

# Non-monotonic dc Stark shifts in the rapidly ionizing orbitals of the water molecule (Supplementary Materials)

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## I. SPHERICAL HARMONIC DECOMPOSITION OF THE EXTERNAL FIELD

The potential for a force oriented in the  $x$  direction can be broken down using spherical harmonics. First, one knows that complex exponentials can be used to express the spherical-polar form of the potential. We write this as,

$$\begin{aligned}
 & -\frac{F_x r}{2} \left( \sin(\theta) \exp(i\phi) + \sin(\theta) \exp(-i\phi) \right) \\
 &= -\frac{F_x r \sin(\theta)}{2} \left( \cos(\phi) + i \sin(\phi) + \cos(\phi) - i \sin(\phi) \right) \\
 &= -F_x r \sin(\theta) \cos(\phi).
 \end{aligned} \tag{1}$$

This will be important for the spherical part of the integrals in the matrix elements, as the first line in Eq. (1) contains a pair of spherical harmonics, but care must be taken of normalization, since we use Wigner  $3j$  coefficients to evaluate the Gaunt integrals which are involved in the matrix elements. The Wigner coefficients are defined for the normalized spherical harmonics involved in the integrals, and thus to retain the result above in Eq. (1) the result from the Wigner coefficients must be multiplied by the appropriate coefficient. A little more clearly, we shall split the integral involved for the DC potential as follows,

$$\begin{aligned}
 & -\frac{F_x}{2} \langle inlm | r \sin \theta \exp i\phi | i'n'l'm' \rangle - \frac{F_x}{2} \langle inlm | r \sin \theta \exp -i\phi | i'n'l'm' \rangle \\
 &= -\frac{F_x}{2} \langle in | r | i'n' \rangle \left( [lm | \sin \theta \exp i\phi | l'm'] + [lm | \sin \theta \exp -i\phi | l'm'] \right).
 \end{aligned} \tag{2}$$

In the first line we have used standard angled Dirac brackets. However, in the second line we have split the matrix elements up into two sets of brackets. In the second line the first angled set is similar to Dirac brackets and indicate integration, but only over the radial variables and radial basis functions, and the square brackets indicate the same but for the spherical parts. The results of these square brackets will be replaced by Wigner  $3j$  coefficients for the corresponding spherical harmonics multiplied by the appropriate constants, which are  $2\sqrt{2\pi/3}$  and  $-2\sqrt{2\pi/3}$  for  $(l, m)$  equal to  $(1, -1)$ , and  $(1, 1)$  respectively. These constants are just the multiplicative inverse of the spherical harmonic normalization coefficients.

