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:

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

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:

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

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_0**	E_{ion}**	IE$_v$**
Ba(H_2O)$_1$	*m*PW1PW91	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**
		6-311++G(d,p)	-101.898964	-101.733282	**4.51**
		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_0**	E_{ion}**	IE$_v$**
Ba(H_2O)$_4$ isomer *(4+0)$_a$*	*m*PW1PW91	6-31G	-331.044265	-330.905847	**3.77**
		6-311G(d)	-331.206237	-331.066652	**3.80**
		6-311G(d,p)	-331.251312	-331.111796	**3.80**
		6-311+G(d,p)	-331.261613	-331.120371	**3.84**
		6-311++G(d,p)	-331.261792	-331.120513	**3.84**
		6-311++G(2d,p)	-331.262055	-331.120854	**3.84**
		6-311++G(3d,p)	-331.264722	-331.123689	**3.84**
		6-311++G(3df,p)	-331.267741	-331.126725	**3.84**
		6-311++G(3df,3pd)	-331.276145	-331.135130	**3.84**
		AUG-cc-PVQZ	-305.835932	-331.164604	**3.83**

* 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	$E_{neutral}$	$E_{ion(+1)}$	IE
Ba	*m*PW1PW91	Bausch. *et al.*	-25.421894	-25.236026	5.06
		SDD	-25.441871	-25.255232	5.08
		Lim *et al.*	-25.445940	-25.258481	5.10
				Experimental value:	5.21

Specie	Theory	RECP	$E_{neutral}$	$E_{ion(+1)}$	IE
Ba	CCSD(T,Full)	Bausch. *et al.*	-25.322073	-25.133532	5.13
		SDD	-25.258984	-25.073281	5.05
		Lim *et al.*	-25.378212	-25.187920	5.18
				Experimental value:	5.21

Specie	Theory	RECP	$E_{ion(+1)}$	$E_{ion(+2)}$	IE
Ba^+	*m*PW1PW91	Bausch. *Et al.*	-25.236026	-24.871354	9.92
		SDD	-25.255232	-24.890441	9.93
		Lim *et al.*	-25.258481	-24.891405	9.99
				Experimental value:	10.00

Specie	Theory	RECP	$E_{ion(+1)}$	$E_{ion(+2)}$	IE
Ba^+	CCSD(T,Full)	Bausch. *et al.*	-25.133532	-24.771889	9.84
		SDD	-25.073281	-24.715209	9.74
		Lim *et al.*	-25.187920	-24.821722	9.96
				Experimental value:	10.00

Specie*	Theory	RECP	E_0**	E_{ion}**	IE_v**
BaO	*m*PW1PW91	Bausch. *et al.*	-100.704981	-100.462628	6.59
		SDD	-100.721548	-100.481590	6.53
		Lim *et al.*	-100.725587	-100.484259	6.57
				Experimental value:	6.91

Specie*	Theory	RECP	E_0**	E_{ion}**	IE_v**
BaO	CCSD(T,Full)	Bausch. *et al.*	-100.551570	-100.305016	6.71
		SDD	-100.478041	-100.237409	6.55
		Lim *et al.*	-100.603934	-100.354486	6.79
				Experimental value:	6.91

* 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:

$(H_2O)_2$:

Theory	$E_0[(H_2O)_2]$	E_{ZPE}	$E[(H_2O)_2]$	$E_0[(H_2O)_1]$	E_{ZPE}	$E[(H_2O)_1]$	D_e	D_0	$D_0/1$
***m*PW1PW91**	-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_{ZPE}	$E[(H_2O)_2]$	$E_0[(H_2O)_1]$	E_{ZPE}	$E[(H_2O)_1]$	D_e	D_0	$D_0/1$
CCSD(T,Full)	-152.621294	0.046923	-152.574371	-76.305850	0.021605	-76.284245	**-6.02**	**-3.69**	**-3.69**

$(H_2O)_3$:

Theory	$E_0[(H_2O)_3]$	E_{ZPE}	$E[(H_2O)_3]$	$E[(H_2O)_2]$	$E[(H_2O)_1]$	D_e	D_0	$D_0/2$
***m*PW1PW91**	-229.332098	0.074047	-229.258051	-152.831962	-76.413183	**-11.56**	**-8.10**	**-4.05**

Theory	$E_0[(H_2O)_3]$	E_{ZPE}	$E[(H_2O)_3]$	$E[(H_2O)_2]$	$E[(H_2O)_1]$	D_e	D_0	$D_0/2$
CCSD(T,Full)	-228.945384	0.074047	-228. 871337	-152.574371	-76.284245	**-11.45**	**-7.98**	**-3.99**

