Photoionization and *ab initio* study of $Ba(H_2O)_n$ (n = 1 - 4) clusters - Supplementary File -

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Basis sets:

O-H: 6-311++G(d,p)
Ba: Relativistic Effective Core Potentials (RECP) and their basis sets:
1.- Bauschlicher *et al.*2.- SDD
3.- Lim *et al.*

Ionization Potentials:

Adiabatic: $IE_a (eV) = \{ E^a [Ba^+(H_2O)_n] - E[Ba(H_2O)_n] \} * 27.2114$ Vertical: $IE_v (eV) = \{ E^v [Ba^+(H_2O)_n] - E[Ba(H_2O)_n] \} * 27.2114$

Where:

 $E[Ba(H_2O)_n]$ is the total energy of the optimized neutral cluster (E_0) corrected by E_{ZPE} (zero point vibrational energy of neutral ground state); $E^a[Ba^+(H_2O)_n]$ is the total energy (E_a) of the optimized cationic cluster, corrected by E^a_{ZPE} (zero-point vibrational energy of ionic state) and $E^v[Ba^+(H_2O)_n]$ is the total energy (E_v) of the cationic cluster with the optimized geometry on the neutral state, also corrected by E^a_{ZPE} .

Binding energy:

 $\Delta E \text{ (kcal mol}^{-1)} = \{ E[Ba^m(H_2O)_n] - E[(H_2O)_n] - E[Ba^m] \} * 627.510$

Where:

m = 0 and +1, in the neutral and ionic state, respectively; $E[(H_2O)_n]$ is the total energy (E_w) of the optimized neutral water cluster corrected by the E^{w}_{ZPE} and E[Ba] is the total energy of the barium atom.

Gibbs free energy of reaction:

$$\Delta_r G^{75 \text{ K}} \text{ (kcal mol}^{-1)} = \Delta_f G [Ba(H_2O)_n] - \Delta_f G [Ba] - n * \Delta_f G [H_2O]$$

Note: All energy values (*E*) are in Hartrees.

Basis sets selection:

H and O atoms:

To analyze basis set effect on the values of calculated ionization energy (IE) for $Ba(H_2O)_n$ clusters, DFT single-point energy calculations with gradually increasing basis set were performed:

Specie	Theory	Basis set	$E_{ heta}^{**}$	E_{ion}^{**}	IE _v **
		6-31G	-101.845409	-101.681922	4.45
		6-311G(d)	-101.884747	-101.720323	4.47
		6-311G(d,p)	-101.895964	-101.731171	4.48
	_	6-311+G(d,p)	-101.898875	-101.733237	4.51
$\mathbf{B}_{\mathbf{D}}(\mathbf{H},\mathbf{O})$	Ba(H ₂ O) ₁ <i>m</i> PW1PW91	6-311++G(d,p)	-101.898964	-101.733282	4.51
	<i>m</i> 1 w 11 w <i>y</i> 1	6-311++G(2d,p)	-101.898771	-101.733009	4.51
		6-311++G(3d,p)	-101.899442	-101.733672	4.51
		6-311++G(3df,p)	-101.900305	-101.734541	4.51
		6-311++G(3df,3pd)	-101.902432	-101.736659	4.51
		AUG-cc-PVQZ	-101.910097	-101.744341	4.51
Specie [*]	Theory	Basis set	E_{o}^{**}	E_{ion}^{**}	IE,**
Specie [*]	Theory	Basis set 6-31G	<i>E₀**</i> -331.044265	<i>E_{ion}**</i> -330.905847	<u>ΙΕ</u> _ν ** 3.77
Specie [*]	Theory	Basis set 6-31G 6-311G(d)	<i>E₀**</i> -331.044265 -331.206237	<u>E</u> ion ^{**} -330.905847 -331.066652	IE _ν ** 3.77 3.80
Specie [*]	Theory	Basis set 6-31G 6-311G(d) 6-311G(d,p)	<i>E</i> ^{**} -331.044265 -331.206237 -331.251312	<i>E</i> _{ion} ** -330.905847 -331.066652 -331.111796	IE _v ** 3.77 3.80 3.80
Specie*	Theory	Basis set 6-31G 6-311G(d) 6-311G(d,p) 6-311+G(d,p)	<i>E</i> ₀ ** -331.044265 -331.206237 -331.251312 -331.261613	<i>E</i> _{ion} ** -330.905847 -331.066652 -331.111796 -331.120371	IE _v ** 3.77 3.80 3.80 3.84
Specie [*] Ba(H ₂ O) ₄	Theory 7700 Theory	Basis set 6-31G 6-311G(d) 6-311G(d,p) 6-311+G(d,p) 6-311++G(d,p)	<i>E</i> ^{**} -331.044265 -331.206237 -331.251312 -331.261613 -331.261792	<i>E</i> _{ion} ** -330.905847 -331.066652 -331.111796 -331.120371 -331.120513	IE _v ** 3.77 3.80 3.80 3.84 3.84
Specie [*] Ba(H ₂ O) ₄ isomer (4+0) ₄	Theory mPW1PW91	Basis set 6-31G 6-311G(d) 6-311G(d,p) 6-311+G(d,p) 6-311++G(d,p) 6-311++G(2d,p)	<i>E</i> ^{**} -331.044265 -331.206237 -331.251312 -331.261613 -331.261792 -331.262055	<i>E</i> _{ion} ** -330.905847 -331.066652 -331.111796 -331.120371 -331.120513 -331.120854	IE,** 3.77 3.80 3.80 3.84 3.84 3.84
Specie [*] Ba(H ₂ O) ₄ isomer (4+0) _a	Theory mPW1PW91	Basis set 6-31G 6-311G(d) 6-311G(d,p) 6-311+G(d,p) 6-311++G(d,p) 6-311++G(d,p) 6-311++G(2d,p) 6-311++G(2d,p)	<i>E</i> ^{**} -331.044265 -331.206237 -331.251312 -331.261613 -331.261792 -331.262055 -331.264722	<i>E</i> _{ion} ** -330.905847 -331.066652 -331.111796 -331.120371 -331.120513 -331.120854 -331.123689	IE,*** 3.77 3.80 3.80 3.84 3.84 3.84 3.84 3.84
Specie [*] Ba(H ₂ O) ₄ isomer $(4+\theta)_a$	Theory mPW1PW91	Basis set 6-31G 6-311G(d) 6-311G(d,p) 6-311+G(d,p) 6-311+G(d,p) 6-311++G(d,p) 6-311++G(2d,p) 6-311++G(2d,p) 6-311++G(3d,p) 6-311++G(3d,p)	<i>E</i> ^{**} -331.044265 -331.206237 -331.251312 -331.261613 -331.261792 -331.262055 -331.264722 -331.264722 -331.267741	E_{ion}^{**} -330.905847 -331.066652 -331.111796 -331.120371 -331.120513 -331.120854 -331.12854 -331.12689 -331.126725	IE,*** 3.77 3.80 3.80 3.84 3.84 3.84 3.84 3.84 3.84
Specie [*] Ba(H ₂ O) ₄ isomer $(4+\theta)_a$	Theory mPW1PW91	Basis set 6-31G 6-311G(d) 6-311G(d,p) 6-311+G(d,p) 6-311+G(d,p) 6-311++G(d,p) 6-311++G(2d,p) 6-311++G(3d,p) 6-311++G(3df,p) 6-311++G(3df,p) 6-311++G(3df,3pd) 6-311++G(3df,3pd)	<i>E</i> ^{**} -331.044265 -331.206237 -331.251312 -331.261613 -331.261792 -331.262055 -331.264722 -331.264724 -331.276145	$\frac{E_{ion}}{^{**}}$ -330.905847 -331.066652 -331.111796 -331.120371 -331.120513 -331.120854 -331.123689 -331.123689 -331.126725 -331.135130	IE _ν ** 3.77 3.80 3.80 3.84 3.84 3.84 3.84 3.84 3.84 3.84

* RECP used for Ba atom: Lim *et al*.

** Note that the values are not corrected by the zero point vibrational energies (E_{ZPE}).

From the results, 6-311++G(d,p) basis set is seen to be able to reproduce the barium-water ionization energy. The ionization energy not changes by the basis set increasing [from the 6-311+G(d,p)], and it indicates that the delocalized electron on the neutral state is well described by the selected basis set. In addition, the calculated binding energies and bond distances for the dimer, trimer and tetramer water clusters, $(H_2O)_n$ (n = 2 - 4) using 6-311++G(d,p) basis sets reproduce reasonably well the experimental values (see Section 5.1).

Basis sets selection:

Ba atom:

The results from the three RECP's and their basis sets were evaluated by comparison to experimental values:

Specie	Theory	RECP	Eneutral	$E_{ion(+1)}$	IE
		Bausch. et al.	-25.421894	-25.236026	5.06
D.		SDD	-25.441871	-25.255232	5.08
Ба	<i>m</i> F w 1F w91	Lim et al.	-25.445940	-25.258481	5.10
_			Experin	ental value:	5.21
Specie	Theory	RECP	$E_{neutral}$	$E_{ion(+1)}$	IE
		Bausch. et al.	-25.322073	-25.133532	5.13
D		SDD	-25.258984	-25.073281	5.05
Ба	CCSD(1,Full)	Lim et al.	-25.378212	-25.187920	5.18
			Experir	nental value:	5 21

Specie	Theory	RECP	$E_{ion(+1)}$	$E_{ion(+2)}$	IE
		Bausch. Et al.	-25.236026	-24.871354	9.92
D.+		SDD	-25.255232	-24.890441	9.93
Ба	<i>m</i> F w 1F w 91	Lim et al.	-25.258481	-24.891405	9.99
			Experin	nental value:	10.00
Specie	Theory	RECP	$E_{ion(+1)}$	$E_{ion(+2)}$	IE
		Bausch. et al.	-25.133532	-24.771889	9.84
$\mathbf{D}_{\mathbf{r}}^{+}$	CCCD/T EII)	SDD	-25.073281	-24.715209	9.74
Ба	CCSD(1,Full)	Lim et al.	-25.187920	-24.821722	9.96
			Experin	nental value:	10.00

Specie [*]	Theory	RECP	E_{θ}^{**}	E_{ion}^{**}	${\rm IE}_{v}^{**}$
		Bausch. et al.	-100.704981	-100.462628	6.59
PaO	mDW/1DW/01	SDD	-100.721548	-100.481590	6.53
DaU	mr wir w91	Lim et al.	-100.725587	-100.484259	6.57
			Experi	mental value:	6.91
Specie*	Theory	RECP	E_{0}^{**}	<i>E</i> _{ion} ***	IE _v **
Specie*	Theory	RECP Bausch. <i>et al</i> .	<i>E</i> ₀ ** -100.551570	<i>E</i> _{ion} ** -100.305016	IE _ν ** 6.71
Specie*	Theory	RECP Bausch. <i>et al.</i> SDD	<i>E</i> ₀ ** -100.551570 -100.478041	<i>E</i> _{ion} ** -100.305016 -100.237409	IE _ν ** 6.71 6.55
Specie [*] BaO	Theory CCSD(T,Full)	RECP Bausch. et al. SDD Lim et al.	<i>E</i> ^{**} -100.551570 -100.478041 -100.603934	<i>E</i> _{ion} ^{**} -100.305016 -100.237409 -100.354486	IE _v ** 6.71 6.55 6.79

Basis set used for O atom: AUG-cc-PVQZ

^{**} Note that the values are not corrected by the zero point vibrational energies (E_{ZPE}).

