Supplementary Information

High pressure structural behaviour of 5, 5′-bitetrazole-1,1′-diolate based energetic materials: a comparative study from first principles calculations

B. Moses Abraham*

Advanced Centre of Research in High Energy Materials (ACRHEM), University of Hyderabad, Prof. C. R. Rao Road, Gachibowli, Hyderabad-500046, Telangana, India.

*E-mail: mosesabrahamb@gmail.com

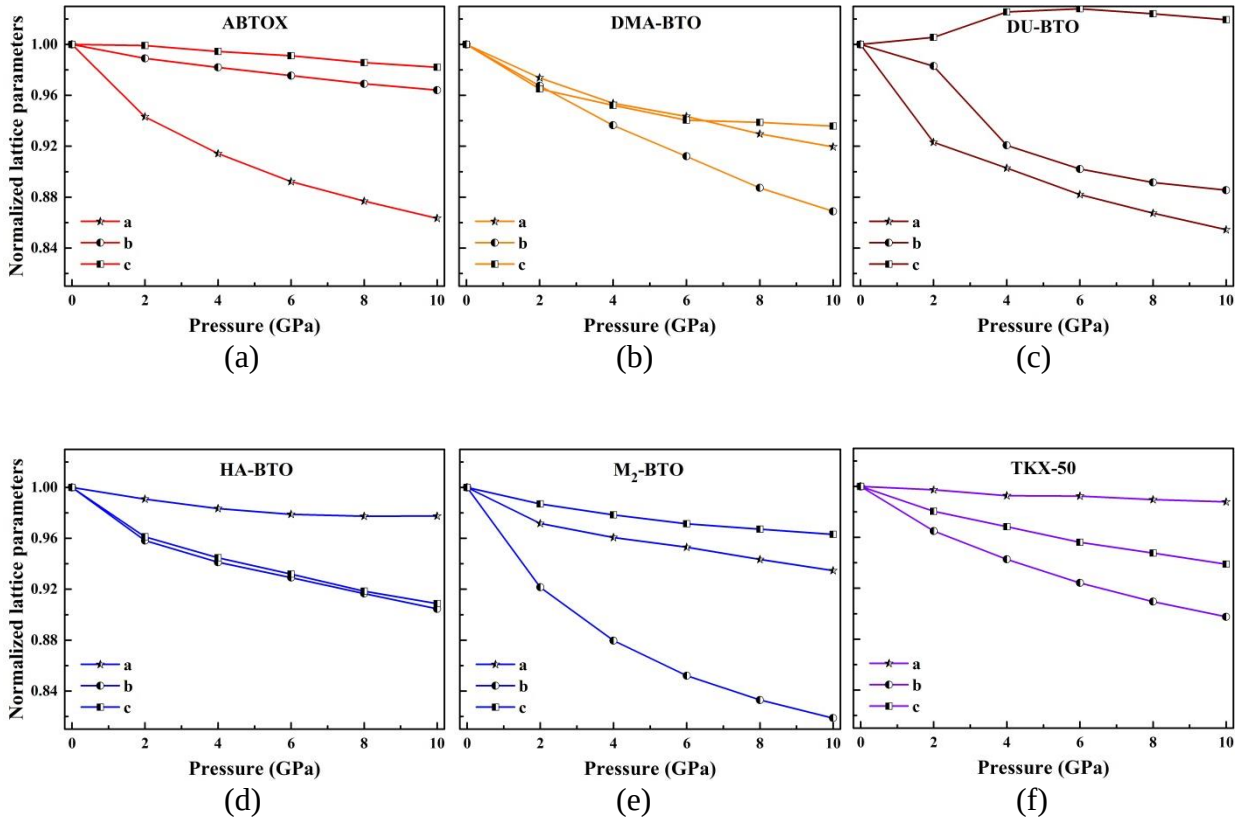
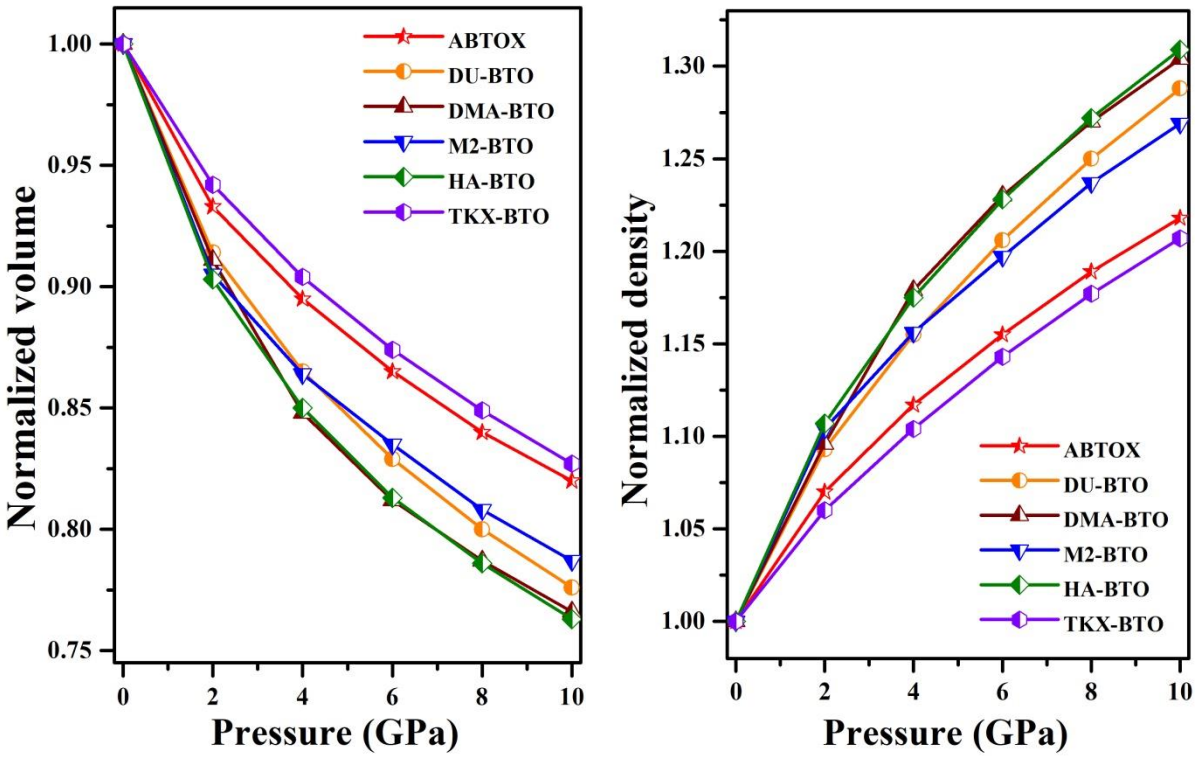
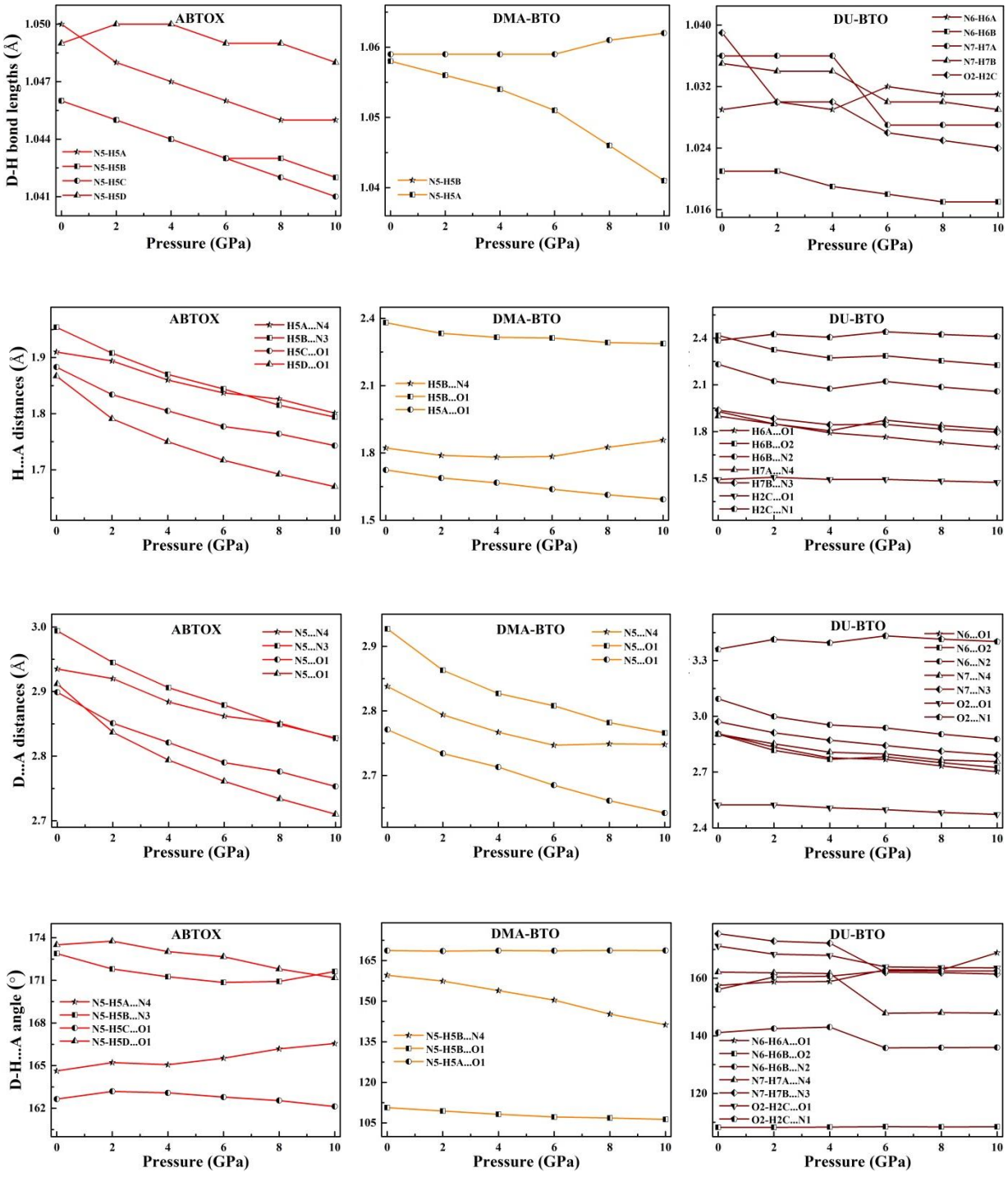