$(H_2O)_4$:

Theory	$E_0[(H_2O)_4]$	E_{ZPE}	$E[(H_2O)_4]$	$E[(H_2O)_3]$	$E[(H_2O)_1]$	D_e	D_0	$D_0/2$
***m*PW1PW91**	-305.788599	0.100305	-305.688295	-229.258051	-76.413183	**-13.63**	**-10.71**	**-5.35**

Theory	$E_0[(H_2O)_4]$	E_{ZPE}	$E[(H_2O)_4]$	$E[(H_2O)_3]$	$E[(H_2O)_1]$	D_e	D_0	$D_0/2$
CCSD(T,Full)	-305.272365	0.100305	-305.172060	-228. 871337	-76.284245	**-13.26**	**-10.34**	**-5.17**

Neutral barium-water clusters:

$Ba(H_2O)_1$: Isomer *1*

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_1]$	$E[(H_2O)_1]$	$E[Ba]$	ΔE	$\Delta_r G^{75K}$
*m*PW1PW91	Bausch. *et al.*	-101.875384	0.022055	-101.853329	-76.413183	-25.421894	**-11.45**	**-10.67**
	SDD	-101.893920	0.022340	-101.871580	-76.413183	-25.441871	**-10.37**	**-9.52**
	Lim *et al.*	-101.898964	0.022009	-101.876955	-76.413183	-25.445940	**-11.19**	**-10.45**
						Average value:	**-11.00**	**-10.21**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_1]$	$E[(H_2O)_1]$	$E[Ba]$	ΔE	$\Delta_r G^{75K}$
CCSD(T,Full)	Bausch. *et al.*	-101.645290	0.022055	-101.623235	-76.284245	-25.322073	**-10.62**	**-9.83**
	SDD	-101.565826	0.022340	-101.543486	-76.284245	-25.258984	**-0.16**	**0.68**
	Lim *et al.*	-101.702281	0.022009	-101.680272	-76.284245	-25.378212	**-11.18**	**-10.44**
						Average value:	**-7.32**	**-6.53**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	Bausch. *et al.*	-101.875384	0.022055	-101.710805	0.023623	-101.710805	**4.52**	**4.52**
	SDD	-101.893920	0.022340	-101.728590	0.023746	-101.728589	**4.54**	**4.54**
	Lim *et al.*	-101.898964	0.022009	-101.733396	0.023608	-101.733396	**4.55**	**4.55**
						Average value:	**4.54**	**4.54**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	Bausch. *et al.*	-101.645290	0.022055	-101.477839	0.023623	-101.477685	**4.60**	**4.60**
	SDD	-101.565826	0.022340	-101.401429	0.023746	-101.401362	**4.51**	**4.51**
	Lim *et al.*	-101.702281	0.022009	-101.533780	0.023608	-101.533601	**4.63**	**4.63**
						Average value:	**4.58**	**4.58**

$Ba(H_2O)_2$: Isomer *(2+0)$_a$*

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba]$	ΔE	$\Delta_r G^{75K}$
*m*PW1PW91	Bausch. *et al.*	-178.331004	0.045450	-178.285554	-152.831963	-25.421894	**-19.89**	**-18.51**
	SDD	-178.349334	0.045389	-178.303945	-152.831963	-25.441871	**-18.89**	**-17.64**
	Lim *et al.*	-178.354136	0.045449	-178.305910	-152.831963	-25.445939	**-17.58**	**-17.93**
						Average value:	**-18.79**	**-17.98**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba]$	ΔE	$\Delta_r G^{75K}$
CCSD(T,Full)	Bausch. *et al.*	-177.971065	0.045450	-177.925615	-152.574371	-25.322073	**-18.31**	**-17.04**
	SDD	-177.891204	0.045389	-177.845815	-152.574371	-25.258984	**-7.82**	**-6.56**
	Lim *et al.*	-178.029627	0.045449	-177.984178	-152.574371	-25.378212	**-19.83**	**-18.56**
						Average value:	**-15.32**	**-14.05**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	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**
	Lim *et al.*	-178.354136	0.045449	-178.203782	0.047550	-178.200782	**4.15**	**4.07**
						Average value:	**4.18**	**4.12**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	Bausch. *et al.*	-177.971065	0.045450	-177.818834	0.047583	-177.816647	**4.26**	**4.20**
	SDD	-177.891204	0.045389	-177.740975	0.047775	-177.740967	**4.15**	**4.15**
	Lim *et al.*	-178.029627	0.045449	-177.875773	0.047550	-177.874537	**4.28**	**4.24**
						Average value:	**4.23**	**4.20**