The RECP developed by Lim *et al.* was selected for the accuracy to reproduce the experimental IE's of ground state Ba, Ba^+ , and the vertical IE of BaO, as compared with the corresponding experimental values.

Water clusters:

(H₂O)₂:

Theory	$E_0[(H_2O)_2]$	$E_{\rm ZPE}$	$E[(H_2O)_2]$	$E_0[(H_2O)_1]$	$E_{\rm ZPE}$	$E[(H_2O)_1]$	D_e	D_{θ}	D ₀ /1
mPW1PW91	-152.878885	0.046923	-152.831962	-76.434787	0.021605	-76.413183	-5.84	-3.51	-3.51
Theory	$E_0[(H_2O)_2]$	$E_{\rm ZPE}$	$E[(H_2O)_2]$	$E_0[(H_2O)_1]$	$E_{\rm ZPE}$	$E[(H_2O)_1]$	D_e	D_{θ}	D ₀ /1
CCSD(T,Full)	-152.621294	0.046923	-152.574371	-76.305850	0.021605	-76.284245	-6.02	-3.69	-3.69

(H₂O)₃:

Theory	$E_0[(H_2O)_3]$	$E_{\rm ZPE}$	$E[(H_2O)_3]$	$E[(H_2O)_2]$	$E[(H_2O)_1]$	D_e	D_{θ}	$D_0/2$
mPW1PW91	-229.332098	0.074047	-229.258051	-152.831962	-76.413183	-11.56	-8.10	-4.05
Theory	$E_0[(H_2O)_3]$	$E_{\rm ZPE}$	$E[(H_2O)_3]$	$E[(H_2O)_2]$	$E[(H_2O)_1]$	D_e	$D_{ heta}$	$D_0/2$
CCSD(T,Full)	-228.945384	0.074047	-228.871337	-152.574371	-76.284245	-11.45	-7.98	-3.99

(H₂O)₄:

Theory	$E_0[(H_2O)_4]$	$E_{\rm ZPE}$	$E[(H_2O)_4]$	$E[(H_2O)_3]$	$E[(H_2O)_1]$	D_e	$D_{ heta}$	D ₀ /2
mPW1PW91	-305.788599	0.100305	-305.688295	-229.258051	-76.413183	-13.63	-10.71	-5.35
Theory	$E_0[(H_2O)_4]$	$E_{\rm ZPE}$	$E[(H_2O)_4]$	$E[(H_2O)_3]$	$E[(H_2O)_1]$	D_e	D_{θ}	D ₀ /2
CCSD(T,Full)	-305.272365	0.100305	-305.172060	-228. 871337	-76.284245	-13.26	-10.34	-5.17

Neutral barium-water clusters:

Ba(H₂O)₁: Isomer 1

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_1]$	$E[(H_2O)_1]$	E[Ba]	ΔE	$\Delta_r G^{75K}$
	Bausch. et al.	-101.875384	0.022055	-101.853329	-76.413183	-25.421894	-11.45	5 -10.67
	SDD	-101.893920	0.022340	-101.871580	-76.413183	-25.441871	-10.37	-9.52
mPW1PW91	Lim et al.	-101.898964	0.022009	-101.876955	-76.413183	-25.445940	-11.19	-10.45
					А	verage value:	-11.00	-10.21
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_1]$	$E[(H_2O)_1]$	E[Ba]	ΔE	$\Delta_r G^{75K}$
	Bausch. et al.	-101.645290	0.022055	-101.623235	-76.28424	5 -25.322073	-10.0	52 -9.83
CCSD(T Enll)	SDD	-101.565826	0.022340	-101.543486	-76.28424	5 -25.258984	-0.1	6 0.68
CCSD(1,Full)	Lim et al.	-101.702281	0.022009	-101.680272	-76.28424	5 -25.378212	-11.1	l8 -10.44
						Average value:	-7.3	2 -6.53
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a_{ ext{ZPE}}$	E_{v}	IE _ν	IE _a
	Bausch. et al.	-101.875384	0.022055	-101.710805	0.023623	101 710805	4.50	1 20
		1011070001	0.0110000		0.025025	-101./10805	4.52	4.52
DIV/1 DIV/0.1	SDD	-101.893920	0.022340	-101.728590	0.023746	-101.728589	4.52 4.54	4.52 4.54
mPW1PW91	SDD Lim <i>et al</i> .	-101.893920 -101.898964	0.022340 0.022009	-101.728590 -101.733396	0.023746 0.023608	-101.728589 -101.733396	4.52 4.54 4.55	4.52 4.54 <u>4.55</u>
mPW1PW91	SDD Lim et al.	-101.893920 -101.898964	0.022340 0.022009	-101.728590 -101.733396	0.023746 0.023608 Av	-101.728589 -101.733396 erage value:	4.52 4.54 4.55 4.54	4.52 4.54 4.55 4.54
mPW1PW91	SDD Lim et al.	-101.893920 -101.898964	0.022340 0.022009	-101.728590 -101.733396	0.023608 0.023608 Av	-101.710805 -101.728589 -101.733396 erage value:	4.52 4.54 4.55 4.55	4.52 4.54 4.55 4.54
mPW1PW91	SDD Lim et al. Basis set Ba	-101.893920 -101.898964	0.022340 0.022009 <i>E</i> _{ZPE}	-101.728590 -101.733396	0.023746 0.023608 Av E ^a _{ZPE}	-101.710303 -101.728589 -101.733396 erage value: E _v	4.52 4.54 4.55 4.54 IE _v	4.52 4.54 4.55 4.54 IE _a
mPW1PW91	SDD Lim et al. Basis set Ba Bausch. et al.	-101.893920 -101.898964 -101.645290	0.022340 0.022009 <u>Ezpe</u> 0.022055	-101.728590 -101.733396 <i>E_a</i> -101.477839	$\frac{0.023623}{0.023746}$ 0.023608 Av $\frac{E^{a}_{ZPE}}{0.023623}$	-101.718803 -101.728589 -101.733396 erage value: <u>E_ν</u> -101.477685	$ 4.52 \\ 4.54 \\ 4.55 \\ 4.54 \\ \overline{1E_{\nu}} \\ 4.60 $	$ \begin{array}{r} 4.52 \\ 4.54 \\ 4.55 \\ 4.54 \\ \hline $
mPW1PW91 Theory CCSD/T E-II)	SDD Lim et al. Basis set Ba Bausch. et al. SDD	-101.893920 -101.898964 -101.645290 -101.565826	0.022340 0.022009 E _{ZPE} 0.022055 0.022340	-101.728590 -101.733396 <u>E_a</u> -101.477839 -101.401429	$\frac{0.023623}{0.023746}$ 0.023608 Av E^{a}_{ZPE} 0.023623 0.023746	-101.728589 -101.733396 erage value: <u>E_v</u> -101.477685 -101.401362		$ \begin{array}{r} 4.52 \\ 4.54 \\ 4.55 \\ 4.54 \\ \hline 4.54 \\ \hline 4.54 \\ \hline IE_a \\ 4.60 \\ 4.51 \\ \end{array} $
mPW1PW91 Theory CCSD(T,Full)	SDD Lim et al. Basis set Ba Bausch. et al. SDD Lim et al.	-101.893920 -101.898964 -101.645290 -101.565826 -101.702281	0.022340 0.022009 <i>E_{ZPE}</i> 0.022055 0.022340 0.022009	-101.728590 -101.733396 -101.477839 -101.401429 -101.533780	0.023746 0.023608 Av <u>E^azpe</u> 0.023623 0.023746 0.023608	$-101.728589 -101.733396 erage value: E_{\nu} -101.477685 -101.401362 -101.533601$		4.52 4.54 4.55 4.54 4.54 4.54 4.60 4.51 4.63 4.63

Ba(H₂O)₂: Isomer $(2+\theta)_a$

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_2]$	$E[(H_2O)_2]$	E[Ba]	ΔΙ	Ξ	$\Delta_r G^{75K}$
	Bausch. et al.	-178.331004	0.045450	-178.285554	-152.83196	3 -25.421894	-19.	89	-18.51
	SDD	-178.349334	0.045389	-178.303945	-152.83196	3 -25.441871	-18.	89	-17.64
mPW1PW91	Lim et al.	-178.354136	0.045449	-178.305910	-152.83196	3 -25.445939	-17.	58	-17.93
						Average value:	-18.	79	-17.98
Theory	Pagis set Pa	F	F	$E[D_{\alpha}(H_{\alpha})]$	E[(H, O)]	$1 E[D_{\alpha}]$		F	A C ^{75K}
Theory	Dasis set Da	E ₀	L ZPE	$E[Ba(H_2O)_2]$	E[(H ₂ O)	$\frac{1}{2} \frac{E[Ba]}{E[Ba]}$	L		Δ _r G
	Bausch. <i>et al.</i>	-1//.9/1065	0.045450	-1//.925615	-152.5743	-25.322073	-13	8.31	-17.04
CCSD(T.Full)	SDD	-177.891204	0.045389	-177.845815	-152.5743	-25.258984	-7	.82	-6.56
	Lim <i>et al</i> .	-1/8.02962/	0.045449	-1//.9841/8	-152.5743	-25.3/8212	-1	9.83	-18.56
						Average value:	-1:	5.32	-14.05
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^{a}{}_{ m ZPE}$	E_{v}	IE _ν	IEa	_
	Bausch. et al.	-178.331004	0.045450	-178.181194	0.047583	-178.178086	4.22	4.13	
	SDD	-178.349334	0.045389	-178.199286	0.047775	-178.198117	4.18	4.15	
<i>mr</i> w1r w91	Lim et al.	-178.354136	0.045449	-178.203782	0.047550	-178.200782	4.15	4.07	
					Av	verage value:	4.18	4.12	
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a_{\rm ZPE}$	E_{v}	IE _v	IE	a
	Bausch. et al.	-177.971065	0.045450	-177.818834	0.047583	-177.816647	4.26	4.2	0
CCSD(T Enll)	SDD	-177.891204	0.045389	-177.740975	0.047775	-177.740967	4.15	4.1	5
CC5D(1,Full)	Lim et al.	-178.029627	0.045449	-177.875773	0.047550	-177.874537	4.28	4.2	4
					Δ	verage value:	4.23	4.2	0

