

Since  $f''$  is related to the absorption cross section by the optical theorem and  $f'$  can be derived from  $f''$  using the Kramers–Kronig dispersion relation, it is possible to estimate the magnitude of anomalous scattering terms from absorption data (Lye, Phillips, Kaplan, Doniach & Hodgson, 1980). Such an estimation for several lanthanides reveals values of  $f''$  as great as 28 electrons and  $f'$  values as large as  $-30$  electrons. The magnitudes of these effects at  $L_{III}$  edges for lanthanides are, for example, even larger than those observed for cesium as described herein. It is expected that these very large effects, which can only be effectively exploited with a synchrotron source, will be increasingly used in protein crystallography.

We wish to thank Professors David Templeton and Seb Doniach and Paul Phizackerley for numerous helpful discussions. This work was supported by the National Institutes of Health through grant CA 16748. Synchrotron radiation beam time was provided by the Stanford Synchrotron Radiation Laboratory which is a National facility supported by the NSF (grant DMR-77-2874) in cooperation with the Stanford Linear Accelerator Center and the US Department of Energy.

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*Acta Cryst.* (1980) **A36**, 864–869

## Classification of Directions in Crystallographic Point Groups According to the Symmetry Principle

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(Received 9 June 1979; accepted 8 April 1980)

### Abstract

It is shown that a complete geometrical classification of directions in crystallographic point groups may be constructed by means of partitioning directions according to connected totalities whose directions possess the same complete group of symmetry. In all

the 32 crystallographic point groups there exist 358 different connected regions of directions.

The set of all symmetry operations of a crystallographic point group which transfer the given direction into itself will be referred to as the *direction group* of

Table 1. Connected regions of directions in crystallographic point groups

Table 1 (cont.)