$Ba(H_2O)_2$: Isomer *(2+0)$_b$*

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba]$	ΔE	$\Delta_r G^{75K}$
*m*PW1PW91	Bausch. *et al.*	-178.328559	0.046694	-178.281865	-152.831963	-25.421894	**-17.58**	**-16.19**
	SDD	-178.346744	0.046889	-178.299855	-152.831963	-25.441871	**-16.33**	**-14.93**
	Lim *et al.*	-178.351660	0.046672	-178.304988	-152.831963	-25.445939	**-17.00**	**-15.62**
						Average value:	**-16.97**	**-15.58**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba]$	ΔE	$\Delta_r G^{75K}$
CCSD(T,Full)	Bausch. *et al.*	-177.969827	0.046694	-177.923133	-152.574371	-25.322073	**-16.75**	**-15.36**
	SDD	-177.889845	0.046889	-177.842956	-152.574371	-25.258984	**-6.02**	**-4.63**
	Lim *et al.*	-178.027492	0.046672	-177.980820	-152.574371	-25.378212	**-17.72**	**-16.35**
						Average value:	**-13.50**	**-12.11**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	Bausch. *et al.*	-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**
	Lim *et al.*	-178.351660	0.046672	-178.203782	0.047550	-178.196471	**4.25**	**4.05**
						Average value:	**4.24**	**4.04**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	Bausch. *et al.*	-177.969827	0.046694	-177.818834	0.047583	-177.813138	**4.29**	**4.13**
	SDD	-177.889845	0.046889	-177.740975	0.047775	-177.735120	**4.23**	**4.08**
	Lim *et al.*	-178.027492	0.046672	-177.875773	0.047550	-177.869896	**4.31**	**4.15**
						Average value:	**4.28**	**4.12**

$Ba(H_2O)_2$: Isomer *(1+1)*

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba]$	ΔE	$\Delta_r G^{75K}$
*m*PW1PW91	Bausch. *et al.*	-178.326657	0.048027	-178.278630	-152.831963	-25.421894	**-15.55**	**-14.24**
	SDD	-178.344897	0.048226	-178.296671	-152.831963	-25.441871	**-14.33**	**-13.07**
	Lim *et al.*	-178.349990	0.048029	-178.301961	-152.831963	-25.445939	**-15.10**	**-13.84**
						Average value:	**-14.99**	**-13.73**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba]$	ΔE	$\Delta_r G^{75K}$
CCSD(T,Full)	Bausch. *et al.*	-177.967008	0.048027	-177.918981	-152.574371	-25.322073	**-14.14**	**-12.84**
	SDD	-177.887456	0.048226	-177.839230	-152.574371	-25.258984	**-3.69**	**-2.38**
	Lim *et al.*	-178.023989	0.048029	-177.975960	-152.574371	-25.378212	**-14.67**	**-13.37**
						Average value:	**-10.83**	**-9.53**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	Bausch. *et al.*	-178.326657	0.048027	-178.172484	0.048990	-178.166128	**4.39**	**4.22**
	SDD	-178.344897	0.048226	-178.190300	0.049047	-178.183748	**4.41**	**4.23**
	Lim *et al.*	-178.349990	0.048029	-178.195104	0.048972	-178.188478	**4.42**	**4.24**
						Average value:	**4.41**	**4.23**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	Bausch. *et al.*	-177.967008	0.048027	-177.810139	0.048990	-177.803443	**4.48**	**4.29**
	SDD	-177.887456	0.048226	-177.733171	0.049047	-177.726796	**4.39**	**4.22**
	Lim *et al.*	-178.023989	0.048029	-177.866257	0.048972	-177.859389	**4.50**	**4.32**
						Average value:	**4.46**	**4.28**

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
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$Ba(H_2O)_3$: Isomer $(3+0)_a$

