Scientia Iranica

A 3D Polyoxoniobate-based Framework Showing Performance in Dye Removal from Aqueous Solution

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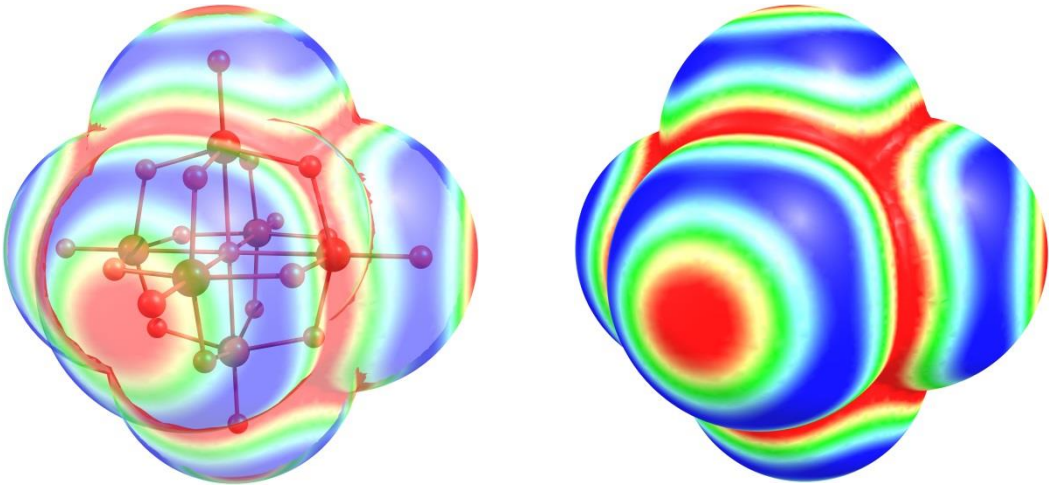
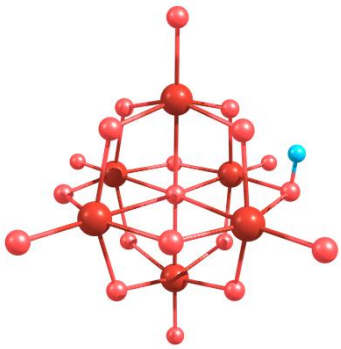


Figure S1 ESP map for $Nb_6O_{19}^{8-}$

$[HNb_6O_{19}]^{7-}$



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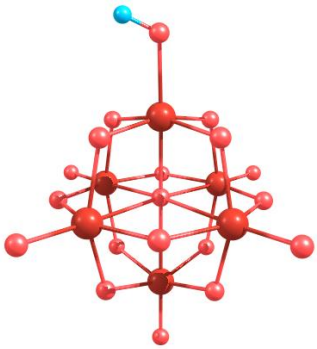

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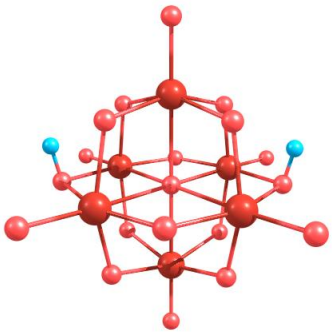
$[H_2Nb_6O_{19}]^{6-}$



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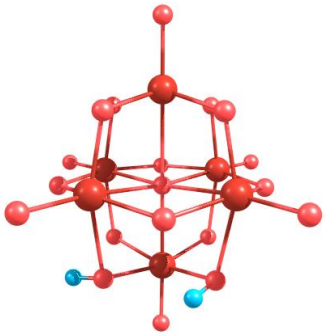

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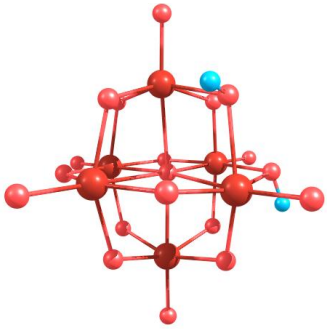

