## Supporting Information

The fully optimized structures calculated at B3LYP/6-311++G(d,p) level of theory for (I) $NO_3^-.H_2O$; (II) $NO_3^-.2H_2O$; (III) $NO_3^-.3H_2O$; (IV) $NO_3^-.4H_2O$; (V) $NO_3^-.5H_2O$, (VI) $NO_3^-.8H_2O$ and (VIII) $NO_3^-.10H_2O$ clusters. Marked alphabets in lower case are used to refer different minimum energy conformers for each hydrated cluster size arranged in order of stability showing 'a' as the most stable one. N atoms are shown by marking 'N' on the spheres, the smallest spheres refer to H atoms and the rest corresponds to O atoms in each structure.
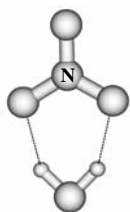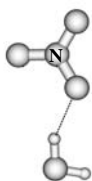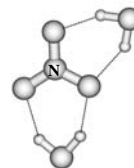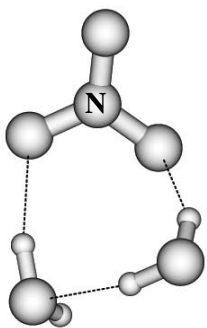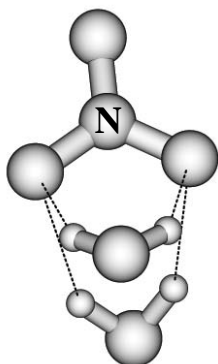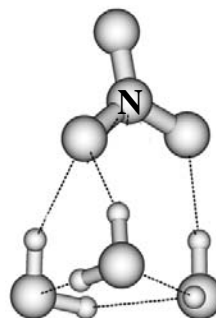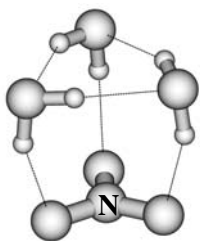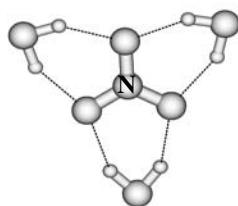
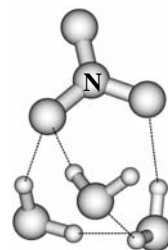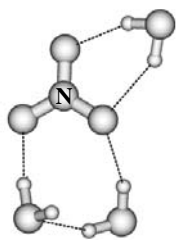**I-a**   **I-b**   **II-a**
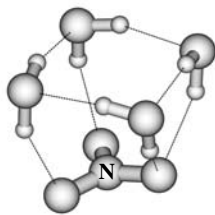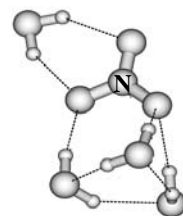
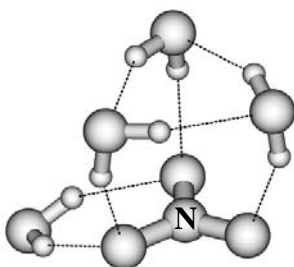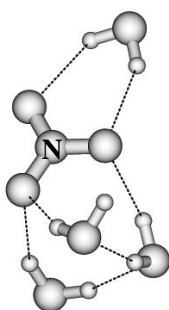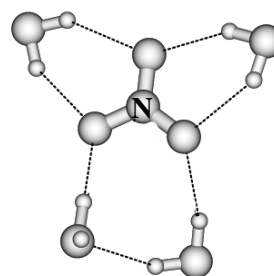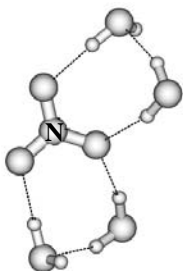**II-b**   **II-c**   **III-a**
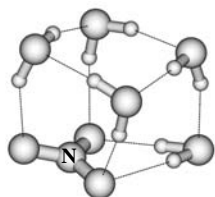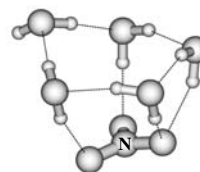
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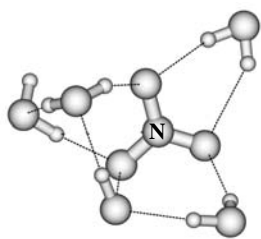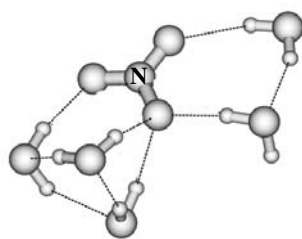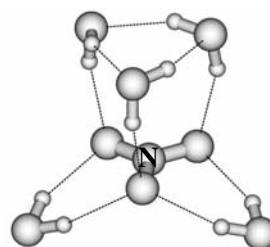
III-d