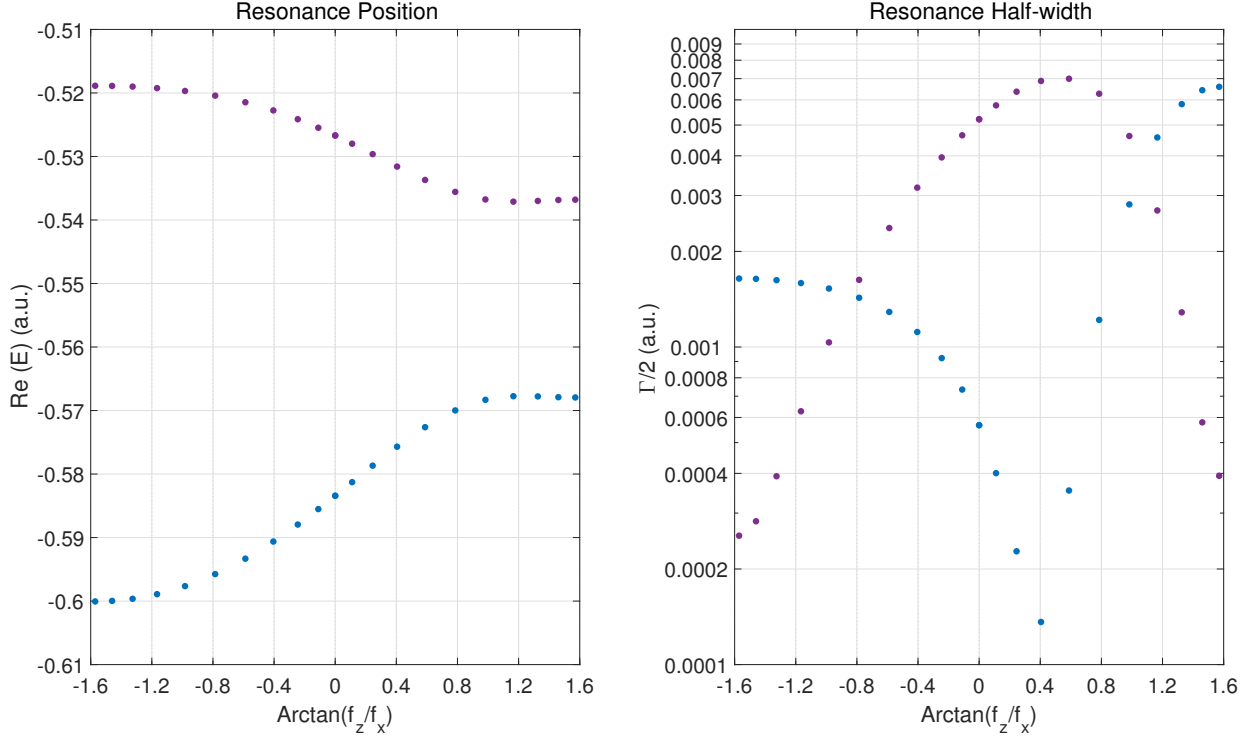


FIG. 1. The left panel contains the resonance positions while the right panel contains half-widths for the  $3a_1$  (blue  $\bullet$ ) and  $1b_1$  (purple  $\bullet$ ) valence orbitals of water in a dc field ( $F_x > 0$ ). The force strengths in each direction are  $F_z = F_o f_z$  and  $F_x = F_o f_x$ , where the lower-case  $\{f_x, f_z\}$  are the dimensionless fractions which determine the projection of  $\vec{F}$  onto the two axes. Hence the angle of the force from the  $x$  to the  $z$  axis is  $\arctan(F_o f_z / F_o f_x) = \arctan(f_z / f_x)$ . Here the vector magnitude is  $|\vec{F}| = F_o \sqrt{f_z^2 + f_x^2} = 0.1$  a.u..  $F_o$  is varied such that  $|\vec{F}|$  is constant for the different values of  $f_z$  and  $f_x$  (see Tables IV-VII).

## II. FIELD ORIENTATION IN THE $x - z$ PLANE: RESONANCE PARAMETERS FOR $1b_1$ AND $3a_1$

Here we present results for different force orientations in the  $x - z$  plane. The resonance parameters are shown in Fig. 1 for both the  $1b_1$  and  $3a_1$  orbitals. Due to symmetry the results would be the same for the force in positive  $x$  axis as negative  $x$  axis, so we choose  $\arctan(f_z/f_x)$  to vary in the range  $-\pi/2$  to  $\pi/2$ , where  $F_x$  and therefore the  $f_x$  are always positive. The lower-case  $\{f_x, f_z\}$  are the (dimensionless) fractions which determine the projection of  $\vec{F}$  onto the two axes. These angles corresponds to  $\pi$  to 0 in terms of the polar

angle. The two extreme values correspond to forces along  $-\hat{z}$  and  $\hat{z}$  respectively, while the force is in the  $\hat{x}$  direction for  $\arctan(f_z/f_x) = 0$ . The force strength itself is chosen to be fixed at  $|\vec{F}| = 0.1$  a.u., not to be confused with  $F_o$  which varies throughout the different values of  $\arctan(f_z/f_x)$ .

The orbital resonance positions get closer to one another as the electric force points towards the  $z$  axis, and farther as it points towards the  $-z$  axis. The  $1b_1$  orbital half-width does not reach a peak when  $\arctan(f_z/f_x) = 0$ . It reaches its peak around 0.4 radians. The  $3a_1$  orbital half-width becomes dominant at larger  $|\arctan|$  for positive angles than negative.