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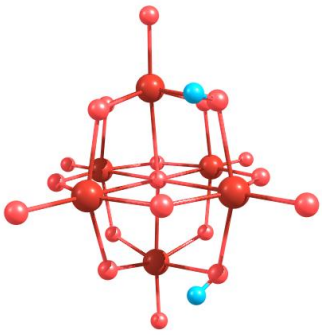

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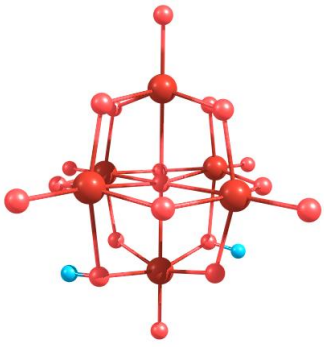

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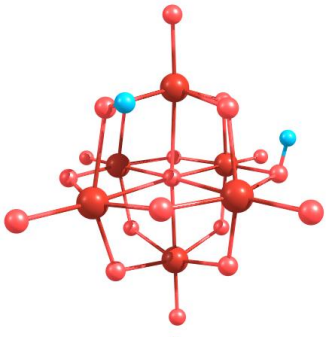

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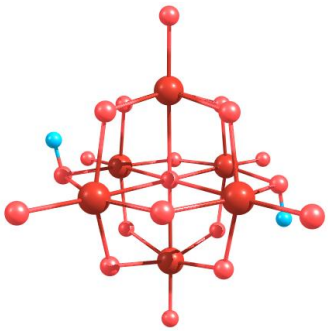

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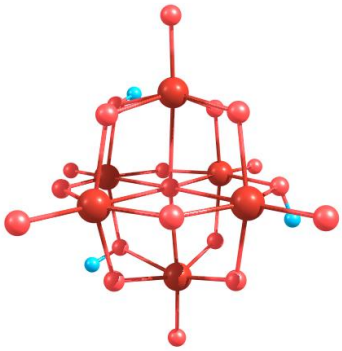
$[H_3Nb_6O_{19}]^{5-}$



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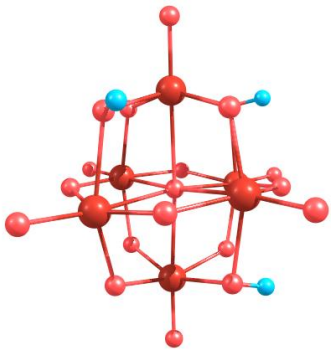

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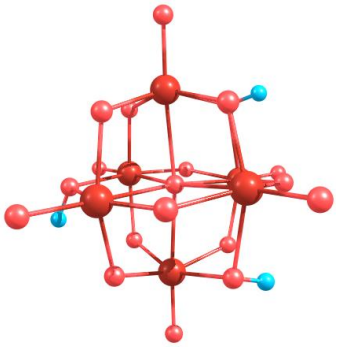

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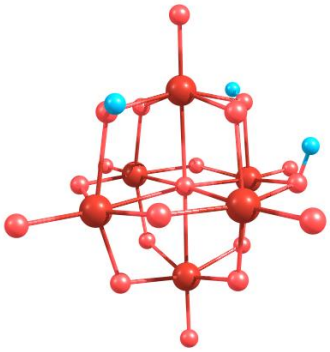

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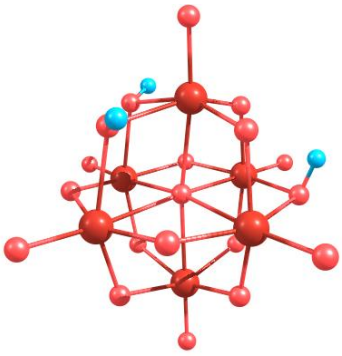

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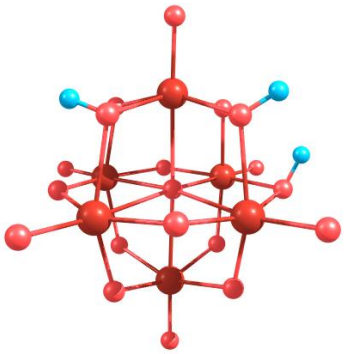

