

# Supplemental Material to: Rovibrational levels of helium hydride ion

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## Abstract

This Supplemental Material contains components of the potentials (18), (19), and (26) used in solving the radial Schrödinger equation (16). In particular,  $\mathcal{E}_a(R)$  is the adiabatic correction to the Born-Oppenheimer interaction energy,  $\mathcal{W}_{\parallel}(R)$  and  $\mathcal{W}_{\perp}(R)$  are the nonadiabatic corrections to the reduced nuclear mass,  $\delta\mathcal{E}_{\text{na}}(R)$  is the nonadiabatic correction to the interaction energy,  $\mathcal{E}^{(n)}$  with  $n = 2, 3,$  and  $4$  are the relativistic, the leading quantum electrodynamics, and the higher order quantum electrodynamics corrections to the interaction energy, respectively. The Born-Oppenheimer interaction energy is not included in the table—it was published in Ref. 17. More details on the methodology of solving the radial Schrödinger equation can be found in Ref. 44.

	$\varepsilon_a (R)$	$\mathcal{W}_{  } (R)$	$\mathcal{W}_{\perp} (R)$	$\delta\varepsilon_{na} (R)$	$\varepsilon^{(2)} (R)$	$\varepsilon^{(3)} (R)$	$\varepsilon^{(4)} (R)$
0.1	5.120201e-4	-2.652557e-8	-7.879834e-9	-8.413331e-6	-3.952852e-4	6.875238e-5	6.309917e-7
0.2	4.798125e-4	-4.364737e-8	-7.431720e-9	-3.952568e-6	-2.553318e-4	4.804173e-5	4.254845e-7
0.3	4.179414e-4	-5.132793e-8	-6.978722e-9	-2.120358e-6	-1.632560e-4	3.361912e-5	2.925348e-7
0.4	3.509248e-4	-5.339009e-8	-6.599032e-9	-1.269233e-6	-1.052129e-4	2.381677e-5	2.050063e-7
0.5	2.892742e-4	-5.260184e-8	-6.324862e-9	-8.268817e-7	-6.827943e-5	1.705119e-5	1.455963e-7
0.6	2.361659e-4	-5.057557e-8	-6.169187e-9	-5.761032e-7	-4.428205e-5	1.228172e-5	1.041073e-7
0.7	1.917959e-4	-4.820154e-8	-6.132095e-9	-4.197298e-7	-2.846694e-5	8.851916e-6	7.444977e-8
0.8	1.552940e-4	-4.591765e-8	-6.204359e-9	-3.149309e-7	-1.788602e-5	6.346218e-6	5.286544e-8
0.9	1.255045e-4	-4.392047e-8	-6.371530e-9	-2.431000e-7	-1.073783e-5	4.493597e-6	3.694963e-8
1.0	1.012902e-4	-4.229799e-8	-6.617407e-9	-1.919068e-7	-5.906277e-6	3.112397e-6	2.510988e-8
1.1	8.164241e-5	-4.108503e-8	-6.926070e-9	-1.542603e-7	-2.653375e-6	2.077300e-6	1.625872e-8
1.2	6.571067e-5	-4.027973e-8	-7.282696e-9	-1.258422e-7	-4.820316e-6	1.300496e-6	9.633397e-9
1.3	5.279757e-5	-3.985401e-8	-7.673829e-9	-1.043696e-7	9.264681e-6	7.183939e-6	4.686764e-9
1.35	4.729232e-5	-3.977118e-8	-7.878545e-9	-9.553175e-8	1.458687e-6	4.842323e-6	2.713279e-9
1.4	4.234082e-5	-3.976842e-8	-8.087551e-9	-8.782027e-8	1.809765e-6	2.846406e-6	1.018993e-9
1.45	3.788912e-5	-3.984133e-8	-8.299641e-9	-8.097470e-8	2.134525e-6	1.112600e-6	-4.313672e-10
1.46	3.705466e-5	-3.986466e-8	-8.342332e-9	-7.969132e-8	2.186122e-6	7.976482e-6	-6.947119e-10
1.5	3.389063e-5	-3.998616e-8	-8.513738e-9	-7.483723e-8	2.317096e-6	-3.552435e-6	-1.666708e-9