Supplementary file

Ba(H₂O)₂: Isomer $(2+\theta)_b$

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_2]$	$E[(H_2O)_2]$	E[Ba]	Δ	E	$\Delta_r G^{75K}$
	Bausch. et al.	-178.328559	0.046694	-178.281865	-152.83196	-25.421894	-17.	58	-16.19
DW1DW01	SDD	-178.346744	0.046889	-178.299855	-152.83196	3 -25.441871	-16.	33	-14.93
mPW1PW91	Lim et al.	-178.351660	0.046672	-178.304988	-152.83196	3 -25.445939	-17.	00	-15.62
						Average value:	-16.	97	-15.58
Theory	Rosis sot Ro	F	F	$F[R_a(H, O)]$	F[(H, O)]	$E[B_{\alpha}]$		F	A C ^{75K}
Theory	Dasis set Da	177.0 (0007	LZPE	$E[Du(\Pi_2 O)_2]$	152 5740	2 $L[Du]$	1		Δ _r θ
	Bausch. <i>et al.</i>	-1//.96982/	0.046694	-1//.923133	-152.5743	5/1 -25.3220/3	-1	0.75	-15.36
CCSD(T,Full)		-1//.889845	0.046889	-1//.842950	-152.5743	271 -25.258984	-0 1/	0.02	-4.03
	Lim et al.	-1/8.02/492	0.046672	-1//.980820	-152.5743	5/1 -25.3/8212	-1	1.12	-10.35
						Average value:	-1	3.50	-12.11
Theory	Rasis set Ra	<i>E</i> ₀	Egne	E.	E^a_{appr}	E	IE	IE	_
Incorg	Bausch <i>et al</i>	-178 328559	0.046694	-178 181194	0.047583	-178 174189	4 22	4.03	_
	SDD	-178.346744	0.046889	-178.199286	0.047775	-178.191916	4.24	4.04	
mPW1PW91	Lim et al.	-178.351660	0.046672	-178.203782	0.047550	-178.196471	4.25	4.05	
-					Av	verage value:	4.24	4.04	
									_
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a{}_{ m ZPE}$	E_v	IE_{v}	IE	a
	Bausch. et al.	-177.969827	0.046694	-177.818834	0.047583	-177.813138	4.29	4.1	3
	SDD	-177 889845	0.046889	-177.740975	0.047775	-177.735120	4.23	4.0	8
CCCD(T EII)	500	177.007045	0.010007	1111110210					
CCSD(T,Full)	Lim et al.	-178.027492	0.046672	-177.875773	0.047550	-177.869896	4.31	4.1	5

Ba(H₂O)₂: Isomer (1+1)

The	Dania ant D	E	E	$E[D_{\pi}(H, O)]$	EL(IL O)	$E[D_{-}]$	A 1		A C 75K
1 neory	Basis set Ba	E_0	E ZPE	$E[Ba(H_2O)_2]$	$E[(H_2O)_2]$	E[Ba]	Δ	5	$\Delta_r \mathbf{G}^{nn}$
	Bausch. <i>et al</i> .	-178.326657	0.048027	-178.278630	-152.831963	3 -25.421894	-15.	55	-14.24
DW/1DW/01	SDD	-178.344897	0.048226	-178.296671	-152.831963	3 -25.441871	-14.	33	-13.07
	Lim et al.	-178.349990	0.048029	-178.301961	-152.831963	3 -25.445939	-15.	10	-13.84
					L	Average value:	-14.	99	-13.73
Theory	Racic cot Ro	F	F	$F[R_{\alpha}(H, \Omega)]$	F[(H, O)]	1 F[Ba]	,	F	A C ^{75K}
Theory	Dasis set Da		LZPE	$E[Bu(\Pi_2 O)_2]$	$E[(H_2O)_2$		1		Δ _r G
	Bausch. <i>et al</i> .	-177.967008	0.048027	-17/.918981	-152.5743	71 -25.322073	-1-	4.14	-12.84
CCSD(T Full)	SDD	-177.887456	0.048226	-177.839230	-152.5743	71 -25.258984	-3	5.69	-2.38
	Lim et al.	-178.023989	0.048029	-177.975960	-152.5743	71 -25.378212	-1	4.67	-13.37
						Average value:	-1	0.83	-9.53
									_
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a_{ m ZPE}$	E_v	IE _ν	IEa	_
Theory	Basis set Ba Bausch. <i>et al</i> .	<i>E</i> ₀ -178.326657	<i>Е</i> _{ZPE} 0.048027	<i>E_a</i> -178.172484	E^{a}_{ZPE} 0.048990	<i>E_v</i> -178.166128	ΙΕ _ν 4.39	IE _a 4.22	-
Theory	Basis set Ba Bausch. <i>et al.</i> SDD	<i>E</i> ₀ -178.326657 -178.344897	<i>E</i> _{ZPE} 0.048027 0.048226	<i>E_a</i> -178.172484 -178.190300	<i>E^a</i> _{ZPE} 0.048990 0.049047	<i>E_v</i> -178.166128 -178.183748	ΙΕ _ν 4.39 4.41	IE _a 4.22 4.23	-
Theory mPW1PW91	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i>	<i>E</i> ₀ -178.326657 -178.344897 -178.349990	<i>E</i> _{ZPE} 0.048027 0.048226 0.048029	<i>E_a</i> -178.172484 -178.190300 -178.195104	<i>E^a_{ZPE}</i> 0.048990 0.049047 0.048972	<i>E_v</i> -178.166128 -178.183748 -178.188478	IE _ν 4.39 4.41 4.42	IE _a 4.22 4.23 4.24	-
Theory mPW1PW91	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i>	<i>E</i> ₀ -178.326657 -178.344897 -178.349990	<i>E</i> _{ZPE} 0.048027 0.048226 0.048029	<i>E_a</i> -178.172484 -178.190300 -178.195104	<i>E^a_{ZPE}</i> 0.048990 0.049047 0.048972 Av	<i>E_ν</i> -178.166128 -178.183748 -178.188478 erage value:	IE _ν 4.39 4.41 4.42 4.41	IE _a 4.22 4.23 4.24 4.23	_ _ _
Theory mPW1PW91	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i> Basis set Ba	E ₀ -178.326657 -178.344897 -178.349990	Е _{ZPE} 0.048027 0.048226 0.048029	<i>E_a</i> -178.172484 -178.190300 -178.195104	E^{a}_{ZPE} 0.048990 0.049047 0.048972 Av	<i>E_ν</i> -178.166128 -178.183748 -178.188478 erage value: <i>E</i>	IE _ν 4.39 4.41 4.42 4.41	IE _a 4.22 4.23 4.24 4.23	-
Theory mPW1PW91 Theory	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i> Basis set Ba	<i>E</i> ₀ -178.326657 -178.344897 -178.349990 <i>E</i> ₀	<u>Егре</u> 0.048027 0.048226 0.048029 <u>Егре</u> 0.048027	<i>E_a</i> -178.172484 -178.190300 -178.195104 <i>E_a</i>	$\frac{E^{a}_{ZPE}}{0.048990}$ 0.049047 0.048972 Av $\frac{E^{a}_{ZPE}}{0.0489000}$	<i>E_ν</i> -178.166128 -178.183748 -178.188478 erage value: <i>E_ν</i> 177.802442	$ IE_{\nu} 4.39 4.41 4.42 4.41 IE_{\nu} 149 $	IE _a 4.22 4.23 4.24 4.23 4.24 4.23	
Theory mPW1PW91 Theory	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i> Basis set Ba Bausch. <i>et al.</i>	E ₀ -178.326657 -178.344897 -178.349990 -177.967008	EZPE 0.048027 0.048226 0.048029 EZPE 0.048027	<i>E_a</i> -178.172484 -178.190300 -178.195104 <i>E_a</i> -177.810139	$\frac{E^{a}_{ZPE}}{0.048990}$ 0.049047 0.048972 Av $\frac{E^{a}_{ZPE}}{0.048990}$	<i>E_v</i> -178.166128 -178.183748 -178.188478 erage value: <i>E_v</i> -177.803443	$ IE_{\nu} 4.39 4.41 4.42 4.41 IE_{\nu} 4.48 4.48 $	IE _a 4.22 4.23 4.24 4.23 IE _a 4.24	
Theory mPW1PW91 Theory CCSD(T E::!!)	Basis set Ba Bausch. et al. SDD Lim et al. Basis set Ba Bausch. et al. SDD	E ₀ -178.326657 -178.344897 -178.349990 -178.349990 -177.967008 -177.887456	E _{ZPE} 0.048027 0.048226 0.048029 E _{ZPE} 0.048027 0.048226	<i>E_a</i> -178.172484 -178.190300 -178.195104 <i>E_a</i> -177.810139 -177.733171	$\frac{E^{a}_{ZPE}}{0.048990}$ 0.049047 0.048972 Av E^{a}_{ZPE} 0.048990 0.049047	<i>E_ν</i> -178.166128 -178.183748 -178.188478 erage value: <i>E_ν</i> -177.803443 -177.726796	$ IE_{\nu} 4.39 4.41 4.42 4.41 IE_{\nu} 4.48 4.39 $	IE _a 4.22 4.23 4.24 4.23 4.24 4.23 IE _a 4.22	<u>a</u> 9 2
Theory mPW1PW91 Theory CCSD(T,Full)	Basis set Ba Bausch. et al. SDD Lim et al. Basis set Ba Bausch. et al. SDD Lim et al.	E ₀ -178.326657 -178.344897 -178.349990 -178.349990 -177.967008 -177.887456 -178.023989	EzPE 0.048027 0.048226 0.048029 EzPE 0.048027 0.048027 0.048226 0.048029	<i>E_a</i> -178.172484 -178.190300 -178.195104 <i>E_a</i> -177.810139 -177.733171 -177.866257	$\frac{E^{a}_{ZPE}}{0.048990}$ 0.049047 0.048972 Av $\frac{E^{a}_{ZPE}}{0.048990}$ 0.049947 0.048972	<i>E_ν</i> -178.166128 -178.183748 -178.188478 erage value: <i>E_ν</i> -177.803443 -177.726796 -177.859389	$\frac{IE_{\nu}}{4.39}$ 4.41 4.42 4.41 IE_{ν} 4.48 4.39 4.50	IE _a 4.22 4.23 4.24 4.23 IE _a 4.2 4.2 4.2	a 9 2 2

