

A Model Order Reduction Algorithm for Estimating the Absorption Spectrum: Supplementary Material

Roel Van Beeumen,^{*,†} David B. Williams-Young,^{*,‡} Joseph M. Kasper,^{*,‡} Chao
Yang,^{*,†} Esmond G. Ng,^{*,†} and Xiaosong Li^{*,‡}

[†]*Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA*

[‡]*Department of Chemistry, University of Washington, Seattle, WA*

E-mail: rvanbeeumen@lbl.gov; dbwy@uw.edu; jkasper2@uw.edu; cyang@lbl.gov; egng@lbl.gov;
xsli@uw.edu

Table 1: Cartesian coordinates of water cluster with 5 waters.

Atom	X (Bohr)	Y (Bohr)	Z (Bohr)
O	-4.48710e+00	-2.47350e+00	6.62500e-01
H	-5.35380e+00	-2.93690e+00	9.03800e-01
H	-4.65770e+00	-1.51860e+00	1.08270e+00
O	-2.82310e+00	-2.76910e+00	-1.28870e+00
H	-3.47920e+00	-2.83120e+00	-4.61600e-01
H	-2.11740e+00	-3.43520e+00	-1.27160e+00
O	-5.50850e+00	-5.09000e-01	2.02740e+00
H	-5.37420e+00	-3.97000e-02	2.93050e+00
H	-6.41140e+00	-9.46000e-01	2.05810e+00
O	-3.13480e+00	-4.35510e+00	1.87100e+00
H	-3.58820e+00	-3.47110e+00	1.55540e+00
H	-2.41990e+00	-4.01880e+00	2.54090e+00
O	-6.48400e+00	-4.32130e+00	1.17760e+00
H	-5.77830e+00	-4.83600e+00	1.74690e+00
H	-7.24410e+00	-4.34120e+00	1.73650e+00

Table 2: Cartesian coordinates of water cluster with 10 waters.

Atom	X (Bohr)	Y (Bohr)	Z (Bohr)
O	-4.48710e+00	-2.47350e+00	6.62500e-01
H	-5.35380e+00	-2.93690e+00	9.03800e-01
H	-4.65770e+00	-1.51860e+00	1.08270e+00
O	-2.82310e+00	-2.76910e+00	-1.28870e+00
H	-3.47920e+00	-2.83120e+00	-4.61600e-01
H	-2.11740e+00	-3.43520e+00	-1.27160e+00
O	-5.50850e+00	-5.09000e-01	2.02740e+00
H	-5.37420e+00	-3.97000e-02	2.93050e+00
H	-6.41140e+00	-9.46000e-01	2.05810e+00
O	-3.13480e+00	-4.35510e+00	1.87100e+00
H	-3.58820e+00	-3.47110e+00	1.55540e+00
H	-2.41990e+00	-4.01880e+00	2.54090e+00
O	-6.48400e+00	-4.32130e+00	1.17760e+00
H	-5.77830e+00	-4.83600e+00	1.74690e+00
H	-7.24410e+00	-4.34120e+00	1.73650e+00
O	-2.18690e+00	-6.30900e-01	1.61100e+00
H	-2.99220e+00	-6.28000e-02	1.63890e+00
H	-2.26630e+00	-1.45380e+00	1.05730e+00
O	-3.47490e+00	-1.75900e-01	-1.19960e+00
H	-3.16900e+00	-1.14630e+00	-1.24930e+00
H	-3.28690e+00	1.10100e-01	-2.20160e+00
O	-3.98120e+00	-5.95140e+00	-3.81500e-01
H	-3.63240e+00	-5.30790e+00	2.89700e-01
H	-4.81450e+00	-6.33960e+00	1.43000e-02
O	-7.80610e+00	-1.46220e+00	2.02370e+00
H	-8.29920e+00	-7.03200e-01	2.54730e+00
H	-8.22400e+00	-2.32000e+00	2.38140e+00
O	-4.34880e+00	-4.58620e+00	-2.63970e+00
H	-3.84540e+00	-3.74830e+00	-2.33010e+00
H	-4.26270e+00	-5.22160e+00	-1.85810e+00

Table 3: Cartesian coordinates of water cluster with 15 waters.

Atom	X (Bohr)	Y (Bohr)	Z (Bohr)
O	-4.48710e+00	-2.47350e+00	6.62500e-01
H	-5.35380e+00	-2.93690e+00	9.03800e-01
H	-4.65770e+00	-1.51860e+00	1.08270e+00
O	-2.82310e+00	-2.76910e+00	-1.28870e+00
H	-3.47920e+00	-2.83120e+00	-4.61600e-01
H	-2.11740e+00	-3.43520e+00	-1.27160e+00

Table 3: Cartesian coordinates of water cluster with 15 waters (Continued).

