

Cambridge Structural Database
6 January 2014

CSD Entries: Summary Statistics

	Structures	%CSD
Total No. of structures	686 944	100.0
No. of different compounds	628 684	-
No. of literature sources	1 578	-
Organic structures	292 661	42.6
Transition metal present	369 682	53.8
Li – Fr or Be – Ra present	34 433	5.0
Main group metal present	41 711	6.1
3D coordinates present	643 032	93.3
Error-free coordinates	630 329	98.0†
Neutron studies	1 616	0.2
Powder diffraction studies	2 930	0.4
Low/high temp. studies	306809	44.7
Absolute configuration determined	14 752	2.1
Disorder present in structure	158 127	23.0
Polymorphic structures	20 753	3.0
R-factor < 0.100	645 809	94.0
R-factor < 0.075	585 333	85.2
R-factor < 0.050	378 391	55.1
R-factor < 0.030	78 594	11.4
No. of atoms with 3D coordinates	53 563 990	-

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