
4/3/c6	$Fd\bar{3}m$ 32*e*	0.06881, 0.06881, 0.06881; 5.13783	0.12354
4/3/c7	$P\bar{4}3m$ 12*i*	0.32513, 0.32513, 0.06250; 2.69243	>0.27768
4/3/c8	$Fm\bar{3}m$ 96*k*	0.19336, 0.19336, 0.08009; 6.24264	0.20662
4/3/c9	$Fd\bar{3}m$ 96*g*	0.15000, 0.15000, −0.02250; 5.54594	>0.27768
4/3/c10	$Im\bar{3}m$ 48*j*	0.00000, 0.41991, 0.30664; 6.24264	0.10331
4/3/c11	$P23$ 12*j*	0.35061, 0.14939, 0.08277; 2.92766	0.25039
4/3/c12	$I2_13$ 24*c*	0.14108, 0.00592, −0.10134; 3.36074	0.33106
4/3/c13	$Pa\bar{3}$ 24*d*	0.17070, 0.10445, −0.17070; 3.53337	0.28487
4/3/c14	$F4_132$ 96*h*	0.14968, 0.08599, −0.00876; 5.78489	0.25965
4/3/c15	$F4_132$ 96*h*	0.15415, 0.06231, 0.04006; 6.75011	0.16343
4/3/c16	$I432$ 48*j*	0.25582, 0.23368, 0.10120; 4.88250	0.21593
4/3/c17	$P4_332$ 24*e*	0.28249, 0.21751, 0.08407; 4.03559	0.19120
4/3/c18	$P4_332$ 24*e*	0.23000, 0.31327, 0.07903; 3.43814	>0.23429
4/3/c19	$I4_132$ 48*i*	0.01273, 0.03274, −0.13943; 4.33581	0.30834
4/3/c20	$I4_132$ 48*i*	0.05500, 0.14971, −0.03706; 4.37141	>0.29923
4/3/c21	$I4_132$ 48*i*	0.12617, 0.01641, −0.06355; 4.28604	0.31921
4/3/c22	$I4_132$ 48*i*	0.14636, 0.03404, −0.02500; 4.68984	>0.17561
4/3/c23	$I4_132$ 48*i*	0.04640, 0.16028, 0.00000; 4.95007	>0.15147
4/3/c24	$I4_132$ 48*i*	0.10019, 0.13419, −0.01500; 5.22114	>0.13884
4/3/c25	$I4_132$ 48*i*	0.13390, 0.10116, 0.00000; 5.84872	0.12562
4/3/c26	$I4_132$ 48*i*	0.16497, 0.04257, 0.03154; 5.51284	0.15001
4/3/c27	$I4_132$ 48*i*	0.17678, 0.17678, 0.00000; 6.82843	0.07894
4/3/c28	$I\bar{4}3d$ 48*e*	0.01258, 0.11716, −0.06487; 4.46896	0.28159
4/3/c29	$Pm\bar{3}n$ 48*l*	0.26057, 0.22169, 0.10154; 4.92436	0.21047
4/3/c30	$Fm\bar{3}c$ 192*j*	0.18311, 0.10347, 0.07077; 7.06514	0.28506
4/3/c31	$Fd\bar{3}c$ 192*h*	0.20384, 0.06338, 0.01568; 7.65860	0.22380
4/3/c32*a*	$Ia\bar{3}d$ 96*h*	0.02636, 0.18542, −0.17433; 7.16777	0.13650
