Supporting Information for “Effects of applied voltage on water at a gold electrode interface from ab initio molecular dynamics”

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1 Additional electrostatic data

The computed electrode potentials for each trajectory presented in the main text follow from the solution and metal potentials $\Phi_S$ and $\Phi_M$, respectively. The values of these quantities at every $\sim$48 fs for each trajectory are given in Figs. S1 and S2. As is mentioned in the main text and is visible here, $\Phi_M$ was the more volatile quantity of these two and contributed to most of the magnitude of the fluctuations in $\Phi_c$.

![Figure S1: Solution potentials $\Phi_S$ as a function of simulation time $t$ for each trajectory, designated by their electrode charges $\sigma$.](image)

![Figure S2: Metal potentials $\Phi_M$ as a function of simulation time $t$ for each trajectory, designated by their electrode charges $\sigma$.](image)

We chose to measure $\Phi_M$ as the value of $\Phi$ in the back 1 Å of the Au(111) slab because of the stability of this quantity relative to alternatives. To illustrate this, we plotted the value of $\Phi_M$ throughout the $\sigma = +0.2$ e trajectory as measured three different ways in
Fig. S3. The relative behaviors of $\Phi_M$ measured each way were similar for each trajectory. These values demonstrate that the method utilized for the data in Fig. S2 and in the main text avoided the very large fluctuations likely associated with the sampling of unusual, or far from equilibrium atomic structures during the dynamics. We can further rationalize this choice by the limitation of relatively short trajectories and our interest in water under bias at thermal equilibrium. The fluctuations of $\Phi_M$ even with our chosen method were large compared to those of $\Phi_S$, underscoring the trade-off between fluctuations in potential vs. charge in fixed-charge and fixed-potential methodologies, respectively.

![Graph](image)

Figure S3: Values of $\Phi_M$ for the $\sigma = +0.2 \, e$ trajectory as computed as the value of $\Phi$ at a fixed $z$ near the middle of the slab (black), the value of $\Phi$ at the average value of $z$ for all Au atoms (green), and as the average value of $\Phi$ in the back 1 Å of the Au slab, within the fixed layer (purple; same as corresponding data in Fig. S2).

The system’s Fermi level $E_F$ exhibits even larger fluctuations than $\Phi_M$, measured any way, during the trajectories, as shown in Fig. S4. While the system’s Fermi energy has been used as a reliable metal potential in static or other applications, it was satisfactory in this work to utilize the more stable $\Phi_M$ as measured at the partially-frozen back of the Au(111) slab.
Figure S4: Computed Fermi energies $E_F$ of the system every 100 MD steps ($\sim$0.48 fs) in each trajectory. Note that the scale on which this quantity is plotted is much larger than that of $\Phi_M$ in Fig. S2.

2 Water hydrogen bonding and orientations

The structural properties of water at the Au(111) interface were further quantified by counting the average numbers of hydrogen bonds formed by water as functions of both its layer and the applied voltage vs. PZC, $\varphi$. Hydrogen bonds were defined by O atoms being less than 3.5 Å apart with an ODO angle within $30^\circ$ of colinear. The average numbers of hydrogen bonds formed by water molecules in each layer were further distinguished by whether the hydrogen bond was formed with another water molecule of the same or of a neighboring layer. These values are reflected in Figs. S5-S7.
Figure S5: Average numbers of hydrogen bonds in layer 1 of water as a function of \( \varphi \), delineated by intra- (cyan) and inter-layer (magenta) contributions. Layer 1 water formed fewer hydrogen bonds than water in layers 2 and 3. Water in this layer formed more hydrogen bonds at \( \varphi \geq 0 \) V vs. PZC and the proportion of intra-layer hydrogen bonds generally increased with \( \varphi \).

Figure S6: Average numbers of hydrogen bonds in layer 2 of water as a function of \( \varphi \), delineated by intra- (cyan) and inter-layer (magenta) contributions. Water in layer 2 demonstrated the most overall hydrogen bonds of the three layers studied. The overall number of hydrogen bonds in this layer was not apparently \( \varphi \)-dependent, although the proportion of intra-layer hydrogen bonds generally decreased with \( \varphi \), in opposition to the trend in layer 1.
Figure S7: Average numbers of hydrogen bonds in layer 3 of water as a function of $\varphi$, delineated by intra- (cyan) and inter-layer (magenta) contributions. Layer 3 water formed slightly fewer hydrogen bonds on average compared to layer 2, and neither the overall number nor the proportion of intra- to inter-layer hydrogen bonds demonstrated a clear dependence on $\varphi$.

From Fig. S5 it is evident that the total average number of hydrogen bonds formed by layer 1 water is lower at negative $\varphi$ than at PZC and positive $\varphi$. Additionally in layer 1, we observed an increase in the number intra-layer hydrogen bonding and a decrease in inter-layer hydrogen bonding when going from negative $\varphi$ to zero and positive $\varphi$. That layer 1 water at $\varphi \geq 0$ V exhibits more overall and intra-layer hydrogen bonds than at $\varphi < 0$ is consistent with the higher densities observed at these potentials. This observation is likely also a consequence of the O atom being more likely than not oriented towards the Au surface at non-negative $\varphi$ given that the O atom typically participates in two hydrogen bonds compared to one for H atoms. Therefore, when O is oriented towards Au and not towards layer 2, its ability to form inter-layer hydrogen bonds is suppressed. The hydrogen bonding similarities between the system at PZC and at $\varphi > 0$ in layer 1 are consistent with their similarities in density as a function of $z$ as well.

Figs. S6 and S7 demonstrate that layer 2 water participates in the most hydrogen bonds overall of the 3 studied. The average overall numbers of hydrogen bonds formed per water in layers 2 and 3 did not show any clear dependence on $\varphi$, consistent with the diminished dependence of $D_\parallel$ and the VDOS spectra on $\varphi$ in these two layers. In addition, the proportion of intra- and inter-layer hydrogen bonds in layer 2 with respect to $\varphi$ was
opposite to that in layer 1. In layer 3, the hydrogen bonding data did not seem to depend on $\varphi$ and the differences with $\varphi$ were likely within the error of the short simulations.

The effects of $\varphi$ on water’s orientation persisted beyond layer 1, the data for which is given in the main text. The orientations of the water bisectors and OD bonds with respect to surface normal for all layers and $\varphi$ are given in Figs. S8 and S9.

Figure S8: Histograms of the cosines of the angles formed between water’s bisector and a unit vector in $z$ for all $\varphi$ and all layers (1: magenta, 2: red, 3: orange, 4: gray). The inset illustration indicates the relevant angle $\theta$ in which the yellow rectangle represents the Au slab, the O atom is red, and the D atoms are white. The effects of $\varphi$ on water’s orientations relative to surface-normal were strongest in layer 1, but persisted into layers 2 and 3.

Figure S9: Histograms of the cosines of the angles formed between OD bond vectors and a unit vector in $z$ for all $\varphi$ and all layers (1: magenta, 2: red, 3: orange, 4: gray). The inset illustration indicates the relevant angles $\theta$ in which the yellow rectangle represents the Au slab, the O atom is red, and the D atoms are white. The effects of $\varphi$ on the orientations of water’s OD bonds relative to surface-normal were strongest in layer 1, but persisted into layers 2 and 3.
3 Mean square displacements

The O atom MSDs in \( x \) and \( y \) up to about half of the total trajectory times for each \( \varphi \) and layers 1-3 were computed to determine the values of \( D_\parallel \) shown in the main text. These are depicted here in Figs. S10-S12. The best fit slopes of the \( xy \) MSDs were used in Einstein’s relation to obtain the 2D diffusion coefficients.

