

# Elastic Coefficients of $\beta$ -HMX as Functions of Pressure and Temperature from Molecular Dynamics

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## Supplemental Material

Table S1. Equilibrium unit-cell volumes and lattice parameters for  $\beta$ -HMX as functions of temperature and pressure.

$T$ (K)	$P$ (GPa)	$a$ (Å)	$b$ (Å)	$c$ (Å)	$\beta$ (deg)	$V$ (Å <sup>3</sup> )
300	$10^{-4}$	6.587	10.468	7.692	98.72	524.27
	5	6.329	9.748	7.319	97.65	447.47
	10	6.253	9.421	7.105	97.24	415.22
	20	6.154	9.024	6.852	96.71	377.95
	30	6.076	8.765	6.698	96.35	354.50
500	$10^{-4}$	6.623	10.667	7.727	98.93	539.25
	5	6.326	9.818	7.346	97.74	452.12
	10	6.252	9.471	7.123	97.33	418.31
	20	6.158	9.061	6.857	96.78	379.90
	30	6.081	8.794	6.698	96.41	355.96
700	$10^{-4}$	6.678	10.967	7.742	99.36	559.39
	5	6.320	9.899	7.373	97.85	456.94
	10	6.250	9.525	7.140	97.43	421.47
	20	6.161	9.100	6.861	96.86	381.86
	30	6.085	8.825	6.698	96.47	357.41
900	5	6.308	9.994	7.399	97.98	461.94
	10	6.243	9.584	7.162	97.55	424.75
	20	6.163	9.141	6.863	96.95	383.83
	30	6.090	8.858	6.696	96.54	358.87
1100	5	6.293	10.111	7.415	98.11	467.10
	10	6.227	9.648	7.192	97.70	428.19
	20	6.165	9.187	6.865	97.05	385.83
	30	6.094	8.894	6.693	96.62	360.35

Table S2. Full 6×6 matrix of elastic coefficients  $C_{ij}$  of  $\beta$ -HMX in units of GPa at 300 K and 1 atm ( $10^{-4}$  GPa). The first column on the left and the top row are indices  $i$  and  $j$ . The matrix is very close to being symmetric. Sixteen coefficients are close to zero as expected for the monoclinic crystal.

	1	2	3	4	5	6
1	<b>22.97 ± 0.04</b>	<b>9.21 ± 0.05</b>	<b>12.35 ± 0.04</b>	-0.01 ± 0.08	<b>-0.43 ± 0.01</b>	-0.004 ± 0.009
2	<b>9.20 ± 0.04</b>	<b>22.62 ± 0.05</b>	<b>12.40 ± 0.04</b>	-0.011 ± 0.009	<b>4.46 ± 0.02</b>	-0.010 ± 0.009
3	<b>12.28 ± 0.04</b>	<b>12.34 ± 0.05</b>	<b>21.67 ± 0.04</b>	-0.001 ± 0.008	<b>1.83 ± 0.01</b>	-0.007 ± 0.008
4	0.00 ± 0.02	0.01 ± 0.03	0.00 ± 0.02	<b>8.645 ± 0.004</b>	0.001 ± 0.006	<b>2.247 ± 0.005</b>
5	<b>-0.43 ± 0.02</b>	<b>4.48 ± 0.02</b>	<b>1.86 ± 0.02</b>	-0.014 ± 0.004	<b>10.407 ± 0.006</b>	-0.003 ± 0.005
6	0.00 ± 0.02	0.00 ± 0.02	-0.02 ± 0.02	<b>2.250 ± 0.004</b>	0.002 ± 0.006	<b>9.527 ± 0.005</b>

Table S3. Full 6×6 matrix of elastic coefficients  $C_{ij}$  of  $\beta$ -HMX in units of GPa at 700 K and 1 atm ( $10^{-4}$  GPa). The first column on the left and the top row are indices  $i$  and  $j$ . The matrix is very close to being symmetric. Sixteen coefficients are close to zero as expected for the monoclinic crystal.

	1	2	3	4	5	6
1	<b>12.78 ± 0.06</b>	<b>4.84 ± 0.07</b>	<b>7.11 ± 0.05</b>	-0.01 ± 0.01	<b>-0.09 ± 0.02</b>	0.03 ± 0.02
2	<b>4.90 ± 0.06</b>	<b>12.09 ± 0.07</b>	<b>6.48 ± 0.05</b>	0.01 ± 0.01	<b>2.92 ± 0.02</b>	0.04 ± 0.02
3	<b>7.08 ± 0.06</b>	<b>6.37 ± 0.08</b>	<b>14.05 ± 0.06</b>	0.02 ± 0.01	<b>0.73 ± 0.02</b>	0.04 ± 0.02
4	-0.02 ± 0.03	-0.02 ± 0.03	0.01 ± 0.02	<b>6.051 ± 0.007</b>	0.010 ± 0.009	<b>1.262 ± 0.009</b>
5	<b>0.09 ± 0.03</b>	<b>2.95 ± 0.04</b>	<b>0.77 ± 0.03</b>	0.005 ± 0.006	<b>6.147 ± 0.009</b>	0.007 ± 0.008
6	0.00 ± 0.03	0.00 ± 0.04	0.01 ± 0.03	<b>1.281 ± 0.007</b>	-0.005 ± 0.008	<b>6.316 ± 0.008</b>

Table S4. Full 6×6 matrix of elastic coefficients  $C_{ij}$  of  $\beta$ -HMX in units of GPa at 1100 K and 30 GPa. The first column on the left and the top row are indices  $i$  and  $j$ . The matrix is very close to being symmetric. Sixteen coefficients are close to zero as expected for the monoclinic crystal.

	1	2	3	4	5	6
1	<b>253.4 ± 0.1</b>	<b>135.0 ± 0.1</b>	<b>165.01 ± 0.07</b>	-0.03 ± 0.04	<b>-24.31 ± 0.04</b>	-0.01 ± 0.04
2	<b>135.0 ± 0.1</b>	<b>200.82 ± 0.09</b>	<b>158.36 ± 0.07</b>	0.06 ± 0.05	<b>25.21 ± 0.05</b>	-0.08 ± 0.04
3	<b>165.10 ± 0.09</b>	<b>158.5 ± 0.1</b>	<b>193.90 ± 0.06</b>	0.00 ± 0.04	<b>7.47 ± 0.04</b>	-0.05 ± 0.04
4	-0.02 ± 0.05	-0.03 ± 0.05	-0.07 ± 0.04	<b>40.52 ± 0.02</b>	-0.01 ± 0.02	<b>13.14 ± 0.02</b>
5	<b>-24.39 ± 0.05</b>	<b>25.17 ± 0.06</b>	<b>7.40 ± 0.05</b>	0.03 ± 0.02	<b>76.64 ± 0.02</b>	0.01 ± 0.02
6	0.01 ± 0.06	0.03 ± 0.06	-0.01 ± 0.04	<b>13.18 ± 0.02</b>	-0.01 ± 0.02	<b>38.21 ± 0.02</b>