Crystal class	Precise independent region of crystal class	Region index	Spherical parameters of region (angles in °)		Number of isohedron type from Table 2	Crystal class	Precise independent region of crystal class	Region index	Spherical parameters of region (angles in °)		Number of isohedron type from Table 2
			1	4					3	4	
1	All sphere	1	$0 \leq \varphi < 360$	$0 \leq \rho \leq 180$	1			1 <sub>1-2</sub> -3	$0 < \varphi < 45$	$0 < \rho < 90$	14
i	Half of sphere	1	$0 \leq \varphi < 180$	$0 \leq \rho < 180$	1			1 <sub>1-2</sub> -3	$45 < \varphi < 90$	$0 < \rho < 90$	14
2		1 <sub>1</sub>		$\rho = 0$	1	mmm		1 <sub>1</sub>	$\rho = 0$	$\rho = 0$	2
		1 <sub>2</sub>		$\rho = 180$	1			1 <sub>2</sub>	$\varphi = 90$	$\rho = 90$	2
		2	$0 \leq \varphi < 180$	$\rho = 90$	2			1 <sub>3</sub>	$\varphi = 0$	$\rho = 90$	2
		1 <sub>1-2</sub>	$0 \leq \varphi < 180$	$0 < \rho < 90$	12			2 <sub>1</sub>	$\varphi = 0$	$\rho = 45$	5
		1 <sub>2-2</sub>	$0 \leq \varphi < 180$	$90 < \rho < 180$	12			2 <sub>2</sub>	$\varphi = 90$	$\rho = 45$	5
m		1		$\rho = 0$	2	2 <sub>3</sub>	$\varphi = 45$	$\rho = 90$	5		
		2	$0 \leq \varphi < 360$	$\rho = 90$	1	3	$\varphi = 45$	$\tan \rho = \sqrt{2}$	34		
		1-2	$0 \leq \varphi < 360$	$0 < \rho < 90$	12	1 <sub>1-2</sub>	$\varphi = 0$	$0 < \rho < 45$	4		
2/m		1		$\rho = 0$	2	1 <sub>1-2</sub>	$\varphi = 90$	$0 < \rho < 45$	4		
		2	$0 \leq \varphi < 180$	$\rho = 90$	2	1 <sub>2-2</sub>	$\varphi = 90$	$45 < \rho < 90$	4		
		A	$0 \leq \varphi < 180$	$\rho = 45$	5	1 <sub>2-3</sub>	$45 < \varphi < 90$	$\rho = 90$	4		
		1-A	$0 \leq \varphi < 180$	$0 < \rho < 45$	4	1 <sub>3-2</sub>	$\varphi = 0$	$45 < \rho < 90$	4		
		A-2	$0 \leq \varphi < 180$	$45 < \rho < 90$	4	1 <sub>3-3</sub>	$0 < \varphi < 45$	$\rho = 90$	4		
222		1 <sub>1</sub>		$\rho = 0$	2	1 <sub>1-3</sub>	$\varphi = 45$	$0 < \tan \rho < \sqrt{2}$	32		
		1 <sub>2</sub>	$\varphi = 90$	$\rho = 90$	2	1 <sub>2-3</sub>	$45 < \varphi < 90$	$\cot \rho = \cos \varphi$	32		
		1 <sub>3</sub>	$\varphi = 0$	$\rho = 90$	2	1 <sub>3-3</sub>	$0 < \varphi < 45$	$\cot \rho = \sin \varphi$	32		
		2 <sub>1</sub>	$\varphi = 0$	$\rho = 45$	5	2 <sub>1-3</sub>	$0 < \varphi < 45$	$\cot \rho = \cos \varphi$	32		
		2 <sub>2</sub>	$\varphi = 90$	$\rho = 45$	5	2 <sub>2-3</sub>	$45 < \varphi < 90$	$\cot \rho = \sin \varphi$	32		
		2 <sub>3</sub>	$\varphi = 45$	$\rho = 90$	5	2 <sub>3-3</sub>	$\varphi = 45$	$\sqrt{2} < \tan \rho < \infty$	32		
		3 <sub>1</sub>	$\varphi = 45$	$\tan \rho = \sqrt{2}$	24	1 <sub>1-2</sub> -3	$0 < \varphi < 45$	$\cot \rho > \cos \varphi$	31		
		3 <sub>2</sub>	$\varphi = 315$	$\tan \rho = \sqrt{2}$	24	1 <sub>1-2</sub> -3	$45 < \varphi < 90$	$\cot \rho > \sin \varphi$	31		
		1 <sub>1-2</sub>	$\varphi = 0$	$0 < \rho < 45$	4	1 <sub>2-2</sub> -3	$45 < \varphi < 90$	$\sin \varphi > \cot \rho > \cos \varphi$	31		
		1 <sub>1-2</sub>	$\varphi = 90$	$0 < \rho < 45$	4	1 <sub>2-2</sub> -3	$45 < \varphi < 90$	$\cot \rho > \cos \varphi$	31		
		1 <sub>2-2</sub>	$45 < \varphi < 90$	$\rho = 90$	4	1 <sub>3-2</sub> -3	$0 < \varphi < 45$	$\cot \rho < \sin \varphi$	31		
		1 <sub>2-2</sub>	$\varphi = 90$	$45 < \rho < 90$	4	1 <sub>3-2</sub> -3	$0 < \varphi < 45$	$\sin \varphi > \cot \rho < \cos \varphi$	31		
		1 <sub>3-2</sub>	$\varphi = 0$	$45 < \rho < 90$	4	1 <sub>3-3</sub>	$0 < \varphi < 45$	$\cot \rho < \cot \rho < \cos \varphi$	31		
		1 <sub>3-2</sub>	$0 < \varphi < 45$	$\rho = 90$	4	1 <sub>1</sub>	$\rho = 0$	$\rho = 0$	1		
		1 <sub>1-3</sub>	$\varphi = 45$	$0 < \tan \rho < \sqrt{2}$	23	1 <sub>2</sub>	$0 \leq \varphi < 120$	$\rho = 180$	1		
		1 <sub>1-3</sub>	$\varphi = 315$	$0 < \tan \rho < \sqrt{2}$	23	2	$0 \leq \varphi < 120$	$\rho = 90$	3		
		1 <sub>2-3</sub>	$45 < \varphi < 90$	$\cot \rho = \cos \varphi$	23	1 <sub>1-2</sub>	$0 \leq \varphi < 120$	$0 < \rho < 90$	13		
		1 <sub>2-3</sub>	$0 < \varphi < 45$	$\cot \rho = \sin \varphi$	23	1 <sub>2-2</sub>	$0 \leq \varphi < 120$	$90 < \rho < 180$	13		
		1 <sub>3-3</sub>	$270 < \varphi < 315$	$\cot \rho = \cos \varphi$	23	3	1	$\rho = 0$	2		
