Powder extinction classes used by X-Cell. For space groups marked with an asterisk, a cell choice or origin choice other than 1 has to be used to obtain the same pattern of systematic absences as for the representative of the powder extinction class.

| Cystal system | Representative | Other space groups |
|---|---|---|
| triclinic | P1 | P-1 |
| monoclinic | P2 | Pm, P2/m |
| monoclinic | $P2_1$ | $P2_1/m$ |
| monoclinic | P2/c | Pc |
| monoclinic | $P2_1/c$ | |
| monoclinic | C2 | Cm, C2/m |
| monoclinic | C2/c | Cc |
| orthorhombic | P222 | Pmm2, Pmmm |
| orthorhombic | $P222_1$ | |
| orthorhombic | $P2_12_12$ | |
| orthorhombic | $P2_12_12_1$ | |
| orthorhombic | Pcc2 | Pccm |
| orthorhombic | Pba2 | Pbam |
| orthorhombic | $Pna2_1$ | Pnma* |
| orthorhombic | Pnn2 | Pnnm |
| orthorhombic | Pnnn | |
| orthorhombic | Pban | |
| orthorhombic | Pmma | Pma2*, $Pmc2_1$* |
| orthorhombic | Pnna | |
| orthorhombic | Pmna | Pnc2* |
| orthorhombic | Pcca | |
| orthorhombic | Pccn | |
| orthorhombic | $Pca2_1$ | Pbcm* |
| orthorhombic | Pmmn | $Pmn2_1$* |
| orthorhombic | Pbcn | |
| orthorhombic | Pbca | |
| orthorhombic | C222 | Cmm2, Cmmm, Amm2* |
| orthorhombic | $C222_1$ | |
| orthorhombic | $Cmc2_1$ | Cmcm, Ama2* |
| orthorhombic | Ccc2 | Cccm |
| orthorhombic | Cmca | Aba2* |
| orthorhombic | Cmma | Abm2* |
| orthorhombic | Ccca | |
| orthorhombic | F222 | Fmm2, Fmmm |
| orthorhombic | Fdd2 | |
| orthorhombic | Fddd | |
| orthorhombic | I222 | $I2_12_12_1$, Imm2, Immm |
| orthorhombic | Iba2 | Ibam |
| orthorhombic | Ima2 | |
| orthorhombic | Ibca | |
| orthorhombic | Imma | |
| tetragonal | P4 | P-4, P4/m, P422, P4mm |
| | | P-42m, P-4m2, P4/mmm |
| tetragonal | $P4_1$ | $P4_3$, $P4_122$, $P4_322$ |
| tetragonal | $P4_2$ | $P4_2/m$, $P4_222$ |
| tetragonal | P4/n | |
| tetragonal | $P4_2/n$ | |
| tetragonal | $P42_12$ | $P-42_1m$ |
| tetragonal | $P4_12_12$ | $P4_32_12$ |
| tetragonal | $P4_22_12$ | |

| | | |
|---|---|---|
| tetragonal | P4bm | P-4b2, P4/mbm |
| tetragonal | $P4_2cm$ | P-4c2, $P4_2/mcm$ |
| tetragonal | $P4_2nm$ | P-4n2, $P4_2/mnm$ |
| tetragonal | P4cc | P/mcc |
| tetragonal | P4nc | |
| tetragonal | $P4_2mc$ | P-42c, $P4_2/mmc$ |
| tetragonal | $P4_2bc$ | $P4_2/mbc$ |
| tetragonal | $P-4_21c$ | |
| tetragonal | P4/nbm | |
| tetragonal | P4/nnc | |
| tetragonal | P4/mnc | |
| tetragonal | P4/nmm | |
| tetragonal | P4/ncc | |
| tetragonal | $P4_2/nbc$ | |
| tetragonal | $P4_2/nnm$ | |
| tetragonal | $P4_2/nmc$ | $P4_2/ncm$ |
| tetragonal | I4 | I4/m, I-4, I422, I4mm |
