

Electronic Supplementary Information for Dalton Transactions  
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**Supplementary Material to: Hydration of Be<sup>2+</sup> in aqueous solutions of simple inorganic salts.  
A combined vibrational spectroscopic and *ab initio* study.**

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**Table S1.** Assignment of tetraaquaberyllium(II) ( $S_4$ )

sym.	description	MP2/6-31G*	MP2/6-31+G*	B3LYP/6-31G*
A	BeO <sub>4</sub> deformation + water twisting	112	140	134
E	BeO <sub>4</sub> deformation + water twisting	136	141	143
B	BeO <sub>4</sub> deformation	154	157	154
A	water twisting	235	246	233
B	BeO <sub>4</sub> deformation	243	247	251
E	water twisting + wagging	255	262	261
B	water twisting	361	373	357
E	water wagging	370	406	382
A	water wagging	375	406	388
B	water wagging	433	457	444
A	BeO <sub>4</sub> stretching	472	471	473
E	water rocking + BeO <sub>4</sub> stretching	613	612	604
B	water rocking + BeO <sub>4</sub> stretching	653	653	643
A	water rocking	680	683	670
E	BeO <sub>4</sub> stretching + water rocking	865	857	856
B	BeO <sub>4</sub> stretching + water rocking	880	872	867
B	water deformation	1728	1723	1707
E	water deformation	1730	1726	1710
A	water deformation	1739	1735	1718
E	water sym stretching	3667	3644	3659
B	water sym stretching	3667	3644	3659
A	water sym stretching	3685	3659	3676
A	water asym stretching	3751	3731	3729
E	water asym stretching	3752	3732	3730
B	water asym stretching	3754	3734	3731

**Table S2.** Total Energies of beryllium species

Level	HF/STO-3G	HF/3-21G	HF/6-31G*
Be <sup>2+</sup>	-13.4397580	-13.530279	-13.6098005
H <sub>2</sub> O C <sub>2v</sub>	-74.9659012	-75.5859598	-76.0107465
Be(H <sub>2</sub> O) <sub>1</sub> <sup>2+</sup> C <sub>2v</sub>	-88.7326468	-89.3858023	-89.8546095
Be(H <sub>2</sub> O) <sub>2</sub> <sup>2+</sup> D <sub>2d</sub>	-163.9838116	-165.2054592	-166.0602912
Be(H <sub>2</sub> O) <sub>3</sub> <sup>2+</sup> D <sub>3</sub>	-239.1495404	-240.9572131	-242.2031810
Be(H <sub>2</sub> O) <sub>4</sub> <sup>2+</sup> S <sub>4</sub>	-314.2503131	-316.6597913	-318.2992010
Be(H <sub>2</sub> O) <sub>5</sub> <sup>2+</sup> C <sub>2v</sub>	-389.2611907	-392.2899325	-394.3364232
Be(H <sub>2</sub> O) <sub>5</sub> <sup>2+</sup> C <sub>2</sub>	-389.2620194	Went to C <sub>2v</sub>	
Be(H <sub>2</sub> O) <sub>5</sub> <sup>2+</sup> [4+1] C <sub>s</sub>		-392.3218256	-394.3606034
Be(H <sub>2</sub> O) <sub>5</sub> <sup>2+</sup> [4+1] C <sub>2</sub>		-392.3220945	-394.3611470
Be(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> T <sub>h</sub>	-464.2801444	-467.9204341	-470.3743458
Be(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> [4+2] D <sub>2d</sub>	-464.3205145	-467.9795149	-470.4203408
Be(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> [4+2] C <sub>s</sub> #1	-464.3121473	-467.9724994	-470.4141716
Be(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> [4+2] C <sub>s</sub> #2	-464.3132687	-467.9731659	-470.4161429
Be(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> [4+2] C <sub>1</sub>		-467.9731767	-470.4162814
Be(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> [4+4] S <sub>4</sub>	-614.3598215	-619.2519722	Went to D <sub>2d</sub> #2
Be(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> [4+4] D <sub>2d</sub> #1	-614.3037082	-619.2141042	-622.4974267
Be(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> [4+4] D <sub>2d</sub> #2			-622.5161435
Be(H <sub>2</sub> O) <sub>12</sub> <sup>2+</sup> [4+8] D <sub>2d</sub>	-914.3576349	-921.7551184	-926.6680404
Be(H <sub>2</sub> O) <sub>12</sub> <sup>2+</sup> [4+8] S <sub>4</sub>	-914.3582058	-921.7872005	-926.6749590
Be(H <sub>2</sub> O) <sub>18</sub> <sup>2+</sup> [6+12] D <sub>2d</sub>		-1375.5002190	-1382.8437815

**Table S2.** Total Energies of beryllium species (continued)

	HF/6-31+G*	MP2/6-31G*	MP2/6-31+G*
Be <sup>2+</sup>	-13.6098066	As HF	As HF
H <sub>2</sub> O C <sub>2v</sub>	-76.0177432	-76.1968478	-76.2097766
Be(H <sub>2</sub> O) <sub>1</sub> <sup>2+</sup> C <sub>2v</sub>	-89.8555961	-90.048141	-90.0503103
Be(H <sub>2</sub> O) <sub>2</sub> <sup>2+</sup> D <sub>2d</sub>	-166.0638598	-166.4468215	-166.4530896
Be(H <sub>2</sub> O) <sub>3</sub> <sup>2+</sup> D <sub>3</sub>	-242.2088940	-242.7824444	-242.7939481
Be(H <sub>2</sub> O) <sub>4</sub> <sup>2+</sup> S <sub>4</sub>	-318.3088383	-319.0715550	-319.0911333
Be(H <sub>2</sub> O) <sub>5</sub> <sup>2+</sup> C <sub>2v</sub>	-394.3510210	-395.3032639	-395.3331264
Be(H <sub>2</sub> O) <sub>5</sub> <sup>2+</sup> [4+1] C <sub>s</sub>	-394.3739105	-395.3276444	-395.3552591
Be(H <sub>2</sub> O) <sub>5</sub> <sup>2+</sup> [4+1] C <sub>2</sub>	-394.3742408	-395.3285773	-395.3558937
Be(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> T <sub>h</sub>	-470.3946568	-471.5359538	-471.5789712
Be(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> [4+2] D <sub>2d</sub>	-470.4377481	-471.5810503	-471.6177118
Be(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> [4+2] S <sub>4</sub>		-471.5811196	
Be(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> [4+2] C <sub>s</sub> #1	-470.4309814	-471.5748335	-471.6107089
Be(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> [4+2] C <sub>s</sub> #2	-470.4330342	-471.5770811	-471.6130773
Be(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> [4+2] C <sub>1</sub>	-470.4332640	-471.	-471.
Be(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> [4+4] S <sub>4</sub>	-622.5375901	Went to D <sub>2d</sub> #2	Went to D <sub>2d</sub> #2
Be(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> [4+4] D <sub>2d</sub> #1	-622.5227534	-624.0463051	-624.1003953
Be(H <sub>2</sub> O) <sub>8</sub> <sup>2+</sup> [4+4] D <sub>2d</sub> #2	-622.5411888	-624.0632065	-624.1176026
Be(H <sub>2</sub> O) <sub>12</sub> <sup>2+</sup> [4+8] D <sub>2d</sub>	-926.7179770	-928.9708655	-929.0763408
Be(H <sub>2</sub> O) <sub>12</sub> <sup>2+</sup> [4+8] S <sub>4</sub>	-926.7227062	-928.9855258	-929.0856764
Be(H <sub>2</sub> O) <sub>18</sub> <sup>2+</sup> [6+12] D <sub>2d</sub>			