

CSD Organic Space Group Statistics – Space Group Number Ordering

Space group number ranking for the 653,326 organic CSD structures for which the space group is fully defined. Statistics for enantiomorphous space groups are as reported in the CSD. 460,797 (71 %) structures adopt centrosymmetric space groups, 192,529 (29 %) adopt non-centrosymmetric space groups, and 157,933 (24 %) structures adopt Sohncke space groups.

| SG No. | Rank | Space Group | No. organics in CSD | % of organics in CSD |
|---------------|-------------|--------------------|----------------------------|-----------------------------|
| 1 | 8 | P1 | 9,160 | 1.4 |
| 2 | 2 | P-1 | 143,374 | 21.9 |
| 3 | 68 | P2 | 133 | <0.3 |
| 4 | 4 | P21 | 54,347 | 8.3 |
| 5 | 9 | C2 | 7,821 | 1.2 |
| 6 | =184 | Pm | 12 | <0.3 |
| 7 | 14 | Pc | 3,427 | 0.5 |
| 8 | =55 | Cm | 184 | <0.3 |
| 9 | 10 | Cc | 6,630 | 1.0 |
| 10 | 121 | P2/m | 37 | <0.3 |
| 11 | 18 | P21/m | 2,248 | 0.3 |
| 12 | 21 | C2/m | 1,653 | <0.3 |
| 13 | 17 | P2/c | 2,820 | 0.4 |
| 14 | 1 | P21/c | 223,278 | 34.2 |
| 15 | 5 | C2/c | 41,165 | 6.3 |
| 16 | =163 | P222 | 19 | <0.3 |
| 17 | =108 | P2221 | 47 | <0.3 |
| 18 | 15 | P21212 | 3,252 | 0.5 |
| 19 | 3 | P212121 | 71,945 | 11.0 |
| 20 | 24 | C2221 | 1,045 | <0.3 |
| 21 | =139 | C222 | 27 | <0.3 |
| 22 | =178 | F222 | 14 | <0.3 |
| 23 | =84 | I222 | 89 | <0.3 |
| 24 | =174 | I212121 | 15 | <0.3 |
| 25 | =212 | Pmm2 | 4 | <0.3 |
| 26 | =84 | Pmc21 | 89 | <0.3 |
| 27 | =172 | Pcc2 | 16 | <0.3 |
| 28 | =201 | Pma2 | 7 | <0.3 |
| 29 | 11 | Pca21 | 6,202 | 0.9 |
| 30 | 101 | Pnc2 | 55 | <0.3 |
| 31 | =47 | Pmn21 | 327 | <0.3 |
| 32 | =87 | Pba2 | 80 | <0.3 |
| 33 | 7 | Pna21 | 10,107 | 1.5 |
| 34 | 73 | Pnn2 | 117 | <0.3 |
| 35 | =206 | Cmm2 | 6 | <0.3 |
| 36 | 27 | Cmc21 | 722 | <0.3 |
| 37 | =95 | Ccc2 | 63 | <0.3 |
| 38 | =174 | Amm2 | 15 | <0.3 |
| 39 | =136 | Abm2 | 28 | <0.3 |
| 40 | 80 | Ama2 | 96 | <0.3 |
| 41 | 33 | Aba2 | 606 | <0.3 |
| 42 | =122 | Fmm2 | 36 | <0.3 |