Supplementary file

Ba(H₂O)₃: Isomer $(3+\theta)_a$

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	E[Ba]	Δ	E
	Bausch. et al.	-254.784611	0.069870	-254.714741	-229.258051	-25.421894	-21.	.83
DIVIDIVA	SDD	-254.802565	0.069914	-254.732651	-229.258051	-25.441871	-20.	.54
mPW1PW91	Lim et al.	-254.807362	0.069875	-254.737487	-229.258051	-25.445939	-21.	.02
					A	verage value:	-21.	.13
Theory	Basis set Ba	E	Ean	$E[Ba(H_2O)_2]$	$E[(H_2O)_2]$	E[Ba]		E
Theory	Bausah at al	254 206516	0.060970	254 226646	22093	2 05 200072	2	0.94
	SDD	-234.290310	0.069870	-234.220040	-220.0/133	7 -23.322075	-20	0.00
CCSD(T,Full)	SDD Lim et al	-254.210202	0.009914	-234.140346	-220.07132	25.250904	-10	0.00 7 80
	Lini et al.	-234.333703	0.009873	-234.203000	-220.07153	-23.378212	-2,	2.00
						Average value:	-1	/.91
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a_{ ext{ZPE}}$	E_{v}	IE _ν	IE _a
Theory	Basis set Ba Bausch. <i>et al</i> .	<i>E</i> ₀ -254.784611	Е _{ZPE} 0.069870	<i>E_a</i> -254.647647	E^{a}_{ZPE} 0.071256	<i>E_v</i> -254.637794	ΙΕ _ν 4.03	IE _a 3.76
Theory	Basis set Ba Bausch. <i>et al.</i> SDD	<i>E</i> ₀ -254.784611 -254.802565	<i>Е</i> _{ZPE} 0.069870 0.069914	<i>E_a</i> -254.647647 -254.666178	<i>E^a</i> _{ZPE} 0.071256 0.071554	E_{ν} -254.637794 -254.657215	IE _v 4.03 4.00	IE _a 3.76 3.76
Theory mPW1PW91	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i>	<i>E</i> ₀ -254.784611 -254.802565 -254.807362	<i>E</i> _{ZPE} 0.069870 0.069914 0.069875	<i>E_a</i> -254.647647 -254.666178 -254.670312	<i>E^a_{ZPE}</i> 0.071256 0.071554 0.071253	<i>E_v</i> -254.637794 -254.657215 -254.660438	IE _ν 4.03 4.00 4.04	IE _a 3.76 3.76 3.77
Theory mPW1PW91	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al</i> .	<i>E</i> ₀ -254.784611 -254.802565 -254.807362	<i>E</i> _{ZPE} 0.069870 0.069914 0.069875	<i>E_a</i> -254.647647 -254.666178 -254.670312	<i>E^a_{ZPE}</i> 0.071256 0.071554 0.071253 Ave	<i>E_v</i> -254.637794 -254.657215 -254.660438 erage value:	IE _ν 4.03 4.00 4.04 4.02	IE _a 3.76 3.76 3.77 3.76
Theory mPW1PW91	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i>	<i>E</i> ₀ -254.784611 -254.802565 -254.807362	<i>E</i> _{ZPE} 0.069870 0.069914 0.069875	<i>E_a</i> -254.647647 -254.666178 -254.670312	<i>E^a_{ZPE}</i> 0.071256 0.071554 0.071253 Ave	<i>E_v</i> -254.637794 -254.657215 -254.660438 erage value:	IE _ν 4.03 4.00 4.04 4.02	IE _a 3.76 3.76 3.77 3.76
Theory mPW1PW91 Theory	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i> Basis set Ba	E ₀ -254.784611 -254.802565 -254.807362 E ₀	<i>E</i> _{ZPE} 0.069870 0.069914 0.069875 <i>E</i> _{ZPE}	<i>E_a</i> -254.647647 -254.666178 -254.670312 <i>E_a</i>	$\frac{E^{a}_{ZPE}}{0.071256}$ 0.071253 0.071253 Ave E^{a}_{ZPE}	<i>E_v</i> -254.637794 -254.657215 -254.660438 erage value: <i>E_v</i>	IE _ν 4.03 4.00 4.04 4.02	IE _a 3.76 3.76 3.77 3.76 IE _a
Theory mPW1PW91 Theory	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i> Basis set Ba Bausch. <i>et al.</i>	<i>E</i> ₀ -254.784611 -254.802565 -254.807362 <i>E</i> ₀ -254.296516	<i>E</i> _{ZPE} 0.069870 0.069914 0.069875 <i>E</i> _{ZPE} 0.069870	<u>E</u> _a -254.647647 -254.666178 -254.670312 <u>E</u> _a -254.156681	$\frac{E^{a}_{ZPE}}{0.071256}$ 0.071253 0.071253 Ave $\frac{E^{a}_{ZPE}}{0.071256}$	<i>E_v</i> -254.637794 -254.657215 -254.660438 erage value: <i>E_v</i> -254.148800	$ IE_{\nu} 4.03 4.00 4.04 4.02 IE_{\nu} 4.06 $	IE _a 3.76 3.76 3.77 3.76 IE _a 3.84
Theory mPW1PW91 Theory	Basis set Ba Bausch. et al. SDD Lim et al. Basis set Ba Bausch. et al. SDD	<i>E</i> ₀ -254.784611 -254.802565 -254.807362 <i>E</i> ₀ -254.296516 -254.216262	E _{ZPE} 0.069870 0.069914 0.069875 E _{ZPE} 0.069870 0.069914	<i>E_a</i> -254.647647 -254.666178 -254.670312 <i>E_a</i> -254.156681 -254.077773	$\frac{E^{a}_{ZPE}}{0.071256}$ 0.071554 0.071253 Ave $\frac{E^{a}_{ZPE}}{0.071256}$ 0.071256 0.071554	<i>E_v</i> -254.637794 -254.657215 -254.660438 erage value: <i>E_v</i> -254.148800 -254.071725	$ IE_{\nu} 4.03 4.00 4.04 4.02 IE_{\nu} 4.06 3.98 $	IE _a 3.76 3.76 3.77 3.76 IE _a 3.84 3.81
Theory mPW1PW91 Theory CCSD(T,Full)	Basis set Ba Bausch. et al. SDD Lim et al. Basis set Ba Bausch. et al. SDD Lim et al.	E ₀ -254.784611 -254.802565 -254.807362 E ₀ -254.296516 -254.216262 -254.355763	E _{ZPE} 0.069870 0.069914 0.069875 E _{ZPE} 0.069870 0.069914 0.069875	<i>E_a</i> -254.647647 -254.666178 -254.670312 <i>E_a</i> -254.156681 -254.077773 -254.214468	$\frac{E^{a}_{ZPE}}{0.071256}$ 0.071554 0.071253 Avo $\frac{E^{a}_{ZPE}}{0.071256}$ 0.071256 0.071554 0.071253	<i>E_v</i> -254.637794 -254.657215 -254.660438 erage value: <i>E_v</i> -254.148800 -254.071725 -254.207698	$\frac{IE_{\nu}}{4.03}$ 4.00 4.04 4.02 $\frac{IE_{\nu}}{4.06}$ 3.98 4.07	IE _a 3.76 3.76 3.77 3.76 IE _a 3.84 3.81 3.88

Ba(H₂O)₃: Isomer $(3+\theta)_b$

Theory	Dogia ant Do	F	F	$E[P_{\alpha}(H, O)]$	E[(H, O)]			R
Theory	Dasis set Da		E ZPE	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$			10
	Bausch. et al.	-254.780616	0.071704	-254.708912	-229.25805	1 -25.421894	-18.	18
mDW1DW01	SDD	-254.798529	0.071965	-254.726564	-229.25805	1 -25.441871	-16.	72
	Lim et al.	-254.803367	0.071576	-254.731791	-229.25805	1 -25.445939	-17.	45
						Average value:	-17.	45
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_3]$	$E[(H_2O)]$	E[Ba]	Δ	E
	Bausch. et al.	-254.295339	0.071704	-254.223635	-228.8713	37 -25.322073	-18	8.97
	SDD	-254.215329	0.071965	-254.143364	-228.8713	37 -25.258984	-8	.18
CCSD(1,Full)	Lim et al.	-254.354288	0.071576	-254.282712	-228.8713	37 -25.378212	-20	0.81
						Average value:	-15	5.99
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a{}_{ m ZPE}$	E_v	IE _v	IEa
	Bausch. et al.	-254.780616	0.071704	-254.647647	0.071256	-254.633435	3.99	3.61
	SDD	-254.798529	0.071965	-254.666178	0.071554	-254.651989	3.98	3.59
mrwirw91	Lim et al.	-254.803367	0.071576	-254.670312	0.071253	-254.656164	4.00	3.61
					Av	verage value:	3.99	3.60
Theory	Basis set Ba	E_0	EZPE	E_a	E^{a}_{ZPE}	E_v	IE _v	IEa
	Bausch. et al.	-254.295339	0.071704	-254.156681	0.071256	-254.146836	4.03	3.76
	SDD	-254.215329	0.071965	-254.077773	0.071554	-254.068925	3.97	3.73
CCSD(T,Full)								
0002(1)1 (11)	Lim et al.	-254.354288	0.071576	-254.214468	0.071253	-254.205461	4.04	3.80

Supplementary file

Ba(H₂O)₃: Isomer (2+1)

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	E[Ba]	Δŀ	Ξ
	Bausch. et al.	-254.779201	0.072033	-254.707168	-229.25805	1 -25.421894	-17.	08
DII/1 DII/01	SDD	-254.796937	0.071874	-254.725063	-229.25805	1 -25.441871	-15.	78
mPW1PW91	Lim et al.	-254.802334	0.072066	-254.730268	-229.25805	1 -25.445939	-16.	49
						Average value:	-16.	45
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	E[Ba]	ΔE	3
	Bausch. et al.	-254.291689	0.072033	-254.219656	-228.87133	7 -25.322073	-16.4	47
	SDD	-254.211514	0.071874	-254.139640	-228.87133	7 -25.258984	-5.8	85
CCSD(1,ull)	Lim et al.	-254.350004	0.072066	-254.277938	-228.87133	7 -25.378212	-17.	81
						Average value:	-13.	38
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a_{\rm ZPE}$	E_{v}	IE _v	IE _a
	Bausch. et al.	-254.779201	0.072033	-254.639968	0.074516	-254.631580	4.08	3.86
DW/1DW/01	SDD	-254.796937	0.071874	-254.658154	0.074790	-254.650314	4.07	3.86
	Lim et al.	-254.802334	0.072066	-254.662580	0.074535	-254.654016	4.10	3.87
					Av	verage value:	4.09	3.86
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a_{ ext{ZPE}}$	E_{v}	IE _v	IEa
	Bausch. et al.	-254.291689	0.072033	-254.151178	0.074516	-254.141097	4.17	3.89
CCSD(T Evil)	SDD	-254.211514	0.071874	-254.073139	0.074790	-254.064096	4.09	3.84
CCSD(1,Full)	Lim et al.	-254.350004	0.072066	-254.208109	0.074535	-254.198769	4.18	3.93
					Δ	verage value	4 1 5	3 80

