How do small differences in geometries affect electrostatic potentials of high-energy molecules? Critical news from critical points.

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Table S1. Crystal structures extracted from Cambridge structural Database containing TNB molecule.

Number	Refcode
1	PYRTNB03
2	PYRTNB04
3	ABUNIU
4	ABUNIU01
5	APANBZ
6	ASKNBZ
7	BDTNBB
8	BZATNB20
9	CAXXII
10	CBZTNB
11	CPCTNB
12	DBTTNB
13	DUGZEL
14	GEXMED
15	HENMOC
16	HQUNBZ
17	HUZSEA
18	IPINEA
19	IPINIE
20	IPINOK
21	IPINUQ
22	IPIPAY
23	JESCAL
24	JIZFEE
25	KIXHEE
26	KOSMUA
27	LIHKUK
28	MESWEP
29	MESWIT
30	MESWOZ
31	MESWUF

32	MIGROJ
33	NAQVOT
34	NIBJUF
35	NIBZAM
36	NIXJOT
37	OJUJIO
38	OJUJOU
39	OJUJUA
40	OJUKAH
41	OJUKEL
42	OJUKIP
43	OJUKOV
44	OJUKUB
45	OJULAI
46	OJULEM
47	ORIMIN
48	ORIMOT
49	PEVKIK
50	PEVKIK01
51	PHNSNB11
52	PHNSNB12
53	POCVIP
54	POJDAT
55	PVVBFD01
56	PVVBKP01
57	PYRTNB
58	RULLUF
59	RUYKUR
60	RUYLAY
61	RUYLEC
62	SESFEE
63	SUGCAY
64	TNBENZ10
65	TNBENZ11
66	TNBENZ12
67	TNBENZ13
68	TNBFBT
69	TNBMSC
70	TNBSCO
71	TNBSCU
72	TNBSNI
73	UQAMIK
74	VEWJIQ

75	VIGKIF
76	VIGKUR
77	VIGLEC
78	VIGLOM
79	VOCJAY
80	WIKTEP
81	WOJWAT
82	WOJWIB
83	WOJWOH
84	WOJWUN
85	WOJXEY
86	XAHZAH
87	YAJGUL
88	YURPAD
89	YURPIL
90	ZAWPUI
91	ZOPGOC
92	ZZZAGS10

Table S2. Crystal structures extracted from Cambridge structural Database containing TNP molecule.

Number	Refcode
1	XOCLOS01
2	ANOTAZ
3	ANTPIC
4	BODSUL
5	BUFCEL01
6	CBCPIC
7	DOGLEQ
8	DUGXOU
9	FIZPEK
10	GIRPON
11	GIYDEX
12	GUNDUP
13	HAGBOG
14	HARJOB
15	KODYIM
16	KORGUV
17	LOFVOS
18	LOWJUC
19	LOWKAJ
20	MIGTEC01
21	NEBFUV

22	NEVKAB
23	NEVKAB01
24	NIXKEK
25	NIXKIO
26	OKUMOY
27	PICRAC
28	PICRAC11
29	PICRAC12
30	PICRAC13
31	PICRAC14
32	PICRAC15
33	PICRAC16
34	PICRAC17
35	PICRAC18
36	PICRAC19
37	POCVOV
38	PUKHEJ
39	PVVBGS01
40	QEGKIW
41	QONYUP
42	QONYUP01
43	QUPNAQ
44	RATBET
45	SASKOO02
46	SEKJAW
47	TERSAK
48	TIHMOO
49	UNUQOK
50	WOBPIN
51	WUPTIK
52	XAGRIJ
53	XEFDAN
54	YECNEZ
55	YEQJEM
56	YUQHEY
57	ZECXEN
58	ZILLUB
59	ZILMAI
60	ZILMEM01
61	ZZZAGV01

Table S3. Crystal structures extracted from Cambridge structural Database containing TNT molecule.

