Ionic Radius Ratio and Coordination Number

Cation-to-anion radius ratio of an ionic compound and the coordination number and geometry predicted by the radius ratio rules.

Method: Pauling's radius ratio rules

Input parameters

Unit system: SI

Parameter	Value	Unit
Cation radius	0.10200	nm
Anion radius	0.18100	nm

Calculated results

Parameter	Value	Unit
Radius ratio	0.56354	
Predicted coordination number	6.0000	
Lower bound of that range	0.41400	
Upper bound of that range	0.73200	

Notes for this case

• Radius ratio rules (Pauling): a cation fits stably among anions that just touch it, which sets lower limits 0.155 (triangular, CN 3), 0.225 (tetrahedral, 4), 0.414 (octahedral, 6), 0.732 (cubic, 8) and 1.0 (12). They are a guide only: covalency and polarisation change the real structure. Use radii for the same coordination from one consistent table. Upper bound shows 0 above a ratio of 1.

Formula and method

$$\frac{r_C}{r_A}:\ 0.155\ (3),\ 0.225\ (4),\ 0.414\ (6),\ 0.732\ (8),\ 1.0\ (12)$$

Variables

r_C	Cation radius	m
r_A	Anion radius	m
r_C/r_A	Radius ratio	-
CN	Predicted coordination number	-
$(r_C/r_A)_{min}$	Lower bound of that range	-
$(r_C/r_A)_{max}$	Upper bound of that range	-

Method and standards

Radius ratio.

Assumptions and limits

- Hard-sphere ions; ionic bonding.

References

Pauling's radius ratio rules

Report details

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Release checks	3 reference cases of this calculator, computed independently, are checked on every release

Results are for engineering estimation. Verify critical designs against the referenced standards and your own data.

This calculator online

https://calc.firecad.com/materials/properties/ionic-radius-ratio

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.