		1 <sub>3-3</sub>	$315 < \varphi < 360$	$\cot \rho = -\sin \varphi$	23	1 <sub>1-1</sub>	2	$0 \leq \varphi < 60$	$\rho = 90$	7	
		2 <sub>1-3</sub>	$0 < \varphi < 45$	$\cot \rho = \cos \varphi$	23	A	$0 \leq \varphi < 120$	$\tan \rho = \sqrt{2}$	28		
		2 <sub>1-3</sub>	$315 < \varphi < 360$	$\cot \rho = \cos \varphi$	23	1-A	$0 \leq \varphi < 120$	$0 < \tan \rho < \sqrt{2}$	27		
		2 <sub>2-3</sub>	$45 < \varphi < 90$	$\cot \rho = \sin \varphi$	23	A-2	$0 \leq \varphi < 120$	$\sqrt{2} < \tan \rho < \infty$	27		
		2 <sub>2-3</sub>	$\varphi = 45$	$\sqrt{2} < \tan \rho < \infty$	23	1	1	$\rho = 0$	2		
		2 <sub>3-3</sub>	$270 < \varphi < 315$	$\cot \rho = -\sin \varphi$	23	2 <sub>1</sub>	$\varphi = 0$	$\rho = 90$	3		
		2 <sub>3-3</sub>	$\varphi = 315$	$\sqrt{2} < \tan \rho < \infty$	23	2 <sub>2</sub>	$\varphi = 60$	$\rho = 90$	3		
		1 <sub>1-2</sub> -3 <sub>1</sub>	$0 < \varphi < 45$	$\cot \rho > \cos \varphi$	22	3	$\varphi = 30$	$\rho = 90$	7		
		1 <sub>1-2</sub> -3 <sub>1</sub>	$45 < \varphi < 90$	$\cot \rho > \sin \varphi$	22	A <sub>1</sub>	$\varphi = 30$	$\tan \rho = \sqrt{2}$	28		
		1 <sub>2-2</sub> -3 <sub>1</sub>	$45 < \varphi < 90$	$\sin \varphi > \cot \rho > \cos \varphi$	22	A <sub>2</sub>	$\varphi = 90$	$\tan \rho = \sqrt{2}$	28		
		1 <sub>2-2</sub> -3 <sub>1</sub>	$45 < \varphi < 90$	$\cot \rho < \cos \varphi$	22	1-A <sub>1</sub>	$\varphi = 30$	$0 < \tan \rho < \sqrt{2}$	27		
		1 <sub>3-2</sub> -3 <sub>1</sub>	$0 < \varphi < 45$	$\cot \rho < \sin \varphi$	22	A <sub>1-3</sub>	$\varphi = 30$	$\sqrt{2} < \tan \rho = \infty$	27		
		1 <sub>3-2</sub> -3 <sub>1</sub>	$0 < \varphi < 45$	$\sin \varphi > \cot \rho < \cos \varphi$	22	1-A <sub>2</sub>	$\varphi = 90$	$0 < \tan \rho < \sqrt{2}$	27		
		1 <sub>1-2</sub> -3 <sub>2</sub>	$315 < \varphi < 360$	$\cot \rho > \cos \varphi$	22	A <sub>2-3</sub>	$\varphi = 90$	$\sqrt{2} < \tan \rho < \infty$	27		
		1 <sub>1-2</sub> -3 <sub>2</sub>	$315 < \varphi < 360$	$-\sin \varphi < \cot \rho < \cos \varphi$	22	1-2 <sub>1</sub>	$\varphi = 0$	$0 < \rho < 90$	25		
		1 <sub>2-2</sub> -3 <sub>2</sub>	$315 < \varphi < 360$	$\cot \rho < -\sin \varphi$	22	1-2 <sub>2</sub>	$\varphi = 60$	$0 < \rho < 90$	25		
		1 <sub>3-2</sub> -3 <sub>2</sub>	$270 < \varphi < 315$	$\cot \rho < \cos \varphi$	22	2 <sub>1-3</sub>	$0 < \varphi < 30$	$\rho = 90$	6		
		1 <sub>3-2</sub> -3 <sub>2</sub>	$270 < \varphi < 315$	$-\sin \varphi > \cot \rho > \cos \varphi$	22	2 <sub>2-3</sub>	$30 < \varphi < 60$	$\rho = 90$	6		
		1 <sub>1-2</sub> -3 <sub>3</sub>	$270 < \varphi < 315$	$\cot \rho > -\sin \varphi$	22	1-2 <sub>1-3</sub>	$0 < \varphi < 30$	$0 < \rho < 90$	26		
		1 <sub>1-2</sub> -3 <sub>3</sub>	$270 < \varphi < 315$		22	1-2 <sub>2-3</sub>	$30 < \varphi < 60$	$0 < \rho < 90$	26		
		mm2		1 <sub>1</sub>		$\rho = 0$	1	1-2 <sub>3</sub>	$60 < \varphi < 90$	$0 < \rho < 90$	26
				1 <sub>2</sub>		$\rho = 180$	1	1-2 <sub>3</sub>	$90 < \varphi < 120$	$0 < \rho < 90$	26
				2 <sub>1</sub>	$\varphi = 0$	$\rho = 90$	2	3m	1 <sub>1</sub>	$\rho = 0$	1
				2 <sub>2</sub>	$\varphi = 90$	$\rho = 90$	2	1 <sub>2</sub>	$\rho = 180$	$\rho = 180$	1
				3	$\varphi = 45$	$\rho = 90$	5	2 <sub>1</sub>	$\varphi = 30$	$\rho = 90$	3
				1 <sub>1-2</sub>	$\varphi = 0$	$0 < \rho < 90$	12	2 <sub>2</sub>	$\varphi = 90$	$\rho = 90$	3
1 <sub>1-2</sub>	$\varphi = 90$			$0 < \rho < 90$	12	3	$\varphi = 60$	$\rho = 90$	7		
1 <sub>2-2</sub>	$\varphi = 0$			$90 < \rho < 180$	12	1 <sub>2-2</sub>	$\varphi = 30$	$0 < \rho < 90$	13		
1 <sub>2-2</sub>	$\varphi = 90$			$90 < \rho < 180$	12	1 <sub>1-2</sub>	$\varphi = 90$	$0 < \rho < 90$	13		
1 <sub>1-3</sub>	$\varphi = 45$			$0 < \rho < 90$	15	1 <sub>2-2</sub>	$\varphi = 30$	$90 < \rho < 180$	13		
1 <sub>2-3</sub>	$\varphi = 45$	$90 < \rho < 180$	15	1 <sub>1-2</sub>	$\varphi = 90$	$90 < \rho < 180$	13				
2 <sub>1-3</sub>	$0 < \varphi < 45$	$\rho = 90$	4	1 <sub>1-3</sub>	$\varphi = 60$	$0 < \rho < 90$	17				
2 <sub>2-3</sub>	$45 < \varphi < 90$	$\rho = 90$	4								