Number	Refcode
1	DIFZOK
2	FETYAE
3	FONHOH
4	IZUZUZ
5	IZUZUZ01
6	IZUZUZ02
7	NIBJUF
8	QINLEH
9	TOZMUS
10	URIHUZ
11	URIJAH
12	URIJEL
13	URIJIP
14	URIJUB
15	URIKAI
16	URIKEM
17	URIKOW
18	URIKUC
19	URILAJ
20	URILEN
21	URILIR
22	URILOX
23	URILUD
24	URIMAK
25	ZZZMUC01
26	ZZZMUC05
27	ZZZMUC06
28	ZZZMUC08
29	ZZZMUC09
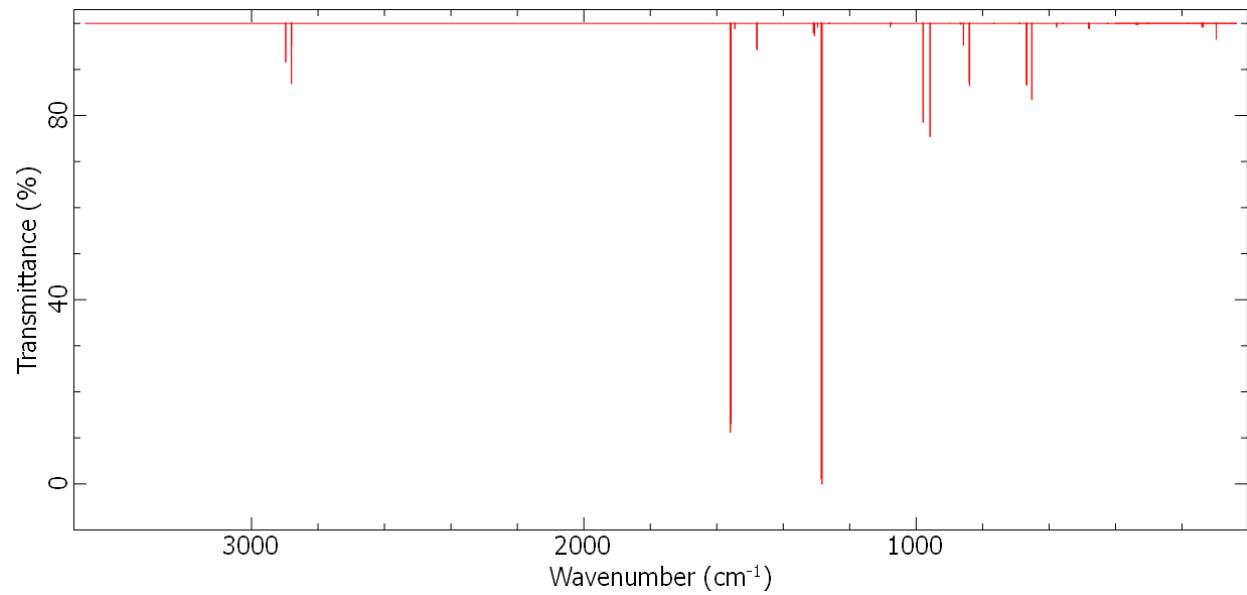
Figure S1. IR spectra calculated for the optimized TNB structure using M06/cc-PVDZ level of theory.
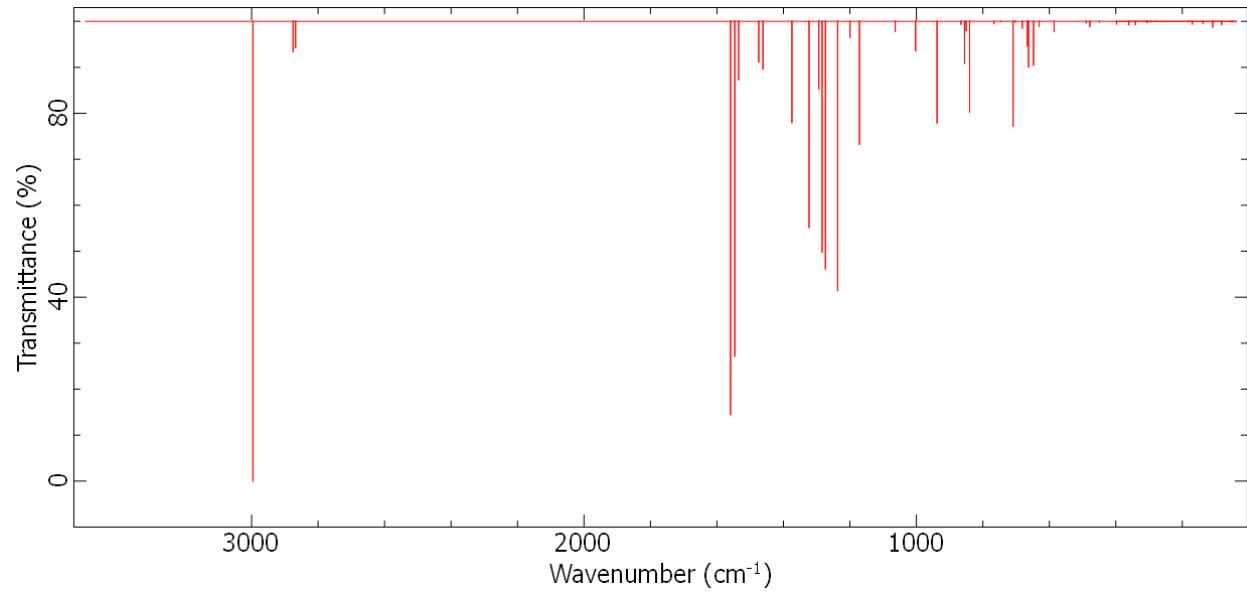