1.6	2.708730e-5	-4.047912e-8	-8.944330e-9	-6.466326e-8	2.587939e-6	-2.676779e-6	-3.593359e-9
1.7	2.163943e-5	-4.122393e-8	-9.373468e-9	-5.636505e-8	2.675917e-6	-4.315341e-6	-4.930713e-9
1.8	1.730743e-5	-4.219167e-8	-9.797419e-9	-4.912381e-8	2.646831e-6	-5.424711e-6	-5.809478e-9
1.9	1.389278e-5	-4.333720e-8	-1.021427e-8	-4.254966e-8	2.539706e-6	-6.121611e-6	-6.331371e-9
2.0	1.122317e-5	-4.459324e-8	-1.062345e-8	-3.664768e-8	2.386996e-6	-6.497974e-6	-6.576828e-9
2.1	9.151340e-6	-4.587146e-8	-1.102522e-8	-3.155460e-8	2.203555e-6	-6.628408e-6	-6.610037e-9
2.2	7.549286e-6	-4.707009e-8	-1.142011e-8	-2.669166e-8	2.006199e-6	-6.569908e-6	-6.482880e-9
2.3	6.307891e-6	-4.808563e-8	-1.180860e-8	-2.192086e-8	1.807058e-6	-6.374048e-6	-6.237816e-9
2.4	5.335850e-6	-4.882532e-8	-1.219075e-8	-1.754819e-8	1.612271e-6	-6.075917e-6	-5.929335e-9
2.5	4.558364e-6	-4.921777e-8	-1.256619e-8	-1.392562e-8	1.425512e-6	-5.711682e-6	-5.520634e-9
2.6	3.918304e-6	-4.921983e-8	-1.293404e-8	-1.085406e-8	1.246194e-6	-5.304712e-6	-5.111184e-9
2.7	3.373273e-6	-4.881903e-8	-1.329305e-8	-8.155419e-9	1.082534e-6	-4.877441e-6	-4.682707e-9
2.8	2.893569e-6	-4.803195e-8	-1.364175e-8	-5.891716e-9	9.342187e-6	-4.446546e-6	-4.255537e-9
2.9	2.463288e-6	-4.689939e-8	-1.397856e-8	-4.052969e-9	7.967928e-6	-4.023043e-6	-3.840465e-9
3.0	2.070217e-6	-4.547971e-8	-1.430198e-8	-2.571955e-9	6.762140e-6	-3.616758e-6	-3.445286e-9
3.1	1.710379e-6	-4.384143e-8	-1.461073e-8	-1.407522e-9	5.695316e-6	-3.237283e-6	-3.075386e-9
3.2	1.382090e-6	-4.205629e-8	-1.490374e-8	-5.199553e-10	4.774149e-6	-2.883054e-6	-2.733839e-9
3.3	1.085885e-6	-4.019331e-8	-1.518031e-8	-1.129514e-10	3.930493e-6	-2.557768e-6	-2.422294e-9
3.4	8.217580e-7	-3.831446e-8	-1.544002e-8	5.005064e-10	3.170127e-6	-2.263530e-6	-2.140581e-9
3.5	5.903320e-7	-3.647180e-8	-1.568280e-8	6.630930e-10	2.474889e-6	-1.997552e-6	-1.888216e-9
3.6	3.904780e-7	-3.470616e-8	-1.590883e-8	6.668656e-10	1.949838e-6	-1.762742e-6	-1.663445e-9
3.7	2.211320e-7	-3.304705e-8	-1.611851e-8	5.856934e-10	1.481635e-6	-1.553846e-6	-1.464535e-9
3.8	8.035700e-8	-3.151345e-8	-1.631247e-8	4.647916e-10	1.097067e-6	-1.370519e-6	-1.289383e-9
3.9	-3.504800e-8	-3.011524e-8	-1.649142e-8	3.074912e-10	6.694890e-6	-1.206154e-6	-1.135641e-9
4.0	-1.266020e-7	-2.885488e-8	-1.665620e-8	1.415994e-10	3.425401e-6	-1.062920e-6	-1.000929e-9
4.1	-1.988200e-7	-2.772917e-8	-1.680769e-8	1.144020e-10	6.279293e-6	-9.386422e-6	-8.834369e-10
4.2	-2.529420e-7	-2.673097e-8	-1.694679e-8	1.393830e-10	-1.450641e-6	-8.308445e-6	-7.809060e-10
4.3	-2.926120e-7	-2.585063e-8	-1.707442e-8	-2.762819e-11	-3.823279e-6	-7.355787e-6	-6.916844e-10
4.4	-3.203830e-7	-2.507720e-8	-1.719147e-8	-4.329589e-12	-5.504822e-6	-6.532566e-6	-6.138117e-10
4.5	-3.379460e-7	-2.439935e-8	-1.729879e-8	-1.755060e-10	-6.792302e-6	-5.818095e-6	-5.459569e-10