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba]$	ΔE
*m*PW1PW91	**Bausch. *et al.***	-254.784611	0.069870	-254.714741	-229.258051	-25.421894	**-21.83**
	SDD	-254.802565	0.069914	-254.732651	-229.258051	-25.441871	**-20.54**
	Lim *et al.*	-254.807362	0.069875	-254.737487	-229.258051	-25.445939	**-21.02**
						Average value:	**-21.13**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba]$	ΔE
CCSD(T,Full)	**Bausch. *et al.***	-254.296516	0.069870	-254.226646	-228.871337	-25.322073	**-20.86**
	SDD	-254.216262	0.069914	-254.146348	-228.871337	-25.258984	**-10.06**
	Lim *et al.*	-254.355763	0.069875	-254.285888	-228.871337	-25.378212	**-22.80**
						Average value:	**-17.91**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	**Bausch. *et al.***	-254.784611	0.069870	-254.647647	0.071256	-254.637794	**4.03**	**3.76**
	SDD	-254.802565	0.069914	-254.666178	0.071554	-254.657215	**4.00**	**3.76**
	Lim *et al.*	-254.807362	0.069875	-254.670312	0.071253	-254.660438	**4.04**	**3.77**
						Average value:	**4.02**	**3.76**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	**Bausch. *et al.***	-254.296516	0.069870	-254.156681	0.071256	-254.148800	**4.06**	**3.84**
	SDD	-254.216262	0.069914	-254.077773	0.071554	-254.071725	**3.98**	**3.81**
	Lim *et al.*	-254.355763	0.069875	-254.214468	0.071253	-254.207698	**4.07**	**3.88**
						Average value:	**4.03**	**3.85**

$Ba(H_2O)_3$: Isomer $(3+0)_b$

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba]$	ΔE
*m*PW1PW91	**Bausch. *et al.***	-254.780616	0.071704	-254.708912	-229.258051	-25.421894	**-18.18**
	SDD	-254.798529	0.071965	-254.726564	-229.258051	-25.441871	**-16.72**
	Lim *et al.*	-254.803367	0.071576	-254.731791	-229.258051	-25.445939	**-17.45**
						Average value:	**-17.45**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba]$	ΔE
CCSD(T,Full)	**Bausch. *et al.***	-254.295339	0.071704	-254.223635	-228.871337	-25.322073	**-18.97**
	SDD	-254.215329	0.071965	-254.143364	-228.871337	-25.258984	**-8.18**
	Lim *et al.*	-254.354288	0.071576	-254.282712	-228.871337	-25.378212	**-20.81**
						Average value:	**-15.99**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	**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**
	Lim *et al.*	-254.803367	0.071576	-254.670312	0.071253	-254.656164	**4.00**	**3.61**
						Average value:	**3.99**	**3.60**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	**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**
	Lim *et al.*	-254.354288	0.071576	-254.214468	0.071253	-254.205461	**4.04**	**3.80**
						Average value:	**4.01**	**3.76**

$Ba(H_2O)_3$: Isomer *(2+1)*

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba]$	ΔE
*m*PW1PW91	Bausch. *et al.*	-254.779201	0.072033	-254.707168	-229.258051	-25.421894	-17.08
	SDD	-254.796937	0.071874	-254.725063	-229.258051	-25.441871	-15.78
	Lim *et al.*	-254.802334	0.072066	-254.730268	-229.258051	-25.445939	-16.49
						Average value:	-16.45

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba]$	ΔE
CCSD(T,ull)	Bausch. *et al.*	-254.291689	0.072033	-254.219656	-228.871337	-25.322073	-16.47
	SDD	-254.211514	0.071874	-254.139640	-228.871337	-25.258984	-5.85
	Lim *et al.*	-254.350004	0.072066	-254.277938	-228.871337	-25.378212	-17.81
						Average value:	-13.38

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	Bausch. *et al.*	-254.779201	0.072033	-254.639968	0.074516	-254.631580	4.08	3.86
	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
						Average value:	4.09	3.86

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	Bausch. *et al.*	-254.291689	0.072033	-254.151178	0.074516	-254.141097	4.17	3.89
	SDD	-254.211514	0.071874	-254.073139	0.074790	-254.064096	4.09	3.84
	Lim *et al.*	-254.350004	0.072066	-254.208109	0.074535	-254.198769	4.18	3.93
						Average value:	4.15	3.89

$Ba(H_2O)_3$: Isomer *(1+1+1)*

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba]$	ΔE
*m*PW1PW91	Bausch. *et al.*	-254.779461	0.073330	-254.706131	-229.258051	-25.421894	-16.43
	SDD	-254.797597	0.073518	-254.724079	-229.258051	-25.441871	-15.16
	Lim *et al.*	-254.802788	0.073360	-254.729428	-229.258051	-25.445939	-15.96
						Average value:	-15.85

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba]$	ΔE
CCSD(T,Full)	Bausch. *et al.*	-254.290498	0.073330	-254.217168	-228.871337	-25.322073	-14.91
	SDD	-254.210417	0.073518	-254.136899	-228.871337	-25.258984	-4.13
	Lim *et al.*	-254.347480	0.073360	-254.274120	-228.871337	-25.378212	-15.42
						Average value:	-11.48

