

SUPPORTING INFORMATION

Article Title:

A Quantum-mechanical Study on the Aquaions and Hydrolyzed species of Po(IV),
Te(IV) and Bi(III) in Water

Authors:

Regla Ayala , Jose M. Martinez, Rafael R. Pappalardo, and Enrique Sanchez Mar-
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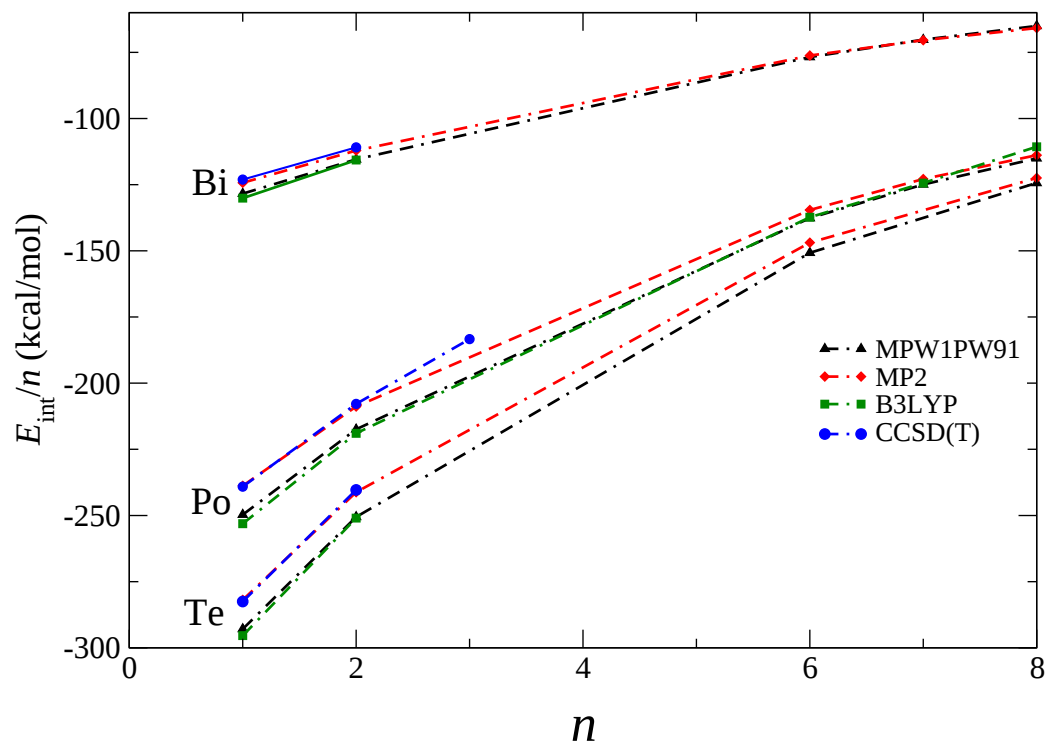


Figure S1. Interaction energy (kcal/mol) per water molecule for different aquaions $[M(H_2O)_n(OH)_m]^{q+}$ at different computational levels.

n	MPW1PW91	MP2	B3LYP	CCSD(T)
Bi				
1	2.17	2.16	2.19	2.17
2	2.20	2.19	2.22	2.20
6	2.42	2.41		
8	2.49	2.48		
Te				
1	1.98	1.96	2.00	2.03
2	2.01	2.00	2.04	2.02
6	2.24	2.23		
8	2.32	2.31		
Po				
1	2.10	2.08	2.12	2.13
2	2.12	2.11	2.15	2.12
6	2.31	2.30	2.31	
8	2.38	2.37	2.40	

Table S1. M-O distances ($\text{\AA}$) of the $[\text{M}(\text{H}_2\text{O})_n]^{q+}$ clusters (M being Te, Bi and Po) optimized at different computational levels in gas phase.

$\frac{m}{n+m}$	0	1	2	3
3	$[\text{Bi}(\text{H}_2\text{O})_3]^{3+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_2(\text{OH})]^{3+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_1(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Bi}(\text{OH})_3]^+$
	-13.8		-1.0	+15.8
4	$[\text{Bi}(\text{H}_2\text{O})_4]^{3+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_3(\text{OH})]^{3+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_2(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_1(\text{OH})_3]^+$
	-7.8		+4.9	+26.2
5	$[\text{Bi}(\text{H}_2\text{O})_5]^{3+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_4(\text{OH})]^{3+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_3(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_2(\text{OH})_3]^+$
	-6.6		+14.4	+30.5
6	$[\text{Bi}(\text{H}_2\text{O})_6]^{3+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_5(\text{OH})]^{3+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_4(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_3(\text{OH})_3]^+$
	+0.7		+21.8	+29.8
7	$[\text{Bi}(\text{H}_2\text{O})_7]^{3+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_6(\text{OH})]^{3+} \longrightarrow$	$[\text{Bi}(\text{H}_2\text{O})_5(\text{OH})_2]^{2+} \longrightarrow$	
	+12.0		+16.7	
8	$[\text{Bi}(\text{H}_2\text{O})_8]^{3+}$			
9	$[\text{Bi}(\text{H}_2\text{O})_9]^{3+}$			

