Supplementary materials

The calculation of thermodynamical parameters of the reaction

$2\ B_3H_6N_{3\ (liq)} + 3\ O_{2\ (gas)} \rightarrow 2\ B_3N_{3\ (gas)} + 6\ H_2O_{\ (gas)}$

Standard thermodynamical parameters of formation of B_3N_3(**I**) $_{(gas)}$, found as a result of calculation by G4 method:

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

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

$B_3H_6N_{3\ (liq)}$: $\Delta_f H^0 = -541.0$ kJ· mol^{-1}, $\Delta_f G^0 = -392.7$ kJ· mol^{-1}, $S^0 = 199.6$ J· mol^{-1}·K^{-1}

$O_{2\ (gas)}$: $\Delta_f H^0 = 0$ kJ· mol^{-1}, $\Delta_f G^0 = 0$ kJ· mol^{-1}, $S^0 = 205.2$ J· mol^{-1}·K^{-1}

$H_2O_{\ (gas)}$: $\Delta_f H^0 = -241.8$ kJ· mol^{-1}, $\Delta_f G^0 = -228.6$ kJ· mol^{-1}, $S^0 = 188.8$ J· mol^{-1}·K^{-1}

$\Delta H^0 = 2$ mol • $\Delta_f H^0$ ($B_3N_{3\ (gas)}$) + 6 mol • $\Delta_f H^0$ ($H_2O_{\ (gas)}$) – 2 mol • $\Delta_f H^0$ ($B_3H_6N_{3\ (liq)}$) – 3 mol • $\Delta_f H^0$ ($O_{2\ (gas)}$) = 2 mol • (192.1 kJ· mol^{-1}) + 6 mol • (-241.8 kJ· mol^{-1}) – 2 mol • (-541.0 kJ· mol^{-1}) – 3 mol • (0) = [384.2 + (-1450.8) – (-1082.0)] kJ = **15.4** kJ

$\Delta S^0 = 2$ mol • S^0 ($B_3N_{3\ (gas)}$) + 6 mol • S^0 ($H_2O_{\ (gas)}$) – 2 mol • S^0 ($B_3H_6N_{3\ (liq)}$) – 3 mol • S^0 ($O_{2\ (gas)}$) = 2 mol • (306.8 J· mol^{-1}·K^{-1}) + 6 mol • (188.8 J· mol^{-1}·K^{-1}) – 2 mol • (199.6 J· mol^{-1}·K^{-1}) – 3 mol • (205.2 J· mol^{-1}·K^{-1}) = [613.6 + 1132.8 – 399.2 – 615.6] J·K^{-1} = **731.6** J·K^{-1}

$\Delta G^0 = 2$ mol • $\Delta_f G^0$ ($B_3N_{3\ (gas)}$) + 6 mol • $\Delta_f G^0$ ($H_2O_{\ (gas)}$) – 2 mol • $\Delta_f G^0$ ($B_3H_6N_{3\ (liq)}$) – 3 mol • $\Delta_f G^0$ ($O_{2\ (gas)}$) = 2 mol • (191.0 kJ· mol^{-1}) + 6 mol • (-228.6 kJ· mol^{-1}) – 2 mol • (-392.7 kJ· mol^{-1}) – 3 mol • (0) = [382.0 + (-1371.6) – (-785.4)] kJ = **-204.2** kJ

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

The calculation of thermodynamical parameters of the reaction

$2\ B_3H_6N_{3\ (gas)} + 3\ O_{2\ (gas)} \rightarrow 2\ B_3N_{3\ (gas)} + 6\ H_2O_{\ (gas)}$

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

$B_3H_6N_{3\ (gas)}$: $\Delta_f H^0$ = -513.7 kJ· mol^{-1}, $\Delta_f G^0$ = -404.8 kJ· mol^{-1}, S_f^0 = 329.1 J· mol^{-1}·K^{-1}

$O_{2\ (gas)}$: $\Delta_f H^0$ = 2.0 kJ· mol^{-1}, $\Delta_f G^0$ = -3.1 kJ· mol^{-1}, S_f^0 = 222.0 J· mol^{-1}·K^{-1}

$H_2O_{\ (gas)}$: $\Delta_f H^0$ = -239.6 kJ· mol^{-1}, $\Delta_f G^0$ = -228.9 kJ· mol^{-1}, S_f^0 = 197.2 J· mol^{-1}·K^{-1}

ΔH^0 = 2 mol • $\Delta_f H^0$ ($B_3N_{3\ (gas)}$) + 6 mol • $\Delta_f H^0$ ($H_2O_{\ (gas)}$) – 2 mol • $\Delta_f H^0$ ($B_3H_6N_{3\ (gas)}$) – 3 mol • $\Delta_f H^0$ ($O_{2\ (gas)}$) = 2 mol • (192.1 kJ· mol^{-1}) + 6 mol • (-239.6 kJ· mol^{-1}) – 2 mol • (-513.7 kJ· mol^{-1}) – 3 mol • (2.0 kJ· mol^{-1}) = [384.2 + (-1437.6) – (-1027.4) – 6.0] kJ = **-32.0** kJ

ΔS^0 = 2 mol • S^0 ($B_3N_{3\ (gas)}$) + 6 mol • S^0 ($H_2O_{\ (gas)}$) – 2 mol • S^0 ($B_3H_6N_{3\ (gas)}$) – 3 mol • S^0 ($O_{2\ (gas)}$) = 2 mol • (306.8 J· mol^{-1}·K^{-1}) + 6 mol • (197.2 J· mol^{-1}·K^{-1}) – 2 mol • (329.1 J· mol^{-1}·K^{-1}) – 3 mol • (222.0 J· mol^{-1}·K^{-1}) = [613.6 + 1183.2 – 658.2 – 666.0] J·K^{-1} = **472.6** J·K^{-1}

ΔG^0 = 2 mol • $\Delta_f G^0$ ($B_3N_{3\ (gas)}$) + 6 mol • $\Delta_f G^0$ ($H_2O_{\ (gas)}$) – 2 mol • $\Delta_f G^0$ ($B_3H_6N_{3\ (gas)}$) – 3 mol • $\Delta_f G^0$ ($O_{2\ (gas)}$) = 2 mol • (191.0 kJ· mol^{-1}) + 6 mol • (-228.9 kJ· mol^{-1}) – 2 mol • (-404.8 kJ· mol^{-1}) – 3 mol • (-3.1 kJ· mol^{-1}) = [382.0 + (-1373.4) –(-809.6) – (-9.3)] kJ = **-172.5** kJ

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

Table S1

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

Compound	($\Delta_{LUMO-HOMO}$), 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