Figure S10: Mean-square displacements in \( x \) and \( y \) for water O atoms in layer 1 for each \( \varphi \) as a function of simulation time \( t \) up to about half of the total BOMD trajectory time. The slopes of the best linear fits to these MSDs were related to the parallel diffusion coefficients \( D_\parallel \) shown in the main text. Water in this layer diffused parallel to the surface most at negative \( \varphi \), consistent with their lower densities and the layer’s greater distance from the surface. That the displacements of O atoms in layer 1 were smaller at positive \( \varphi \) is also consistent with the O atom being electrostatically attracted to the surface. Note that deviations from linearity for some trajectories are reflected in the large error bars in Fig. 7.
Figure S11: Mean-square displacements in $x$ and $y$ for water O atoms in layer 2 for each $\phi$ as a function of simulation time $t$ up to about half of the total BOMD trajectory time. The slopes of the best linear fits to these MSDs were related to the parallel diffusion coefficients $D_\parallel$ shown in the main text. Water in layer 2 diffused parallel to the surface most at small, non-zero $\phi$, regardless of sign. At the largest in magnitude values of $\phi$, water diffused parallel to the surface more than at PZC. Note that deviations from linearity for some trajectories are reflected in the large error bars in Fig. 7.

Figure S12: Mean-square displacements in $x$ and $y$ for water O atoms in layer 3 for each $\phi$ as a function of simulation time $t$ up to about half of the total BOMD trajectory time. The slopes of the best linear fits to these MSDs were related to the parallel diffusion coefficients $D_\parallel$ shown in the main text. Water in layer 3 diffused parallel to the surface most at small, non-zero $\phi$, regardless of sign. At the largest in magnitude values of $\phi$, water diffused parallel to the surface more than at PZC. Note that deviations from linearity for some trajectories are reflected in the large error bars in Fig. 7.
4 Velocity autocorrelation functions

The velocity autocorrelation functions of all water atoms for each $\varphi$ and layers 1-3 were computed and shown in Figs. S13-S15. The first 1200 fs of each were Fourier transformed to obtain the corresponding VDOS spectra.

Figure S13: Velocity autocorrelation functions $\langle v(0)v(t) \rangle$ of water O and D atoms in layer 1 for each $\varphi$. The first 1200 fs were Fourier transformed to obtained the VDOS spectra shown in the main text.

Figure S14: Velocity autocorrelation functions $\langle v(0)v(t) \rangle$ of water O and D atoms in layer 2 for each $\varphi$. The first 1200 fs were Fourier transformed to obtained the VDOS spectra shown in the main text.
Figure S15: Velocity autocorrelation functions $\langle v(0)v(t) \rangle$ of water O and D atoms in layer 3 for each $\phi$. The first 1200 fs were Fourier transformed to obtained the VDOS spectra shown in the main text.

5 Additional VDOS spectra and analysis

The VDOS spectra shown in the main text were obtained from the Fourier-transformed velocity autocorrelation functions, followed by Gaussian convolution. The resolution of the VDOS spectra that corresponds to the $\sim$0.48 fs time step was about $\sim$27 cm$^{-1}$. We further note here that the interpretations of the VDOS spectra are limited to mainly qualitative observations regarding the effects of distance from the surface and $\phi$ given the relatively short BOMD trajectories.

Figs. S16-S18 show the referenced VDOS spectra for layers 1-3 corresponding to those in the main text, with the $\phi = 0$ V spectrum of each layer as the reference. These referenced spectra are all plotted on the same scale. The referenced spectra highlight shifts and differences in intensity at different $\phi$ for each of the first three layers of water from the electrode. These spectra are clearly most intense in layer 1, where the effects of the electrode electrification are greatest. The referenced spectra for layer 1 demonstrate that both the $\delta$DOD and $\nu$OD peaks are blue shifted at non-zero $\phi$. The referenced $\nu$OD signals in layers 2 and 3 for non-zero $\phi$ are slightly negative at the lower frequencies characteristic of $\nu$OD and slightly positive at the higher frequencies characteristic of $\nu$OD. This is consistent of water molecules in layers 2 and 3 being somewhat oriented according to the screened electric field (Figs. S8 and S9).
Figure S16: VDOS spectra at each $\varphi$ for layer 1 water referenced to PZC (black; zero by construction). Negative intensities at lower frequencies and positive intensities at higher frequencies around both regions of interest are representative of blue shifts of both peaks at non-zero $\varphi$.

Figure S17: VDOS spectra at each $\varphi$ for layer 2 water referenced to PZC (black; zero by construction). The lower intensities relative to layer 1 are indicative of a lesser effect of the electrode potential on the vibrational spectra.
Figure S18: VDOS spectra at each $\varphi$ for layer 3 water referenced to PZC (black; zero by construction). The lower intensities relative to layer 1 are indicative of a lesser effect of the electrode potential on the vibrational spectra.

For the purposes of measuring the positions and integrating the intensities of the two VDOS peaks of interest despite the $\sim 27$ cm$^{-1}$ resolution, we interpolated between data points for the appropriate portions of each spectra. The positions of the $\delta$DOD peaks were sensitive to both $\varphi$ and the layer. These data are shown in Fig. S19. In layer 1, the peak occurs at a higher frequency at all non-zero $\varphi$, as discussed in the main text. We observed blue shifts of this vibrational mode's frequency in layer 1 was up to about 10 cm$^{-1}$ at modest positive and negative $\varphi$. Layer 2 demonstrated very little effect of $\varphi$ on the $\delta$DOD peak position and the $\delta$DOD peak position in layer 3 appeared to blue shift with increasing $\varphi$. Moreover, the position of the $\delta$DOD peak in layer 1 was red-shifted relative to those of layers 2 an 3. This is characteristic of water with a weakened hydrogen bonding network,$^6$ consistent with the observation of the least number of hydrogen bonds formed on average in layer 1 (Figs. S5,$^7$ S7).
Figure S19: Positions of the water $\delta$DOD peaks for each $\varphi$ and layers 1-3 as determined by the maximum values of the interpolating functions in this region of the spectra.

The positions of the water $\nu$OD peaks for each $\varphi$ and layers 1-3 were also determined via interpolation are shown in Fig. S20. We only investigated the global maxima of the interpolating functions for each spectrum despite there likely being several characteristic $\nu$OD peaks. These data also demonstrate that in layer 1 the position of the peak was blue-shifted at all non-zero $\varphi$, with shifts of the positions of maximum frequency of over 100 cm$^{-1}$. There was no discernible pattern in the $\nu$OD peak positions beyond layer 1.

Figure S20: Positions of the water $\nu$OD peaks for each $\varphi$ and layers 1-3 as determined by the maximum values of the interpolating functions in this region of the spectra.

We also integrated the total intensities of the $\delta$DOD peaks using the interpolated spectra. These integrated intensities are shown in Fig. S21. For layer 1, we observed a minimum integrated spectral intensity for $\delta$DOD at the PZC, which was also observed for SEIRAS spectra of aqueous electrolytes on Au(111). We observed a maximal integrated
δDOD peak intensity at the most negative φ studied. There were no discernible patterns observed among the integrated intensities of the δDOD peaks in layers 2 and 3.

Figure S21: Integrated intensities (arbitrary units) of the water δDOD peaks for each φ and layers 1-3. The integration range was 1000-1400 cm\(^{-1}\).

For comparison, we also computed the VDOS spectra from the velocity autocorrelation functions only in the surface-normal dimension \(z\) given the importance of surface-normal dipoles in many surface-enhanced spectroscopies. These are shown alongside their corresponding 3D VDOS spectra in Figs. S22-S24. For the most part, the \(z\)-only VDOS spectra hew closely to the full VDOS spectra, especially in the second and third layers. In layer 1, the \(z\)-only VDOS spectra demonstrate some subtle differences from the 3D spectra: The δDOD peaks appear slightly red-shifted in the \(z\)-only spectra relative to the full spectra. In addition, the \(z\)-only spectra for layer 1 generally hew to only the second \(\nu\)OD peaks of the full spectra for \(\varphi \neq 0\) V. That this is more evident when there is a non-zero potential is consistent with the observation of water molecules that are more oriented along the surface-normal electric fields associated with the applied biases. This difference between the full and \(z\)-only spectra furthermore suggests that there are more than one characteristic \(\nu\)OD mode in this heterogeneous environment. However, it is likely that all vibrational modes are strongly coupled between the (arbitrary) Cartesian dimensions given the overall similarities between the spectra.
Figure S22: Layer 1 water VDOS spectra obtained from the 3D velocity autocorrelation functions (solid; same as main text) and from the $z$ velocity autocorrelation functions (dashed). The spectra for each $\varphi$ are shifted arbitrarily for clarity.