Table 1 (cont.)

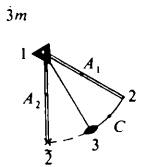
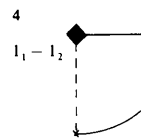
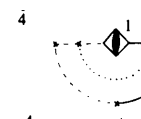
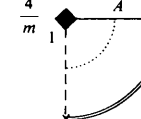
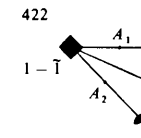
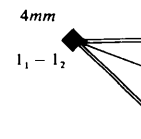
Crystal class	Precise independent region of crystal class	Region index	Spherical parameters of region (angles in °)		Number of isohedron type from Table 2	
			3	4		
$3m$ 	1	1 <sub>1-3</sub>	$\varphi = 60$	$90 < \rho < 180$	17	
	2	2 <sub>1-3</sub>	$0 < \varphi < 60$	$\rho = 90$	6	
	3	2 <sub>2-3</sub>	$30 < \varphi < 90$	$\rho = 90$	6	
	A <sub>1</sub>	1 <sub>1-2,1-3</sub>	$0 < \varphi < 60$	$0 < \rho < 90$	16	
	A <sub>2</sub>	1 <sub>1-2,2-3</sub>	$30 < \varphi < 90$	$0 < \rho < 90$	16	
	C	1 <sub>2-1,2-3</sub>	$0 < \varphi < 60$	$90 < \rho < 180$	16	
	1-A <sub>1</sub>	1 <sub>2-2,2-3</sub>	$30 < \varphi < 90$	$90 < \rho < 180$	16	
	A <sub>1</sub> -2	1	$\rho = 0$		2	
	1-A <sub>2</sub>	2	$\varphi = 30$	$\rho = 90$	7	
	A <sub>2</sub> -2	3	$\varphi = 60$	$\rho = 90$	7	
$4$ 	1 <sub>1</sub>	1 <sub>1</sub>	$\rho = 0$		1	
	1 <sub>2</sub>	1 <sub>2</sub>	$\rho = 180$		1	
	2	2	$0 \leq \varphi < 90$	$\rho = 90$	5	
	1-2	1-2	$0 \leq \varphi < 90$	$0 < \rho < 90$	15	
	1 <sub>2</sub> -2	1 <sub>2</sub> -2	$0 \leq \varphi < 90$	$90 < \rho < 180$	15	
	$\bar{4}$ 	1	1	$\rho = 0$		2
		2	2	$0 \leq \varphi < 90$	$\rho = 90$	5
		A	A	$0 \leq \varphi < 180$	$\tan \rho = \sqrt{2}$	24
		1-A	1-A	$0 \leq \varphi < 180$	$0 < \tan \rho < \sqrt{2}$	23
		A-2	A-2	$0 < \varphi < 180$	$\sqrt{2} < \tan \rho < \infty$	23
$\frac{4}{m}$ 	1	1	$\rho = 0$		2	
	2	2	$0 \leq \varphi < 90$	$\rho = 90$	5	
	A	A	$0 \leq \varphi < 90$	$\tan \rho = \sqrt{2}$	34	
	1-A	1-A	$0 \leq \varphi < 90$	$0 < \tan \rho < \sqrt{2}$	32	
	A-2	A-2	$0 \leq \varphi < 90$	$\sqrt{2} \tan \rho < \infty$	32	
$422$ 	1	1	$\rho = 0$		2	
	2 <sub>1</sub>	2 <sub>1</sub>	$\varphi = 0$	$\rho = 90$	5	
	2 <sub>2</sub>	2 <sub>2</sub>	$\varphi = 45$	$\rho = 90$	5	
	3	3	$\varphi = 22.5$	$\rho = 90$	9	
	A <sub>1</sub>	A <sub>1</sub>	$\varphi = 0$	$\tan \rho = \sqrt{2}$	34	
	A <sub>2</sub>	A <sub>2</sub>	$\varphi = 45$	$\tan \rho = \sqrt{2}$	34	
	1-A <sub>1</sub>	1-A <sub>1</sub>	$\varphi = 0$	$0 < \tan \rho < \sqrt{2}$	32	
	A <sub>1</sub> -2 <sub>1</sub>	A <sub>1</sub> -2 <sub>1</sub>	$\varphi = 0$	$\sqrt{2} < \tan \rho < \infty$	32	
	1-3	1-3	$\varphi = 22.5$	$0 < \rho < 90$	30	
	$\bar{1}$ -3	$\bar{1}$ -3	$\varphi = 22.5$	$90 < \rho < 180$	30	
	2 <sub>1</sub> -3	2 <sub>1</sub> -3	$0 < \varphi < 22.5$	$\rho = 90$	8	
	2 <sub>2</sub> -3	2 <sub>2</sub> -3	$22.5 < \varphi < 45$	$\rho = 90$	8	
	1-A <sub>2</sub>	1-A <sub>2</sub>	$\varphi = 45$	$0 < \tan \rho < \sqrt{2}$	32	
	A <sub>2</sub> -2 <sub>2</sub>	A <sub>2</sub> -2 <sub>2</sub>	$\varphi = 45$	$\sqrt{2} < \tan \rho < \infty$	32	
	1-2 <sub>1</sub> -3	1-2 <sub>1</sub> -3	$0 < \varphi < 22.5$	$0 < \rho < 90$	29	
1-2 <sub>2</sub> -3	1-2 <sub>2</sub> -3	$22.5 < \varphi < 45$	$0 < \rho < 90$	29		
$\bar{1}$ -2 <sub>1</sub> -3	$\bar{1}$ -2 <sub>1</sub> -3	$0 < \varphi < 22.5$	$90 < \rho < 180$	29		
$\bar{1}$ -2 <sub>2</sub> -3	$\bar{1}$ -2 <sub>2</sub> -3	$22.5 < \varphi < 45$	$90 < \rho < 180$	29		
$4mm$ 	1 <sub>1</sub>	1 <sub>1</sub>	$\rho = 0$		1	
	1 <sub>2</sub>	1 <sub>2</sub>	$\rho = 180$		1	
	2 <sub>1</sub>	2 <sub>1</sub>	$\varphi = 0$	$\rho = 90$	5	
	2 <sub>2</sub>	2 <sub>2</sub>	$\varphi = 45$	$\rho = 90$	5	
	3	3	$\varphi = 22.5$	$\rho = 90$	9	
	1 <sub>1</sub> -2 <sub>1</sub>	1 <sub>1</sub> -2 <sub>1</sub>	$\varphi = 0$	$0 < \rho < 90$	15	
	1 <sub>1</sub> -2 <sub>2</sub>	1 <sub>1</sub> -2 <sub>2</sub>	$\varphi = 45$	$0 < \rho < 90$	15	
	1 <sub>2</sub> -2 <sub>1</sub>	1 <sub>2</sub> -2 <sub>1</sub>	$\varphi = 0$	$90 < \rho < 180$	15	
	1 <sub>2</sub> -2 <sub>2</sub>	1 <sub>2</sub> -2 <sub>2</sub>	$\varphi = 45$	$90 < \rho < 180$	15	
	1 <sub>1</sub> -3	1 <sub>1</sub> -3	$\varphi = 22.5$	$0 < \rho < 90$	19	