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|----|------|--------|--------|------|
| 43 | | Fdd2 | 2,030 | 0.3 |
| 44 | =160 | Imm2 | 20 | <0.3 |
| 45 | 45 | Iba2 | 373 | <0.3 |
| 46 | 106 | Ima2 | 50 | <0.3 |
| 47 | =195 | Pmmm | 8 | <0.3 |
| 48 | =167 | Pnnn | 18 | <0.3 |
| 49 | =220 | Pccm | 2 | <0.3 |
| 50 | =136 | Pban | 28 | <0.3 |
| 51 | =160 | Pmma | 20 | <0.3 |
| 52 | 52 | Pnna | 294 | <0.3 |
| 53 | 102 | Pmna | 53 | <0.3 |
| 54 | 58 | Pcca | 170 | <0.3 |
| 55 | 79 | Pbam | 101 | <0.3 |
| 56 | 20 | Pccn | 1,944 | <0.3 |
| 57 | 41 | Pbcm | 458 | <0.3 |
| 58 | 57 | Pnnm | 183 | <0.3 |
| 59 | 74 | Pmmn | 114 | <0.3 |
| 60 | 13 | Pbcn | 4,440 | 0.7 |
| 61 | 6 | Pbca | 22,827 | 3.5 |
| 62 | 12 | Pnma | 4,762 | 0.7 |
| 63 | 49 | Cmcm | 313 | <0.3 |
| 64 | 35 | Cmca | 600 | <0.3 |
| 65 | =160 | Cmmm | 20 | <0.3 |
| 66 | =157 | Cccm | 21 | <0.3 |
| 67 | 124 | Cmma | 34 | <0.3 |
| 68 | 63 | Ccca | 146 | <0.3 |
| 69 | =163 | Fmmm | 19 | <0.3 |
| 70 | 51 | Fddd | 298 | <0.3 |
| 71 | =145 | Immm | 24 | <0.3 |
| 72 | 69 | Ibam | 129 | <0.3 |
| 73 | 81 | Ibca | 95 | <0.3 |
| 74 | =151 | Imma | 23 | <0.3 |
| 75 | 144 | P4 | 25 | <0.3 |
| 76 | 29 | P41 | 708 | <0.3 |
| 77 | =92 | P42 | 69 | <0.3 |
| 78 | 31 | P43 | 676 | <0.3 |
| 79 | 59 | I4 | 167 | <0.3 |
| 80 | =64 | I41 | 143 | <0.3 |
| 81 | =76 | P-4 | 110 | <0.3 |
| 82 | 36 | I-4 | 571 | <0.3 |
| 83 | =201 | P4/m | 7 | <0.3 |
| 84 | =116 | P42/m | 42 | <0.3 |
| 85 | =47 | P4/n | 327 | <0.3 |
| 86 | 34 | P42/n | 602 | <0.3 |
| 87 | 70 | I4/m | 127 | <0.3 |
| 88 | 22 | I41/a | 1,643 | <0.3 |
| 89 | =212 | P422 | 4 | <0.3 |
| 90 | =114 | P4212 | 44 | <0.3 |
| 91 | =145 | P4122 | 24 | <0.3 |
| 92 | 23 | P41212 | 1,260 | <0.3 |
| 93 | =220 | P4222 | 2 | <0.3 |
| 94 | 91 | P42212 | 72 | <0.3 |
| 95 | =169 | P4322 | 17 | <0.3 |
| 96 | 25 | P43212 | 1,015 | <0.3 |
| 97 | =182 | I422 | 13 | <0.3 |
| 98 | =169 | I4122 | 17 | <0.3 |

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|-----|------|---------|-------|------|
| 99 | =216 | P4mm | 3 | <0.3 |
| 100 | =209 | P4bm | 5 | <0.3 |
| 101 | =216 | P42cm | 3 | <0.3 |
| 102 | =201 | P42nm | 7 | <0.3 |
| 103 | =182 | P4cc | 13 | <0.3 |
| 104 | =163 | P4nc | 19 | <0.3 |
| 105 | =220 | P42mc | 2 | <0.3 |
| 106 | 98 | P42bc | 57 | <0.3 |
| 107 | =195 | I4mm | 8 | <0.3 |
| 108 | =195 | I4cm | 8 | <0.3 |
| 109 | =174 | I41md | 15 | <0.3 |
| 110 | 60 | I41cd | 164 | <0.3 |
| 112 | =174 | P-42c | 15 | <0.3 |
| 113 | 54 | P-421m | 192 | <0.3 |
| 114 | 38 | P-421c | 526 | <0.3 |
| 115 | =220 | P-4m2 | 2 | <0.3 |
| 116 | =184 | P-4c2 | 12 | <0.3 |
| 117 | 143 | P-4b2 | 26 | <0.3 |
| 118 | =103 | P-4n2 | 51 | <0.3 |
| 119 | 227 | I-4m2 | 1 | <0.3 |
| 120 | =131 | I-4c2 | 29 | <0.3 |
| 121 | =116 | I-42m | 42 | <0.3 |
| 122 | =55 | I-42d | 184 | <0.3 |
| 123 | =153 | P4/mmm | 22 | <0.3 |
| 124 | =131 | P4/mcc | 29 | <0.3 |
| 125 | =220 | P4/nbm | 2 | <0.3 |
| 126 | 94 | P4/nnc | 64 | <0.3 |
| 127 | =209 | P4/mbm | 5 | <0.3 |
| 128 | 118 | P4/mnc | 41 | <0.3 |
| 129 | 67 | P4/nmm | 135 | <0.3 |
| 130 | =87 | P4/ncc | 80 | <0.3 |
| 131 | =212 | P42/mmc | 4 | <0.3 |
| 133 | =145 | P42/nbc | 24 | <0.3 |
| 134 | =209 | P42/nnm | 5 | <0.3 |
| 135 | =131 | P42/mbc | 29 | <0.3 |
| 136 | 107 | P42/mnm | 49 | <0.3 |
| 137 | =95 | P42/nmc | 63 | <0.3 |
| 138 | =128 | P42/ncm | 31 | <0.3 |
| 139 | =122 | I4/mmm | 36 | <0.3 |
| 140 | =169 | I4/mcm | 17 | <0.3 |
| 141 | =103 | I41/amd | 51 | <0.3 |
| 142 | =64 | I41/acd | 143 | <0.3 |
| 143 | 83 | P3 | 90 | <0.3 |
| 144 | 30 | P31 | 690 | <0.3 |
| 145 | 28 | P32 | 714 | <0.3 |
| 146 | 26 | R3 | 908 | <0.3 |
| 147 | 46 | P-3 | 355 | <0.3 |
| 148 | 16 | R-3 | 2,959 | 0.5 |
| 149 | =212 | P312 | 4 | <0.3 |
| 150 | =92 | P321 | 69 | <0.3 |
| 151 | 194 | P3112 | 10 | <0.3 |
| 152 | 40 | P3121 | 494 | <0.3 |
| 153 | =178 | P3212 | 14 | <0.3 |
| 154 | 43 | P3221 | 409 | <0.3 |
| 155 | 71 | R32 | 125 | <0.3 |
| 157 | =206 | P31m | 6 | <0.3 |