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	Bausch. *et al.*	-254.779461	0.073330	-254.628024	0.073661	-254.617845	4.41	4.13
	SDD	-254.797597	0.073518	-254.645922	0.073851	-254.634803	4.44	4.14
	Lim *et al.*	-254.802788	0.073360	-254.650715	0.073699	-254.640029	4.44	4.15
						Average value:	4.43	4.14

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	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
	Lim *et al.*	-254.347480	0.073360	-254.192495	0.073699	-254.180691	4.55	4.23
						Average value:	4.50	4.19

$Ba(H_2O)_4$: Isomer $(4+0)_a$

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
mPW1PW91	**Bausch. et al.**	-331.239428	0.094029	-331.145399	-305.688295	-25.421894	**-22.09**
	SDD	-331.257195	0.094541	-331.162654	-305.688295	-25.441871	**-20.39**
	Lim et al.	-331.261792	0.093975	-331.167817	-305.688295	-25.445939	**-21.07**
						Average value:	**-21.19**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
CCSD(T,Full)	**Bausch. et al.**	-330.623683	0.094029	-330.529654	-305.172060	-25.322073	**-22.29**
	SDD	-330.542879	0.094541	-330.448338	-305.172060	-25.258984	**-10.85**
	Lim et al.	-330.682883	0.093975	-330.588908	-305.172060	-25.378212	**-24.24**
						Average value:	**-19.13**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
mPW1PW91	**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**
	Lim et al.	-331.261792	0.093975	-331.130648	0.094304	-331.120513	**3.85**	**3.58**
						Average value:	**3.84**	**3.57**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	**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**
	Lim et al.	-330.682883	0.093975	-330,549527	0.094304	-330.540675	**3.88**	**3.64**
						Average value:	**3.85**	**3.61**

$Ba(H_2O)_4$: Isomer $(4+0)_b$

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
mPW1PW91	**Bausch. et al.**	-331.236234	0.094422	-331.141812	-305.688295	-25.421894	**-19.84**
	SDD	-331.254094	0.094788	-331.159306	-305.688295	-25.441871	**-18.29**
	Lim et al.	-331.258707	0.094684	-331.164023	-305.688295	-25.445939	**-18.69**
						Average value:	**-18.94**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
CCSD(T,Full)	**Bausch. et al.**	-330.622409	0.094422	-330.527987	-305.172060	-25.322073	**-21.24**
	SDD	-330.542019	0.094788	-330.447231	-305.172060	-25.258984	**-10.16**
	Lim et al.	-330.682413	0.094684	-330.587729	-305.172060	-25.378212	**-23.50**
						Average value:	**-18.30**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
mPW1PW91	**Bausch. et al.**	-331.236234	0.094422	-331.107980	0.094301	-331.097515	**3.77**	**3.49**
	SDD	-331.254094	0.094788	-331.126638	0.094529	-331.116517	**3.74**	**3.46**
	Lim et al.	-331.258707	0.094684	-331.130648	0.094304	-331.119889	**3.77**	**3.47**
						Average value:	**3.76**	**3.47**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	**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**
	Lim et al.	-330.682413	0.094684	-330,549527	0.094304	-330,543490	**3,77**	**3.61**
						Average value:	**3,75**	**3.57**

$Ba(H_2O)_4$: Isomer $(3+1)_a$

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
*m*PW1PW91	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**
	Lim *et al.*	-331.258474	0.094860	-331.158720	-305.688295	-25.445939	**-15.37**
						Average value:	**-17.44**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
CCSD(T,Full)	Bausch. *et al.*	-330.618458	0.095020	-330.523438	-305.172060	-25.322073	**-18.39**
	SDD	-330.537651	0.094681	-330.442970	-305.172060	-25.258984	**-7.48**
	Lim *et al.*	-330.677921	0.094860	-330.580128	-305.172060	-25.378212	**-18.73**
						Average value:	**-14.87**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	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**
	Lim *et al.*	-331.258474	0.094860	-331.128157	0.097947	-331.117698	**3.78**	**3.50**
						Average value:	**3.84**	**3.58**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	Bausch. *et al.*	-330.618458	0.095020	-330.488888	0.097963	-330.475472	**3.97**	**3.61**
	SDD	-330.537651	0.094681	-330.410619	0.098176	-330.391428	**4.07**	**3.55**
	Lim *et al.*	-330.677921	0.094860	-330,546817	0.097947	-330.535006	**3.89**	**3.57**
						Average value:	**3.98**	**3.58**

