

Formation Enthalpies and Entropies for Frenkel and Schottky Defects

The following table contains some numbers found in the literature. It is not complete, eventually it might get "fuller".

Illustration

Schottky Disorder

| Crystal | H_F [eV] | S_F [k] | H_M Cation vacancy [eV] | H_M Anion vacancy [eV] |
|---------|---|-------------------|---------------------------|--------------------------|
| LiF | 2.5 ¹⁾ 2.34 ^{2), 3)} | 9.6 ¹⁾ | 0.7 ¹⁾ | 0.7 ¹⁾ |
| LiCl | 2.12 ^{2), 3)} | | | |
| LiBr | 1.8 ³⁾ | | | |
| LiI | 1,3 ³⁾ | | | |
| NaCl | 2.3 ^{1), 2), 3)} | 6 ¹⁾ | 0.7 ¹⁾ | 1.0 ¹⁾ |
| KCl | 2.3 ¹⁾ 2.26 ³⁾ | 6.5 ¹⁾ | 0.7 ¹⁾ | 1.0 ¹⁾ |
| KBr | 2.4 ¹⁾ | 8.6 ¹⁾ | 0.6 ¹⁾ | 0.9 ¹⁾ |
| CsI | 1.9 ¹⁾ | - | 0.6 ¹⁾ | 0.3 ¹⁾ |
| MgO | 6.6 ²⁾ | | | |
| CaO | 6.1 | | | |

Frenkel Disorder

| | H_F [eV] | S_F [k] | H_m Anion interstitial [eV] | H_M Anion vacancy [eV] |
|------------------|--|-----------|-------------------------------|--------------------------|
| AgCl | 1.6 ^{2), 3)} | | | |
| AgBr | 1,20 ³⁾ | | | |
| β - AgI | 0,7 ³⁾ | | | |
| CaF ₂ | 2.7 ¹⁾ 2.8 ^{2), 3)} | - | ≈ 1.0 ¹⁾ | 0.6 ¹⁾ |
| SrF ₂ | 2.3 ¹⁾ 0.7 ³⁾ | - | 0.8 ¹⁾ | 0.9 ¹⁾ |
| BaF ₂ | 1.9 ¹⁾ | - | 0.7 ¹⁾ | 0.6 ¹⁾ |
| PbF ₂ | 1.1 ¹⁾ | - | - | - |

| | | | | |
|-------------------------|-------------------|---|---|---|
| SrCl₂ | 1.7 ¹⁾ | - | - | - |
| ZrO₂ | 4.1 ²⁾ | | | |
| UO₂ | 3.4 ²⁾ | | | |

- 1) From "[Hayes and Stoneham](#)"; Defects and Defect Processes in Nonmetallic Solids
- 2) [From University of Hull, Lectures](#)
- 3) [From Uni Lethbridge; California.](#)