### III. TABLES

#### A. Resonance parameters corresponding to molecular orbitals ( $x$ directed force)

For all the following subsections, the number of significant digits has been controlled at 4 in accord with the findings of Fig. 1 of Ref. [1]. This applies foremost to the real part of the energy eigenvalues. The imaginary parts have been controlled to the same number of digits under the **siunitx** tabular environment. In any case the small imaginary values (below  $10^{-7}$ ) should be trusted to fewer digits. Some of the numbers have been cut off before 4 significant digits by the **siunitx** tabular environment due to trailing zeroes. The real parts of the energy eigenvalues (Re) are the resonance widths, and the imaginary parts (Im) are the resonance half-widths.

MO:  $1b_1$ 

$F_x$	$\Re$	$\Im$
0.02	-0.5214	$-1.266 \times 10^{-12}$
0.04	-0.5216	$-4.242 \times 10^{-7}$
0.06	-0.5226	$-1.252 \times 10^{-4}$
0.08	-0.5246	$-1.475 \times 10^{-3}$
0.10	-0.5267	$-5.213 \times 10^{-3}$
0.12	-0.5274	$-1.097 \times 10^{-2}$
0.14	-0.5263	$-1.797 \times 10^{-2}$
0.16	-0.5232	$-2.552 \times 10^{-2}$
0.18	-0.5181	$-3.294 \times 10^{-2}$
0.20	-0.5112	$-3.958 \times 10^{-2}$
0.22	-0.5032	$-4.502 \times 10^{-2}$
0.24	-0.4947	$-4.908 \times 10^{-2}$
0.26	-0.4862	$-5.195 \times 10^{-2}$
0.28	-0.4780	$-5.394 \times 10^{-2}$
0.30	-0.4704	$-5.540 \times 10^{-2}$

TABLE I. Resonance positions and half-widths for the molecular orbital  $1b_1$  of  $H_2O$ .MO:  $3a_1$ 

$F_x$	$\Re$	$\Im$
0.02	-0.5723	$-1.623 \times 10^{-12}$
0.04	-0.5736	$-1.663 \times 10^{-9}$
0.06	-0.5759	$-2.424 \times 10^{-6}$
0.08	-0.5791	$-7.967 \times 10^{-5}$
0.10	-0.5834	$-5.673 \times 10^{-4}$
0.12	-0.5884	$-1.850 \times 10^{-3}$
0.14	-0.5936	$-3.909 \times 10^{-3}$
0.16	-0.5987	$-6.471 \times 10^{-3}$
0.18	-0.6038	$-9.345 \times 10^{-3}$
0.20	-0.6088	$-1.247 \times 10^{-2}$
0.22	-0.6138	$-1.584 \times 10^{-2}$
0.24	-0.6187	$-1.946 \times 10^{-2}$
0.26	-0.6236	$-2.334 \times 10^{-2}$
0.28	-0.6284	$-2.745 \times 10^{-2}$
0.30	-0.6330	$-3.177 \times 10^{-2}$

TABLE II. Resonance positions and half-widths for the molecular orbital  $3a_1$  of  $H_2O$ .

MO:  $1b_2$

$F_x$	$\Re$	$\Im$
0.02	-0.7100	NA
0.04	-0.7105	NA
0.06	-0.7113	$-1.001 \times 10^{-10}$
0.08	-0.7124	$-6.274 \times 10^{-8}$
0.10	-0.7139	$-2.565 \times 10^{-6}$
0.12	-0.7158	$-2.749 \times 10^{-5}$
0.14	-0.7181	$-1.394 \times 10^{-4}$
0.16	-0.7210	$-4.486 \times 10^{-4}$
0.18	-0.7244	$-1.076 \times 10^{-3}$
0.20	-0.7282	$-2.115 \times 10^{-3}$
0.22	-0.7322	$-3.622 \times 10^{-3}$
0.24	-0.7365	$-5.613 \times 10^{-3}$
0.26	-0.7410	$-8.082 \times 10^{-3}$
0.28	-0.7454	$-1.101 \times 10^{-2}$
0.30	-0.7499	$-1.435 \times 10^{-2}$

TABLE III. Resonance positions and half-widths for the molecular orbital  $1b_2$  of  $H_2O$ .