$Ba(H_2O)_4$: Isomer $(3+1)_b$

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
*m*PW1PW91	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**
	Lim *et al.*	-331.253580	0.097010	-331.158720	-305.688295	-25.445939	**-15.37**
						Average value:	**-15.48**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
CCSD(T,Full)	Bausch. *et al.*	-330.616439	0.097133	-330.521419	-305.172060	-25.322073	**-17.12**
	SDD	-330.536540	0.097510	-330.441859	-305.172060	-25.258984	**-6.79**
	Lim *et al.*	-330.674988	0.097010	-330.580128	-305.172060	-25.378212	**-18.73**
						Average value:	**-14.21**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	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**
	Lim *et al.*	-331.253580	0.097010	-331.127276	0.096055	-331.107344	**4.01**	**3.47**
						Average value:	**4.00**	**3.46**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	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**
	Lim *et al.*	-330.674988	0.097010	-330,542696	0.096055	-330.527111	**4.06**	**3.63**
						Average value:	**3.95**	**3.61**

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$Ba(H_2O)_4$: Isomer *(2+2)*

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
*m*PW1PW91	Bausch. *et al.*	-331.228696	0.097733	-331.130963	-305.688295	-25.421894	**-13.04**
	SDD	-331.246009	0.097907	-331.148102	-305.688295	-25.441871	**-11.25**
	Lim *et al.*	-331.251568	0.097738	-331.153830	-305.688295	-25.445939	**-12.30**
						Average value:	**-12.20**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
CCSD(T,Full)	Bausch. *et al.*	-330.612760	0.097733	-330.515027	-305.172060	-25.322073	**-13.11**
	SDD	-330.531946	0.097907	-330.434039	-305.172060	-25.258984	**-1.88**
	Lim *et al.*	-330.670762	0.097738	-330.573024	-305.172060	-25.378212	**-14.28**
						Average value:	**-9.76**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	Bausch. *et al.*	-331.228696	0.097733	-331.087648	0.099707	-331.083043	**4.02**	**3.89**
	SDD	-331.246009	0.097907	-331.104869	0.099707	-331.100016	**4.02**	**3.89**
	Lim *et al.*	-331.251568	0.097738	-331.110105	0.099687	-331.105368	**4.03**	**3.90**
						Average value:	**4.02**	**3.89**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	Bausch. *et al.*	-330.612760	0.097733	-330.469647	0.099707	-330.463626	**4.11**	**3.95**
	SDD	-330.531946	0.097907	-330.390560	0.099707	-330.384611	**4.06**	**3.90**
	Lim *et al.*	-330.670762	0.097738	-330,527619	0.099687	-330.521251	**4.12**	**3,95**
						Average value:	**4.10**	**3.93**

$Ba(H_2O)_4$: Isomer *(1+2+1)*

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
*m*PW1PW91	Bausch. *et al.*	-331.226797	0.098123	-331.128674	-305.688295	-25.421894	**-11.60**
	SDD	-331.244948	0.098326	-331.146622	-305.688295	-25.441871	**-10.33**
	Lim *et al.*	-331.250131	0.098165	-331.151966	-305.688295	-25.445939	**-11.13**
						Average value:	**-11.02**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
CCSD(T,Full)	Bausch. *et al.*	-330.609833	0.098123	-330.511710	-305.172060	-25.322073	**-11.03**
	SDD	-330.529795	0.098326	-330.431469	-305.172060	-25.258984	**-0.27**
	Lim *et al.*	-330.666853	0.098165	-330.568688	-305.172060	-25.378212	**-11.56**
						Average value:	**-7.62**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
*m*PW1PW91	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**
	Lim *et al.*	-331.250131	0.098165	-331.106221	0.098553	-331.092231	**4.31**	**3.93**
						Average value:	**4.29**	**3.92**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	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**
	Lim *et al.*	-330.666853	0.098165	-330,520200	0.098553	-330.505260	**4.41**	**4.00**
						Average value:	**4,37**	**3.97**

$Ba(H_2O)_4$: Isomer *(1+1+1+1)*

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
***m*PW1PW91**	**Bausch. *et al.***	-331.229827	0.098272	-331.131555	-305.688295	-25.421894	**-13.41**
	SDD	-331.247955	0.098466	-331.149489	-305.688295	-25.441871	**-12.13**
	Lim *et al.*	-331.253093	0.098241	-331.154852	-305.688295	-25.445939	**-12.94**
						Average value:	**-12.82**