Ba(H₂O)₃: Isomer (1+1+1)

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	E[Ba]	Δŀ	Ξ
	Bausch. et al.	-254.779461	0.073330	-254.706131	-229.25805	51 -25.421894	-16.	43
DIVIDIVOI	SDD	-254.797597	0.073518	-254.724079	-229.25805	51 -25.441871	-15.	16
mPW1PW91	Lim et al.	-254.802788	0.073360	-254.729428	-229.25805	51 -25.445939	-15.	96
						Average value:	-15.	85
Theory	Pagia sot Pa	F	F	$E[D_{\alpha}(H_{\alpha})]$				E
Theory	Dasis set Da	E	E ZPE	$E[Ba(H_2O)_3]$	$E[(\Pi_2 U)]$		Δ	
	Bausch. et al.	-254.290498	0.073330	-254.217168	-228.8713	-25.322073	-14	4.91
CCSD(T Full)	SDD	-254.210417	0.073518	-254.136899	-228.8713	-25.258984	-4	.13
CCSD(1,Full)	Lim et al.	-254.347480	0.073360	-254.274120	-228.8713	337 -25.378212	-15	5.42
						Average value:	-11	1.48
T)	D 1 (D	E			74	T	W	T
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	E^{u}_{ZPE}	E_v	IΕ _ν	IE_a
	Bausch. et al.	-254.779461	0.073330	-254.628024	0.073661	-254.617845	4.41	4.13
DW/1DW/01	SDD	-254.797597	0.073518	-254.645922	0.073851	-254.634803	4.44	4.14
mPw1Pw91	Lim et al.	-254.802788	0.073360	-254.650715	0.073699	-254.640029	4.44	4.15
					A	verage value:	4.43	4.14
Theory	Basis set Ba	E_0	EZPE	E_a	$E^a_{\rm ZPE}$	E_{v}	IE _v	IE _a
•	Bausch. et al.	-254.290498	0.073330	-254.136138	0.073661	-254.124850	4.52	4.21
	SDD	-254.210417	0.073518	-254.059150	0.073851	-254.047392	4.45	4.13
I I SIMI MULL								
CCSD(1,Full)	Lim et al.	-254.347480	0.073360	-254.192495	0.073699	-254.180691	4.55	4.23

Supplementary file

Ba(H₂O)₄: Isomer $(4+\theta)_a$

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	E[Ba]	ΔI	Ξ
	Bausch. et al.	-331.239428	0.094029	-331.145399	-305.688293	5 -25.421894	-22.	09
	SDD	-331.257195	0.094541	-331.162654	-305.688295	5 -25.441871	-20.	39
mPW1PW91	Lim et al.	-331.261792	0.093975	-331.167817	-305.688295	5 -25.445939	-21.	07
					1	Average value:	-21.	19
Theory	Basis set Ba	E	EZPE	$E[Ba(H_2O)_4]$	$E[(H_2O)]_4$	E[Ba]	٨	E
	Bausch <i>et al</i>	-330 623683	0.09/029	-330 529654	-305 1720	50 _25 322073	-22	2 29
	SDD	-330 542879	0.094541	-330.448338	-305 1720	50 -25.322073	-22) 85
CCSD(T,Full)	Lim et al	-330 682883	0.093975	-330 588908	-305 1720	50 -25.250004	-10	1 24
	Lini ti ui.	330.002003	0.073713	550.500700	505.1720	Average value:	-19	9.13
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a_{ m ZPE}$	E_{v}	IE _v	IE_a
	Bausch. et al.	-331.239428	0.094029	-331.107980	0.094301	-331.098366	3.85	3.58
	SDD	-331.257195	0.094541	-331.126638	0.094529	-331.116814	3.82	3.55
mP w IP w 91	Lim et al.	-331.261792	0.093975	-331.130648	0.094304	-331.120513	3.85	3.58
-					Av	erage value:	3.84	3.57
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	E^{a}_{ZPE}	E_{v}	IE _v	IEa
	Bausch. et al.	-330.623683	0.094029	-330.490068	0.094301	-330.481882	3.87	3.64
	SDD	-330.542879	0.094541	-330.412556	0.094529	-330.403396	3.80	3.55
CCSD(T,Full)	SDD Lim <i>et al</i> .	-330.542879 -330.682883	0.094541 0.093975	-330.412556 -330,549527	0.094529 0.094304	-330.403396 -330.540675	3.80 3.88	3.55 3.64

Ba(H₂O)₄: Isomer $(4+\theta)_b$

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	E[Ba]	ΔΙ	3
•	Bausch. et al.	-331.236234	0.094422	-331.141812	-305.68829	5 -25.421894	-19.	84
	SDD	-331.254094	0.094788	-331.159306	-305.688295	5 -25.441871	-18.29	
mPW1PW91	Lim et al.	-331.258707	0.094684	-331.164023	-305.688295	5 -25.445939	-18.	69
•					1	Average value:	-18.	94
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_4]$	$E[(H_2O)_4$] <i>E</i> [<i>Ba</i>]	Δ	E
	Bausch. et al.	-330.622409	0.094422	-330.527987	-305.1720	50 -25.322073	-21	1.24
	SDD	-330.542019	0.094788	-330.447231	-305.1720	50 -25.258984	-1().16
CCSD(1,Full)	Lim et al.	-330.682413	0.094684	-330.587729	-305.1720	50 -25.378212	-23	3.50
						Average value:	-18	8.30
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a{}_{ m ZPE}$	E_{v}	IE _v	IE _a
	Bausch. et al.	-331.236234	0.094422	-331.107980	0.094301	-331.097515	3.77	3.49
DU11 DU101	SDD	-331.254094	0.094788	-331.126638	0.094529	-331.116517	3.74	3.46
mPw1Pw91	Lim et al.	-331.258707	0.094684	-331.130648	0.094304	-331.119889	3.77	3.47
					Av	erage value:	3.76	3.47
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a{}_{ m ZPE}$	E_{v}	IE_{ν}	IE_a
	Bausch. et al.	-330.622409	0.094422	-330.490068	0.094301	-330,483870	3,77	3.60
	SDD	-330.542019	0.094788	-330.412556	0.094529	-330,405620	3,70	3.52
CCSD(1,FUII)	Lim et al.	-330.682413	0.094684	-330,549527	0.094304	-330,543490	3,77	3.61
					А	verage value:	3,75	3.57

Supplementary file

Ba(H₂O)₄: Isomer (3+1)_a

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	E[Ba]	Δ	Ξ
	Bausch. et al.	-331.235734	0.095020	-331.140714	-305.688295	-25.421894	-19.	15
	SDD	-331.253213	0.094681	-331.158532	-305.688295	-25.441871	-17.	80
mPW1PW91	Lim et al.	-331.258474	0.094860	-331.158720	-305.688295	-25.445939	-15.	37
					A	verage value:	-17.	44
Theory	Basis set Ba	E	EZPE	$E[Ba(H_2O)_4]$	$E[(H_2O)_A]$	E[Ba]		E
	Bausch <i>et al</i>	-330 618458	0.095020	-330 523438	-305 17206	0 _25 322073	-19	3 3 9
	SDD	-330 537651	0.094681	-330 442970	-305 17206	-25.322073	-10	48
CCSD(T,Full)	Lim et al.	-330.677921	0.094860	-330.580128	-305.17206	0 -25.378212	-18	.40 3.73
						Average value:	-14	1.87
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a_{\ \rm ZPE}$	E_v	IE _v	IE _a
	Bausch. et al.	-331.235734	0.095020	-331.105578	0.097963	-331.094837	3.91	3.62
	SDD	-331.253213	0.094681	-331.124040	0.098176	-331.115979	3.83	3.61
mP w IP w 91	Lim et al.	-331.258474	0.094860	-331.128157	0.097947	-331.117698	3.78	3.50
•					Av	erage value:	3.84	3.58
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a_{ ext{ZPE}}$	E_{v}	IE _v	IE_a
Theory	Basis set Ba Bausch. <i>et al</i> .	<i>E</i> ₀ -330.618458	<i>Е</i> _{ZPE} 0.095020	<i>E</i> _a -330.488888	E^{a}_{ZPE} 0.097963	E_{ν} -330.475472	IE _ν 3.97	IE _a 3.61
Theory	Basis set Ba Bausch. <i>et al.</i> SDD	<i>E</i> ₀ -330.618458 -330.537651	Е _{ZPE} 0.095020 0.094681	<i>E_a</i> -330.488888 -330.410619	<i>E^a</i> _{ZPE} 0.097963 0.098176	<i>E_v</i> -330.475472 -330.391428	IE _ν 3.97 4.07	IE _a 3.61 3.55
Theory CCSD(T,Full)	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i>	<i>E</i> ₀ -330.618458 -330.537651 -330.677921	<i>E</i> _{ZPE} 0.095020 0.094681 0.094860	<i>E_a</i> -330.488888 -330.410619 -330,546817	<i>E^a</i> _{ZPE} 0.097963 0.098176 0.097947	<i>E_v</i> -330.475472 -330.391428 -330.535006	IE _ν 3.97 4.07 3.89	IE _a 3.61 3.55 3.57