Fig. S1. Normalized lattice parameters under progressing pressure for (a) ABTOX, (b) DMA-BTO, (c) DU-BTO, (d) HA-BTO, (e) M_2-BTO and (f) TKX-50.

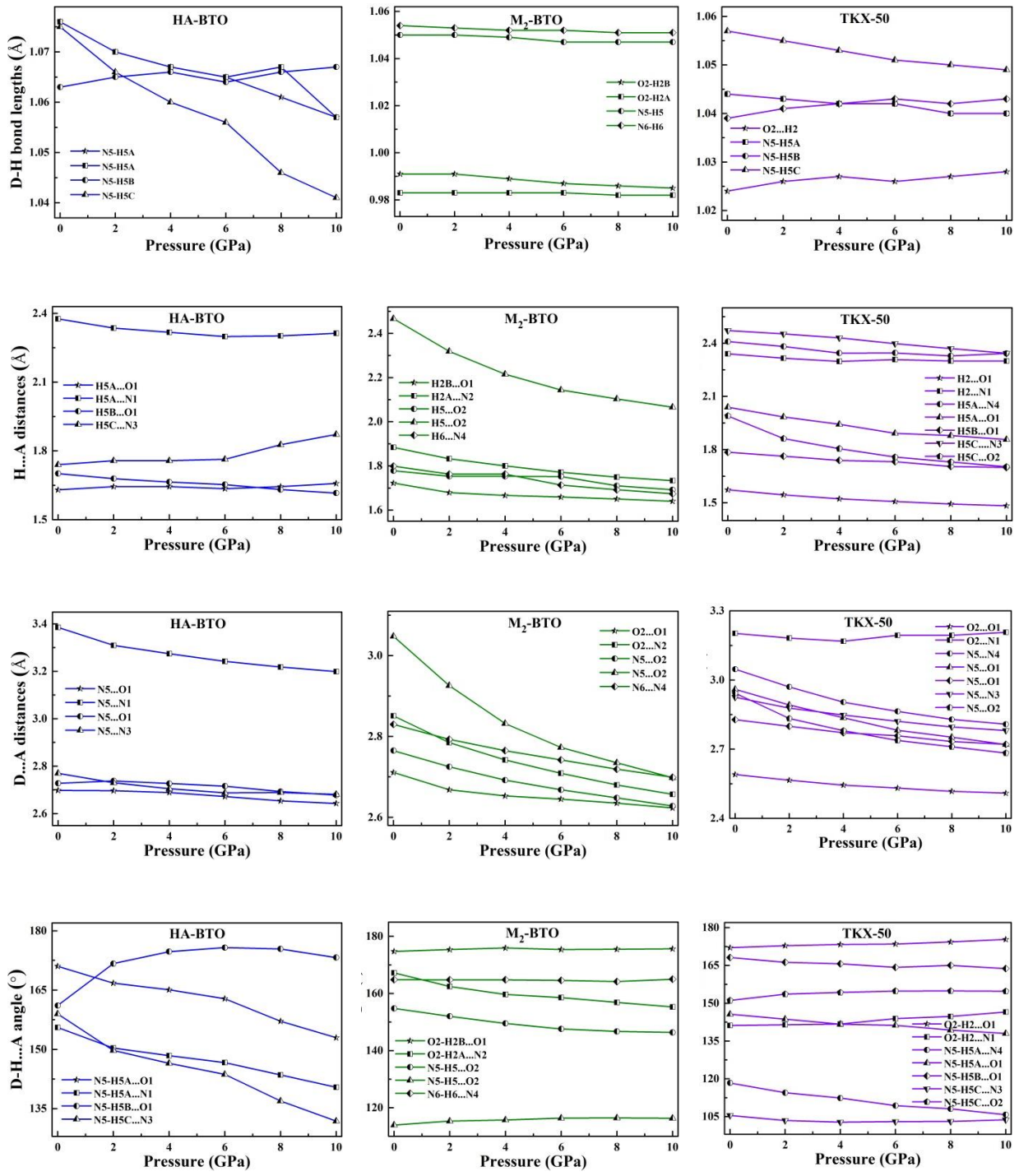


(a) (b)

Fig. S2. Normalized (a) volume and (b) density as a function of pressure for the studied six BTO- based energetic materials.