## B. Dominant resonance parameters vs the force orientation in $x - z$ plane

MO: $1b_1$			
$(f_z, f_x)$	$\arctan(f_z/f_x)$	$\Re$	$\Im$
(0.0, 1.0)	0 rad	-0.5267	$-5.213 \times 10^{-3}$
(0.1, 0.9)	0.1107 rad	-0.5280	$-5.766 \times 10^{-3}$
(0.2, 0.8)	0.2450 rad	-0.5296	$-6.367 \times 10^{-3}$
(0.3, 0.7)	0.4049 rad	-0.5316	$-6.882 \times 10^{-3}$
(0.4, 0.6)	0.5880 rad	-0.5337	$-6.995 \times 10^{-3}$
(0.5, 0.5)	0.7854 rad	-0.5356	$-6.274 \times 10^{-3}$
(0.6, 0.4)	0.9828 rad	-0.5368	$-4.618 \times 10^{-3}$
(0.7, 0.3)	1.166 rad	-0.5371	$-2.692 \times 10^{-3}$
(0.8, 0.2)	1.326 rad	-0.5370	$-1.286 \times 10^{-3}$
(0.9, 0.1)	1.460 rad	-0.5368	$-5.792 \times 10^{-4}$
(1.0, 0.0)	1.571 rad	-0.5368	$-3.930 \times 10^{-4}$

TABLE IV. Resonance positions and half-widths for the molecular orbital  $1b_1$  of  $\text{H}_2\text{O}$ . The force strengths in each direction are  $F_z = F_o f_z$  and  $F_x = F_o f_x$ . Hence the angle of the force from the  $x$  to the  $z$  axis is  $\arctan(F_o f_z / F_o f_x) = \arctan(f_z / f_x)$ . Here the vector magnitude is  $|\vec{F}| = F_o \sqrt{f_z^2 + f_x^2} = 0.1$  a.u..  $F_o$  is varied such that  $|\vec{F}|$  is constant.

MO: $3a_1$			
$(f_z, f_x)$	$\arctan(f_z/f_x)$	$\Re$	$\Im$
(0.0, 1.0)	0 rad	-0.5834	$-5.673 \times 10^{-4}$
(0.1, 0.9)	0.1107 rad	-0.5813	$-4.008 \times 10^{-4}$
(0.2, 0.8)	0.2450 rad	-0.5787	$-2.274 \times 10^{-4}$
(0.3, 0.7)	0.4049 rad	-0.5757	$-1.362 \times 10^{-4}$
(0.4, 0.6)	0.5880 rad	-0.5726	$-3.533 \times 10^{-4}$
(0.5, 0.5)	0.7854 rad	-0.5700	$-1.217 \times 10^{-3}$
(0.6, 0.4)	0.9828 rad	-0.5683	$-2.812 \times 10^{-3}$
(0.7, 0.3)	1.166 rad	-0.5677	$-4.570 \times 10^{-3}$
(0.8, 0.2)	1.326 rad	-0.5678	$-5.819 \times 10^{-3}$
(0.9, 0.1)	1.460 rad	-0.5679	$-6.436 \times 10^{-3}$
(1.0, 0.0)	1.571 rad	-0.5679	$-6.598 \times 10^{-3}$

TABLE V. Resonance positions and half-widths for the molecular orbital  $3a_1$  of  $\text{H}_2\text{O}$ . The force strengths in each direction are  $F_z = F_o f_z$  and  $F_x = F_o f_x$ . Hence the angle of the force from the  $x$  to the  $z$  axis is  $\arctan(F_o f_z / F_o f_x) = \arctan(f_z / f_x)$ . Here the vector magnitude is  $|\vec{F}| = F_o \sqrt{f_z^2 + f_x^2} = 0.1$  a.u..  $F_o$  is varied such that  $|\vec{F}|$  is constant.

MO: $1b_1$			
$(f_z, f_x)$	$\arctan(f_z/f_x)$	$\Re$	$\Im$
(0.0, 1.0)	0 rad	-0.5267	$-5.213 \times 10^{-3}$
(-0.1, 0.9)	-0.1107 rad	-0.5255	$-4.642 \times 10^{-3}$
(-0.2, 0.8)	-0.2450 rad	-0.5241	$-3.954 \times 10^{-3}$
(-0.3, 0.7)	-0.4049 rad	-0.5227	$-3.176 \times 10^{-3}$
(-0.4, 0.6)	-0.5880 rad	-0.5215	$-2.370 \times 10^{-3}$
(-0.5, 0.5)	-0.7854 rad	-0.5204	$-1.628 \times 10^{-3}$
(-0.6, 0.4)	-0.9828 rad	-0.5197	$-1.034 \times 10^{-3}$
(-0.7, 0.3)	-1.166 rad	-0.5192	$-6.275 \times 10^{-4}$
(-0.8, 0.2)	-1.326 rad	-0.5190	$-3.919 \times 10^{-4}$
(-0.9, 0.1)	-1.460 rad	-0.5189	$-2.827 \times 10^{-4}$
(-1.0, 0.0)	-1.571 rad	-0.5189	$-2.546 \times 10^{-4}$