Figure S23: Layer 2 water VDOS spectra obtained from the 3D velocity autocorrelation functions (solid; same as main text) and from the $z$ velocity autocorrelation functions (dashed). The spectra for each $\varphi$ are shifted arbitrarily for clarity.

Figure S24: Layer 3 water VDOS spectra obtained from the 3D velocity autocorrelation functions (solid; same as main text) and from the $z$ velocity autocorrelation functions (dashed). The spectra for each $\varphi$ are shifted arbitrarily for clarity.
The integrated intensities of the $\delta$DOD peaks for the 3D and $z$-only VDOS spectra for layer 1 water are shown in Fig. S25. These integrals show discrepancies only at positive $\varphi$, and for the $z$-only spectra the integrated intensity is no longer minimal at PZC.

Figure S25: Integrated intensities (arbitrary units) of the water $\delta$DOD peaks in the 3D (magenta) and $z$-only (light pink) VDOS spectra for layer 1 water.

6 Representative input files and initial Cartesian coordinates

Example Quantum-ESPRESSO PWscf input file, including initial coordinates, for the $\sigma = -0.4 e$ trajectory:

```plaintext
&CONTROL
  restart_mode = 'restart',
  calculation = 'md',
  max_seconds = 3520,
  prefix = 'AuH2O',
  outdir = './',
  pseudo_dir = '/home/zkg/ONCV-pseudos/',
  etot_conv_thr = 1.0D-4,
  forcc_conv_thr = 1.0D-3,
  dt = 10.0,
  wf_collect = .TRUE.,
  tefield = .true.,
  dipfield = .true.,
  gate = .true.,
/
&SYSTEM
  ibrav = 0,
  !      celldm(1) = 7.89223,
  nspin = 1,
  tot_charge = -0.4,
```

S17
nat = 216,
ntyp = 3,
ecutwfc = 60,
occupations = 'smearing', smearing = 'cold', degauss = 0.01,
edir = 3,
emaxpos = 0.99,
eopreg = 0.95,
zgate = 0.87,
block = .true.,
block_1 = 0.743665,
block_2 = 0.91,
block_height = 0.25,
/
&ELECTRONS
conv_thr = 1.D-4,
mixing_mode = 'plain',
mixing_beta = 0.5D0,
startingwfc = 'file',
startingpot = 'file',
electron_maxstep = 150,
/
&IONS
ion_dynamics = 'verlet',
pot_extrapolation = 'first_order',
wfc_extrapolation = 'none',
ion_temperature = 'rescaling',
tempw = 330.D0,
tolp = 100.D0,
/
K_POINTS { gamma }

ATOMIC_SPECIES
Au 196.96657 Au_ONCV_PBE-1.0.UPF
H 2.00 H_ONCV_PBE-1.0.UPF
O 15.999 O_ONCV_PBE-1.0.UPF

CELL_PARAMETERS (angstrom)
10.226698060 0.000000000 0.000000000
0.000000000 11.808773755 0.000000000
0.000000000 0.000000000 36.000000000

ATOMIC_POSITIONS (angstrom)
Au 5.113345000 0.000000000 6.410460000 1 1 0
Au 7.670027730 1.476096250 6.410460000 1 1 0
Au 5.113345000 2.952192500 6.410460000 1 1 0
Au 7.670027730 4.428288750 6.410460000 1 1 0
Au 5.113345000 5.904385000 6.410460000 1 1 0
Au 7.670027730 7.380481250 6.410460000 1 1 0
Au 5.113345000 8.856672500 6.410460000 1 1 0
Au 7.670027730 10.32673750 6.410460000 1 1 0
Au 0.000000000 0.000000000 6.410460000 1 1 0
Au 2.556672500 1.476096250 6.410460000 1 1 0
Au 0.000000000 2.952192500 6.410460000 1 1 0
Au 2.556672500 4.428288750 6.410460000 1 1 0
Au 0.000000000 5.904385000 6.410460000 1 1 0
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Au 0.000000000 8.856577500 6.410460000 1 1 0
Au 2.556672500 10.332673750 6.410460000 1 1 0
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Au 6.817796740 2.952192500 8.820910000
Au 9.374469240 4.428288750 8.820910000
Au 6.817796740 5.904385000 8.820910000
Au 9.374469240 7.380481250 8.820910000
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Au 1.704451740 2.952192500 8.820910000
Au 4.261124240 4.428288750 8.820910000
Au 1.704451740 5.904385000 8.820910000
Au 4.261124240 7.380481250 8.820910000
Au 1.704451740 8.856577500 8.820910000
Au 4.261124240 10.332673750 8.820910000
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Au 5.965575980 1.476096250 11.231400000
Au 8.522248480 2.952192500 11.231400000
Au 5.965575980 4.428288750 11.231400000
Au 8.522248480 5.904385000 11.231400000
Au 5.965575980 7.380481250 11.231400000
Au 8.522248480 8.856577500 11.231400000
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Au 3.408903480 2.952192500 11.231400000
Au 0.852224850 4.428288750 11.231400000
Au 3.408903480 5.904385000 11.231400000
Au 0.852224850 7.380481250 11.231400000
Au 3.408903480 8.856577500 11.231400000
Au 0.852224850 10.332673750 11.231400000
O 3.474117948 8.795442378 23.759914278
H 3.580137747 7.833496774 23.759914278
H 2.541373385 8.908932147 23.759914278
O 4.097545029 4.670815939 20.864088030
H 3.303533920 4.11578906 20.873099898
H 4.764900793 4.050070607 20.505774890
O 2.90912584 8.542762202 17.217268989
H 3.396052387 7.683220980 17.289937227
H 2.312305576 8.508994790 16.416936571
O 0.232576032 4.304660875 21.044962170
H 0.685409235 3.895099936 21.810698945
O 0.571792465 3.830027377 20.266290198
O 2.040303802 9.224822479 21.022950338
H 2.565430742 8.461253552 20.633679016
H 2.440159050 9.357660497 21.894829355
O 3.814232983 7.519272386 14.513869883
H 3.861329045 6.691738014 15.054334810
H 3.740420357 7.178721275 13.597302711
O  8.784266081  8.106721185  22.922853506
H  7.861763259  7.871519202  22.132015071
H  7.702839380  8.357769686  15.292888970
O  1.248163681  7.390322464  14.849388600
H  1.104129925  8.635969590  15.616902938
O  10.082773089  7.106780784  20.737625620
H  0.763857614  7.480847628  20.760174626
H  0.006667415  6.136304498  20.700411653
O  5.340199259  11.240543292  14.919425159
H  5.731463722  10.363702970  14.807367800
H  4.368268790  11.058476767  14.892990557
O  7.187144861  2.890747058  23.681981996
H  8.090164596  2.938478766  24.021221265
H  6.928916285  1.939348005  23.735326136
O  4.777842336  3.950702741  18.053653533
H  5.535400463  9.616309354  18.075493438
H  4.068274911  9.715285417  17.606037243
O  4.643734084  3.357215799  17.488688572
H  4.650260212  2.532359508  16.956464823
H  5.321849959  3.189297114  18.169821351
O  1.357360322  6.196853128  14.571333565
H  0.527620207  5.693428033  14.813738514
H  1.686111298  5.775095878  13.750884539
O  8.701744661  2.890747058  23.681981996
H  7.424519336  7.537135286  15.367479610
H  9.037741243  6.817169423  15.072826007
O  9.696677435  5.427750273  24.025243758
H  10.273246478  4.508601130  23.928956051
H  9.825442120  5.739686861  23.120100759
O  2.188042220  1.037771562  17.156754963
H  2.406764988  0.773520384  16.245266186
H  2.044255473  12.029971974  17.683522319
O  6.108185019  8.772426972  14.332849826
H  6.512706917  7.998699955  13.88221341
H  5.206968795  8.377215444  14.512851591
H  2.406270430  3.237531190  20.368124086
H  1.820377219  1.626642689  20.719900776
O  3.211567483  1.860979536  20.111648467
H  4.710720305  2.125566874  14.820277806
H  5.119816000  1.254770380  14.663086060
H  3.763570969  1.928102807  14.656994079
O  5.928667169  0.732223829  17.371483246
H  6.091221470  12.376808279  16.426037003
H  5.453171943  11.708238437  17.622063179
O  3.915635019  0.708999047  23.001575333
O  2.982259975  0.458710579  23.117278009
H  4.057554913  0.651962033  22.034145573
O  4.187830893  4.866586562  14.830041757
H  4.624640332  4.175668730  15.364559229
H  3.350304101  4.430239194  14.530929367
Accompanying Environ\textsuperscript{1213} input file for the $\sigma = -0.4 \, e$ trajectory:

