

Cambridge Structural Database
1 January 2021

CSD Entries: Summary Statistics

	Structures	%CSD
Total No. of structures	1,112,278	100.0
No. of different compounds	1,004,974	-
No. of literature sources	2,036	-
Organic structures	488,628	43.9
Transition metal present	532,217	47.8
Li – Fr or Be – Ra present	54,417	4.9
Main group metal present	115,311	10.4
3D coordinates present	1,052,406	94.6
Error-free coordinates	1,041,407	98.9†
Neutron studies	2,360	0.2
Powder diffraction studies	8,014	0.7
Low/high temp. studies	587,799	52.8
Absolute configuration determined	39,327	3.5
Disorder present in structure	297,757	26.8
Polymorphic structures	32,834	3.0
R-factor < 0.100	1,068,635	96.1
R-factor < 0.075	967,769	87.0
R-factor < 0.050	636,823	57.3
R-factor < 0.030	154,880	13.9
No. of atoms with 3D coordinates	94,176,969	-

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