

Cambridge Structural Database
16 February 2015

CSD Entries: Summary Statistics

	Structures	%CSD
Total No. of structures	758844	100.0
No. of different compounds	695828	-
No. of literature sources	1649	-
Organic structures	323149	42.6
Transition metal present	375561	49.5
Li – Fr or Be – Ra present	37331	4.9
Main group metal present	79955	10.5
3D coordinates present	713353	94.0
Error-free coordinates	694541	97.4†
Neutron studies	1719	0.2
Powder diffraction studies	3326	0.4
Low/high temp. studies	352454	46.4
Absolute configuration determined	17991	2.4
Disorder present in structure	178898	23.6
Polymorphic structures	22854	3.0
R-factor < 0.100	714920	94.2
R-factor < 0.075	647957	85.4
R-factor < 0.050	420330	55.4
R-factor < 0.030	89060	11.7
No. of atoms with 3D coordinates	60478168	-

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