**Figure S2. IR spectra calculated for the optimized TNP structure using M06/cc-PVDZ level of theory.**
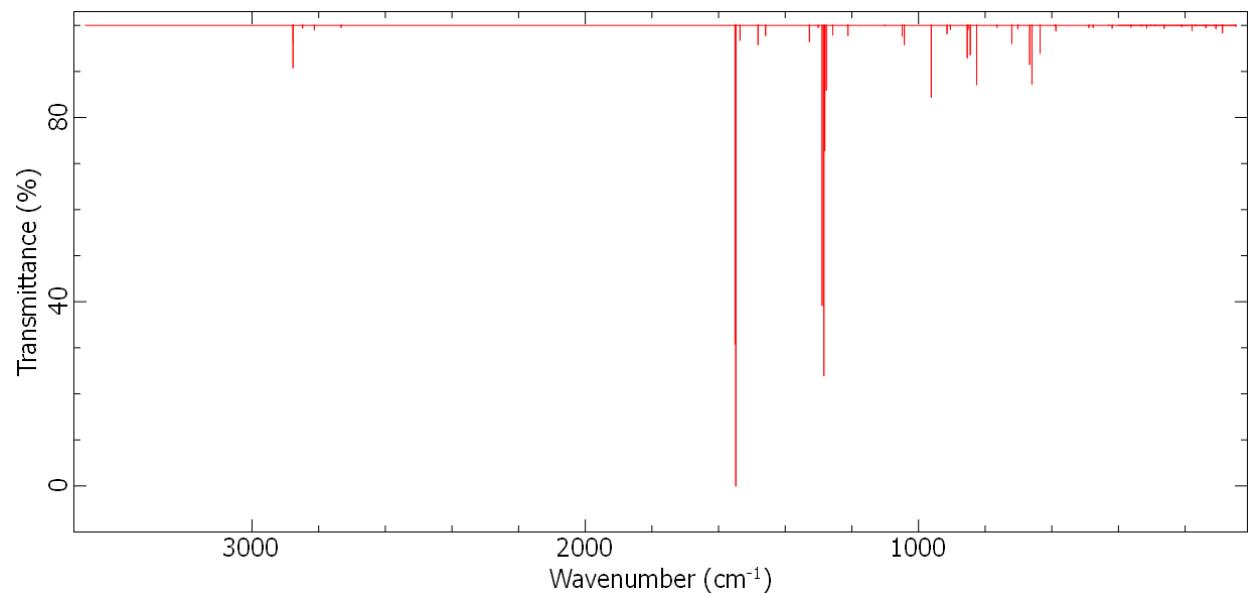
Figure S3. IR spectra calculated for the optimized TNT structure using M06/cc-PVDZ level of theory.
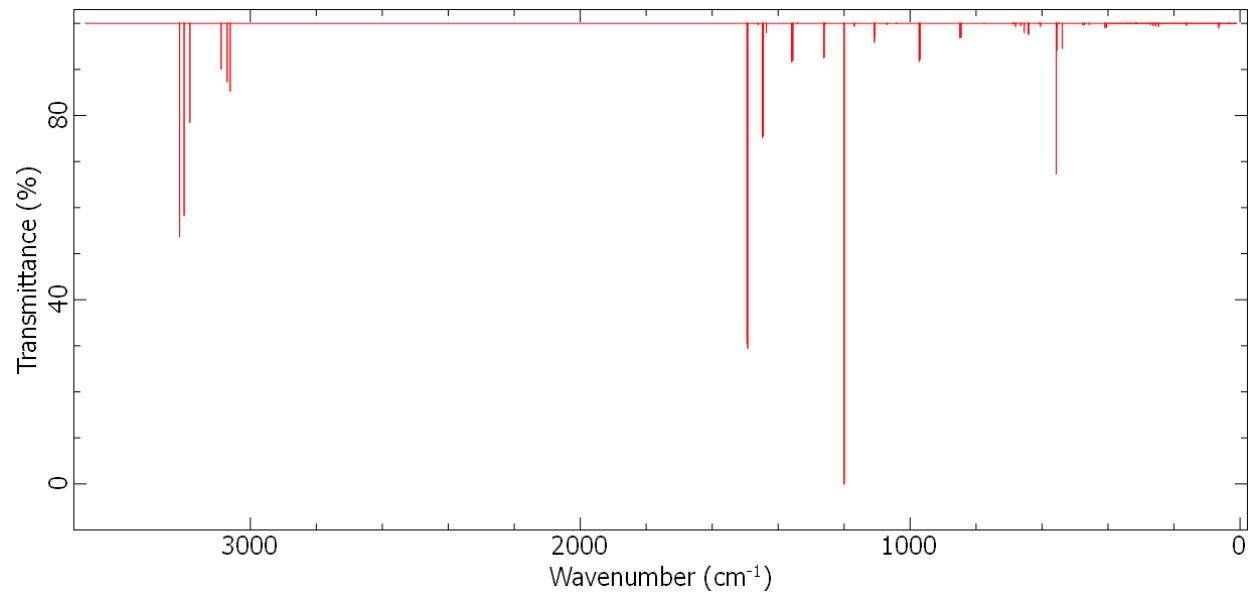

