

Cambridge Structural Database
1 January 2012

CSD Entries: Summary Statistics

| | Structures | %CSD |
|-----------------------------------|-------------------|-------------|
| Total No. of structures | 596 810 | 100.0 |
| No. of different compounds | 544 565 | - |
| No. of literature sources | 1 429 | - |
| Organic structures | 254 475 | 42.6 |
| Transition metal present | 319 188 | 53.5 |
| Li – Fr or Be – Ra present | 30 134 | 5.0 |
| Main group metal present | 36 923 | 6.2 |
| 3D coordinates present | 554 760 | 93.0 |
| Error-free coordinates | 545 085 | 98.3† |
| Neutron studies | 1 534 | 0.3 |
| Powder diffraction studies | 2 354 | 0.4 |
| Low/high temp. studies | 250 328 | 41.9 |
| Absolute configuration determined | 11 111 | 1.9 |
| Disorder present in structure | 132 349 | 22.2 |
| Polymorphic structures | 18 486 | 3.1 |
| R-factor < 0.100 | 559 093 | 93.6 |
| R-factor < 0.075 | 506 465 | 84.9 |
| R-factor < 0.050 | 325 440 | 54.5 |
| R-factor < 0.030 | 65 897 | 11.0 |
| No. of atoms with 3D coordinates | 45 048 092 | - |

† Taken as a percentage of structures for which 3D coordinates are present in the CSD