Ba(H₂O)₄: Isomer $(3+1)_b$

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	E[Ba]	ΔΙ	Ξ
v	Bausch. et al.	-331.230934	0.097133	-331.135914	-305.688295	-25.421894	-16.	14
	SDD	-331.248629	0.097510	-331.153948	-305.688295	-25.441871	-14.	92
mPW1PW91	Lim et al.	-331.253580	0.097010	-331.158720	-305.688295	-25.445939	-15.	37
					A	verage value:	-15.	48
Theorem	Pagis set Po	F	F	$E[D_{\alpha}(H_{\alpha})]$	$\mathbf{F}[(\mathbf{H},\mathbf{O})]$	$E[D_{\alpha}]$		F
Theory	Dasis set Da		LZPE	$E[Bu(H_2O)_4]$	$E[(\Pi_2 O)_4]$		4	
	Bausch. <i>et al</i> .	-330.616439	0.097133	-330.521419	-305.17206	0 -25.322073	-17	7.12
CCSD(T.Full)	SDD	-330.536540	0.097510	-330.441859	-305.17206	0 -25.258984	-6	.79
CC5D(1,1 un)	Lim <i>et al</i> .	-330.674988	0.097010	-330.580128	-305.17206	0 -25.378212	-18	3.73
						Average value:	-14	1.21
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a_{ m ZPE}$	E_{v}	IE _ν	IE_a
	Bausch. et al.	-331.230934	0.097133	-331.104664	0.095992 ·	331.085037	4.00	3.46
	SDD	-331.248629	0.097510	-331.123153	0.096374 ·	331.103458	4.00	3.46
mPw1Pw91	Lim et al.	-331.253580	0.097010	-331.127276	0.096055 ·	331.107344	4.01	3.47
					Ave	erage value:	4.00	3.46
Theory	Basis set Ba	E_0	EZPE	E_{a}	E^{a}_{zpe}	E_{v}	IE _v	IEa
•	Bausch. et al.	-330.616439	0.097133	-330.484941	0.095992	-330.469132	4.03	3.60
	SDD	-330.536540	0.097510	-330.405811	0.096374	-330.400240	3.75	3.60
CCSD(T,Full)	Lim et al.	-330.674988	0.097010	-330,542696	0.096055	-330.527111	4.06	3.63
						-		

Supplementary file

Ba(H₂O)₄: Isomer (2+2)

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	E[Ba]	Δ	Ε
	Bausch. et al.	-331.228696	0.097733	-331.130963	-305.68829	5 -25.421894	-13.	04
DIVIDIVA	SDD	-331.246009	0.097907	-331.148102	-305.68829	5 -25.441871	-11.	25
mPW1PW91	Lim et al.	-331.251568	0.097738	-331.153830	-305.68829	5 -25.445939	-12.	30
•						Average value:	-12.	20
Theory	Basis sot Ba	F	F	$F[R_{a}(H, O)]$	F[(H, O)]	$1 F[B_{\alpha}]$		F
Theory	Dasis set Da	220 (127(0	E ZPE	<i>E</i> [<i>Du</i> (<i>H</i> ₂ <i>O</i>) ₄]	205.1720	$\frac{1}{10} \frac{1}{10} \frac{1}{10} $	1/	2 1 1
	Bausch. <i>et al.</i>	-330.612/60	0.097733	-330.515027	-305.1720	60 -25.322073	-1.	5.11
CCSD(T.Full)	SDD	-330.531946	0.09/90/	-330.434039	-305.1720	60 -25.258984	-1	.88
005D(1,1 ull)	Lim et al.	-330.670762	0.097738	-330.573024	-305.1720	60 -25.378212	-14	1.28
						Average value:	-9	.76
Theory	Rasis set Ra	E	E	E	ra			
Theory	Dusis set Du	\boldsymbol{L}_0	$\boldsymbol{L}_{\text{ZPE}}$	L_a	E ZPE	E_{v}	IE _ν	IE_a
	Bausch. <i>et al</i> .	-331.228696	<i>L</i> _{ZPE} 0.097733	-331.087648	<u>е</u> _{ZPE} 0.099707	<i>E_v</i> -331.083043	1Ε _ν 4.02	IE _a 3.89
DW/1 DW/01	Bausch. <i>et al.</i> SDD	-331.228696 -331.246009	Е _{ZPE} 0.097733 0.097907	-331.087648 -331.104869	<u>е _{ZPE}</u> 0.099707 0.099707	<i>E_v</i> -331.083043 -331.100016	1E _ν 4.02 4.02	IE _a 3.89 3.89
mPW1PW91	Bausch. <i>et al.</i> SDD Lim <i>et al.</i>	-331.228696 -331.246009 -331.251568	EZPE 0.097733 0.097907 0.097738	<i>E_a</i> -331.087648 -331.104869 -331.110105	<u>Е _{ZPE}</u> 0.099707 0.099707 0.099687	<i>E_v</i> -331.083043 -331.100016 -331.105368	$ 1E_{\nu} 4.02 4.02 4.03 $	IE _a 3.89 3.89 3.90
<i>m</i> PW1PW91	Bausch. <i>et al.</i> SDD Lim <i>et al.</i>	-331.228696 -331.246009 -331.251568	<i>E</i> _{ZPE} 0.097733 0.097907 0.097738	<i>E_a</i> -331.087648 -331.104869 -331.110105	<u>E zpe</u> 0.099707 0.099707 0.099687 <u>Av</u>	<i>E_v</i> -331.083043 -331.100016 -331.105368 erage value:	$ 1E_{\nu} 4.02 4.02 4.03 4.02 4.02 4.02 4.02 $	IE _a 3.89 3.89 3.90 3.89
<i>m</i> PW1PW91	Bausch. <i>et al.</i> SDD Lim <i>et al.</i>	-331.228696 -331.246009 -331.251568	<i>E</i> _{ZPE} 0.097733 0.097907 0.097738	<i>L_a</i> -331.087648 -331.104869 -331.110105	<u>Е zpe</u> 0.099707 0.099707 0.099687 Ау	<i>E_v</i> -331.083043 -331.100016 -331.105368 rerage value:	IE _ν 4.02 4.02 4.03 4.02	IE _a 3.89 3.89 3.90 3.89
mPW1PW91	Bausch. <i>et al.</i> SDD Lim <i>et al.</i> Basis set Ba	<i>E</i> ₀ -331.228696 -331.246009 -331.251568 <i>E</i> ₀	<i>E</i> _{ZPE} 0.097733 0.097907 0.097738 <i>E</i> _{ZPE}	<i>E_a</i> -331.087648 -331.104869 -331.110105 <i>E_a</i>	<u>Е zpe</u> 0.099707 0.099707 0.099687 <u>А</u> у	<i>E_v</i> -331.083043 -331.100016 -331.105368 rerage value: <i>E_v</i>	$ \frac{1E_{\nu}}{4.02} \\ 4.02 \\ 4.03 \\ 4.02 \\ IE_{\nu} $	IE _a 3.89 3.89 3.90 3.89 IE _a
mPW1PW91 Theory	Bausch. <i>et al.</i> SDD Lim <i>et al.</i> Basis set Ba Bausch. <i>et al.</i>	<i>E</i> ₀ -331.228696 -331.246009 -331.251568 <i>E</i> ₀ -330.612760	<i>Е</i> _{ZPE} 0.097733 0.097907 0.097738 <i>Е</i> _{ZPE} 0.097733	<i>E_a</i> -331.087648 -331.104869 -331.110105 <i>E_a</i> -330.469647	<u>Е гре</u> 0.099707 0.099707 0.099687 <u>А</u> у <u>Е^{<i>a</i>}гре</u> 0.099707	<i>E_ν</i> -331.083043 -331.100016 -331.105368 rerage value: <i>E_ν</i> -330.463626	$\frac{\text{IE}_{\nu}}{4.02}$ $\frac{4.02}{4.03}$ $\frac{4.03}{4.02}$ $\overline{\text{IE}_{\nu}}$ 4.11	IE _a 3.89 3.89 3.90 3.89 3.89 IE _a 3.95
mPW1PW91 Theory CCSD/T Enilly	Bausch. et al. SDD Lim et al. Basis set Ba Bausch. et al. SDD	<i>E</i> ₀ -331.228696 -331.246009 -331.251568 <i>E</i> ₀ -330.612760 -330.531946	<i>Е</i> _{ZPE} 0.097733 0.097907 0.097738 <i>Е</i> _{ZPE} 0.097733 0.097907	<i>E_a</i> -331.087648 -331.104869 -331.110105 <i>E_a</i> -330.469647 -330.390560	<u>Е гре</u> 0.099707 0.099707 0.099687 <u>Ау</u> <u>Е^{<i>a</i>}гре</u> 0.099707 0.099707	<i>E_ν</i> -331.083043 -331.100016 -331.105368 rerage value: <i>E_ν</i> -330.463626 -330.384611	$ \begin{array}{r} IE_{\nu} \\ 4.02 \\ 4.03 \\ 4.03 \\ 4.02 \\ IE_{\nu} \\ 4.11 \\ 4.06 \\ \end{array} $	IE _a 3.89 3.89 3.90 3.89 IE _a 3.95 3.90
mPW1PW91 Theory CCSD(T,Full)	Bausch. et al. SDD Lim et al. Basis set Ba Bausch. et al. SDD Lim et al.	<i>E</i> ⁰ -331.228696 -331.246009 -331.251568 <i>E</i> ⁰ -330.612760 -330.531946 -330.670762	EZPE 0.097733 0.097907 0.097738 EZPE 0.097733 0.097733 0.097733 0.097733 0.097733	<i>E_a</i> -331.087648 -331.104869 -331.110105 <i>E_a</i> -330.469647 -330.390560 -330,527619	<u>Е гре</u> 0.099707 0.099707 0.099687 <u>Ач</u> 0.099707 0.099707 0.099707	E_{ν} -331.083043 -331.100016 -331.105368 rerage value: E_{ν} -330.463626 -330.384611 -330.521251	$\frac{\text{IE}_{\nu}}{4.02}$ 4.02 4.03 4.02 $\overline{\text{IE}_{\nu}}$ 4.11 4.06 4.12	IE _a 3.89 3.89 3.90 3.89 3.89 3.89 IE _a 3.95 3.90 3.95

Ba(H₂O)₄: Isomer (1+2+1)

Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	E[Ba]	ΔI	E
	Bausch. et al.	-331.226797	0.098123	-331.128674	-305.688295	5 -25.421894	-11.	60
DIVIDUU	SDD	-331.244948	0.098326	-331.146622	-305.688295	5 -25.441871	-10.	33
mPW1PW91	Lim et al.	-331.250131	0.098165	-331.151966	-305.688295	5 -25.445939	-11.	13
					1	Average value:	-11.	02
	D 1 / D							-
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	E[Ba]	Δ	E
	Bausch. et al.	-330.609833	0.098123	-330.511710	-305.1720	60 -25.322073	-11	1.03
CCSD(T Full)	SDD	-330.529795	0.098326	-330.431469	-305.1720	60 -25.258984	-0	.27
CCSD(1,Full)	Lim et al.	-330.666853	0.098165	-330.568688	-305.1720	60 -25.378212	-11	1.56
						Average value:	-7	.62
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	E_a	$E^a{}_{ m ZPE}$	E_v	IE _ν	IEa
	Bausch. et al.	-331.226797	0.098123	-331.083506	0.098530	-331.069665	4.29	3.91
	SDD	-331.244948	0.098326	-331.101302	0.098654	-331.087650	4.29	3.92
<i>mr</i> w 1r w 91	Lim et al.	-331.250131	0.098165	-331.106221	0.098553	-331.092231	4.31	3.93
					Av	erage value:	4.29	3.92
Theory	Basis set Ba	E_0	EZPE	Ea	$E^{a}_{7\rm PF}$	E_{v}	IE,	IE,
	Bausch, et al.	-330,609833	0.098123	-330.463824	0.098530	-330,448997	4.39	3.98
	SDD	-330.529795	0.098326	-330.386147	0.098654	-330.372046	4.30	3.92
CCSD(T,Full)	Lim et al.	-330.666853	0.098165	-330,520200	0.098553	-330.505260	4.41	4.00
					А	verage value:	4,37	3.97

