Chemical bonding in energetic materials : β–NTO

by

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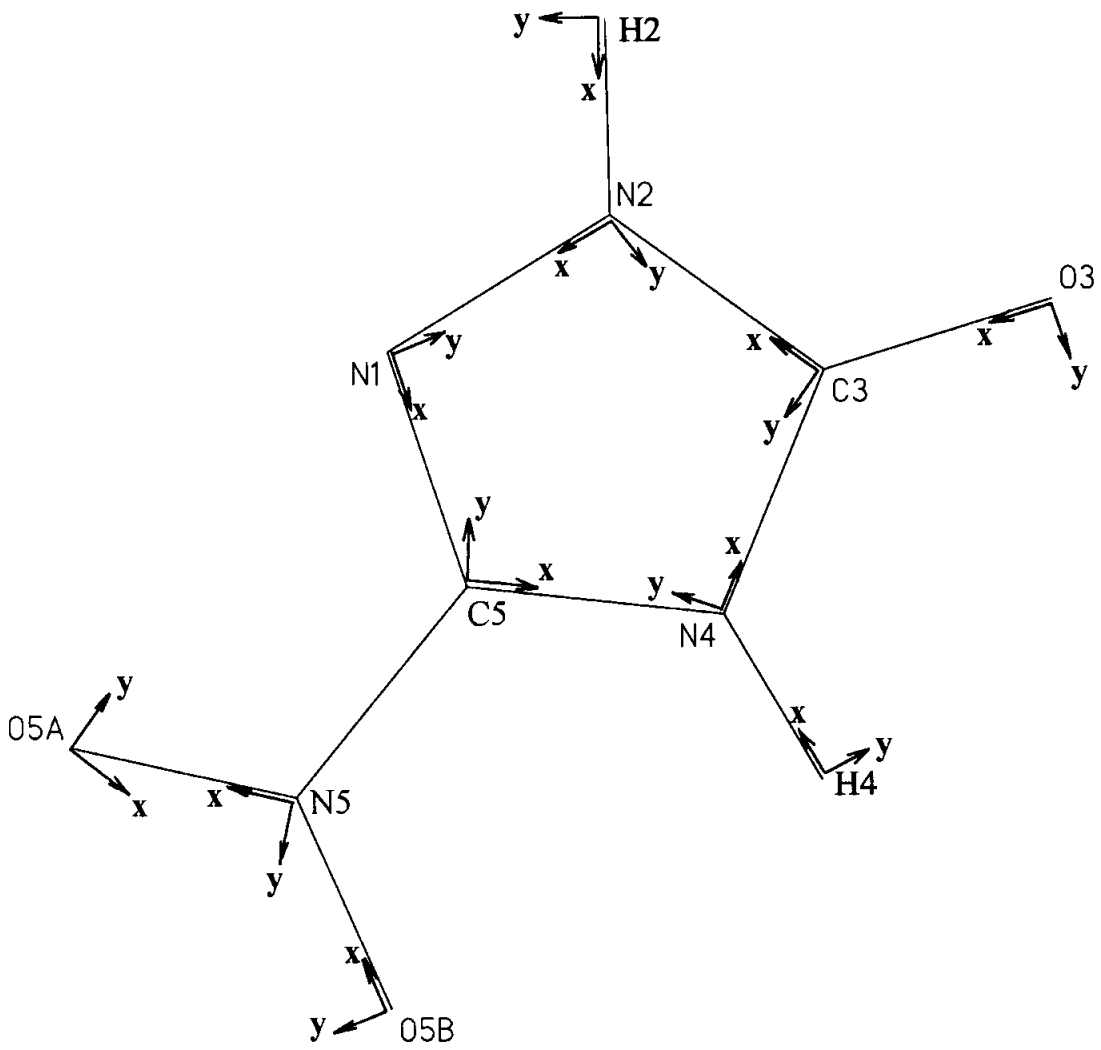
Deposition material

Table D1. Experimental setup

run No.	2θ	ω_{start}	φ	No. of frames
1	0	350	0	530
2	0	350	45	530
3	0	350	90	530
4	0	350	180	530
5	0	350	270	530
6	-45	300	0	500
7	-45	300	30	500
8	-45	300	90	500
9	-45	300	135	500
10	-45	300	225	500
11	-45	300	315	500
12	0	350	0	100

Table D2. The results of the multipole refinement.