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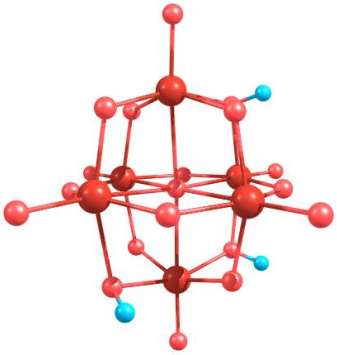

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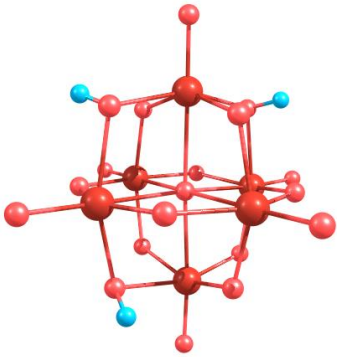

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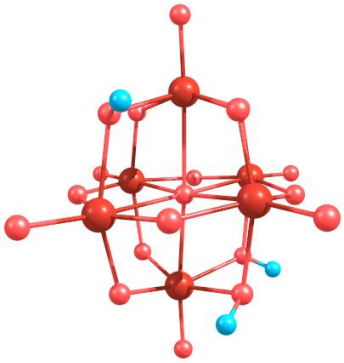

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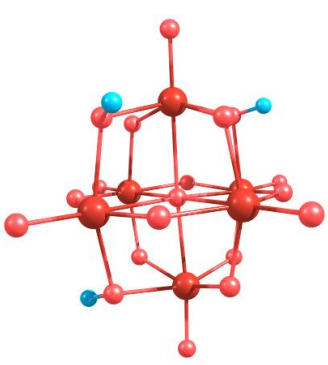
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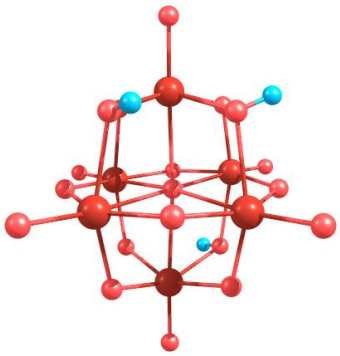
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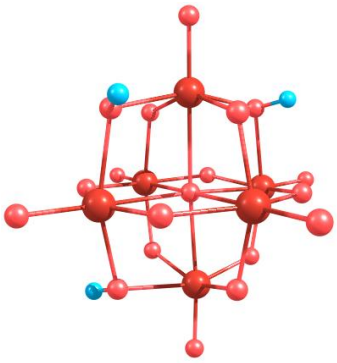
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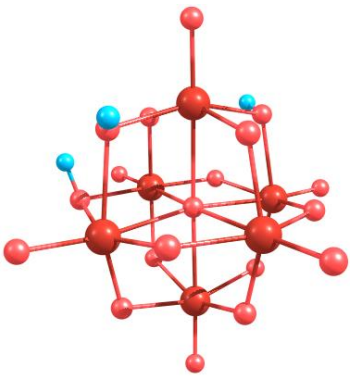
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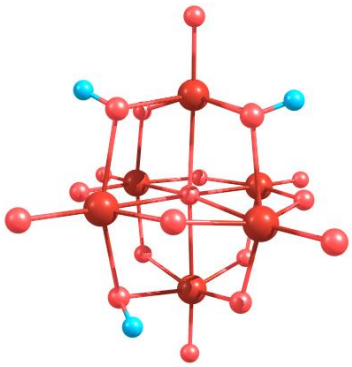
