The FORTRAN 77 program named QCP2.FOR was compiled and run on a 32-bit Windows 7 personal computer. Editing and execution was performed within the Command Prompt window. The executable program is named QCP2.EXE. In our work, an earlier version of this program was used to vary parameters, but this program uses the final set of parameters to give outputs.

Sixty small molecules in our work are computed and the outputs are written in about 10 seconds. The compiler that I used was RM/FORTRAN by Ryan-McFarland, Version 2.10, ~1986. The input file is INPUT.

The output files are FORT8 and OUTPUT. Backup copies of these last three files are INPUT.SAV, FORT8.SAV, and OUTPUT.SAV.

Another FORTRAN 77 program named QCP3.FOR varies the bond lengths of the input from Re -0.4 Å to Re +0.4 Å in steps of 0.1 Å. The executable program is QCP3.EXE. The input program is the same file INPUT as above and the output programs are FORT9, FORT8, and OUTPUT. A backup copy of FORT9 is FORT9.SAV. The labels of the output of FORT9 are specific to the INPUT file of this work. The unlabeled files at the end of FORT9 are O**2** calculations at additional bond lengths (used to create Figure 2).