Supporting information for "A long-range-corrected density functional that performs well for both ground-state properties and time-dependent density functional theory excitation energies, including charge-transfer excited states"

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Summary

This Supporting Information consists of three parts: ω- and C_{HF}-dependent vertical excitation energies (VEEs) for our database of excited states, charge-transfer (CT) VEEs in the C_2H_4–C_2F_4 heterodimer, and ω-dependent excitation energy curves (with $C_{\mathrm{HF}} = 0$) for a subset of molecules in the database of Peach *et al.* [J. Chem. Phys. **128** 044118 (2008)].

VEEs for the excited-state database are given first, starting on page 3. Each figure plots the VEEs, as a function of ω, for one molecule and one value of C_{HF}. Plots for $C_{\mathrm{HF}} = 0$ begin on page 3, while those for $C_{\mathrm{HF}} = 0.1$, 0.2, and 0.3 a_0^{-1} begin on pages 28, 53, and 78, respectively. Only singlet excitation are shown. The grey circles represent the raw data from the Q-Chem output and the horizontal lines correspond to the "best estimate" values from Table 1 of Schreiber *et al.* [J. Chem. Phys. **128** 134110 (2008)]. The curved lines indicate our ω-dependent state assignments, where the color matches that of the corresponding benchmark value from Schreiber *et al.*

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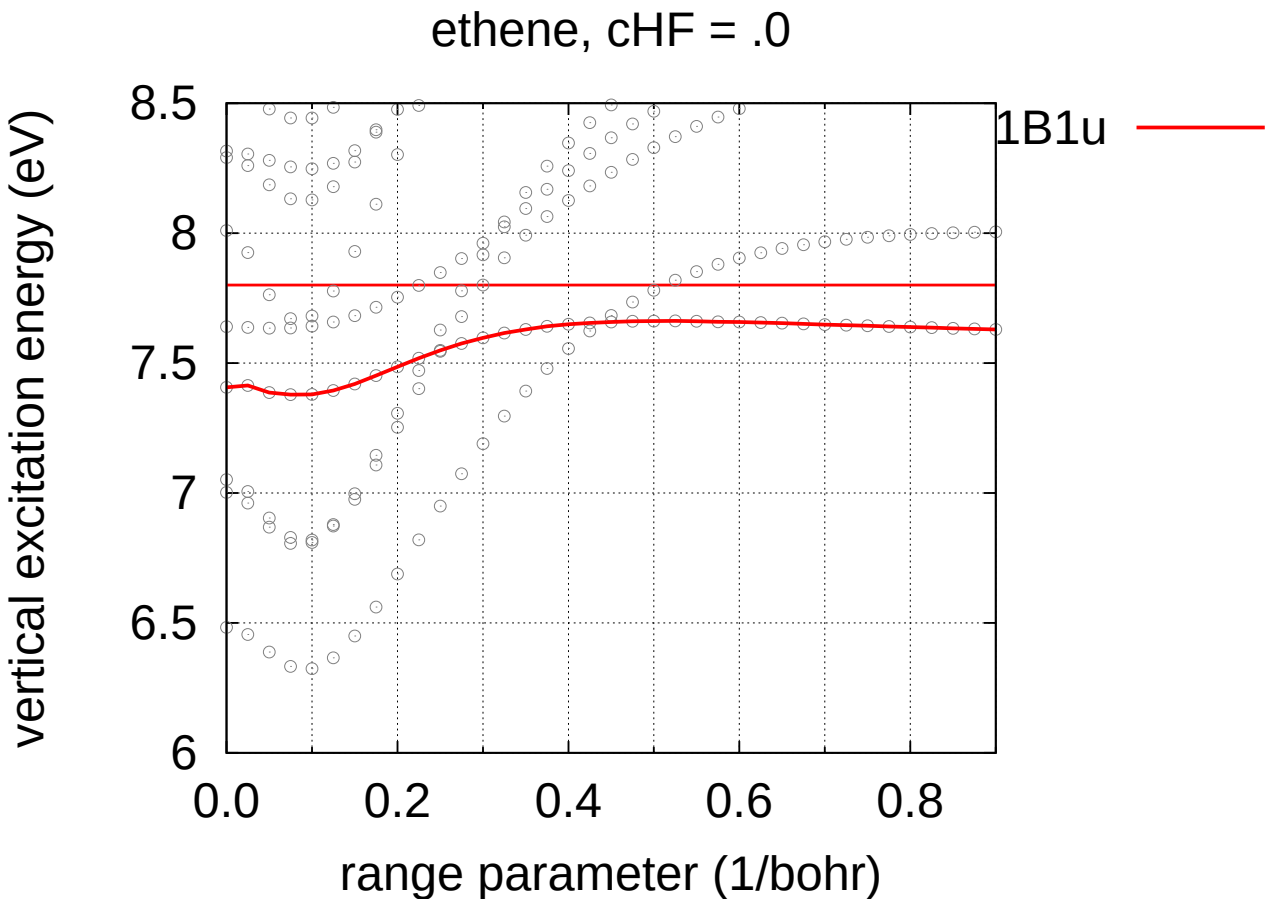
These calculations employed the aug-cc-pVDZ basis set and SG-1 quadrature the grid. The diffuse functions present in aug-cc-pVDZ sometimes give rise to spuriously low lying Rydberg states (for the same reasons as the spuriously low-lying charge transfer states). Also, some of the graphs exhibit avoided crossings between states of the same symmetry (which cannot cross as ω is varied). State assignments in these case were made based on the irreducible representations, oscillator strengths, and radii of gyration of the virtual orbitals. In many cases, we repeated the calculations using the cc-pVDZ basis set, in order to confirm the identity of putative Rydberg excitations.

The CT excitation energy plots for C_2H_4–C_2F_4 begin on page 103. Each graph plots the lowest CT excitation energy as a function of the inter-monomer distance, R. In each figure, the excitation energies have been shifted to a common value of zero at $R = 5.0$ Å. These calculations use the cc-pVDZ basis and the SG-1 quadrature grid.