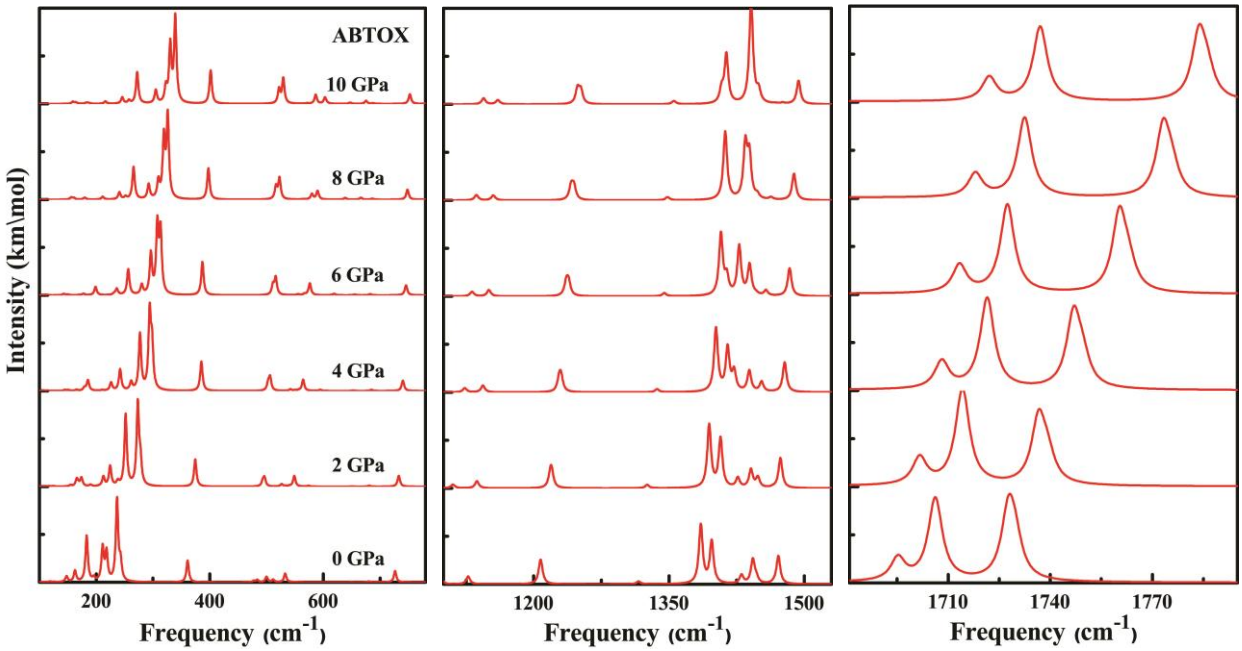

ABTOX
DMA-BTO
DU-BTO
D-H bond lengths (Å)
H...A distances (Å)
D...A distances (Å)
D-H...A angle (°)
Pressure (GPa)
N5-H5A
N5-H5B
N5-H5C
N5-H5D
N6-H6A
N6-H6B
N7-H7A
N7-H7B
O2-H2C
H5A...N4
H5B...N3
H5C...O1
H5D...O1
H5B...N4
H5B...O1
H5A...O1
H6A...O1
H6B...O2
H6B...N2
H7A...N4
H7B...N3
H2C...O1
H2C...N1
N5...N4
N5...N3
N5...O1
N5...O1
N5...N4
N5...O1
N5...O1
N6...O1
N6...O2
N6...N2
N7...N4
N7...N3
O2...O1
O2...N1
N5-H5A...N4
N5-H5B...N3
N5-H5C...O1
N5-H5D...O1
N5-H5B...N4
N5-H5B...O1
N5-H5A...O1
N6-H6A...O1
N6-H6B...O2
N6-H6B...N2
N7-H7A...N4
N7-H7B...N3
O2-H2C...O1
O2-H2C...N1

(a) (b) (c)

