

**CSD Space Group Statistics – Space Group Frequency Ordering**

Space group frequency ranking for the 1,231,575 CSD structures for which the space group is fully defined. Statistics for enantiomorphous space groups are as reported in the CSD. 965,978 (78 %) of structures adopt centrosymmetric space groups, 265,597 (22 %) adopt non-centrosymmetric space groups, and 199,748 (16 %) structures adopt Sohncke space groups.

| <b>Rank</b> | <b>SG No.</b> | <b>Space Group</b> | <b>No. in CSD</b> | <b>% of CSD</b> |
|-------------|---------------|--------------------|-------------------|-----------------|
| 1           | 14            | P21/c              | 420,364           | 34.1            |
| 2           | 2             | P-1                | 309,600           | 25.1            |
| 3           | 15            | C2/c               | 101,754           | 8.3             |
| 4           | 19            | P212121            | 85,542            | 6.9             |
| 5           | 4             | P21                | 63,321            | 5.1             |
| 6           | 61            | Pbca               | 39,615            | 3.2             |
| 7           | 33            | Pna21              | 16,805            | 1.4             |
| 8           | 9             | Cc                 | 12,791            | 1.0             |
| 9           | 62            | Pnma               | 12,343            | 1.0             |
| 10          | 1             | P1                 | 12,197            | 1.0             |
| 11          | 5             | C2                 | 10,461            | 0.8             |
| 12          | 60            | Pbcn               | 10,134            | 0.8             |
| 13          | 148           | R-3                | 10,002            | 0.8             |
| 14          | 29            | Pca21              | 9,339             | 0.8             |
| 15          | 13            | P2/c               | 8,019             | 0.7             |
| 16          | 12            | C2/m               | 6,265             | 0.5             |
| 17          | 11            | P21/m              | 5,686             | 0.5             |
| 18          | 7             | Pc                 | 5,564             | 0.5             |
| 19          | 18            | P21212             | 4,943             | 0.4             |
| 20          | 88            | I41/a              | 4,376             | 0.4             |
| 21          | 56            | Pccn               | 4,338             | 0.4             |
| 22          | 43            | Fdd2               | 4,078             | 0.3             |
| 23          | 92            | P41212             | 2,314             | <0.3            |
| 24          | 167           | R-3c               | 2,228             | <0.3            |
| 25          | 20            | C2221              | 2,127             | <0.3            |
| 26          | 96            | P43212             | 2,090             | <0.3            |
| 27          | 146           | R3                 | 1,664             | <0.3            |
| 28          | 36            | Cmc21              | 1,663             | <0.3            |
| 29          | 82            | I-4                | 1,655             | <0.3            |
| 30          | 86            | P42/n              | 1,575             | <0.3            |
| 31          | 64            | Cmca               | 1,506             | <0.3            |
| 32          | 114           | P-421c             | 1,413             | <0.3            |
| 33          | 147           | P-3                | 1,389             | <0.3            |
| 34          | 70            | Fddd               | 1,376             | <0.3            |
| 35          | 176           | P63/m              | 1,337             | <0.3            |
| 36          | 52            | Pnna               | 1,314             | <0.3            |
| 37          | 41            | Aba2               | 1,282             | <0.3            |
| 38          | 161           | R3c                | 1,213             | <0.3            |
| 39          | 57            | Pbcm               | 1,184             | <0.3            |

