

Cambridge Structural Database
5 January 2017

CSD Entries: Summary Statistics

	Structures	%CSD
Total No. of structures	869,295	100.0
No. of different compounds	795,368	-
No. of literature sources	1705	-
Organic structures	374,246	43.1
Transition metal present	425,881	49.0
Li – Fr or Be – Ra present	42,398	4.9
Main group metal present	90,308	10.4
3D coordinates present	820,543	94.4
Error-free coordinates	809,942	98.7†
Neutron studies	1910	0.2
Powder diffraction studies	4124	0.5
Low/high temp. studies	424,018	48.8
Absolute configuration determined	24,005	2.7
Disorder present in structure	212,700	24.5
Polymorphic structures	26,223	3.0
R-factor < 0.100	820,518	94.4
R-factor < 0.075	743,222	85.6
R-factor < 0.050	483,997	55.7
R-factor < 0.030	104,563	12.0
No. of atoms with 3D coordinates	71,065,827	-

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