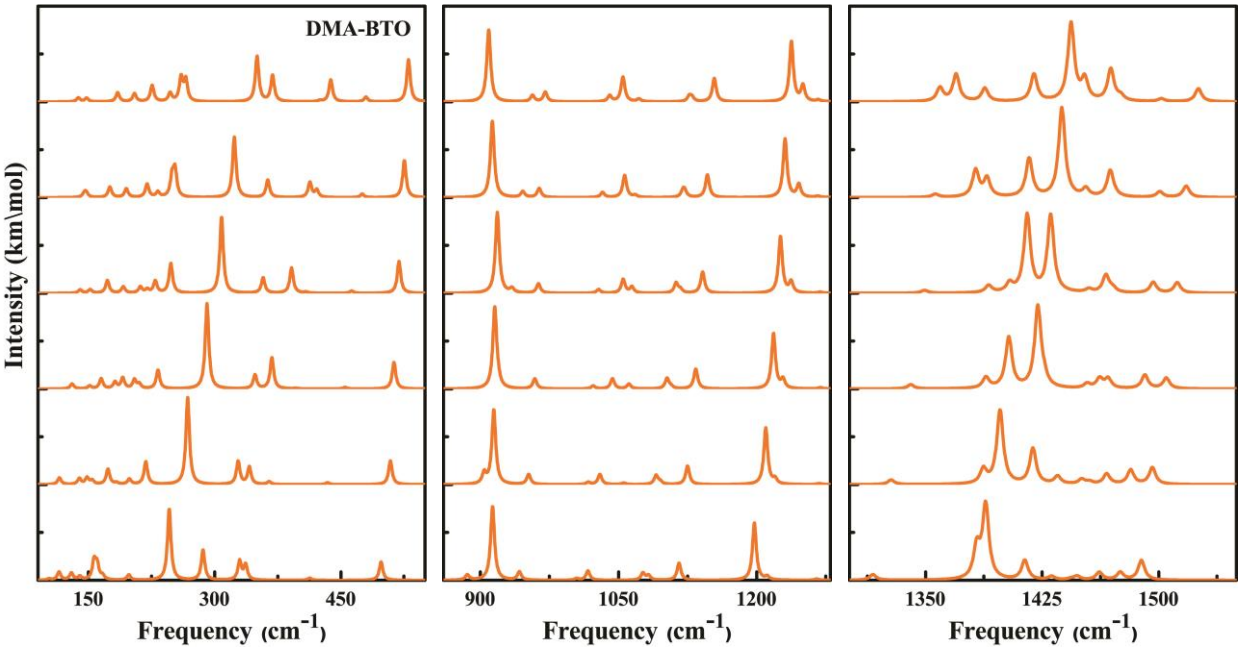


(d) (e) (f)

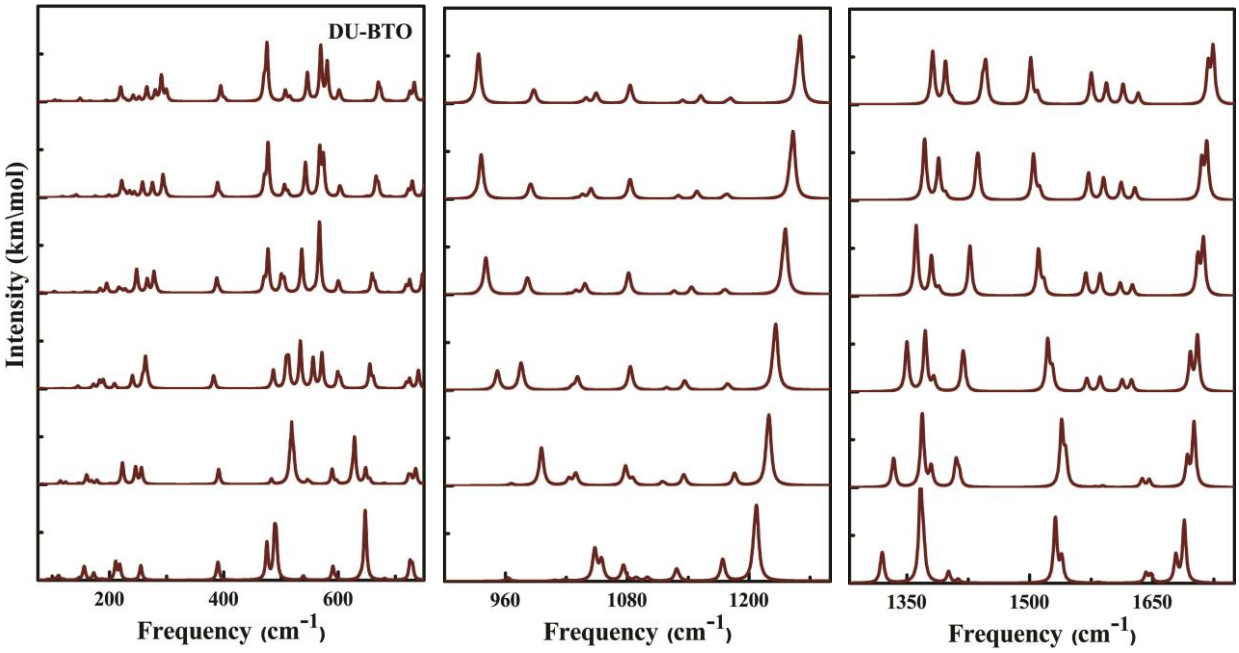
Fig. S3. Calculated intramolecular D-H bond length, intermolecular D…H and H…A distances, and D-H…A bond angle as a function of pressure for (a) ABTOX, (b) DMA-BTO, (c) DU-BTO, (d) HA-BTO, (e) M_2-BTO and (f) TKX-50.