|     |     |         |       |      |
|-----|-----|---------|-------|------|
| 40  | 63  | Cmcm    | 1,180 | <0.3 |
| 41  | 205 | Pa-3    | 1,135 | <0.3 |
| 42  | 225 | Fm-3m   | 1,124 | <0.3 |
| 43  | 152 | P3121   | 1,102 | <0.3 |
| 44  | 76  | P41     | 1,097 | <0.3 |
| 45  | 85  | P4/n    | 1,042 | <0.3 |
| 46  | 78  | P43     | 968   | <0.3 |
| 47  | 87  | I4/m    | 916   | <0.3 |
| 48  | 173 | P63     | 895   | <0.3 |
| 49  | 145 | P32     | 890   | <0.3 |
| =50 | 144 | P31     | 887   | <0.3 |
| =50 | 154 | P3221   | 887   | <0.3 |
| 52  | 165 | P-3c1   | 871   | <0.3 |
| 53  | 58  | Pnnm    | 857   | <0.3 |
| 54  | 166 | R-3m    | 823   | <0.3 |
| 55  | 169 | P61     | 809   | <0.3 |
| 56  | 170 | P65     | 780   | <0.3 |
| 57  | 122 | I-42d   | 770   | <0.3 |
| 58  | 198 | P213    | 724   | <0.3 |
| 59  | 45  | Iba2    | 712   | <0.3 |
| 60  | 31  | Pmn21   | 707   | <0.3 |
| 61  | 142 | I41/acd | 653   | <0.3 |
| 62  | 130 | P4/ncc  | 615   | <0.3 |
| 63  | 54  | Pcca    | 578   | <0.3 |
| 64  | 155 | R32     | 576   | <0.3 |
| 65  | 163 | P-31c   | 570   | <0.3 |
| 66  | 68  | Ccca    | 568   | <0.3 |
| 67  | 194 | P63/mmc | 538   | <0.3 |
| 68  | 72  | Ibam    | 512   | <0.3 |
| 69  | 217 | I-43m   | 494   | <0.3 |
| 70  | 110 | I41cd   | 486   | <0.3 |
| 71  | 159 | P31c    | 436   | <0.3 |
| 72  | 8   | Cm      | 434   | <0.3 |
| 73  | 221 | Pm-3m   | 399   | <0.3 |
| 74  | 160 | R3m     | 368   | <0.3 |
| 75  | 220 | I-43d   | 365   | <0.3 |
| 76  | 55  | Pbam    | 364   | <0.3 |
| =77 | 113 | P-421m  | 360   | <0.3 |
| =77 | 139 | I4/mmm  | 360   | <0.3 |
| 79  | 34  | Pnn2    | 355   | <0.3 |
| 80  | 74  | Imma    | 352   | <0.3 |
| =81 | 59  | Pmmn    | 346   | <0.3 |
| =81 | 73  | Ibca    | 346   | <0.3 |
| 83  | 178 | P6122   | 344   | <0.3 |
| 84  | 79  | I4      | 341   | <0.3 |
| 85  | 141 | I41/amd | 317   | <0.3 |
| =86 | 80  | I41     | 298   | <0.3 |
| =86 | 126 | P4/nnc  | 298   | <0.3 |
| 88  | 23  | I222    | 293   | <0.3 |
| 89  | 143 | P3      | 289   | <0.3 |