Supplementary file

Ba(H₂O)₄: Isomer (1+1+1+1)

		F	T					
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	E[Ba]	ΔΙ	5
	Bausch. et al.	-331.229827	0.098272	-331.131555	-305.68829	5 -25.421894	-13.	41
DW/1DW/01	SDD	-331.247955	0.098466	-331.149489	-305.68829	5 -25.441871	-12.	13
mPw1Pw91	Lim et al.	-331.253093	0.098241	-331.154852	-305.68829	5 -25.445939	-12.	94
						Average value:	-12.	82
Theory	Basis set Ba	E_0	$E_{\rm ZPE}$	$E[Ba(H_2O)_4]$	$E[(H_2O)]$	E[Ba]	Δ	E
	Bausch. et al.	-330.612015	0.098272	-330.513743	-305.1720	60 -25.322073	-12	2.31
	SDD	-330.532068	0.098466	-330.433602	-305.1720	60 -25.258984	-1	.61
CCSD(T,Full)	Lim et al.	-330.668715	0.098241	-330.570474	-305.1720	60 -25.378212	-12	2.68
						Average value:	-8	.86
Theory	Basis set Ba	E	Ezpe	E	E^{a}_{TPF}	E.	IE.	IE.
Theory	Basis set Ba Bausch, <i>et al.</i>	<i>E</i> ₀ -331,229827	<i>Е</i> _{ZPE} 0.098272	E_a -331.080818	$\frac{E^a_{ZPE}}{0.098474}$	E_{ν} -331.067843	IE _v 4.41	IE _a 4.06
Theory	Basis set Ba Bausch. <i>et al.</i> SDD	<i>E</i> ₀ -331.229827 -331.247955	<i>E</i> _{ZPE} 0.098272 0.098466	<i>E_a</i> -331.080818 -331.098643	<i>E^a_{ZPE}</i> 0.098474 0.098642	<i>E_v</i> -331.067843 -331.085296	ΙΕ _ν 4.41 4.43	IE _a 4.06 4.07
Theory mPW1PW91	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i>	<i>E</i> ₀ -331.229827 -331.247955 -331.253093	<i>E</i> _{ZPE} 0.098272 0.098466 0.098241	<i>E_a</i> -331.080818 -331.098643 -331.103501	E^{a}_{ZPE} 0.098474 0.098642 0.098452	<i>E_v</i> -331.067843 -331.085296 -331.090110	IE _ν 4.41 4.43 4.44	IE _a 4.06 4.07 4.08
Theory mPW1PW91	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al</i> .	<i>E</i> ₀ -331.229827 -331.247955 -331.253093	<i>E</i> _{ZPE} 0.098272 0.098466 0.098241	<i>E_a</i> -331.080818 -331.098643 -331.103501	<i>E^a_{ZPE}</i> 0.098474 0.098642 0.098452	<i>E_v</i> -331.067843 -331.085296 -331.090110 verage value:	IE _ν 4.41 4.43 4.44 4.43	IE _a 4.06 4.07 4.08 4.07
Theory mPW1PW91	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i>	<i>E</i> ₀ -331.229827 -331.247955 -331.253093	<i>E</i> _{ZPE} 0.098272 0.098466 0.098241	<i>E_a</i> -331.080818 -331.098643 -331.103501	E ^a _{ZPE} 0.098474 0.098642 0.098452 Au	<i>E_v</i> -331.067843 -331.085296 -331.090110 /erage value:	IE _ν 4.41 4.43 4.44 4.43	IE _a 4.06 4.07 4.08 4.07
Theory mPW1PW91 Theory	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i> Basis set Ba	E ₀ -331.229827 -331.247955 -331.253093 E ₀	<i>Е</i> _{ZPE} 0.098272 0.098466 0.098241 <i>Е</i> _{ZPE}	<i>E_a</i> -331.080818 -331.098643 -331.103501 <i>E_a</i>	$\frac{E^{a}_{ZPE}}{0.098474}$ 0.098642 0.098452 Av E^{a}_{ZPE}	<i>E_v</i> -331.067843 -331.085296 -331.090110 /erage value: <i>E_v</i>	IE _ν 4.41 4.43 4.44 4.43 IE _ν	IE _a 4.06 4.07 4.08 4.07 IE _a
Theory mPW1PW91 Theory	Basis set Ba Bausch. <i>et al.</i> SDD Lim <i>et al.</i> Basis set Ba Bausch. <i>et al.</i>	<i>E</i> ₀ -331.229827 -331.247955 -331.253093 <i>E</i> ₀ -330.612015	<i>Е</i> _{ZPE} 0.098272 0.098466 0.098241 <i>Е</i> _{ZPE} 0.098272	<i>E_a</i> -331.080818 -331.098643 -331.103501 <i>E_a</i> -330.459614	$\frac{E^{a}_{ZPE}}{0.098474}$ 0.098642 0.098452 Au E^{a}_{ZPE} 0.098474	<i>E_v</i> -331.067843 -331.085296 -331.090110 /erage value: <i>E_v</i> -330.446258	$ IE_{\nu} 4.41 4.43 4.44 4.43 IIE_{\nu} 4.52 $	IE _a 4.06 4.07 4.08 4.07 IE _a 4.15
Theory mPW1PW91 Theory	Basis set Ba Bausch. et al. SDD Lim et al. Basis set Ba Bausch. et al. SDD	<i>E</i> ₀ -331.229827 -331.247955 -331.253093 <i>E</i> ₀ -330.612015 -330.532068	<i>Е</i> _{ZPE} 0.098272 0.098466 0.098241 <i>Е</i> _{ZPE} 0.098272 0.098466	<i>E_a</i> -331.080818 -331.098643 -331.103501 <i>E_a</i> -330.459614 -330.382364	$\frac{E^{a}_{ZPE}}{0.098474}$ 0.098642 0.098452 Au E^{a}_{ZPE} 0.098474 0.098474 0.098642	<i>E_v</i> -331.067843 -331.085296 -331.090110 /erage value: <i>E_v</i> -330.446258 -330.369215	$ IE_{\nu} 4.41 4.43 4.44 4.43 IIE_{\nu} 4.52 4.44 $	IE _a 4.06 4.07 4.08 4.07 IE _a 4.15 4.08
Theory mPW1PW91 Theory CCSD(T,Full)	Basis set Ba Bausch. et al. SDD Lim et al. Basis set Ba Bausch. et al. SDD Lim et al.	E ₀ -331.229827 -331.247955 -331.253093 E ₀ -330.612015 -330.532068 -330.668715	EzPE 0.098272 0.098466 0.098241 EzPE 0.098272 0.098466 0.098241	<i>E_a</i> -331.080818 -331.098643 -331.103501 <i>E_a</i> -330.459614 -330.382364 -330,515888	$\frac{E^{a}_{ZPE}}{0.098474}$ 0.098642 0.098452 $\frac{E^{a}_{ZPE}}{0.098474}$ 0.098474 0.098642 0.098452	E _v -331.067843 -331.085296 -331.090110 /erage value: E _v -330.446258 -330.369215 -330.501893	$\frac{IE_{\nu}}{4.41}$ 4.43 4.44 4.43 $\overline{IE_{\nu}}$ 4.52 4.44 4.55	IE _a 4.06 4.07 4.08 4.07 IE _a 4.15 4.08 4.16

Neutral barium-water clusters:

Ba⁺(**H**₂**O**)₁: Isomer 1^+

Theory	Basis set Ba	E_a	$E^{a}_{ m ZPE}$	$E [Ba^+(H_2O)_1]$	$E[(H_2O)_1]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-101.710805	0.023623	-101.687182	-76.413183	-25.236026	-23.83
	SDD	-101.728590	0.023746	-101.704844	-76.413183	-25.255232	-22.86
mPW1PW91	Lim et al.	-101.733396	0.023608	-101.709788	-76.413183	-25.258481	-23.92
-					Ave	erage value:	-23.54
Theory	Basis set Ba	E_a	$E^a_{\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ $	$E [Ba^+(H_2O)_1]$	$E[(H_2O)_1]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-101.477839	0.023623	-101.454216	-76.284245	-25.133532	-22.87
	SDD	-101.401429	0.023746	-101.377683	-76.284245	-25.073281	-12.65
CCSD(1,Full)	Lim et al.	-101.533780	0.023608	-101.510172	-76.284245	-25.187920	-23.85
					A	verage value:	-19.79

Ba⁺(H₂O)₂: Isomer $(2+\theta)^+$

Theory	Basis set Ba	E_a	$E^a_{\rm ZPE}$	$E[Ba^+(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-178.181194	0.047583	-178.133611	-152.831962	-25.236026	-41.18
	SDD	-178.199286	0.047775	-178.151511	-152.831962	-25.255232	-40.36
mrw1rw91	Lim et al.	-178.203782	0.047550	-178.156232	-152.831962	-25.258481	-41.28
					Av	erage value:	-40.94
Theory	Basis set Ba	E_a	$E^a_{\ m ZPE}$	$E [Ba^+(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-177.818834	0.047583	-177.771251	-152.574371	-25.133532	-39.75
	SDD	-177.740975	0.047775	-177.693200	-152.574371	-25.073281	-28.58
CCSD(1,Full)	Lim et al.	-177.875773	0.047550	-177.828223	-152.574371	-25.187920	-41.37
					A	verage value:	-36.57

Ba⁺(H₂O)₂: Isomer (1+1)⁺

Theory	Basis set Ba	E_a	$E^a_{ ext{ZPE}}$	$E[Ba^+(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-178.172484	0.048990	-178.123494	-152.831962	-25.236026	-34.83
	SDD	-178.190300	0.049047	-178.141253	-152.831962	-25.255232	-33.92
mPW1PW91	Lim et al.	-178.195104	0.048972	-178.146132	-152.831962	-25.258481	-34.95
					Av	erage value:	-34.57
Theory	Basis set Ba	E_a	$E^{a}_{ m ZPE}$	$E^{Ba^+}(H_2O)_2$]	$E[(H_2O)_2]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-177.810139	0.048990	-177.761149	-152.574371	-25.133532	-33.41
CCCD/T EII)	SDD	-177.733171	0.049047	-177.684124	-152.574371	-25.073281	-22.89
CCSD(1,Full)	Lim et al.	-177.866257	0.048972	-177.817285	-152.574371	-25.187920	-34.51
					A	verage value:	-30.27