Table 1 (cont.)

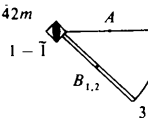
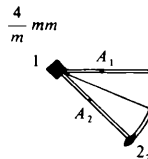
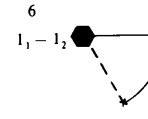
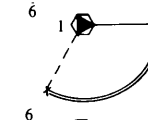
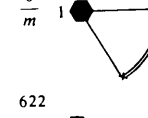
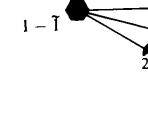
Crystal class	Precise independent region of crystal class	Region index	Spherical parameters of region (angles in °)		Number of isohedron type from Table 2	
			3	4		
$42m$ 	1	1	$\rho = 0$		2	
	2	2	$\varphi = 0$	$\rho = 90$	5	
	3	3	$\varphi = 45$	$\rho = 90$	5	
	A	A	$\varphi = 0$	$\tan \rho = \sqrt{2}$	34	
	B <sub>1</sub>	B <sub>1</sub>	$\varphi = 45$	$\tan \rho = \sqrt{2}$	24	
	B <sub>2</sub>	B <sub>2</sub>	$\varphi = 45$	$\tan \rho = -\sqrt{2}$	24	
	C	C	$\varphi = 22.5$	$\rho = 90$	9	
	1-A	1-A	$\varphi = 0$	$0 < \tan \rho < \sqrt{2}$	32	
	A-2	A-2	$\varphi = 0$	$\sqrt{2} < \tan \rho < \infty$	32	
	1-B <sub>1</sub>	1-B <sub>1</sub>	$\varphi = 45$	$0 < \tan \rho < \sqrt{2}$	23	
	$\bar{1}$ -B <sub>1</sub>	$\bar{1}$ -B <sub>1</sub>	$\varphi = 45$	$\sqrt{2} < \tan \rho < \infty$	23	
	$\bar{1}$ -B <sub>2</sub>	$\bar{1}$ -B <sub>2</sub>	$\varphi = 45$	$0 > \tan \rho > -\sqrt{2}$	23	
	B <sub>2</sub> -3	B <sub>2</sub> -3	$\varphi = 45$	$-\sqrt{2} > \tan \rho > -\infty$	23	
	2-C	2-C	$0 < \varphi < 22.5$	$\rho = 90$	8	
	C-3	C-3	$22.5 < \varphi < 45$	$\rho = 90$	8	
1-2-3	1-2-3	$0 < \varphi < 45$	$0 < \rho < 90$	33		
$\bar{1}$ -2-3	$\bar{1}$ -2-3	$0 < \varphi < 45$	$90 < \rho < 180$	33		
$\frac{4}{m}mm$ 	1	1	$\rho = 0$		2	
	2 <sub>1</sub>	2 <sub>1</sub>	$\varphi = 0$	$\rho = 90$	5	
	2 <sub>2</sub>	2 <sub>2</sub>	$\varphi = 45$	$\rho = 90$	5	
	3	3	$\varphi = 22.5$	$\rho = 90$	9	
	A <sub>1</sub>	A <sub>1</sub>	$\varphi = 0$	$\tan \rho = \sqrt{2}$	34	
	A <sub>2</sub>	A <sub>2</sub>	$\varphi = 45$	$\tan \rho = \sqrt{2}$	34	
	1-A <sub>1</sub>	1-A <sub>1</sub>	$\varphi = 0$	$0 < \tan \rho < \sqrt{2}$	32	
	A <sub>1</sub> -2	A <sub>1</sub> -2	$\varphi = 0$	$\sqrt{2} < \tan \rho < \infty$	32	
	1-A <sub>2</sub>	1-A <sub>2</sub>	$\varphi = 45$	$0 < \tan \rho < \sqrt{2}$	32	
	A <sub>2</sub> -2	A <sub>2</sub> -2	$\varphi = 45$	$\sqrt{2} < \tan \rho < \infty$	32	
	1-3	1-3	$\varphi = 22.5$	$0 < \rho < 90$	47	
	2 <sub>1</sub> -3	2 <sub>1</sub> -3	$0 < \varphi < 22.5$	$\rho = 90$	8	
	2 <sub>2</sub> -3	2 <sub>2</sub> -3	$22.5 < \varphi < 45$	$\rho = 90$	8	
	1-2 <sub>1</sub> -3	1-2 <sub>1</sub> -3	$0 < \varphi < 22.5$	$0 < \rho < 90$	46	
	1-2 <sub>2</sub> -3	1-2 <sub>2</sub> -3	$22.5 < \varphi < 45$	$0 < \rho < 90$	46	
$6$ 	1 <sub>1</sub>	1 <sub>1</sub>	$\rho = 0$		1	
	1 <sub>2</sub>	1 <sub>2</sub>	$\rho = 180$		1	
	2	2	$0 \leq \varphi < 60$	$\rho = 90$	7	
	1-2	1-2	$0 \leq \varphi < 60$	$0 < \rho < 90$	17	
	2-1 <sub>1</sub>	2-1 <sub>1</sub>	$0 \leq \varphi < 60$	$90 < \rho < 180$	17	
	$\bar{6}$ 	1	1	$\rho = 0$		2
		2	2	$0 \leq \varphi < 120$	$\rho = 90$	3
1-2		1-2	$0 \leq \varphi < 120$	$0 < \rho < 90$	25	
$\frac{6}{m}$ 	1	1	$\rho = 0$		2	
	2	2	$0 \leq \varphi < 60$	$\rho = 90$	7	
	1-2	1-2	$0 \leq \varphi < 60$	$0 < \rho < 90$	37	
$622$ 	1	1	$\rho = 0$		2	
	2 <sub>1</sub>	2 <sub>1</sub>	$\varphi = 0$	$\rho = 90$	7	
	2 <sub>2</sub>	2 <sub>2</sub>	$\varphi = 30$	$\rho = 90$	7	
	1-3	1-3	$\varphi = 15$	$\rho = 90$	11	
	1-2 <sub>1</sub>	1-2 <sub>1</sub>	$\varphi = 0$	$0 < \rho < 90$	37	
	1-2 <sub>2</sub>	1-2 <sub>2</sub>	$\varphi = 30$	$0 < \rho < 90$	37	
	1-3	1-3	$\varphi = 15$	$0 < \rho < 90$	39	
	$\bar{1}$ -3	$\bar{1}$ -3	$\varphi = 15$	$90 < \rho < 180$	39	
	2 <sub>1</sub> -3	2 <sub>1</sub> -3	$0 < \varphi < 15$	$\rho = 90$	10	
	2 <sub>2</sub> -3	2 <sub>2</sub> -3	$15 < \varphi < 30$	$\rho = 90$	10	
	1-2 <sub>1</sub> -3	1-2 <sub>1</sub> -3	$0 < \varphi < 15$	$0 < \rho < 90$	38	
	1-2 <sub>2</sub> -3	1-2 <sub>2</sub> -3	$15 < \varphi < 30$	$0 < \rho < 90$	38	
	$\bar{1}$ -2 <sub>1</sub> -3	$\bar{1}$ -2 <sub>1</sub> -3	$0 < \varphi < 15$	$90 < \rho < 180$	38	
	$\bar{1}$ -2 <sub>2</sub> -3	$\bar{1}$ -2 <sub>2</sub> -3	$15 < \varphi < 30$	$90 < \rho < 180$	38	

Table 1 (cont.)