4/3/c32*b*		0.06000, 0.16278, −0.05014; 4.72299	>0.43599
4/4/c1	$Im\bar{3}m$ 12*d*	0.25000, 0.00000, 0.50000; 2.82843	0.27768
4/4/c2	$Im\bar{3}m$ 16*f*	0.15849, 0.15849, 0.15849; 3.15470	0.26684
4/4/c3	$Im\bar{3}m$ 24*h*	0.00000, 0.33333, 0.33333; 3.46410	0.30230
4/4/c4	$Im\bar{3}m$ 48*i*	0.25000, 0.10355, 0.39645; 4.82843	0.22327
4/4/c5	$Ia\bar{3}d$ 48*g*	0.12500, 0.33333, −0.08333; 4.38178	0.29874
4/4/c6	$Pm\bar{3}m$ 24*k*	0.00000, 0.36940, 0.18470; 3.82843	0.22395
4/4/c7	$Pn\bar{3}m$ 24*k*	0.37500, 0.37500, 0.05178; 3.69552	0.24899
4/4/c8	$Im\bar{3}m$ 48*k*	0.37385, 0.37385, 0.16000; 3.96366	>0.39270
4/4/c9	$I23$ 24*f*	0.32000, 0.18000, 0.01660; 2.76604	>0.58006
4/4/c10	$Pn\bar{3}$ 24*h*	0.35000, 0.15000, 0.05000; 3.16228	>0.31575
4/4/c11	$Ia\bar{3}$ 48*e*	0.00942, 0.12212, −0.21089; 3.89928	0.42392
4/4/c12	$P432$ 24*k*	0.36759, 0.19481, 0.09000; 3.29506	>0.33828
4/4/c13	$Im\bar{3}m$ 48*j*	0.00000, 0.37000, 0.17121; 4.12995	>0.32910
4/4/c14	$I432$ 48*j*	0.33229, 0.16843, 0.03896; 4.09029	0.36726
4/4/c15	$I432$ 48*j*	0.40299, 0.14603, 0.05002; 4.58087	0.26145
4/4/c16	$I432$ 48*j*	0.38000, 0.12947, 0.11122; 4.14280	>0.26372
4/4/c17	$Fd\bar{3}m$ 192*i*	0.17753, 0.08876, 0.00000; 7.96626	0.19886
4/4/c18	$Im\bar{3}m$ 96*l*	0.42678, 0.32322, 0.07322; 6.82843	0.15787
4/4/c19	$Im\bar{3}m$ 96*l*	0.31994, 0.20175, 0.08357; 5.98313	0.23468
4/4/c20	$Ia\bar{3}d$ 96*h*	0.09911, 0.01072, −0.13572; 5.86926	0.24861
4/4/c21	$Ia\bar{3}d$ 96*h*	0.14370, 0.02842, −0.10900; 5.17617	0.36245
4/4/c22	$Ia\bar{3}d$ 96*h*	0.10786, 0.20701, −0.08431; 5.45643	0.30942
4/4/c23	$Ia\bar{3}d$ 96*h*	0.15528, 0.02487, −0.04689; 4.73068	0.47479
4/5/c1	$Fd\bar{3}c$ 192*h*	0.16816, 0.08089, −0.01703; 6.04876	0.45426
4/5/c2	$Ia\bar{3}d$ 96*h*	0.00000, 0.04640, −0.16028; 4.95007	>0.33732
4/5/c3	$Ia\bar{3}d$ 96*h*	0.05116, 0.14877, −0.04200; 4.40834	>0.56714
4/6/c1	$Fd\bar{3}m$ 8*a*	0.00000, 0.00000, 0.00000; 2.30941	0.34009
