

Cambridge Structural Database  
1 January 2020

*CSD Entries: Summary Statistics*

	<b>Structures</b>	<b>%CSD</b>
Total No. of structures	1,050,466	100.0
No. of different compounds	951,854	-
No. of literature sources	2,020	-
Organic structures	459,193	43.7
Transition metal present	505,916	48.2
Li – Fr or Be – Ra present	51,243	4.9
Main group metal present	108,593	10.3
3D coordinates present	994,494	94.7
Error-free coordinates	983,859	98.9†
Neutron studies	2,283	0.2
Powder diffraction studies	7,378	0.7
Low/high temp. studies	544,730	51.9
Absolute configuration determined	35,191	3.4
Disorder present in structure	276,456	26.3
Polymorphic structures	31,223	3.0
R-factor < 0.100	1,009,743	96.1
R-factor < 0.075	914,711	87.1
R-factor < 0.050	600,910	57.2
R-factor < 0.030	145,755	13.9
No. of atoms with 3D coordinates	88,500,008	-

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