\begin{verbatim}
&ENVIRON
  !
  verbose = 2
  environ_thr = 1.d-1
  environ_type = 'input'
  env_electrostatic = .true.
  env_static_permittivity = 78.3D0
  env_dielectric_regions = 1
\end{verbatim}

S22
&BOUNDARY
    solvent_mode = 'electronic'
    solvent_radius = 7.0D0,
/
&ELECTROSTATIC
    !
    pbc_correction = 'none'
    pbc_dim = 2
    pbc_axis = 3
    !
    tol = 1.d-7
    mix = 0.6
    solver = 'iterative'
    auxiliary = 'full'
/
DIELECTRIC_REGIONS {angstrom}
1.0 1.0 5.5 5.5 6.4104 6.4104 0.5 2 3

Initial coordinates of the $\sigma = -0.2$ e trajectory:

|     |          |          |          |          |          |          |          |          |          |
|-----|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| Au  | 5.113345000 | 0.000000000 | 6.410460000 |          |          |          |          |          |          |
| Au  | 7.670027730 | 1.476096250 | 6.410460000 |          |          |          |          |          |          |
| Au  | 5.113345000 | 2.952192500 | 6.410460000 |          |          |          |          |          |          |
| Au  | 7.670027730 | 4.428288750 | 6.410460000 |          |          |          |          |          |          |
| Au  | 5.113345000 | 5.904385000 | 6.410460000 |          |          |          |          |          |          |
| Au  | 7.670027730 | 7.380481250 | 6.410460000 |          |          |          |          |          |          |
| Au  | 5.113345000 | 8.856577500 | 6.410460000 |          |          |          |          |          |          |
| Au  | 7.670027730 | 10.332673750 | 6.410460000 |          |          |          |          |          |          |
| Au  | 0.000000000 | 0.000000000 | 6.410460000 |          |          |          |          |          |          |
| Au  | 2.556672500 | 1.476096250 | 6.410460000 |          |          |          |          |          |          |
| Au  | 0.000000000 | 2.952192500 | 6.410460000 |          |          |          |          |          |          |
| Au  | 2.556672500 | 4.428288750 | 6.410460000 |          |          |          |          |          |          |
| Au  | 0.000000000 | 5.904385000 | 6.410460000 |          |          |          |          |          |          |
| Au  | 2.556672500 | 7.380481250 | 6.410460000 |          |          |          |          |          |          |
| Au  | 0.000000000 | 8.856577500 | 6.410460000 |          |          |          |          |          |          |
| Au  | 2.556672500 | 10.332673750 | 6.410460000 |          |          |          |          |          |          |
| Au  | 6.817796740 | 0.000000000 | 8.820910000 |          |          |          |          |          |          |
| Au  | 9.374469240 | 1.476096250 | 8.820910000 |          |          |          |          |          |          |
| Au  | 6.817796740 | 2.952192500 | 8.820910000 |          |          |          |          |          |          |
| Au  | 9.374469240 | 4.428288750 | 8.820910000 |          |          |          |          |          |          |
| Au  | 6.817796740 | 5.904385000 | 8.820910000 |          |          |          |          |          |          |
| Au  | 9.374469240 | 7.380481250 | 8.820910000 |          |          |          |          |          |          |
| Au  | 6.817796740 | 8.856577500 | 8.820910000 |          |          |          |          |          |          |
| Au  | 9.374469240 | 10.332673750 | 8.820910000 |          |          |          |          |          |          |
| Au  | 1.704451740 | 0.000000000 | 8.820910000 |          |          |          |          |          |          |
| Au  | 4.261124240 | 1.476096250 | 8.820910000 |          |          |          |          |          |          |
| Au  | 1.704451740 | 2.952192500 | 8.820910000 |          |          |          |          |          |          |
| Au  | 4.261124240 | 4.428288750 | 8.820910000 |          |          |          |          |          |          |
| Au  | 1.704451740 | 5.904385000 | 8.820910000 |          |          |          |          |          |          |
| Au  | 4.261124240 | 7.380481250 | 8.820910000 |          |          |          |          |          |          |

