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适用于 TATB, RDX, HMX 含能材料的全原子力场的建立与验证

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Development and Validation of an All-Atom Force Field for the Energetic Materials TATB, RDX and HM

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表s1　力场键参数

Table s1　Bond stretching parameters

		b_0/(nm)	k_b/(kJ·mol^{-1}·nm^{-2})
c_3an	c_3ani	0.13950	188362.62
c_3an	n_3h2	0.13000	102838.94
c_3ani	n_3o	0.13050	150041.10
c_4h2	h_1	0.10890	156787.79
c_4h2	n_3no	0.14400	110748.56
h_1n	n_3h2	0.10100	207121.29
n_3no	n_3o	0.13925	151374.88
n_3o	o_1n	0.12235	282284.31

c, d in formula (1): c=2 nm^{-1}, d=7/3 nm^{-2}

表 s2　力场角参数

Table s2　Angle bending parameters

			θ/(°)	k_a/(kJ·mol^{-1})
c_3an	c_3ani	c_3an	119.99920	188.92
c_3an	c_3ani	n_3o	120.00800	476.06
c_3an	n_3h2	h_1n	120.48610	131.66
c_3ani	c_3an	c_3ani	115.99920	188.92
c_3ani	c_3an	n_3h2	122.98490	261.51
c_3ani	n_3o	o_1n	120.60340	209.34
c_4h2	n_3no	c_4h2	119.05920	445.22
c_4h2	n_3no	n_3o	115.57740	349.07
h_1	c_4h2	h_1	106.77020	177.97
h_1	c_4h2	n_3no	109.81840	191.89
h_1n	n_3h2	h_1n	128.80830	164.14
n_3no	c_4h2	n_3no	113.84240	300.08
n_3no	n_3o	o_1n	117.49170	44.43
o_1n	n_3o	o_1n	123.83850	576.22

e, *f* in formula (1): if $\theta_0 \neq (0,\ \pi)$, $e = -\frac{2(\pi-2\theta_0)}{3\theta_0(\pi-\theta_0)}$, $f = -\frac{1}{2\theta_0(\pi-\theta_0)}$; when $\theta_0 = (0,\ \pi)$, $e = f = 0$.

表 s3　力场二面角参数

Table s3　Torsion parameters

				n_1	k_t/(kJ·mol^{-1})	n_2	k_t/(kJ·mol^{-1})	n_3	k_t/(kJ·mol^{-1})
c_3an	c_3ani	c_3an	c_3ani	2.00000	22.0146				
c_3an	c_3ani	c_3an	n_3h2	2.00000	22.0146				
c_3an	c_3ani	n_3o	o_1n	2.00000	19.3824				
c_3ani	c_3an	c_3ani	n_3o	2.00000	22.0146				
c_3ani	c_3an	n_3h2	h_1n	2.00000	6.2802				
c_4h2	n_3no	c_4h2	h_1	3.00000	0.8838	1.00000	-8.7131	2.00000	-0.9986
c_4h2	n_3no	c_4h2	n_3no	2.00000	1.3528	1.00000	35.3990	3.00000	-0.5627
c_4h2	n_3no	n_3o	o_1n	2.00000	10.1002				
h_1	c_4h2	n_3no	n_3o	3.00000	3.1991				
n_3h2	c_3an	c_3ani	n_3o	2.00000	22.0146				
n_3no	c_4h2	n_3no	n_3o	2.00000	-6.8814				

表 s4　力场面外键角参数

Table s4　Out of plane angle parameters

				χ/(°)	k_0/(kJ·mol^{-1})
c_3ani	c_3an	c_3ani	n_3h2	0.00000	43.3547
c_3an	n_3h2	h_1n	h_1n	0.00000	0.00000
c_3ani	n_3o	o_1n	o_1n	0.00000	0.00000

表 s5　键-键交叉项参数

Table s5　Bond bond couple parameters

			k_{bb}/(kJ·mol^{-1}·nm^{-2})
h_1	c_4h2	h_1	2976.0193

表 s6　键-角交叉项参数

Table s6　Bond angle couple parameters

			k_{ba}/(kJ·mol^{-1}·nm^{-1})
h_1	c_4h2	h_1	746.7576