

Cambridge Structural Database
1 January 2022

CSD Entries: Summary Statistics

	Structures	%CSD
Total No. of structures	1,175,551	100.0
No. of different compounds	1,059,813	-
No. of literature sources	2,052	-
Organic structures	520,813	44.2
Transition metal present	557,546	47.4
Li – Fr or Be – Ra present	57,828	4.9
Main group metal present	122,285	10.4
3D coordinates present	1,113,076	94.7
Error-free coordinates	1,098,316	98.6†
Neutron studies	2,488	0.2
Powder diffraction studies	8,390	0.7
Low/high temp. studies	623,104	53.0
Absolute configuration determined	42,968	3.7
Disorder present in structure	320,700	27.2
Polymorphic structures	36,298	3.1
R-factor < 0.100	1,128,781	96.0
R-factor < 0.075	1,021,862	86.9
R-factor < 0.050	673,388	57.3
R-factor < 0.030	164,349	14.0
No. of atoms with 3D coordinates	100,294,256	-

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