S23
|   | 1.704451740 | 8.856577500 | 8.820910000 |
|---|-------------|-------------|-------------|
| Au | 4.261124240 | 10.332673750 | 8.820910000 |
| Au | 8.522248480 | 0.000000000 | 11.231400000 |
| Au | 5.965575980 | 1.476096250 | 11.231400000 |
| Au | 8.522248480 | 2.952192500 | 11.231400000 |
| Au | 5.965575980 | 4.428288750 | 11.231400000 |
| Au | 8.522248480 | 5.904385000 | 11.231400000 |
| Au | 5.965575980 | 7.380481250 | 11.231400000 |
| Au | 8.522248480 | 8.856577500 | 11.231400000 |
| Au | 3.408903480 | 0.000000000 | 11.231400000 |
| Au | 0.852224850 | 1.476096250 | 11.231400000 |
| Au | 3.408903480 | 2.952192500 | 11.231400000 |
| Au | 0.852224850 | 4.428288750 | 11.231400000 |
| Au | 3.408903480 | 5.904385000 | 11.231400000 |
| Au | 0.852224850 | 7.380481250 | 11.231400000 |
| O | 3.392863129 | 8.809062166 | 23.694277586 |
| H | 3.430799695 | 7.839672957 | 23.699482202 |
| H | 2.626849334 | 9.025043682 | 24.247672842 |
| O | 4.100611148 | 6.083639381 | 20.958175486 |
| H | 3.305030210 | 4.076227276 | 21.104107817 |
| H | 4.720366595 | 3.941982484 | 20.572508445 |
| O | 2.935248419 | 8.581025711 | 17.307817174 |
| H | 3.415418403 | 7.718988414 | 17.427422307 |
| H | 2.313723223 | 8.502514644 | 16.541552606 |
| O | 0.437671013 | 4.235117830 | 21.080796629 |
| H | 0.326780003 | 3.663175735 | 21.839836725 |
| H | 0.446468981 | 3.846553181 | 20.283516859 |
| O | 2.053216842 | 9.154859539 | 21.151462693 |
| H | 2.554193247 | 8.429780061 | 20.687025652 |
| H | 2.403155132 | 9.145631908 | 22.070556559 |
| O | 3.853716830 | 7.542815393 | 14.472981998 |
| H | 3.907300409 | 6.706933215 | 14.999745493 |
| H | 3.781369607 | 7.217562682 | 13.550791354 |
| O | 6.473315818 | 0.334455691 | 23.730797688 |
| H | 5.489615292 | 0.354077254 | 23.613836238 |
| H | 6.88796059 | 11.284056986 | 24.128087026 |
| O | 4.286365818 | -0.170391849 | 20.270686922 |
| H | 4.682366286 | 10.933117828 | 20.826425418 |
| H | 4.312497523 | 11.178936379 | 19.385526174 |
| O | 7.524145072 | 1.010448944 | 21.159860074 |
| H | 7.519535202 | 12.049643567 | 20.550862367 |
| H | 7.217591943 | 0.648071430 | 22.019052206 |
| O | 9.650007722 | 10.857217229 | 17.519543852 |
| H | 8.279748643 | 9.596753942 | 17.555849014 |
| H | 10.462272859 | 10.747420244 | 18.093434563 |
| O | 6.963775444 | 3.437084455 | 14.019763645 |
| H | 7.476723509 | 2.639431914 | 14.265397769 |
| H | 6.035444876 | 3.137927626 | 14.172662914 |
| O | 1.329990906 | 6.008963153 | 17.708314185 |
| H | 1.439540820 | 5.023047747 | 17.834839378 |
| H | 1.725984397 | 6.195214516 | 16.835494068 |
|   |          |          |          |
|---|----------|----------|----------|
| O | 6.926793040 | 5.628968384 | 18.481327681 |
| H | 7.007642900 | 5.213697184 | 19.370352132 |
| H | 7.613598452 | 5.135907020 | 17.970201902 |
| O | 1.316216476 | 0.185395956 | 21.802899021 |
| H | 1.952418702 | 11.356222185 | 21.435172873 |
| H | 0.474874147 | 17.970201902 | 21.948713118 |
| O | 5.622012454 | 2.436962203 | 19.976765160 |
| H | 6.450571807 | 2.070638301 | 20.402117659 |
| H | 5.126813352 | 1.600497822 | 19.851215938 |
| O | -0.008905920 | 11.608006841 | 15.053907039 |
| H | 9.833822714 | 10.885075591 | 14.496058497 |
| H | 10.077150175 | 11.283038586 | 15.990474517 |
| O | 5.528242653 | 5.116966623 | 24.070739598 |
| H | 6.121384421 | 4.326029090 | 23.965343833 |
| H | 4.686313923 | 4.853525377 | 23.663942226 |
| O | 9.255197468 | 5.103843294 | 15.195698020 |
| H | 9.079881481 | 4.656453434 | 16.082406413 |
| H | 9.078323586 | 4.354410241 | 14.594598157 |
| O | 7.596080062 | 4.635257600 | 21.011763902 |
| H | 8.565895657 | 4.447180378 | 20.940339315 |
| O | 7.234783876 | 3.844400687 | 21.447387692 |
| O | 9.357856864 | 10.691429072 | 22.278343105 |
| H | 8.817783639 | 10.593623132 | 21.460746789 |
| H | 9.297614336 | 9.779554327 | 22.659371911 |
| O | 9.824590544 | 2.516453493 | 14.447823756 |
| H | 9.810996843 | 2.201957951 | 13.515122005 |
| H | 9.672774004 | 1.687898062 | 14.947470257 |
| O | 8.268927126 | 1.491772945 | 18.164085701 |
| H | 8.819579384 | 0.713024541 | 17.946563594 |
| H | 7.339351085 | 1.196165445 | 17.963693050 |
| O | 8.724775263 | 9.698252297 | 13.752235477 |
| O | 7.762307946 | 9.814977406 | 13.631640597 |
| O | 8.767108227 | 8.843797781 | 14.280003116 |
| O | 1.764631539 | 10.526622372 | 18.679232030 |
| O | 2.087374875 | 9.706718072 | 18.216716035 |
| O | 1.806512004 | 10.29391924 | 19.632245159 |
| H | 8.853747948 | 8.069654454 | 22.951234712 |
| H | 7.927049371 | 7.751061533 | 22.800270443 |
| H | 9.309255230 | 7.733396344 | 22.132968847 |
| O | 6.989953918 | 8.365873024 | 18.116662787 |
| H | 6.770824868 | 7.441304356 | 18.37843980 |
| H | 7.955520514 | 8.241522690 | 17.894974801 |
| O | 1.053967993 | 8.645789514 | 15.382081848 |
| H | 1.209663668 | 7.800699039 | 14.860895591 |
| O | 0.132225488 | 8.526715978 | 15.681775221 |
| O | 10.139208894 | 7.116857470 | 20.782128882 |
| O | 0.784326853 | 7.563713795 | 20.860579526 |
| O | 0.105728238 | 6.155229322 | 20.794425456 |
| H | 5.277516347 | 11.160116836 | 14.952820512 |
| H | 5.768883669 | 10.326974559 | 14.761892774 |
| H | 4.326823362 | 10.89478025 | 14.841257633 |
| O | 7.151405578 | 2.944582173 | 23.794734224 |
| H | 8.063446340 | 3.011237069 | 24.117787306 |
| H | 6.896383048 | 1.991081299 | 23.877506162 |
| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| O       | 6.511785937 | 6.858680157 | 22.168856232 |
| H       | 6.915481590 | 6.172327444 | 21.580777368 |
| H       | 6.080576255 | 6.296940853 | 22.866949849 |
| O       | 7.491547808 | 10.140862092 | 20.254360561 |
| H       | 6.778815182 | 9.909798768 | 20.890372087 |
| H       | 7.368491283 | 9.491002566 | 19.510204876 |
| O       | 6.562176495 | 6.125539028 | 14.299793150 |
| H       | 5.645246329 | 5.784018822 | 14.390471858 |
| H       | 7.082562613 | 5.291349371 | 14.285570749 |
| O       | 1.990671462 | 3.599797976 | 13.948932693 |
| H       | 2.191071726 | 2.709355297 | 13.583077951 |
| H       | 1.146612387 | 3.398942355 | 14.428755345 |
| O       | 4.369673646 | 6.247919763 | 17.483694310 |
| H       | 5.297479272 | 6.108315818 | 17.778203041 |
| H       | 4.606848038 | 5.329108943 | 17.358884859 |
| O       | 1.328804172 | 3.414979642 | 18.159122664 |
| H       | 1.795740487 | 3.063743493 | 18.960224625 |
| H       | 1.538678698 | 2.672561728 | 17.536195169 |
| O       | 7.567350980 | 0.752360432 | 14.542420580 |
| H       | 8.297254609 | 11.923804937 | 14.614202639 |
| H       | 6.768183665 | 0.222694492 | 14.341589562 |
| O       | 8.801305411 | 3.919271356 | 17.517617612 |
| H       | 8.567605006 | 2.955303556 | 17.62661670 |
| H       | 9.798259779 | 3.880242941 | 17.866917282 |

Initial coordinates of the $\sigma = 0$ e trajectory:

| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| Au      | 5.173900970 | 0.285728353 | 6.410460002 |
| Au      | 7.867060373 | 1.441943922 | 6.410460002 |
| Au      | 5.365586323 | 3.177701420 | 6.410460002 |
| Au      | 7.666171977 | 4.526538966 | 6.410460002 |
| Au      | 5.044124624 | 6.001230585 | 6.410460002 |
| Au      | 7.558271223 | 7.427015362 | 6.410460002 |
| Au      | 5.159361938 | 9.121919196 | 6.410460002 |
| Au      | 7.565397734 | 10.442693153 | 6.410460002 |
| Au      | -0.072087954 | 0.021347949 | 6.410460002 |
| Au      | 2.429646017 | 1.326647058 | 6.410460002 |
| Au      | 0.036836371 | 3.202833250 | 6.410460002 |
| Au      | 2.701797208 | 4.395996953 | 6.410460002 |
| Au      | -0.107874575 | 6.001697787 | 6.410460002 |
| Au      | 2.599128080 | 7.433233039 | 6.410460002 |
| Au      | -0.168108525 | 8.959495892 | 6.410460002 |
| Au      | 2.403573037 | 10.269330105 | 6.410460002 |
| Au      | 7.015335516 | 0.015058390 | 8.921855987 |
| Au      | 9.690183836 | 1.453864232 | 9.114868978 |
| Au      | 7.249581800 | 2.896182233 | 8.808896377 |
| Au      | 9.634691706 | 4.489380036 | 8.947297284 |
| Au      | 7.038029855 | 5.734501999 | 9.492410842 |
| Au      | 9.412766271 | 7.486525446 | 8.782613508 |
| Au      | 6.912689379 | 8.518094413 | 8.914351224 |
| Au      | 9.504088221 | 10.237350958 | 9.314531462 |
| Au      | 1.800434634 | 0.069655412 | 9.246583933 |
| Au      | 4.144759654 | 1.603168820 | 8.675883287 |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| H | 5.336033234 | 0.709336603 | 14.095992105 |
| O | 0.930527190  | 4.486536465  | 17.586099790  |
| H | 0.144632243  | 3.935756735  | 17.493859620  |
| H | 1.249701582  | 4.592671841  | 16.669398648  |
| O | 7.248755798  | 4.833896080  | 18.541366465  |
| H | 7.603810340  | 4.694177329  | 19.465138264  |
| H | 7.655471228  | 4.042749394  | 18.12447202  |
| O | 2.162237841  | -0.124970478 | 21.234109422 |
| H | 3.079516317  | 11.674197624 | 21.566845018 |
| H | 1.522265531  | 11.833132814 | 22.011082054 |
| O | 5.626374724  | 1.824307990  | 19.866219732  |
| H | 6.603634288  | 1.988291140  | 20.175910812  |
| H | 5.571344920  | 0.825282443  | 19.942950454  |
| O | 0.576069496  | 11.302009790 | 17.446648245  |
| H | 9.814600797  | 11.269285691 | 17.362855364  |
| H | 10.788021414 | 10.725035520 | 18.303323587  |
| O | 6.265158232  | 6.234045200  | 22.744571647  |
| H | 5.733415717  | 5.772747134  | 23.434367591  |
| H | 5.708816897  | 6.312874768  | 21.941660530  |
| O | 8.867423324  | 4.854729148  | 14.381319618  |
| H | 8.791134829  | 3.911042169  | 14.351024350  |
| H | 9.247951274  | 4.956512494  | 13.495113684  |
| O | 8.207059133  | 5.302567252  | 20.970701492  |
| H | 9.064914871  | 5.128297697  | 21.379687459  |
| H | 7.633044258  | 5.573090314  | 21.732279439  |
| O | 10.880352415 | 12.196561346 | 23.115128212  |
| H | 9.978481759  | 11.925311307 | 22.735529358  |
| H | 10.937735727 | 11.452735607 | 23.714853933  |
| O | 8.928654199  | 2.147204557  | 14.854833326  |
| O | 8.594436062  | 1.419760898  | 14.330751146  |
| H | 8.631613435  | 2.222338480  | 15.805110456  |
| O | 8.177048907  | -0.871629142 | 17.690466448  |
| O | 8.003558383  | -1.134096999 | 18.635810028  |
| H | 7.642658501  | -1.514342013 | 17.224436578  |
| O | 9.618764363  | 9.153628434  | 15.025097060  |
| H | 9.912789032  | 8.649973173  | 14.260992399  |
| H | 8.694271201  | 8.682213299  | 15.212660694  |
| O | 1.059487048  | 9.716508213  | 19.947634735  |
| H | 1.578420125  | 9.226805432  | 19.234852193  |
| H | 1.638793192  | 10.363878874 | 20.465734805  |
| O | 10.356059809 | 8.431276024  | 25.278778062  |
| H | 9.681474000  | 7.903293959  | 24.752943046  |
| H | 10.871160898 | 8.791970295  | 24.548647670  |
| O | 8.605127329  | 7.375965169  | 18.390586512  |
| H | 8.195581540  | 6.488458101  | 18.488754845  |
| H | 9.505812399  | 7.170585243  | 18.113937479  |
| O | 0.903902547  | 7.654699701  | 17.780457922  |
| H | 1.245702437  | 6.904773061  | 16.186473285  |
| O | 0.430838317  | 8.318904861  | 16.141898043  |
| H | 12.181140212 | 6.916444423  | 22.835605726  |
| O | 2.609181937  | 6.391237108  | 22.308341142  |
| H | 1.199417800  | 6.294103191  | 22.825220571  |
| O | 5.962666929  | 9.789913444  | 14.086203817  |
| H | 5.258909737  | 9.389116261  | 14.634592212  |
Initial coordinates of the $\sigma = +0.2 \ e$ trajectory:

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| Au   | 5.113345000 | 0.000000000 | 6.410460000 |
| Au   | 7.670027730  | 1.476096250 | 6.410460000 |
| Au   | 5.113345000 | 2.952192500 | 6.410460000 |
| Au   | 7.670027730  | 4.428288750 | 6.410460000 |
| Au   | 5.113345000 | 5.904385000 | 6.410460000 |
| Au   | 7.670027730  | 7.380481250 | 6.410460000 |
| Au   | 5.113345000 | 8.856577500 | 6.410460000 |
| Au   | 7.670027730  | 10.332673750 | 6.410460000 |
| Au   | 0.000000000  | 0.000000000 | 6.410460000 |
| Au   | 2.556672500  | 1.476096250 | 6.410460000 |
| Au   | 0.000000000  | 2.952192500 | 6.410460000 |
| Au   | 2.556672500  | 4.428288750 | 6.410460000 |
| Au   | 0.000000000  | 5.904385000 | 6.410460000 |
| Au   | 2.556672500  | 7.380481250 | 6.410460000 |
| Au   | 0.000000000  | 8.856577500 | 6.410460000 |
| Au   | 2.556672500  | 10.332673750 | 6.410460000 |
| Au   | 6.817796740  | 0.000000000 | 8.820910000 |
| Au   | 9.374469240  | 1.476096250 | 8.820910000 |
| Au   | 6.817796740  | 2.952192500 | 8.820910000 |
| Au   | 9.374469240  | 4.428288750 | 8.820910000 |
| Au   | 6.817796740  | 5.904385000 | 8.820910000 |
| Au   | 9.374469240  | 7.380481250 | 8.820910000 |
Au  6.817796740  8.856577500  8.820910000
Au  9.374469240  10.332673750  8.820910000
Au  1.704451740  0.000000000  8.820910000
Au  4.261124240  1.476096250  8.820910000
Au  1.704451740  2.952192500  8.820910000
Au  4.261124240  4.428288750  8.820910000
Au  1.704451740  5.904385000  8.820910000
Au  4.261124240  7.380481250  8.820910000
Au  1.704451740  8.856577500  8.820910000
Au  4.261124240 10.332673750  8.820910000
Au  8.522248480  0.000000000  11.231400000
Au  5.965575980  1.476096250  11.231400000
Au  8.522248480  2.952192500  11.231400000
Au  5.965575980  4.428288750  11.231400000
Au  8.522248480  5.904385000  11.231400000
Au  5.965575980  7.380481250  11.231400000
Au  8.522248480  8.856577500  11.231400000
Au  3.408903480  0.000000000  11.231400000
Au  0.852224850  1.476096250  11.231400000
Au  3.408903480  2.952192500  11.231400000
Au  0.852224850  4.428288750  11.231400000
Au  3.408903480  5.904385000  11.231400000
Au  0.852224850  7.380481250  11.231400000
Au  3.408903480  8.856577500  11.231400000
Au  0.852224850 10.332673750  11.231400000
H  3.174407839  8.885569710  23.565253910
H  3.342207432  7.952912601  23.744873124
H  2.850875803  9.219891126  24.416345793
O  4.045390418  4.564254159  21.053039948
H  3.254557215  4.024715490  21.053039948
H  3.254557215  4.024715490  21.053039948
O  2.925694174  8.619463630  17.327172869
H  3.361680847  7.745339415  17.481433402
H  2.752734922  8.522864611  16.584907151
O  0.019128389  4.221716935  21.156563057
H  0.351771044  3.673066368  21.923824640
H  0.410792674  3.833135653  20.365612681
O  1.977407831  9.134484178  21.143035037
H  2.587030188  8.499260820  20.703324062
H  2.77561138  9.104801876  22.089138368
O  3.824997750  7.569418352  14.500374096
H  3.974948611  6.849644564  15.155430001
O  3.702137537  7.07723995  13.668288046
H  6.515683450  0.370385412  23.677411977
H  5.52916664  0.364406763  23.62635381
H  6.764180066  11.498704418  24.317034866
O  4.310563661 -0.157887890  20.262897573
H  4.759965008  10.996012409  20.83420226
H  4.34954581  11.167912986  19.398795031
O  7.528682452  1.021536352  21.137073918
H  7.49019261  12.050235265  20.549904112
H  7.269166112  0.662435834  22.013510412
O  9.673971258  10.848214868  17.532034007

