

Cambridge Structural Database  
1 January 2024

*CSD Entries: Summary Statistics*

|                                   | <b>Structures</b> | <b>%CSD</b> |
|-----------------------------------|-------------------|-------------|
| Total No. of structures           | 1,298,446         | 100.0       |
| No. of different compounds        | 1,163,733         | -           |
| No. of literature sources         | 2,065             | -           |
| Organic structures                | 584,008           | 45.0        |
| Transition metal present          | 604,327           | 46.5        |
| Li – Fr or Be – Ra present        | 63,715            | 4.9         |
| Main group metal present          | 136,067           | 10.5        |
| 3D coordinates present            | 1,227,959         | 94.6        |
| Error-free coordinates            | 1,215,773         | 99.0†       |
| Neutron studies                   | 2,616             | 0.2         |
| Powder diffraction studies        | 9,432             | 0.7         |
| Low/high temp. studies            | 714,796           | 55.1        |
| Absolute configuration determined | 53,222            | 4.1         |
| Disorder present in structure     | 365,338           | 28.1        |
| Polymorphic structures            | 40,915            | 3.2         |
| R-factor < 0.100                  | 1,244,817         | 95.9        |
| R-factor < 0.075                  | 1,125,974         | 86.7        |
| R-factor < 0.050                  | 743,857           | 57.3        |
| R-factor < 0.030                  | 182,749           | 14.1        |
| No. of atoms with 3D coordinates  | 111,915,402       | -           |

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