ABTOX
10 GPa
8 GPa
6 GPa
4 GPa
2 GPa
0 GPa
Intensity (km\mol)
200
400
600
Frequency (cm-1)
1200
1350
1500
Frequency (cm-1)
1710
1740
1770
Frequency (cm-1)

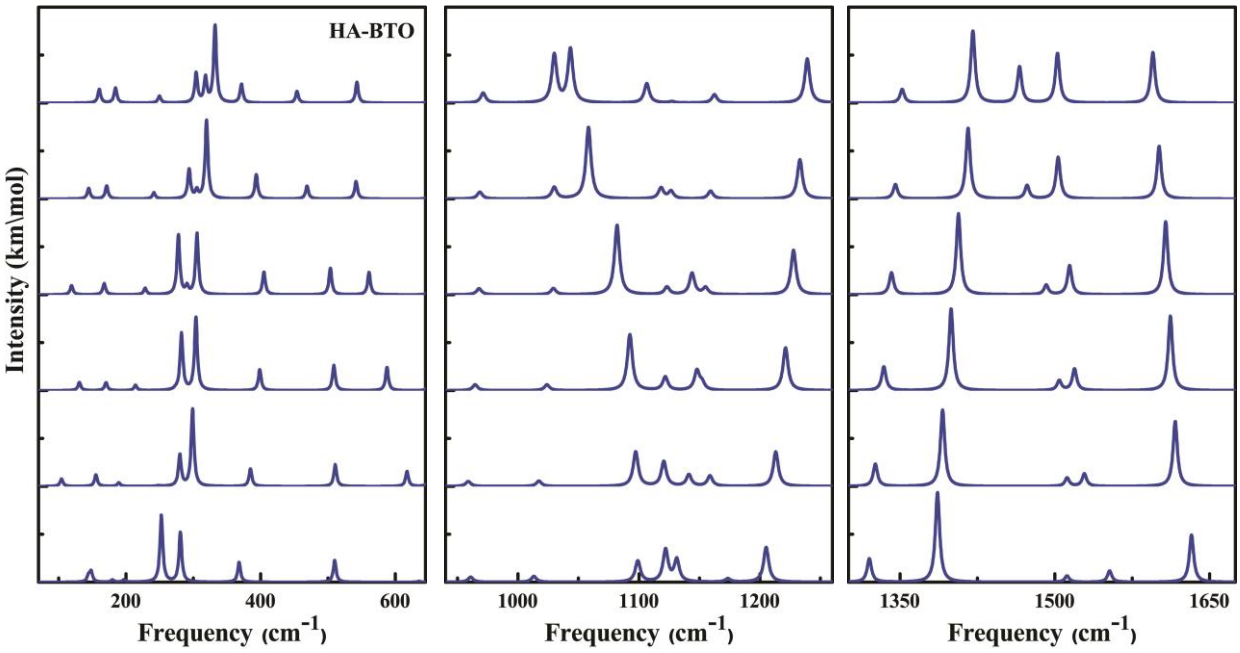
(a) (b) (c)


DMA-BTO
Intensity (km\mol)
150
300
450
Frequency (cm-1)
900
1050
1200
Frequency (cm-1)
1350
1425
1500
Frequency (cm-1)

(d) (e) (f)


DU-BTO
Intensity (km\mol)
200
400
600
Frequency (cm-1)
960
1080
1200
Frequency (cm-1)
1350
1500
1650
Frequency (cm-1)

(g) (h) (i)


HA-BTO
Intensity (km\mol)
200
400
600
Frequency (cm-1)
1000
1100
1200
Frequency (cm-1)
1350
1500
1650
Frequency (cm-1)

(j) (k) (l)

