

Cambridge Structural Database
5 January 2018

CSD Entries: Summary Statistics

	Structures	%CSD
Total No. of structures	931,333	100.0
No. of different compounds	848,492	-
No. of literature sources	1,717	-
Organic structures	402,533	43.2
Transition metal present	454,079	48.8
Li – Fr or Be – Ra present	46,116	5.0
Main group metal present	96,590	10.4
3D coordinates present	880,576	94.6
Error-free coordinates	870,113	98.8†
Neutron studies	2,074	0.2
Powder diffraction studies	4,619	0.5
Low/high temp. studies	464,662	49.9
Absolute configuration determined	27,658	3.0
Disorder present in structure	236,615	25.4
Polymorphic structures	27,998	3.0
R-factor < 0.100	879,656	94.4
R-factor < 0.075	796,564	85.5
R-factor < 0.050	519,513	55.8
R-factor < 0.030	113,636	12.2
No. of atoms with 3D coordinates	77,074,097	-

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