TABLE VI. Resonance positions and half-widths for the molecular orbital  $1b_1$  of  $\text{H}_2\text{O}$ . The force strengths in each direction are  $F_z = F_o f_z$  and  $F_x = F_o f_x$ . Hence the angle of the force from the  $x$  to the  $z$  axis is  $\arctan(F_o f_z / F_o f_x) = \arctan(f_z / f_x)$ . Here the vector magnitude is  $|\vec{F}| = F_o \sqrt{f_z^2 + f_x^2} = 0.1$  a.u..  $F_o$  is varied such that  $|\vec{F}|$  is constant.



MO:  $3a_1$ 

$(f_z, f_x)$	$\arctan(f_z/f_x)$	$\Re$	$\Im$
(0.0, 1.0)	0 rad	-0.5834	$-5.673 \times 10^{-4}$
(-0.1, 0.9)	-0.1107 rad	-0.5855	$-7.345 \times 10^{-4}$
(-0.2, 0.8)	-0.2450 rad	-0.5879	$-9.227 \times 10^{-4}$
(-0.3, 0.7)	-0.4049 rad	-0.5906	$-1.115 \times 10^{-3}$
(-0.4, 0.6)	-0.5880 rad	-0.5933	$-1.290 \times 10^{-3}$
(-0.5, 0.5)	-0.7854 rad	-0.5958	$-1.429 \times 10^{-3}$
(-0.6, 0.4)	-0.9828 rad	-0.5976	$-1.528 \times 10^{-3}$
(-0.7, 0.3)	-1.166 rad	-0.5989	$-1.590 \times 10^{-3}$
(-0.8, 0.2)	-1.326 rad	-0.5996	$-1.624 \times 10^{-3}$
(-0.9, 0.1)	-1.460 rad	-0.6000	$-1.639 \times 10^{-3}$
(-1.0, 0.0)	-1.571 rad	-0.6001	$-1.643 \times 10^{-3}$

TABLE VII. Resonance positions and half-widths for the molecular orbital  $3a_1$  of  $\text{H}_2\text{O}$ . The force strengths in each direction are  $F_z = F_o f_z$  and  $F_x = F_o f_x$ . Hence the angle of the force from the  $x$  to the  $z$  axis is  $\arctan(F_o f_z / F_o f_x) = \arctan(f_z / f_x)$ . Here the vector magnitude is  $|\vec{F}| = F_o \sqrt{f_z^2 + f_x^2} = 0.1 \text{ a.u.}$ .  $F_o$  is varied such that  $|\vec{F}|$  is constant.

C. Resonance parameters corresponding to molecular orbitals ( $y$  directed force)

MO: $1b_1$		
$F_y$	$\Re$	$\Im$
0.02	-0.5216	NA
0.04	-0.5223	$-4.658 \times 10^{-10}$
0.06	-0.5236	$-1.186 \times 10^{-6}$
0.08	-0.5255	$-4.532 \times 10^{-5}$
0.10	-0.5282	$-3.426 \times 10^{-4}$
0.12	-0.5317	$-1.205 \times 10^{-3}$
0.14	-0.5356	$-2.825 \times 10^{-3}$
0.16	-0.5397	$-5.227 \times 10^{-3}$
0.18	-0.5439	$-8.347 \times 10^{-3}$
0.20	-0.5480	$-1.209 \times 10^{-2}$
0.22	-0.5519	$-1.635 \times 10^{-2}$
0.24	-0.5556	$-2.105 \times 10^{-2}$
0.26	-0.5590	$-2.611 \times 10^{-2}$
0.28	-0.5622	$-3.146 \times 10^{-2}$
0.30	-0.5651	$-3.706 \times 10^{-2}$

TABLE VIII. Resonance positions and half-widths for the molecular orbital  $1b_1$  of  $\text{H}_2\text{O}$ .