4/6/c2	$Im\bar{3}m$ 6*b*	0.00000, 0.50000, 0.50000; 2.00000	0.39270
4/6/c3	$Ia\bar{3}d$ 24*d*	0.37500, 0.00000, 0.25000; 3.26599	0.36072
4/6/c4	$Ia\bar{3}$ 16*c*	0.10355, 0.10355, 0.10355; 2.78769	0.38671
5/3/c1	$Im\bar{3}$ 12*e*	0.18301, 0.00000, 0.50000; 2.73205	0.30812
5/3/c2	$I\bar{4}3d$ 24*d*	0.03958, 0.00000, 0.25000; 3.03807	0.44814
5/3/c3	$Pm\bar{3}m$ 6*e*	0.29289, 0.00000, 0.00000; 2.41421	0.22327
5/3/c4	$Fm\bar{3}m$ 48*h*	0.00000, 0.16667, 0.16667; 4.24264	0.32910
5/3/c5	$Pm\bar{3}$ 12*j*	0.00000, 0.30400, 0.23872; 2.55102	>0.35015
5/3/c6	$Im\bar{3}$ 24*g*	0.00000, 0.35505, 0.32247; 3.44949	0.30616
5/3/c7	$P\bar{4}3m$ 12*i*	0.37500, 0.37500, 0.12500; 2.82843	0.27768
5/3/c8	$Pm\bar{3}m$ 24*m*	0.35355, 0.35355, 0.14645; 3.41421	0.31575
5/3/c9	$Pn\bar{3}m$ 24*k*	0.39645, 0.39645, 0.10355; 3.41421	0.31575
5/3/c10	$Fd\bar{3}m$ 96*g*	0.19643, 0.19643, 0.08929; 6.59966	0.17487
5/3/c11	$Fd\bar{3}m$ 96*g*	0.18119, 0.18119, −0.04356; 5.13783	0.37062
5/3/c12	$I23$ 24*f*	0.31000, 0.18267, 0.01209; 2.73114	>0.58006
5/3/c13	$I23$ 24*f*	0.35631, 0.16829, 0.08816; 2.96596	0.48163
5/3/c14	$Fd\bar{3}$ 96*g*	0.17500, 0.09584, −0.01625; 5.14338	>0.32345
5/3/c15	$Ia\bar{3}$ 48*e*	0.06154, 0.15123, −0.15577; 4.29649	0.31688
5/3/c16	$Ia\bar{3}$ 48*e*	0.12000, 0.15786, −0.06225; 3.46892	>0.59741
5/3/c17	$Ia\bar{3}$ 48*e*	0.11350, 0.16250, −0.06018; 3.48895	>0.58652
5/3/c18	$P432$ 24*k*	0.37399, 0.19579, 0.08110; 3.33667	0.33828
5/3/c19	$F4_132$ 96*h*	0.13390, 0.10116, 0.00000; 5.84872	0.25124
5/3/c20	$I432$ 48*j*	0.29800, 0.14572, 0.10227; 3.97189	0.40110
5/3/c21	$Im\bar{3}m$ 48*j*	0.00000, 0.38215, 0.16667; 4.24264	0.32910
5/3/c22	$I432$ 48*j*	0.40795, 0.14302, 0.05924; 4.56770	0.26372
5/3/c23	$P4_332$ 24*e*	0.27698, 0.48100, 0.34555; 3.93210	0.20670
5/3/c24	$P4_332$ 24*e*	0.20462, 0.35855, 0.09304; 3.06230	0.43759