| | | I-4m2, I-42m, I4/mmm |
| tetragonal | $I4_1$ | $I4_122$ |
| tetragonal | $I4_1/a$ | |
| tetragonal | I4cm | I-4c2, I4/mcm |
| tetragonal | $I4_1md$ | $I-4_2d$ |
| tetragonal | $I4_1cd$ | |
| tetragonal | $I4_1/amd$ | |
| tetragonal | $I4_1/acd$ | |
| cubic | P23 | Pm-3, P432, P-43m, Pm-3m |
| cubic | $P2_13$ | $P4_232$ |
| cubic | Pn-3 | Pn-3m |
| cubic | Pa-3 | |
| cubic | $P4_332$ | $P4_132$ |
| cubic | P-43n | Pm-3n |
| cubic | Pn-3n | |
| cubic | F23 | Fm-3, F432, F-43m, Fm-3m |
| cubic | Fd-3 | Fd-3m |
| cubic | $F4_132$ | |
| cubic | F-43c | Fm-3c |
| cubic | Fd-3c | |
| cubic | I23 | I213, Im-3, I432, I-43m, Im-3m |
| cubic | Ia-3 | |
| cubic | $I4_132$ | |
| cubic | I-43d | |
| cubic | Ia-3d | |
| hex/trigonal | P3 | P-3, P312, P321, P3m1 |
| | | P31m, P-31m, P-3m1, P6 |
| | | P-6, P6/m, P622, P6mm |
| | | P-6m2, P-62m, P6/mmm |
| hex/trigonal | $P3_1$ | $P32, P3_112, P3_121, P3_212$ |
| | | $P3_221$, P62, P64, $P6_222$, $P6_422$ |
| hex/trigonal | P3c1 | P-3c1, $P6_3cm$, P-6c2, $P6_3/mcm$ |
| hex/trigonal | P31c | P-31c, $P6_3mc$, P-62c, $P6_3/mmc$ |
| hex/trigonal | $P6_1$ | $P6_5, P6_122, P6_522$ |
| hex/trigonal | $P6_3$ | $P6_3/m, P6_322$ |
| hex/trigonal | P6cc | P6/mcc |
| hex/trigonal | R3 | R-3, R32, R3m, R-3m |
| hex/trigonal | R3c | R-3c |

| Compound | nb | s.g. | wavelength | a | b | c | alpha | beta | gamma | peak1 | peak2 | peak3 | peak4 | peak5 | peak6 | peak7 | peak8 | peak9 | peak10 | peak11 | peak12 | peak13 | peak14 | peak15 | peak16 | peak17 | peak18 | peak19 | peak20 | peak21 | peak22 | peak23 | peak24 | peak25 | peak26 | peak27 | peak28 | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| beta-l-glutamic-acid | 1 | $P2_12_12_1$ | 1.5406 | 5.191 | 17.403 | 6.994 | 90.000 | 90.000 | 90.000 | 10.1729 | 13.6480 | 17.8298 | 19.9013 | 20.4046 | 21.3146 | 21.9147 | 22.9795 | 23.6571 | 24.0637 | 25.4576 | 25.9803 | 26.3094 | 26.7257 | 27.4710 | 28.6326 | 29.8136 | 30.8203 | 31.2462 | 32.5337 | 32.8338 | 33.5114 | 34.5568 | 35.4280 | | | | | |
| fluorapatite | 2 | $P6_3/m$ | 1.5406 | 9.369 | 9.369 | 6.884 | 90.000 | 90.000 | 120.000 | 16.8200 | 18.8824 | 21.8400 | 22.8800 | 25.4100 | 25.8000 | 28.0800 | 29.0400 | 31.8600 | 32.1900 | 33.0400 | 34.0800 | 35.5800 | 39.2600 | 39.9800 | 40.6000 | 42.1600 | 42.4170 | 43.8400 | 44.5777 | 45.3200 | 46.8200 | 48.2200 | 48.8300 | 49.5178 | | | | |