Figure S4. IR spectra calculated for the optimized TATB structure using M06/cc-PVDZ level of theory.
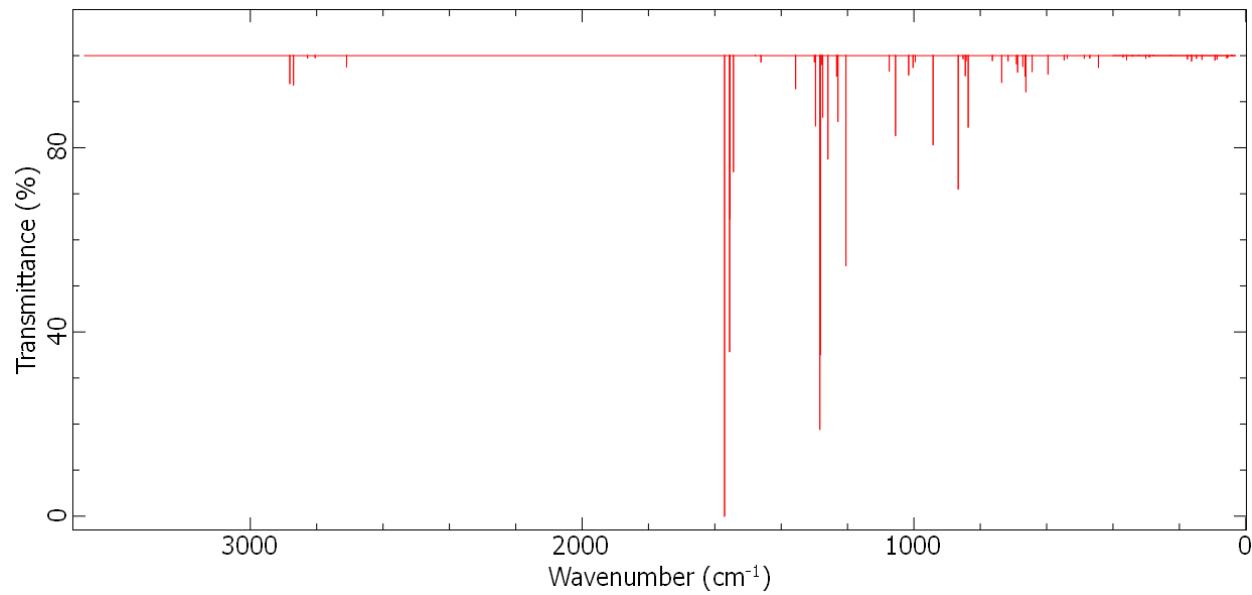
Figure S5. IR spectra calculated for the optimized TETRYL structure using M06/cc-PVDZ level of theory.
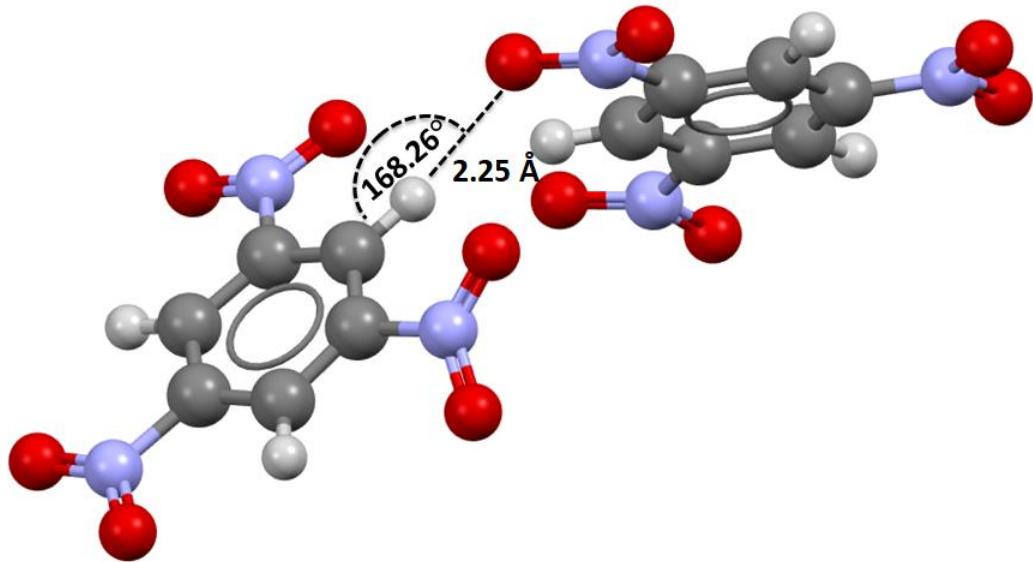

Figure S6. C-H/O interactions between TNB molecules in the crystal structure TNBENZ10. The distance between interacting H and O atoms in this interaction is 2.25Å, while C-H-O angle is 168.26°.