MO: $3a_1$		
$F_y$	$\Re$	$\Im$
0.02	-0.5721	NA
0.04	-0.5730	$-2.840 \times 10^{-11}$
0.06	-0.5746	$-1.694 \times 10^{-7}$
0.08	-0.5770	$-1.243 \times 10^{-5}$
0.10	-0.5802	$-1.429 \times 10^{-4}$
0.12	-0.5845	$-6.626 \times 10^{-4}$
0.14	-0.5897	$-1.869 \times 10^{-3}$
0.16	-0.5956	$-3.935 \times 10^{-3}$
0.18	-0.6020	$-6.894 \times 10^{-3}$
0.20	-0.6087	$-1.069 \times 10^{-2}$
0.22	-0.6156	$-1.520 \times 10^{-2}$
0.24	-0.6227	$-2.025 \times 10^{-2}$
0.26	-0.6300	$-2.556 \times 10^{-2}$
0.28	-0.6374	$-3.066 \times 10^{-2}$
0.30	-0.6441	$-3.503 \times 10^{-2}$

TABLE IX. Resonance positions and half-widths for the molecular orbital  $3a_1$  of  $\text{H}_2\text{O}$ .

MO: $1b_2$		
$F_y$	$\Re$	$\Im$
0.02	-0.7099	$-3.147 \times 10^{-12}$
0.04	-0.7100	$-5.100 \times 10^{-12}$
0.06	-0.7102	$-1.897 \times 10^{-7}$
0.08	-0.7108	$-2.218 \times 10^{-5}$
0.10	-0.7122	$-3.260 \times 10^{-4}$
0.12	-0.7147	$-1.719 \times 10^{-3}$
0.14	-0.7177	$-5.139 \times 10^{-3}$
0.16	-0.7204	$-1.101 \times 10^{-2}$
0.18	-0.7217	$-1.921 \times 10^{-2}$
0.20	-0.7211	$-2.929 \times 10^{-2}$
0.22	-0.7180	$-4.071 \times 10^{-2}$
0.24	-0.7123	$-5.292 \times 10^{-2}$
0.26	-0.7042	$-6.564 \times 10^{-2}$
0.28	-0.6938	$-7.881 \times 10^{-2}$
0.30	-0.6822	$-9.270 \times 10^{-2}$

TABLE X. Resonance positions and half-widths for the molecular orbital  $1b_2$  of  $\text{H}_2\text{O}$ .

#### D. Comparison with HF total ionization rates

Table XI contains a direct sums of energy eigenvalues to obtain total Stark shifts and resonance widths, to be compared with with the HF results of Jagau [2]. We carry out a direct sum (written DS (2) for a sum of the occupied orbitals, where the two indicates double occupation due to spin degeneracy) to find the net energy and shifts. The innermost two orbitals ( $1a_1$  and  $2a_1$ ) are left out when their values are too small, which only happens for the widths and not the Stark shifts. The HF row references Jagau [2].