For the molecules discussed in Section IV of the paper, ω-dependent excitation energy curves are presented, for $C_{\mathrm{HF}} = 0$, beginning on page 107. These calculations were performed using the SG-1 quadrature grid and the cc-pVDZ basis set. In each graph, the excitation energy at $\omega = 0.45\ a_0^{-1}$ is highlighted, as this is the best choice of ω for ground-state properties, when $C_{\mathrm{HF}} = 0$, and this is the functional that we call "$C_{\mathrm{HF}} = 0$" in Table II of the paper. Benchmark excitation energies, taken from the study by Peach *et al.* [J. Chem. Phys. **128** 044118 (2008)] are indicated in the figures by horizontal lines.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7
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6
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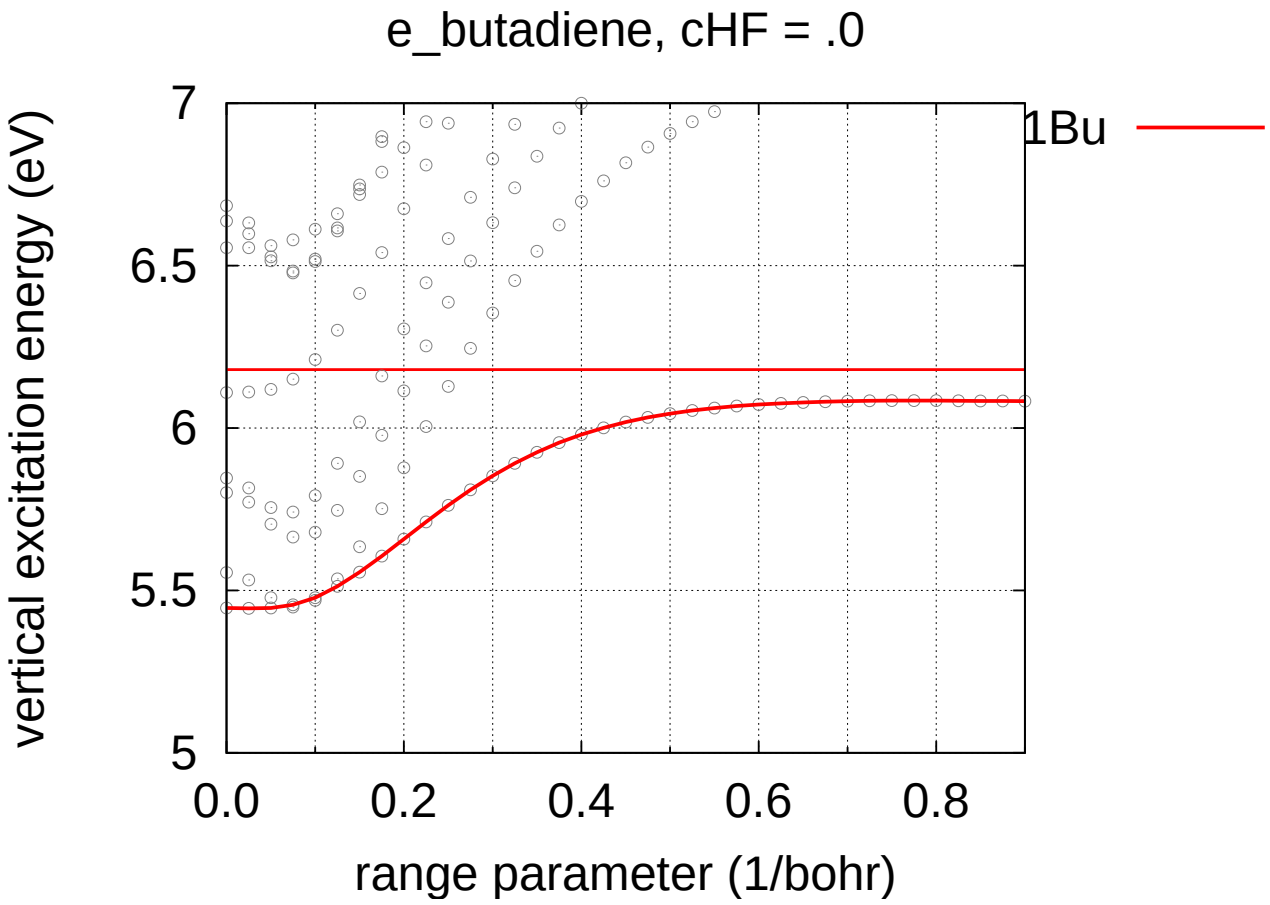
0.2
0.4
0.6
0.8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vertical excitation energy (eV)
range parameter (1/bohr)
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6
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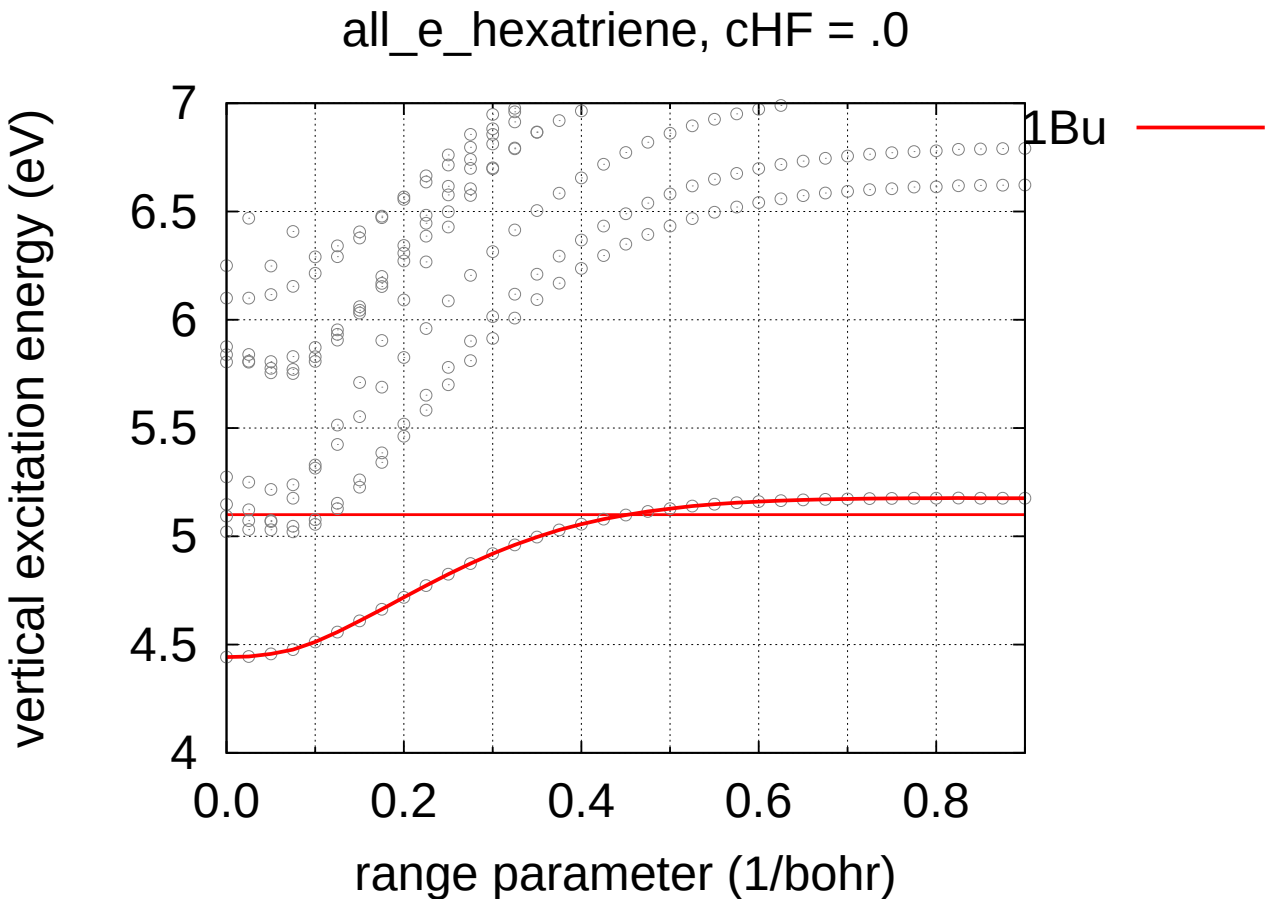
0.2
0.4
0.6
0.8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range parameter (1/bohr)
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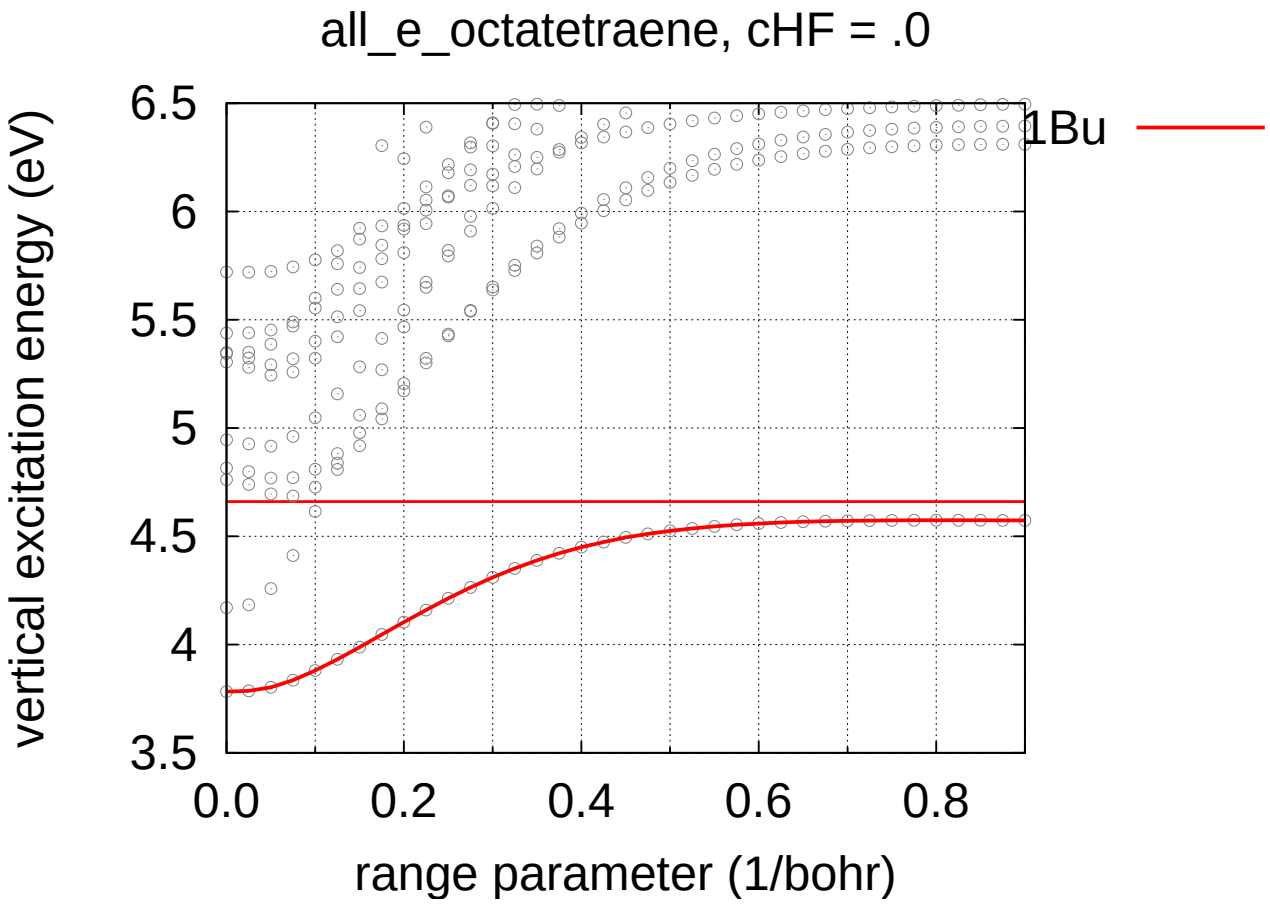
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8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range parameter (1/bohr)
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6
5.5
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4.5
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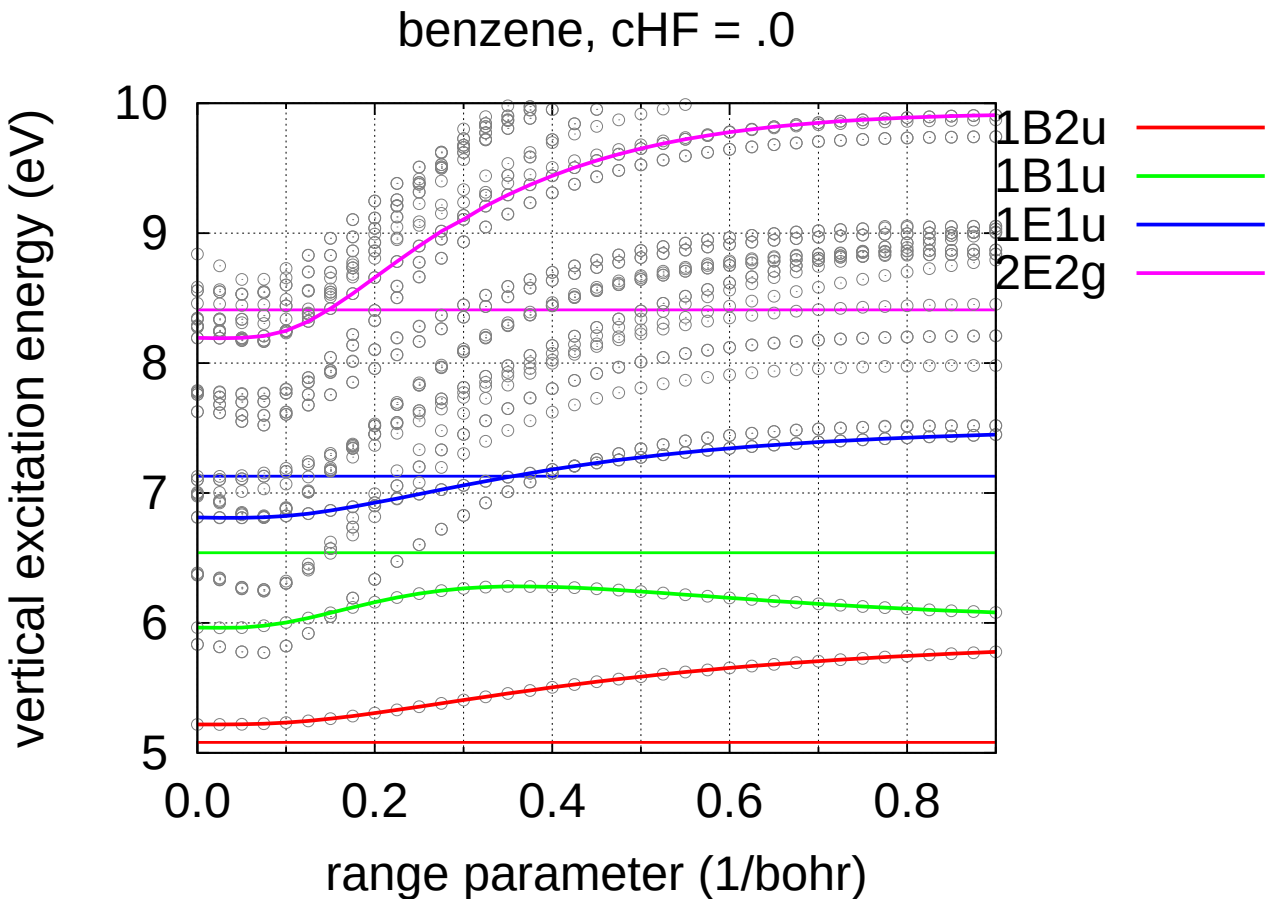
3.5
0.0
0.2
0.4
0.6
0.8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range parameter (1/bohr)
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9
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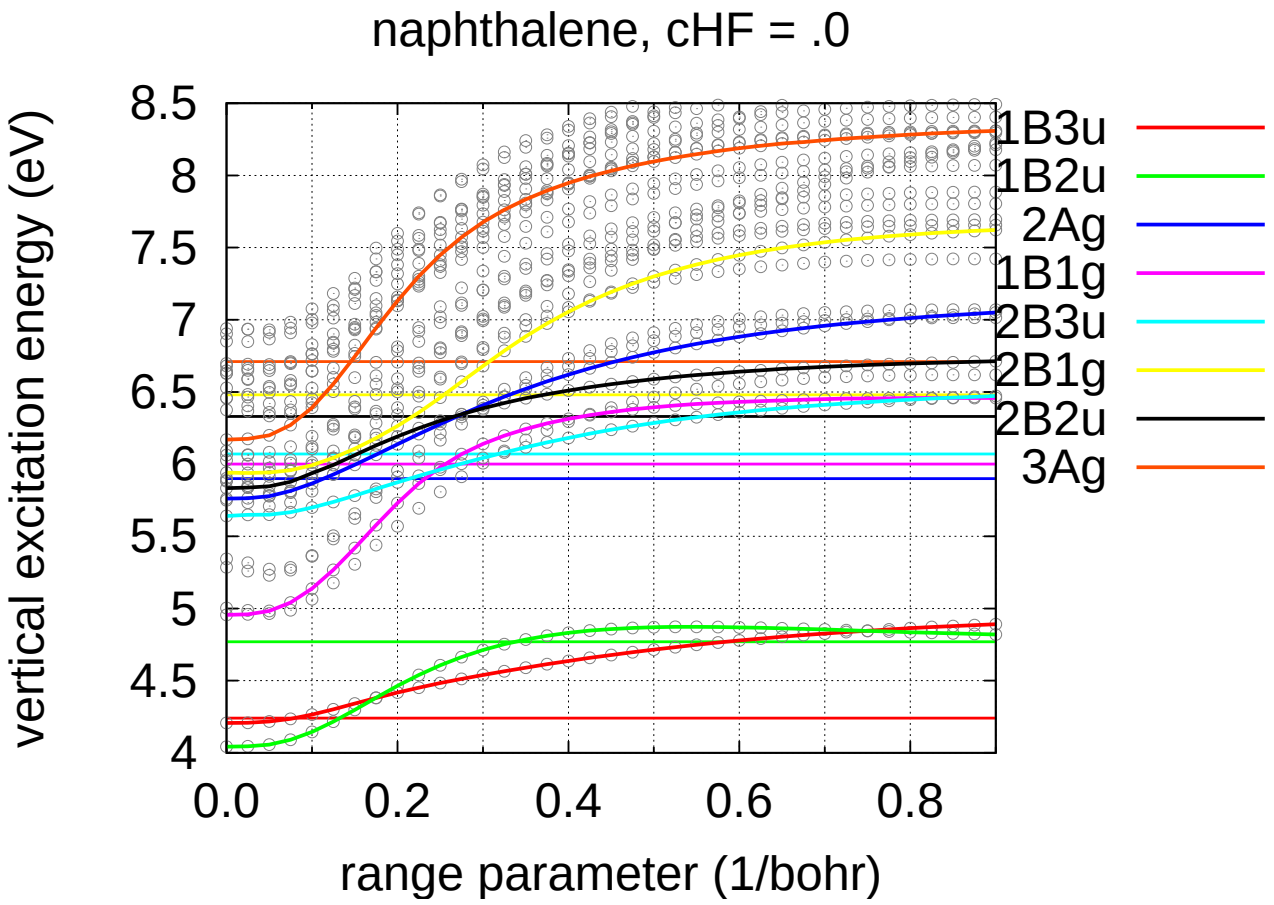
0.2
0.4
0.6
0.8
1B2u
1B1u
1E1u
2E2g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range parameter (1/bohr)
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8
7.5
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
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0.8
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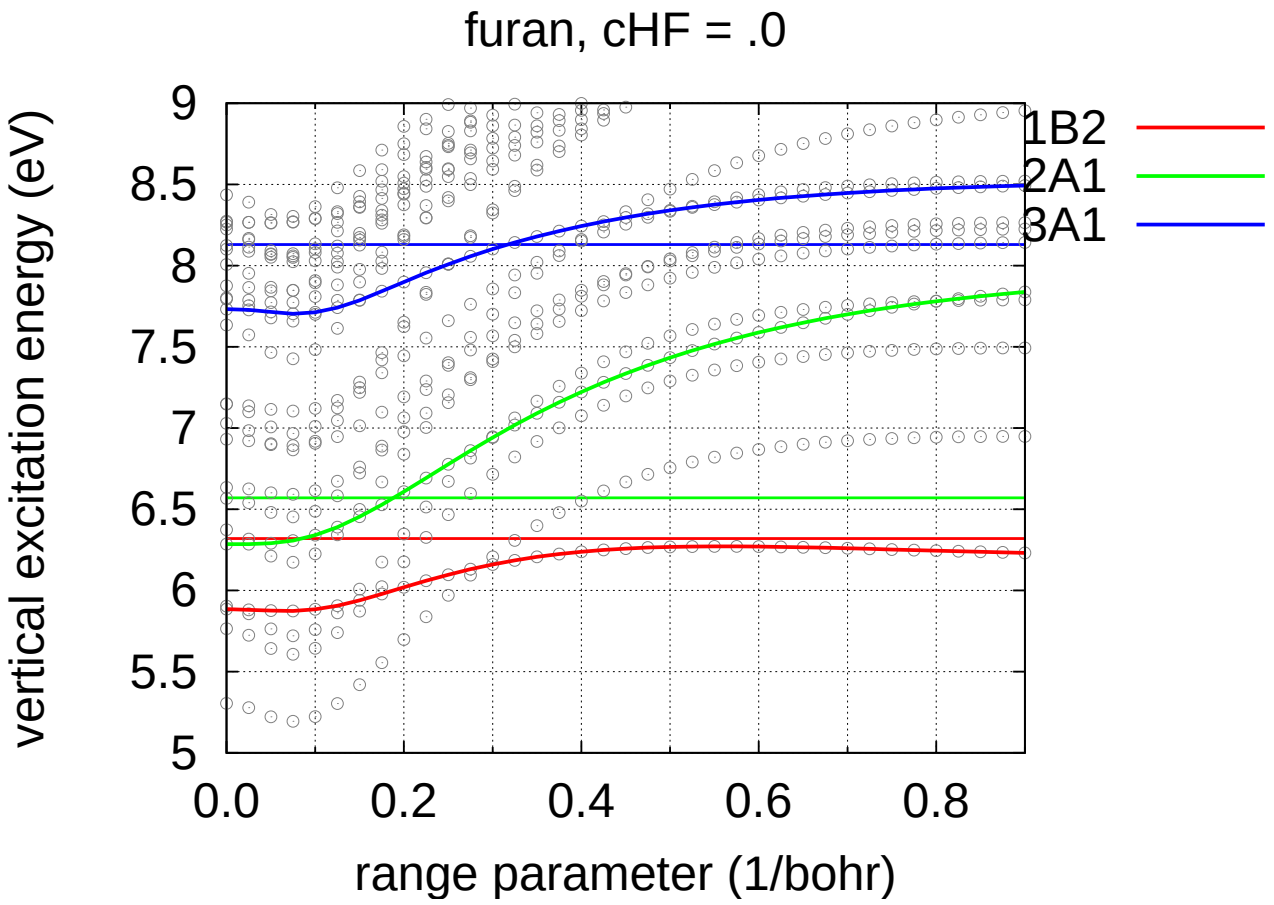
1B2u
2Ag
1B1g
2B3u
2B1g
2B2u
3Ag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range parameter (1/bohr)
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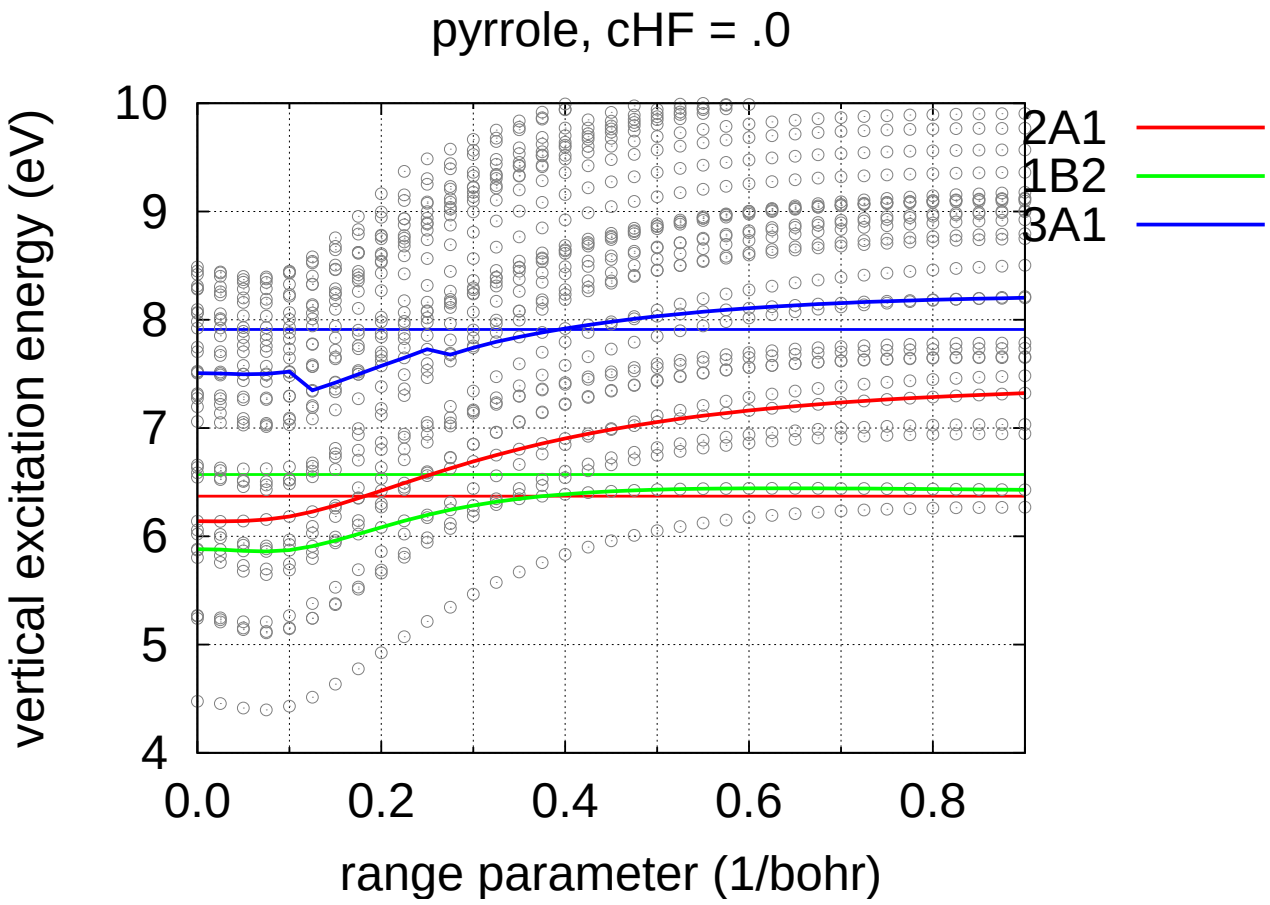
8.5
8
7.5
7
6.5
6
5.5
5
0.0
0.2
0.4
0.6
0.8
1B2
2A1
3A1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range parameter (1/bohr)
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9
8
7
6
5
4
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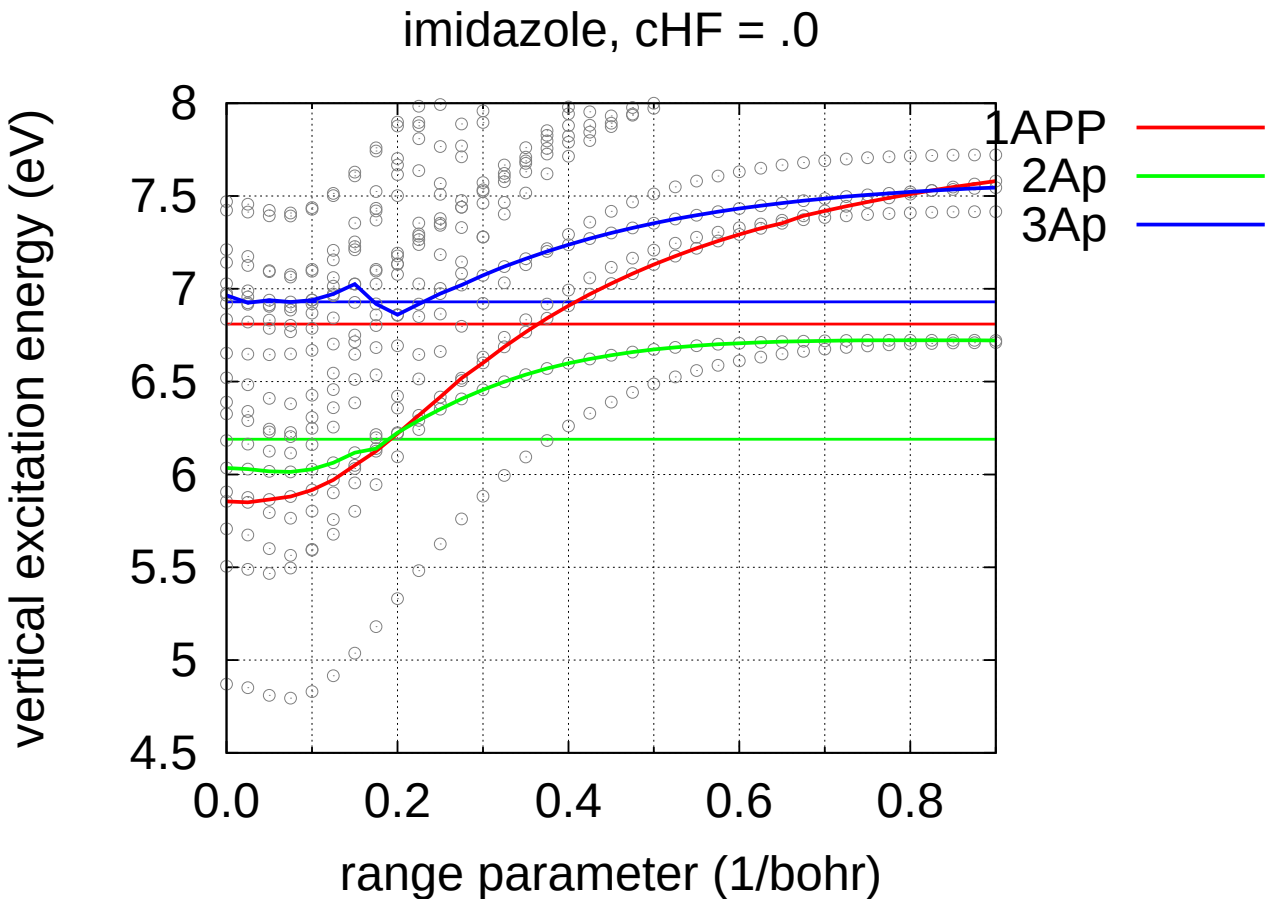
0.2
0.4
0.6
0.8
2A1
1B2
3A1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range parameter (1/bohr)
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7.5
7
6.5
6
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5
4.5
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0.2
0.4
0.6
0.8
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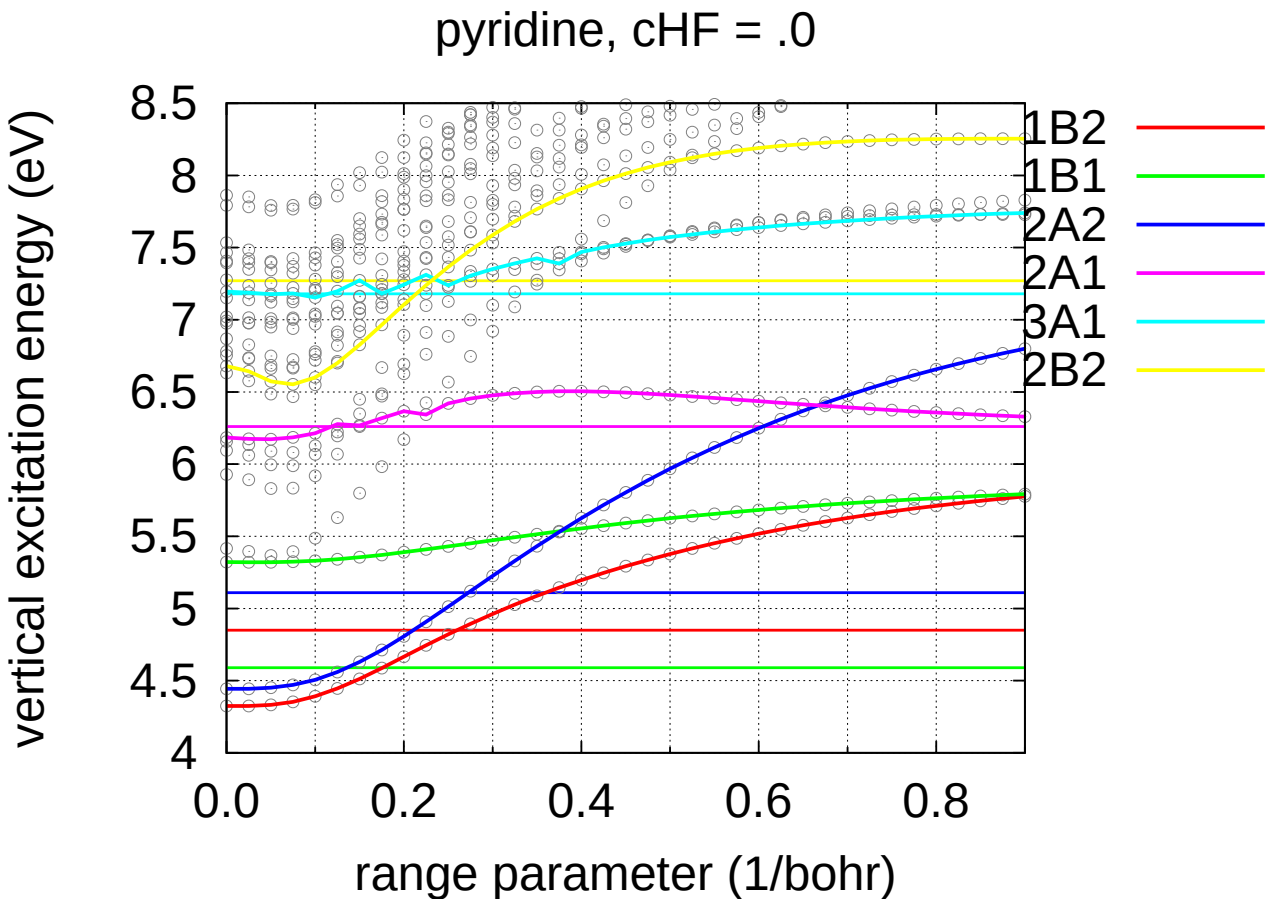
2Ap
3Ap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vertical excitation energy (eV)
range parameter (1/bohr)
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8
7.5
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8
1B2
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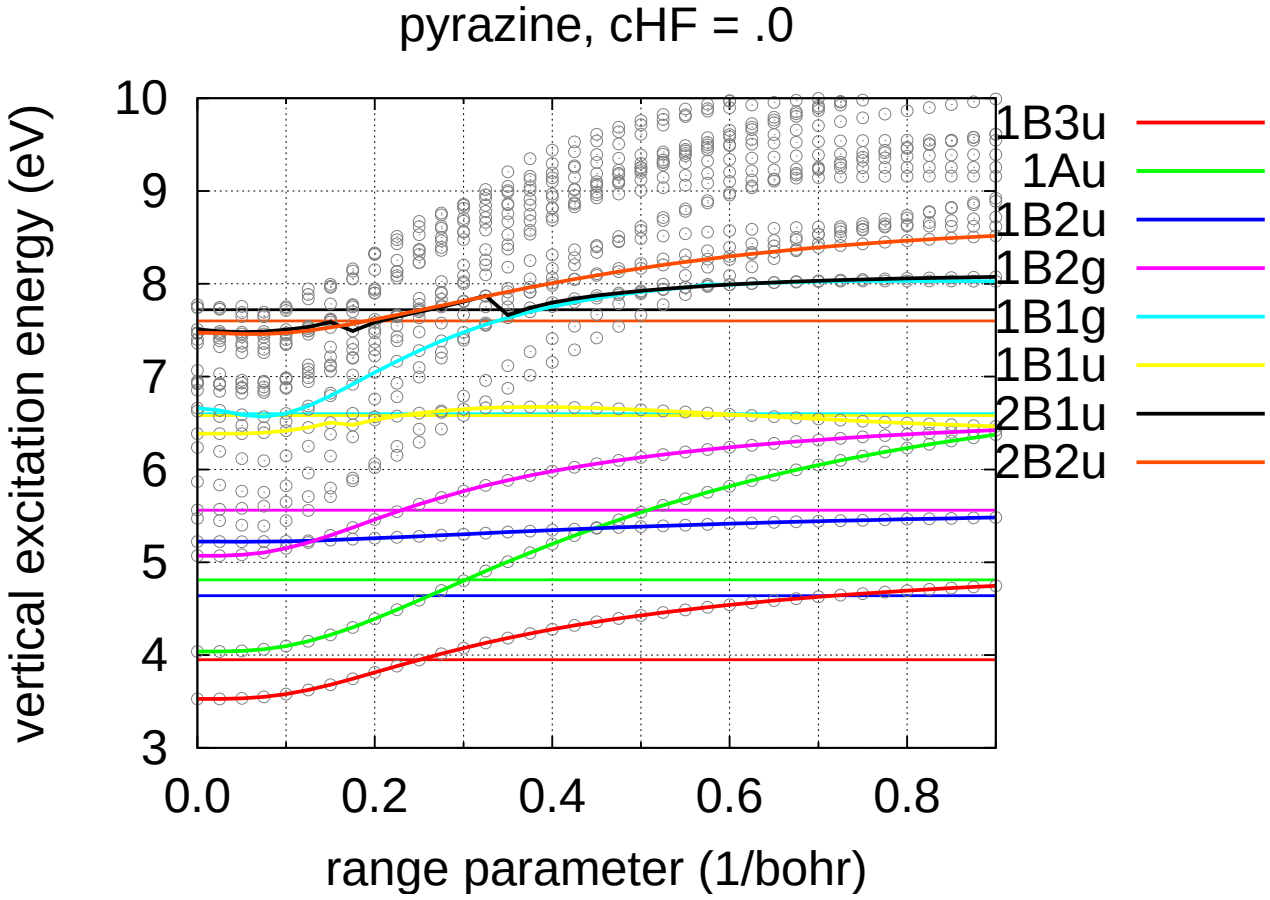
2A2
2A1
3A1
2B2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range parameter (1/bohr)
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9
8
7
6
5
4
3
0.0
0.2
0.4
0.6
0.8
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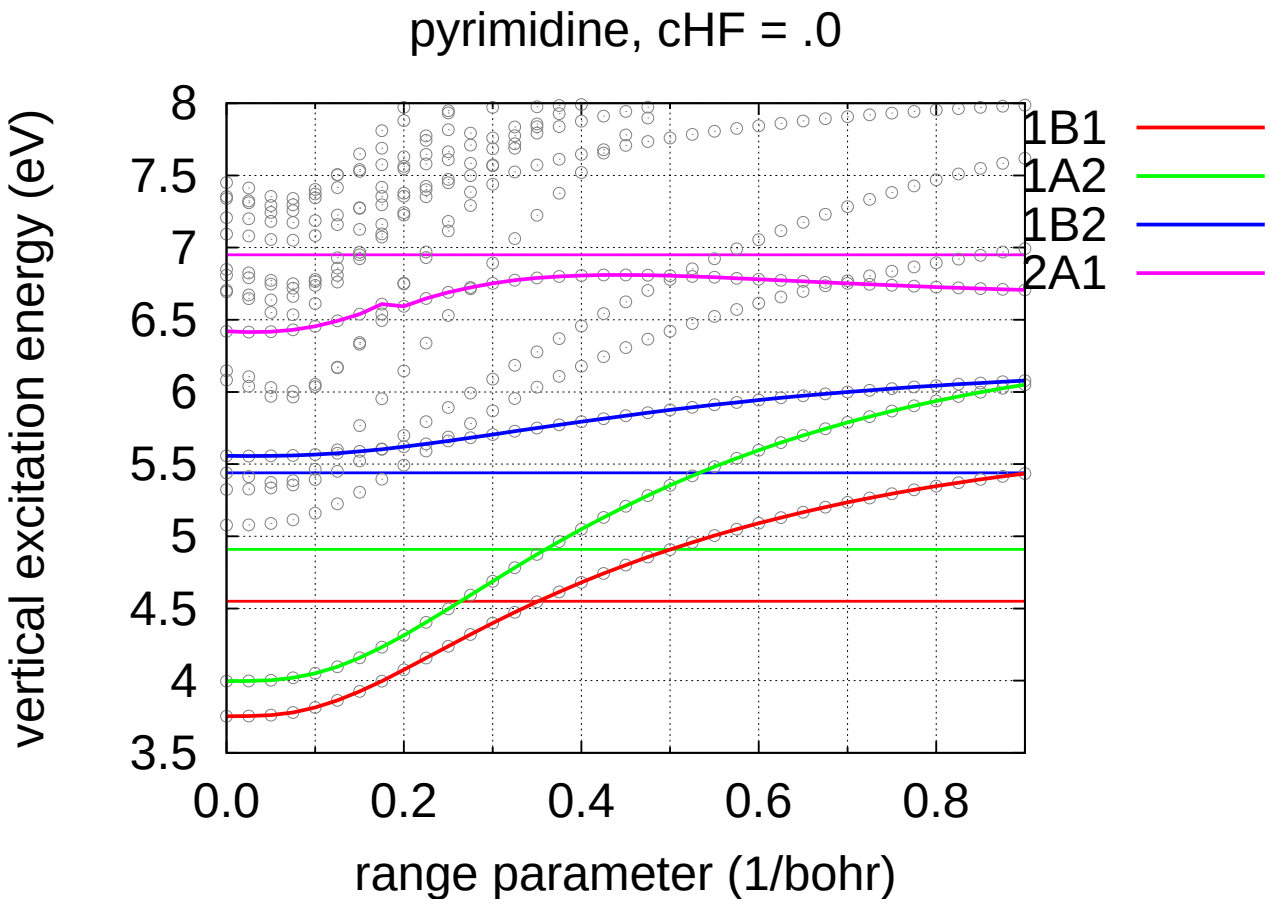