|      |     |         |     |      |
|------|-----|---------|-----|------|
| 90   | 179 | P6522   | 285 | <0.3 |
| 91   | 81  | P-4     | 273 | <0.3 |
| 92   | 65  | Cmmm    | 271 | <0.3 |
| 93   | 129 | P4/nmm  | 265 | <0.3 |
| =94  | 94  | P42212  | 259 | <0.3 |
| =94  | 229 | Im-3m   | 259 | <0.3 |
| 96   | 227 | Fd-3m   | 258 | <0.3 |
| 97   | 98  | I4122   | 256 | <0.3 |
| 98   | 128 | P4/mnc  | 244 | <0.3 |
| 99   | 136 | P42/mnm | 240 | <0.3 |
| 100  | 40  | Ama2    | 235 | <0.3 |
| 101  | 123 | P4/mmm  | 234 | <0.3 |
| 102  | 190 | P-62c   | 232 | <0.3 |
| 103  | 121 | I-42m   | 231 | <0.3 |
| =104 | 182 | P6322   | 222 | <0.3 |
| =104 | 197 | I23     | 222 | <0.3 |
| 106  | 3   | P2      | 219 | <0.3 |
| 107  | 32  | Pba2    | 209 | <0.3 |
| 108  | 118 | P-4n2   | 208 | <0.3 |
| 109  | 26  | Pmc21   | 202 | <0.3 |
| 110  | 218 | P-43n   | 193 | <0.3 |
| 111  | 204 | Im-3    | 192 | <0.3 |
| 112  | 222 | Pn-3n   | 189 | <0.3 |
| 113  | 10  | P2/m    | 186 | <0.3 |
| 114  | 228 | Fd-3c   | 185 | <0.3 |
| 115  | 71  | Immm    | 183 | <0.3 |
| 116  | 53  | Pmna    | 182 | <0.3 |
| 117  | 30  | Pnc2    | 177 | <0.3 |
| =118 | 46  | Ima2    | 175 | <0.3 |
| =118 | 186 | P63mc   | 175 | <0.3 |
| 120  | 164 | P-3m1   | 173 | <0.3 |
| =121 | 191 | P6/mmm  | 172 | <0.3 |
| =121 | 206 | Ia-3    | 172 | <0.3 |
| =123 | 131 | P42/mmc | 170 | <0.3 |
| =123 | 138 | P42/ncm | 170 | <0.3 |
| 125  | 69  | Fmmm    | 169 | <0.3 |
| 126  | 140 | I4/mcm  | 167 | <0.3 |
| 127  | 66  | Cccm    | 161 | <0.3 |
| 128  | 199 | I213    | 157 | <0.3 |
| 129  | 137 | P42/nmc | 154 | <0.3 |
| 130  | 203 | Fd-3    | 153 | <0.3 |
| 131  | 192 | P6/mcc  | 152 | <0.3 |
| 132  | 230 | Ia-3d   | 150 | <0.3 |
| 133  | 37  | Ccc2    | 148 | <0.3 |
| 134  | 104 | P4nc    | 147 | <0.3 |
| 135  | 196 | F23     | 142 | <0.3 |
| 136  | 77  | P42     | 132 | <0.3 |
| =137 | 50  | Pban    | 126 | <0.3 |
| =137 | 84  | P42/m   | 126 | <0.3 |
| =139 | 106 | P42bc   | 124 | <0.3 |

|      |     |         |     |      |
|------|-----|---------|-----|------|
| =139 | 120 | I-4c2   | 124 | <0.3 |
| =139 | 135 | P42/mbc | 124 | <0.3 |
| =139 | 215 | P-43m   | 124 | <0.3 |
| 143  | 97  | I422    | 123 | <0.3 |
| 144  | 219 | F-43c   | 122 | <0.3 |
| =145 | 90  | P4212   | 120 | <0.3 |
| =145 | 150 | P321    | 120 | <0.3 |
| =145 | 223 | Pm-3n   | 120 | <0.3 |
| 148  | 158 | P3c1    | 119 | <0.3 |
| 149  | 124 | P4/mcc  | 117 | <0.3 |
| 150  | 17  | P2221   | 112 | <0.3 |
| 151  | 91  | P4122   | 111 | <0.3 |
| 152  | 95  | P4322   | 110 | <0.3 |
| 153  | 226 | Fm-3c   | 106 | <0.3 |
| 154  | 117 | P-4b2   | 102 | <0.3 |
| 155  | 42  | Fmm2    | 97  | <0.3 |
| 156  | 67  | Cmma    | 95  | <0.3 |
| 157  | 48  | Pnnn    | 94  | <0.3 |
| =158 | 127 | P4/mbm  | 93  | <0.3 |
| =158 | 171 | P62     | 93  | <0.3 |
| =158 | 180 | P6222   | 93  | <0.3 |
| 161  | 21  | C222    | 92  | <0.3 |
| 162  | 44  | Imm2    | 91  | <0.3 |
| 163  | 193 | P63/mcm | 89  | <0.3 |
| =164 | 51  | Pmma    | 88  | <0.3 |
| =164 | 211 | I432    | 88  | <0.3 |
| 166  | 209 | F432    | 86  | <0.3 |
| 167  | 24  | I212121 | 84  | <0.3 |
| 168  | 213 | P4132   | 75  | <0.3 |
| =169 | 75  | P4      | 74  | <0.3 |
| =169 | 202 | Fm-3    | 74  | <0.3 |
| =169 | 210 | F4132   | 74  | <0.3 |
| =172 | 39  | Abm2    | 73  | <0.3 |
| =172 | 162 | P-31m   | 73  | <0.3 |
| 174  | 125 | P4/nbm  | 72  | <0.3 |
| 175  | 212 | P4332   | 71  | <0.3 |
| 176  | 134 | P42/nnm | 70  | <0.3 |
| 177  | 172 | P64     | 69  | <0.3 |
| 178  | 201 | Pn-3    | 67  | <0.3 |
| 179  | 216 | F-43m   | 64  | <0.3 |
| =180 | 109 | I41md   | 62  | <0.3 |
| =180 | 175 | P6/m    | 62  | <0.3 |
| 182  | 38  | Amm2    | 61  | <0.3 |
| 183  | 83  | P4/m    | 60  | <0.3 |
| 184  | 181 | P6422   | 58  | <0.3 |
| =185 | 108 | I4cm    | 55  | <0.3 |
| =185 | 177 | P622    | 55  | <0.3 |
| =187 | 133 | P42/nbc | 54  | <0.3 |
| =187 | 189 | P-62m   | 54  | <0.3 |
| =189 | 116 | P-4c2   | 52  | <0.3 |