5/3/c25	$P4_332$ 24*e*	0.25000, 0.25000, 0.06250; 3.77124	0.23429
5/3/c26	$I4_132$ 48*i*	0.07721, 0.00440, −0.12479; 3.99072	0.39545
5/3/c27	$I4_132$ 48*i*	0.14198, 0.01576, −0.04647; 4.25191	0.32696
5/3/c28	$I4_132$ 48*i*	0.05908, 0.15230, −0.03414; 4.37935	0.29923
5/3/c29	$I4_132$ 48*i*	0.15441, 0.05741, 0.00000; 5.23077	0.17561
5/3/c30	$I4_132$ 48*i*	0.12500, 0.12500, 0.00000; 5.65685	0.13884
5/3/c31	$I4_132$ 48*i*	0.03921, 0.16789, 0.03921; 5.49509	0.15147
5/3/c32	$P\bar{4}3n$ 24*i*	0.32294, 0.15287, 0.05900; 3.05139	0.44230
5/3/c33	$I\bar{4}3d$ 48*e*	0.03850, 0.09950, −0.17883; 4.08731	0.36807
5/3/c34	$I\bar{4}3d$ 48*e*	−0.01396, 0.06901, −0.14064; 3.86666	0.43474
5/3/c35	$I\bar{4}3d$ 48*e*	0.04469, −0.01992, −0.13818; 4.40222	0.29459
5/3/c36	$I\bar{4}3d$ 48*e*	0.12209, 0.16816, −0.04027; 3.72868	0.48481
5/3/c37	$Pn\bar{3}n$ 48*i*	0.37500, 0.27294, 0.07912; 4.66883	0.24695
5/3/c38	$Fd\bar{3}c$ 192*h*	0.22858, 0.07802, −0.04972; 7.26387	0.26230
5/3/c39	$Fd\bar{3}c$ 192*h*	0.14378, 0.10260, −0.00906; 5.91407	0.48601
5/3/c40	$Ia\bar{3}d$ 96*h*	−0.02177, 0.15871, −0.05864; 5.32760	0.33241
5/3/c41	$Ia\bar{3}d$ 96*h*	0.09454, 0.03843, −0.14109; 5.73656	0.26627
5/3/c42	$Ia\bar{3}d$ 96*h*	0.01294, 0.12843, −0.11389; 5.73656	0.26627
5/3/c43	$Ia\bar{3}d$ 96*h*	0.09353, 0.07974, −0.04304; 5.42956	0.31403
5/3/c44	$Ia\bar{3}d$ 96*h*	0.07264, 0.17736, −0.05236; 4.86704	0.43600
5/4/c1	$Ia\bar{3}d$ 48*g*	0.12500, 0.40052, −0.15052; 3.55405	0.55985
5/4/c2	$Im\bar{3}$ 24*g*	0.00000, 0.30900, 0.18445; 2.71070	>0.61623
5/4/c3	$Im\bar{3}m$ 48*j*	0.00000, 0.35505, 0.17753; 3.98313	0.39771
5/4/c4	$Im\bar{3}m$ 48*k*	0.37500, 0.37500, 0.12500; 4.00000	0.39270
5/4/c5	$Pn\bar{3}n$ 48*i*	0.31159, 0.16778, 0.08643; 3.74660	0.47789
5/4/c6	$Pn\bar{3}n$ 48*i*	0.39000, 0.16399, 0.07378; 3.93213	>0.38476
5/4/c7	$Ia\bar{3}d$ 96*h*	0.15945, 0.02204, −0.05505; 4.71802	0.47862

