

Referee's Report

Title: How Large are Nonadiabatic Effects in Atomic and Diatomic Systems?

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This paper reports the first non-adiabatic Quantum Monte Carlo benchmarks for first row atoms and hydrides, as measured by the diagonal Born-Oppenheimer correction (DBOC) plus the contributions from excited eigenstates. As noted in the text, the DBOC is by far the larger component. Most of the work focuses on total energies for atoms and atomic ions, which are normally not of particular interest to chemists. Beginning on page 6 (out of 8.5 pages of text) the discussion turns to hydrides. Agreement with reference values taken from the literature is good ($< 1 \text{ mE}_h$) with the exception of HF where the difference grows to 2.4 mE_h . In the case of CH the authors believe they have an unusually large fixed-node error.

On page 6 the text states, "...the nonadiabatic results agree closely with their adiabatic counterparts...". That is as expected, but because the dissociation energies in Table II are given as D_e and then later as D_0 it is not possible to tell exactly how large the non-adiabatic corrects actually are. They are quite small. In addition, the DBOCs are relatively insensitive to the level of theory. Perhaps a comment to that effect would be helpful for the reader to put things into perspective.

The lack of line numbers in the manuscript makes it difficult to indicate where changes or questions are located in the text.

I find the paper to be acceptable for publication after addressing the small number of minor issues below.

Minor comments and/or suggests are as follows:

Pg. 2	The abbreviation ECG appears to be undefined at this point in the text. Please define. I assume it means "explicitly correlated Gaussian".
Pg. 4	Sometimes the term "non-adiabatic" appears in the text and other times it uses "nonadiabatic". Please be consistent.
Pg. 6	"Finding accurate reference data...is not straightforward. We will use highly converged ECG data when available." Break the sentence for the sake of improving the readability.
Pg. 7	In the title to Table II it should be made clear that both the total energies and dissociation energies are given in Hartrees. It's relatively unconventional to report D_e values in Hartrees.
Pg. 9	An extraneous lower case "p" appears in reference 57.