1Au
1B2u
1B2g
1B1g
1B1u
2B1u
2B2u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vertical excitation energy (eV)
range parameter (1/bohr)
8
7.5
7
6.5
6
5.5
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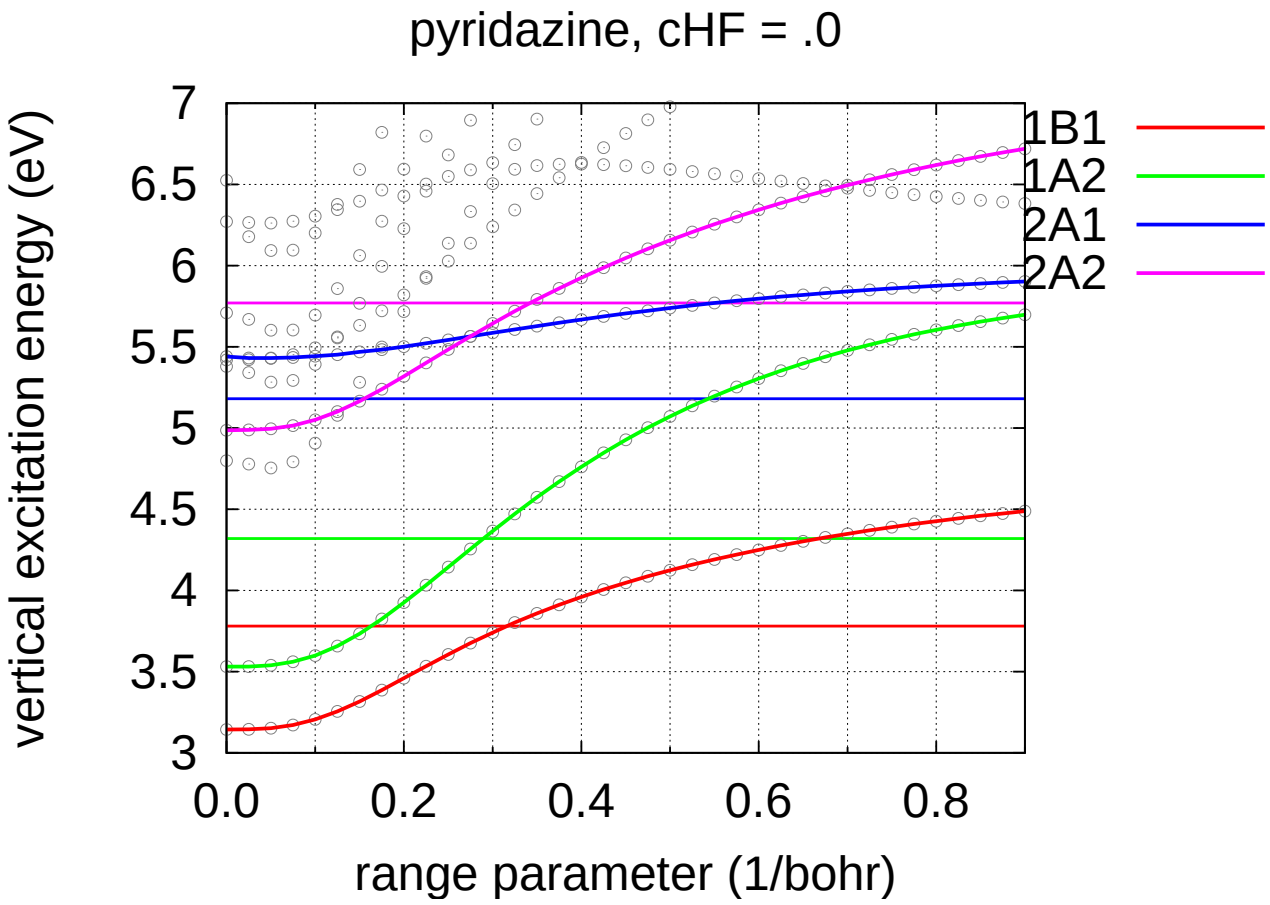
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8
1B1
1A2
1B2
2A1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vertical excitation energy (eV)
range parameter (1/bohr)
7
6.5
6
5.5
5
4.5
4
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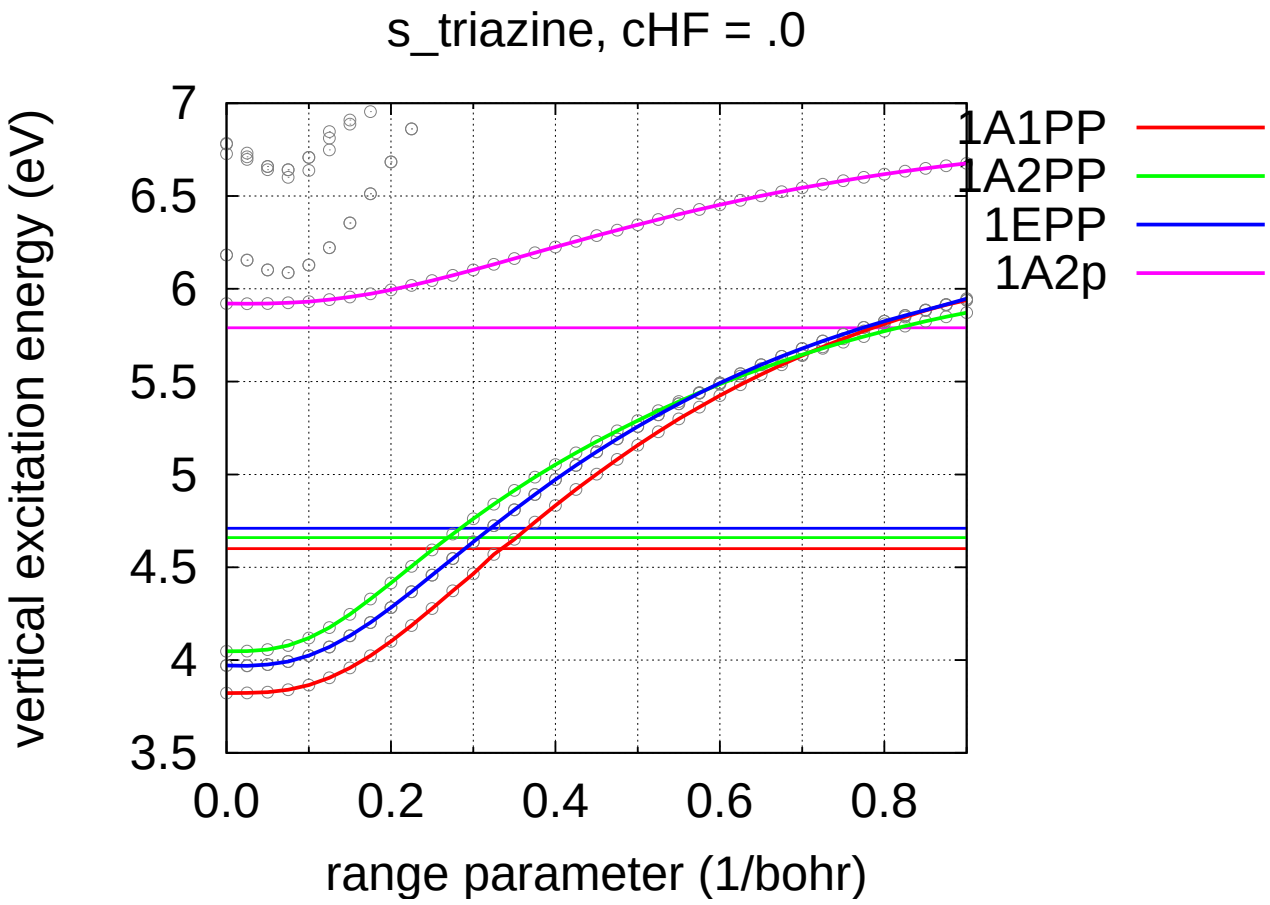
3
0.0
0.2
0.4
0.6
0.8
1B1
1A2
2A1
2A2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range parameter (1/bohr)
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6
5.5
5
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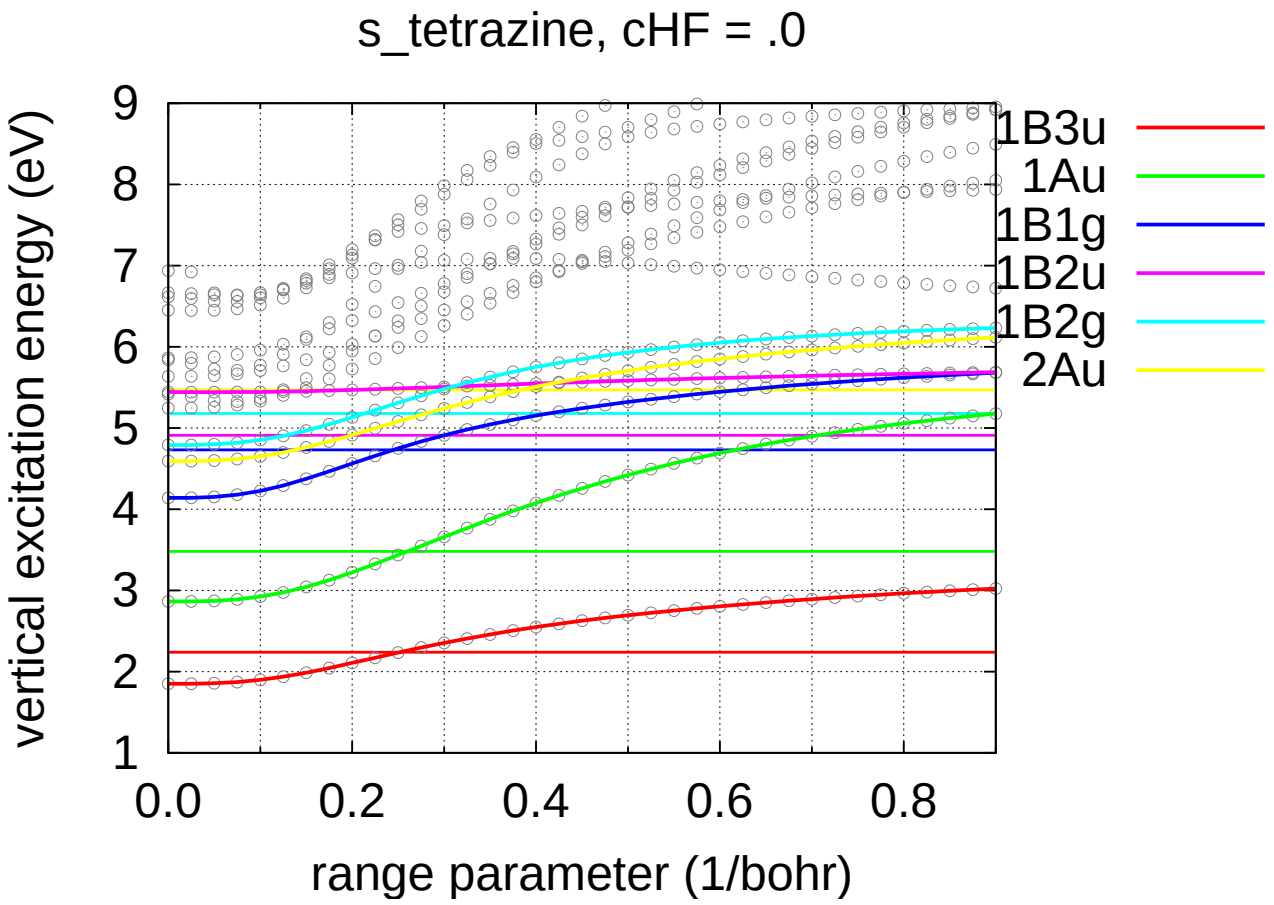
0.4
0.6
0.8
1A1PP
1A2PP
1EPP
1A2p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range parameter (1/bohr)
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2
3
4
5
6
7
8
9
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0.4
0.6
0.8
1B3u
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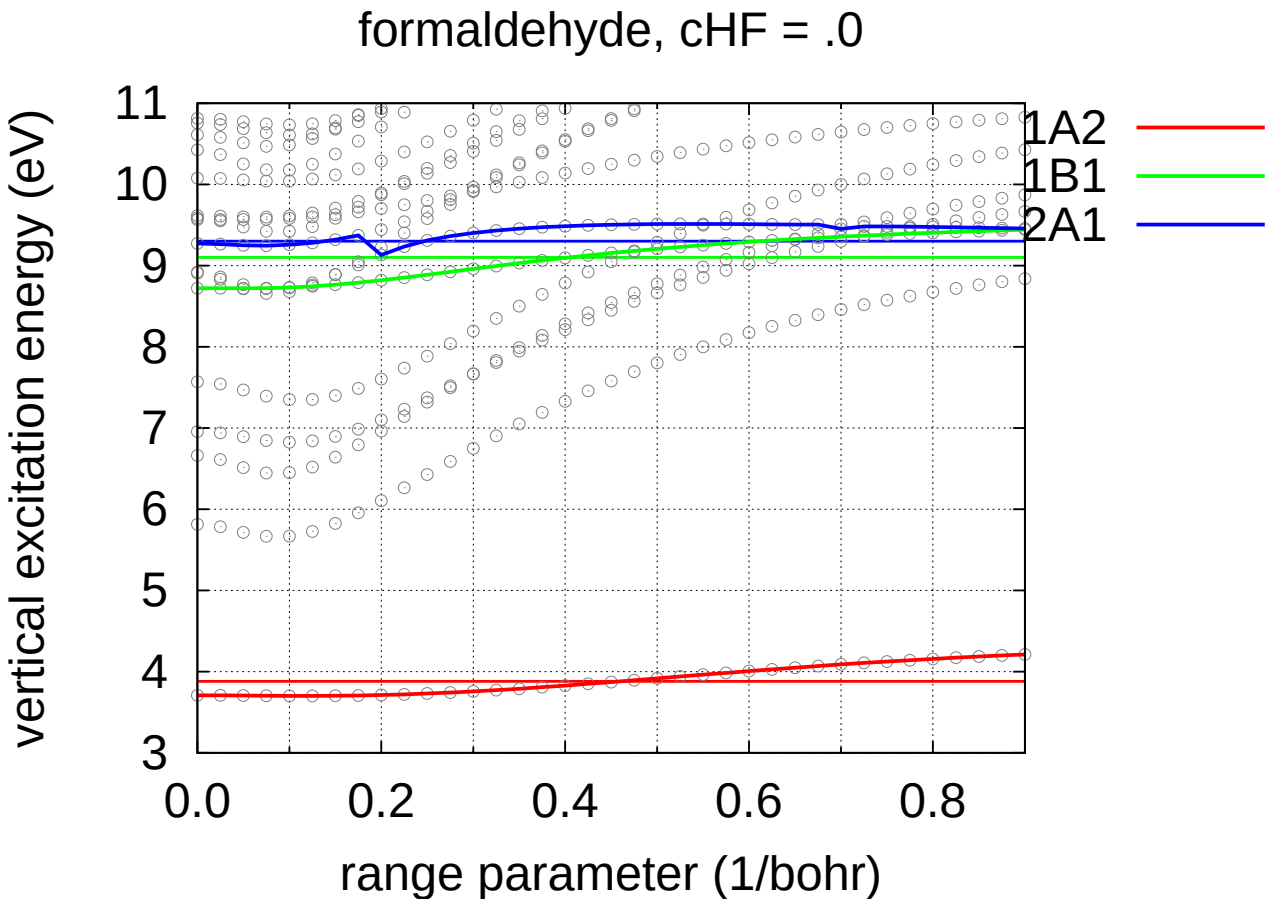
1B1g
1B2u
1B2g
2Au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range parameter (1/bohr)
11
10
9
8
7
6
5
4
3
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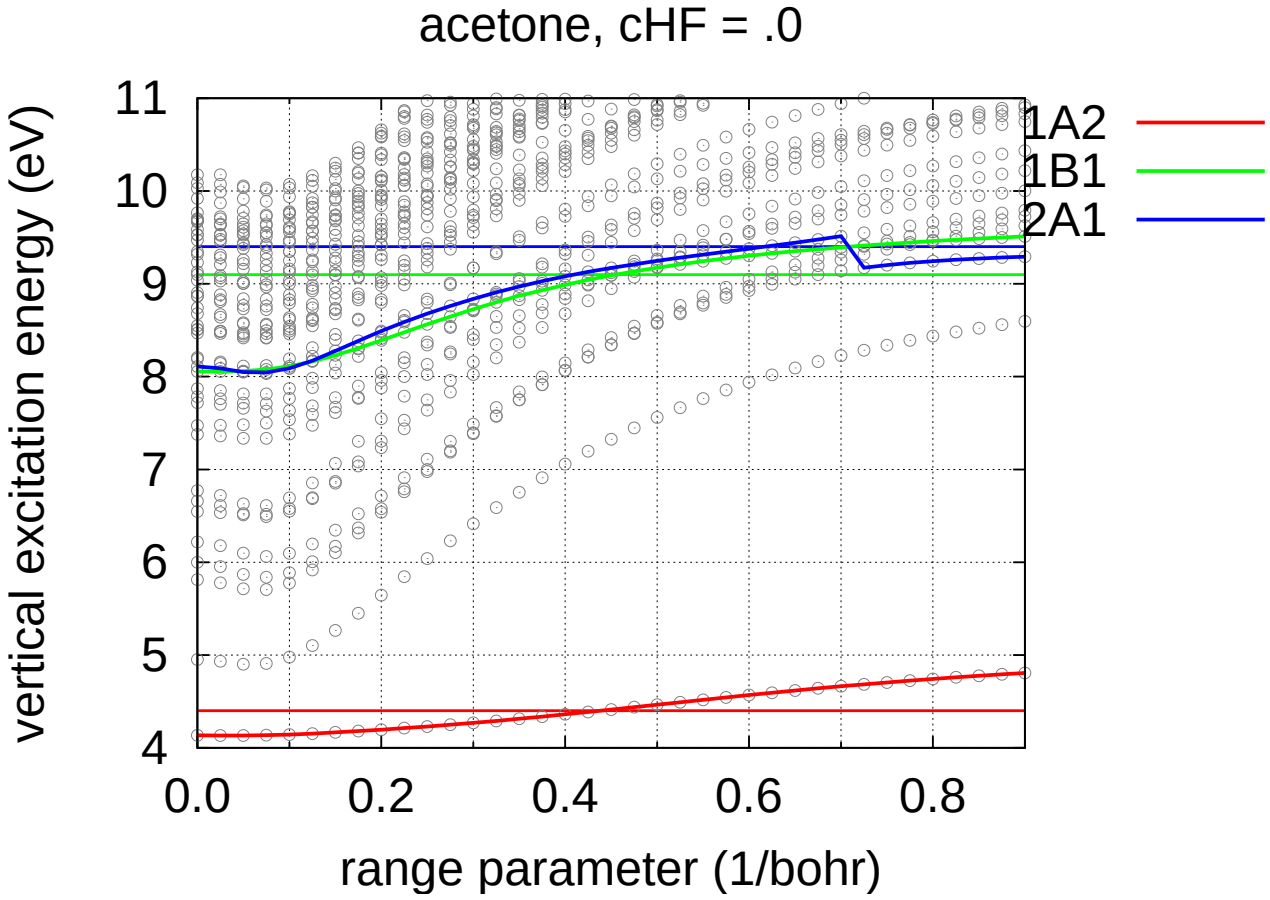
0.6
0.8
1A2
1B1
2A1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range parameter (1/bohr)
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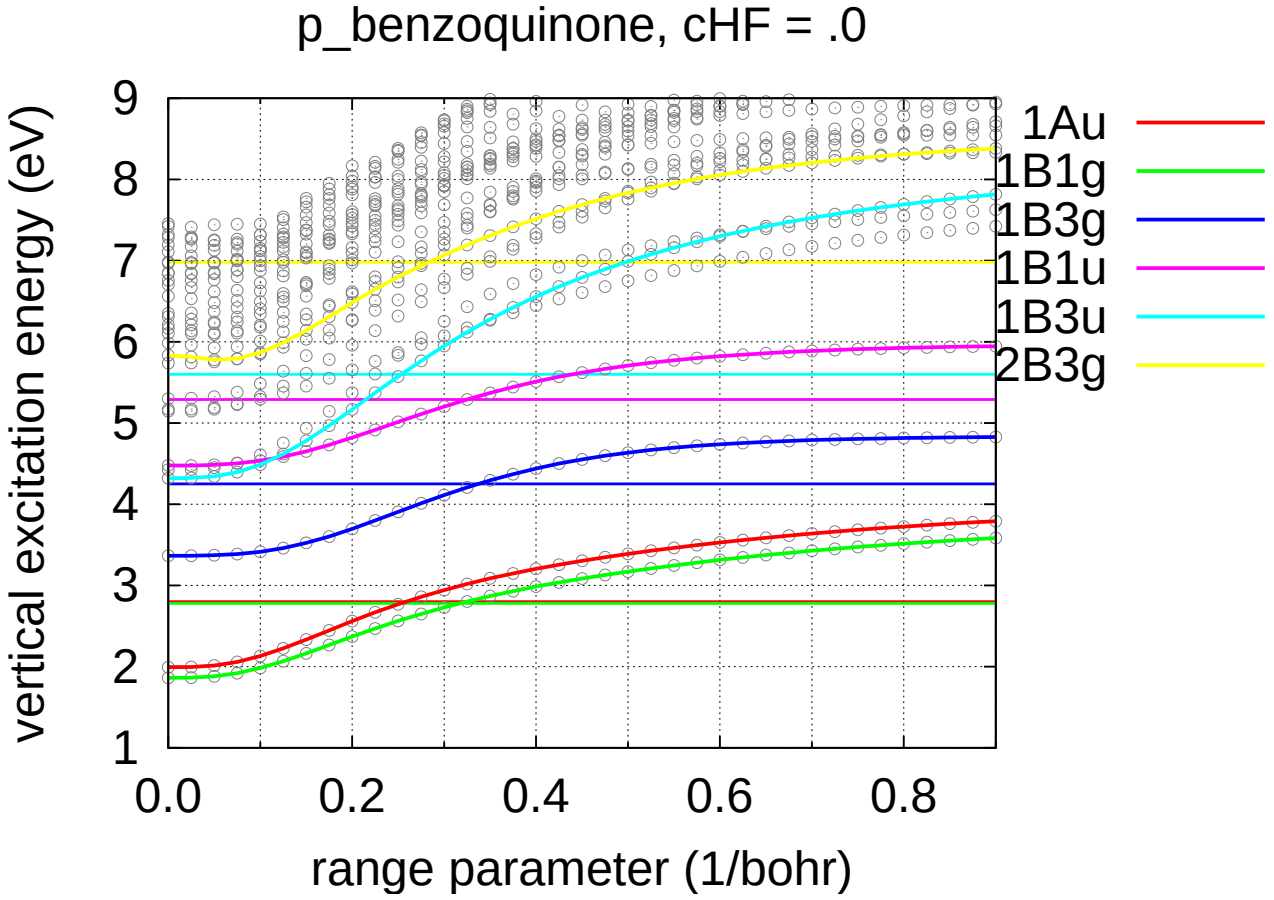
2A1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range parameter (1/bohr)
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2
3
4
5
6
7
8
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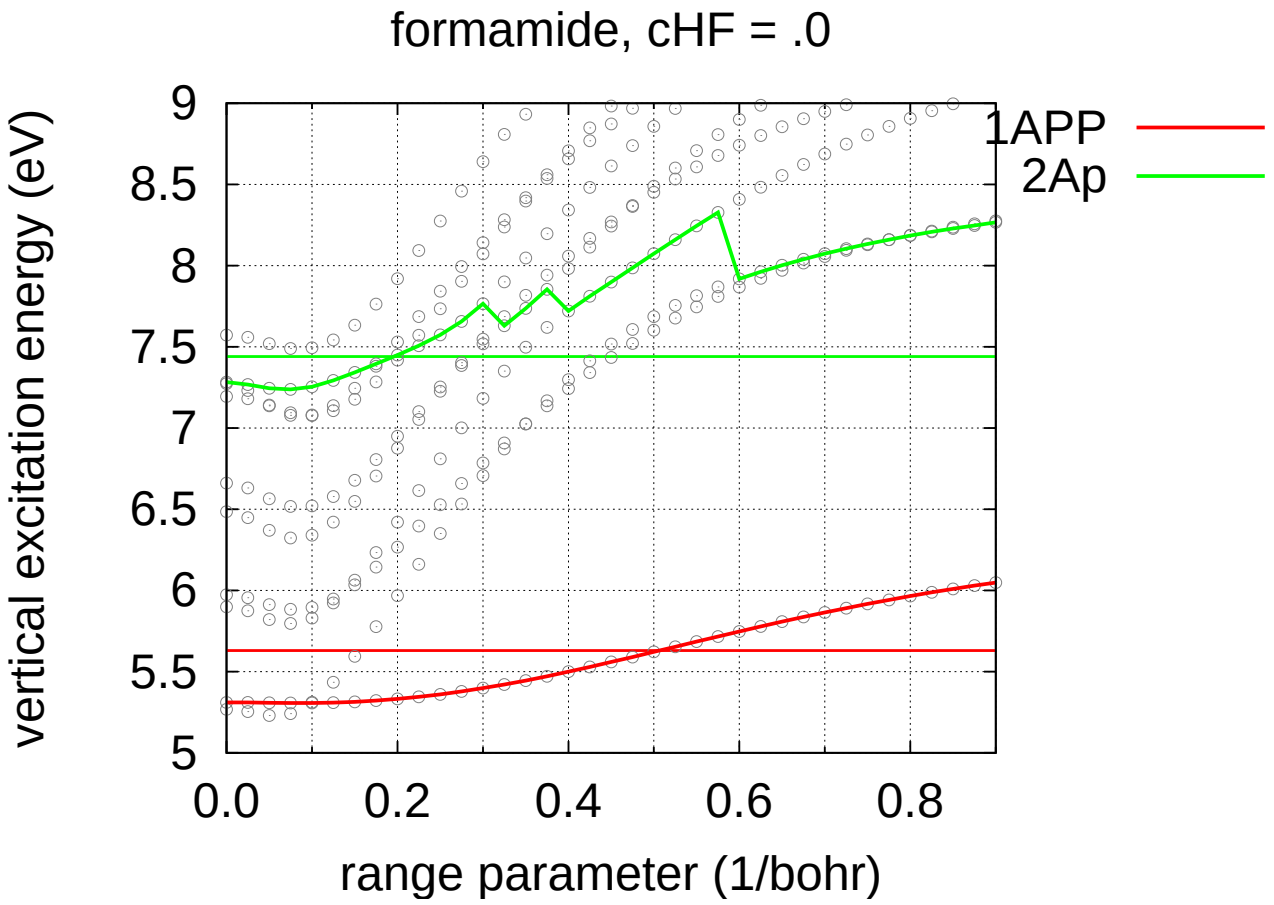
0.4
0.6
0.8
1Au
1B1g
1B3g
1B1u
1B3u
2B3g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2Ap
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7.5
7
6.5
6
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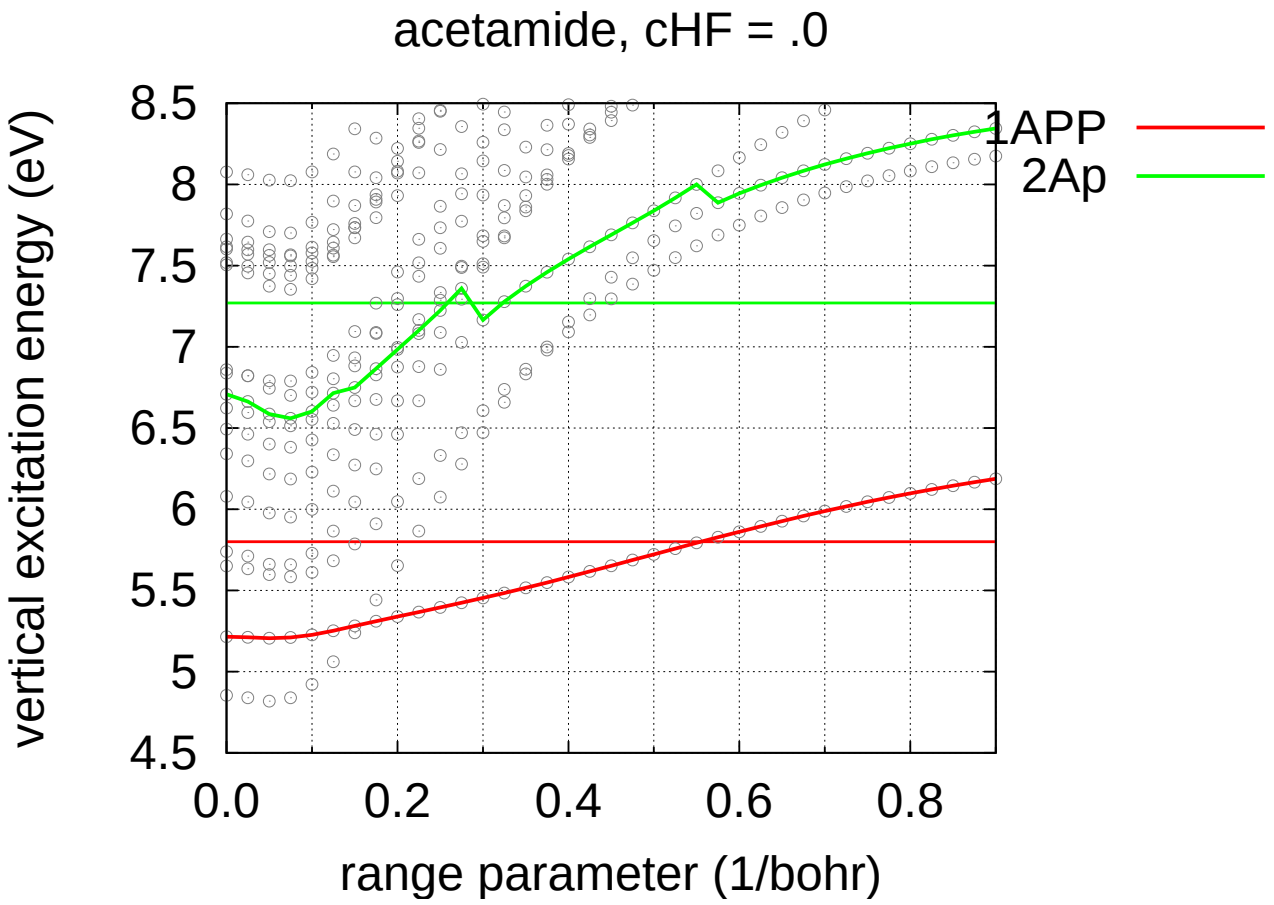
0.8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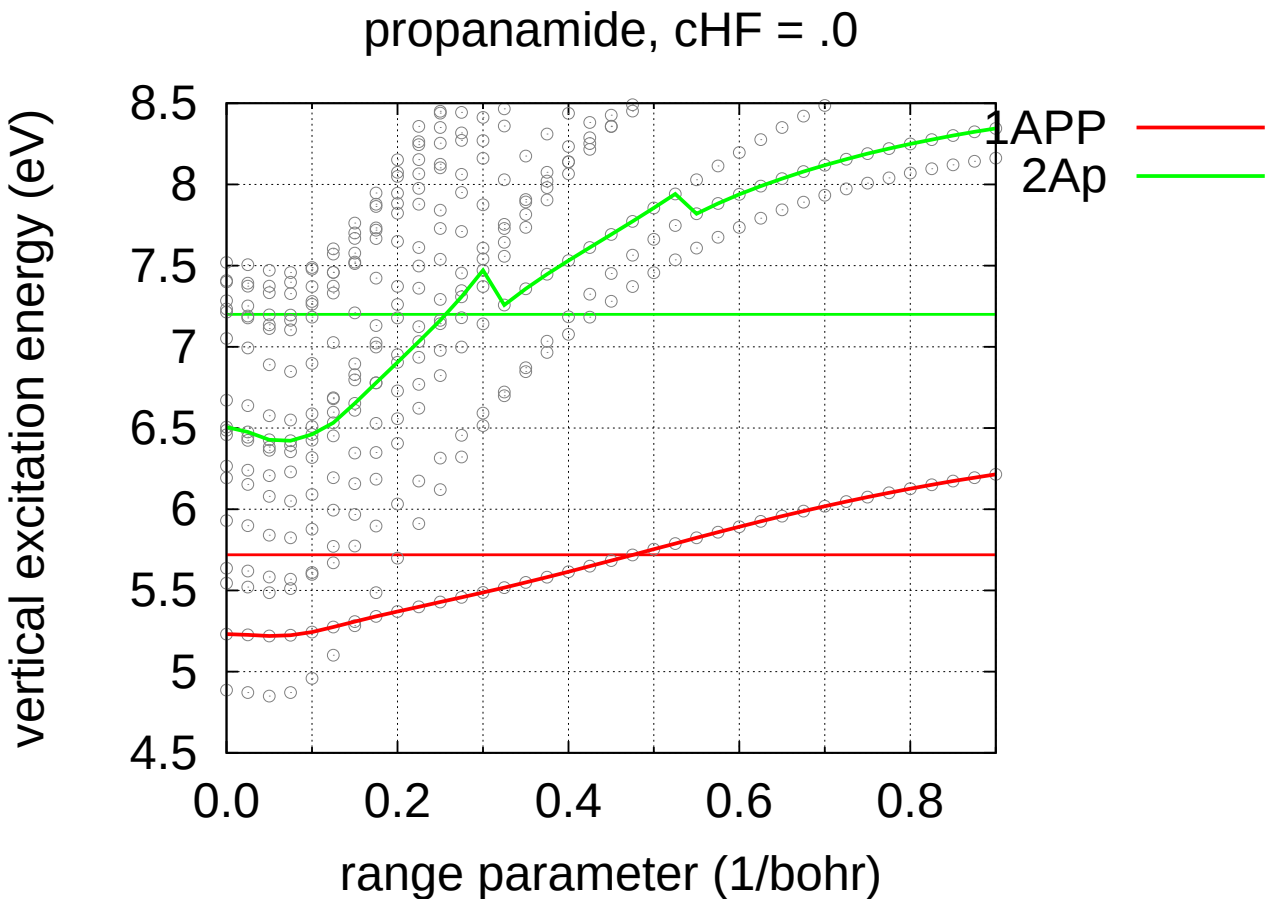
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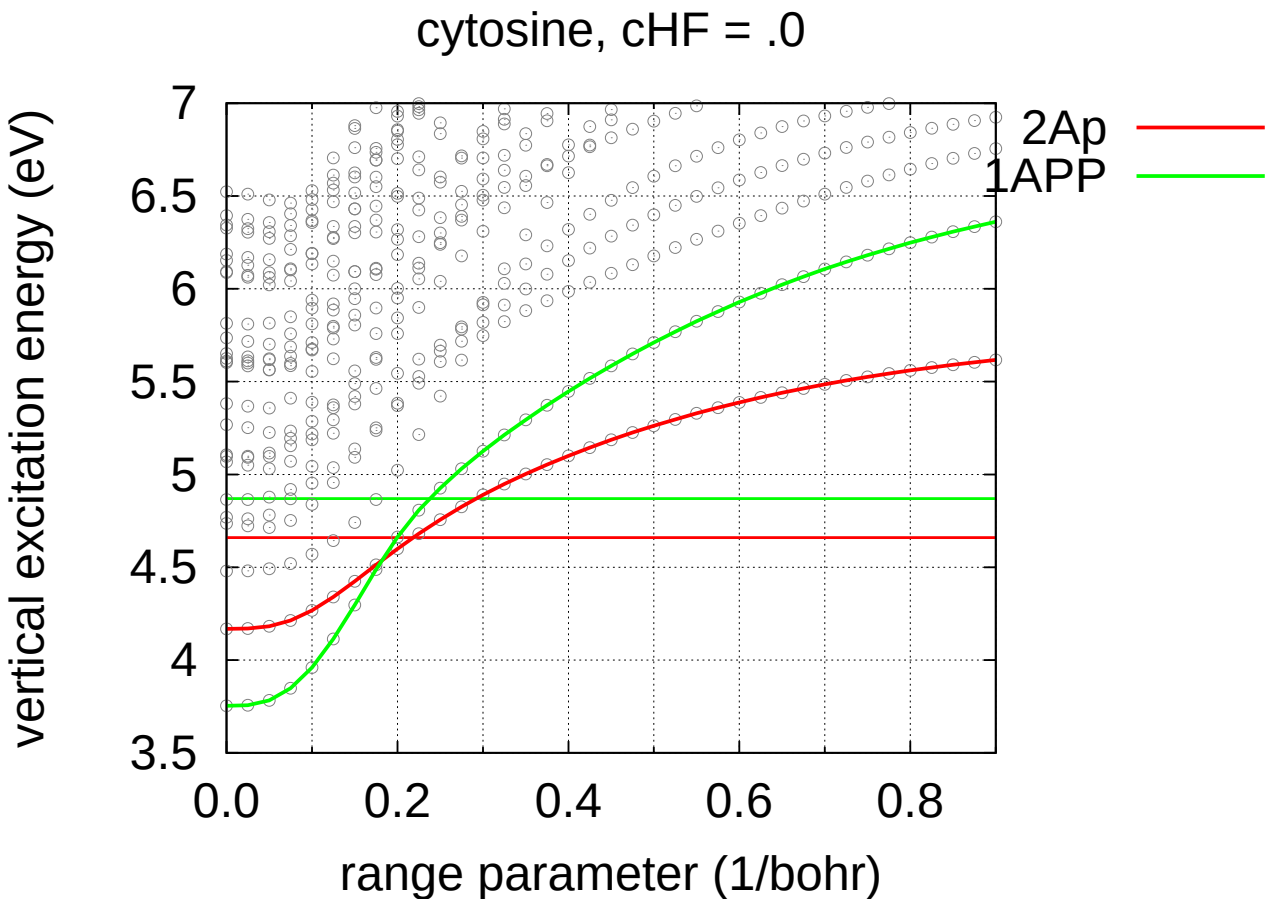
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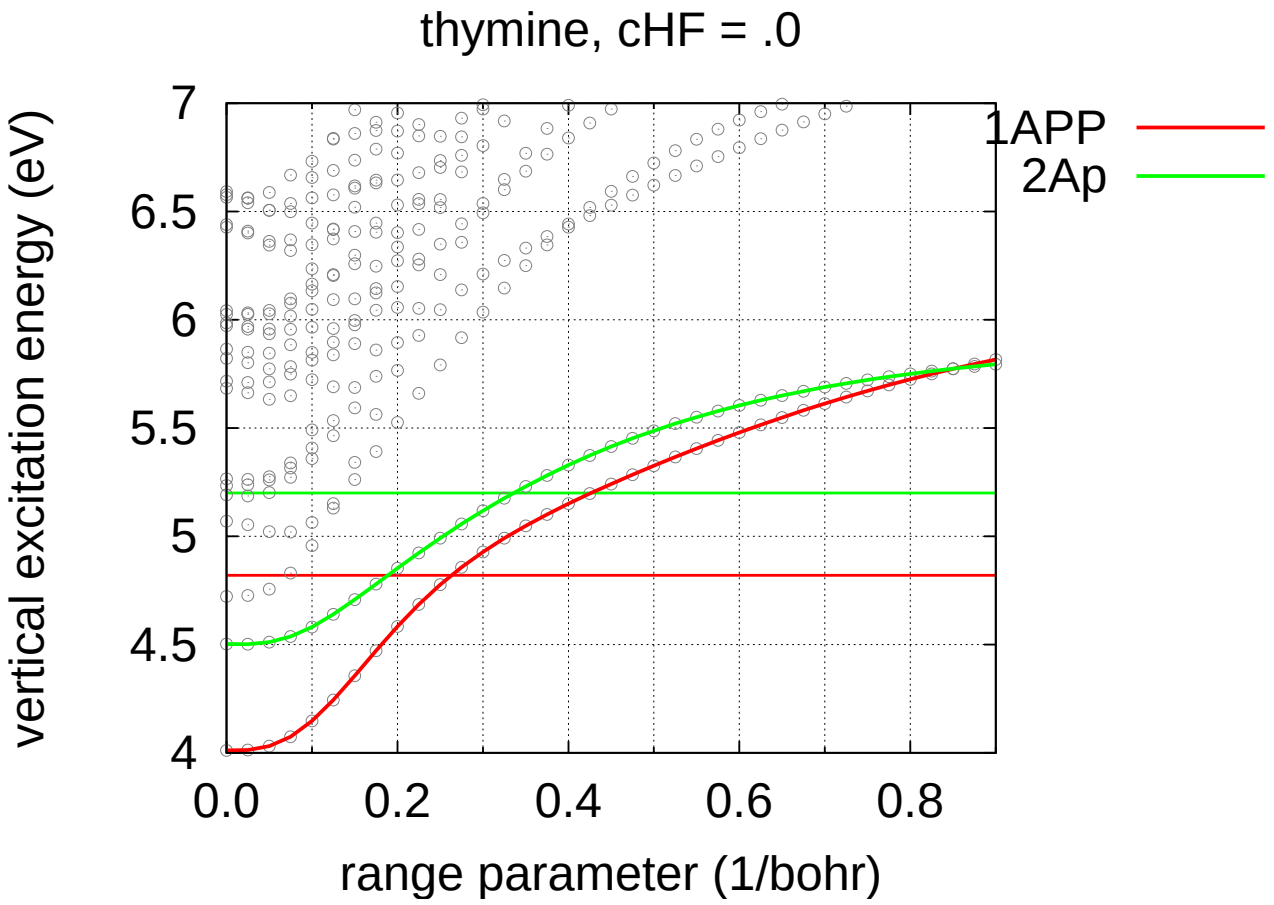
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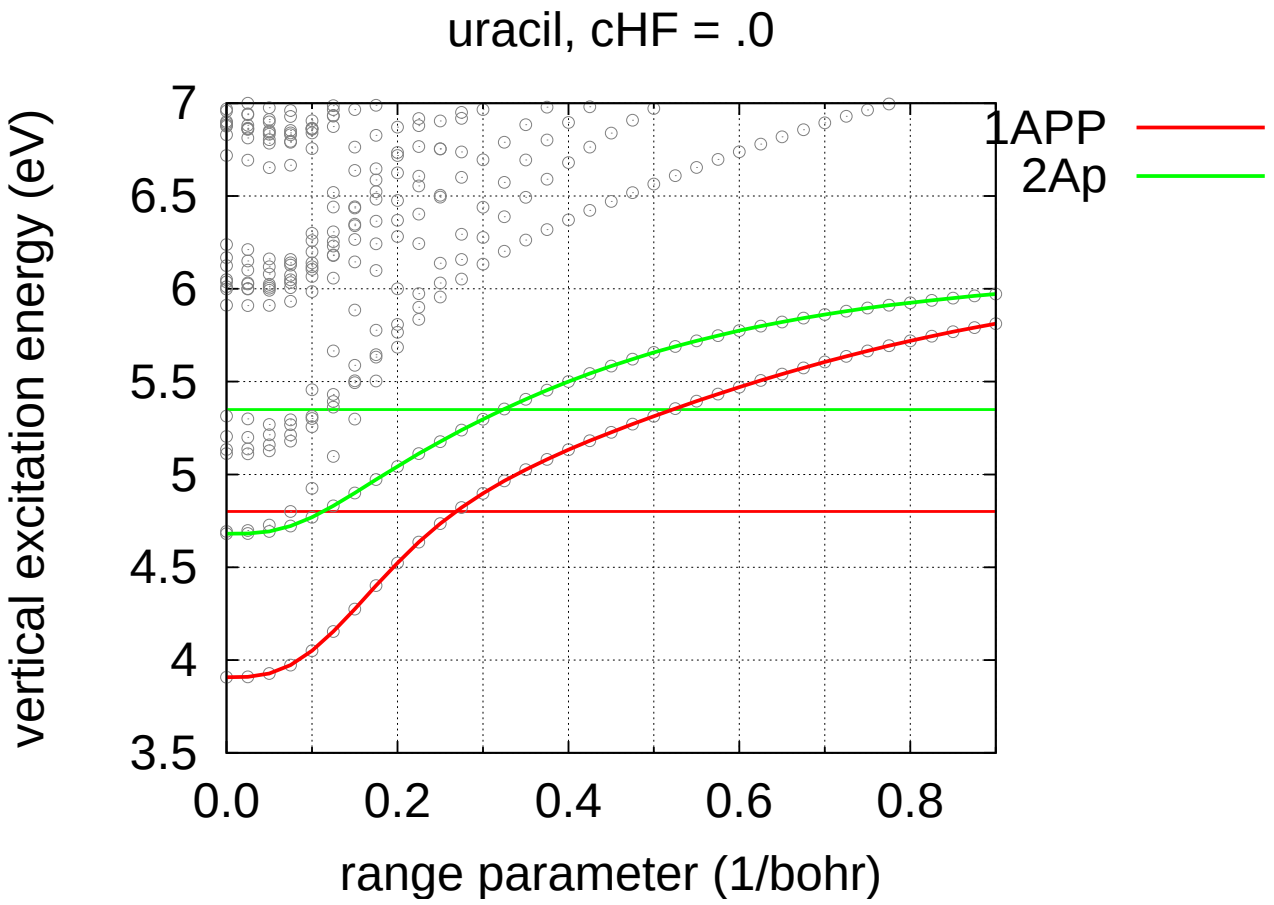
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5.5
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4.5
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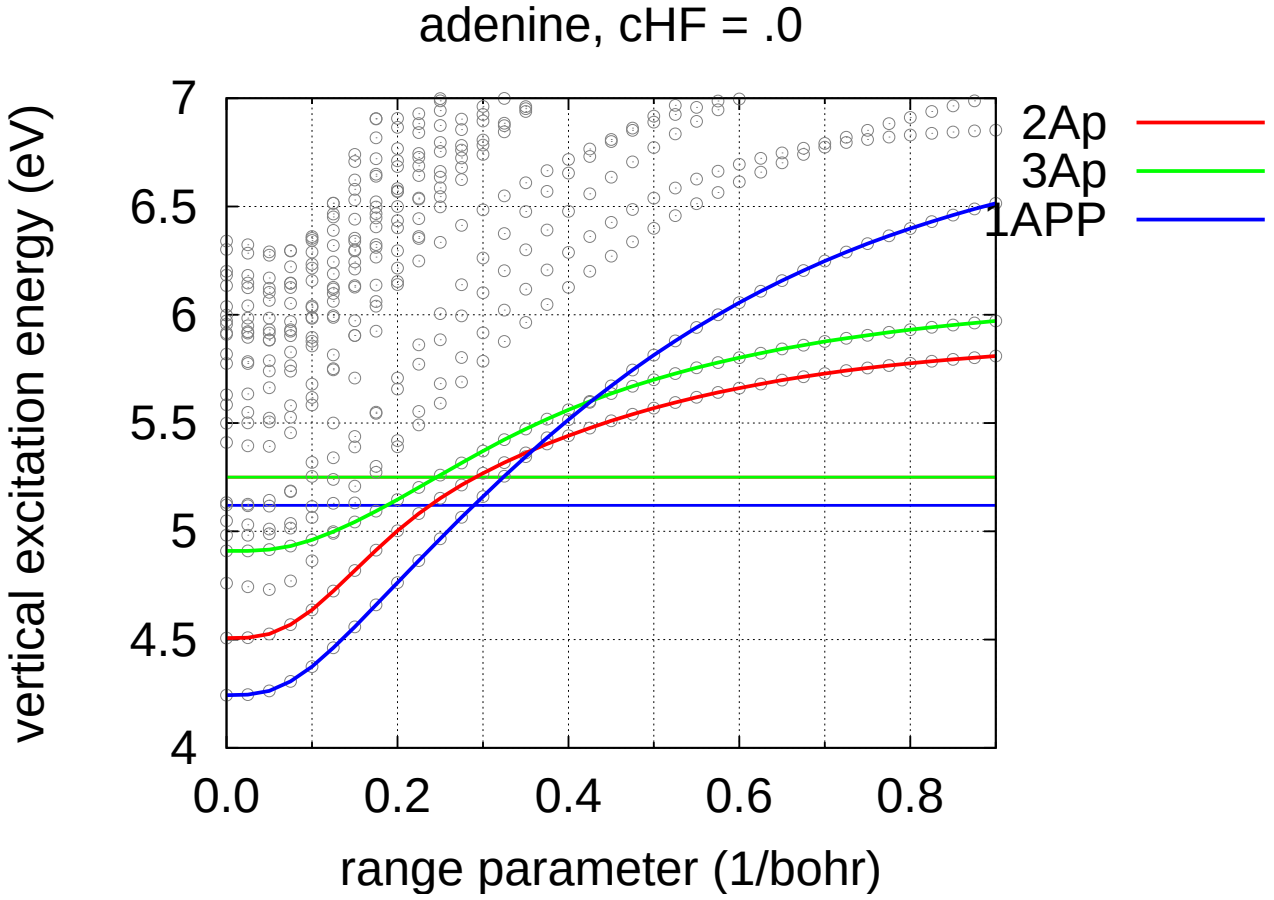
0.4
0.6
0.8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3Ap
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5
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0.0
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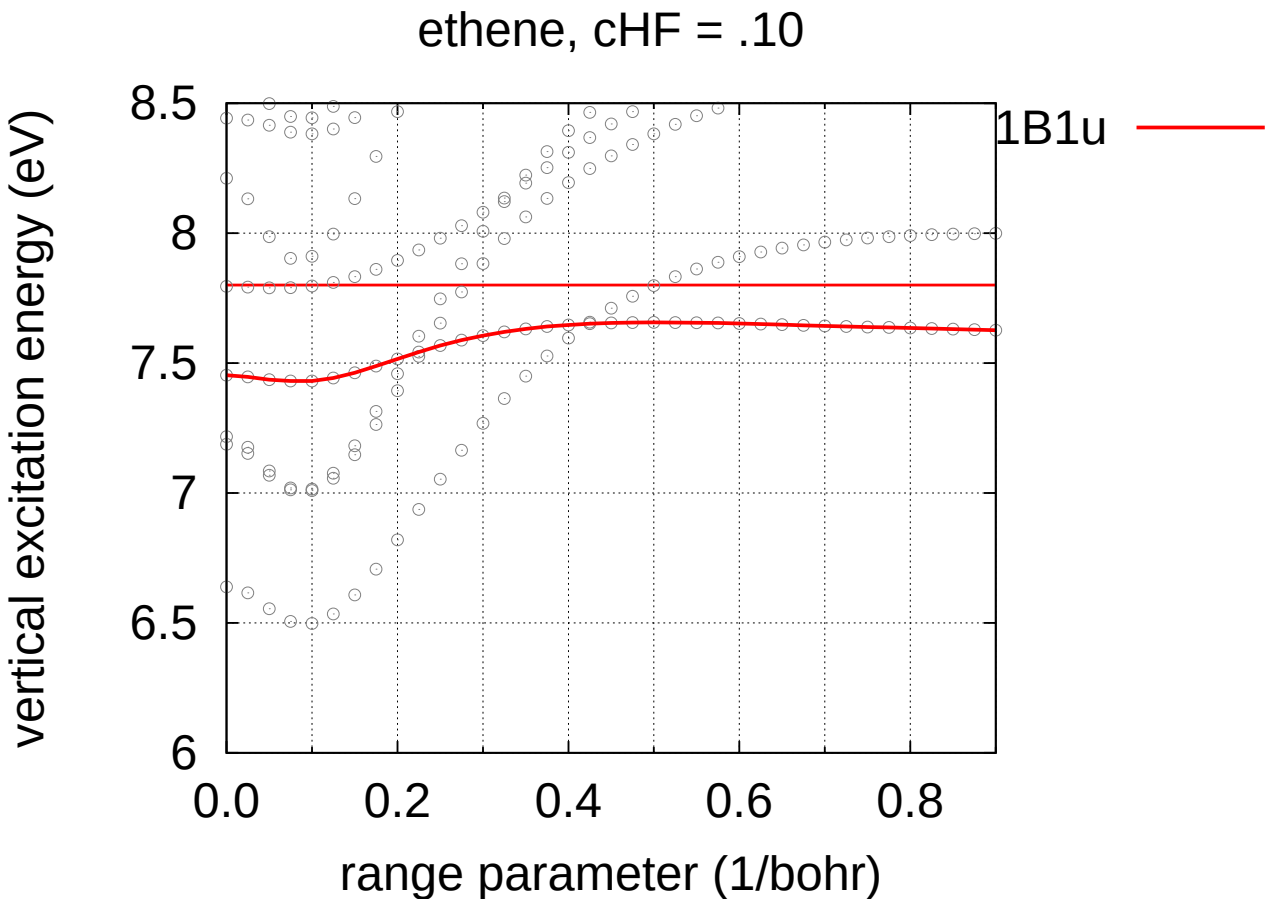
0.4
0.6
0.8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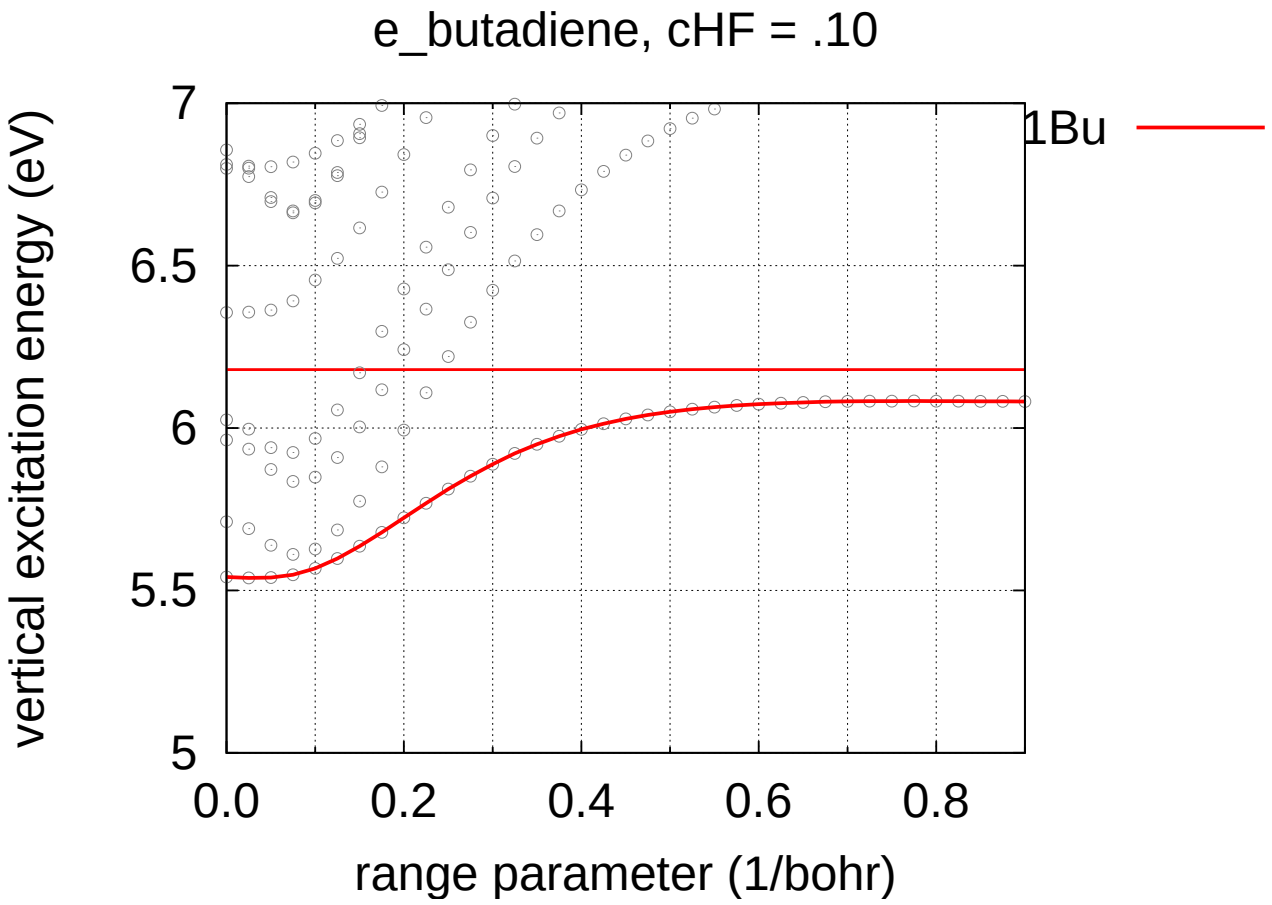
0.2
0.4
0.6
0.8
range parameter (1/bohr)
1B1u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vertical excitation energy (eV)
range parameter (1/bohr)
1Bu
7
6.5
6
5.5
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0.0
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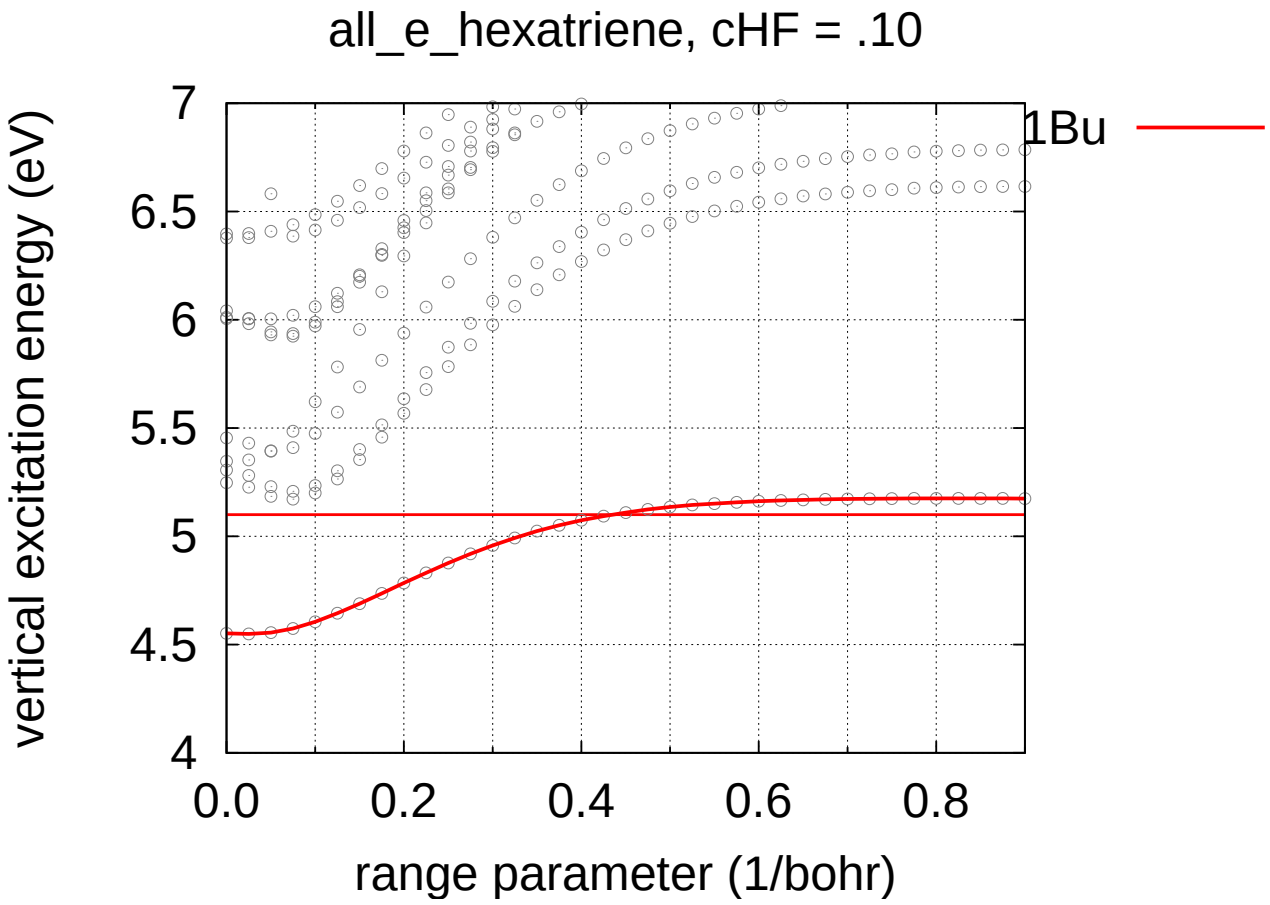
0.4
0.6
0.8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6
5.5
5
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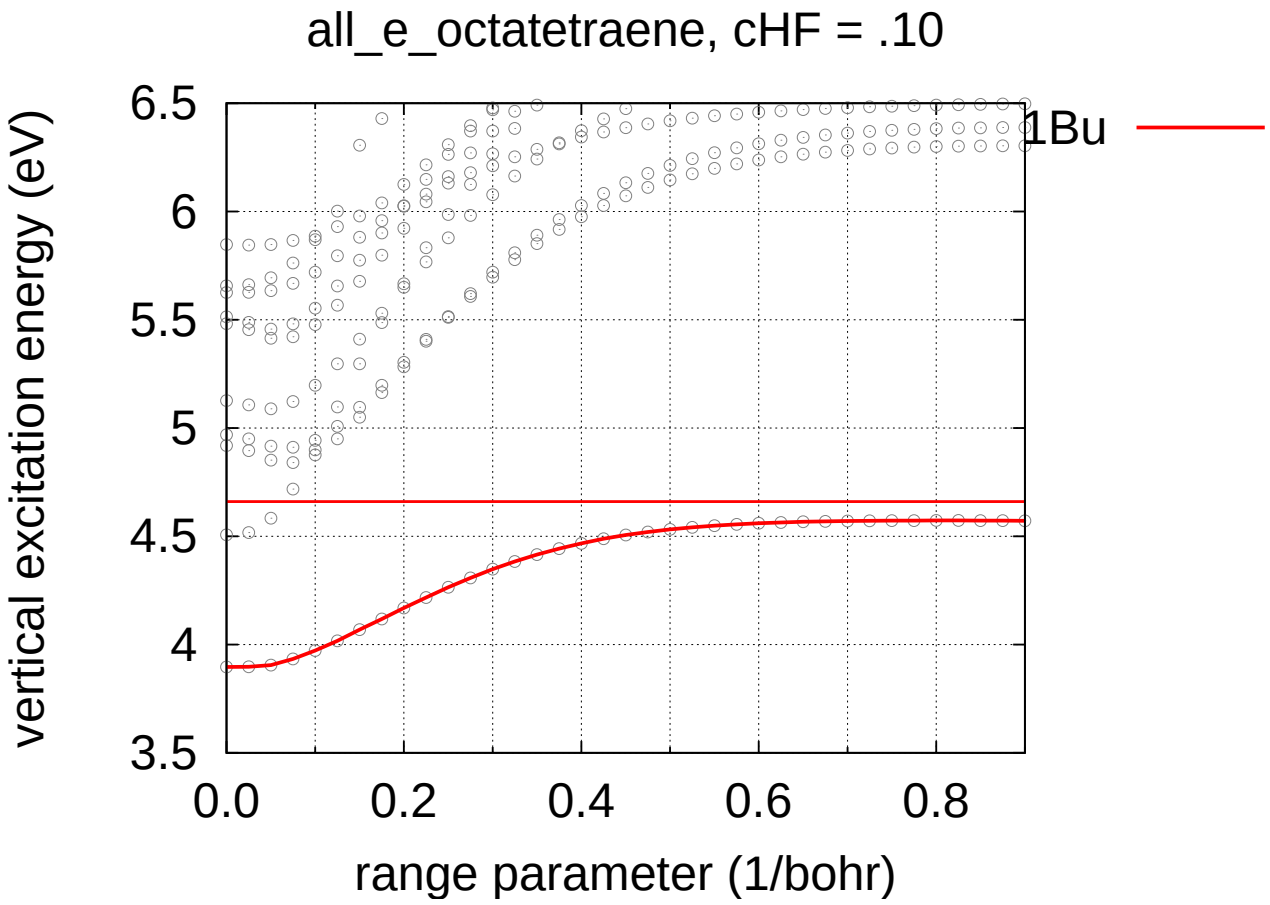
0.4
0.6
0.8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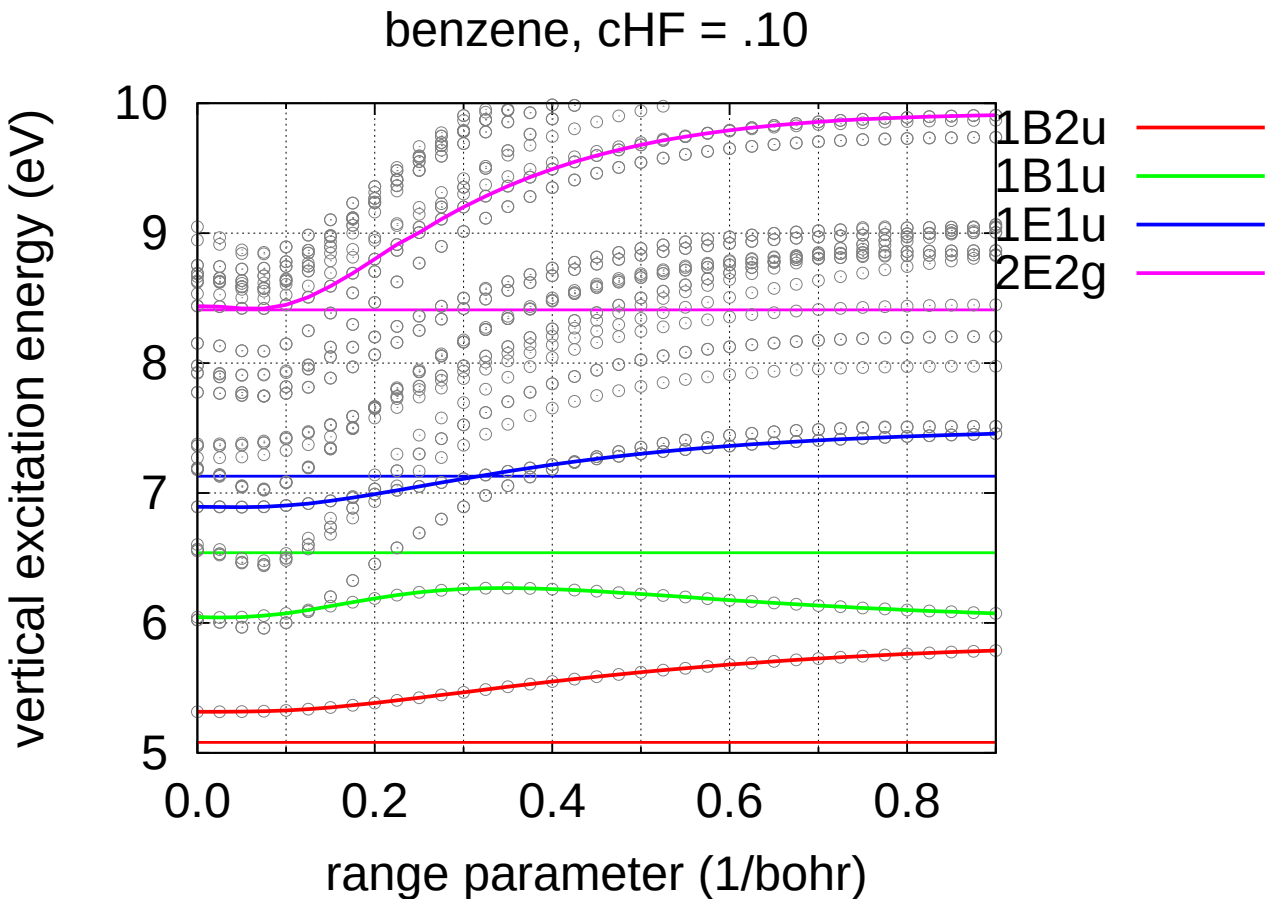
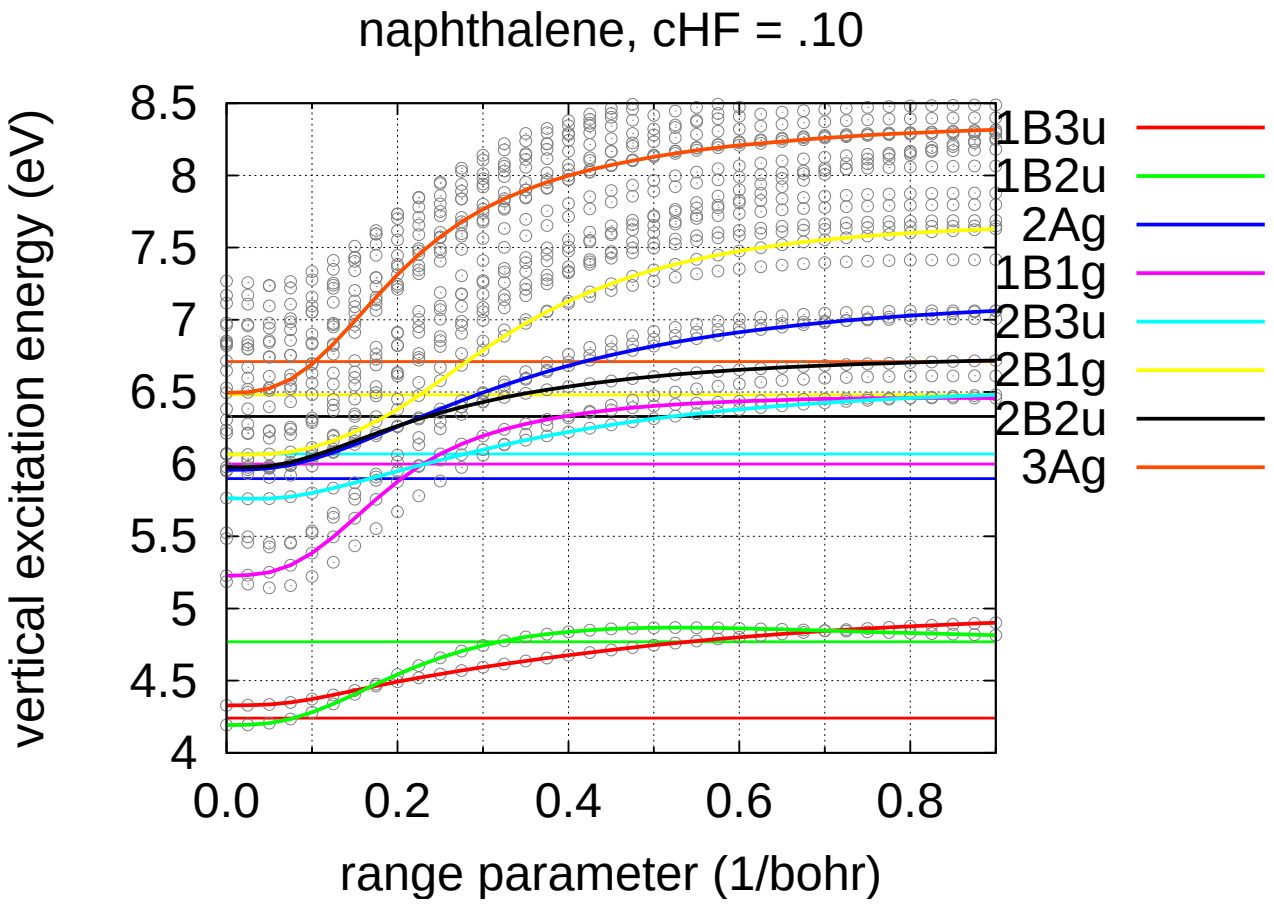
vertical excitation energy (eV)
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8
range parameter (1/bohr)
1Bu