| red fluorescein | 3 | $Pna2_1$ | 1.4000 | 10.459 | 13.218 | 10.566 | 90.000 | 90.000 | 90.000 | 9.7300 | 10.8050 | 12.1600 | 12.4000 | 15.2300 | 16.2965 | 16.5550 | 17.0700 | 17.1750 | 18.1350 | 18.2285 | 19.8375 | 21.0200 | 21.0950 | 21.2874 | 23.9800 | 24.4303 | 24.9842 | 25.1900 | 27.1792 | 27.3547 | 27.7342 | 28.5279 | | | | | | |
| formylurea | 4 | $Pna2_1$ | 1.5406 | 16.813 | 6.050 | 3.669 | 90.000 | 90.000 | 90.000 | 10.5500 | 18.0600 | 21.1567 | 24.8400 | 25.8000 | 26.5100 | 28.4400 | 28.9400 | 29.4700 | 30.4000 | 31.3800 | 31.9400 | 32.7000 | 35.2800 | 35.7000 | 36.5500 | 39.2600 | 40.0400 | 41.8800 | 43.0315 | 43.2799 | 44.0000 | 44.3511 | 45.1152 | 45.6800 | 46.2100 | | | |
| o-thymotic acid | 5 | $P2_12_12_1$ | 1.5406 | 11.094 | 8.155 | 11.771 | 90.000 | 100.162 | 90.000 | 10.1207 | 12.1051 | 13.2958 | 13.5765 | 14.8542 | 15.3133 | 16.2869 | 19.3845 | 19.5843 | 19.9523 | 22.0658 | 23.0629 | 24.3182 | 24.9928 | 25.5313 | 25.8121 | 26.7219 | 27.1672 | 27.5738 | 28.0578 | 28.7547 | | | | | | | | |
| sodium-chloro-acetate | 6 | $P2_12_12_1$ | 1.3950 | 7.093 | 5.342 | 10.776 | 90.000 | 92.454 | 90.000 | 7.4300 | 16.7675 | 20.0900 | 20.4400 | 22.7100 | 23.7862 | 24.2300 | 24.3800 | 27.0888 | 27.3300 | 28.0900 | 28.6216 | 29.0509 | 29.7944 | 30.0400 | 30.2758 | 31.2152 | 31.4218 | 32.4107 | 33.7327 | | | | | | | | | |
| piv-pro-gly-NHMe | 7 | $P2_1$ | 1.5406 | 7.975 | 9.299 | 5.846 | 105.139 | 99.425 | 63.674 | 10.8574 | 12.4016 | 12.5840 | 15.7138 | 17.1152 | 17.6605 | 19.5152 | 19.6784 | 20.0432 | 20.6096 | 20.9840 | 21.8204 | 21.9632 | 22.5968 | 24.0656 | 24.2192 | 24.9296 | 25.3712 | 26.4701 | 28.8368 | 29.4512 | 29.8710 | 30.3595 | 31.2752 | 31.9184 | | | | |
| 4-toluenesulphonhydrazide | 8 | $P2_12_12_1$ | 1.5406 | 18.5971 | 5.6390 | 8.5334 | 90.000 | 106.2182 | 90.000 | 9.9300 | 10.5595 | 13.1000 | 15.7900 | 16.5000 | 18.6300 | 18.9800 | 19.9100 | 20.1000 | 20.5200 | 20.7600 | 21.1900 | 21.7200 | 22.3400 | 22.9388 | 24.2600 | 25.0911 | 25.4500 | 26.2403 | 26.4800 | 26.9000 | 27.6800 | 28.4800 | 29.0200 | 29.6100 | 29.8800 | | | |
| 3-chloro-trans-cinnamic acid | 9 | $P2_12_12_1$ | 1.5406 | 12.385 | 4.950 | 13.928 | 90.000 | 94.293 | 90.000 | 6.3326 | 12.7048 | 14.3000 | 15.2200 | 16.0900 | 18.4600 | 18.9900 | 19.2782 | 19.9000 | 20.1400 | 20.4800 | 22.0000 | 22.9800 | 23.4800 | 23.5700 | 24.1684 | 24.8200 | 25.8200 | 26.3100 | 26.8900 | 27.6800 | 28.5023 | 28.8700 | 29.2547 | 30.3184 | 30.7600 | | | |
| 1-methylfluorene | 10 | $P2_12_12_1$ | 1.5406 | 14.294 | 5.699 | 12.371 | 90.000 | 95.106 | 90.000 | 9.0900 | 9.9547 | 12.4669 | 16.7700 | 17.1500 | 18.2000 | 19.4600 | 19.9000 | 20.6400 | 21.6200 | 22.0032 | 22.5200 | 24.0271 | 24.4194 | 25.0200 | 25.3400 | 25.9600 | 26.7600 | 27.4200 | 27.8200 | 28.9847 | 29.3000 | 29.6000 | 29.9994 | 30.4183 | | | | |