Atom	X (Bohr)	Y (Bohr)	Z (Bohr)
O	-5.50850e+00	-5.09000e-01	2.02740e+00
H	-5.37420e+00	-3.97000e-02	2.93050e+00
H	-6.41140e+00	-9.46000e-01	2.05810e+00
O	-3.13480e+00	-4.35510e+00	1.87100e+00
H	-3.58820e+00	-3.47110e+00	1.55540e+00
H	-2.41990e+00	-4.01880e+00	2.54090e+00
O	-6.48400e+00	-4.32130e+00	1.17760e+00
H	-5.77830e+00	-4.83600e+00	1.74690e+00
H	-7.24410e+00	-4.34120e+00	1.73650e+00
O	-2.18690e+00	-6.30900e-01	1.61100e+00
H	-2.99220e+00	-6.28000e-02	1.63890e+00
H	-2.26630e+00	-1.45380e+00	1.05730e+00
O	-3.47490e+00	-1.75900e-01	-1.19960e+00
H	-3.16900e+00	-1.14630e+00	-1.24930e+00
H	-3.28690e+00	1.10100e-01	-2.20160e+00
O	-3.98120e+00	-5.95140e+00	-3.81500e-01
H	-3.63240e+00	-5.30790e+00	2.89700e-01
H	-4.81450e+00	-6.33960e+00	1.43000e-02
O	-7.80610e+00	-1.46220e+00	2.02370e+00
H	-8.29920e+00	-7.03200e-01	2.54730e+00
H	-8.22400e+00	-2.32000e+00	2.38140e+00
O	-4.34880e+00	-4.58620e+00	-2.63970e+00
H	-3.84540e+00	-3.74830e+00	-2.33010e+00
H	-4.26270e+00	-5.22160e+00	-1.85810e+00
O	-8.22900e+00	-1.66300e+00	-5.38900e-01
H	-8.07880e+00	-2.68720e+00	-7.43100e-01
H	-8.10440e+00	-1.65740e+00	4.55500e-01
O	-6.34760e+00	1.16210e+00	3.33600e-01
H	-6.50270e+00	4.40700e-01	-3.37700e-01
H	-5.89870e+00	7.00700e-01	1.13370e+00
O	-7.82670e+00	-4.42320e+00	-1.13690e+00
H	-7.21330e+00	-4.52700e+00	-3.30000e-01
H	-8.86290e+00	-4.40900e+00	-8.69300e-01
O	-1.16190e+00	-3.67190e+00	3.41730e+00
H	-1.25930e+00	-4.23210e+00	4.28070e+00
H	-8.05000e-01	-2.77090e+00	3.79850e+00
O	-6.93910e+00	1.68000e-01	-2.27340e+00
H	-6.78620e+00	-3.14000e-01	-3.18380e+00
H	-7.44570e+00	-5.49900e-01	-1.75170e+00

Table 4: Cartesian coordinates of water cluster with 20 waters.