benzene, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
10
9
8
7
6
5
0.0
0.2
0.4
0.6
0.8
1B2u
1B1u
1E1u
2E2g


naphthalene, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8
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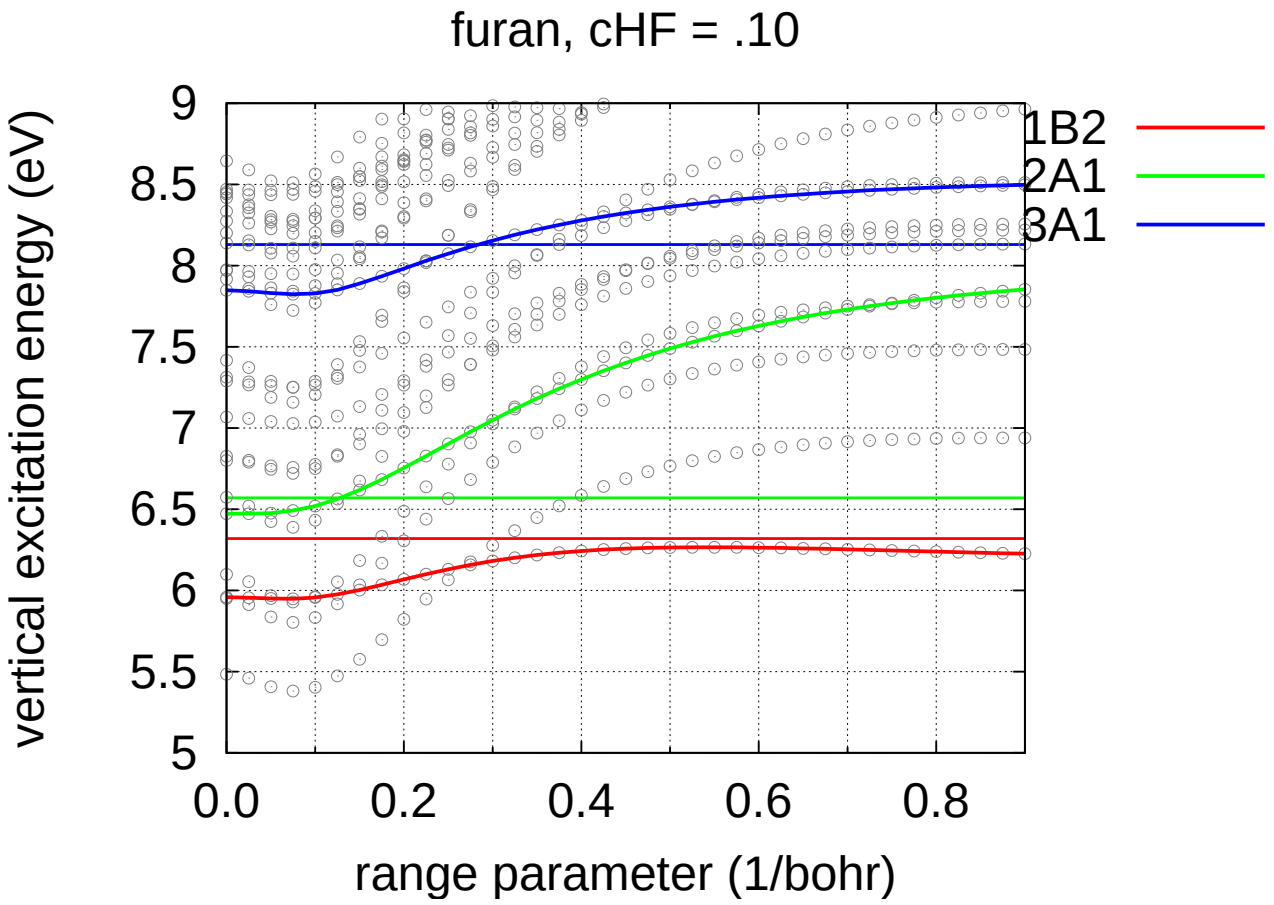
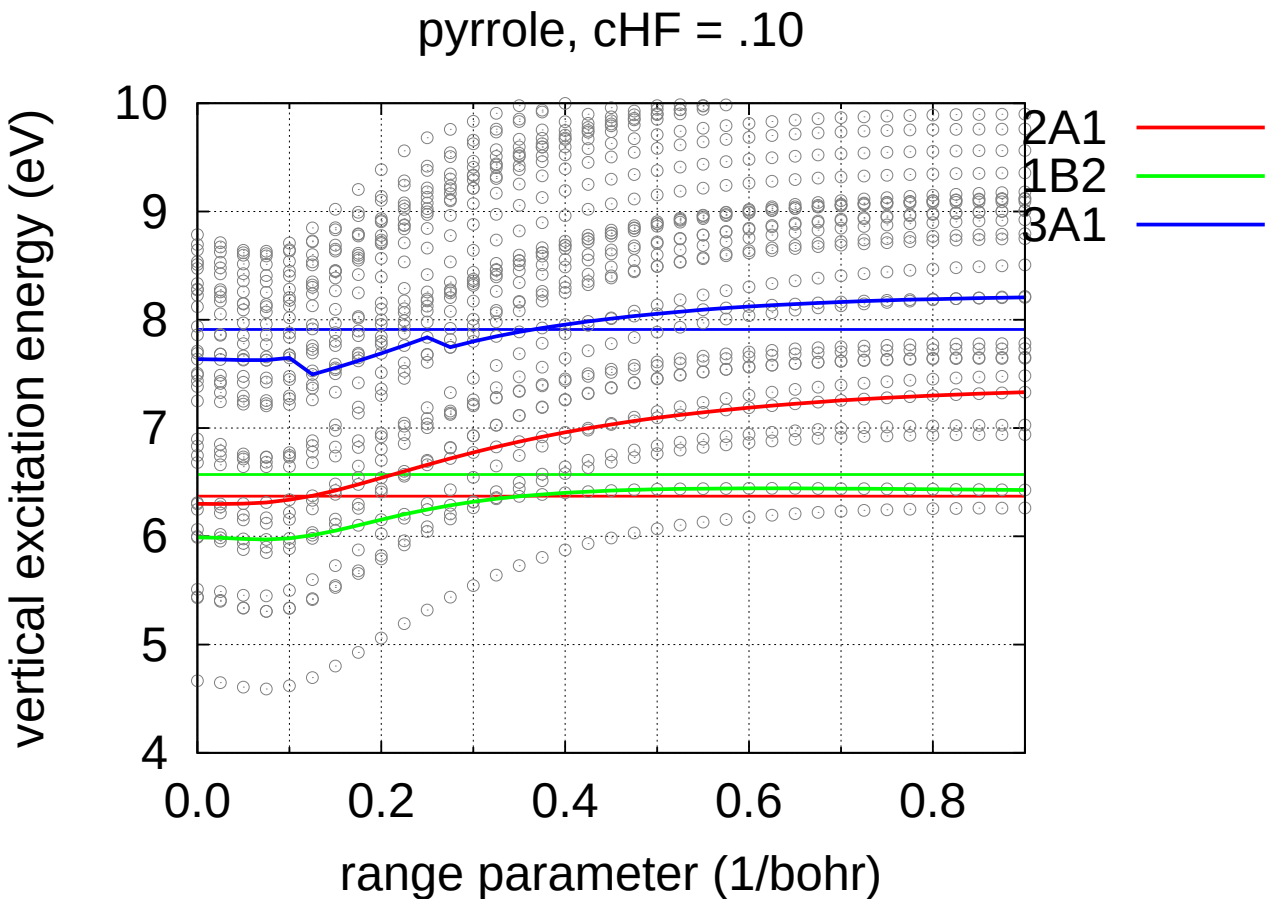
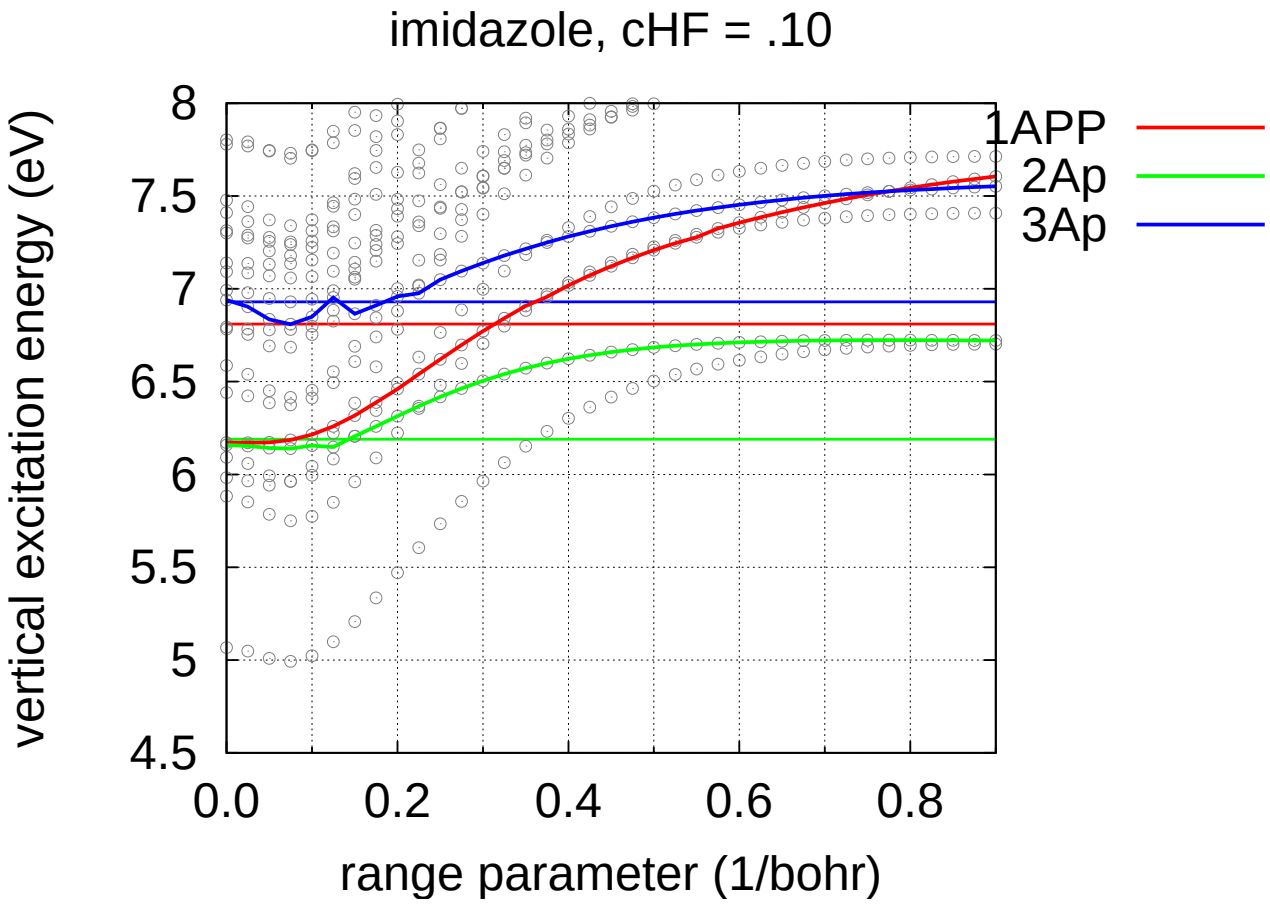
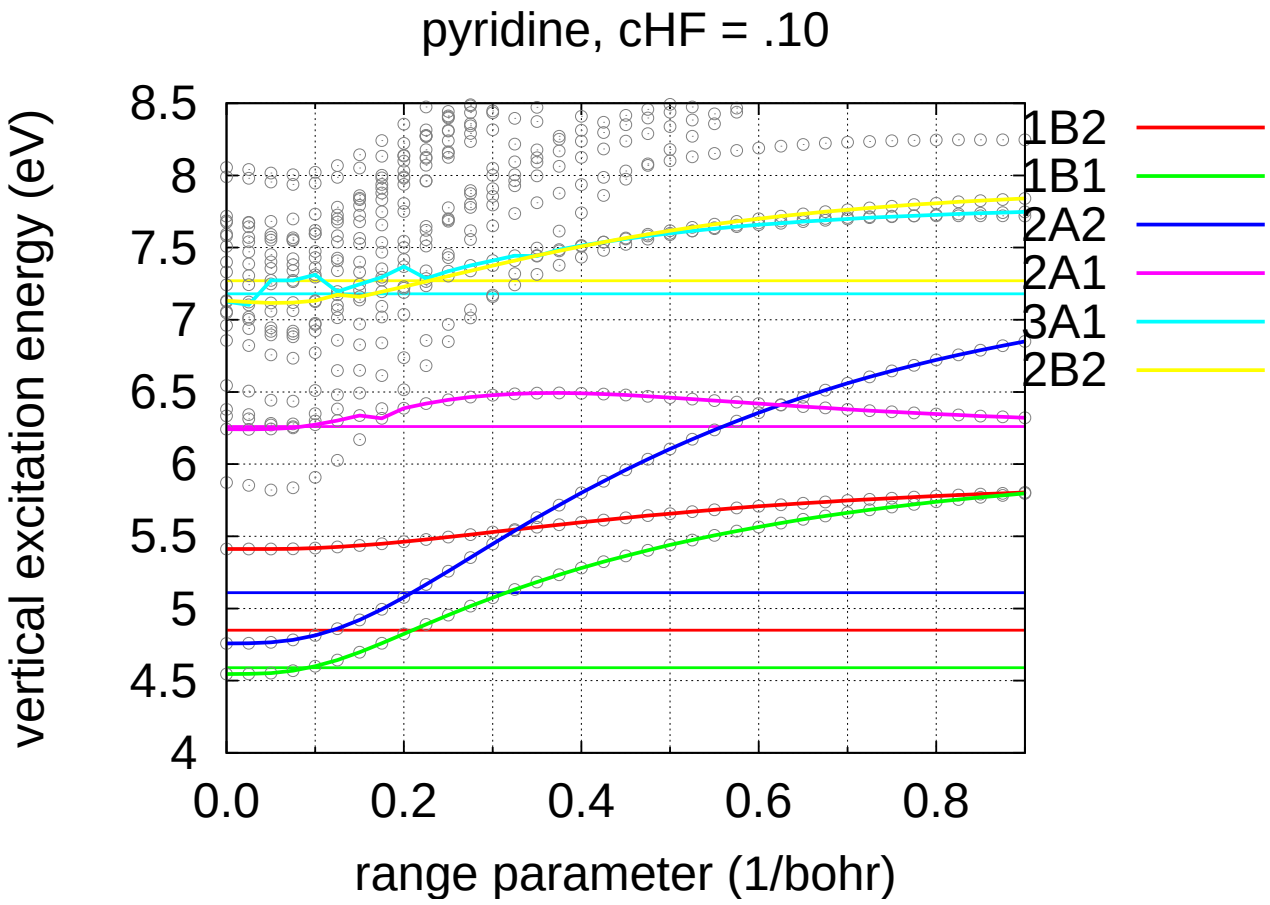
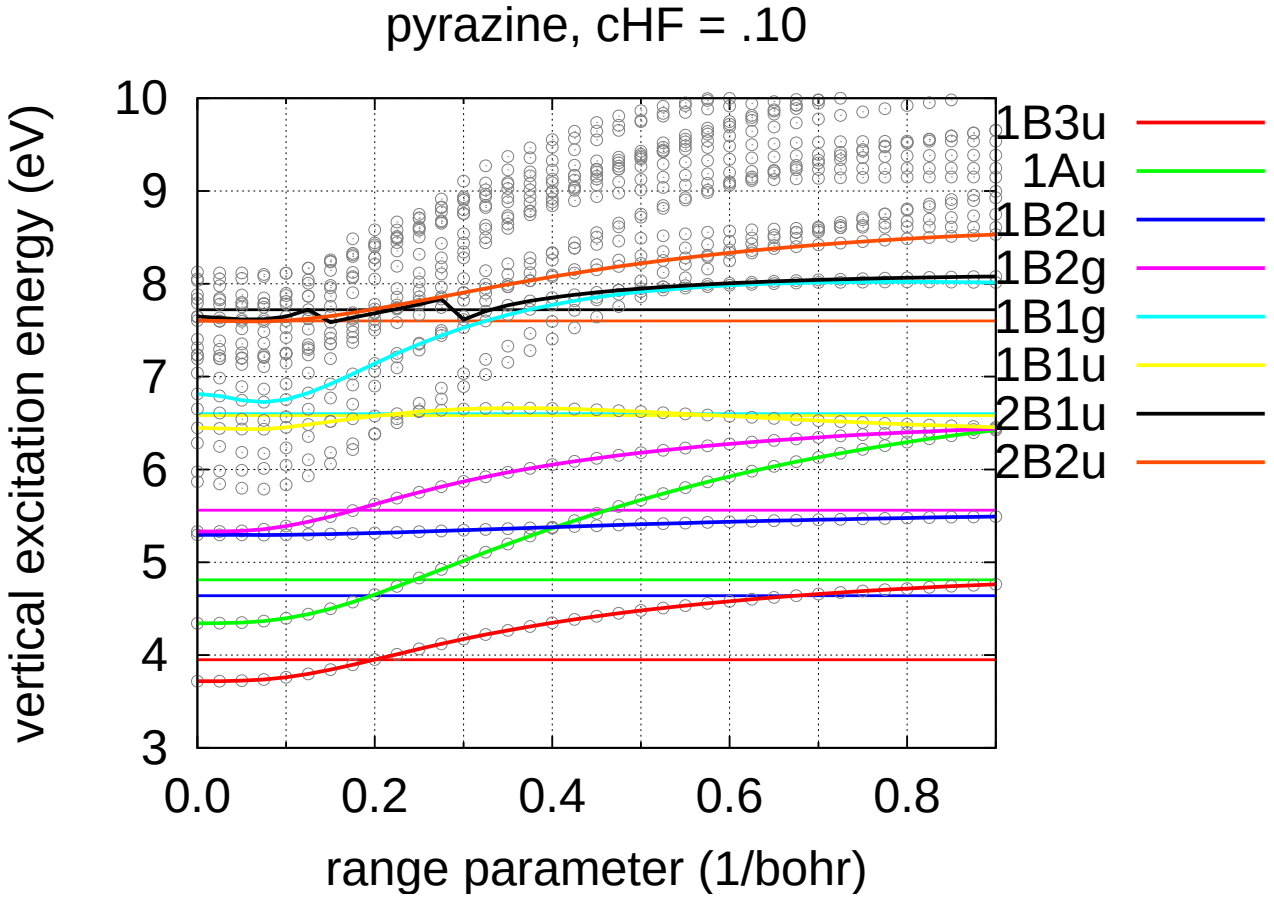
1B2u
2Ag
1B1g
2B3u
2B1g
2B2u
3Ag

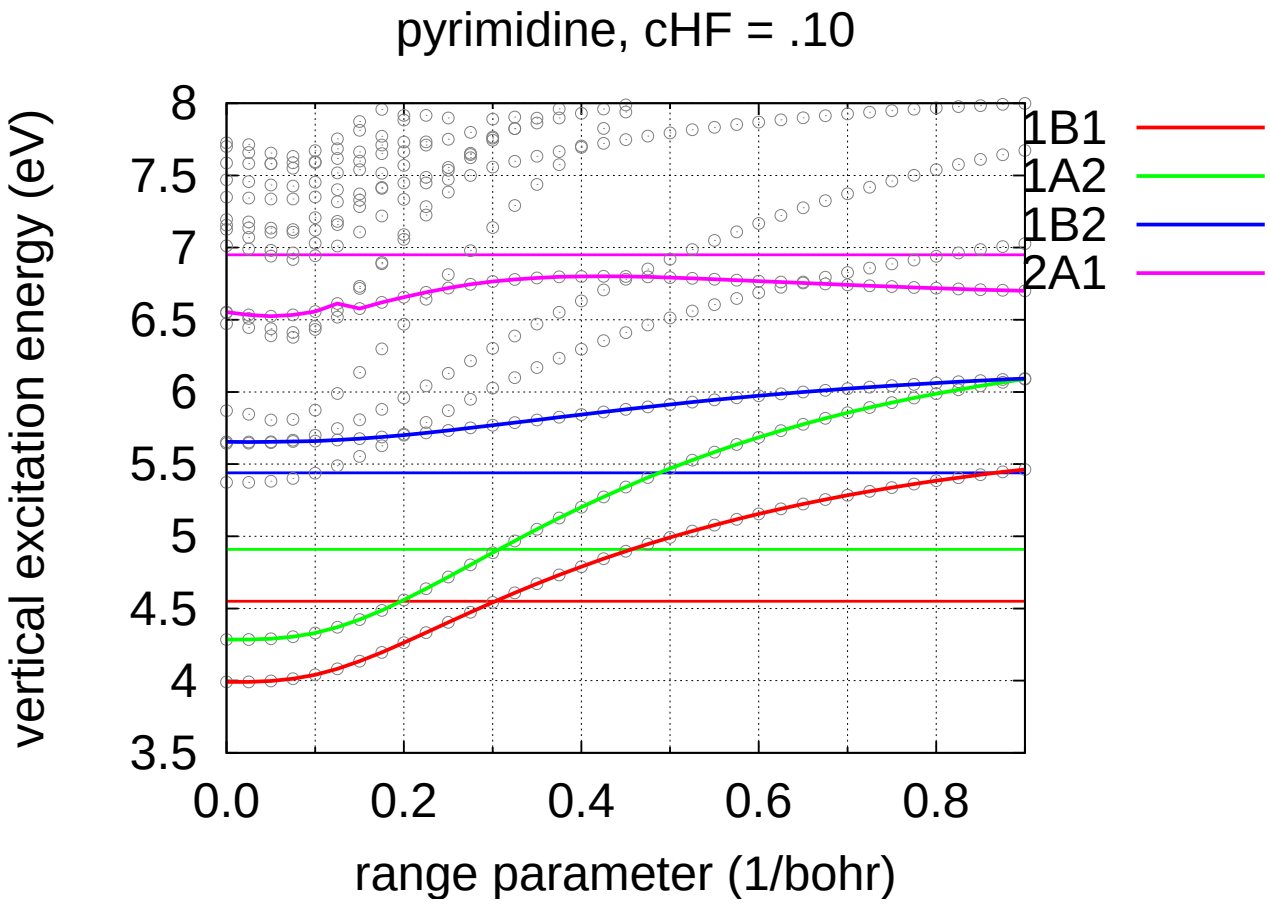

furan, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
9
8.5
8
7.5
7
6.5
6
5.5
5
0.0
0.2
0.4
0.6
0.8
1B2
2A1
3A1

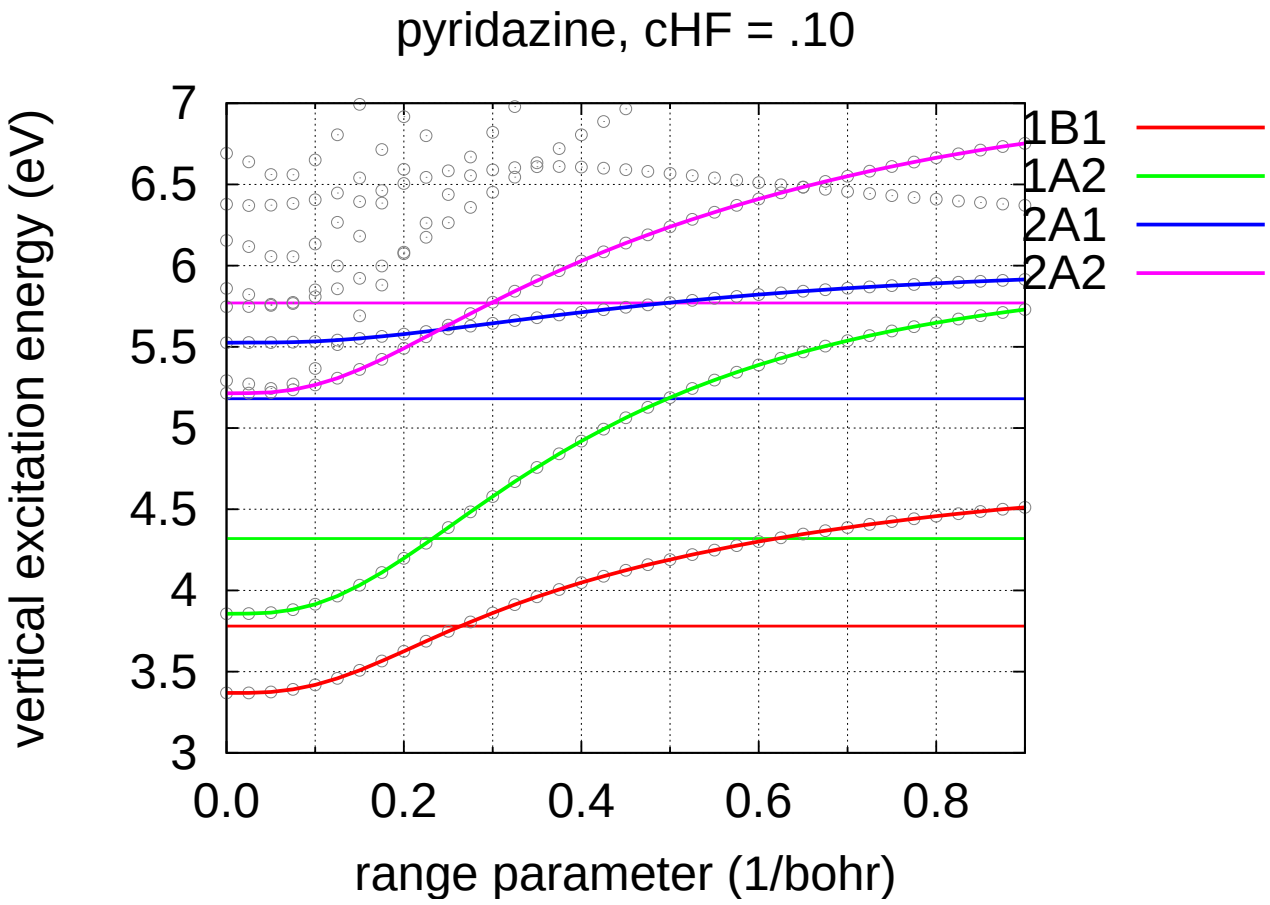

pyrrole, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
10
9
8
7
6
5
4
0.0
0.2
0.4
0.6
0.8
2A1
1B2
3A1