Precise independent region of crystal class		Region index	Spherical parameters of region (angles in °)		Number of isohedron type from Table 2
Crystal class 1	Crystal class 2		3	4	
6mm		1 <sub>1</sub>	$\rho = 0$	1	
		1 <sub>2</sub>	$\rho = 180$	1	
		2 <sub>1</sub>	$\varphi = 0$	$\rho = 90$	7
		2 <sub>2</sub>	$\varphi = 30$	$\rho = 90$	7
		3	$\varphi = 15$	$\rho = 90$	11
		1 <sub>1</sub> -2 <sub>1</sub>	$\varphi = 0$	$0 < \rho < 90$	17
		1 <sub>1</sub> -2 <sub>2</sub>	$\varphi = 30$	$0 < \rho < 90$	8
		1 <sub>2</sub> -2 <sub>1</sub>	$\varphi = 0$	$90 < \rho < 180$	8
		1 <sub>2</sub> -2 <sub>2</sub>	$\varphi = 30$	$90 < \rho < 180$	8
		2 <sub>1</sub> -3	$0 < \varphi < 15$	$\rho = 90$	10
		2 <sub>2</sub> -3	$15 < \varphi < 30$	$\rho = 90$	10
		1 <sub>1</sub> -3	$\varphi = 15$	$0 < \rho < 90$	21
		1 <sub>2</sub> -3	$\varphi = 15$	$90 < \rho < 180$	21
		1 <sub>1</sub> -2 <sub>1</sub> -3	$0 < \varphi < 15$	$0 < \rho < 90$	20
		1 <sub>1</sub> -2 <sub>2</sub> -3	$15 < \varphi < 30$	$0 < \rho < 90$	20
		1 <sub>2</sub> -2 <sub>1</sub> -3	$0 < \varphi < 15$	$90 < \rho < 180$	20
		1 <sub>2</sub> -2 <sub>2</sub> -3	$15 < \varphi < 30$	$90 < \rho < 180$	20
62m		1	$\rho = 0$	2	
		2 <sub>1</sub>	$\varphi = 0$	$\rho = 90$	3
		2 <sub>2</sub>	$\varphi = 60$	$\rho = 90$	3
		3	$\varphi = 30$	$\rho = 90$	7
		1-2 <sub>1</sub>	$\varphi = 0$	$0 < \rho < 90$	25
		1-2 <sub>2</sub>	$\varphi = 60$	$0 < \rho < 90$	25
		1-3	$\varphi = 30$	$0 < \rho < 90$	37
		2 <sub>1</sub> -3	$0 < \varphi < 30$	$\rho = 90$	6
		2 <sub>2</sub> -3	$30 < \varphi < 60$	$\rho = 90$	6
		1-2 <sub>1</sub> -3	$0 < \varphi < 30$	$0 < \rho < 90$	36
		1-2 <sub>2</sub> -3	$30 < \varphi < 60$	$0 < \rho < 90$	36
6/m mm		1	$\rho = 0$	2	
		2 <sub>1</sub>	$\varphi = 0$	$\rho = 90$	7
		2 <sub>2</sub>	$\varphi = 30$	$\rho = 90$	7
		3	$\varphi = 15$	$\rho = 90$	11
		1-2 <sub>1</sub>	$\varphi = 0$	$0 < \rho < 90$	37
		1-2 <sub>2</sub>	$\varphi = 30$	$0 < \rho < 90$	37
		1-3	$\varphi = 15$	$0 < \rho < 90$	49
		2 <sub>1</sub> -3	$0 < \varphi < 15$	$\rho = 90$	10
		2 <sub>2</sub> -3	$15 < \varphi < 30$	$\rho = 90$	10
		1-2 <sub>1</sub> -3	$0 < \varphi < 15$	$0 < \rho < 90$	48
1-2 <sub>2</sub> -3	$15 < \varphi < 30$	$0 < \rho < 90$	48		
23		1	$\rho = 0$	28	
		2	$\varphi = 0$	$\rho = 45$	42
		3 <sub>1</sub>	$\varphi = 45$	$\tan \rho = \sqrt{2}$	24
		3 <sub>2</sub>	$\varphi = 315$	$\tan \rho = \sqrt{2}$	24
		A <sub>1</sub>	$\varphi = 0$	$\tan \rho = \frac{1}{2} \cos \frac{\pi}{5}$	45
		A <sub>2</sub>	$\varphi = 90$	$\tan \rho = \frac{1}{2} \cos \frac{\pi}{5}$	45
		1-A <sub>1</sub>	$\varphi = 0$	$0 < \tan \rho < \frac{1}{2} \cos \frac{\pi}{5}$	44
		A <sub>1</sub> -2	$\varphi = 0$	$\frac{1}{2} \cos \frac{\pi}{5} < \tan \rho < 1$	44
		1-A <sub>2</sub>	$\varphi = 90$	$0 < \tan \rho < \frac{1}{2} \cos \frac{\pi}{5}$	44
		A <sub>2</sub> -2	$\varphi = 90$	$\frac{1}{2} \cos \frac{\pi}{5} < \tan \rho < 1$	44
1-3 <sub>1</sub>	$\varphi = 45$	$0 < \tan \rho < \sqrt{2}$	40		
1-3 <sub>2</sub>	$\varphi = 315$	$0 < \tan \rho < \sqrt{2}$	40		
2-3 <sub>1</sub>	$0 < \varphi < 45$	$\cot \rho = \cos \varphi$	41		
2-3 <sub>2</sub>	$315 < \varphi < 360$	$\cot \rho = \cos \varphi$	41		
1-2-3 <sub>1</sub>	$0 < \varphi < 45$	$\cot \rho > \cos \varphi$	43		
1-2-3 <sub>2</sub>	$315 < \varphi < 360$	$\cot \rho > \cos \varphi$	43		
1-2-3 <sub>1</sub>	$45 < \varphi < 90$	$\cot \rho > \sin \varphi$	43		
1-2-3 <sub>2</sub>	$315 < \varphi < 360$	$\cot \rho > \cos \varphi$	43		
1-2-3 <sub>2</sub>	$270 < \varphi < 315$	$-\sin \varphi < \cot \rho$	43		

Table 1 (cont.)

Precise independent region of crystal class		Region index	Spherical parameters of region (angles in °)		Number of isohedron type from Table 2		
Crystal class 1	Crystal class 2		3	4			
m3		1	$\rho = 0$	28			
		2	$\varphi = 0$	$\rho = 45$	42		
		3	$\varphi = 45$	$\tan \rho = \sqrt{2}$	34		
		A <sub>1</sub>	$\varphi = 0$	$\tan \rho = \frac{1}{2} \cos \frac{\pi}{5}$	45		
		A <sub>2</sub>	$\varphi = 90$	$\tan \rho = \frac{1}{2} \cos \frac{\pi}{5}$	45		
		1-A <sub>1</sub>	$\varphi = 0$	$0 < \tan \rho < \frac{1}{2} \cos \frac{\pi}{5}$	44		
		A <sub>1</sub> -2	$\varphi = 0$	$\frac{1}{2} \cos \frac{\pi}{5} < \tan \rho < 1$	44		
		1-A <sub>2</sub>	$\varphi = 90$	$0 < \tan \rho < \frac{1}{2} \cos \frac{\pi}{5}$	44		
		A <sub>2</sub> -2	$\varphi = 90$	$\frac{1}{2} \cos \frac{\pi}{5} < \tan \rho < 1$	44		
		1-3	$\varphi = 45$	$0 < \tan \rho < \sqrt{2}$	53		
		2-3	$0 < \varphi < 45$	$\cot \rho = \cos \varphi$	54		
		1-2-3	$0 < \varphi < 45$	$\cot \rho > \cos \varphi$	52		
		1-2-3	$45 < \varphi < 90$	$\cot \rho > \sin \varphi$	52		
		432		1	$\rho = 0$	28	
				2	$\varphi = 0$	$\rho = 45$	42
				3	$\varphi = 45$	$\tan \rho = \sqrt{2}$	34
				1-2	$\varphi = 0$	$0 < \rho < 45$	51
1-3	$\varphi = 45$			$0 < \tan \rho < \sqrt{2}$	33		
2-3	$0 < \varphi < 45$			$\cot \rho = \cos \varphi$	54		
1-2-3	$0 < \varphi < 45$			$\cot \rho > \cos \varphi$	55		
1-2-3	$45 < \varphi < 90$			$\cot \rho > \sin \varphi$	55		
43m				1	$\rho = 0$	28	
				2	$\varphi = 0$	$\rho = 45$	42
		3 <sub>1</sub>	$\varphi = 45$	$\tan \rho = \sqrt{2}$	24		
		3 <sub>2</sub>	$\varphi = 315$	$\tan \rho = \sqrt{2}$	24		
		1-2	$\varphi = 0$	$0 < \rho < 45$	51		
		1-3 <sub>1</sub>	$\varphi = 45$	$0 < \tan \rho < \sqrt{2}$	40		
		1-3 <sub>2</sub>	$\varphi = 315$	$0 < \tan \rho < \sqrt{2}$	40		
		2-3 <sub>1</sub>	$0 < \varphi < 45$	$\cot \rho = \cos \varphi$	48		
		2-3 <sub>2</sub>	$315 < \varphi < 360$	$\cot \rho = \cos \varphi$	48		
		1-2-3 <sub>1</sub>	$0 < \varphi < 45$	$\cot \rho > \cos \varphi$	30		
1-2-3 <sub>2</sub>	$315 < \varphi < 360$	$\cot \rho > \cos \varphi$	30				
m3m		1	$\rho = 0$	28			
		2	$\varphi = 0$	$\rho = 45$	42		
		3	$\varphi = 45$	$\tan \rho = \sqrt{2}$	34		
		1-2	$\varphi = 0$	$0 < \rho < 45$	51		
		1-3	$\varphi = 45$	$0 < \tan \rho < \sqrt{2}$	53		
		2-3	$0 < \varphi < 45$	$\cot \rho = \cos \varphi$	54		
		1-2-3	$0 < \varphi < 45$	$\cot \rho > \cos \varphi$	56		