Table 1 (continued)

Type	Symmetry	*x*, *y*, *z*; *a*	ρ_{min}
5/5/c1	$I\bar{4}3d$ 16*c*	0.03661, 0.03661, 0.03661; 2.30940	0.68017
6/3/c1	$P4_332$ 4*a*	0.12500, 0.12500, 0.12500; 1.63299	0.48096
6/3/c2	$Fd\bar{3}m$ 16*c*	0.12500, 0.12500, 0.12500; 2.82843	0.37024
6/3/c3	$Pm\bar{3}m$ 12*i*	0.00000, 0.29289, 0.29289; 2.41421	0.44653
6/3/c4	$Fm\bar{3}m$ 32*f*	0.14645, 0.14645, 0.14645; 3.41421	0.42099
6/3/c5	$Fd\bar{3}c$ 96*g*	0.12500, 0.04167, 0.20833; 4.89898	0.42752
6/3/c6	$Im\bar{3}m$ 24*h*	0.00000, 0.35355, 0.35355; 3.41421	0.31575
6/3/c7	$Ia\bar{3}d$ 48*g*	0.12500, 0.28349, −0.03349; 3.86370	0.43574
6/3/c8	$Pm\bar{3}$ 12*j*	0.00000, 0.30902, 0.19098; 2.61803	0.35015
6/3/c9	$Fm\bar{3}$ 48*h*	0.00000, 0.20797, 0.12853; 3.89005	0.42695
6/3/c10	$Im\bar{3}$ 24*g*	0.00000, 0.31699, 0.18301; 2.73205	0.61623
6/3/c11	$I\bar{4}3m$ 24*i*	0.30619, 0.30619, 0.08144; 3.14626	0.40348
6/3/c12	$Pm\bar{3}n$ 24*k*	0.00000, 0.26779, 0.20232; 2.92436	0.50248
6/3/c13	$Fm\bar{3}c$ 96*j*	0.00000, 0.17500, 0.11071; 4.61191	>0.49984
6/3/c14	$Fd\bar{3}m$ 96*g*	0.12500, 0.12500, 0.00000; 5.65685	0.27768
6/3/c15	$Im\bar{3}m$ 48*k*	0.37132, 0.37132, 0.18934; 3.88562	0.42841
6/3/c16	$I23$ 24*f*	0.32322, 0.17678, 0.03033; 2.78769	0.58006
6/3/c17	$P4_332$ 12*d*	0.12500, 0.29654, −0.04654; 2.37997	0.46609
6/3/c18	$Pa\bar{3}$ 24*d*	0.07367, 0.23226, −0.17070; 3.05998	0.43858
6/3/c19	$Pa\bar{3}$ 24*d*	0.19451, 0.09665, −0.06457; 3.12062	0.41351
6/3/c20	$Pa\bar{3}$ 24*d*	0.06101, 0.22272, −0.04789; 2.99818	0.46627
6/3/c21	$Pa\bar{3}$ 24*d*	0.19164, 0.22216, −0.03434; 2.91369	0.50802
6/3/c22	$Ia\bar{3}$ 48*e*	0.11500, 0.15390, −0.06582; 3.48182	>0.58652
6/3/c23	$Ia\bar{3}$ 48*e*	0.11766, 0.16740, −0.05617; 3.47794	0.59741
6/3/c24	$P432$ 24*k*	0.35692, 0.19405, 0.10550; 3.20135	0.38301
6/3/c25	$F4_132$ 96*h*	0.14017, 0.08663, 0.00000; 5.77186	0.26141
6/3/c26	$I432$ 48*j*	0.29038, 0.15788, 0.08584; 3.93483	0.41254
6/3/c27	$P4_332$ 24*e*	0.21201, 0.35608, 0.08953; 3.05980	0.43866
6/3/c28	$I\bar{4}3d$ 48*e*	0.06035, 0.07844, −0.11264; 3.87023	0.43354
6/3/c29	$I\bar{4}3d$ 48*e*	0.11845, 0.18554, −0.02965; 3.70780	0.49305
6/3/c30	$Pn\bar{3}n$ 48*i*	0.35000, 0.17984, 0.06509; 3.69710	>0.44593
6/3/c31	$Pn\bar{3}n$ 48*i*	0.39560, 0.16221, 0.06719; 4.02734	0.38476