Ba⁺(**H**₂**O**)₃: Isomer $(3+\theta)^+$

Theory	Basis set Ba	E_a	$E^a_{ ext{ZPE}}$	$E [Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-254.647647	0.071256	-254.576391	-229.258051	-25.236026	-51.65
D11/1 D11/01	SDD	-254.666178	0.071554	-254.594624	-229.258051	-25.255232	-51.04
mPW1PW91	Lim et al.	-254.670312	0.071253	-254.599059	-229.258051	-25.258481	-51.79
					Ave	erage value:	-51.49
Theory	Basis set Ba	E_a	$E^a{}_{ m ZPE}$	$E [Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-254.156681	0.071256	-254.085425	-228.871337	-25.133532	-50.55
	SDD	-254.077773	0.071554	-254.006219	-228.871337	-25.073281	-38.65
CCSD(1,Full)	Lim et al.	-254.214468	0.071253	-254.143215	-228.871337	-25.187920	-52.68
					A	verage value:	-47.30

Ba⁺(H₂O)₃: Isomer (2+1)⁺

Theory	Basis set Ba	E_a	$E^a_{\rm ZPE}$	$E [Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-254.639968	0.074516	-254.565452	-229.258051	-25.236026	-44.79
	SDD	-254.658154	0.074790	-254.583364	-229.258051	-25.255232	-43.98
mrw1rw91	Lim et al.	-254.662580	0.074535	-254.588045	-229.258051	-25.258481	-44.88
					Ave	erage value:	-44.55
Theory	Basis set Ba	E_a	$E^a_{ ext{ZPE}}$	$E [Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-254.151178	0.074516	-254.076662	-228.871337	-25.133532	-45.05
	SDD	-254.073139	0.074790	-253.998349	-228.871337	-25.073281	-33.72
CCSD(1,Full)	Lim et al.	-254.208109	0.074535	-254.133574	-228.871337	-25.187920	-46.63
					A	verage value:	-41.80

Ba⁺(**H**₂**O**)₃: Isomer (1+1+1)⁺

Theory	Basis set Ba	E_a	$E^a_{\rm ZPE}$	$E [Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-254.628024	0.073661	-254.554363	-229.258051	-25.236026	-37.83
	SDD	-254.645922	0.073851	-254.572071	-229.258051	-25.255232	-36.89
<i>mrw</i> 1 <i>rw</i> 91	Lim et al.	-254.650715	0.073699	-254.577016	-229.258051	-25.258481	-37.95
					Av	-37.56	
Theory	Basis set Ba	E_a	$E^{a}{}_{ m ZPE}$	$E [Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-254.136138	0.073661	-254.062477	-228.871337	-25.133532	-36.15
	SDD	-254.059150	0.073851	-253.985299	-228.871337	-25.073281	-25.53
CCSD(1,Full)	Lim et al.	-254.192495	0.073699	-254.118796	-228.871337	-25.187920	-37.36
					A	-33.01	

Ba⁺(H₂O)₄: Isomer $(4+\theta)^+$

Theory	Basis set Ba	E_a	$E^{a}_{ m ZPE}$	$E [Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-331.107980	0.094301	-331.013679	-305.688295	-25.236026	-56.07
	SDD	-331.126638	0.094529	-331.032109	-305.688295	-25.255232	-55.59
mPw1Pw91	Lim et al.	-331.130648	0.094304	-331.036344	-305.688295	-25.258481	-56.20
					Ave	-55.95	
Theory	Basis set Ba	E_a	$E^{a}_{ m ZPE}$	$E [Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-330.490068	0.094301	-330.395767	-305.172060	-25.133532	-56.59
	SDD	-330.412556	0.094529	-330.318027	-305.172060	-25.073281	-45.61
CCSD(1,Full)	Lim et al.	-330,549527	0.094304	-330,455223	-305.172060	-25.187920	-59.77
					A	verage value:	-53.99

Ba⁺(**H**₂**O**)₄: Isomer $(3+1)_a^+$

Theory	Basis set Ba	E_a	$E^a_{ ext{ZPE}}$	$E [Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE		
	Bausch. et al.	-331.104664	0.095992	-331.008672	-305.688295	-25.236026	-52.93		
DW/1DW/01	SDD	-331.123153	0.096374	-331.026779	-305.688295	-25.255232	-52.24		
mP w IP w 91	Lim et al.	-331.127276	0.096055	-331.031221	-305.688295	-25.258481	-52.99		
					Av	Average value:			
Theory	Basis set Ba	E_a	$E^a_{ ext{ZPE}}$	$E [Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE		
	Bausch. et al.	-330.484941	0.095992	-330.388949	-305.172060	-25.133532	-52.31		
	SDD	-330.405811	0.096374	-330.309437	-305.172060	-25.073281	-40.22		
CCSD(1,Full)	Lim et al.	-330,542696	0.096055	-330,446641	-305.172060	-25.187920	-54,38		
					A	verage value:	-48,97		

Supplementary file

Ba⁺(**H**₂**O**)₄: Isomer $(3+1)_b^+$

Theory	Basis set Ba	E_a	$E^a_{ m ZPE}$	<i>E`</i> [<i>B</i>	$a^{+}(H_2O)_4]$	$E[(H_2$	O) ₄]	E[Ba	+]	ΔE	
	Bausch. et al.	-331.105578	0.097963	-33	1.007615	-305.68	38295	-25.236	026	-52.27	
	SDD	-331.124040	0.098176	-33	1.025864	-305.68	38295	-25.255	232	-51.67	
mrw1rw91	Lim et al.	-331.128157	0.097947	-33	1.030210	-305.68	38295	-25.258	481	-52.36	_
							Av	erage va	lue:	-52.10	-
Theory	Basis set Ba	E_a	E^{a}	ZPE	E^{Ba^+}	$[I_2O)_4]$	E[(H	$[_{2}O)_{4}]$	E[Ba	a ⁺]	ΔE
	Bausch. et al.	-330.48888	38 0.09	7963	-330.39	0925	-305.1	72060	-25.13	3532	-53.55
	SDD	-330.41061	9 0.09	8176	-330.31	2443	-305.1	72060	-25.07	3281	-42.11
CCSD(T,Full)	Lim et al.	-330,5468	817 0.09	7947	-330,44	8870	-305.1	72060	-25.18	7920	-55.78
								Av	erage va	alue:	-50.48

Ba⁺(**H**₂**O**)₄: Isomer $(2+2)_a^+$

Theory	Basis set Ba	E_a	$E^{a}_{ m ZPE}$	$E [Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-331.098052	0.097715	-331.000337	-305.688295	-25.236026	-47.70
	SDD	-331.116183	0.097907	-331.018276	-305.688295	-25.255232	-46.91
mr wirw91	Lim et al.	-331.120654	0.097764	-331.022890	-305.688295	-25.258481	-47.76
					Average value:		-47.46
Theory	Basis set Ba	E_a	$E^{a}_{ m ZPE}$	$E [Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-330.478809	0.097715	-330.381094	-305.172060	-25.133532	-47.38
	SDD	-330.400879	0.097907	-330.302972	-305.172060	-25.073281	-36.16
CCSD(1,Full)	Lim et al.	-330,536113	0.097764	-330,438349	-305.172060	-25.187920	-49,18
					A	-44,24	

Ba⁺(**H**₂**O**)₄: Isomer $(2+2)_b^+$

Bausch. et al. -331.087648 0.099707 -330.987941 -305.688295 -25.236026 -39. SDD -331.104869 0.099707 -331.005162 -305.688295 -25.255232 -38. Lim et al. -331.110105 0.099687 -331.010418 -305.688295 -25.258481 -39. Average value: -39. -39. -39. -39. -39. -39.).92 3.68).94).51
SDD -331.104869 0.099707 -331.005162 -305.688295 -25.255232 -38. mPW1PW91 Lim et al. -331.110105 0.099687 -331.010418 -305.688295 -25.258481 -39. Average value: -39.	8.68 9.94 9.51
Important Lim et al. -331.110105 0.099687 -331.010418 -305.688295 -25.258481 -39. Average value: -39.).94).51
Average value: -39.	9.51
Theory Basis set Ba E_a E^a_{ZPE} $E[Ba^+(H_2O)_4]$ $E[(H_2O)_4]$ $E[Ba^+]$	ΔΕ
Bausch. et al330.469647 0.099707 -330.369940 -305.172060 -25.133532 -44	10.38
SDD -330.390560 0.099707 -330.290853 -305.172060 -25.073281 -24	28.56
Lim et al330,527619 0.099687 -330,427932 -305.172060 -25.187920 -4	12,64
Average value: -3'	37,19

Ba⁺(H₂O)₄: Isomer (1+2+1)⁺

Theory	Basis set Ba	E_a	$E^a_{\rm ZPE}$	$E [Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-331.083506	0.098530	-330.984976	-305.688295	-25.236026	-38.06
	SDD	-331.101302	0.098654	-331.002648	-305.688295	-25.255232	-37.10
mPw1Pw91	Lim et al.	-331.106221	0.098553	-331.007668	-305.688295	-25.258481	-38.21
•					Av	-37.79	
Theory	Basis set Ba	E_a	$E^{a}{}_{ m ZPE}$	$E [Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-330.463824	0.098530	-330.365294	-305.172060	-25.133532	-37.46
	SDD	-330.386147	0.098654	-330.287493	-305.172060	-25.073281	-26.45
CCSD(1,Full)	Lim et al.	-330,520200	0.098553	-330,421647	-305.172060	-25.187920	-38.70
					A	-34.20	

Supplementary file

Ba⁺(**H**₂**O**)₄: Isomer $(1+1+1+1)^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E [Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-331.080818	0.098474	-330.982344	-305.688295	-25.236026	-36.41
DW1DW01	SDD	-331.098643	0.098642	-331.000001	-305.688295	-25.255232	-35.44
<i>mP</i> w1P w91	Lim et al.	-331.103501	0.098452	-331.005049	-305.688295	-25.258481	-36.57
					Av	erage value:	-36.14
Theory	Basis set Ba	E_a	$E^a_{\rm ZPE}$	$E [Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
	Bausch. et al.	-330.459614	0.098474	-330.361140	-305.172060	-25.133532	-34.86
	SDD	-330.382364	0.098642	-330.283722	-305.172060	-25.073281	-24.08
CCSD(1,Full)	Lim et al.	-330,515888	0.098452	-330,417436	-305.172060	-25.187920	-36.05
					A	-31.67	

Comparison of different RECP's used for the Ba atom:

