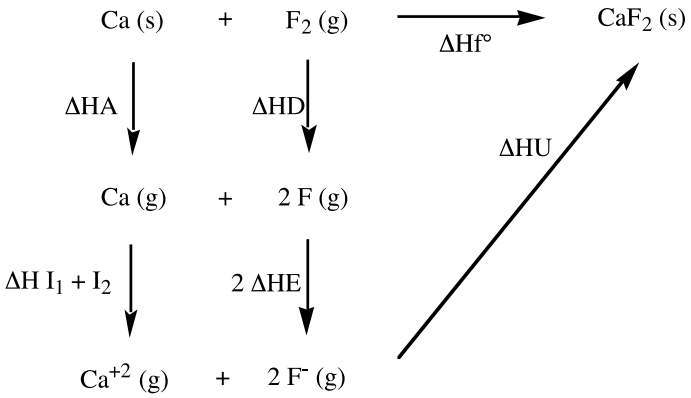
CICLOS DE BORN-HABER

1. Halogenuros MX_2. Ejemplo CaF_2.



$$\Delta H_f^\circ = \Delta H_A + \Delta H_{I1 + I2} + \Delta H_D + 2\,\Delta H_E + \Delta H_U$$

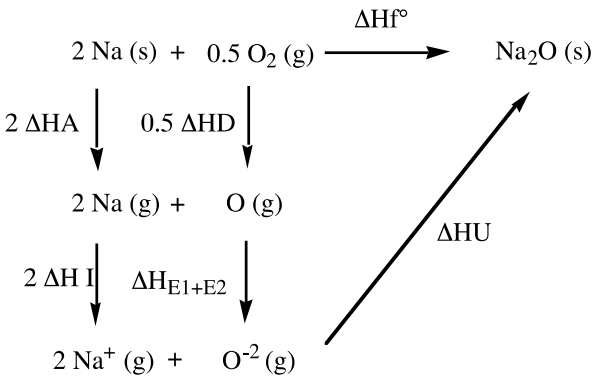
$$= 178 + 590 + 1146 + 157 - 2 \times 328 + \Delta H_U.$$

$$\Delta HU = -1389.2 \frac{A\,[Z+]\,[Z-]}{do\ (Å)} \left(1 - \frac{1}{n}\right)$$

$A = 2.519$; $Z+ = 2$; $Z- = 1$; $do = 1.19 + 1.14$; $n = (9+7) / 2$; $\Delta H_U = -2628.3$

$\Delta H_f^\circ = -1201$ KJmol^{-1}. (ΔH_f°experimental = -1243 KJmol^{-1}).

2. Óxidos M_2O. Ejemplo Na_2O.



$$\Delta H_f^{\circ}(Na_2O) = 2x\Delta H_A + 2x\Delta H_I + 0.5\,\Delta H_D + \Delta H_{E1+E2} + \Delta H_U$$

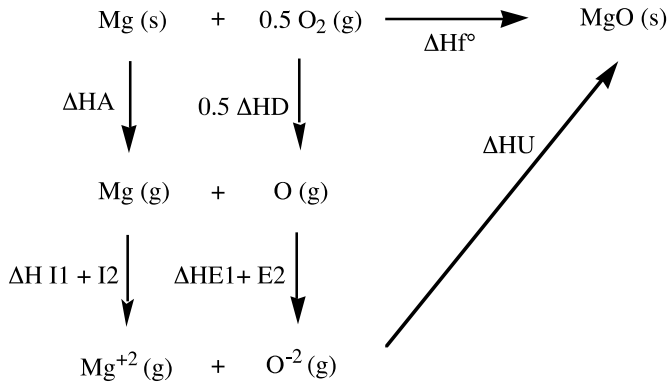
$$\Delta H_f^{\circ}(Na_2O) = 2x110 + 2x495.7 + 0.5 \times 493.4 - 141.1 + 780 + \Delta H_U$$

Estructura: antifluorita.

$$A = 2.5194;\ Z+ = 1;\ Z- = 2;\ do = 1.26 + 1.16;\ n = 7;\ \Delta H_U = -2479.30$$

$$\Delta H_f^{\circ}(Na_2O) = -383.6\ KJmol^{-1}$$

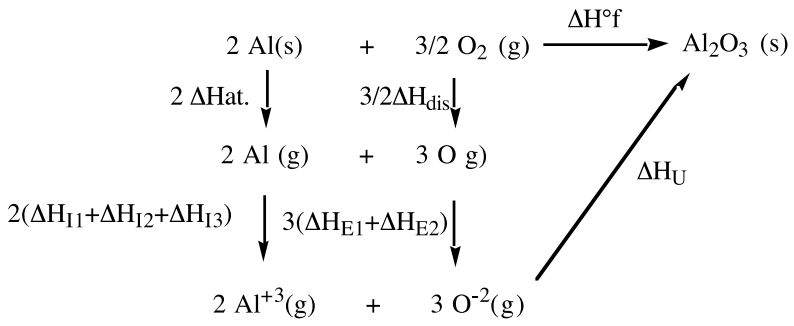
3. Óxidos MO. Ejemplo MgO.



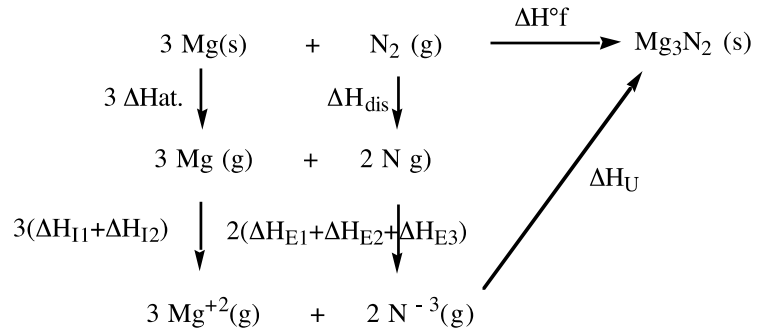
$$\Delta H_f^{\circ} = \Delta H_A + \Delta H_{I1+I2} + 0.5\,\Delta H_D + \Delta H_{E1+E2} + \Delta H_U$$

$$= 146 + 737 + 1450 + 246.7 - 141.1 + 780 - 3926.2 = -707.6\ KJmol^{-1}$$

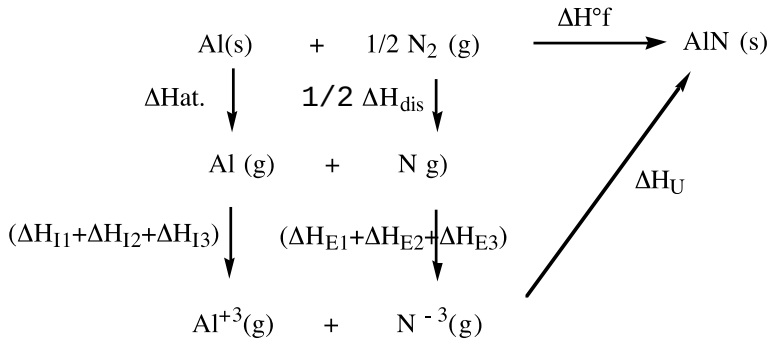
4. Óxidos M_2O_3. Ejemplo Al_2O_3.



5. Nitruros M_3N_2. Ejemplo Mg_3N_2.



6. Nitruros MN. Ejemplo AlN.



6. Sulfuros M_2S. Ejemplo Tl_2S.