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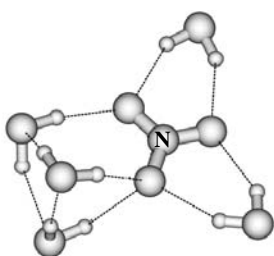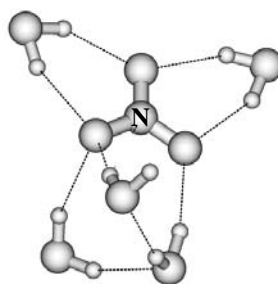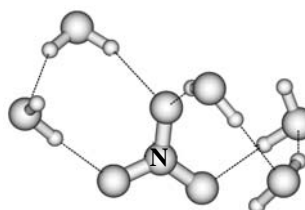
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IV-b

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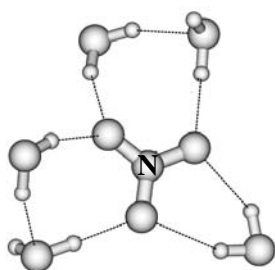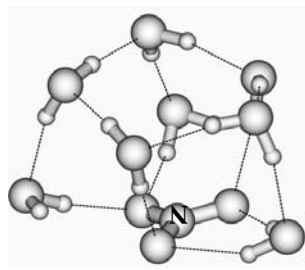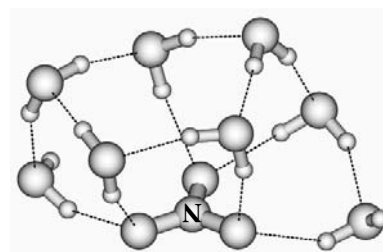
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IV-e

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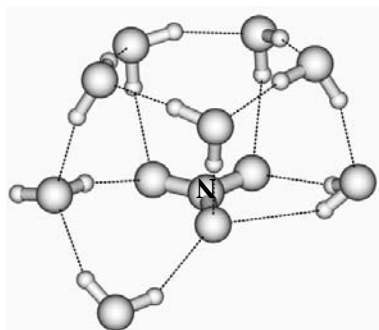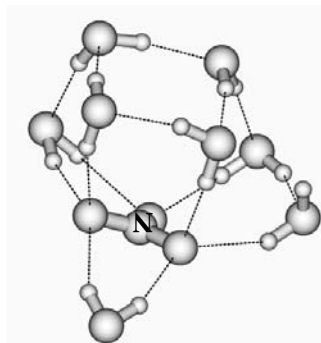
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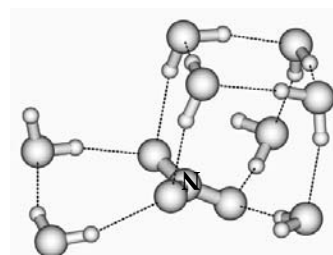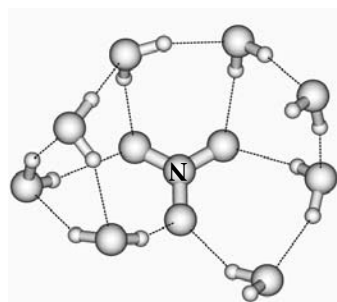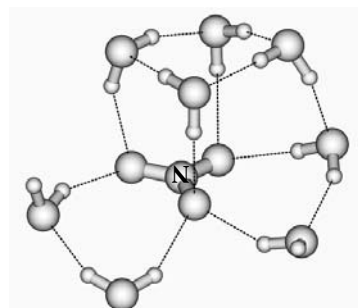
V-d