the crystallographic point group. It is evident that all such different groups are described by the ten crystallographic point groups of the plane: 1, 2, 3, 4, 6, m, mm2, 3m, 4mm, 6mm.

Let the magnitude of some property depend only on the relative positions of the direction and crystallographic point group. In such cases this magnitude will also be identical in directions which are equivalent by symmetry transformations transferring the crystallographic point group into itself, i.e. in directions equivalent by the normalizer of the crystallographic point group in the group of the sphere. It

follows that the normalizer of the corresponding crystallographic point group will be the symmetry group of the indicatory surface of such a property. Seven different normalizers correspond to the 32 crystallographic point groups:

$\frac{\infty}{\infty}m$	1, $\bar{1}$
$\frac{\infty}{m}m$	2, 3, 4, 6, $m$ , $\bar{3}$ , $\bar{4}$ , $\bar{6}$ , $\frac{2}{m}$ , $\frac{4}{m}$ , $\frac{6}{m}$
$\frac{12}{m}mm$	622, $6mm$ , $\frac{6}{m}mm$
$\frac{8}{m}mm$	422, $4mm$ , $\frac{4}{m}mm$
$\frac{6}{m}mm$	32, $3m$ , $\bar{3}m$ , $\bar{6}2m$
$\frac{4}{m}mm$	$mm2$ , $\bar{4}2m$
$m3m$	222, $mmm$ , 23, $m3$ , $432$ , $\bar{4}3m$ , $m3m$ .

In the projection sphere the independent region of the  $\frac{\infty}{\infty}m$  normalizer consists of one zero-dimensional simplex, that of the  $\frac{\infty}{m}m$  normalizer, of two zero-dimensional simplexes and one unidimensional simplex. The independent regions of the remaining normalizers consist of one two-dimensional, three unidimensional and three zero-dimensional simplexes. Since a crystallographic point group is a normal subgroup of its corresponding normalizer the simplexes of an independent region of the normalizer form a partition of the precise independent region of the crystallographic point group.

We shall refer to the totality of symmetry transformations transferring into itself both the given direction and the complete set of symmetry elements of the given crystallographic point group as *the group of the given direction by the normalizer*. It is evident that this group is a subgroup of the normalizer. In order to find all such different groups, it is sufficient to take one point from each of the simplexes of the independent region of the normalizer, as directions corresponding to the same simplex possess the same group. In all the 32 crystallographic point groups there are nine different direction groups by the normalizer: 1,  $m$ ,  $mm2$ ,  $3m$ ,  $4mm$ ,  $6mm$ ,  $8mm$ ,  $12mm$ ,  $\infty m$ .

We shall refer two directions to the same *geometrical sort* with respect to a point group if they belong to the same simplex or equivalent simplexes by the normalizer. Such a classification of directions in terms

of geometry results from the fact that all the directions of the same geometric sort are located similarly relative to the symmetry elements of the crystallographic point group. In all the 32 crystallographic point groups there exist 168 different geometric sorts of directions.

The direction is called a *general* one if it belongs to the internal points of the independent region of the normalizer, and a *particular* one if it belongs to its boundary.

It should be noted now that in the projection of the independent regions of the normalizers  $\frac{8}{m}mm$  and  $\frac{12}{m}mm$  one edge and one corner are formed of directions with irrational indices and whose groups by the normalizer are not crystallographic ones. We shall call the 12 sorts corresponding to such simplexes *irrational* ones. In the crystallographic point groups  $mm2$ ,  $222$  and  $mmm$  there are geometric sorts whose end groups of directions by the normalizer are higher than the holohedries of the considered groups. We shall term such ten sorts *real* ones. The remaining 146 sorts (*rational sorts*) in one-to-one manner correspond to 146 crystallographic varieties of the simple forms obtained by Bokiy (1940) and successfully used by Shuvalov (1970) for the classification of possible types of phase transitions in ferroelectrics.

We shall refer to the complete totality of equivalent directions according to the crystallographic point group as the *direction star*. The complete group of symmetry which is transforming into itself both the direction star and some direction of this star we call *complete groups* of this *direction*. In all the 32 crystallographic point groups there are seven different complete groups of the directions: 1,  $m$ ,  $mm2$ ,  $3m$ ,  $4mm$ ,  $5m$ ,  $\infty m$ .

We shall call directions in which the group by the normalizer and the complete group do not coincide *instantaneous* ones. An increase of symmetry in a complete group is obtained because the star is considered separately from the crystallographic point group which generated it.

We shall refer two directions in the same crystallographic point group to the same *connected region* if the complete group of directions does not change during a continuous transition from the first direction to the second one. In order to find all different connected regions of directions, we can take advantage of the fact that each connected region is either a simplex of the independent region of the normalizer, or an instantaneous direction, or part of a simplex separated by an instantaneous direction. In all the 32 crystallographic point groups there exist 358 different connected regions (Table 1).