	N(2)	H(2)	O(3)	N(1)	N(4)	H(4)	C(3)	O(5b)	O(5a)	N(5)	C(5)
M1	5.20(4)	0.77(2)	6.48(5)	5.06(4)	5.35(5)	0.70(2)	3.63(6)	6.14(4)	6.19(4)	4.68(6)	3.79(7)
D1+	-0.030(6)	0.063(7)	-0.090(10)	-0.051(7)	0	0.039(7)	-0.041(10)	-0.067(9)	-0.066(8)	-0.018(8)	0
D1-	-0.013(6)	0	0.019(7)	-0.143(8)	-0.040(6)	0.022(8)	-0.071(10)	-0.021(7)	0	0.015(8)	0.087(10)
D0	0	-0.028(8)	0	0	0.015(6)	0	0	0	0	0.028(8)	0.035(8)
Q0	0	0	-0.022(8)	-0.099(8)	-0.060(7)	0	-0.216(11)	-0.048(8)	-0.041(7)	-0.173(10)	-0.124(10)
Q1+	0.013(6)	0	0	0	0	0	0	0	0	0.015(7)	0
Q1-	0.016(6)	0	0.011(7)	0	0.020(6)	0	0	-0.018(8)	0.012(7)	0	0
Q2+	-0.047(6)	0	-0.056(9)	0.066(7)	-0.019(7)	0	-0.027(9)	-0.137(10)	-0.066(7)	0.026(8)	-0.045(9)
Q2-	0.011(6)	0	-0.021(8)	0.083(8)	0.046(7)	0	0.103(9)	0	-0.096(7)	-0.064(8)	-0.036(10)
O0	0	0	0	0.015(9)	0	0	0	-0.016(10)	0	0	0
O1+	-0.014(8)	0	0	-0.035(9)	0	0	0.033(11)	-0.048(9)	-0.012(9)	0.012(10)	0
O1-	0.018(8)	0	0	-0.040(9)	0	0	0	0	0	0	0.034(11)
O2+	0	0	0	0	0	0	0.025(11)	-0.017(9)	0.015(9)	0	-0.012(11)
O2-	0.014(8)	0	0	0	0	0	-0.012(11)	-0.017(10)	0	0.015(10)	-0.013(11)
O3+	0.174(11)	0	0.035(10)	0.107(10)	0.159(10)	0	0.236(15)	0.029(9)	0.018(8)	0.281(15)	0.287(15)
O3-	-0.018(8)	0	0	-0.075(9)	-0.045(9)	0	-0.105(12)	0.014(9)	0.038(8)	0.035(11)	-0.117(13)
H0	-0.012(11)	0	0	0	0	0	0.022(14)	0	0	0	0.041(16)
H1+	-0.016(10)	0	0	0.021(11)	0.053(10)	0	0	0.034(12)	0	0	0
H1-	0	0	-0.022(12)	0	0	0	-0.019(13)	0	0	-0.035(12)	0
H2+	0	0	0.031(13)	0	0	0	-0.031(13)	0	-0.020(11)	0.032(12)	0.035(14)
H2-	0.044(10)	0	0	0	0	0	-0.011(13)	0	0	0	-0.052(14)
H3+	0	0	0.014(11)	-0.024(11)	0.011(10)	0	0	0	-0.030(11)	0.025(12)	-0.037(14)
H3-	-0.018(10)	0	-0.026(12)	0.013(12)	0	0	0	0	-0.026(11)	0.036(14)	0.033(14)
H4+	0.011(9)	0	0.026(12)	0.032(11)	0.029(10)	0	0.067(16)	-0.015(12)	0	-0.020(12)	0
H4-	0.027(10)	0	0.022(11)	0	0	0	0	0	0	0	-0.023(15)
κ'	1.006(5)	1.22(3)	0.981(4)	1.013(5)	1.004(5)	1.22(3)	1.058(9)	1.005(4)	1.002(4)	1.034(6)	1.048(9)
κ''	1.09(4)	1.29(4)	0.80(4)	0.98(2)	1.03(3)	1.29(4)	1.01(2)	0.84(3)	1.02(5)	0.93(2)	0.98(2)



FigD1. Local coordinate system for multipole refinement