$\Re \Delta E$						
$F_x$	0.04	0.06	0.08	0.10	0.12	0.14
$1a_1$	-0.000001	-0.000002	-0.000004	-0.000006	-0.000009	-0.000012
$2a_1$	-0.000978	-0.002202	-0.003920	-0.006135	-0.008853	-0.012085
$1b_2$	-0.000611	-0.001386	-0.002494	-0.003968	-0.005862	-0.008238
$3a_1$	-0.001789	-0.004039	-0.007292	-0.011596	-0.016597	-0.021781
$1b_1$	-0.000306	-0.001228	-0.003288	-0.005356	-0.0060933	-0.004985
DS (2)	-0.007371	-0.017715	-0.033998	-0.054121	-0.074829	-0.094203
HF	-0.006510	-0.015381	-0.028639	-0.045285	-0.063967	-0.083259
$\Gamma$						
$F_x$	0.04	0.06	0.08	0.10	0.12	0.14
$1b_2$	0.000000	0.000000	0.000000	0.000005	0.000055	0.000279
$3a_1$	0.000000	0.000005	0.000160	0.001135	0.003700	0.007818
$1b_1$	0.000000	0.000250	0.002950	0.010426	0.021947	0.035945
DS (2)	0.000002	0.000510	0.006218	0.023132	0.051405	0.088084
HF	0.000004	0.000523	0.004346	0.014036	0.030614	0.052159
$\Re \Delta E$						
$F_y$	0.04	0.06	0.08	0.10	0.12	0.14
$1a_1$	-0.000001	-0.000002	-0.000004	-0.000006	-0.000009	-0.000012
$2a_1$	-0.001984	-0.004459	-0.007918	-0.012355	-0.017767	-0.024154
$1b_2$	-0.000001	-0.000334	-0.000941	-0.002349	-0.004809	-0.007848
$3a_1$	-0.001222	-0.002800	-0.005134	-0.008387	-0.012660	-0.017853
$1b_1$	-0.000966	-0.002233	-0.004162	-0.006885	-0.010334	-0.014261
DS (2)	-0.008545	-0.019657	-0.036318	-0.059966	-0.091157	-0.128257
HF	-0.007442	-0.016968	-0.030838	-0.049445	-0.072722	-0.100332
$\Gamma$						
$F_y$	0.04	0.06	0.08	0.10	0.12	0.14
$1b_2$	0.000000	0.000000	0.000000	0.000005	0.000055	0.000279
$3a_1$	0.000000	0.000005	0.000160	0.001135	0.003700	0.007818
$1b_1$	0.000000	0.000250	0.002950	0.010426	0.021947	0.035945
DS (2)	0.000000	0.000006	0.000220	0.003246	0.014347	0.039327
HF	0.000000	0.000019	0.000387	0.002354	0.007550	0.017486

TABLE XI. Stark shifts and widths for the valence orbitals of the water molecule for different force strengths. The total molecular Stark shifts and widths calculated using a direct sum of the complex energy eigenvalues of the occupied orbitals, and are labeled DS (2). All results are from the current work except for HF which references Jagau [2].

E. Tabulations of  $\ell$  max = 4 calculations

MO: $1b_1$		
$F_z$	$\Re$	$\Im$
-0.30	-0.5359	$-2.216 \times 10^{-2}$
-0.28	-0.5341	$-1.878 \times 10^{-2}$
-0.26	-0.5323	$-1.558 \times 10^{-2}$
-0.24	-0.5305	$-1.258 \times 10^{-2}$
-0.22	-0.5287	$-9.825 \times 10^{-3}$
-0.20	-0.5268	$-7.335 \times 10^{-3}$
-0.18	-0.5250	$-5.158 \times 10^{-3}$
-0.16	-0.5233	$-3.332 \times 10^{-3}$
-0.14	-0.5217	$-1.900 \times 10^{-3}$
-0.12	-0.5203	$-8.898 \times 10^{-4}$
-0.10	-0.5193	$-2.997 \times 10^{-4}$
-0.08	-0.5187	$-5.453 \times 10^{-5}$
-0.06	-0.5188	$-2.669 \times 10^{-6}$
-0.04	-0.5194	NA
-0.02	-0.5204	NA
0.00	-0.5219	0
0.02	-0.5239	NA
0.04	-0.5263	$-5.906 \times 10^{-9}$
0.06	-0.5293	$-4.275 \times 10^{-6}$
0.08	-0.5330	$-9.197 \times 10^{-5}$
0.10	-0.5376	$-5.255 \times 10^{-4}$
0.12	-0.5428	$-1.605 \times 10^{-3}$
0.14	-0.5485	$-3.489 \times 10^{-3}$
0.16	-0.5544	$-6.200 \times 10^{-3}$
0.18	-0.5603	$-9.667 \times 10^{-3}$
0.20	-0.5661	$-1.381 \times 10^{-2}$
0.22	-0.5717	$-1.852 \times 10^{-2}$
0.24	-0.5771	$-2.374 \times 10^{-2}$
0.26	-0.5822	$-2.934 \times 10^{-2}$
0.28	-0.5870	$-3.530 \times 10^{-2}$
0.30	-0.5916	$-4.155 \times 10^{-2}$

TABLE XII. Resonance positions and half-widths for the molecular orbital  $1b_1$  of  $\text{H}_2\text{O}$ .