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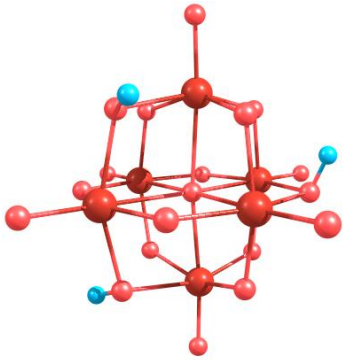
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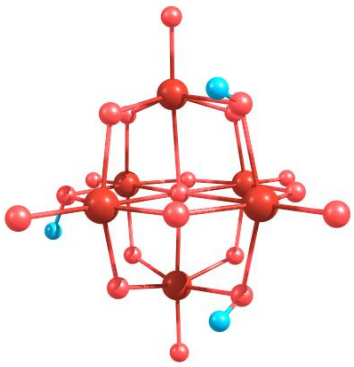
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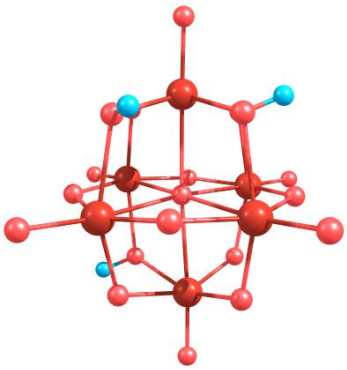
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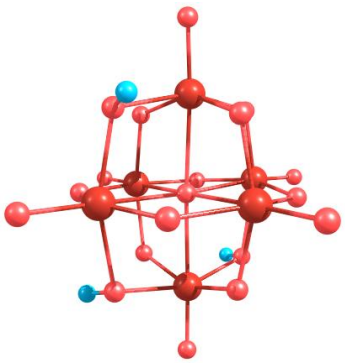
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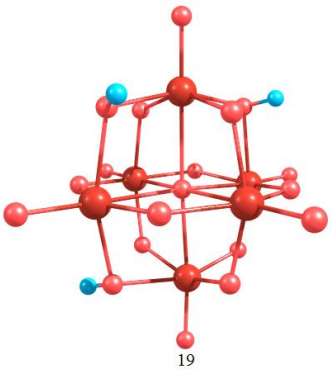
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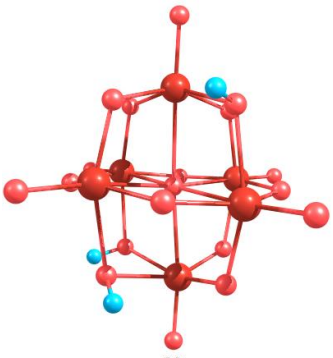
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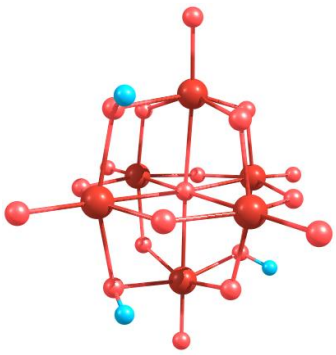
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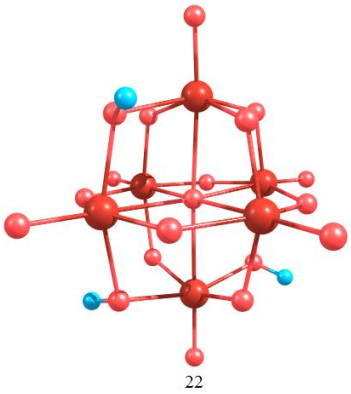