| p-methoxybenzoic acid | 11 | $P2_12_12_1$ | 1.5406 | 16.942 | 10.943 | 3.963 | 90.000 | 98.099 | 90.000 | 9.6400 | 10.5400 | 13.2900 | 16.1700 | 17.0200 | 19.3513 | 22.6500 | 23.6001 | 23.9600 | 24.9824 | 25.3400 | 26.7400 | 27.0800 | 27.7800 | 28.7753 | 29.0600 | 29.9911 | 30.6100 | 31.0835 | 31.2512 | 31.7180 | 31.9732 | 32.4838 | 32.6807 | | | | | |
| alpha-l-glutamic-acid | 12 | $P2_12_12_1$ | 1.5406 | 10.335 | 8.827 | 7.111 | 90.000 | 90.000 | 90.000 | 15.1194 | 15.9906 | 17.1425 | 18.1589 | 19.9013 | 20.0949 | 21.2758 | 21.8857 | 23.5216 | 25.2446 | 25.4479 | 25.9803 | 26.4934 | 27.0118 | 27.7808 | 28.3810 | 29.8090 | 30.5106 | 30.8106 | 32.1658 | 32.9499 | 33.4726 | 34.0728 | | | | | | |
| ekermanite | 13 | $P-42_1m$ | 1.5406 | 7.852 | 7.852 | 5.018 | 90.000 | 90.000 | 90.000 | 16.0000 | 17.6800 | 21.0250 | 22.6600 | 23.9050 | 25.3750 | 28.8850 | 29.8000 | 31.1050 | 32.2750 | 35.8150 | 36.2050 | 37.0300 | 37.6600 | 38.8450 | 39.4450 | 40.5537 | 42.7802 | 44.3800 | 45.3849 | 46.2400 | 47.7400 | 48.9100 | 49.2100 | 50.3254 | 51.2800 | 51.7600 | 52.0450 | 52.6600 |
| tetrahexylsexithiophene | 14 | C2 | 1.5406 | 24.951 | 7.515 | 13.869 | 90.000 | 117.244 | 90.000 | 7.1530 | 7.8925 | 12.8370 | 13.3880 | 14.1710 | 15.9400 | 17.5640 | 18.1988 | 19.2605 | 20.3236 | 21.4355 | 22.6220 | 23.2915 | 23.6250 | 24.0310 | 24.7270 | 24.9524 | 25.4674 | 26.0262 | | | | | | | | | | |
| erythromycin A dihydrate | 15 | $P2_12_12_1$ | 1.5406 | 9.191 | 9.629 | 47.146 | 90.000 | 90.000 | 90.000 | 7.4650 | 9.3250 | 9.7900 | 10.2850 | 10.7200 | 11.1400 | 12.1600 | 13.0900 | 13.3484 | 13.7800 | 14.4250 | 14.7850 | 15.2438 | 16.2550 | 17.4250 | 17.5996 | 17.8300 | 18.3668 | 18.6975 | 19.2250 | 20.0675 | 20.8606 | 21.4652 | | | | | | |
| 4-nitrophenylhexylurethane | 16 | $P2_1$ | 1.5406 | 5.613 | 5.762 | 21.500 | 90.000 | 96.863 | 90.000 | 8.2598 | 12.4287 | 16.5876 | 16.8703 | 18.7950 | 20.7600 | 21.3657 | 22.6847 | 22.9808 | 24.4883 | 24.9728 | 25.9284 | 26.5879 | 29.1587 | 29.4413 | | | | | | | | | | | | | | |
| (E)-2-(4,6-Difluoroindan-1-ylidene)acetamide I | 17 | $P2_12_12_1$ | 1.5406 | 14.257 | 5.112 | 15.048 | 90.000 | 116.885 | 90.000 | 6.8900 | 11.7500 | 13.1300 | 13.8650 | 14.1500 | 16.2287 | 17.1236 | 17.4500 | 18.5191 | 18.7100 | 18.9841 | 20.8850 | 21.3200 | 21.7955 | 22.4300 | 23.6600 | 24.9200 | 25.2500 | 25.7900 | 26.4950 | 27.5900 | 27.9950 | 28.5650 | 29.0576 | 31.4000 | | | | |