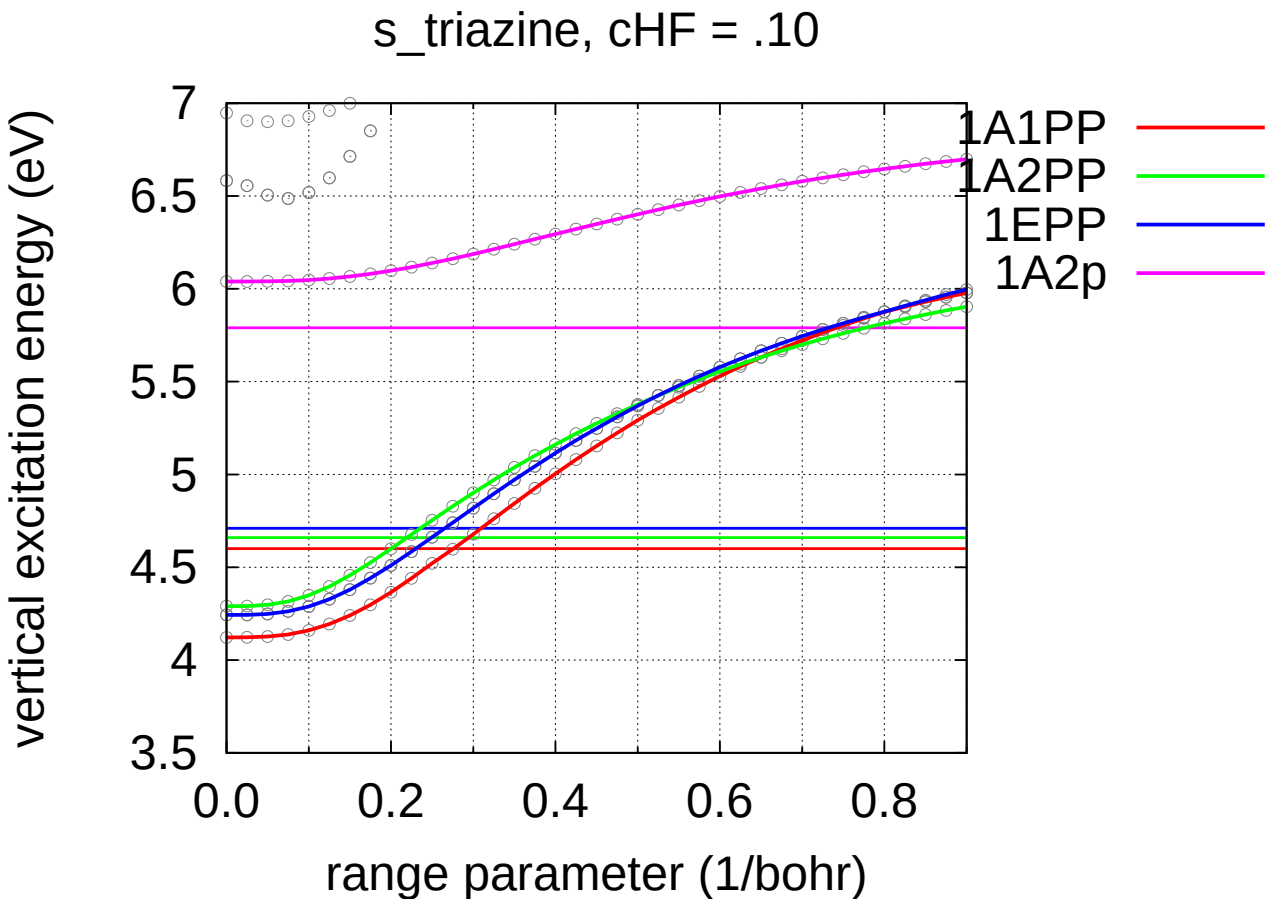

imidazole, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
8
7.5
7
6.5
6
5.5
5
4.5
0.0
0.2
0.4
0.6
0.8
1APP
2Ap
3Ap

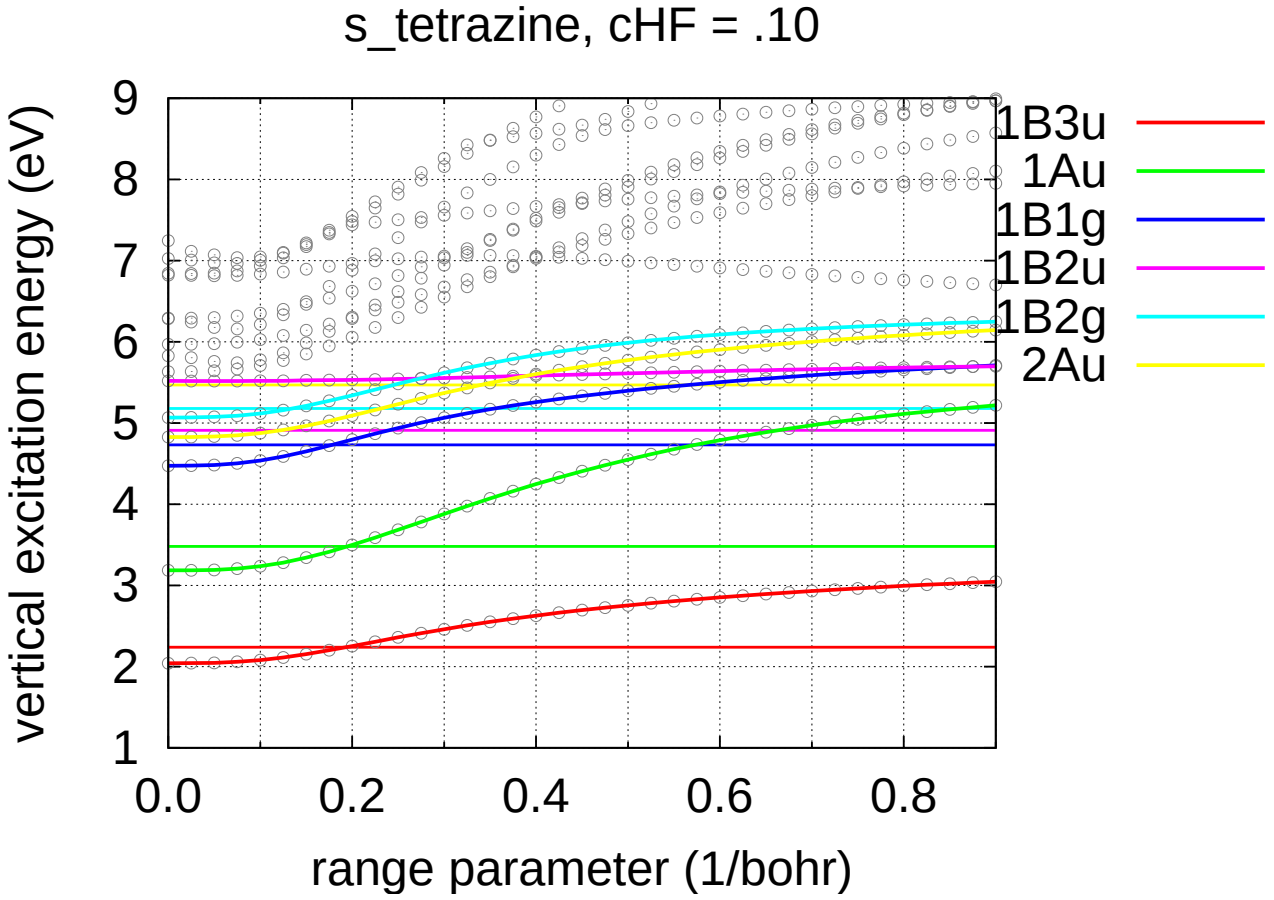

pyridine, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8
1B2
1B1
2A2
2A1
3A1
2B2

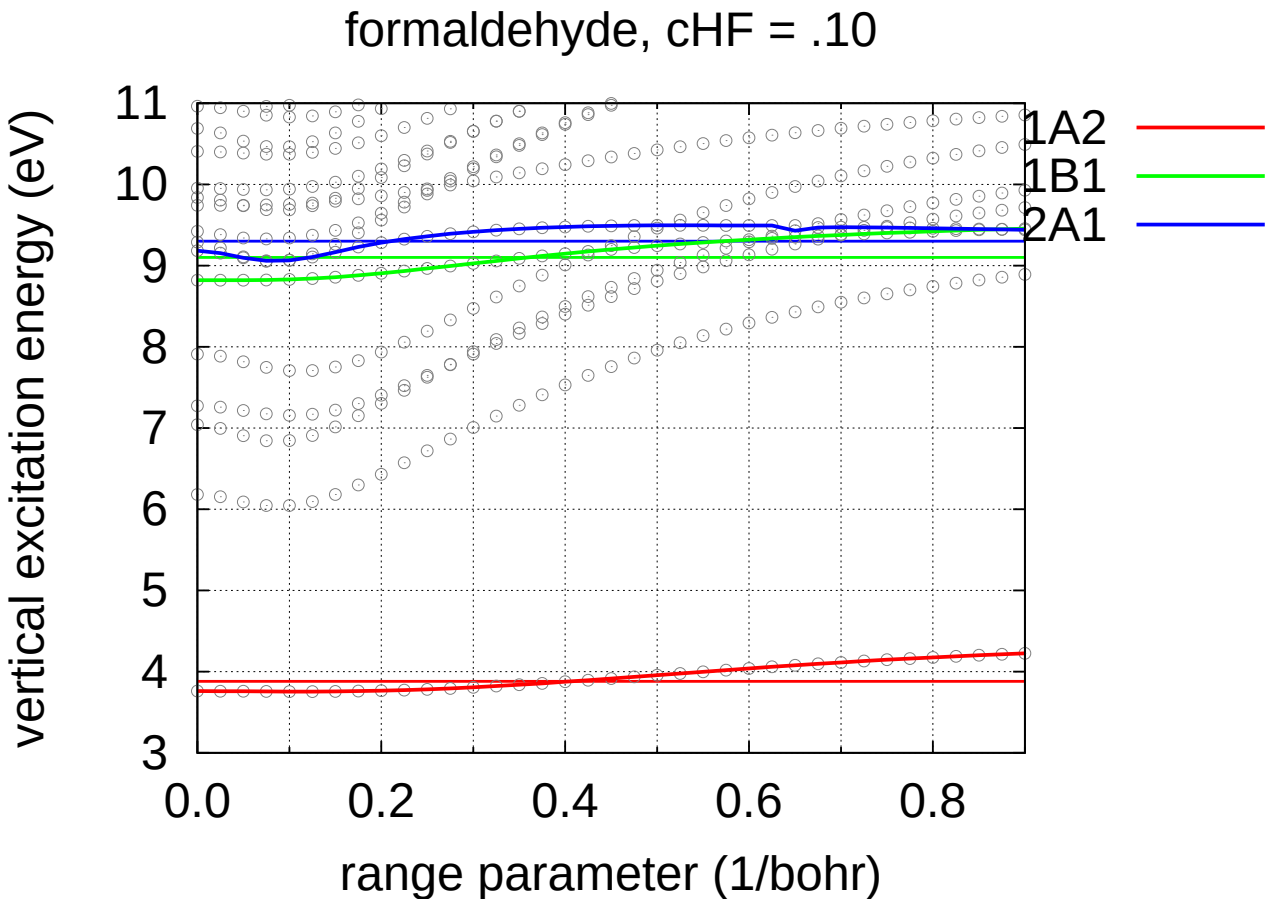

pyrazine, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
10
9
8
7
6
5
4
3
0.0
0.2
0.4
0.6
0.8
1B3u
1Au
1B2u
1B2g
1B1g
1B1u
2B1u
2B2u

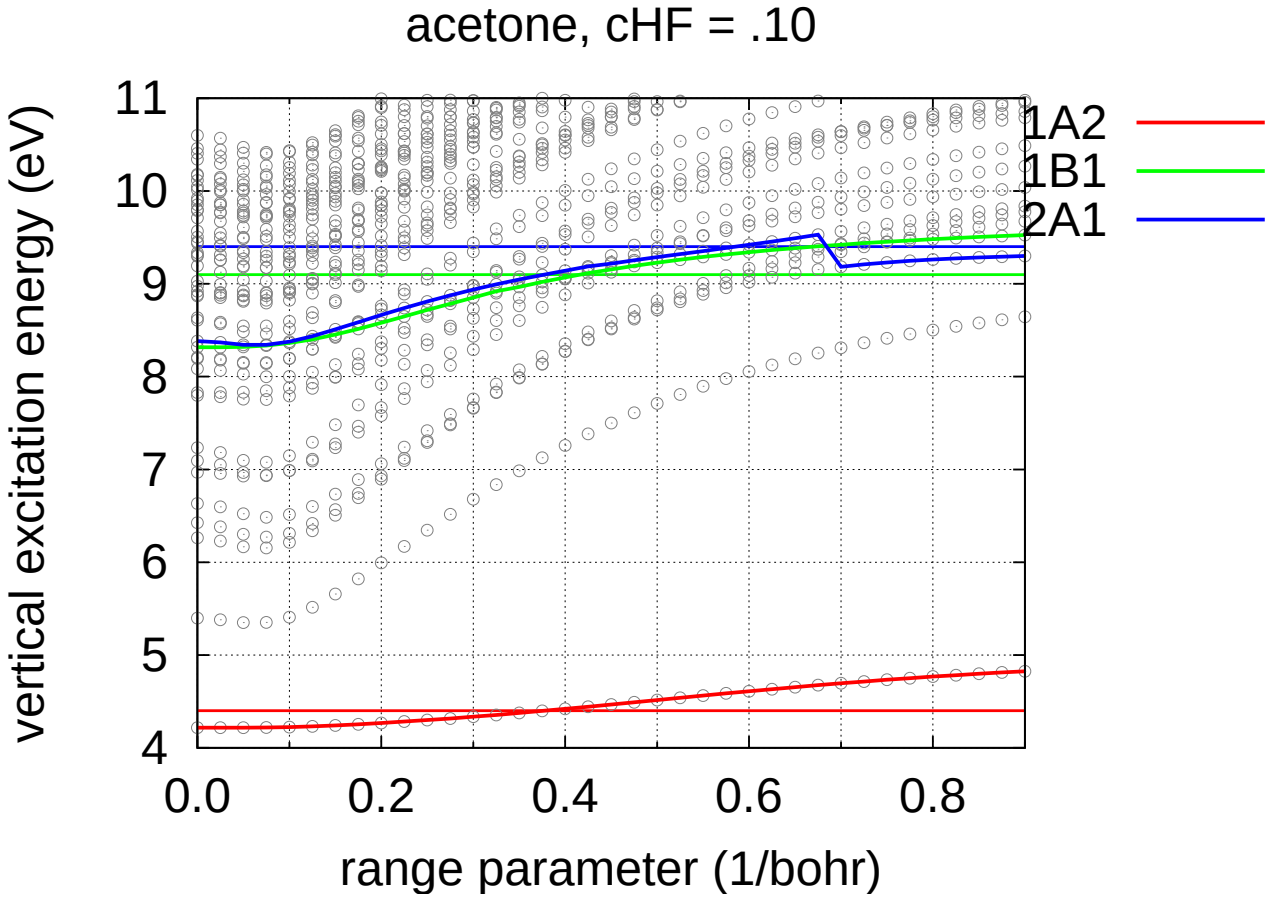

pyrimidine, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8
1B1
1A2
1B2
2A1

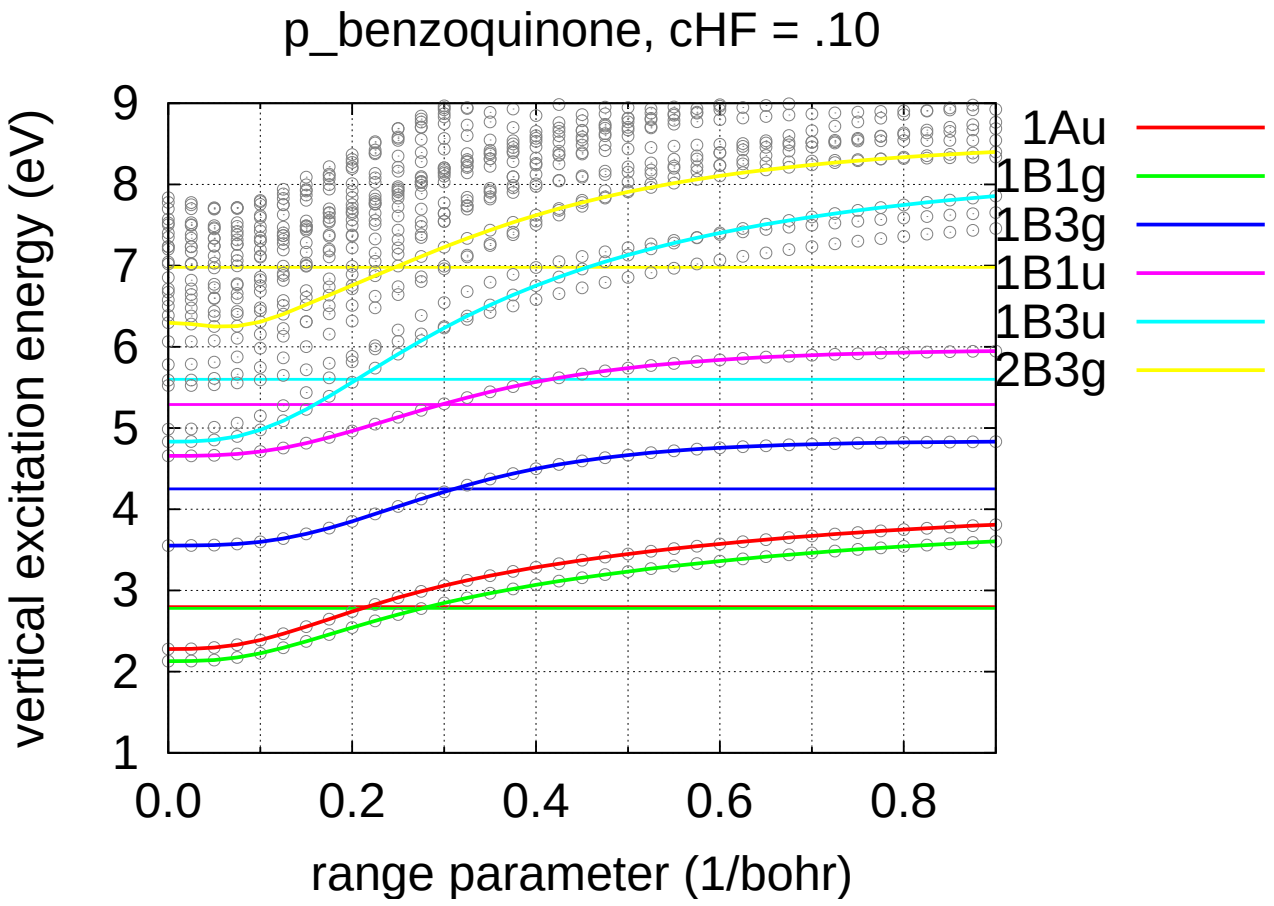

pyridazine, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
7
6.5
6
5.5
5
4.5
4
3.5
3
0.0
0.2
0.4
0.6
0.8
1B1
1A2
2A1
2A2

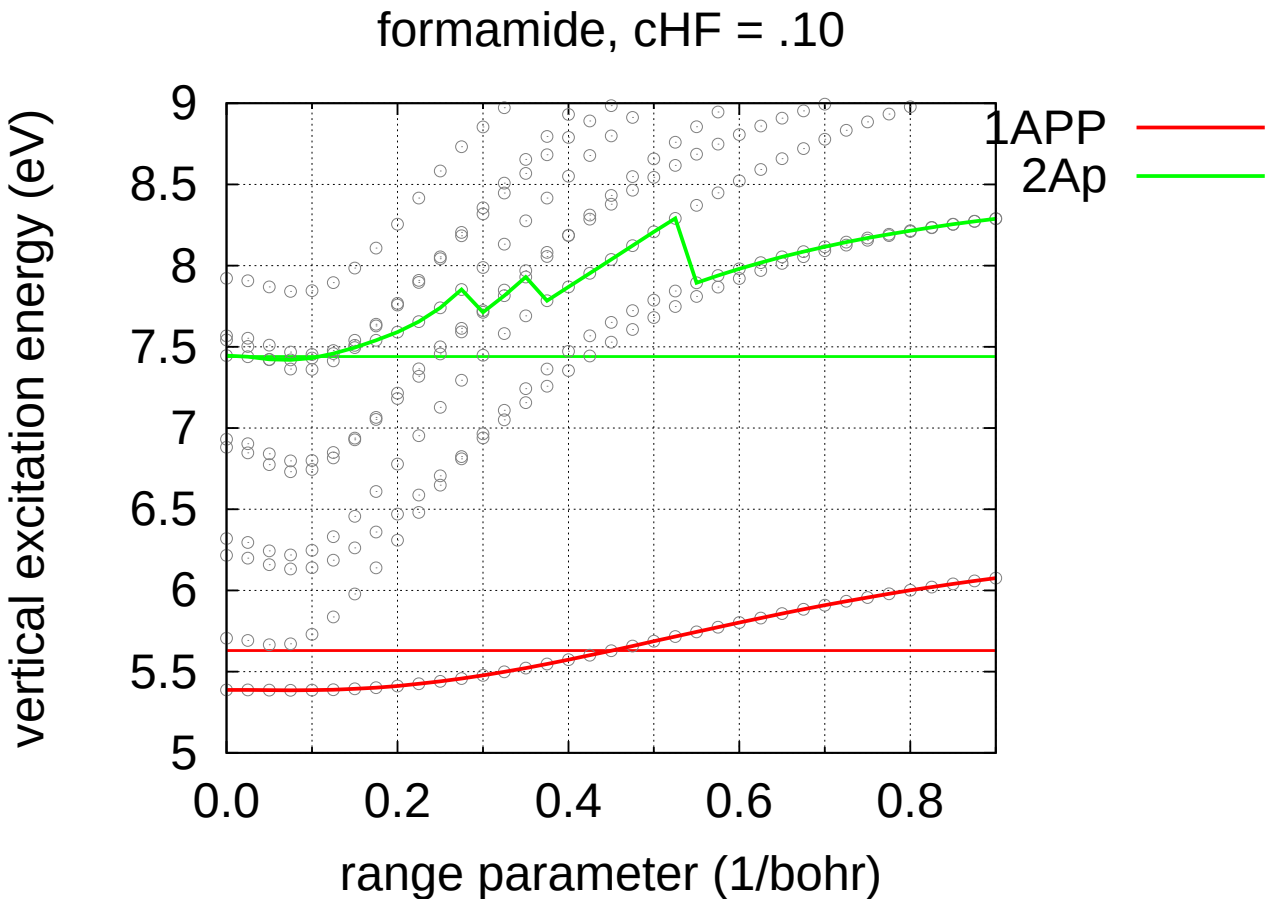

s_triazine, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8
1A1PP
1A2PP
1EPP
1A2p

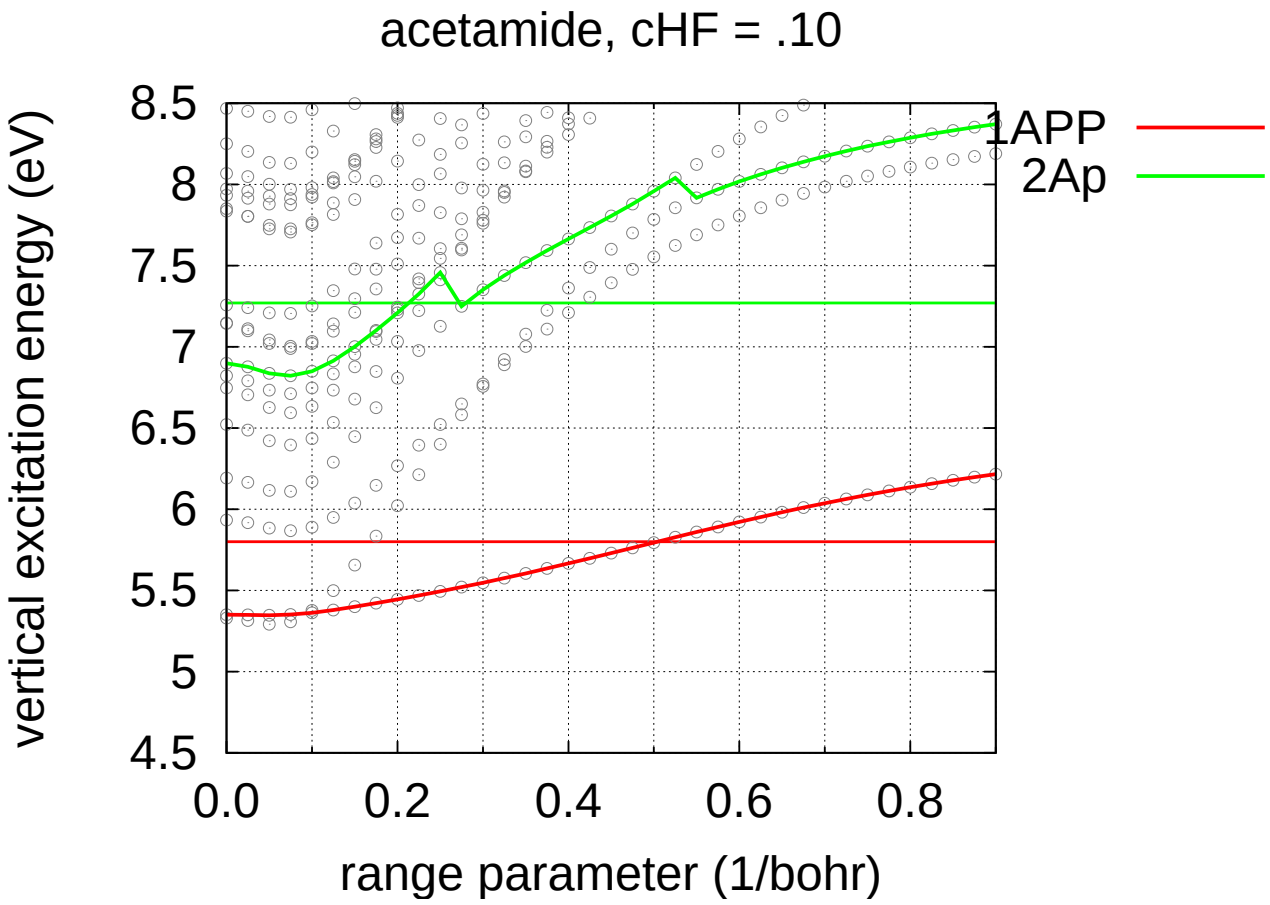

s_tetrazine, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
1
2
3
4
5
6
7
8
9
0.0
0.2
0.4
0.6
0.8
1B3u
1Au
1B1g
1B2u
1B2g
2Au

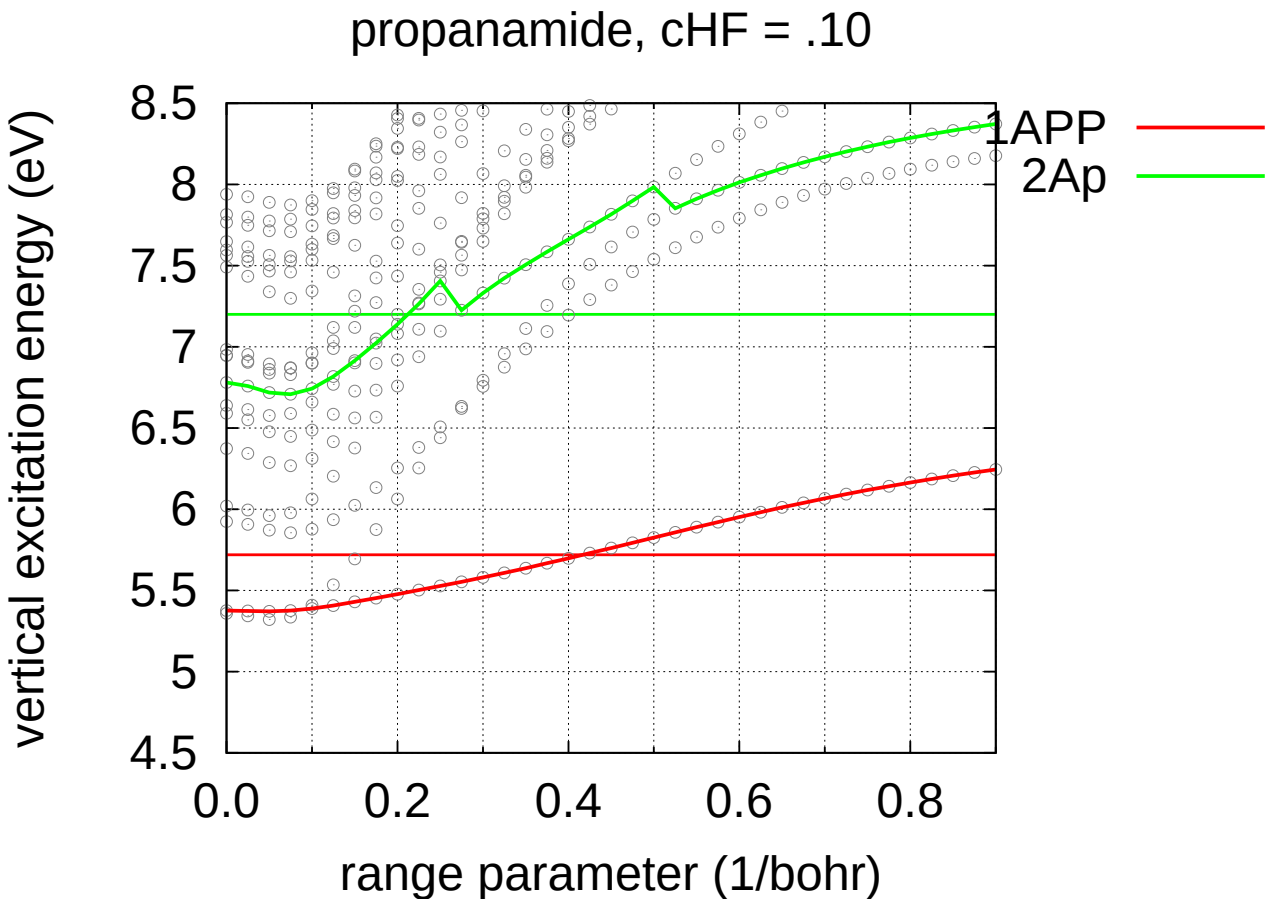

formaldehyde, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
11
10
9
8
7
6
5
4
3
0.0
0.2
0.4
0.6
0.8
1A2
1B1
2A1

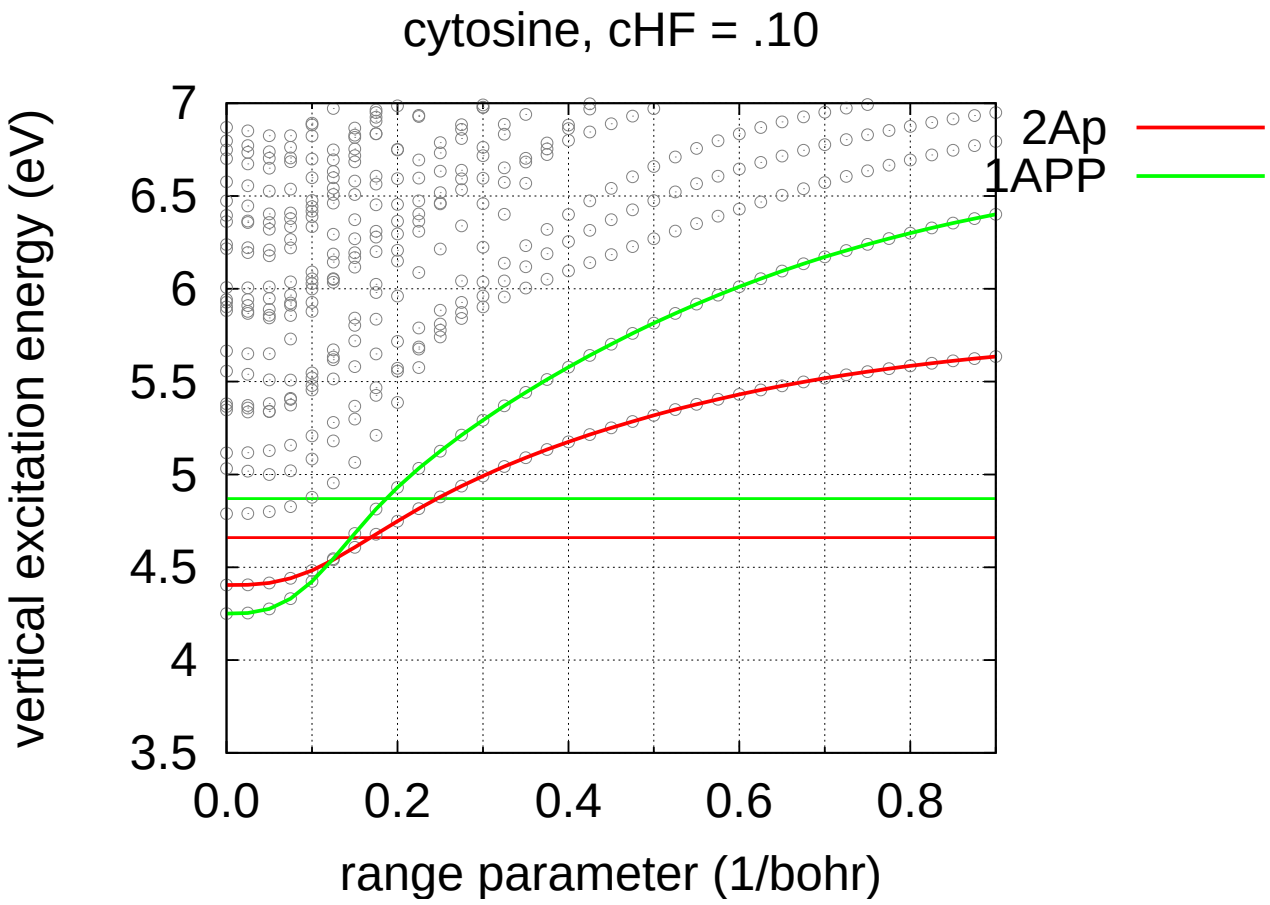

acetone, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
11
10
9
8
7
6
5
4
0.0
0.2
0.4
0.6
0.8
1A2
1B1
2A1