Table S2. Gibbs energy for the successive hydrolysis reactions $[\text{Bi}(\text{H}_2\text{O})_n(\text{OH})_m]^{q+} + \text{H}_2\text{O} \longrightarrow [\text{Bi}(\text{H}_2\text{O})_n(\text{OH})_m]^{q+} + \text{H}_3\text{O}^+$

$\frac{m}{n+m}$	0	1	2	3	4
4	$[\text{Po}(\text{H}_2\text{O})_4]^{4+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_3(\text{OH})]^{3+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_2(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_1(\text{OH})_3]^+ \longrightarrow$	$[\text{Po}(\text{OH})_4]$
	-56.5	-32.3	-5.2	+22.6	
5	$[\text{Po}(\text{H}_2\text{O})_5]^{4+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_4(\text{OH})]^{3+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_3(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_2(\text{OH})_3]^+ \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_1(\text{OH})_4]$
	-45.5	-14.3	-0.1	+29.3	
6	$[\text{Po}(\text{H}_2\text{O})_6]^{4+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_5(\text{OH})]^{3+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_4(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_3(\text{OH})_3]^+ \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_2(\text{OH})_4]$
	-31.2	-11.1	+4.2	+30.8	
7	$[\text{Po}(\text{H}_2\text{O})_7]^{4+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_6(\text{OH})]^{3+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_5(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_4(\text{OH})_3]^+ \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_3(\text{OH})_4]$
	-23.8	-5.8	12.1	+36.2	
8	$[\text{Po}(\text{H}_2\text{O})_8]^{4+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_7(\text{OH})]^{3+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_6(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_5(\text{OH})_3]^+ \longrightarrow$	
	-15.6	+3.4	+12.7		
9	$[\text{Po}(\text{H}_2\text{O})_9]^{4+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_8(\text{OH})]^{3+} \longrightarrow$	$[\text{Po}(\text{H}_2\text{O})_7(\text{OH})_2]^{2+} \longrightarrow$		
	-5.4	+3.3			

Table S3. Gibbs energy for the successive hydrolysis reactions $[\text{Po}(\text{H}_2\text{O})_n(\text{OH})_m]^{q+} + \text{H}_2\text{O} \longrightarrow [\text{Po}(\text{H}_2\text{O})_{n+1}(\text{OH})_{m+1}]^{q+} + \text{H}_3\text{O}^+$

$\frac{m}{n+m}$	0	1	2	3	4
4	$[\text{Te}(\text{H}_2\text{O})_4]^{4+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_3(\text{OH})]^{3+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_2(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_1(\text{OH})_3]^+ \longrightarrow$	$[\text{Te}(\text{OH})_4]$
	-63.6	-37.1	-10.7	+19.3	
5	$[\text{Te}(\text{H}_2\text{O})_5]^{4+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_4(\text{OH})]^{3+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_3(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_2(\text{OH})_3]^+ \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_1(\text{OH})_4]$
	-51.6	-19.5	-4.6	+26.1	
6	$[\text{Te}(\text{H}_2\text{O})_6]^{4+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_5(\text{OH})]^{3+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_4(\text{OH})_2]^{2+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_3(\text{OH})_3]^+$	
	-45.1	-18.3	-0.1		
7	$[\text{Te}(\text{H}_2\text{O})_7]^{4+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_6(\text{OH})]^{3+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_5(\text{OH})_2]^{2+}$		
	-31.3	-16.4			
8	$[\text{Te}(\text{H}_2\text{O})_8]^{4+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_7(\text{OH})]^{3+} \longrightarrow$	$[\text{Te}(\text{H}_2\text{O})_6(\text{OH})_2]^{2+}$		
	-19.0	-2.1			
9	$[\text{Te}(\text{H}_2\text{O})_9]^{4+}$				

Table S4. Gibbs energy for the successive hydrolysis reactions $[\text{Te}(\text{H}_2\text{O})_n(\text{OH})_m]^{q+} + \text{H}_2\text{O} \longrightarrow [\text{Te}(\text{H}_2\text{O})_{n+1}(\text{OH})_{m+1}]^{q+} + \text{H}_3\text{O}^+$