Figure S2 The lowest energy isomers for each protonation state

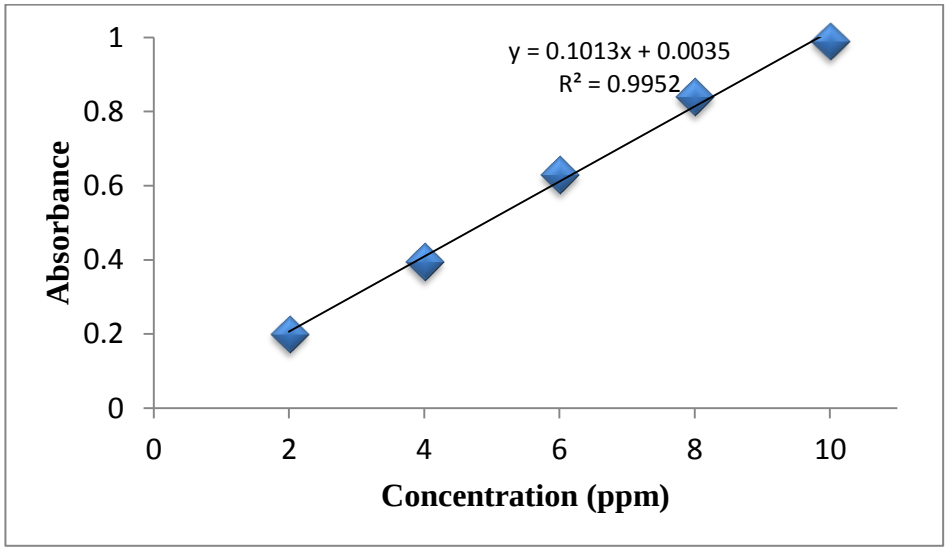


Figure S3 UV-Vis calibration curve

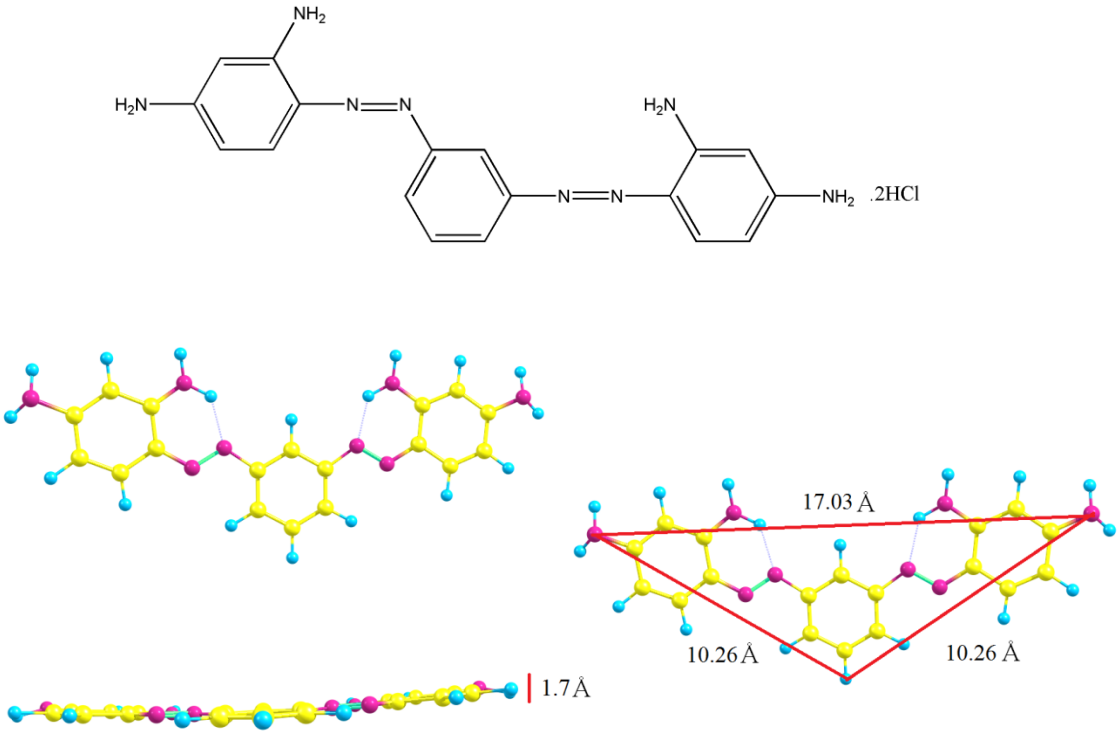
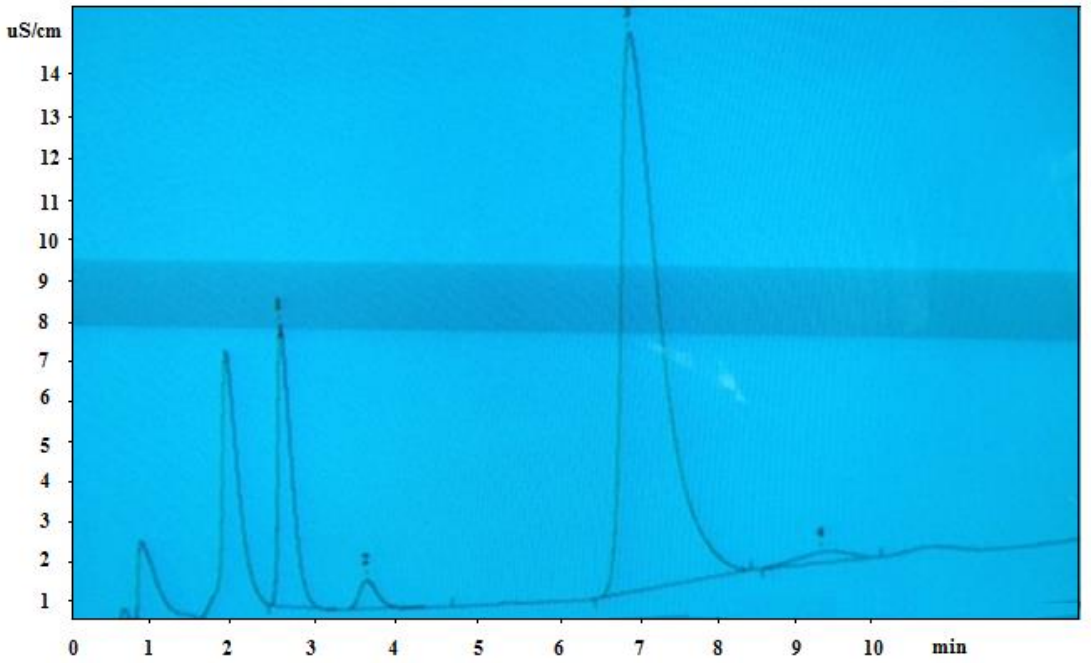