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|-----|------|---------|-----|------|
| 158 | =114 | P3c1 | 44 | <0.3 |
| 159 | 75 | P31c | 111 | <0.3 |
| 160 | 61 | R3m | 160 | <0.3 |
| 161 | 42 | R3c | 443 | <0.3 |
| 162 | =184 | P-31m | 12 | <0.3 |
| 163 | 89 | P-31c | 74 | <0.3 |
| 164 | =128 | P-3m1 | 31 | <0.3 |
| 165 | =76 | P-3c1 | 110 | <0.3 |
| 166 | 66 | R-3m | 141 | <0.3 |
| 167 | 39 | R-3c | 499 | <0.3 |
| 168 | =167 | P6 | 18 | <0.3 |
| 169 | 32 | P61 | 640 | <0.3 |
| 170 | 37 | P65 | 551 | <0.3 |
| 171 | =103 | P62 | 51 | <0.3 |
| 172 | =108 | P64 | 47 | <0.3 |
| 173 | 50 | P63 | 301 | <0.3 |
| 174 | =184 | P-6 | 12 | <0.3 |
| 175 | =139 | P6/m | 27 | <0.3 |
| 176 | 44 | P63/m | 390 | <0.3 |
| 177 | =201 | P622 | 7 | <0.3 |
| 178 | 78 | P6122 | 103 | <0.3 |
| 179 | 90 | P6522 | 73 | <0.3 |
| 180 | =131 | P6222 | 29 | <0.3 |
| 181 | =190 | P6422 | 11 | <0.3 |
| 182 | =119 | P6322 | 39 | <0.3 |
| 183 | =220 | P6mm | 2 | <0.3 |
| 184 | =201 | P6cc | 7 | <0.3 |
| 185 | =184 | P63cm | 12 | <0.3 |
| 186 | 97 | P63mc | 61 | <0.3 |
| 187 | =125 | P-6m2 | 33 | <0.3 |
| 188 | =206 | P-6c2 | 6 | <0.3 |
| 189 | =190 | P-62m | 11 | <0.3 |
| 190 | =112 | P-62c | 45 | <0.3 |
| 191 | =125 | P6/mmm | 33 | <0.3 |
| 192 | =195 | P6/mcc | 8 | <0.3 |
| 193 | =153 | P63/mcm | 22 | <0.3 |
| 194 | 82 | P63/mmc | 92 | <0.3 |
| 195 | =190 | P23 | 11 | <0.3 |
| 196 | =184 | F23 | 12 | <0.3 |
| 197 | =112 | I23 | 45 | <0.3 |
| 198 | 72 | P213 | 118 | <0.3 |
| 199 | =157 | I213 | 21 | <0.3 |
| 200 | =220 | Pm-3 | 2 | <0.3 |
| 201 | =178 | Pn-3 | 14 | <0.3 |
| 202 | =163 | Fm-3 | 19 | <0.3 |
| 203 | =139 | Fd-3 | 27 | <0.3 |
| 204 | =145 | Im-3 | 24 | <0.3 |
| 205 | 53 | Pa-3 | 268 | <0.3 |
| 206 | =119 | Ia-3 | 39 | <0.3 |
| 207 | =136 | P432 | 28 | <0.3 |
| 208 | =195 | P4232 | 8 | <0.3 |
| 209 | =216 | F432 | 3 | <0.3 |
| 210 | =110 | F4132 | 46 | <0.3 |
| 211 | =125 | I432 | 33 | <0.3 |
| 212 | =190 | P4332 | 11 | <0.3 |
| 213 | =178 | P4132 | 14 | <0.3 |

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|-----|------|-------|-----|------|
| 214 | =172 | I4132 | 16 | <0.3 |
| 215 | =153 | P-43m | 22 | <0.3 |
| 216 | =195 | F-43m | 8 | <0.3 |
| 217 | 62 | I-43m | 148 | <0.3 |
| 218 | =131 | P-43n | 29 | <0.3 |
| 219 | =153 | F-43c | 22 | <0.3 |
| 220 | =110 | I-43d | 46 | <0.3 |
| 221 | =99 | Pm-3m | 56 | <0.3 |
| 222 | =157 | Pn-3n | 21 | <0.3 |
| 223 | =151 | Pm-3n | 23 | <0.3 |
| 224 | =216 | Pn-3m | 3 | <0.3 |
| 225 | =84 | Fm-3m | 89 | <0.3 |
| 226 | =145 | Fm-3c | 24 | <0.3 |
| 227 | =99 | Fd-3m | 56 | <0.3 |
| 228 | =145 | Fd-3c | 24 | <0.3 |
| 229 | 130 | Im-3m | 30 | <0.3 |
| 230 | =139 | Ia-3d | 27 | <0.3 |