V-e

V-f

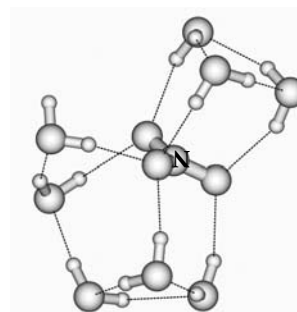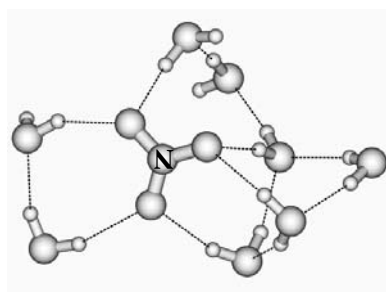**V-g**

V-h

V-i

VI-a

VI-b

VI-c   **VI-d**   **VI-e**

VI-f   **VI-g**   **VI-h**
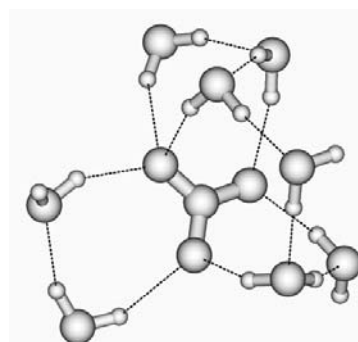
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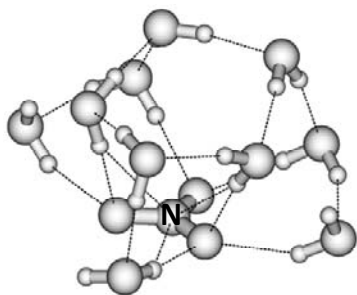
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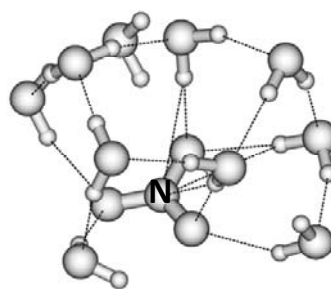
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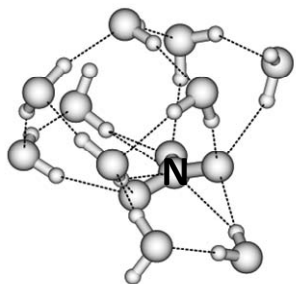
VII-c

2. Table 1

Calculated vertical detachment energy in eV of all the conformers of a particular size for

$NO_3^-.nH_2O$ (n=1-5, 8 &10) clusters at B3LYP/6-311++G(d,p) level of theory.

Clusters	Conformers	Vertical detachment energy (eV)
$NO_3^-.H_2O$	I-A	4.93
	I-b	4.75
$NO_3^-.2H_2O$	II-a	5.52
	II-B	5.30
	II-c	5.45
$NO_3^-.3H_2O$	III-a	5.66
	III-b	5.55
	III-c	6.00
	III-d	5.73
	III-e	5.95
$NO_3^-.4H_2O$	IV-a	5.86
	IV-b	6.20
	IV-c	6.11
	IV-d	6.50
	IV-e	6.33
	IV-f	6.09

$NO_3^-.5H_2O$	V-a	6.18
	V-b	5.95
	V-c	6.43
	V-d	6.34
	V-e	6.56
	V-f	6.62
	V-g	6.85
	V-h	6.33
	V-I	6.49
$NO_3^-.8H_2O$	VI-a	7.00
	VI-b	6.72
	VI-c	6.70
	VI-d	6.81
	VI-e	6.70
	VI-f	6.80
	VI-g	6.75
	VI-h	7.10
	VI-i	6.65
	VI-j	7.09
$NO_3^-.10H_2O$	VII-a	7.10
	VII-a	7.04
	VII-a	6.97