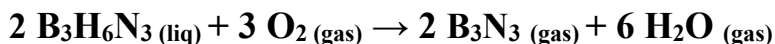


The calculation of thermodynamical parameters of the reaction



Standard thermodynamical parameters of formation of $\text{B}_3\text{N}_3(\text{I})$ (gas), found as a result of calculation by G4 method:

$$\Delta_f H^0 = 192.1 \text{ kJ}\cdot\text{mol}^{-1}, \Delta_f G^0 = 191.0 \text{ kJ}\cdot\text{mol}^{-1}, S^0 = 306.8 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$$

Standard thermodynamical parameters of formation of chemical compounds participating in the above-mentioned reaction which were found in experiment:

$$\text{B}_3\text{H}_6\text{N}_3 (\text{liq}): \Delta_f H^0 = -541.0 \text{ kJ}\cdot\text{mol}^{-1}, \Delta_f G^0 = -392.7 \text{ kJ}\cdot\text{mol}^{-1}, S^0 = 199.6 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$$

$$\text{O}_2 (\text{gas}): \Delta_f H^0 = 0 \text{ kJ}\cdot\text{mol}^{-1}, \Delta_f G^0 = 0 \text{ kJ}\cdot\text{mol}^{-1}, S^0 = 205.2 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$$

$$\text{H}_2\text{O} (\text{gas}): \Delta_f H^0 = -241.8 \text{ kJ}\cdot\text{mol}^{-1}, \Delta_f G^0 = -228.6 \text{ kJ}\cdot\text{mol}^{-1}, S^0 = 188.8 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$$

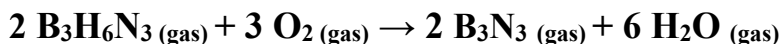
$$\begin{aligned} \Delta H^0 &= 2 \text{ mol} \cdot \Delta_f H^0 (\text{B}_3\text{N}_3 (\text{gas})) + 6 \text{ mol} \cdot \Delta_f H^0 (\text{H}_2\text{O} (\text{gas})) - 2 \text{ mol} \cdot \Delta_f H^0 (\text{B}_3\text{H}_6\text{N}_3 (\text{liq})) - 3 \\ &\text{mol} \cdot \Delta_f H^0 (\text{O}_2 (\text{gas})) = 2 \text{ mol} \cdot (192.1 \text{ kJ}\cdot\text{mol}^{-1}) + 6 \text{ mol} \cdot (-241.8 \text{ kJ}\cdot\text{mol}^{-1}) - \\ &2 \text{ mol} \cdot (-541.0 \text{ kJ}\cdot\text{mol}^{-1}) - 3 \text{ mol} \cdot (0) = [384.2 + (-1450.8) - (-1082.0)] \text{ kJ} = \mathbf{15.4 \text{ kJ}} \end{aligned}$$

$$\begin{aligned} \Delta S^0 &= 2 \text{ mol} \cdot S^0 (\text{B}_3\text{N}_3 (\text{gas})) + 6 \text{ mol} \cdot S^0 (\text{H}_2\text{O} (\text{gas})) - 2 \text{ mol} \cdot S^0 (\text{B}_3\text{H}_6\text{N}_3 (\text{liq})) - 3 \text{ mol} \cdot S^0 \\ &(\text{O}_2 (\text{gas})) = 2 \text{ mol} \cdot (306.8 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}) + 6 \text{ mol} \cdot (188.8 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}) - \\ &2 \text{ mol} \cdot (199.6 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}) - 3 \text{ mol} \cdot (205.2 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}) = [613.6 + 1132.8 - 399.2 - \\ &615.6] \text{ J}\cdot\text{K}^{-1} = \mathbf{731.6 \text{ J}\cdot\text{K}^{-1}} \end{aligned}$$

$$\begin{aligned} \Delta G^0 &= 2 \text{ mol} \cdot \Delta_f G^0 (\text{B}_3\text{N}_3 (\text{gas})) + 6 \text{ mol} \cdot \Delta_f G^0 (\text{H}_2\text{O} (\text{gas})) - 2 \text{ mol} \cdot \Delta_f G^0 (\text{B}_3\text{H}_6\text{N}_3 (\text{liq})) - 3 \\ &\text{mol} \cdot \Delta_f G^0 (\text{O}_2 (\text{gas})) = 2 \text{ mol} \cdot (191.0 \text{ kJ}\cdot\text{mol}^{-1}) + 6 \text{ mol} \cdot (-228.6 \text{ kJ}\cdot\text{mol}^{-1}) - \\ &2 \text{ mol} \cdot (-392.7 \text{ kJ}\cdot\text{mol}^{-1}) - 3 \text{ mol} \cdot (0) = [382.0 + (-1371.6) - (-785.4)] \text{ kJ} = \mathbf{-204.2 \text{ kJ}} \end{aligned}$$

$$\Delta G (T) = \Delta H^0 - T\Delta S^0 = 15.4 - 0.7316T$$

The calculation of thermodynamical parameters of the reaction



Standard thermodynamical parameters of formation of chemical compounds participating in the above-mentioned reaction which were calculated by G4 method:

$$\text{B}_3\text{H}_6\text{N}_3 (\text{gas}): \Delta_f H^0 = -513.7 \text{ kJ} \cdot \text{mol}^{-1}, \Delta_f G^0 = -404.8 \text{ kJ} \cdot \text{mol}^{-1}, S_f^0 = 329.1 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$$

$$\text{O}_2 (\text{gas}): \Delta_f H^0 = 2.0 \text{ kJ} \cdot \text{mol}^{-1}, \Delta_f G^0 = -3.1 \text{ kJ} \cdot \text{mol}^{-1}, S_f^0 = 222.0 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$$

$$\text{H}_2\text{O} (\text{gas}): \Delta_f H^0 = -239.6 \text{ kJ} \cdot \text{mol}^{-1}, \Delta_f G^0 = -228.9 \text{ kJ} \cdot \text{mol}^{-1}, S_f^0 = 197.2 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$$

$$\begin{aligned} \Delta H^0 &= 2 \text{ mol} \cdot \Delta_f H^0 (\text{B}_3\text{N}_3 (\text{gas})) + 6 \text{ mol} \cdot \Delta_f H^0 (\text{H}_2\text{O} (\text{gas})) - 2 \text{ mol} \cdot \Delta_f H^0 (\text{B}_3\text{H}_6\text{N}_3 (\text{gas})) - \\ & 3 \text{ mol} \cdot \Delta_f H^0 (\text{O}_2 (\text{gas})) = 2 \text{ mol} \cdot (192.1 \text{ kJ} \cdot \text{mol}^{-1}) + 6 \text{ mol} \cdot (-239.6 \text{ kJ} \cdot \text{mol}^{-1}) - \\ & 2 \text{ mol} \cdot (-513.7 \text{ kJ} \cdot \text{mol}^{-1}) - 3 \text{ mol} \cdot (2.0 \text{ kJ} \cdot \text{mol}^{-1}) = [384.2 + (-1437.6) - (-1027.4) - \\ & 6.0] \text{ kJ} = \mathbf{-32.0 \text{ kJ}} \end{aligned}$$

$$\begin{aligned} \Delta S^0 &= 2 \text{ mol} \cdot S^0 (\text{B}_3\text{N}_3 (\text{gas})) + 6 \text{ mol} \cdot S^0 (\text{H}_2\text{O} (\text{gas})) - 2 \text{ mol} \cdot S^0 (\text{B}_3\text{H}_6\text{N}_3 (\text{gas})) - \\ & 3 \text{ mol} \cdot S^0 (\text{O}_2 (\text{gas})) = 2 \text{ mol} \cdot (306.8 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}) + 6 \text{ mol} \cdot (197.2 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}) - \\ & 2 \text{ mol} \cdot (329.1 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}) - 3 \text{ mol} \cdot (222.0 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}) = [613.6 + 1183.2 - 658.2 - \\ & 666.0] \text{ J} \cdot \text{K}^{-1} = \mathbf{472.6 \text{ J} \cdot \text{K}^{-1}} \end{aligned}$$

$$\begin{aligned} \Delta G^0 &= 2 \text{ mol} \cdot \Delta_f G^0 (\text{B}_3\text{N}_3 (\text{gas})) + 6 \text{ mol} \cdot \Delta_f G^0 (\text{H}_2\text{O} (\text{gas})) - 2 \text{ mol} \cdot \Delta_f G^0 (\text{B}_3\text{H}_6\text{N}_3 (\text{gas})) - \\ & 3 \text{ mol} \cdot \Delta_f G^0 (\text{O}_2 (\text{gas})) = 2 \text{ mol} \cdot (191.0 \text{ kJ} \cdot \text{mol}^{-1}) + 6 \text{ mol} \cdot (-228.9 \text{ kJ} \cdot \text{mol}^{-1}) - \\ & 2 \text{ mol} \cdot (-404.8 \text{ kJ} \cdot \text{mol}^{-1}) - 3 \text{ mol} \cdot (-3.1 \text{ kJ} \cdot \text{mol}^{-1}) = [382.0 + (-1373.4) - (-809.6) - (- \\ & 9.3)] \text{ kJ} = \mathbf{-172.5 \text{ kJ}} \end{aligned}$$

$$\Delta G (T) = \Delta H^0 - T \Delta S^0 = \mathbf{-32.0 - 0.4726T}$$

Table S1

Energy differences between LUMO and HOMO ($\Delta_{\text{LUMO-HOMO}}$) for various modifications of B_3N_3 .

Compound	($\Delta_{\text{LUMO-HOMO}}$), eV
B_3N_3 (I)	11.946
B_3N_3 (II)	9.226
B_3N_3 (III)	8.589
B_3N_3 (IV)	9.126
B_3N_3 (V)	9.290
B_3N_3 (VI)	9.108
B_3N_3 (VII)	9.334