





















**Table B8.** Density and energy of  $\alpha$ -HMX, calculated with two double bonds in the  $\text{NO}_2$  group.

| Space group                                   | Density | Total energy | van der Waals energy | Electrostatic energy |
|---|---------|--------------|----------------------|----------------------|
| P2 <sub>1</sub> /c                            | 1.759   | -619.65      | -84.77               | -406.31              |
| P1  | 1.811   | -617.64      | -91.63               | -405.43              |
| P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> | 1.756   | -616.09      | -86.65               | -399.95              |
| P2 <sub>1</sub>                               | 1.740   | -615.47      | -81.17               | -402.67              |
| Pbca  | 1.792   | -615.09      | -92.55               | -400.58              |
| C2/c  | 1.764   | -614.00      | -85.56               | -402.21              |

**Table B9.** Density and energy of  $\beta$ -HMX.

| Space group                                   | Density | Total energy | van der Waals energy | Electrostatic energy |
|---|---------|--------------|----------------------|----------------------|
| P2 <sub>1</sub> /c                            | 1.967   | -1107.34     | -31.80               | -1062.15             |
| P2 <sub>1</sub>                               | 1.975   | -1106.67     | -24.69               | -1071.82             |
| P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> | 1.924   | -1103.24     | -28.28               | -1058.80             |
| Pbca  | 1.938   | -1102.74     | -30.54               | -1058.80             |
| C2/c  | 1.894   | -1101.73     | -23.56               | -1063.91             |
| P1  | 1.870   | -1101.15     | -22.51               | -1063.99             |

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