| (E)-2-(4,6-Difluoroindan-1-ylidene)acetamide II | 18 | $P-1$ | 1.5406 | 15.084 | 13.909 | 4.959 | 86.851 | 97.742 | 111.039 | 6.2150 | 7.3678 | 10.7150 | 11.9600 | 12.5600 | 13.5200 | 14.8550 | 16.2950 | 16.8650 | 17.6900 | 18.9500 | 19.7600 | 20.3900 | 21.6350 | 22.3550 | 23.4650 | 23.7800 | 24.1979 | 25.3400 | 25.7300 | 26.3792 | 27.0200 | 27.4400 | | | | | | |
| (E)-2-(4,6-Difluoroindan-1-ylidene)acetamide II | 19 | $P2_12_12_1$ | 1.5406 | 12.790 | 5.100 | 29.334 | 90.000 | 96.565 | 90.000 | 6.0000 | 6.9055 | 8.6326 | 9.6700 | 12.0800 | 13.2300 | 13.8600 | 14.4783 | 14.6146 | 15.7600 | 17.3600 | 17.5600 | 18.1800 | 18.3400 | 19.4700 | 20.2200 | 21.0800 | 21.6454 | 22.4292 | 22.6900 | 23.5448 | 24.2110 | 24.6900 | 25.4322 | 26.1900 | 26.6800 | 27.5693 | 27.9487 | |
| octane | 20 | $P-1$ | 1.5943 | 4.099 | 9.388 | 11.515 | 71.080 | 90.009 | 105.744 | 8.4534 | 16.9052 | 20.4687 | 21.6735 | 22.6604 | 23.4750 | 24.2000 | 25.7500 | 27.0500 | 27.6514 | 28.8500 | 29.4250 | 30.0500 | 30.4000 | 31.8500 | 33.4250 | 34.1500 | 35.1568 | 35.9886 | 36.4750 | 37.5141 | | | | | | | | |
| pentadecane | 21 | $Pbcm$ | 1.5943 | 4.088 | 4.630 | 24.810 | 97.228 | 91.004 | 74.980 | 14.8500 | 3.7248 | 7.3836 | 20.5750 | 21.0750 | 22.3312 | 22.8500 | 23.5000 | 24.0000 | 24.3500 | 24.8002 | 25.7000 | 26.9250 | 27.4750 | 28.5750 | 29.7500 | 30.1897 | 31.6301 | 32.0174 | 32.5750 | 34.4250 | 35.0765 | 36.1500 | 36.7427 | 37.2112 | | | | |
| nonane | 22 | $P-1$ | 1.5943 | | 4.847 | 7.098 | 41.594 | 90.000 | 90.000 | 90.000 | 23.0500 | 4.3466 | 8.7749 | 13.1905 | 17.6355 | 23.9250 | 25.4962 | 26.0000 | 26.7791 | 27.8000 | 28.3097 | 30.5500 | 32.3250 | 33.7250 | 37.2000 | 38.4000 | 40.7500 | 42.9000 | 43.9091 | 44.7000 | 46.6500 | 47.0000 | 48.9250 | 50.7500 | 53.4000 | | | | |
| aigh (alpha phase) | 23 | $P-1$ | 1.5406 | 10.715 | 7.764 | 7.420 | 71.025 | 82.789 | 78.871 | 8.4597 | 12.2001 | 12.6772 | 14.1159 | 14.7529 | 15.7229 | 15.9633 | 16.9204 | 18.3513 | 18.6879 | 19.2530 | 20.4915 | 21.8718 | 22.3648 | 23.7475 | 24.6607 | 25.4940 | 26.3981 | 27.0908 | 27.8051 | 28.1326 | | | | | | | | |
| indigo (alpha phase) | 24 | $P2_1$ | 1.5406 | 10.882 | 5.831 | 12.252 | 90.000 | 130.147 | 90.000 | 10.6150 | 14.4999 | 17.0455 | 17.3766 | 18.5849 | 18.8906 | 21.3237 | 22.7163 | 23.7847 | 24.3641 | 26.2813 | 28.9586 | 30.1239 | 31.1053 | 32.1787 | 33.0677 | 33.8825 | 35.8053 | 37.6630 | 38.4973 | 39.7684 | | | | | | | | |