6/3/c32	$Fm\bar{3}c$ 192*j*	0.19860, 0.15545, 0.07610; 6.57045	0.35442
6/3/c33	$Fd\bar{3}c$ 192*h*	0.19528, 0.07284, −0.02613; 6.46100	0.37274
6/3/c34	$Fd\bar{3}c$ 192*h*	0.15420, 0.08550, −0.01300; 5.78170	0.52016
6/3/c35	$Ia\bar{3}d$ 96*h*	0.05831, 0.03311, −0.16169; 5.30161	0.33732
6/3/c36	$Ia\bar{3}d$ 96*h*	0.13193, 0.22163, −0.10828; 5.16133	0.36558
6/3/c37	$Ia\bar{3}d$ 96*h*	0.04949, 0.14937, −0.04570; 4.45854	0.56714
6/3/c38	$Ia\bar{3}d$ 96*h*	0.05257, 0.14823, −0.03881; 4.36508	0.60436
6/3/c39	$Ia\bar{3}d$ 96*h*	0.14595, 0.03259, −0.02664; 4.65518	0.49827
6/4/c1	$Pm\bar{3}m$ 1*a*	0.00000, 0.00000, 0.00000; 1.00000	0.52360
7/3/c1	$Pm\bar{3}n$ 24*k*	0.00000, 0.28033, 0.17325; 2.88593	0.52282
7/3/c2	$Fm\bar{3}c$ 96*j*	0.00000, 0.17397, 0.10752; 4.65028	0.49984
7/3/c3	$Fd\bar{3}$ 96*g*	0.20022, 0.09842, −0.03232; 4.82664	0.44703
7/3/c4	$Fd\bar{3}$ 96*g*	0.15048, 0.09300, 0.00000; 5.37633	0.32345
7/3/c5	$Ia\bar{3}$ 48*e*	0.12188, 0.14998, −0.06724; 3.45567	0.60904
7/3/c6	$Ia\bar{3}$ 48*e*	0.10893, 0.15754, −0.06440; 3.49933	0.58652
7/3/c7	$I\bar{4}3d$ 48*e*	0.03151, 0.06631, −0.13562; 3.78180	0.46467
7/3/c8	$I\bar{4}3d$ 48*e*	0.13177, 0.11001, −0.08051; 3.49558	0.58841
7/3/c9	$Pn\bar{3}n$ 48*i*	0.34884, 0.18039, 0.06455; 3.69072	0.49993
7/3/c10	$Pn\bar{3}n$ 48*i*	0.38438, 0.16589, 0.08059; 3.83406	0.44593
7/3/c11	$Pn\bar{3}n$ 48*i*	0.30511, 0.16588, 0.09019; 3.74493	0.47853
7/4/c1	$Pa\bar{3}$ 8*c*	0.15451, 0.15451, 0.15451; 1.86834	0.64227
8/3/c1	$I\bar{4}3d$ 12*a*	0.37500, 0.00000, 0.25000; 2.13809	0.64284
8/3/c2	$Pm\bar{3}m$ 3*c*	0.00000, 0.50000, 0.50000; 1.41421	0.55536
8/3/c3	$Fd\bar{3}m$ 48*f*	0.18750, 0.00000, 0.00000; 3.77124	0.46859
8/3/c4	$Fm\bar{3}c$ 96*j*	0.00000, 0.17610, 0.11408; 4.57045	0.52649
8/3/c5	$Pa\bar{3}$ 24*d*	0.13361, 0.19581, −0.07942, 2.82843	0.55536
8/4/c1	$Im\bar{3}m$ 2*a*	0.00000, 0.00000, 0.00000; 1.15470	0.68017
9/3/c1	$I4_132$ 24*h*	0.12500, 0.37500, −0.12500; 2.82843	0.55536
9/3/c2	$I\bar{4}3m$ 8*c*	0.18750, 0.18750, 0.18750; 1.88562	0.62478
9/3/c3	$Im\bar{3}$ 24*g*	0.00000, 0.30096, 0.18600; 2.68817	0.64691
9/3/c4	$I\bar{4}3m$ 24*i*	0.37500, 0.37500, 0.12500; 2.82843	0.55536
12/3/c1	$Fm\bar{3}m$ 4*a*	0.00000, 0.00000, 0.00000; 1.41421	0.74048

