

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