4.6	-3.475480e-7	-2.380601e-8	-1.739720e-8	-1.933825e-10	-8.230059e-6	-5.189567e-6	-4.869715e-10
4.7	-3.503710e-7	-2.328685e-8	-1.748747e-8	-1.943495e-10	-9.291408e-6	-4.642571e-6	-4.353995e-10
4.8	-3.491770e-7	-2.283245e-8	-1.757033e-8	-2.007805e-10	-1.014454e-6	-4.171091e-6	-3.903657e-10
4.9	-3.428950e-7	-2.243444e-8	-1.764645e-8	-2.105872e-10	-1.067690e-6	-3.765000e-6	-3.510459e-10
5.0	-3.347190e-7	-2.208549e-8	-1.771644e-8	-2.215262e-10	-1.141512e-6	-3.398560e-6	-3.165212e-10
5.2	-3.131180e-7	-2.151021e-8	-1.784030e-8	-2.423531e-10	-1.274014e-6	-2.793208e-6	-2.595328e-10
5.4	-2.872090e-7	-2.106540e-8	-1.794588e-8	-2.640002e-10	-1.381312e-6	-2.320364e-6	-2.150726e-10
5.6	-2.601270e-7	-2.072009e-8	-1.803643e-8	-2.846225e-10	-1.465306e-6	-1.947307e-6	-1.800365e-10
5.8	-2.341750e-7	-2.045051e-8	-1.811456e-8	-3.034819e-10	-1.520889e-6	-1.651046e-6	-1.522386e-10
6.0	-2.102140e-7	-2.023803e-8	-1.818233e-8	-3.203524e-10	-1.564752e-6	-1.411986e-6	-1.298414e-10
6.2	-1.876850e-7	-2.006796e-8	-1.824139e-8	-3.352376e-10	-1.436562e-6	-1.192738e-6	-1.095120e-10
6.4	-1.678830e-7	-1.992892e-8	-1.829423e-8	-3.482345e-10	-1.311623e-6	-1.013505e-6	-9.291238e-11
6.6	-1.502130e-7	-1.981238e-8	-1.833898e-8	-3.594754e-10	-1.188527e-6	-8.643600e-6	-7.912600e-11
6.8	-1.362490e-7	-1.970275e-8	-1.837806e-8	-3.690982e-10	-1.071132e-6	-7.397515e-6	-6.762805e-11
7.0	-1.207720e-7	-1.961750e-8	-1.841258e-8	-3.772371e-10	-9.615972e-6	-6.352434e-6	-5.800071e-11
7.2	-1.090250e-7	-1.954386e-8	-1.844332e-8	-3.840194e-10	-8.609410e-6	-5.472717e-6	-4.990928e-11
7.4	-9.808600e-8	-1.947949e-8	-1.847088e-8	-3.895574e-10	-7.694431e-6	-4.729583e-6	-4.308420e-11
7.6	-8.839900e-8	-1.942269e-8	-1.849572e-8	-3.939623e-10	-6.869195e-6	-4.099688e-6	-3.730731e-11
7.8	-7.993700e-8	-1.937216e-8	-1.851820e-8	-3.973349e-10	-6.129111e-6	-3.564019e-6	-3.240127e-11
8.0	-7.282467e-8	-1.932691e-8	-1.853860e-8	-3.997689e-10	-5.468098e-6	-3.107030e-6	-2.822136e-11
9.0	-4.620242e-8	-1.915771e-8	-1.861676e-8	-4.007040e-10	-3.114363e-6	-1.626161e-6	-1.472128e-11
10.0	-3.070027e-8	-1.904984e-8	-1.866752e-8	-3.888756e-10	-1.819786e-6	-9.007655e-6	-8.143603e-12
12.0	-1.510153e-8	-1.892888e-8	-1.872458e-8	-3.482768e-10	-6.836050e-6	-3.168757e-6	-2.873544e-12
15.0	-6.312248e-9	-1.885191e-8	-1.876061e-8	-2.815236e-10	-1.952147e-6	-8.538120e-6	-7.861147e-12
20.0	-2.035490e-9	-1.881066e-8	-1.877972e-8	-1.958709e-10	-3.654286e-6	-1.502387e-6	-1.446182e-13
30.0	-4.083584e-10	-1.879385e-8	-1.878743e-8	-1.055623e-10	-3.143978e-6	-1.131730e-6	-1.299900e-14
40.0	-1.299644e-10	-1.879086e-8	-1.878879e-8	-6.494470e-11	-5.097347e-6	-1.329697e-6	-2.332668e-15
50.0	-5.338157e-11	-1.879002e-8	-1.878917e-8	-4.377413e-11	-1.143491e-6	-5.727894e-6	-6.138277e-16
60.0	-2.578284e-11	-1.878972e-8	-1.878931e-8	-3.144274e-11	-3.008596e-6	1.243096e-6	-2.059952e-16