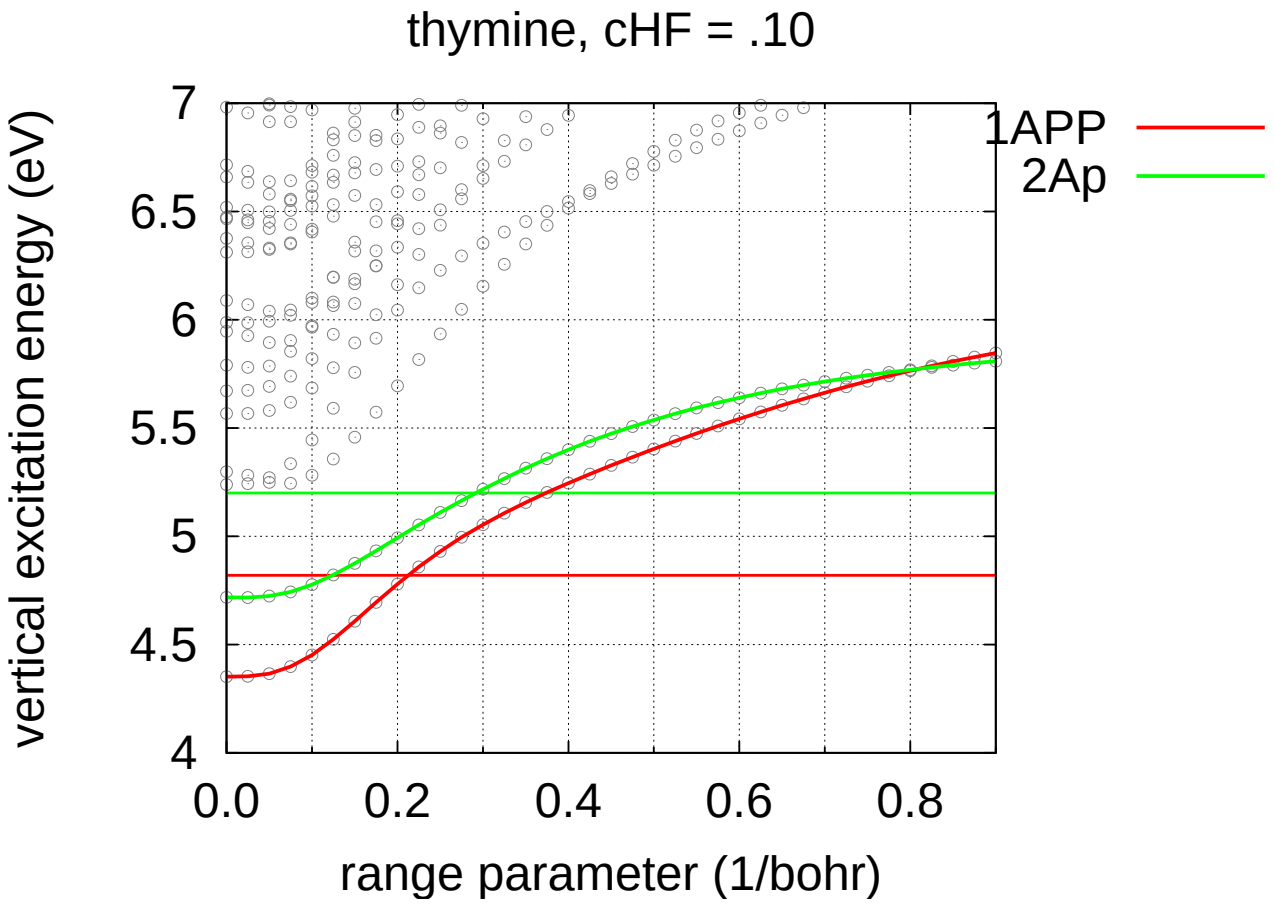

p_benzoquinone, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
1
2
3
4
5
6
7
8
9
0.0
0.2
0.4
0.6
0.8
1Au
1B1g
1B3g
1B1u
1B3u
2B3g

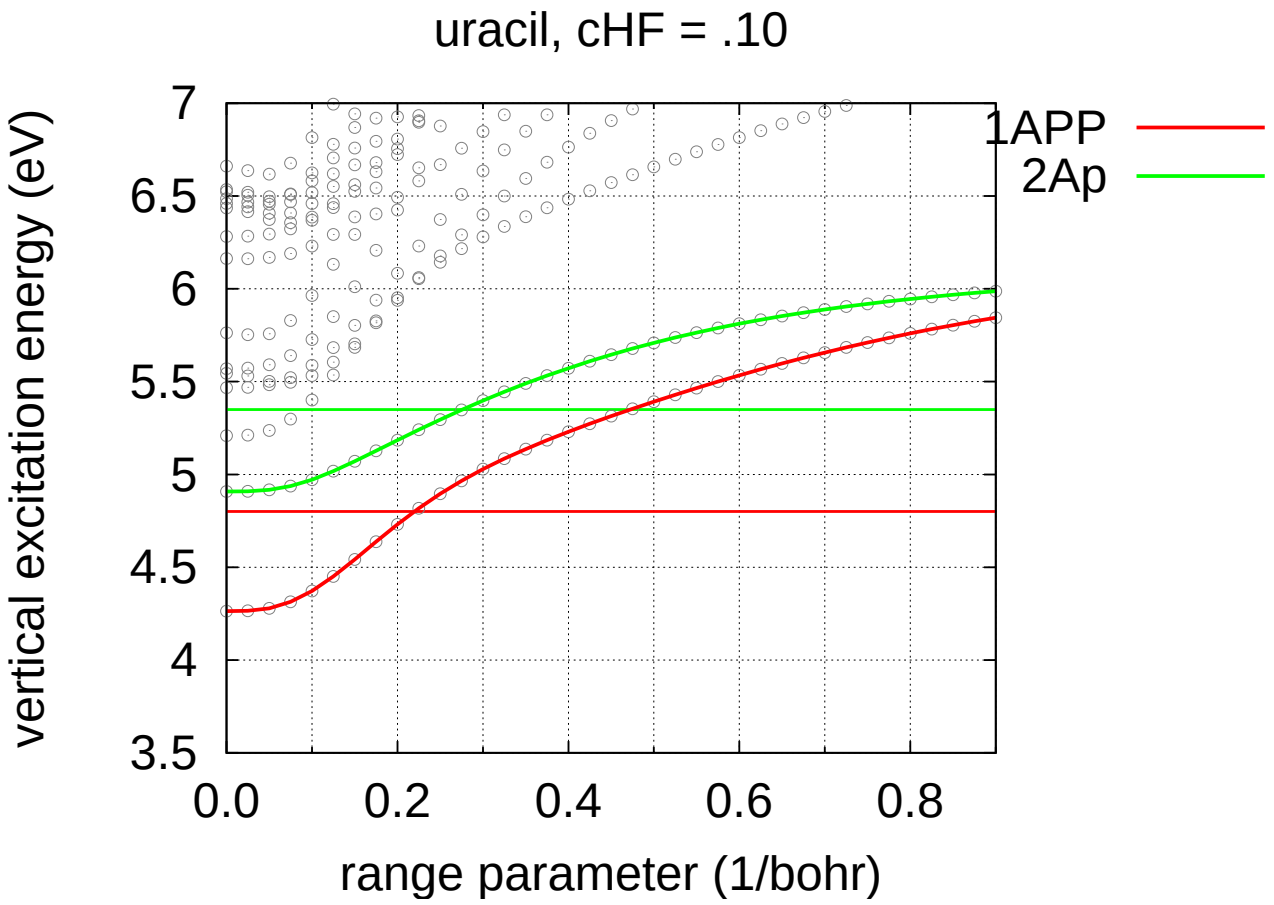

formamide, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
9
8.5
8
7.5
7
6.5
6
5.5
5
0.0
0.2
0.4
0.6
0.8

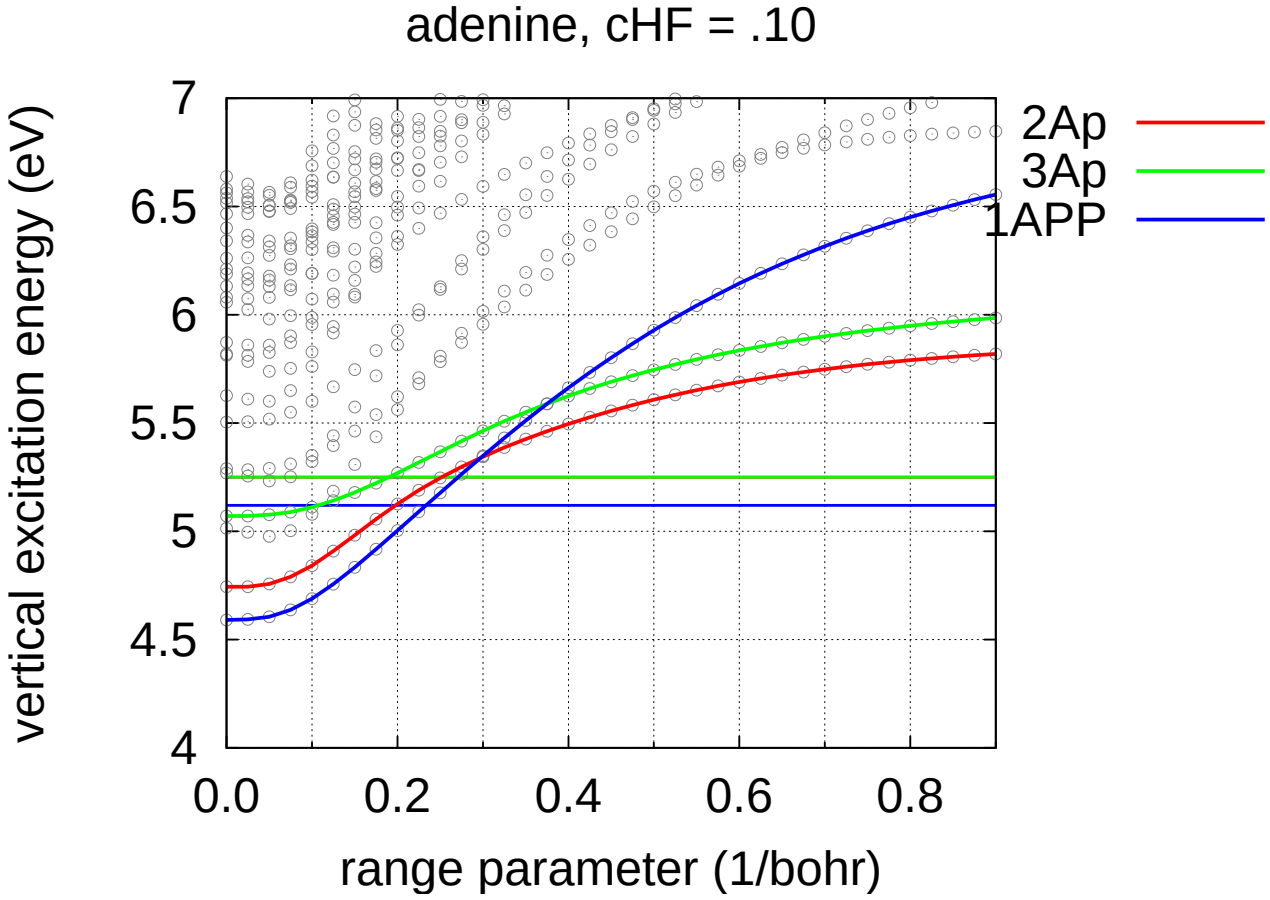

acetamide, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
8.5
8
7.5
7
6.5
6
5.5
5
4.5
0.0
0.2
0.4
0.6
0.8
1APP
2Ap

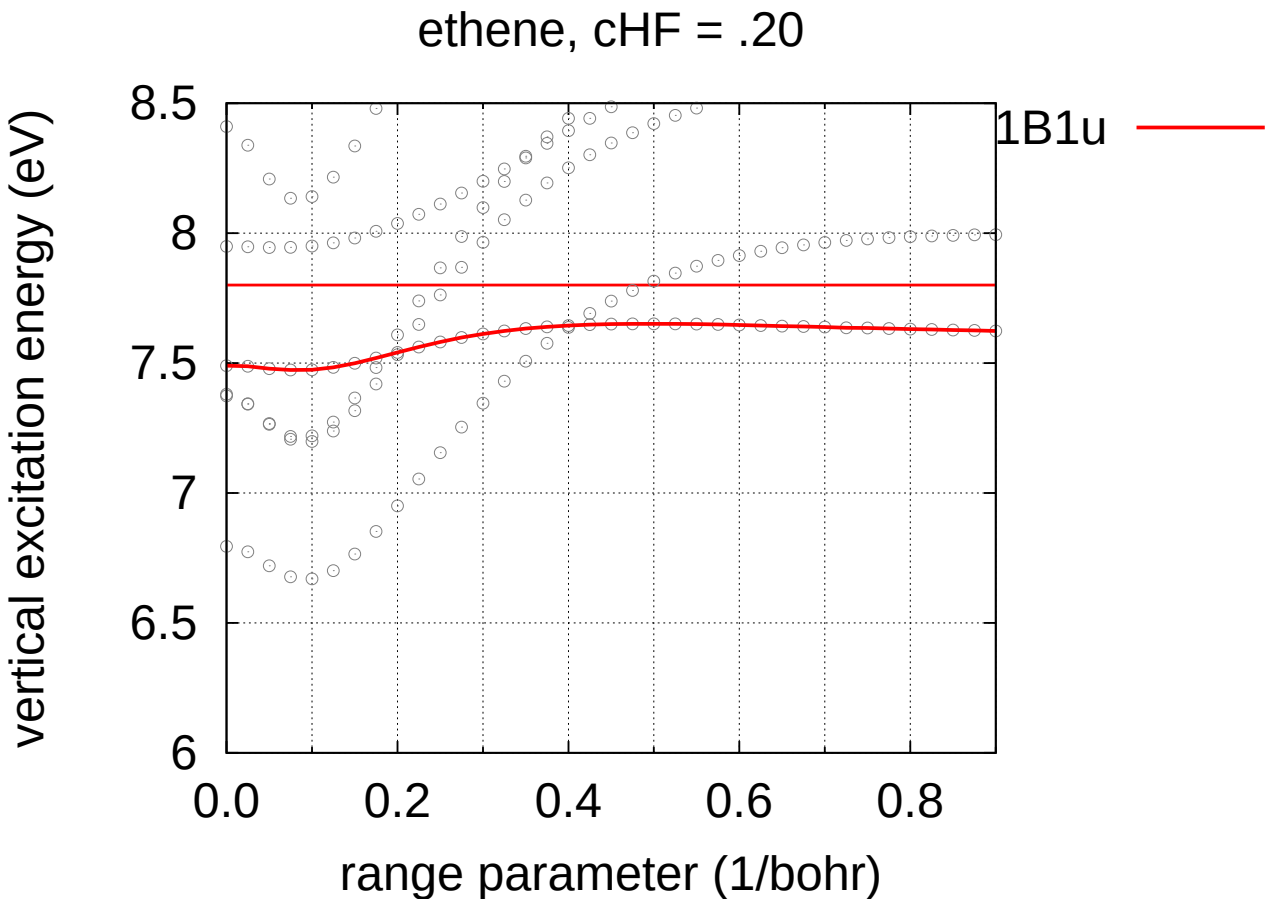

propanamide, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
8.5
8
7.5
7
6.5
6
5.5
5
4.5
0.0
0.2
0.4
0.6
0.8
1APP
2Ap

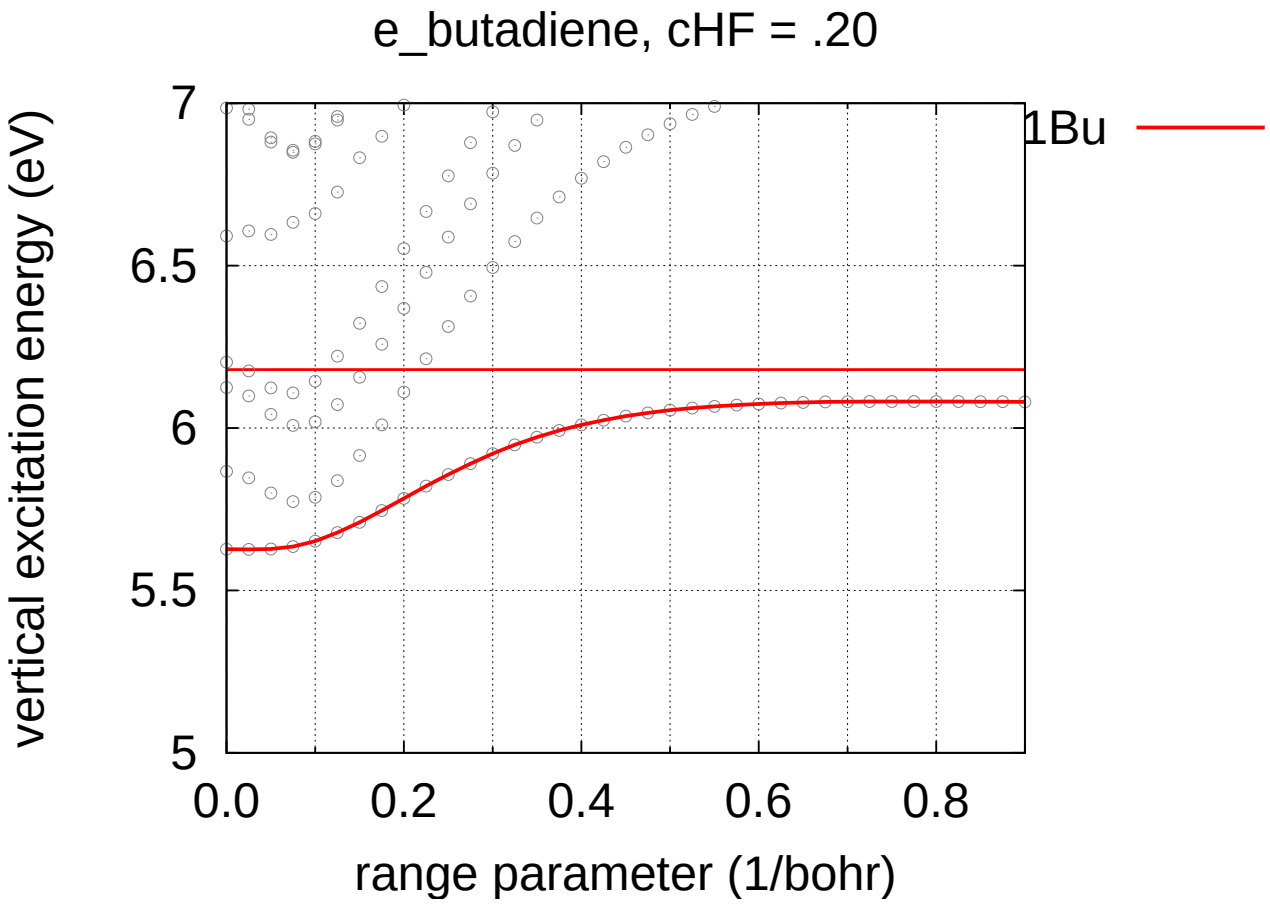

cytosine, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
2Ap
1APP
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8

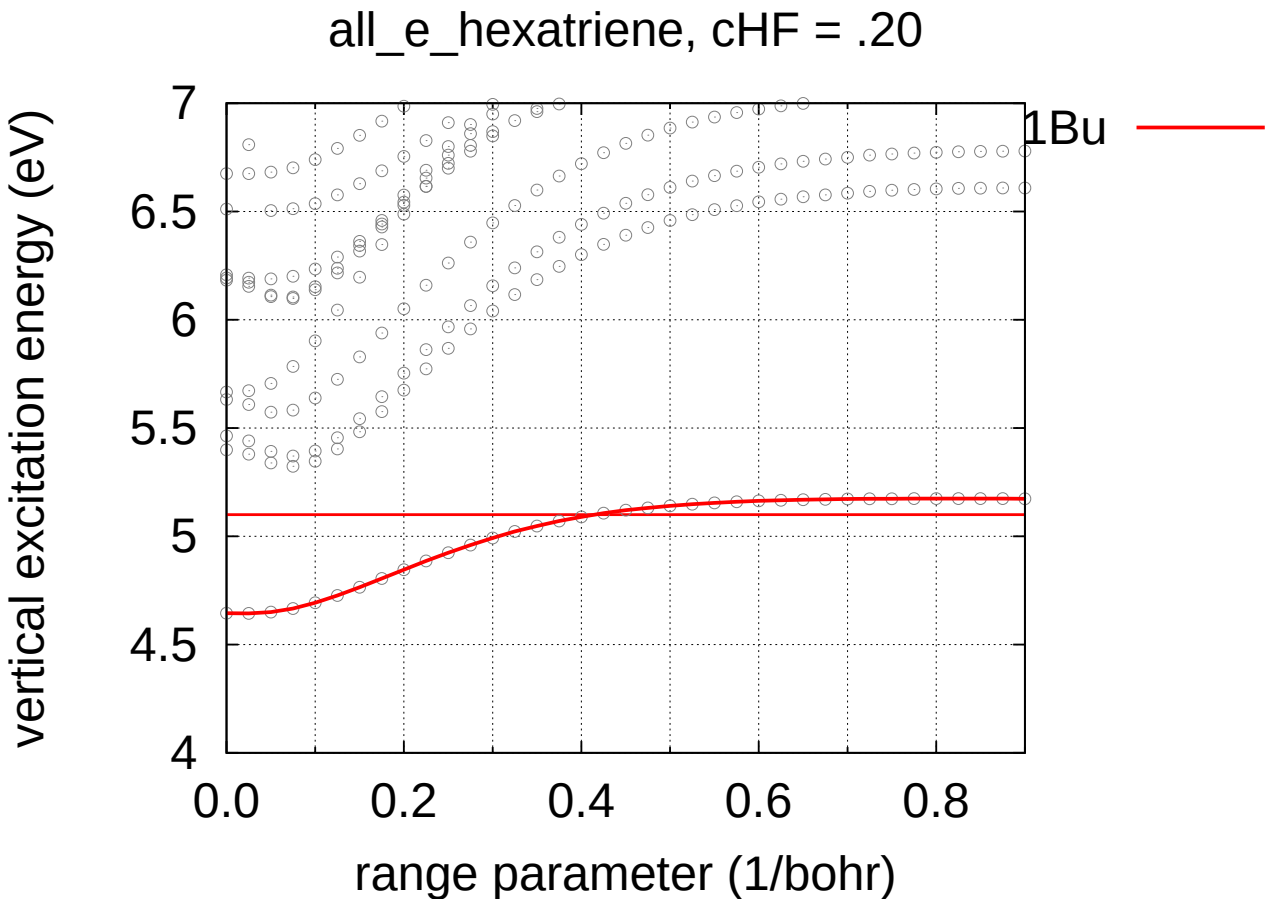

thymine, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8

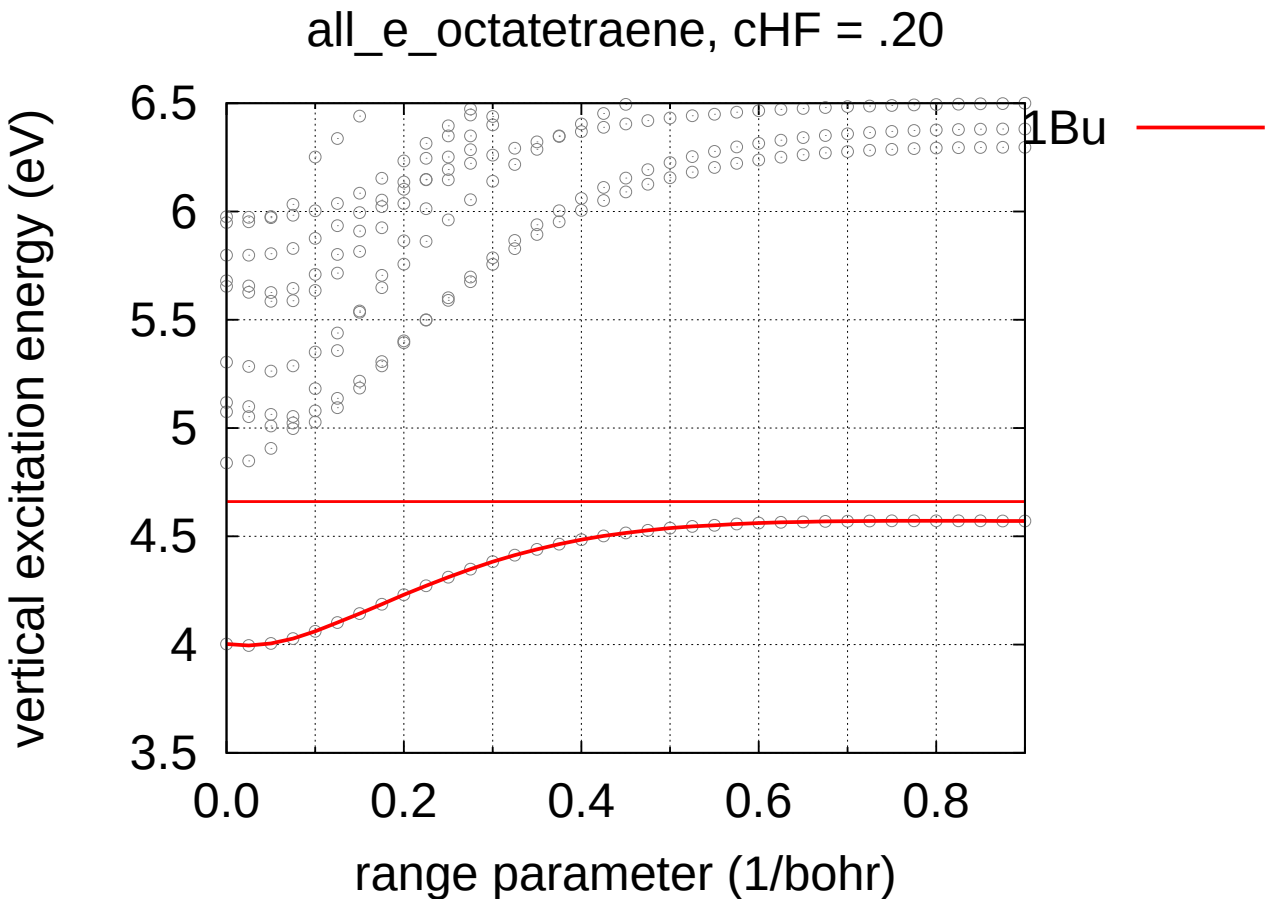

uracil, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8

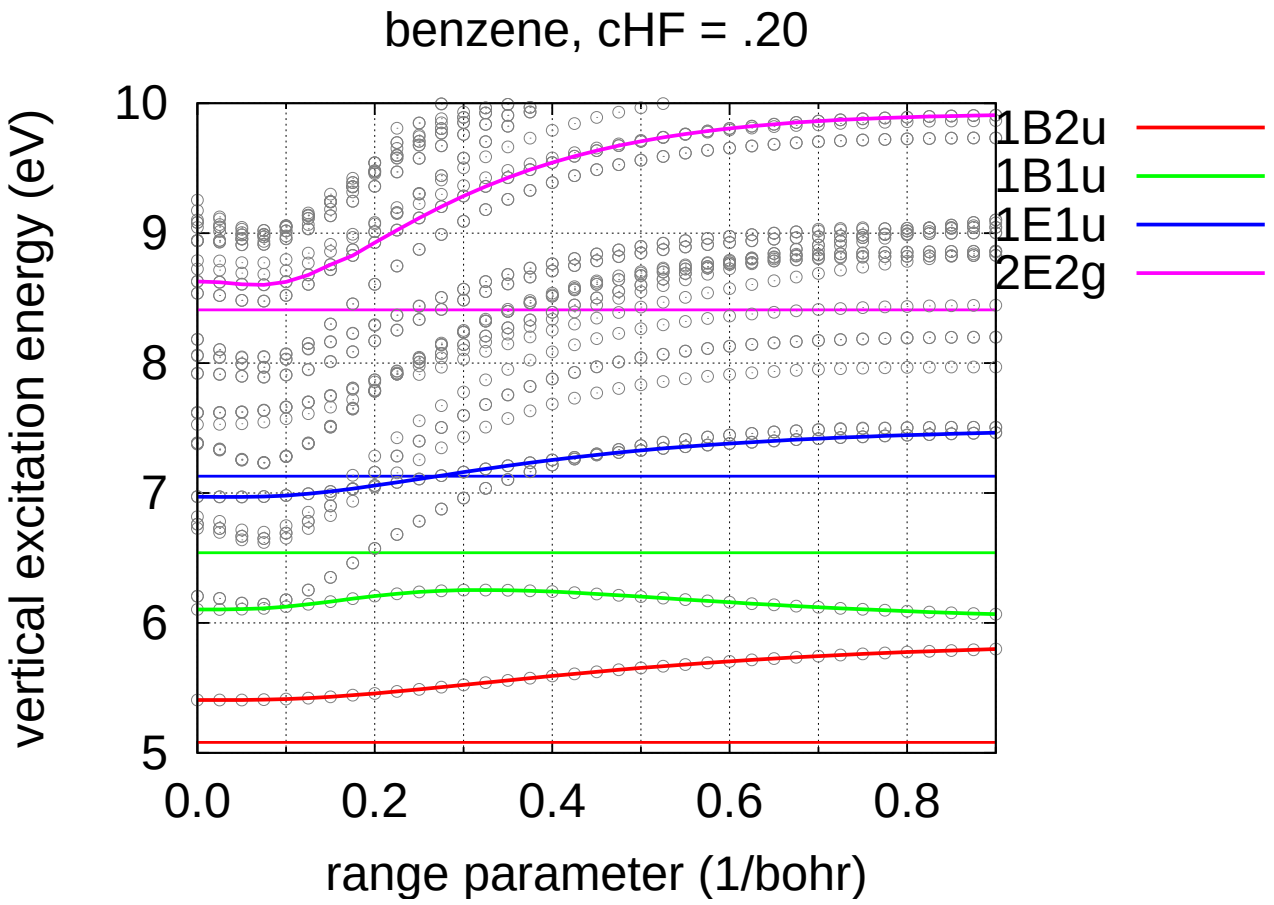

adenine, cHF = .10
vertical excitation energy (eV)
range parameter (1/bohr)
2Ap
3Ap
1APP
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8

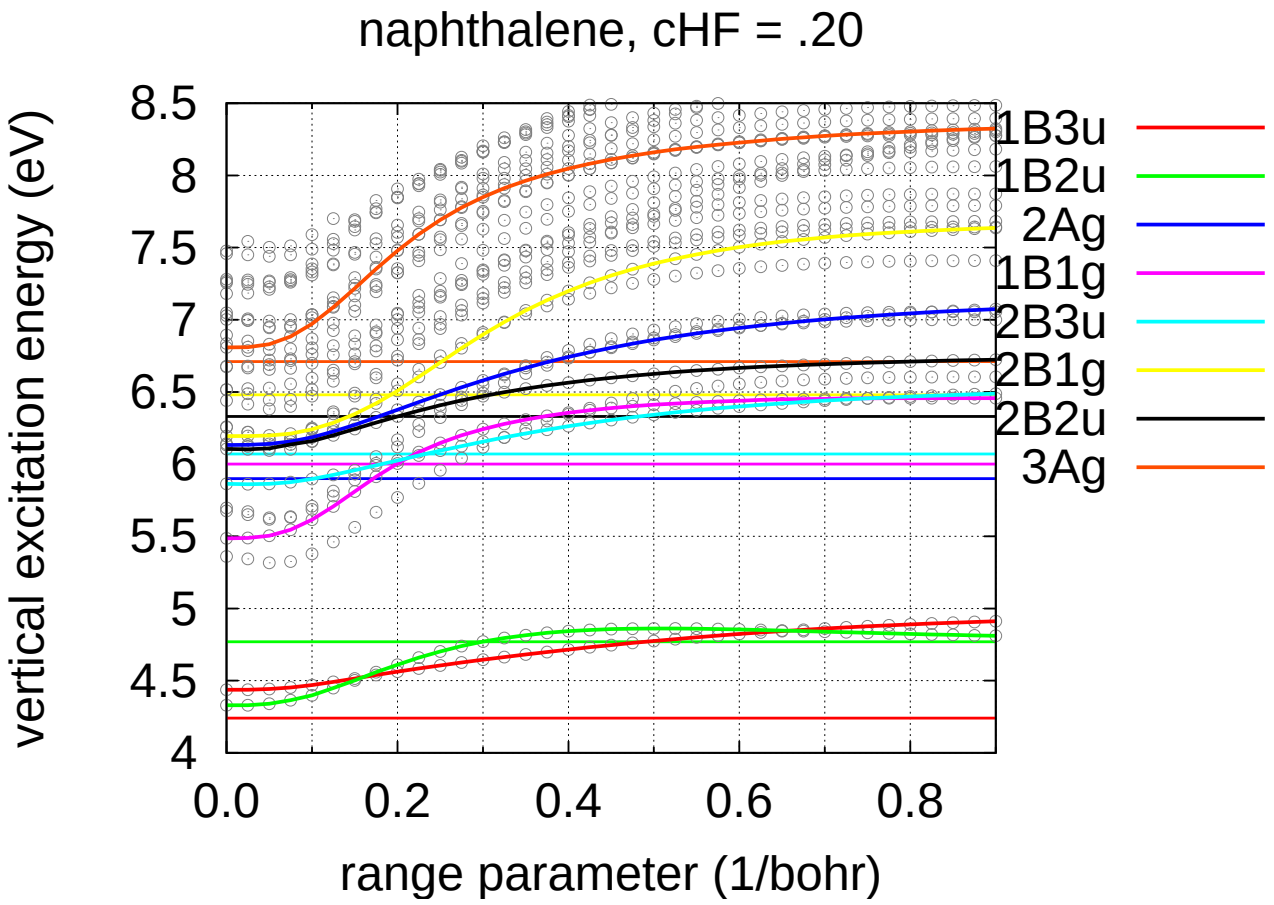

ethene, cHF = .20
vertical excitation energy (eV)
8.5
8
7.5
7
6.5
6
0.0
0.2
0.4
0.6
0.8
range parameter (1/bohr)
1B1u

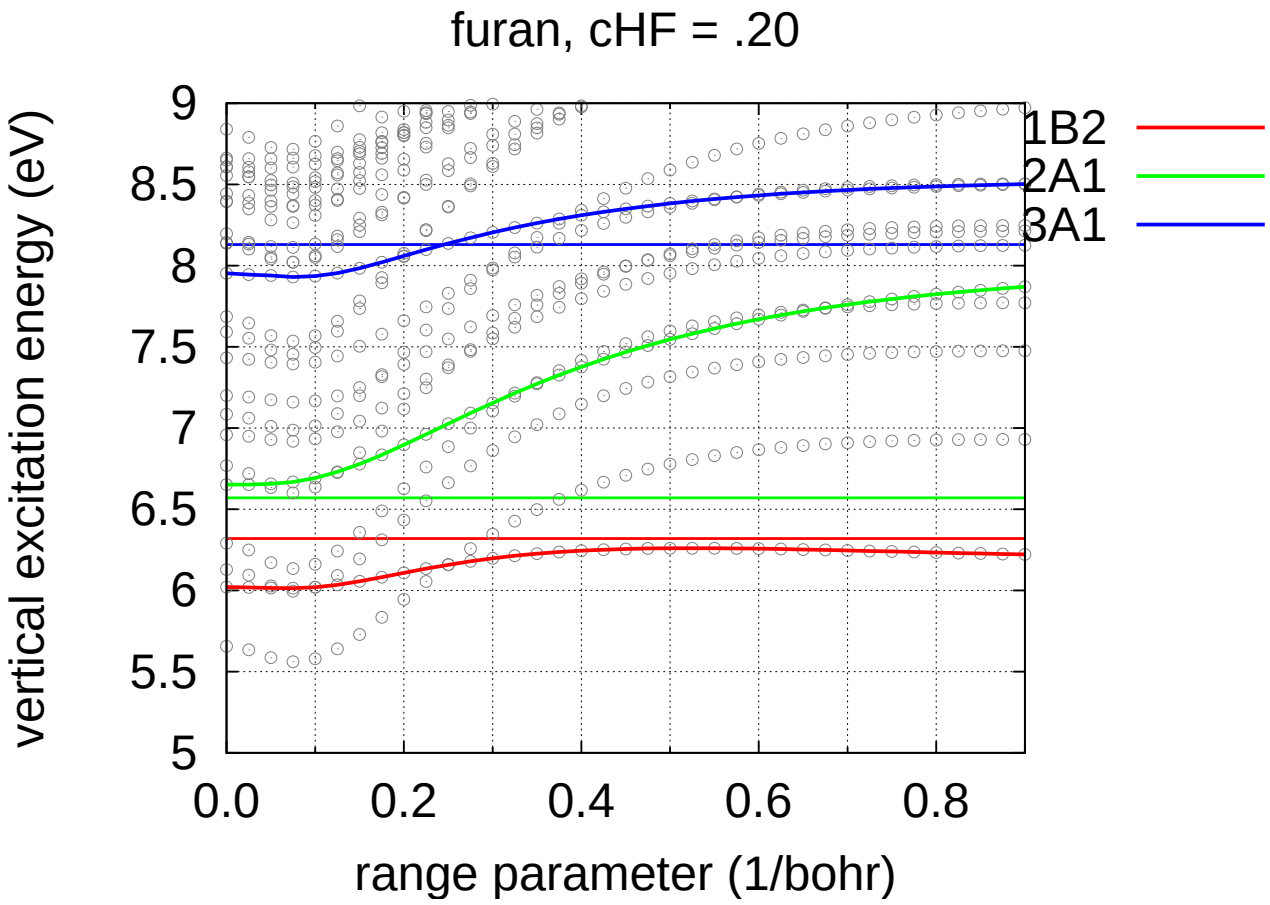

e_butadiene, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
1Bu
7
6.5
6
5.5
5
0.0
0.2
0.4
0.6
0.8

