CSIRO NANOSTRUCTURE DATABANK

Header List – Silver Nanoparticle Data Set

ID	File name and unique identifier
Structural Feature	
Shape	The zonohedron of the polyhedral nanoparticle
N Atoms	Total number of atoms
N Bulk	Total number of bulk atoms
N Surface	Total number of surface atoms
R min	Minimum radius, in Å
R max	Maximum radius, in Å
R_diff	Difference between minimum and maximum radius, in Å
R_avg	Average radius, in Å
R_std	Standard deviation of the radius, in Å
R_skew	Skewness of the radius, in Å
R kurt	Kurtosis of the radius, in Å
Anisotropy	Aspect ratio
S 100	Number of atoms on (100) surface facet
S_111	Number of atoms on (111) surface facet
S 110	Number of atoms on (110) surface facet
S_311	Number of atoms on (311) surface facet
N_facets	Number of surface facets
Curve 0-10	Surface curvature angle between 1 and 10 degrees
Curve_11-20	Surface curvature angle between 11 and 20 degrees
Curve_21-30	Surface curvature angle between 21 and 30 degrees
Curve_31-40	Surface curvature angle between 31 and 40 degrees
Curve_41-50	Surface curvature angle between 41 and 50 degrees
Curve_51-60	Surface curvature angle between 51 and 60 degrees
Curve_61-70	Surface curvature angle between 61 and 70 degrees
Curve_71-80	Surface curvature angle between 71 and 80 degrees
Curve_81-90	Surface curvature angle between 81 and 90 degrees
Curve_91-100	Surface curvature angle between 91 and 100 degrees
Curve_101-110	Surface curvature angle between 101 and 110 degrees
Curve_111-120	Surface curvature angle between 111 and 120 degrees
Curve_121-130	Surface curvature angle between 121 and 130 degrees
Curve_131-140	Surface curvature angle between 131 and 140 degrees
Curve_141-150	Surface curvature angle between 141 and 150 degrees
Curve_151-160	Surface curvature angle between 151 and 160 degrees
Curve_161-170	Surface curvature angle between 161 and 170 degrees
Curve_171-180	Surface curvature angle between 171 and 180 degrees
Avg_total	Coordination statistics, average Ag coordination number
Avg_bulk	Coordination statistics, average bulk Ag coordination number
Avg_surf	Coordination statistics, average surface Ag coordination number
SCN1	Degree of under-coordination number of surface atoms, surface coordination number 1
SCN2	Degree of under-coordination number of surface atoms, surface coordination number 2
SCN3	Degree of under-coordination number of surface atoms, surface coordination number 3
SCN4	Degree of under-coordination number of surface atoms, surface coordination number 4
SCN5	Degree of under-coordination number of surface atoms, surface coordination number 5

SCN6 Degree of under-coordination number of surface atoms, surface coordination number 6 SCN7 Degree of under-coordination number of surface atoms, surface coordination number 7 SCN8 Degree of under-coordination number of surface atoms, surface coordination number 8 SCN9 Degree of under-coordination number of surface atoms, surface coordination number 9 SCN10 Degree of under-coordination number of surface atoms, surface coordination number 10 SCN11 Degree of under-coordination number of surface atoms, surface coordination number 11 SCN12 Degree of under-coordination number of surface atoms, surface coordination number 12 Avg Average Ag-Ag bond length, in Å Std dev Standard deviations of the Ag-Ag bond length, in Å Max Maximum Ag-Ag bond length, in Å Min Min Minimum Ag-Ag bond length, in Å Min Min Minimum Ag-Ag bond length, in Å N_Bonds Total number of Ag-Ag bonds FCC Total number of FCC atoms HCP Total number of HCP atoms HCP Total number of HCP atoms HCP Total number of HCD atoms			
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T1 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 1 T2 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 2 T3 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 3 T4 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 4 T5 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 5 T6 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 6 T7 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 7 T8 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 8 T9 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 9 T10 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 10 T11 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 11 T12 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T13 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order param	Avg_surf	Spherical harmonics q6.q6 > 0.7 coordination, average order parameter or surface atoms	
T2 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 2 T3 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 3 T4 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 4 T5 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 5 T6 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 6 T7 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 7 T8 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 8 T9 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 9 T10 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 10 T11 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 11 T12 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T13 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 Target Property Labels Formation _E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV EA Electron affinity, in eV	T0	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 0	
Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 3 T4 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 4 T5 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 5 T6 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 6 T7 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 7 T8 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 8 T9 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 9 T10 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 10 T11 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 11 T12 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T13 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T=20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T=20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T=20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T=20 Spherical harmonics q6.q6 > 0.7 coord	T1	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 1	
T4 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 4 T5 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 5 T6 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 6 T7 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 7 T8 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 8 T9 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 9 T10 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 10 T11 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 11 T12 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T13 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with ord	T2	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 2	
T5 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 5 T6 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 6 T7 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 7 T8 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 8 T9 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 9 T10 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 10 T11 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 11 T12 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T13 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >0 Target Property Labels Formation_E Formation_energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV	T3	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 3	
T6 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 6 T7 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 7 T8 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 8 T9 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 9 T10 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 10 T11 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 11 T12 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T13 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV EP Ionisation potential, in eV	T4		
T7 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 7 T8 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 8 T9 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 9 T10 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 10 T11 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 11 T12 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T13 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >00 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >00 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >00 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >00 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >00 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >00 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >00 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >00 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >00 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >00 T=10 Spherical harmonics q6.q6 > 0.7 coo	T5	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 5	
Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 8 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 9 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 10 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 11 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 The spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 The spherical harmonics q6.q6 > 0.7			
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T10 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 10 T11 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 11 T12 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T13 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV EA Electron affinity, in eV			
T11 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 11 T12 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T13 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV	T9	Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 9	
Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 12 T13 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV	T10		
Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 13 T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV			
T14 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 14 T15 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV EA Electron affinity, in eV			
Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 15 T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV			
T16 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 16 T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV			
T17 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 17 T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV			
T18 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 18 T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV			
T19 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 19 T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV			
T20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of 20 T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV			
T>20 Spherical harmonics q6.q6 > 0.7 coordination, atoms with order parameter of >20 Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV			
Target Property Labels Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV			
Formation_E Formation energy, (E_np-E_bulk)/N_atoms, in eV EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV			
EF Energy of the Fermi level, in eV IP Ionisation potential, in eV EA Electron affinity, in eV	· · · ·		
IP Ionisation potential, in eV EA Electron affinity, in eV			
EA Electron affinity, in eV			
EG Electronic band gap, in eV			
	EG	Electronic band gap, in eV	