Theory	Basis set Ba	E_0	E_{ZPE}	$E[Ba(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba]$	ΔE
CCSD(T,Full)	**Bausch. *et al.***	-330.612015	0.098272	-330.513743	-305.172060	-25.322073	**-12.31**
	SDD	-330.532068	0.098466	-330.433602	-305.172060	-25.258984	**-1.61**
	Lim *et al.*	-330.668715	0.098241	-330.570474	-305.172060	-25.378212	**-12.68**
						Average value:	**-8.86**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
***m*PW1PW91**	**Bausch. *et al.***	-331.229827	0.098272	-331.080818	0.098474	-331.067843	**4.41**	**4.06**
	SDD	-331.247955	0.098466	-331.098643	0.098642	-331.085296	**4.43**	**4.07**
	Lim *et al.*	-331.253093	0.098241	-331.103501	0.098452	-331.090110	**4.44**	**4.08**
						Average value:	**4.43**	**4.07**

Theory	Basis set Ba	E_0	E_{ZPE}	E_a	E^a_{ZPE}	E_v	IE_v	IE_a
CCSD(T,Full)	**Bausch. *et al.***	-330.612015	0.098272	-330.459614	0.098474	-330.446258	**4.52**	**4.15**
	SDD	-330.532068	0.098466	-330.382364	0.098642	-330.369215	**4.44**	**4.08**
	Lim *et al.*	-330.668715	0.098241	-330,515888	0.098452	-330.501893	**4.55**	**4.16**
						Average value:	**4.50**	**4.13**

Neutral barium-water clusters:

$Ba^+(H_2O)_1$: Isomer *1*$^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_1]$	$E[(H_2O)_1]$	$E[Ba^+]$	ΔE
***m*PW1PW91**	**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**
	Lim *et al.*	-101.733396	0.023608	-101.709788	-76.413183	-25.258481	**-23.92**
						Average value:	**-23.54**

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_1]$	$E[(H_2O)_1]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	**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**
	Lim *et al.*	-101.533780	0.023608	-101.510172	-76.284245	-25.187920	**-23.85**
						Average value:	**-19.79**

$Ba^+(H_2O)_2$: Isomer *(2+0)*$^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba^+]$	ΔE
***m*PW1PW91**	**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**
	Lim *et al.*	-178.203782	0.047550	-178.156232	-152.831962	-25.258481	**-41.28**
						Average value:	**-40.94**

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	**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**
	Lim *et al.*	-177.875773	0.047550	-177.828223	-152.574371	-25.187920	**-41.37**
						Average value:	**-36.57**

$Ba^+(H_2O)_2$: Isomer *(1+1)*$^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba^+]$	ΔE
***m*PW1PW91**	**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**
	Lim *et al.*	-178.195104	0.048972	-178.146132	-152.831962	-25.258481	**-34.95**
						Average value:	**-34.57**

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_2]$	$E[(H_2O)_2]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	**Bausch. *et al.***	-177.810139	0.048990	-177.761149	-152.574371	-25.133532	**-33.41**
	SDD	-177.733171	0.049047	-177.684124	-152.574371	-25.073281	**-22.89**
	Lim *et al.*	-177.866257	0.048972	-177.817285	-152.574371	-25.187920	**-34.51**
						Average value:	**-30.27**

$Ba^+(H_2O)_3$: Isomer *(3+0)*$^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
***m*PW1PW91**	**Bausch. *et al.***	-254.647647	0.071256	-254.576391	-229.258051	-25.236026	**-51.65**
	SDD	-254.666178	0.071554	-254.594624	-229.258051	-25.255232	**-51.04**
	Lim *et al.*	-254.670312	0.071253	-254.599059	-229.258051	-25.258481	**-51.79**
						Average value:	**-51.49**

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	**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**
	Lim *et al.*	-254.214468	0.071253	-254.143215	-228.871337	-25.187920	**-52.68**
						Average value:	**-47.30**

$Ba^+(H_2O)_3$: Isomer *(2+1)*$^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	E`$[Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
*m*PW1PW91	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**
	Lim *et al.*	-254.662580	0.074535	-254.588045	-229.258051	-25.258481	**-44.88**
						Average value:	**-44.55**

Theory	Basis set Ba	E_a	E^a_{ZPE}	E`$[Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	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**
	Lim *et al.*	-254.208109	0.074535	-254.133574	-228.871337	-25.187920	**-46.63**
						Average value:	**-41.80**

$Ba^+(H_2O)_3$: Isomer *(1+1+1)*$^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	E`$[Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
*m*PW1PW91	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**
	Lim *et al.*	-254.650715	0.073699	-254.577016	-229.258051	-25.258481	**-37.95**
						Average value:	**-37.56**

Theory	Basis set Ba	E_a	E^a_{ZPE}	E`$[Ba^+(H_2O)_3]$	$E[(H_2O)_3]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	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**
	Lim *et al.*	-254.192495	0.073699	-254.118796	-228.871337	-25.187920	**-37.36**
						Average value:	**-33.01**