S32
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | 9.32125818 | 9.945077558 | 17.607073582 |
| H       | 10.47486373 | 10.78524219 | 18.127586147 |
| O       | 6.957732802 | 3.450519383 | 13.998534942 |
| H       | 7.492112243 | 2.674184164 | 14.255682290 |
| H       | 6.043641531 | 3.125019791 | 14.167297053 |
| O       | 1.335704574 | 6.009769557 | 17.718789636 |
| H       | 1.431659097 | 5.021391939 | 17.854036583 |
| H       | 1.816532170 | 6.213858472 | 16.904873543 |
| O       | 6.838267138 | 5.575973705 | 18.515721058 |
| H       | 6.942084913 | 5.178034809 | 19.411143054 |
| H       | 7.527098838 | 5.097472171 | 18.003501160 |
| O       | 1.288615077 | 0.190984759 | 21.713651255 |
| H       | 1.934924645 | 11.297457571 | 21.536900709 |
| H       | 0.443725847 | 11.468438782 | 21.901141110 |
| O       | 5.585084079 | 2.411616137 | 19.932470532 |
| H       | 6.443895241 | 2.114616269 | 20.339944030 |
| H       | 5.106228313 | 1.554559036 | 19.919411764 |
| O       | 0.019346633 | 11.58264213 | 15.070027473 |
| H       | 9.093388411 | 10.845021815 | 14.519107445 |
| H       | 10.082371459 | 11.27732638 | 16.009421132 |
| O       | 5.597326039 | 5.132919383 | 24.030835780 |
| H       | 6.140016601 | 4.306541910 | 23.916301790 |
| H       | 4.675640644 | 4.860097692 | 23.906682646 |
| O       | 9.264574830 | 5.114461995 | 15.203277648 |
| H       | 9.102884338 | 4.678840885 | 16.103804463 |
| H       | 9.082638829 | 4.351941626 | 14.626945630 |
| O       | 7.581404963 | 4.592699974 | 21.011307029 |
| H       | 8.555226160 | 4.433026163 | 21.008522520 |
| H       | 7.255621589 | 3.890792312 | 21.596221293 |
| O       | 9.365780827 | 10.702902811 | 22.250009159 |
| H       | 8.821781346 | 10.624720608 | 21.440147807 |
| H       | 9.282095786 | 9.789102161 | 22.622029647 |
| O       | 9.816906301 | 2.518210398 | 14.492927706 |
| H       | 9.754412126 | 2.130077612 | 13.599149109 |
| H       | 9.589143596 | 1.775713901 | 15.080089687 |
| O       | 8.269797391 | 1.498805887 | 18.115317078 |
| H       | 8.803790824 | 0.697431404 | 17.956553325 |
| H       | 7.335577597 | 1.207934201 | 17.949628501 |
| O       | 8.700277747 | 9.681798407 | 13.735487521 |
| H       | 7.736752368 | 9.757506527 | 13.587805542 |
| H       | 8.745984777 | 8.828006235 | 14.258965707 |
| O       | 1.749611932 | 10.582472458 | 18.747810174 |
| H       | 2.076823947 | 9.758712879 | 18.300626197 |
| O       | 1.758904114 | 10.367762921 | 19.709599186 |
| H       | 8.824897452 | 8.137105161 | 22.895300690 |
| H       | 7.914841253 | 7.785862514 | 22.767032160 |
| H       | 9.299424739 | 7.757277016 | 22.120336391 |
| H       | 7.032150474 | 8.308273733 | 17.998367847 |
| H       | 6.746606843 | 7.419881134 | 18.307229576 |
| H       | 8.030252232 | 8.168247536 | 17.977772780 |
| O       | 1.045815637 | 8.638291708 | 15.400872936 |
| H       | 1.232941708 | 7.862248654 | 14.806422002 |
| O       | 0.132835201 | 8.450380366 | 15.687744215 |
| H       | 10.163033710 | 7.118710243 | 20.718058394 |
H 0.792456873  7.589025151  20.861249102
H 0.129096716  6.160232316  20.767730951
O 5.332783408  11.102276394  14.901001969
H 5.812094317  10.250295400  14.787792166
H 4.380664269  10.838330133  14.852984648
O 7.207214834  2.965356359  23.744907436
H 7.973861128  3.056170024  24.327539937
H 6.935164673  2.012627150  23.804727148
O 4.870470756  10.190112669  18.042712518
H 5.612839237  9.547419788  18.052225102
H 4.124986850  9.708303115  17.600159199
O 4.687032156  3.414827361  13.369065580
H 4.763263912  2.530717928  16.965902111
H 5.191545849  3.086585999  18.20599794
O 1.173927458  6.321231247  14.217037180
H 0.452528775  5.761829214  14.609881099
H 1.685054765  5.764072845  13.602147959
O 8.684119020  7.650356264  15.386705986
H 7.819371468  7.768017371  15.819566810
H 8.753705515  6.92633940  15.184828295
O 10.152413133  5.588666682  24.113170035
H 10.172560066  4.655167304  24.333566837
H 9.767236946  5.656858766  23.226861624
O 2.185802519  1.051385528  17.132638144
H 2.463458597  0.768018900  16.247393621
H 2.10238116  12.066835913  17.703563082
O 6.168796242  8.696546776  14.076367758
H 6.10766963  7.808600223  14.102321176
H 5.232799715  8.380120945  14.220661865
O 2.319047149  2.232903354  20.281880578
H 1.768097850  1.53960367  20.732089648
H 3.10399821  1.742540635  19.979218572
O 4.727049532  2.027895630  14.656006505
H 5.010209612  1.097311886  14.738095452
H 3.761894766  1.945450794  14.545021848
O 5.840259714  0.779399620  17.254931795
H 6.167467450  12.379924164  16.362118609
H 5.451400759  11.719201399  15.527330007
O 3.963833758  0.763463592  23.108586635
H 3.124950690  0.474596689  23.490242681
H 3.863836958  0.670892632  22.146349796
O 4.205301977  4.843716105  14.910043337
H 4.530704023  4.321237468  15.671002632
H 3.445303384  4.326797821  14.556975186
H 2.855596229  6.849044051  20.02995751
H 2.349794306  6.649682345  19.207815158
H 3.447633355  6.070800583  20.167221264
H 5.282203406  9.293489016  21.700791721
H 4.675075344  9.358342664  22.467180818
H 5.602133253  8.356070092  21.729516780
O 1.137273384  2.655282159  23.145547520
H 1.199740104  1.754906854  22.757097210
H 0.734668599  2.489619210  24.008083335
O 2.902422400  10.205364531  14.382547280