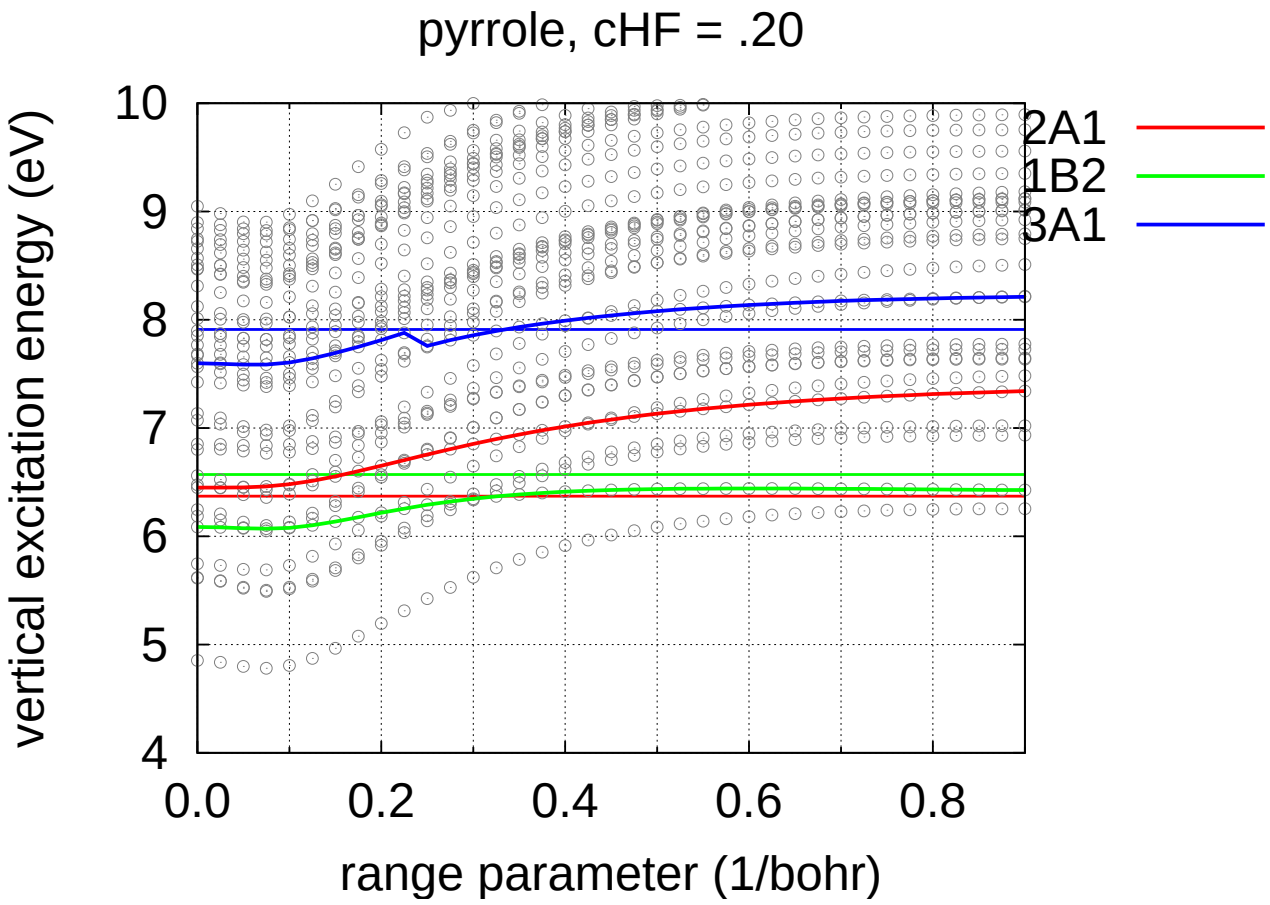

all_e_hexatriene, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
1Bu
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8

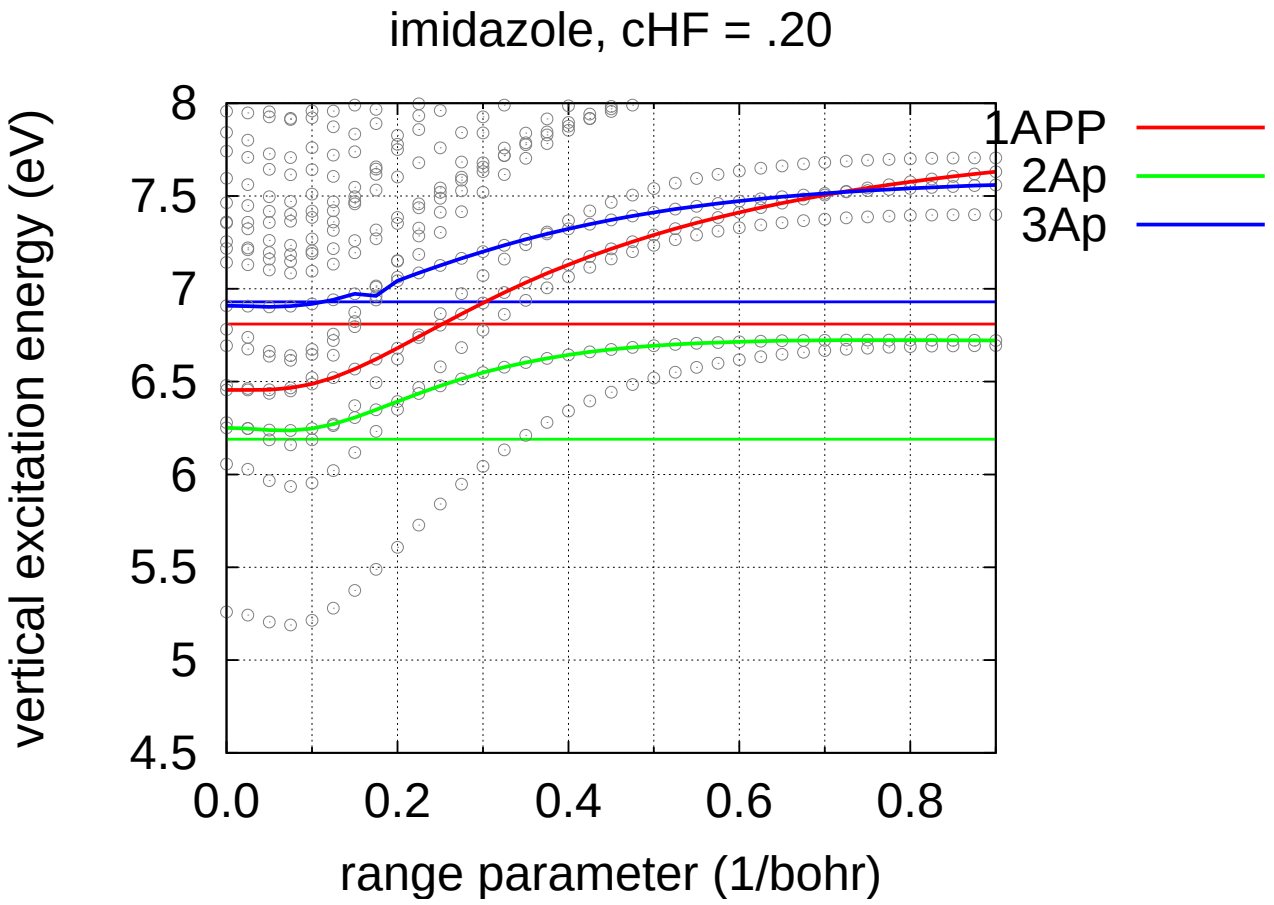

all_e_octatetraene, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
1Bu
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8

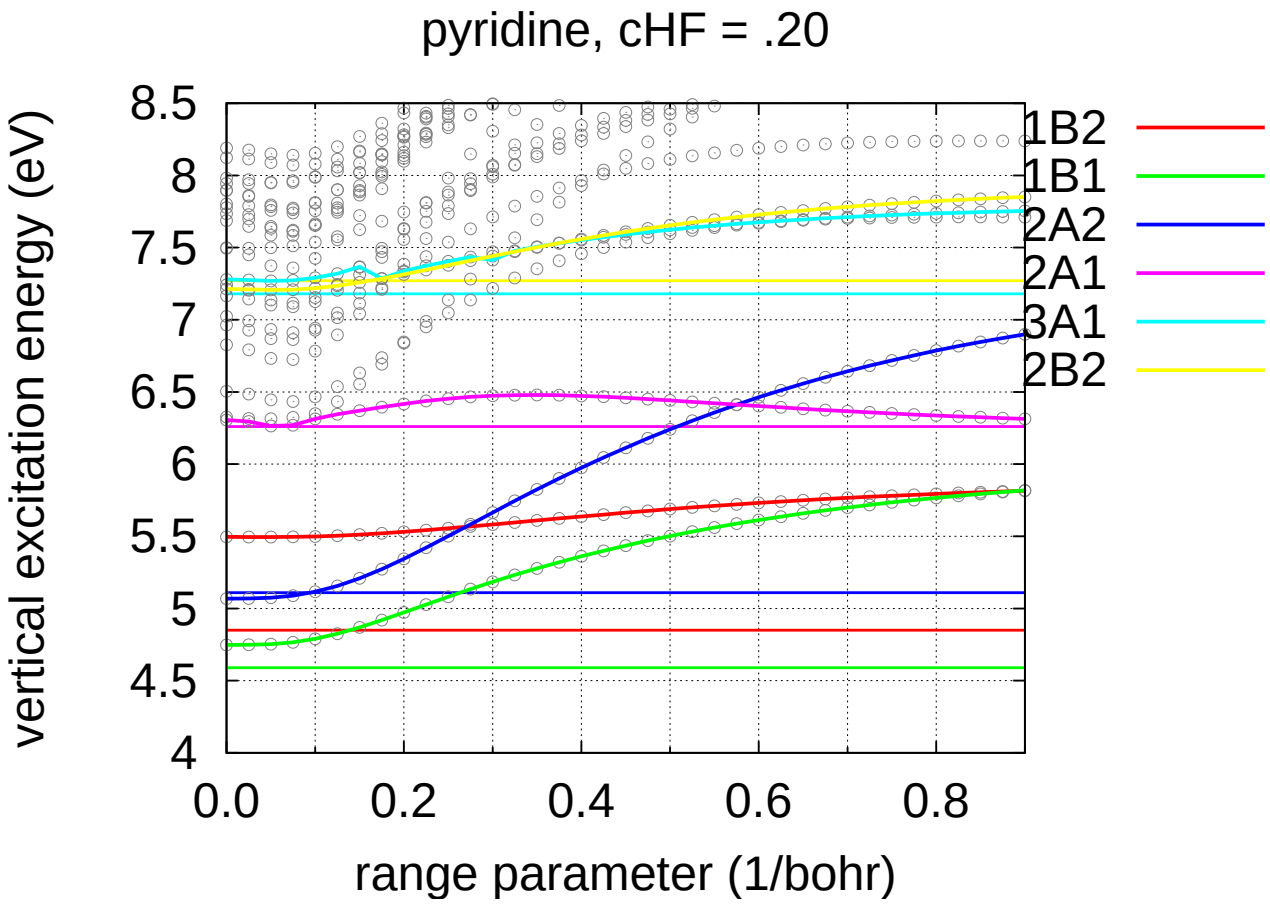

benzene, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
10
9
8
7
6
5
0.0
0.2
0.4
0.6
0.8
1B2u
1B1u
1E1u
2E2g

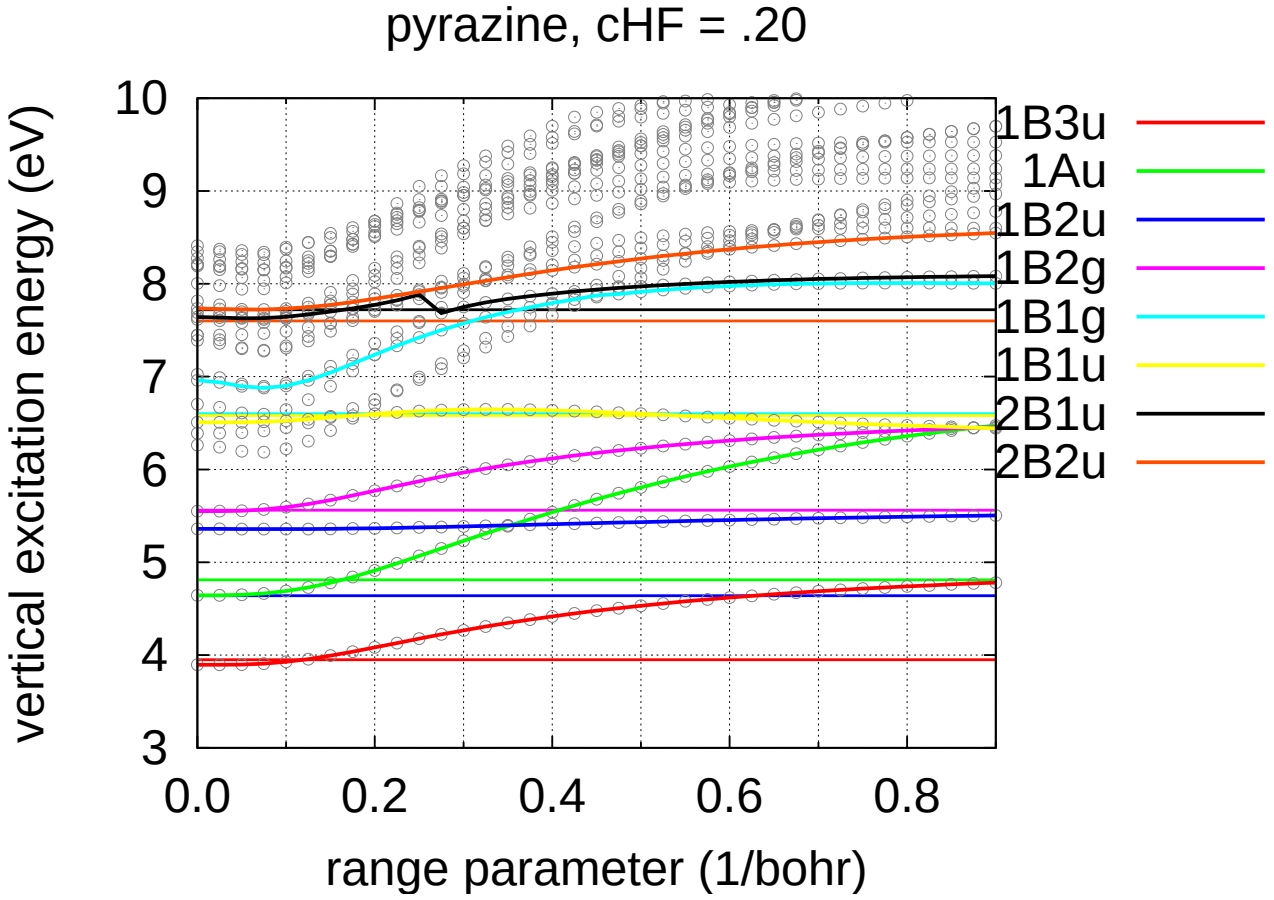

naphthalene, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8
1B3u
1B2u
2Ag
1B1g
2B3u
2B1g
2B2u
3Ag

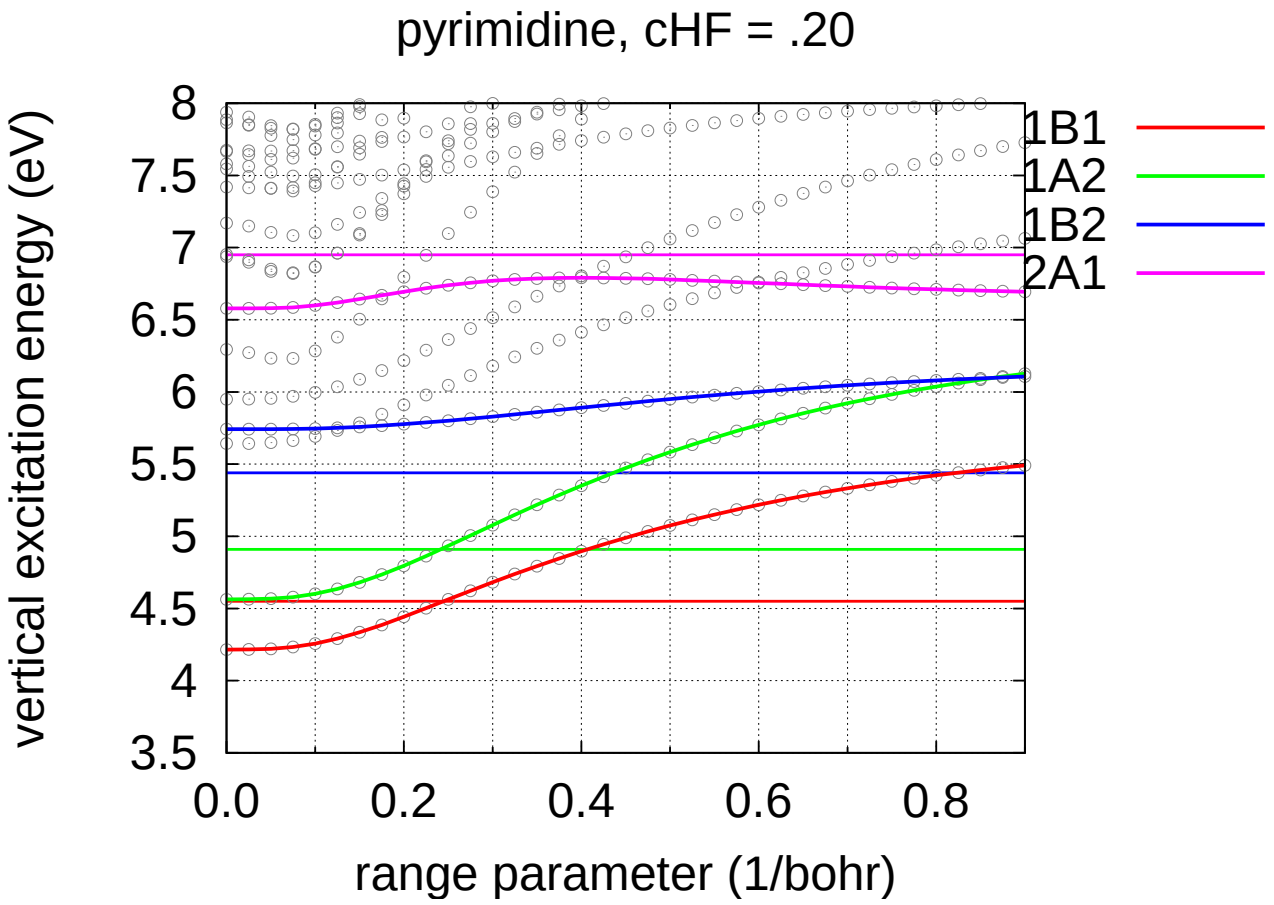

furan, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
9
8.5
8
7.5
7
6.5
6
5.5
5
0.0
0.2
0.4
0.6
0.8
1B2
2A1
3A1

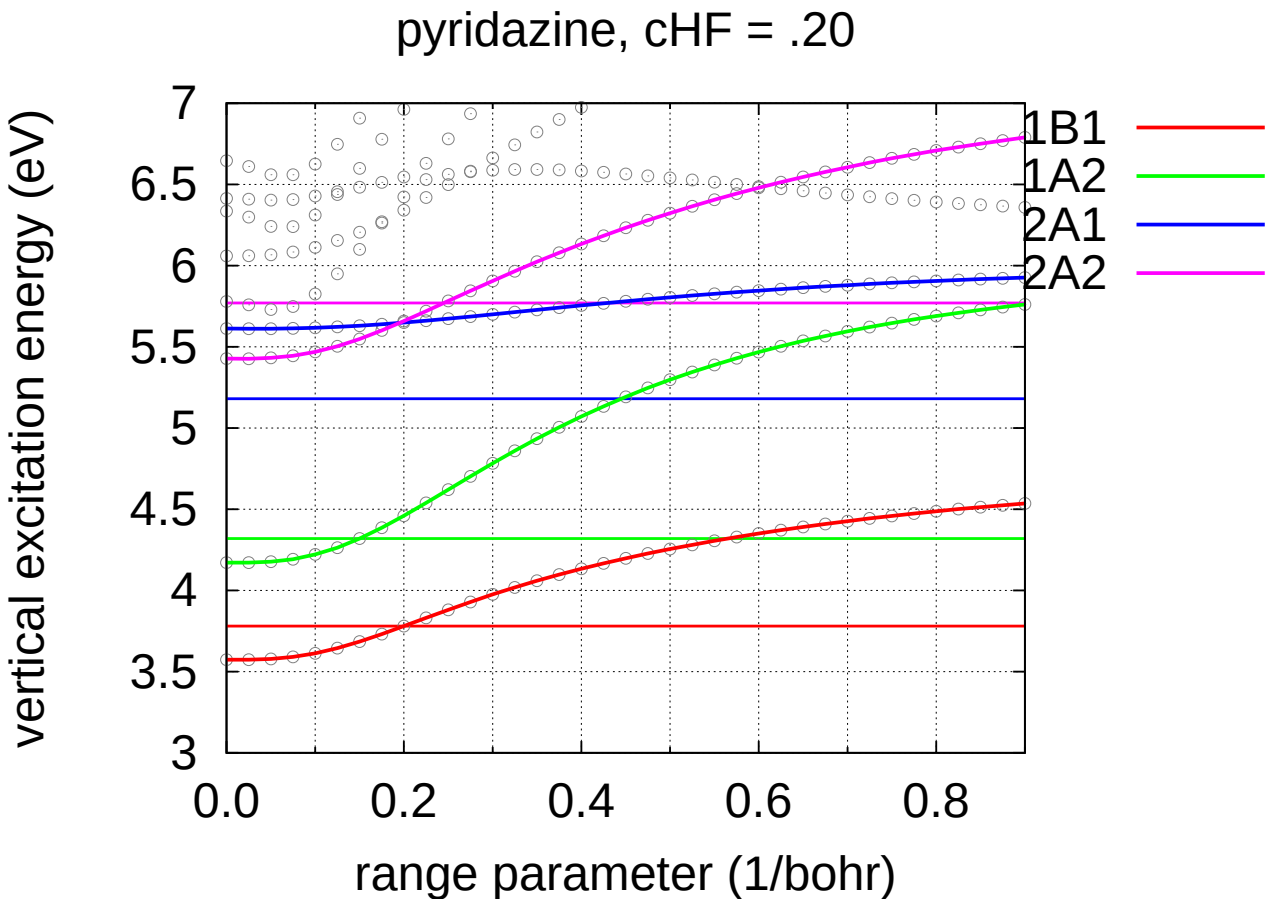

pyrrole, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
10
9
8
7
6
5
4
0.0
0.2
0.4
0.6
0.8
2A1
1B2
3A1

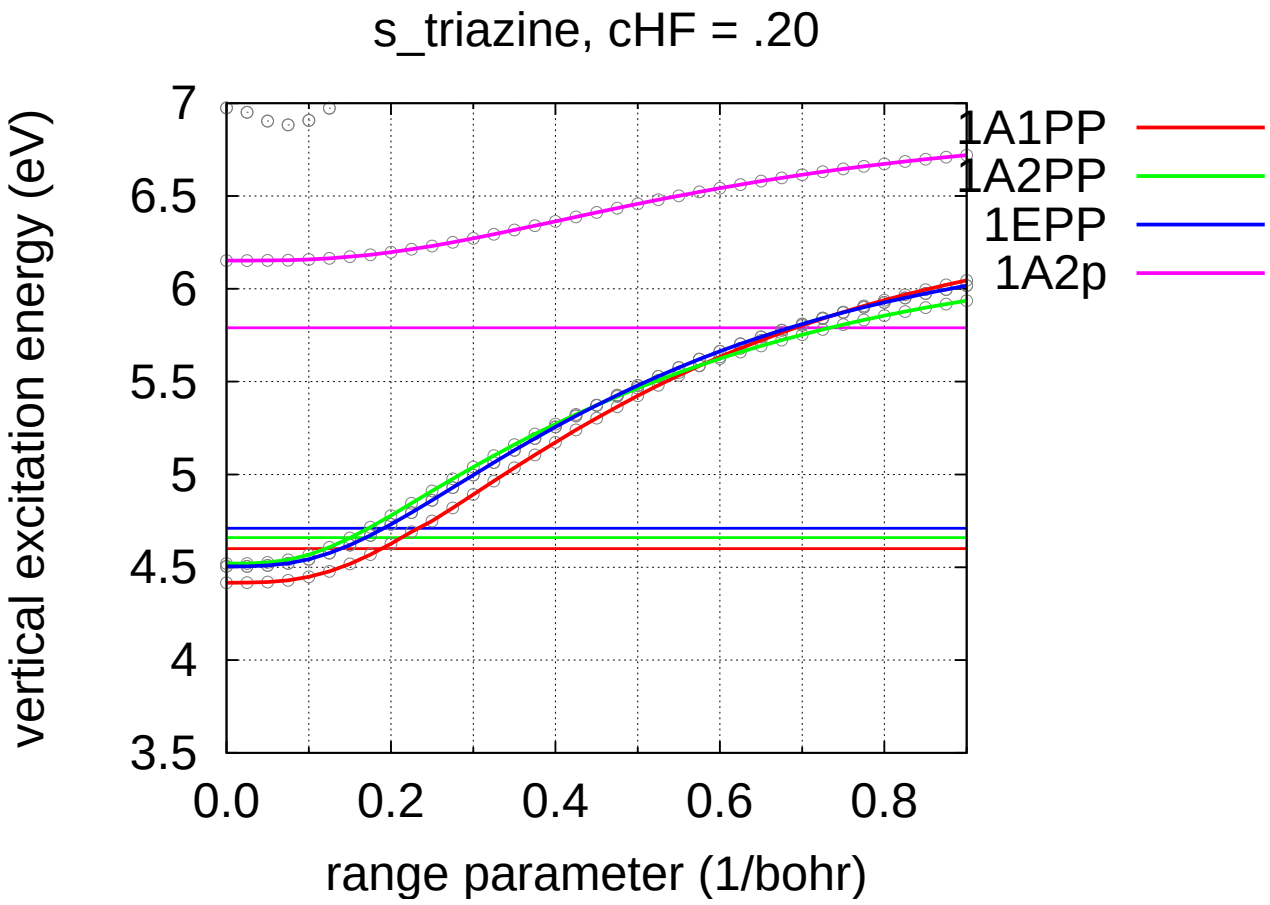

imidazole, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
8
7.5
7
6.5
6
5.5
5
4.5
0.0
0.2
0.4
0.6
0.8
1APP
2Ap
3Ap

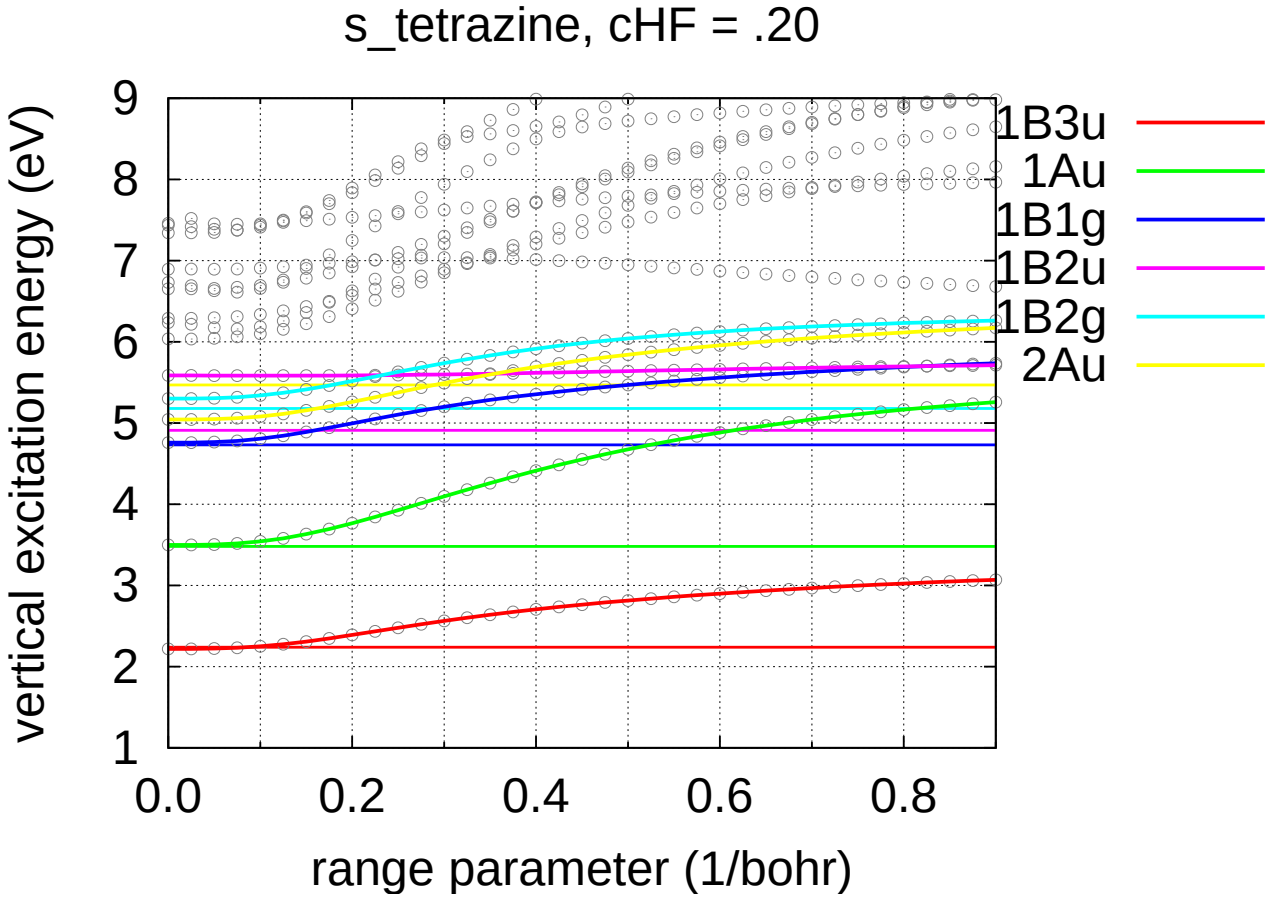

pyridine, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8
1B2
1B1
2A2
2A1
3A1
2B2

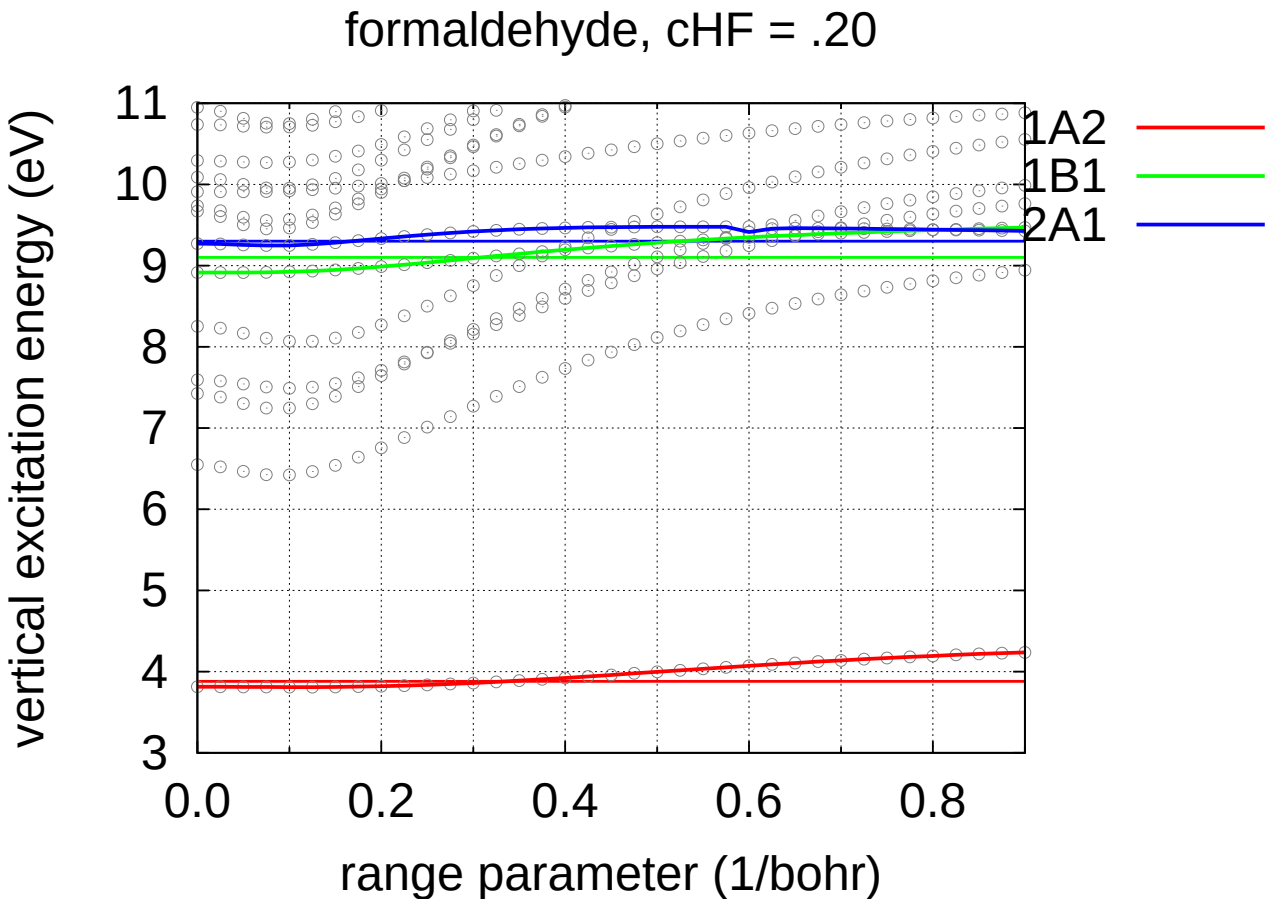

pyrazine, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
10
9
8
7
6
5
4
3
0.0
0.2
0.4
0.6
0.8
1B3u
1Au
1B2u
1B2g
1B1g
1B1u
2B1u
2B2u