$Ba^+(H_2O)_4$: Isomer *(4+0)*$^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	E`$[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
*m*PW1PW91	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**
	Lim *et al.*	-331.130648	0.094304	-331.036344	-305.688295	-25.258481	**-56.20**
						Average value:	**-55.95**

Theory	Basis set Ba	E_a	E^a_{ZPE}	E`$[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	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**
	Lim *et al.*	-330,549527	0.094304	-330,455223	-305.172060	-25.187920	**-59.77**
						Average value:	**-53.99**

$Ba^+(H_2O)_4$: Isomer *(3+1)*$_a^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	E`$[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
*m*PW1PW91	Bausch. *et al.*	-331.104664	0.095992	-331.008672	-305.688295	-25.236026	**-52.93**
	SDD	-331.123153	0.096374	-331.026779	-305.688295	-25.255232	**-52.24**
	Lim *et al.*	-331.127276	0.096055	-331.031221	-305.688295	-25.258481	**-52.99**
						Average value:	**-52.72**

Theory	Basis set Ba	E_a	E^a_{ZPE}	E`$[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	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**
	Lim *et al.*	-330,542696	0.096055	-330,446641	-305.172060	-25.187920	**-54,38**
						Average value:	**-48,97**

$Ba^+(H_2O)_4$: Isomer $(3+1)_b^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
*m*PW1PW91	Bausch. *et al.*	-331.105578	0.097963	-331.007615	-305.688295	-25.236026	**-52.27**
	SDD	-331.124040	0.098176	-331.025864	-305.688295	-25.255232	**-51.67**
	Lim *et al.*	-331.128157	0.097947	-331.030210	-305.688295	-25.258481	**-52.36**
						Average value:	**-52.10**

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	Bausch. *et al.*	-330.488888	0.097963	-330.390925	-305.172060	-25.133532	**-53.55**
	SDD	-330.410619	0.098176	-330.312443	-305.172060	-25.073281	**-42.11**
	Lim *et al.*	-330,546817	0.097947	-330,448870	-305.172060	-25.187920	**-55.78**
						Average value:	**-50.48**

$Ba^+(H_2O)_4$: Isomer $(2+2)_a^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
*m*PW1PW91	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**
	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_{ZPE}	$E`[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	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**
	Lim *et al.*	-330,536113	0.097764	-330,438349	-305.172060	-25.187920	**-49,18**
						Average value:	**-44,24**

$Ba^+(H_2O)_4$: Isomer $(2+2)_b^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
*m*PW1PW91	Bausch. *et al.*	-331.087648	0.099707	-330.987941	-305.688295	-25.236026	**-39.92**
	SDD	-331.104869	0.099707	-331.005162	-305.688295	-25.255232	**-38.68**
	Lim *et al.*	-331.110105	0.099687	-331.010418	-305.688295	-25.258481	**-39.94**
						Average value:	**-39.51**

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	Bausch. *et al.*	-330.469647	0.099707	-330.369940	-305.172060	-25.133532	**-40.38**
	SDD	-330.390560	0.099707	-330.290853	-305.172060	-25.073281	**-28.56**
	Lim *et al.*	-330,527619	0.099687	-330,427932	-305.172060	-25.187920	**-42,64**
						Average value:	**-37,19**

$Ba^+(H_2O)_4$: Isomer $(1+2+1)^+$

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
*m*PW1PW91	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**
	Lim *et al.*	-331.106221	0.098553	-331.007668	-305.688295	-25.258481	**-38.21**
						Average value:	**-37.79**

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	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**
	Lim *et al.*	-330,520200	0.098553	-330,421647	-305.172060	-25.187920	**-38.70**
						Average value:	**-34.20**

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

$Ba^{+}(H_2O)_4$: 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
***m*PW1PW91**	**Bausch. *et al.***	-331.080818	0.098474	-330.982344	-305.688295	-25.236026	**-36.41**
	SDD	-331.098643	0.098642	-331.000001	-305.688295	-25.255232	**-35.44**
	Lim *et al.*	-331.103501	0.098452	-331.005049	-305.688295	-25.258481	**-36.57**
						Average value:	**-36.14**

Theory	Basis set Ba	E_a	E^a_{ZPE}	$E`[Ba^+(H_2O)_4]$	$E[(H_2O)_4]$	$E[Ba^+]$	ΔE
CCSD(T,Full)	**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**
	Lim *et al.*	-330,515888	0.098452	-330,417436	-305.172060	-25.187920	**-36.05**
						Average value:	**-31.67**

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