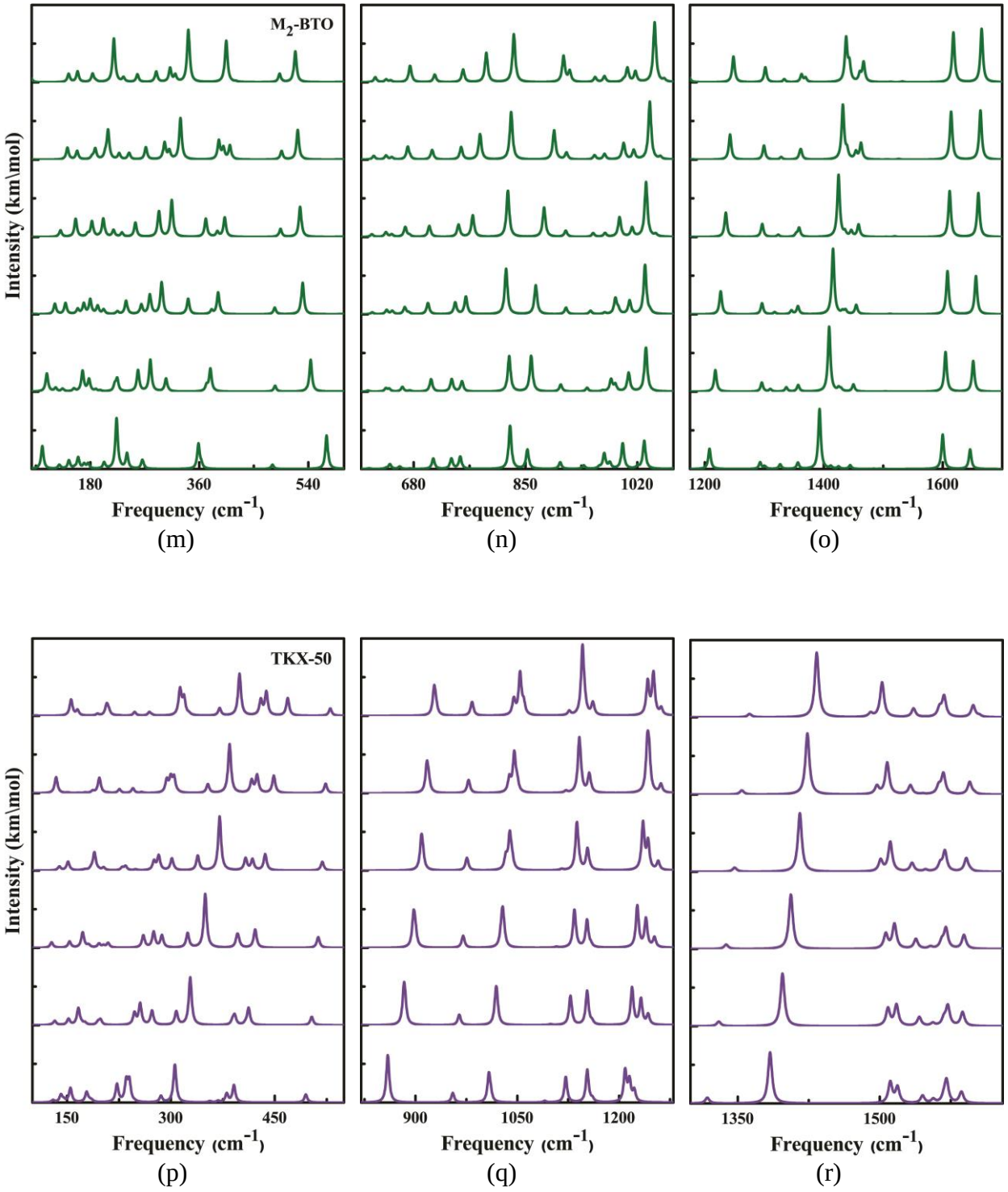


Fig. S4. Calculated IR spectra of (a-c) ABTO, (d-f) DMA-BTO, (g-i) DU-BTO, (j-l) HA-BTO, (m-o) M_2-BTO and (p-r) TKX-50 without high frequency symmetric/asymmetric stretching vibrations.