MO: $3a_1$		
$F_z$	$\Re$	$\Im$
-0.30	-0.6252	$-5.477 \times 10^{-2}$
-0.28	-0.6283	$-5.012 \times 10^{-2}$
-0.26	-0.6306	$-4.484 \times 10^{-2}$
-0.24	-0.6318	$-3.904 \times 10^{-2}$
-0.22	-0.6319	$-3.281 \times 10^{-2}$
-0.20	-0.6306	$-2.634 \times 10^{-2}$
-0.18	-0.6278	$-1.990 \times 10^{-2}$
-0.16	-0.6236	$-1.380 \times 10^{-2}$
-0.14	-0.6180	$-8.451 \times 10^{-3}$
-0.12	-0.6113	$-4.250 \times 10^{-3}$
-0.10	-0.6041	$-1.522 \times 10^{-3}$
-0.08	-0.5970	$-2.869 \times 10^{-4}$
-0.06	-0.5907	$-1.390 \times 10^{-5}$
-0.04	-0.5853	$-1.998 \times 10^{-8}$
-0.02	-0.5805	NA
0.00	-0.5762	0
0.02	-0.5725	NA
0.04	-0.5696	$-8.946 \times 10^{-8}$
0.06	-0.5681	$-6.134 \times 10^{-5}$
0.08	-0.5692	$-1.219 \times 10^{-3}$
0.10	-0.5725	$-6.149 \times 10^{-3}$
0.12	-0.5755	$-1.651 \times 10^{-2}$
0.14	-0.5750	$-3.221 \times 10^{-2}$
0.16	-0.5678	$-5.195 \times 10^{-2}$
0.18	-0.5503	$-7.072 \times 10^{-2}$
0.20	-0.5259	$-7.921 \times 10^{-2}$
0.22	-0.5056	$-7.948 \times 10^{-2}$
0.24	-0.4896	$-7.729 \times 10^{-2}$
0.26	-0.4765	$-7.498 \times 10^{-2}$
0.28	-0.4651	$-7.280 \times 10^{-2}$
0.30	-0.4550	$-7.104 \times 10^{-2}$

TABLE XIII. Resonance positions and half-widths for the molecular orbital  $3a_1$  of  $\text{H}_2\text{O}$ .

MO:  $1b_2$

$F_z$	$\Re$	$\Im$
-0.30	-0.6763	$-9.022 \times 10^{-3}$
-0.28	-0.6768	$-7.007 \times 10^{-3}$
-0.26	-0.6775	$-5.240 \times 10^{-3}$
-0.24	-0.6783	$-3.735 \times 10^{-3}$
-0.22	-0.6794	$-2.500 \times 10^{-3}$
-0.20	-0.6809	$-1.539 \times 10^{-3}$
-0.18	-0.6826	$-8.446 \times 10^{-4}$
-0.16	-0.6848	$-3.939 \times 10^{-4}$
-0.14	-0.6874	$-1.442 \times 10^{-4}$
-0.12	-0.6905	$-3.632 \times 10^{-5}$
-0.10	-0.6942	$-4.914 \times 10^{-6}$
-0.08	-0.6983	$-2.153 \times 10^{-7}$
-0.06	-0.7029	$-9.155 \times 10^{-10}$
-0.04	-0.7079	NA
-0.02	-0.7134	NA
0.00	-0.7194	0
0.02	-0.7259	NA
0.04	-0.7329	NA
0.06	-0.7405	$-1.275 \times 10^{-9}$
0.08	-0.7486	$-3.397 \times 10^{-7}$
0.10	-0.7575	$-8.667 \times 10^{-6}$
0.12	-0.7671	$-7.048 \times 10^{-5}$
0.14	-0.7776	$-3.028 \times 10^{-4}$
0.16	-0.7891	$-8.821 \times 10^{-4}$
0.18	-0.8015	$-1.992 \times 10^{-3}$
0.20	-0.8147	$-3.781 \times 10^{-3}$
0.22	-0.8286	$-6.341 \times 10^{-3}$
0.24	-0.8431	$-9.724 \times 10^{-3}$
0.26	-0.8580	$-1.393 \times 10^{-2}$
0.28	-0.8733	$-1.895 \times 10^{-2}$
0.30	-0.8889	$-2.475 \times 10^{-2}$

TABLE XIV. Resonance positions and half-widths for the molecular orbital  $1b_2$  of  $\text{H}_2\text{O}$ .

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