|      |     |         |    |      |
|------|-----|---------|----|------|
| =189 | 200 | Pm-3    | 52 | <0.3 |
| =189 | 207 | P432    | 52 | <0.3 |
| 192  | 187 | P-6m2   | 51 | <0.3 |
| 193  | 47  | Pmmm    | 49 | <0.3 |
| 194  | 6   | Pm      | 48 | <0.3 |
| 195  | 22  | F222    | 46 | <0.3 |
| =196 | 119 | I-4m2   | 45 | <0.3 |
| =196 | 174 | P-6     | 45 | <0.3 |
| 198  | 16  | P222    | 41 | <0.3 |
| 199  | 103 | P4cc    | 40 | <0.3 |
| =200 | 27  | Pcc2    | 39 | <0.3 |
| =200 | 185 | P63cm   | 39 | <0.3 |
| =200 | 224 | Pn-3m   | 39 | <0.3 |
| 203  | 214 | I4132   | 38 | <0.3 |
| =204 | 112 | P-42c   | 37 | <0.3 |
| =204 | 168 | P6      | 37 | <0.3 |
| 206  | 102 | P42nm   | 35 | <0.3 |
| 207  | 151 | P3112   | 31 | <0.3 |
| 208  | 195 | P23     | 30 | <0.3 |
| 209  | 107 | I4mm    | 29 | <0.3 |
| 210  | 157 | P31m    | 28 | <0.3 |
| 211  | 132 | P42/mcm | 27 | <0.3 |
| 212  | 153 | P3212   | 26 | <0.3 |
| 213  | 49  | Pccm    | 23 | <0.3 |
| 214  | 28  | Pma2    | 21 | <0.3 |
| 215  | 188 | P-6c2   | 19 | <0.3 |
| =216 | 89  | P422    | 18 | <0.3 |
| =216 | 149 | P312    | 18 | <0.3 |
| 218  | 184 | P6cc    | 16 | <0.3 |
| 219  | 35  | Cmm2    | 14 | <0.3 |
| 220  | 25  | Pmm2    | 12 | <0.3 |
| =221 | 93  | P4222   | 9  | <0.3 |
| =221 | 99  | P4mm    | 9  | <0.3 |
| =221 | 100 | P4bm    | 9  | <0.3 |
| =221 | 101 | P42cm   | 9  | <0.3 |
| =221 | 111 | P-42m   | 9  | <0.3 |
| =226 | 156 | P3m1    | 8  | <0.3 |
| =226 | 208 | P4232   | 8  | <0.3 |
| 228  | 115 | P-4m2   | 7  | <0.3 |
| 229  | 183 | P6mm    | 4  | <0.3 |
| 230  | 105 | P42mc   | 3  | <0.3 |