Figure S4 The chemical structure of Bismarck brown



Quantitation method: Custom

No	Retention min	Height uS/cm	Area uS/cm*sec	Conc. mg/L	Name
1	2.69	7.09	78.666	6.050	chloride
2	3.66	0.73	12.102	1.392	nitrite
3	6.97	14.16	469.475	55.107	nirate
4	9.30	0.28	13.248	1.176	sulfate
4	13.01	22.26	573.491	63.724	

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Figure S5 The IC Chromatogram and respected concentrations

Table S1 Relative energies of hydrogenated hexaniobate

$[HNb_6O_{19}]^{7-}$	Relative energy($kJmol^{-1}$)	$[H_2Nb_6O_{19}]^{6-}$	Relative energy($kJmol^{-1}$)	$[H_3Nb_6O_{19}]^{5-}$	Relative energy($kJmol^{-1}$)
$[HNb_6O_{19}]^{7-}$(1)	0.0	$[H_2Nb_6O_{19}]^{6-}$(1)	13.7	$[H_3Nb_6O_{19}]^{6-}$ (1)	21.1
$[HNb_6O_{19}]^{7-}$(2)	45.0	$[H_2Nb_6O_{19}]^{6-}$(2)	3.3	$[H_3Nb_6O_{19}]^{6-}$ (2)	20.3
-	-	$[H_2Nb_6O_{19}]^{6-}$(3)	10.9	$[H_3Nb_6O_{19}]^{6-}$ (3)	0.0
-	-	$[H_2Nb_6O_{19}]^{6-}$(4)	19.9	$[H_3Nb_6O_{19}]^{6-}$ (4)	21.4
-	-	$[H_2Nb_6O_{19}]^{6-}$(5)	21.4	$[H_3Nb_6O_{19}]^{6-}$ (5)	4.8
-	-	$[H_2Nb_6O_{19}]^{6-}$(6)	0.0	$[H_3Nb_6O_{19}]^{6-}$ (6)	11.7
-	-	$[H_2Nb_6O_{19}]^{6-}$(7)	13.3	$[H_3Nb_6O_{19}]^{6-}$ (7)	49.5
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (8)	50.6
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (9)	11.7
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (10)	49.4
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (11)	12.5
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (12)	49.3
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (13)	21.4
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (14)	27.7
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (15)	22.3
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (16)	20.3
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (17)	12.0
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (18)	49.5
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (19)	49.3
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (20)	11.7
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (21)	49.4
-	-	-	-	$[H_3Nb_6O_{19}]^{6-}$ (22)	50.5