Supporting Information for:

Theoretical infrared and terahertz spectra of an RDX/Aluminum complex

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Supporting Information

According to NBO analysis by the second order perturbation theory analysis (charge transfer), six main interactions are observed between RDX molecules. All of them are described as stabilizing lone pair (LP) to C-H antibond (BD^*), $n_{\text{O}} \rightarrow \sigma^*_{\text{C-Hec}}$ interactions, as shown in Figure S1.

As can be seen, the lowest energy Lewis structure is the one with three LP in one oxygen belonging to the only equatorial NO_2 . In this structure all of the three pairs of electrons in the interacting oxygen, interact with the C-H antibonding orbital of the neighbor molecule. All the interactions make a total of 4.42 kcal (second order estimate) as calculated from the third column, $E(2)$ in the Table S1. The C-Hec antibonding orbital plot is shown in Figure S2.

Figure S1. Simplified graphic representation of the six $n_{\text{O}} \rightarrow \sigma^*_{\text{C-Hec}}$ interactions calculated by NBO theory. Also oxygen and hydrogen natural charges are shown.

Natural charges also show that the interacting oxygen is the most negative charged and the interacting hydrogen is the most positive charged, making both molecules to interact and form a theoretical dimer. This kind of interaction may be responsible for crystal formation.

Figure S2. Calculated NBO C-H antibonding orbital

Table S1. Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol (Intermolecular threshold: 0.05 kcal/mol)

						E(2)	E(j)-E(i)	F(i,j)
Donor NBO (i)			Acceptor NBO (j)			kcal/mol	a.u.	a.u.
from unit 1 to unit 2								
93.	LP(1)	O6	/595.	BD*(1)	C26 - H30	0.88	1.22	0.029
94.	LP(2)	O6	/595.	BD*(1)	C26 - H30	0.19	0.73	0.011
95.	LP (3)	O6	/595.	BD*(1)	C26 - H30	1.14	0.71	0.029
561.	BD*(1)	O1 - N10	/358.	RY*(8)	N23	0.07	0.86	0.019
561.	BD*(1)	O1 - N10	/364.	RY*(1)	N24	0.07	0.30	0.011
562.	BD*(2)	O1 - N10	/364.	RY*(1)	N24	0.10	0.31	0.014
from unit 2 to unit 1								
99.	LP (1)	O22	/584.	BD*(1)	C14 - H19	0.19	0.73	0.011
100.	LP (2)	O22	/584.	BD*(1)	C14 - H19	0.88	1.22	0.029
101.	LP (3)	O22	/584.	BD*(1)	C14 - H19	1.14	0.71	0.029
603.	BD*(1)	N34 - O37	/219.	RY*(1)	N9	0.07	0.30	0.011
603.	BD*(1)	N34 - O37	/263.	RY*(8)	N12	0.07	0.86	0.019
604.	BD*(2)	N34 - O37	/219.	RY*(1)	N9	0.10	0.31	0.014

Note: Atom numbers in this table correspond to the structure shown in Figure 2S.