Supporting Information for "Evaluation of range-separated hybrid density functionals for the prediction of vibrational frequencies, infrared intensities, and Raman activities"

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TABLE I: Basis set dependence of the harmonic vibrational frequencies (in cm^{-1}), infrared intensities (in $km\,mol^{-1}$), and Raman activities (in $Å^4\,amu^{-1}$) for the vibrational modes of water computed with the PBEh density functional.

	a_1			a_1			b_2			
basis set	ω	I_{IR}	I_{Raman}	ω	I_{IR}	I_{Raman}	ω	I_{IR}	I_{Raman}	CPU[a]
Sadlej pVTZ	1645.68	74.90	0.98	3858.30	5.71	99.55	3975.03	66.05	24.04	2
cc-pVDZ	1664.85	58.73	5.80	3825.85	6.33	70.84	3930.73	30.30	34.84	1
cc-pVTZ	1644.41	70.51	4.05	3863.18	4.50	70.55	3966.35	46.76	26.63	2
cc-pVQZ	1639.78	73.87	2.52	3865.01	5.12	77.72	3968.47	57.02	25.93	8
cc-pV5Z	1636.07	75.63	1.76	3866.67	6.06	81.89	3971.21	63.93	25.29	78
aug-cc-pVDZ	1628.43	72.27	1.67	3853.56	4.76	95.76	3966.49	62.83	25.32	2
aug-cc-pVTZ	1633.48	76.68	0.96	3856.70	5.58	97.54	3962.05	66.88	24.93	4
aug-cc-pVQZ	1635.14	77.04	0.77	3863.06	5.64	98.08	3967.81	67.42	24.55	38
aug-cc-pV5Z	1635.32	77.13	0.72	3865.46	5.62	98.57	3970.45	67.27	24.47	327
d-aug-cc-pVDZ	1634.54	75.41	0.72	3853.61	5.36	99.66	3968.39	64.71	24.95	2
d-aug-cc-pVTZ	1634.30	76.97	0.69	3857.40	5.36	100.15	3961.73	66.39	24.63	9
d-aug-cc-pVQZ	1635.08	77.08	0.69	3862.95	5.64	99.28	3967.74	67.25	24.47	96
d-aug-cc-pV5Z	1635.30	77.17	0.69	3865.49	5.64	99.22	3970.47	67.30	24.43	944
Experimental[b]	1649	64.0	0.9	3832	2.98	108.0	3943	43.3	19.2	

[a]Relative CPU time for a frequency calculation at the optimized structure.

[b]Experimental harmonic frequencies from Ref. 1, vibrational intensities from Ref. 2, and Raman activities from Refs. 3, 4.

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TABLE II: Basis set dependence of the harmonic vibrational frequencies computed with the PBE density functional. Details as in Table I.

	a_1			a_1			b_2			
basis set	ω	$I_{\rm IR}$	$I_{\rm Raman}$	ω	$I_{\rm IR}$	$I_{\rm Raman}$	ω	$I_{\rm IR}$	$I_{\rm Raman}$	CPU[a]
Sadlej pVTZ	1602.63	65.58	1.10	3695.97	1.94	110.02	3812.08	49.87	25.50	2
cc-pVDZ	1626.35	48.04	6.41	3646.82	1.06	75.01	3753.06	14.05	36.74	1
cc-pVTZ	1606.59	61.22	4.43	3700.48	0.99	74.70	3803.00	30.12	28.32	2
cc-pVQZ	1600.81	64.54	2.82	3704.71	1.47	82.43	3807.75	39.78	27.73	8
cc-pV5Z	1595.80	66.65	1.94	3707.47	2.26	86.71	3811.58	47.41	26.95	64
aug-cc-pVDZ	1585.00	62.81	1.82	3689.02	1.50	104.82	3802.13	47.83	26.95	1
aug-cc-pVTZ	1592.75	67.57	1.04	3696.35	2.01	106.86	3800.84	51.31	26.47	5
aug-cc-pVQZ	1594.49	68.07	0.82	3703.33	2.05	108.07	3807.75	51.74	26.06	24
aug-cc-pV5Z	1594.43	68.16	0.76	3705.95	2.03	108.81	3810.63	51.56	25.97	210
d-aug-cc-pVDZ	1591.17	66.04	0.79	3689.01	1.80	110.40	3804.09	49.25	26.24	2
d-aug-cc-pVTZ	1593.44	68.00	0.73	3696.68	1.87	111.13	3800.21	50.75	26.09	8
d-aug-cc-pVQZ	1594.36	68.17	0.73	3703.10	2.04	110.14	3807.55	51.55	25.95	64
d-aug-cc-pV5Z	1594.40	68.24	0.73	3706.02	2.04	110.05	3810.66	51.59	25.91	500
Experimental[b]	1649	64.0	0.9	3832	2.98	108.0	3943	43.3	19.2	

[a]Relative CPU time for a frequency calculation at the optimized structure.

[b]Experimental harmonic frequencies from Ref. 1, vibrational intensities from Ref. 2, and Raman activities from Refs. 3, 4.

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