The first column of Table 1 shows the symbol of the crystallographic point group and the second one its precise independent region (Galiulin, 1978). For crystallographic point groups with normalizers of finite

Table 2. Fifty six types of isohedron

No.	Isohedron type	Complete group of direction star	Complete group of direction	A set of expansions
1	2	3	4	5
1	Monohedron	$\infty m$	$\infty m$	1
2	Pinkakoid	$\infty m$	$\infty m$	1, 2, $m$
3	Trigonal prism	$62m$	$mm2$	3
4	Rhombic prism	$mmm$	$m$	$\frac{2}{m}, 222, mm2$
5	Tetragonal prism	$\frac{4}{m}mm$	$mm2$	$\frac{2}{m}, 222, mm2, 4, \bar{4}$
6	Ditrigonal prism	$62m$	$m$	32, $3m$
7	Hexagonal prism	$\frac{6}{m}mm$	$mm2$	$\bar{3}, 32, 3m, 6$
8	Ditetragonal prism	$\frac{4}{m}mm$	$m$	422, $4mm, \bar{4}2m$
9*	Octagonal prism	$\frac{8}{m}mm$	$mm2$	422, $4mm, 42m, 8, \bar{8}$
10	Dihexagonal prism	$\frac{6}{m}mm$	$m$	$\bar{3}m, 622, 6mm$
11*	Dodecagonal prism	$\frac{12}{m}mm$	$mm2$	$\bar{3}m, 622, 6mm, 12, \bar{1}2$
12	Dihedron	$mm2$	$m$	2, $m$
13	Trigonal pyramid	$3m$	$m$	3
14	Rhombic pyramid	$mm2$	1	$mm2$
15	Tetragonal pyramid	$4mm$	$m$	$mm2, 4$
16	Ditrigonal pyramid	$3m$	1	$3m$
17	Hexagonal pyramid	$6mm$	$m$	$3m, 6$
18	Ditetragonal pyramid	$4mm$	1	$4mm$
19*	Octagonal pyramid	$8mm$	$m$	$4mm, 8$
20	Dihexagonal pyramid	$6mm$	1	$6mm$
21*	Dodecagonal pyramid	$12mm$	$m$	$6mm, 12$
22e	Rhombic tetrahedron	222	1	222
23	Tetragonal tetrahedron	$42m$	$m$	222, $\bar{4}$
24	Tetrahedron	$43m$	$3m$	222, $\bar{4}$
25	Trigonal dipyramid	$62m$	$m$	32, $6$
26e	Trigonal trapezohedron	32	1	32
27	Rhombohedron	$\bar{3}m$	$m$	$\bar{3}, 32$
28	Cube	$m3m$	$4mm$	$\bar{3}, 32$
29e	Tetragonal trapezohedron	422	1	422
30*	Octagonal deltohedron	$82m$	$m$	422, $4mm, 8$
31	Rhombic dipyramid	$mmm$	1	$mmm$
32	Tetragonal dipyramid	$\frac{4}{m}mm$	$m$	$mmm, \frac{4}{m}, 422, \bar{4}2m$
33	Tetragonal scalenohedron	$\bar{4}2m$	1	$\bar{4}2m$
34	Octahedron	$m3m$	$3m$	$mmm, \frac{4}{m}, 422, \bar{4}2m$
35	Trigonal scalenohedron	$\frac{6}{m}mm$	1	$\frac{6}{m}mm$
36	Ditrigonal dipyramid	$62m$	1	$62m$
37	Hexagonal dipyramid	$\frac{6}{m}mm$	$m$	$\bar{3}m, \frac{6}{m}, 622, \bar{6}2m$
38e	Hexagonal trapezohedron	622	1	622
39*	Dodecagonal deltohedron	$\bar{1}22m$	$m$	$\bar{3}m, \frac{6}{m}, 62m, 622, 12$
40	Trigon-tritrahedron	$\bar{4}3m$	$m$	23
41	Tetragon-tritrahedron	$43m$	$m$	23
42	Rhombododecahedron	$m3m$	$mm2$	23
43e	Pentagon-tritrahedron	23	1	23
44	Pentagon-dodecahedron	$m3$	$m$	23
45*	Dodecahedron	$m5m$	$5m$	23
46	Ditetragonal dipyramid	$\frac{4}{m}mm$	1	$\frac{4}{m}mm$
47*	Octagonal dipyramid	$\frac{8}{m}mm$	$m$	$\frac{4}{m}mm, \frac{8}{m}, 822, 82m$
48	Dihexagonal dipyramid	$\frac{6}{m}mm$	1	$\frac{6}{m}mm$
49*	Dodecagonal dipyramid	$\frac{12}{m}mm$	$m$	$\frac{6}{m}mm, \frac{12}{m}, 1222, 122m$

\* Irrational directions; e enantiomorphous directions.

Table 2 (cont.)

No.	Isohedron type	Complete group of direction star	Complete group of direction	A set of expansions
1	2	3	4	5
50	Hexatetrahedron	$43m$	1	$43m$
51	Tetrahexahedron	$m3m$	$m$	$43m, 432$
52	Didodecahedron	$m3$	1	$m3$
53	Tetragon-trioctahedron	$m3m$	$m$	$m3, 432$
54	Trigon tritrahedron	$m3m$	$m$	$m3, 432$
55e	Pentagon-trioctahedron	432	1	432
56	Hexaoctahedron	$m3m$	1	$m3m$

order, the table indicates the separation of the precise independent region of the crystallographic point group by independent regions of the normalizer. The vertices of the initial independent region of the normalizer are indicated by the numbers 1, 2 (in the case of the normalizer  $\frac{\infty}{m}$ ) and 1, 2, 3 (in the case of the normalizers of the finite order). Vertices equivalent by the normalizer are designated by identical numbers with digital subindices. If these vertices are not included in the precise independent region of the crystallographic point group, curved lines are put above the numbers which designate them. Instantaneous directions are designated by the letters *A, B, C*. Each connected region of the type is designated by the numbers or letters of the sides which limit it. The fourth column shows the spherical parameters of the region. The  $\rho$  values in the figures of the table are read off from the positive direction perpendicular to the drawing plane, and the  $\varphi$  values from the right horizontal direction clockwise. The fifth column indicates the number of the isohedron (a polyhedron with equivalent faces) of Table 2 whose faces are perpendicular to the star vectors. In all the 32 crystallographic point groups there are 56 different types of isohedra (Galiulin, 1978). The fifth column of Table 2 shows expansions of the crystallographic point group according to the direction group. The order of the expansions corresponds to the number of equivalent directions. If it equals unity, the direction is termed a particular one. A set of expansions contains all the subgroups of the crystallographic point group transferring any two vectors of the star into each other, but leaving neither vector in its position.

The author wishes to express his thanks to N. V. Belov, Z. G. Pinsker and L. A. Shuvalov whose comments and advice were very helpful when solving the present problem.

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