minimal density ρ_{min} are given in columns 3 and 4, respectively.

(II) For 30 sphere-packing types, however, the density decreases towards at least one border and, therefore, no sphere packing with minimal density exists. Accordingly, only a limiting value for ρ_{min} is tabulated in column 4. It has to be stressed that the coordinates in column 3 then refer to an arbitrary point inside the parameter region. Even in such a case, the distance to the next-nearest neighbours may be considerably longer than to the nearest neighbours (*e.g.* 29% for type 4/3/*c*32).

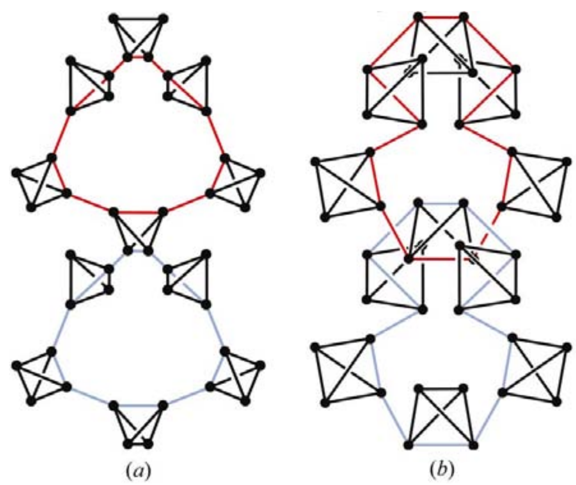

Figure 1
(*a*) Sphere packing of type 4/3/*c*32*a* with minimal density; (*b*) sphere packing of type 4/3/*c*32*b* with coordinates 0.06, 0.16278, −0.05014. The red and blue meshes of length 12 are separate in 4/3/*c*32*a* and interlocked in 4/3/*c*32*b*.

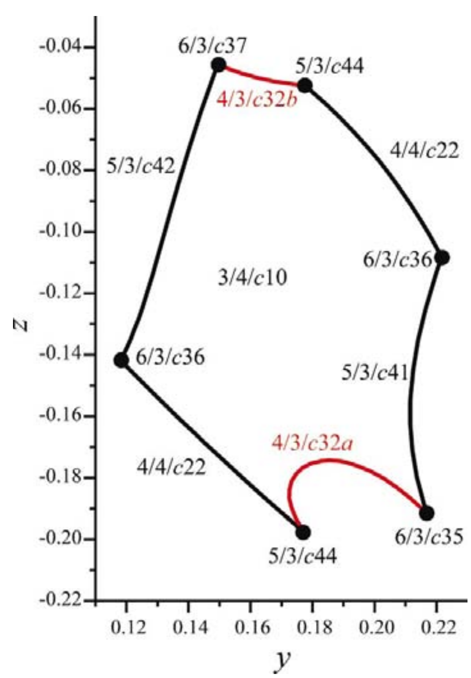

Figure 2
Projection of the parameter regions of 4/3/*c*32*a* and 4/3/*c*32*b*.

Table 2
Absolute minimal sphere-packing densities for each value of k.

k	$\rho_{\rm absmin}$	Type
3	0.05552	3/3/*c*1
4	0.07894	4/3/*c*27
5	0.13884	5/3/*c*30
6	0.26141	6/3/*c*25
7	0.32345	7/3/*c*4
8	0.46859	8/3/*c*3
9	0.55536	9/3/*c*1, 9/3/*c*5
12	0.74048	12/3/*c*1

The given coordinates always refer 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. Therefore, the lattice parameter a referred to $d = 1$ is added to the coordinates in column 3.

As one of the referees pointed out, there was a discrepancy with respect to the minimal density of sphere-packing type 4/3/*c*32. On closer inspection, it turned out that this type has to be split into two variants, *i.e.* 4/3/*c*32*a* and 4/3/*c*32*b*, as first described by Koch & Sowa (2004) for three hexagonal sphere-packing types: All sphere packings of both variants are generated by the same set of symmetry operations, so the sphere-packing graphs are isomorphic. There exist, however, meshes of length 12 that are separate in 4/3/*c*32*a*, but interlocked in 4/3/*c*32*b* (*cf*. Fig. 1). Fig. 2 shows the corresponding parameter regions.

For all types of sphere packings with the same number k of contacts, the lowest minimal density $\rho_{\rm absmin}(k)$ is given in Table 2. Naturally, these values increase with k. Calculating the corresponding linear regression results in

$$\rho_{\rm absmin}(k) = c_1 k - c_2$$
$$\text{with} \quad c_1 = 0.083 \pm 0.005, \quad c_2 = 0.233 \pm 0.035$$

and a correlation coefficient of $R = 0.99$.

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