Atom	X (Bohr)	Y (Bohr)	Z (Bohr)
O	-4.48710e+00	-2.47350e+00	6.62500e-01
H	-5.35380e+00	-2.93690e+00	9.03800e-01
H	-4.65770e+00	-1.51860e+00	1.08270e+00
O	-2.82310e+00	-2.76910e+00	-1.28870e+00
H	-3.47920e+00	-2.83120e+00	-4.61600e-01
H	-2.11740e+00	-3.43520e+00	-1.27160e+00
O	-5.50850e+00	-5.09000e-01	2.02740e+00
H	-5.37420e+00	-3.97000e-02	2.93050e+00
H	-6.41140e+00	-9.46000e-01	2.05810e+00
O	-3.13480e+00	-4.35510e+00	1.87100e+00
H	-3.58820e+00	-3.47110e+00	1.55540e+00
H	-2.41990e+00	-4.01880e+00	2.54090e+00
O	-6.48400e+00	-4.32130e+00	1.17760e+00
H	-5.77830e+00	-4.83600e+00	1.74690e+00
H	-7.24410e+00	-4.34120e+00	1.73650e+00
O	-2.18690e+00	-6.30900e-01	1.61100e+00
H	-2.99220e+00	-6.28000e-02	1.63890e+00
H	-2.26630e+00	-1.45380e+00	1.05730e+00
O	-3.47490e+00	-1.75900e-01	-1.19960e+00
H	-3.16900e+00	-1.14630e+00	-1.24930e+00
H	-3.28690e+00	1.10100e-01	-2.20160e+00
O	-3.98120e+00	-5.95140e+00	-3.81500e-01
H	-3.63240e+00	-5.30790e+00	2.89700e-01
H	-4.81450e+00	-6.33960e+00	1.43000e-02
O	-7.80610e+00	-1.46220e+00	2.02370e+00
H	-8.29920e+00	-7.03200e-01	2.54730e+00
H	-8.22400e+00	-2.32000e+00	2.38140e+00
O	-4.34880e+00	-4.58620e+00	-2.63970e+00
H	-3.84540e+00	-3.74830e+00	-2.33010e+00
H	-4.26270e+00	-5.22160e+00	-1.85810e+00
O	-8.22900e+00	-1.66300e+00	-5.38900e-01
H	-8.07880e+00	-2.68720e+00	-7.43100e-01
H	-8.10440e+00	-1.65740e+00	4.55500e-01
O	-6.34760e+00	1.16210e+00	3.33600e-01
H	-6.50270e+00	4.40700e-01	-3.37700e-01
H	-5.89870e+00	7.00700e-01	1.13370e+00
O	-7.82670e+00	-4.42320e+00	-1.13690e+00
H	-7.21330e+00	-4.52700e+00	-3.30000e-01
H	-8.86290e+00	-4.40900e+00	-8.69300e-01
O	-1.16190e+00	-3.67190e+00	3.41730e+00
H	-1.25930e+00	-4.23210e+00	4.28070e+00

Table 4: Cartesian coordinates of water cluster with 20 waters (Continued).

Atom	X (Bohr)	Y (Bohr)	Z (Bohr)
H	-8.05000e-01	-2.77090e+00	3.79850e+00
O	-6.93910e+00	1.68000e-01	-2.27340e+00
H	-6.78620e+00	-3.14000e-01	-3.18380e+00
H	-7.44570e+00	-5.49900e-01	-1.75170e+00
O	-5.82000e+00	-6.13400e+00	3.20270e+00
H	-6.54790e+00	-6.59770e+00	3.74380e+00
H	-5.15660e+00	-5.69990e+00	3.84380e+00
O	-2.80110e+00	1.87130e+00	5.41900e-01
H	-2.97300e+00	1.06070e+00	2.19000e-02
H	-2.37300e+00	2.47720e+00	-1.19700e-01
O	-6.14800e-01	-4.25610e+00	-1.46110e+00
H	2.78800e-01	-4.41350e+00	-2.04670e+00
H	-3.30400e-01	-4.21210e+00	-5.00200e-01
O	2.03500e-01	-3.77510e+00	1.05100e+00
H	-2.71300e-01	-3.63360e+00	1.93430e+00
H	9.34000e-01	-3.09220e+00	8.98900e-01
O	-6.77310e+00	-3.87270e+00	-3.48050e+00
H	-5.79630e+00	-3.98210e+00	-3.26330e+00
H	-7.25490e+00	-4.03450e+00	-2.59030e+00

Table 5: Cartesian coordinates of water cluster with 25 waters.

Atom	X (Bohr)	Y (Bohr)	Z (Bohr)
O	-4.48710e+00	-2.47350e+00	6.62500e-01
H	-5.35380e+00	-2.93690e+00	9.03800e-01
H	-4.65770e+00	-1.51860e+00	1.08270e+00
O	-2.82310e+00	-2.76910e+00	-1.28870e+00
H	-3.47920e+00	-2.83120e+00	-4.61600e-01
H	-2.11740e+00	-3.43520e+00	-1.27160e+00
O	-5.50850e+00	-5.09000e-01	2.02740e+00
H	-5.37420e+00	-3.97000e-02	2.93050e+00
H	-6.41140e+00	-9.46000e-01	2.05810e+00
O	-3.13480e+00	-4.35510e+00	1.87100e+00
H	-3.58820e+00	-3.47110e+00	1.55540e+00
H	-2.41990e+00	-4.01880e+00	2.54090e+00
O	-6.48400e+00	-4.32130e+00	1.17760e+00
H	-5.77830e+00	-4.83600e+00	1.74690e+00
H	-7.24410e+00	-4.34120e+00	1.73650e+00
O	-2.18690e+00	-6.30900e-01	1.61100e+00
H	-2.99220e+00	-6.28000e-02	1.63890e+00

Table 5: Cartesian coordinates of water cluster with 25 waters (Continued).

