Attribute name	Description	Unit	Value origin	Citation keys
atomic_number	Atomic number		stored	
atomic_radius_rahm	Atomic radius by Rahm et al.	pm	stored	[45, 46]
atomic_radius	Atomic radius	pm	stored	[53]
atomic_volume	Atomic volume	cm^3/mol	stored	
atomic_weight_uncertainty	Atomic weight uncertainty	Da	stored	[34, 63]
atomic_weight	Relative atomic weight ([11])	Da	stored	[34, 63]
block	Block in periodic table		stored	
covalent_radius_bragg	Covalent radius by Bragg	pm	stored	[10]
covalent_radius_cordero	Covalent radius by Cerdero et al. ([2])	pm	stored	[16]
covalent_radius_pyykko_double	Double bond covalent radius by Pyykko et al.	pm	stored	[42]
covalent_radius_pyykko_triple	Triple bond covalent radius by Pyykko et al.	pm	stored	[44]
covalent_radius_pyykko	Single bond covalent radius by Pyykko et al.	pm	stored	[43]
electron_affinity	Electron affinity ([4])	eV	stored	[6, 23]
electronegativity_allen	Allen's scale of electronegativity ([5])	eV	stored	[30, 31]
electronegativity_mulliken	Mulliken's scale of electronegativity	eV	computed	[35]
electrophilicity	Parr's electrophilicity index		computed	[39]
group	Group in the periodic table		stored	
hardness	Absolute hardness. Can also be calcualted for ions.	eV	computed	[38]
ionenergy	See IonizationEnergy class documentation		stored	
mass_number	Mass number of the most abundant isotope		computed	
melting_point	Melting point	K	stored	[22]
mendeleev_number	Mendeleev's number ([6])		stored	[41, 57]
name	Name in English		stored	
nist_webbook_url	URL for the NIST Chemistry WebBook		computed	[37]
nvalence	Number of valence electrons		computed	

Attribute name	Description	Unit	Value origin	Citation keys
oxistates	See OxidationState class documentation		stored	
period	Period in periodic table		stored	
proton_affinity	Proton affinity	kJ/mol	stored	[23]
softness	Absolute softness. Can also be calculated for ions.	1/eV	computed	
vdw_radius_alvarez	Van der Waals radius according to Alvarez ([8])	pm	stored	[5, 58]
vdw_radius_batsanov	Van der Waals radius according to Batsanov	pm	stored	[8]
vdw_radius_bondi	Van der Waals radius according to Bondi	pm	stored	[9]
vdw_radius_dreiding	Van der Waals radius from the DREIDING FF	pm	stored	[33]
vdw_radius_mm3	Van der Waals radius from the MM3 FF	pm	stored	[3]
vdw_radius_rt	Van der Waals radius according to Rowland and Taylor	pm	stored	[48]
vdw_radius_truhlar	Van der Waals radius according to Truhlar	pm	stored	[32]
vdw_radius_uff	Van der Waals radius from the UFF	pm	stored	[47]
vdw_radius	Van der Waals radius	pm	stored	[23]
zeff	Effective nuclear charge		computed	