

Cambridge Structural Database
1 January 2023

CSD Entries: Summary Statistics

	Structures	%CSD
Total No. of structures	1,235,232	100.0
No. of different compounds	1,109,868	-
No. of literature sources	2,058	-
Organic structures	550,745	44.6
Transition metal present	581,041	47
Li – Fr or Be – Ra present	60,769	4.9
Main group metal present	128,883	10.4
3D coordinates present	1,168,675	94.6
Error-free coordinates	1,156,756	98.9†
Neutron studies	2,545	0.2
Powder diffraction studies	8,928	0.7
Low/high temp. studies	675,320	54.6
Absolute configuration determined	48,399	3.9
Disorder present in structure	342,250	27.7
Polymorphic structures	38,375	3.1
R-factor < 0.100	1,185,360	96.0
R-factor < 0.075	1,072,641	86.8
R-factor < 0.050	707,829	57.3
R-factor < 0.030	173,337	14.0
No. of atoms with 3D coordinates	105,821,374	-

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