Atom	X (Bohr)	Y (Bohr)	Z (Bohr)
H	-2.26630e+00	-1.45380e+00	1.05730e+00
O	-3.47490e+00	-1.75900e-01	-1.19960e+00
H	-3.16900e+00	-1.14630e+00	-1.24930e+00
H	-3.28690e+00	1.10100e-01	-2.20160e+00
O	-3.98120e+00	-5.95140e+00	-3.81500e-01
H	-3.63240e+00	-5.30790e+00	2.89700e-01
H	-4.81450e+00	-6.33960e+00	1.43000e-02
O	-7.80610e+00	-1.46220e+00	2.02370e+00
H	-8.29920e+00	-7.03200e-01	2.54730e+00
H	-8.22400e+00	-2.32000e+00	2.38140e+00
O	-4.34880e+00	-4.58620e+00	-2.63970e+00
H	-3.84540e+00	-3.74830e+00	-2.33010e+00
H	-4.26270e+00	-5.22160e+00	-1.85810e+00
O	-8.22900e+00	-1.66300e+00	-5.38900e-01
H	-8.07880e+00	-2.68720e+00	-7.43100e-01
H	-8.10440e+00	-1.65740e+00	4.55500e-01
O	-6.34760e+00	1.16210e+00	3.33600e-01
H	-6.50270e+00	4.40700e-01	-3.37700e-01
H	-5.89870e+00	7.00700e-01	1.13370e+00
O	-7.82670e+00	-4.42320e+00	-1.13690e+00
H	-7.21330e+00	-4.52700e+00	-3.30000e-01
H	-8.86290e+00	-4.40900e+00	-8.69300e-01
O	-1.16190e+00	-3.67190e+00	3.41730e+00
H	-1.25930e+00	-4.23210e+00	4.28070e+00
H	-8.05000e-01	-2.77090e+00	3.79850e+00
O	-6.93910e+00	1.68000e-01	-2.27340e+00
H	-6.78620e+00	-3.14000e-01	-3.18380e+00
H	-7.44570e+00	-5.49900e-01	-1.75170e+00
O	-5.82000e+00	-6.13400e+00	3.20270e+00
H	-6.54790e+00	-6.59770e+00	3.74380e+00
H	-5.15660e+00	-5.69990e+00	3.84380e+00
O	-2.80110e+00	1.87130e+00	5.41900e-01
H	-2.97300e+00	1.06070e+00	2.19000e-02
H	-2.37300e+00	2.47720e+00	-1.19700e-01
O	-6.14800e-01	-4.25610e+00	-1.46110e+00
H	2.78800e-01	-4.41350e+00	-2.04670e+00
H	-3.30400e-01	-4.21210e+00	-5.00200e-01
O	2.03500e-01	-3.77510e+00	1.05100e+00
H	-2.71300e-01	-3.63360e+00	1.93430e+00
H	9.34000e-01	-3.09220e+00	8.98900e-01
O	-6.77310e+00	-3.87270e+00	-3.48050e+00

Table 5: Cartesian coordinates of water cluster with 25 waters (Continued).

Atom	X (Bohr)	Y (Bohr)	Z (Bohr)
H	−5.79630e+00	−3.98210e+00	−3.26330e+00
H	−7.25490e+00	−4.03450e+00	−2.59030e+00
O	−9.01120e+00	−3.87530e+00	2.26300e+00
H	−9.29850e+00	−4.71850e+00	2.82290e+00
H	−9.56970e+00	−3.93700e+00	1.39390e+00
O	−5.14190e+00	7.10500e−01	4.58560e+00
H	−4.79090e+00	2.69700e−01	5.43750e+00
H	−4.44250e+00	1.44500e+00	4.35530e+00
O	−6.22730e+00	−7.41940e+00	7.15200e−01
H	−6.57610e+00	−8.37610e+00	8.25500e−01
H	−6.60640e+00	−6.91160e+00	1.49820e+00
O	−1.60250e+00	−6.85310e+00	1.49550e+00
H	−2.10090e+00	−7.53270e+00	1.99720e+00
H	−2.08600e+00	−6.03330e+00	1.78320e+00
O	−4.37650e+00	−5.18340e+00	5.43180e+00
H	−4.67860e+00	−5.67210e+00	6.28820e+00
H	−4.36120e+00	−4.21060e+00	5.85520e+00