S34
Initial coordinates of the $\sigma = +0.4\ e$ trajectory:

| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| Au      | 5.799776829 | -0.158542157 | 6.410460017 |
| Au      | 8.484172050  | 1.407882777  | 6.410460017 |
| Au      | 6.122186702  | 2.926058435  | 6.410460017 |
| Au      | 8.573679878  | 4.576814038  | 6.410460017 |
| Au      | 6.122546608  | 6.073008003  | 6.410460017 |
| Au      | 8.656684160  | 7.482968567  | 6.410460017 |
| Au      | 6.260444383  | 8.884357166  | 6.410460017 |
| Au      | 8.782948805  | 10.384701912 | 6.410460017 |
| Au      | 0.864699091  | 0.229869785  | 6.410460017 |
| Au      | 3.518459656  | 1.667466093  | 6.410460017 |
| Au      | 0.898062719  | 3.076684134  | 6.410460017 |
| Au      | 3.628981003  | 4.563718576  | 6.410460017 |
| Au      | 1.102728579  | 5.920505115  | 6.410460017 |
| Au      | 3.839037014  | 7.640788576  | 6.410460017 |
| Au      | 1.000347462  | 8.696670428  | 6.410460017 |
| Au      | 3.249749737  | 10.633727989 | 6.410460017 |
| Au      | 8.142020248  | -0.054556550 | 8.965861111 |
| Au      | 10.575515669 | 1.624901402 | 9.026385755 |
Au 7.913313523  2.909946746  9.059004516  8.843276392
Au 10.090753067  5.824733553  8.78613322  8.990134219
Au 7.928759140  8.915124688  9.27166991  8.797772881
Au 10.591282129  10.283552926  8.92734942  8.93380567
Au 2.862533729  0.216037557  8.933880567  8.89472921
Au 5.418968532  1.426741492  9.12462144  8.96240654
Au 2.337246418  3.259453982  8.933724942  8.85173004
Au 5.035318191  4.32954498  8.933724942  8.89472921
Au 2.834098834  3.259453982  8.881573004  8.85173004
Au 5.035318191  6.134843839  8.933724942  8.85173004
Au 2.832263932  4.32954498  8.933724942  8.85173004
Au 5.298765450  10.283552926  8.797772881  8.810888419
Au 9.728466898  0.071866192  11.431029755  11.433997647
Au 6.675029246  1.875058290  11.55751471  11.320144174
Au 9.784118388  3.117898406  11.320144174  11.433997647
Au 7.157275295  4.51286016  11.827056979  11.433997647
Au 9.618127078  6.184731482  11.475463026  11.433997647
Au 7.149007869  7.540630506  11.226378753  11.433997647
Au 9.689022826  9.042710609  11.519900955  11.433997647
Au 7.269678541  10.326953997  11.542049665  11.433997647
Au 4.621129224  -0.146224698  11.433997647  11.433997647
Au 1.883226656  1.510450848  11.433997647  11.433997647
Au 4.172652600  3.250950344  11.433997647  11.433997647
Au 1.830909190  4.612753625  11.433997647  11.433997647
Au 4.535871582  5.974348075  11.433997647  11.433997647
Au 1.958505324  7.457927486  11.433997647  11.433997647
Au 4.632188918  8.963142798  11.433997647  11.433997647
Au 2.012425723  10.557902512  11.433997647  11.433997647
O  1.909546471  9.460504051  22.144395451  22.144395451
H  1.501061692  9.467645863  23.115328772  23.115328772
H  2.763831335  9.986823442  22.177953399  22.177953399
O  3.162031844  3.279639528  17.656298377  17.656298377
H  2.196458902  3.377715755  17.401880805  17.401880805
O  3.478936087  2.386680009  17.745916436  17.745916436
H  1.262437898  6.116699576  17.926863797  17.926863797
O  0.524282468  5.881252683  18.615510426  18.615510426
H  1.93124902  5.263765450  17.33292940  17.33292940
O  -5.687484221  1.355968333  26.00832219  26.00832219
H  -5.508168764  1.403312599  26.917924249  26.917924249
H  -5.896929949  0.433013434  25.999244602  25.999244602
O  7.229642090  7.683588593  20.893980453  20.893980453
H  7.940799740  7.046263729  21.302157794  21.302157794
H  7.789487953  8.358162473  20.44228406  20.44228406
O  2.463193876  5.353481519  14.065129248  14.065129248
H  2.851440983  5.172361625  14.949609685  14.949609685
H  2.924692113  4.710278248  13.537664158  13.537664158
O  5.901669303  2.037906900  20.934024173  20.934024173
H  4.987723797  1.779155106  21.023401674  21.023401674
H  6.495688620  13.223541711  20.684282959  20.684282959
O  4.878358301  -0.873445981  19.471816854  19.471816854
H  4.998362463  10.418970972  20.25727940  20.25727940
H  5.430316184  10.508897084  18.737143623  18.737143623

S36
|Atom| X    | Y    | Z    |
|----|------|------|------|
|O   | 9.181151475 | -0.934041110 | 25.240579928 |
|H   | 9.383754206  | 11.697446116 | 25.667972626 |
|H   | 8.271202197  | -0.899041601 | 17.329526846 |
|O   | 10.541375249 | 8.568836588  | 16.966303289 |
|H   | 11.21546304  | 9.248711067  | 16.899541435 |
|O   | 6.371645188  | 1.766648649  | 13.779302649 |
|H   | 7.018727165  | 0.962117313  | 14.065310897 |
|H   | 5.650951453  | 1.916976121  | 14.162006540 |
|O   | 1.955498796  | 3.788260547  | 20.20039811 |
|H   | 2.386715967  | 3.587138569  | 19.315216612 |
|O   | 1.630904938  | 2.941165938  | 20.467414165 |
|H   | 5.989188425  | 3.541113866  | 18.424564310 |
|H   | 6.155976341  | 4.468091832  | 18.559306487 |
|O   | 5.944971630  | 3.239721239  | 19.404495698 |
|H   | 0.911073238  | -1.104803402 | 19.519374445 |
|O   | 1.404290221  | 10.572894558 | 18.692658783 |
|H   | 0.954849217  | 9.906827671  | 20.184418047 |
|O   | 4.317263222  | 0.912375909  | 17.708459151 |
|H   | 4.659370264  | 0.610360359  | 16.848539929 |
|O   | 4.753610746  | 0.452105387  | 18.421135970 |
|O   | 0.388595640  | 9.12883681   | 14.51450051 |
|H   | 10.066258329 | 8.635539967  | 15.358953532 |
|H   | 9.063124466  | 8.643920594  | 14.072093830 |
|O   | 0.926726310  | 9.304234589  | 24.543496710 |
|H   | 0.130446551  | 9.833896742  | 24.854225296 |
|H   | 1.746790470  | 9.491957786  | 25.105295177 |
|O   | 7.349687574  | 3.955253659  | 15.533255439 |
|H   | 7.807068466  | 4.721704410  | 15.961527032 |
|O   | 6.832094348  | 4.454106549  | 14.836886947 |
|H   | 6.848207273  | 3.910297339  | 22.857659949 |
|O   | 6.016707566  | 4.406039376  | 23.064927509 |
|H   | 6.535099630  | 3.17542363   | 22.190310765 |
|O   | 9.967109682  | 2.055510707  | 22.895502302 |
|H   | 10.724412112 | 1.973749039  | 23.515972553 |
|H   | 9.717312945  | 2.982667030  | 22.938795267 |
|O   | 9.403331882  | 2.940393554  | 14.435651355 |
|H   | 8.523018873  | 3.314352714  | 14.870205918 |
|H   | 9.223544705  | 2.04510016   | 14.077440167 |
|O   | 6.201420155  | -2.033425809 | 17.320280697 |
|H   | 7.008346475  | -2.15322261  | 17.883229453 |
|H   | 6.511097726  | -1.988074197 | 16.379823722 |
|O   | 4.233044088  | 11.375346694 | 14.908501743 |
|H   | 4.620421846  | 12.182695464 | 14.566758515 |
|H   | 4.912742815  | 10.662338065 | 14.706270746 |
|O   | 2.838773744  | 8.734848978  | 18.835173735 |
|H   | 3.237925314  | 7.888293020  | 19.164862727 |
|H   | 3.533682784  | 9.438748473  | 19.091701349 |
|O   | 16.861553888 | 9.767756195  | 23.557492063 |
|H   | 17.482423825 | 9.085089920  | 23.317947024 |
|O   | 16.577716075 | 9.521392039  | 24.447119144 |
|H   | 6.768598981  | 6.416790851  | 18.612802678 |
|H   | 5.852913304  | 6.576216071  | 18.454358558 |
|H   | 6.947151543  | 6.753200499  | 19.629224014 |
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