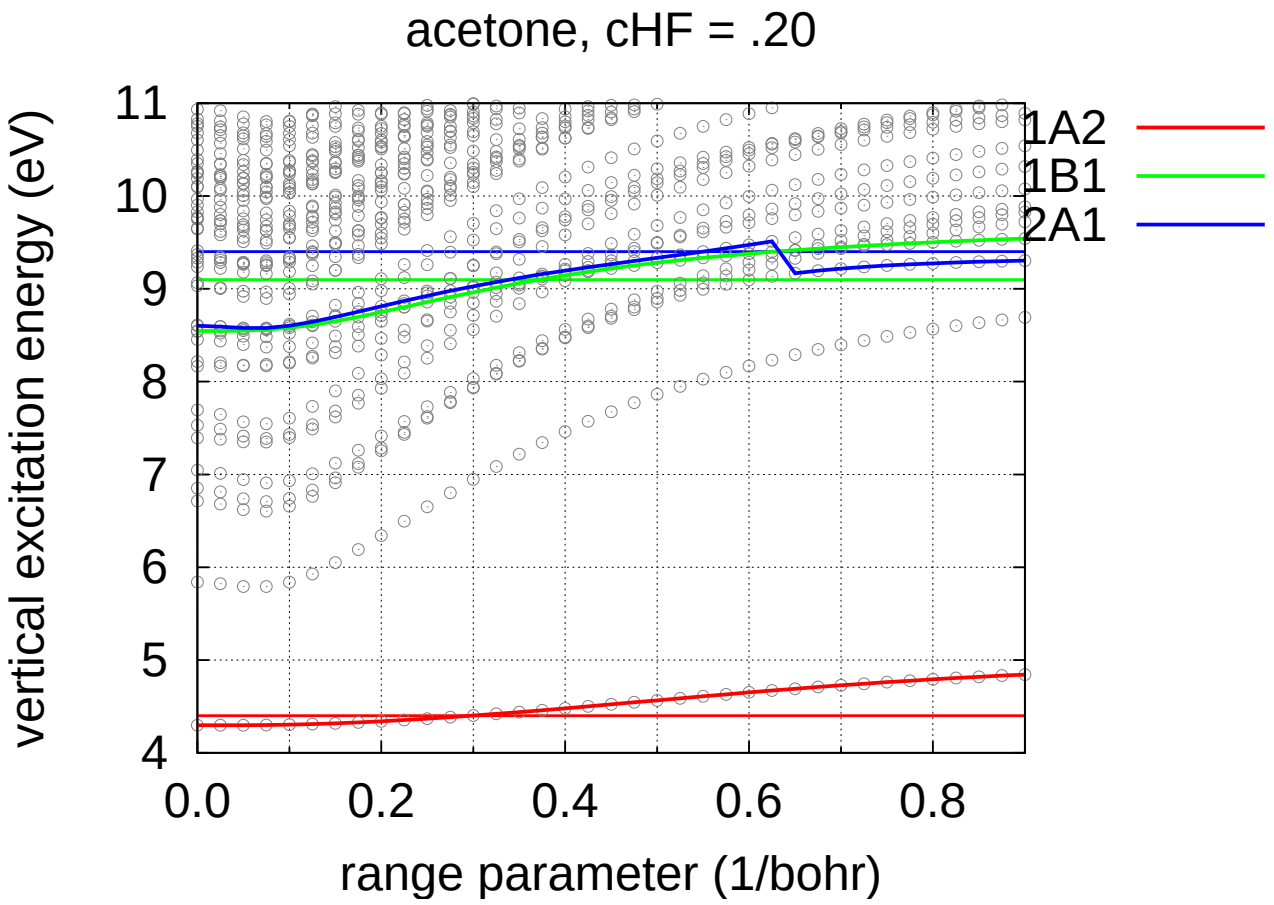

pyrimidine, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8
1B1
1A2
1B2
2A1

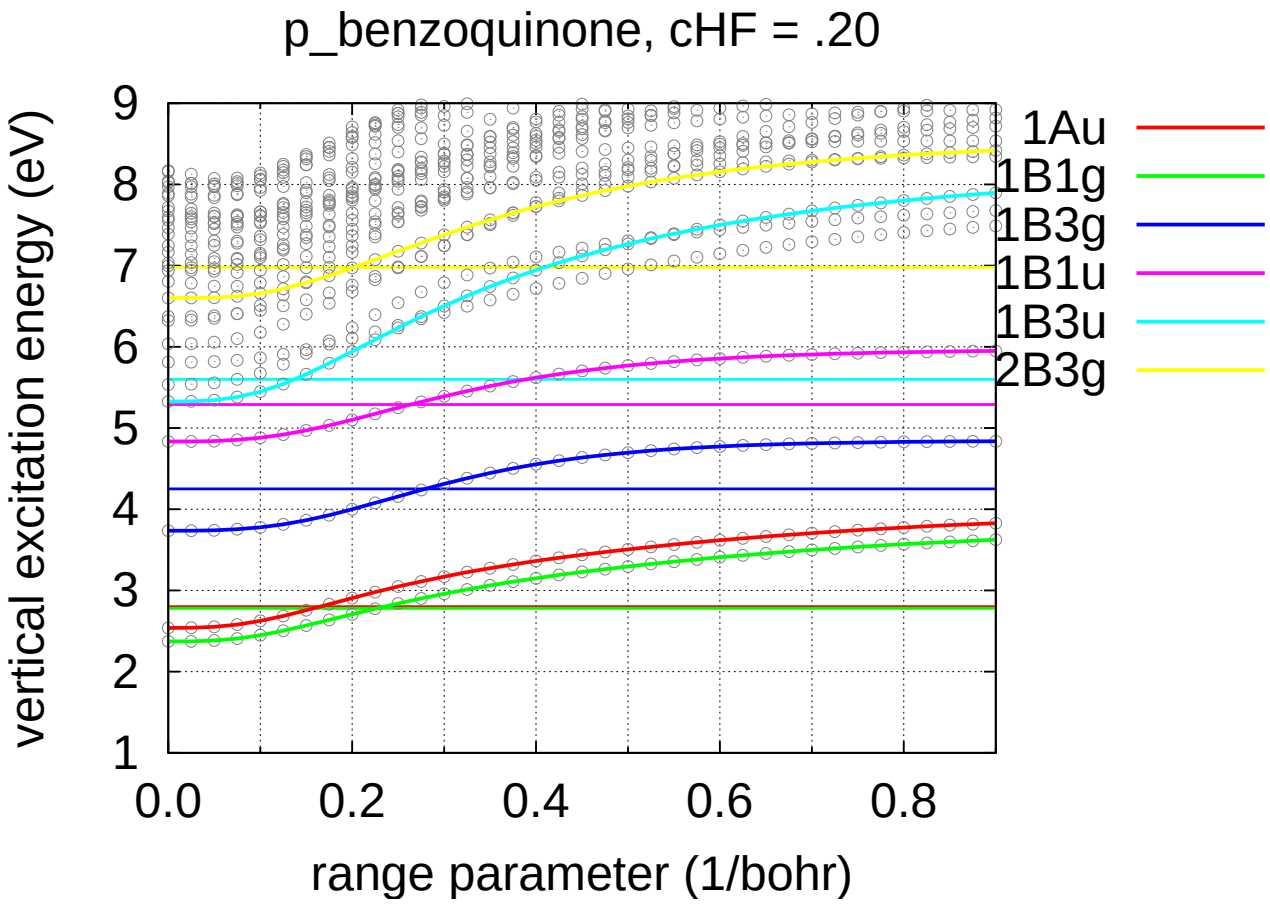

pyridazine, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
7
6.5
6
5.5
5
4.5
4
3.5
3
0.0
0.2
0.4
0.6
0.8
1B1
1A2
2A1
2A2

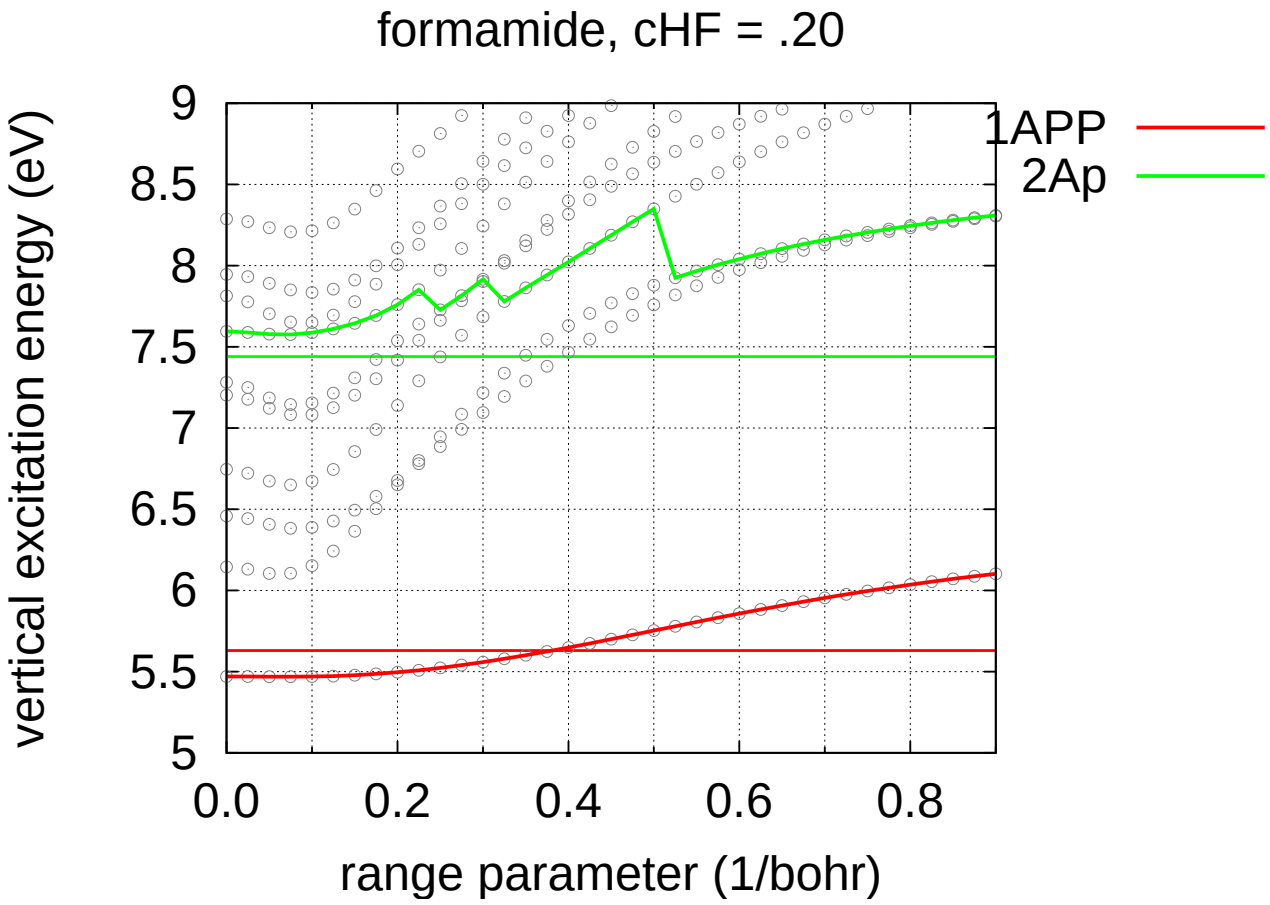

s_triazine, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8
1A1PP
1A2PP
1EPP
1A2p

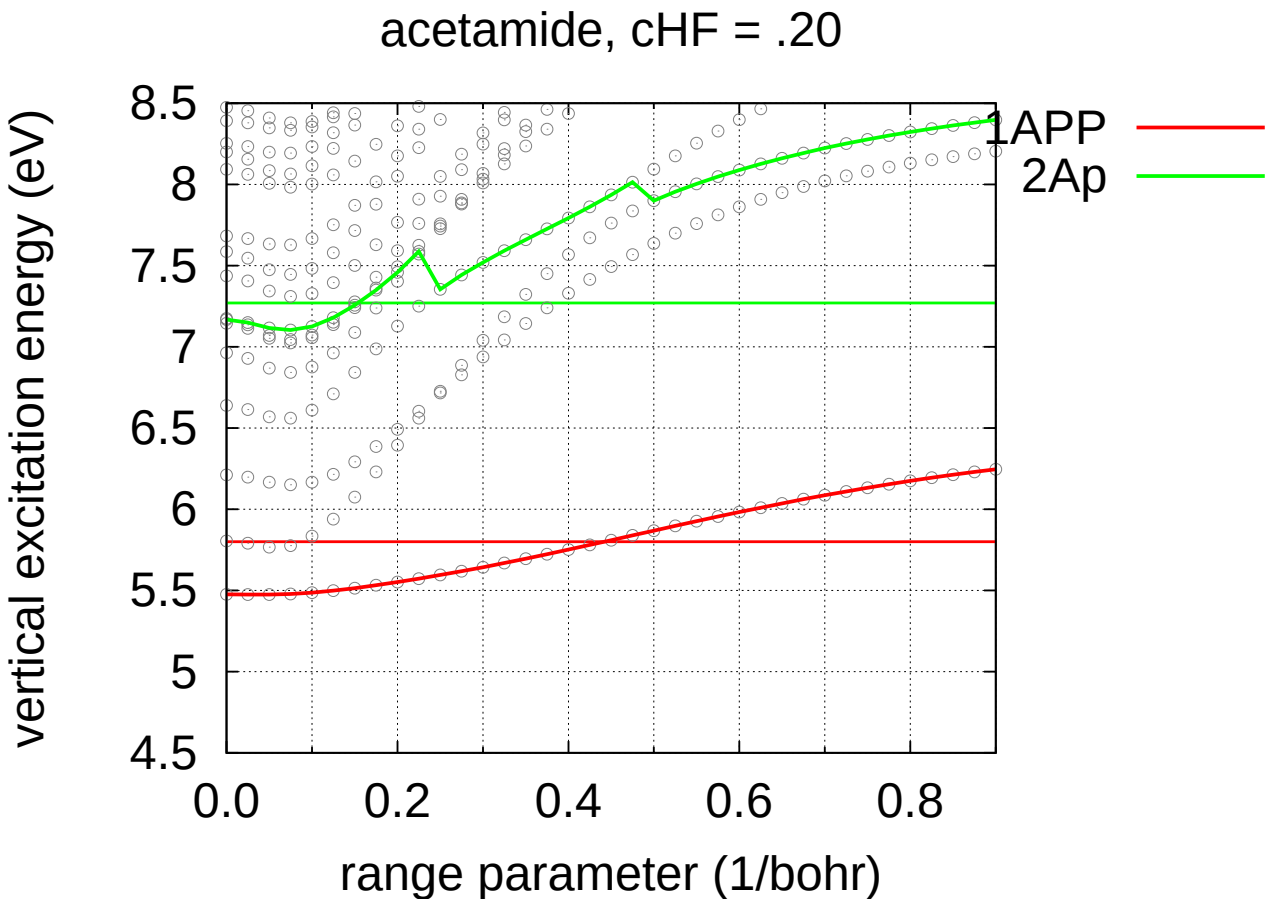

s_tetrazine, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
1
2
3
4
5
6
7
8
9
0.0
0.2
0.4
0.6
0.8
1B3u
1Au
1B1g
1B2u
1B2g
2Au

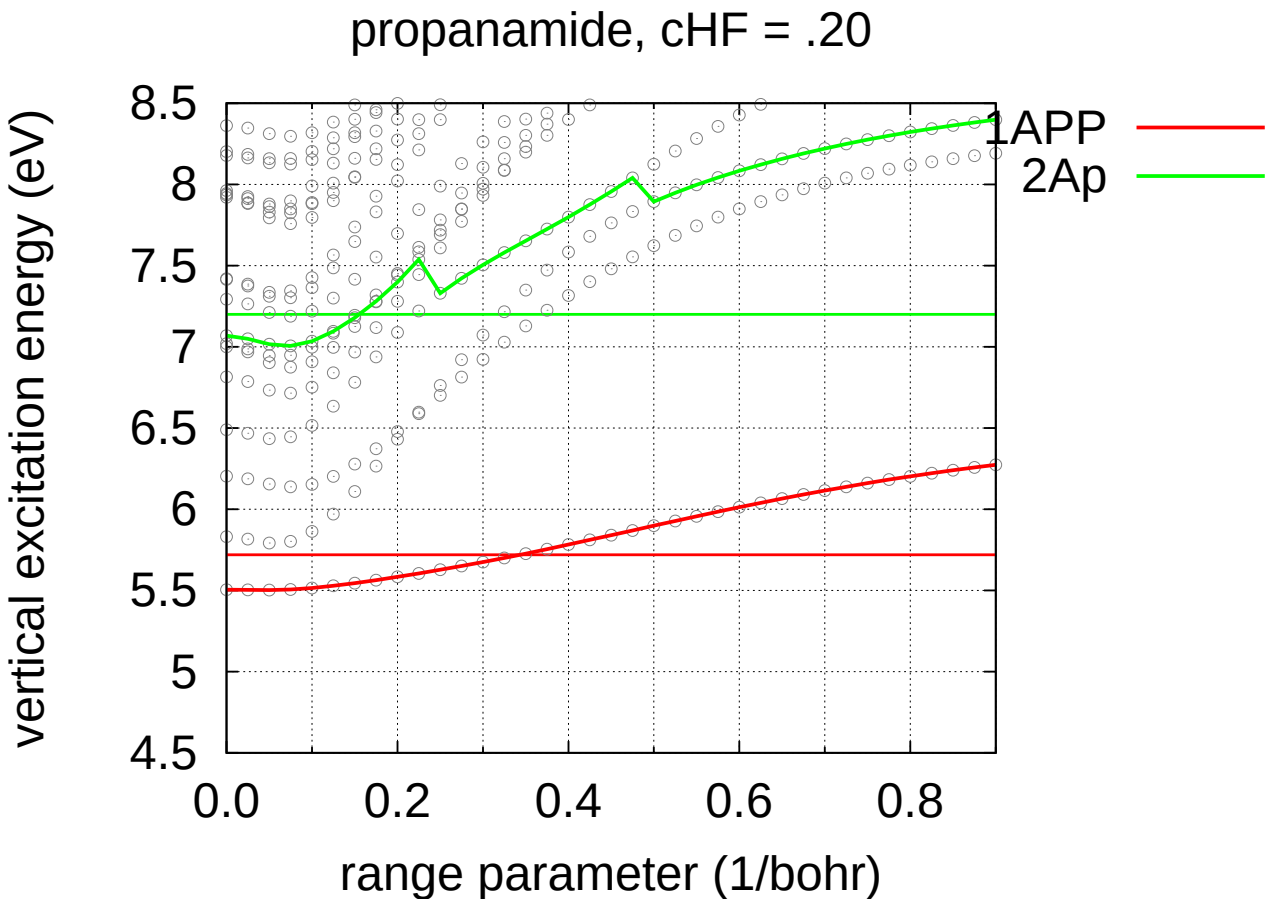

formaldehyde, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
11
10
9
8
7
6
5
4
3
0.0
0.2
0.4
0.6
0.8
1A2
1B1
2A1

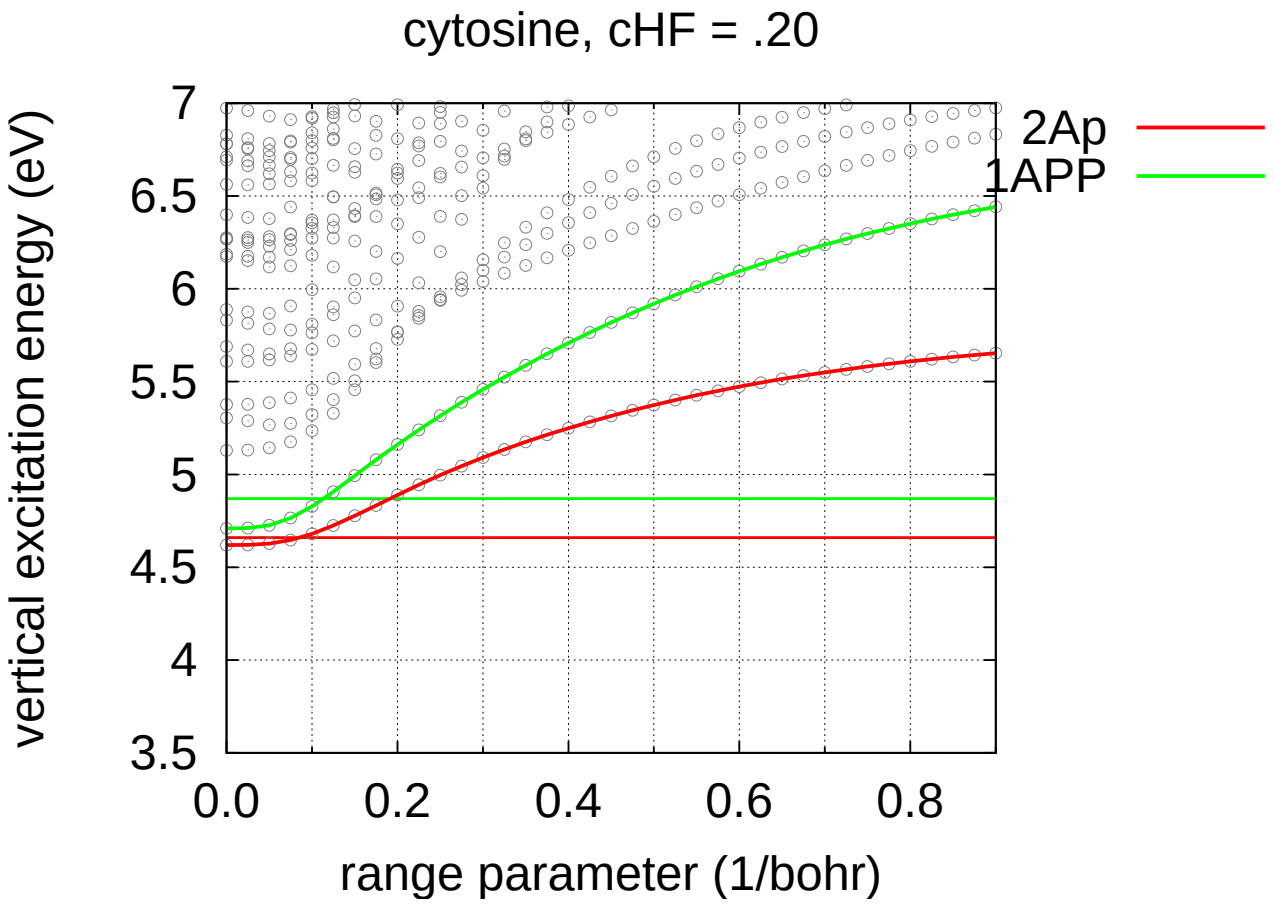

acetone, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
11
10
9
8
7
6
5
4
0.0
0.2
0.4
0.6
0.8
1A2
1B1
2A1

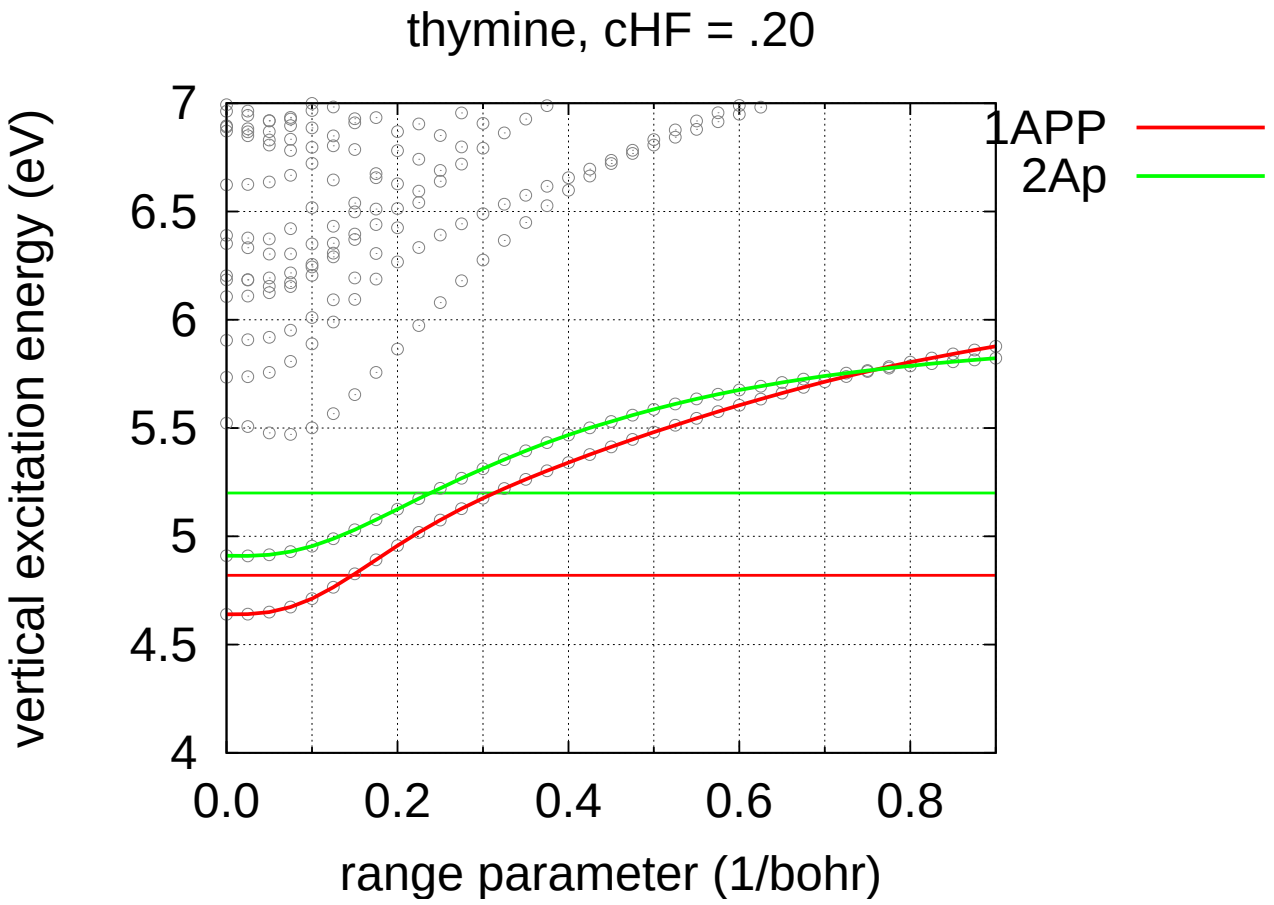

p_benzoquinone, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
1
2
3
4
5
6
7
8
9
0.0
0.2
0.4
0.6
0.8
1Au
1B1g
1B3g
1B1u
1B3u
2B3g

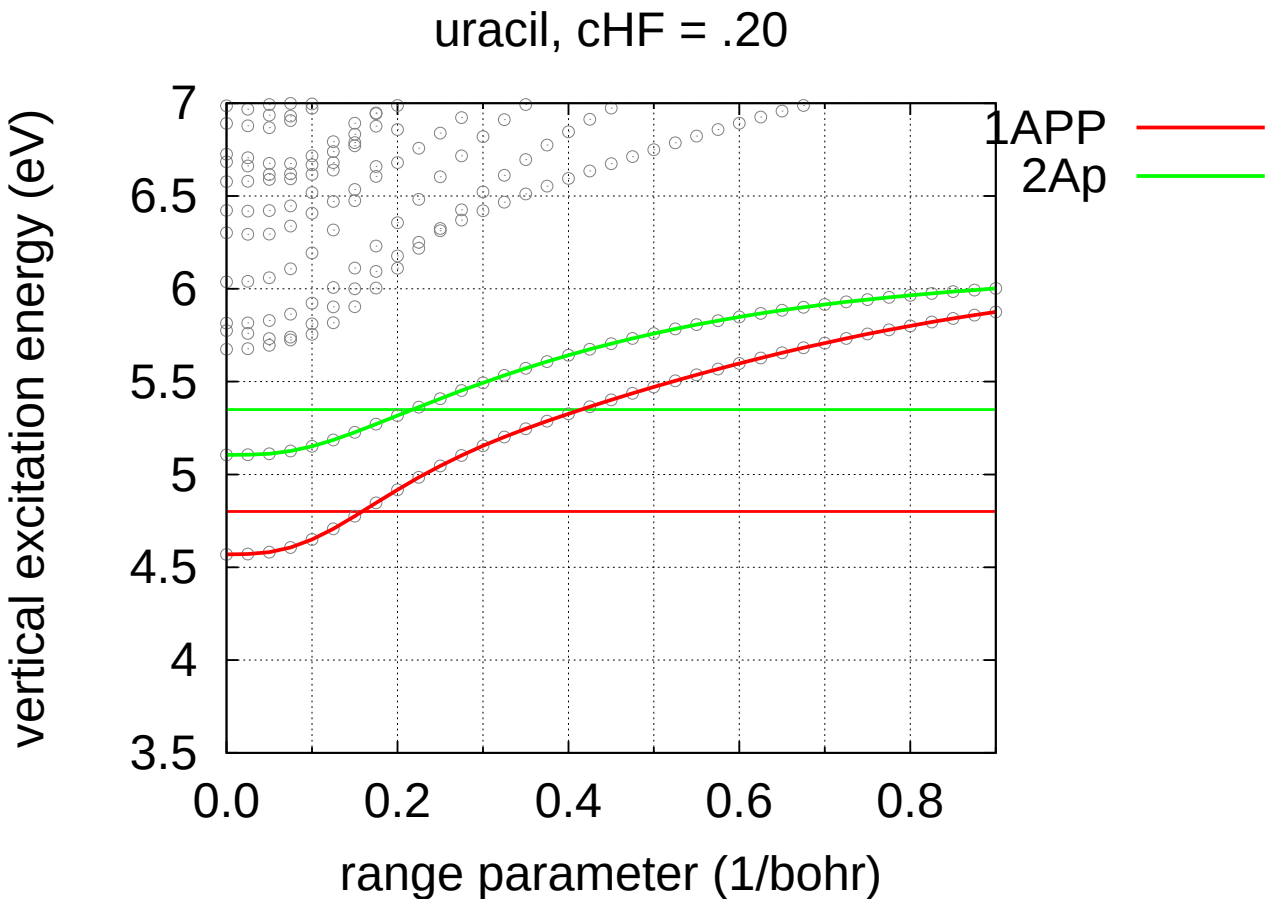

formamide, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
9
8.5
8
7.5
7
6.5
6
5.5
5
0.0
0.2
0.4
0.6
0.8

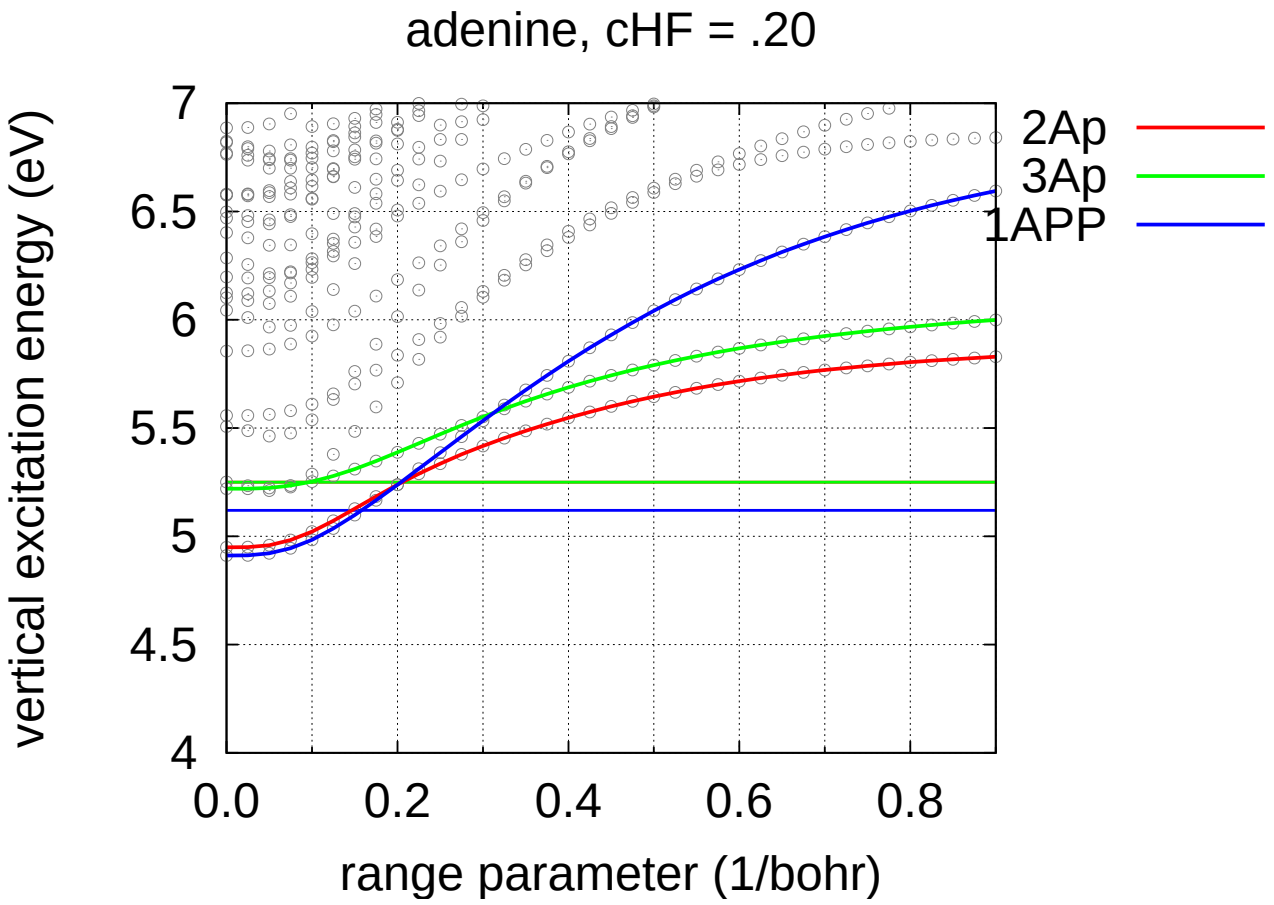

acetamide, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
8.5
8
7.5
7
6.5
6
5.5
5
4.5
0.0
0.2
0.4
0.6
0.8

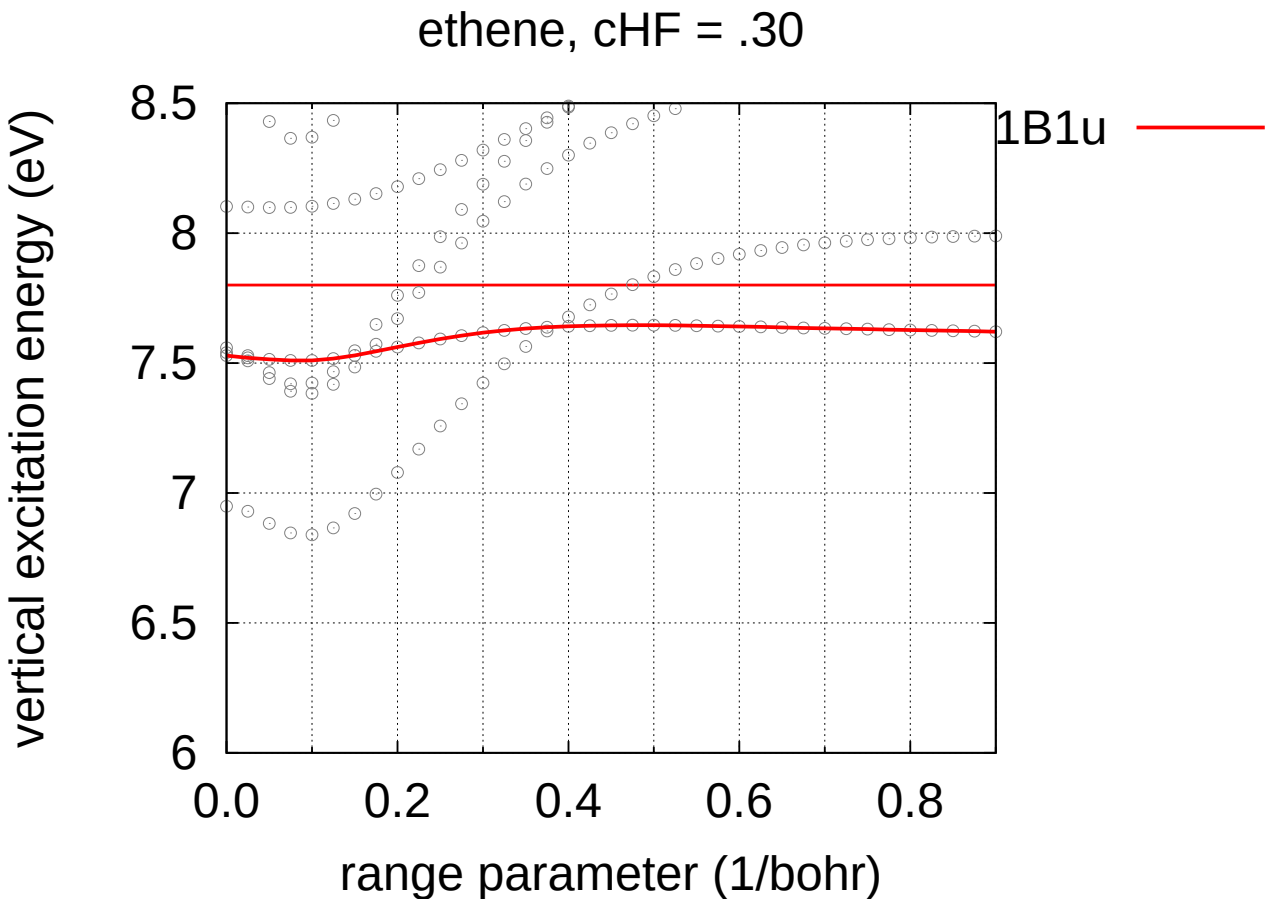

propanamide, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
8.5
8
7.5
7
6.5
6
5.5
5
4.5
0.0
0.2
0.4
0.6
0.8

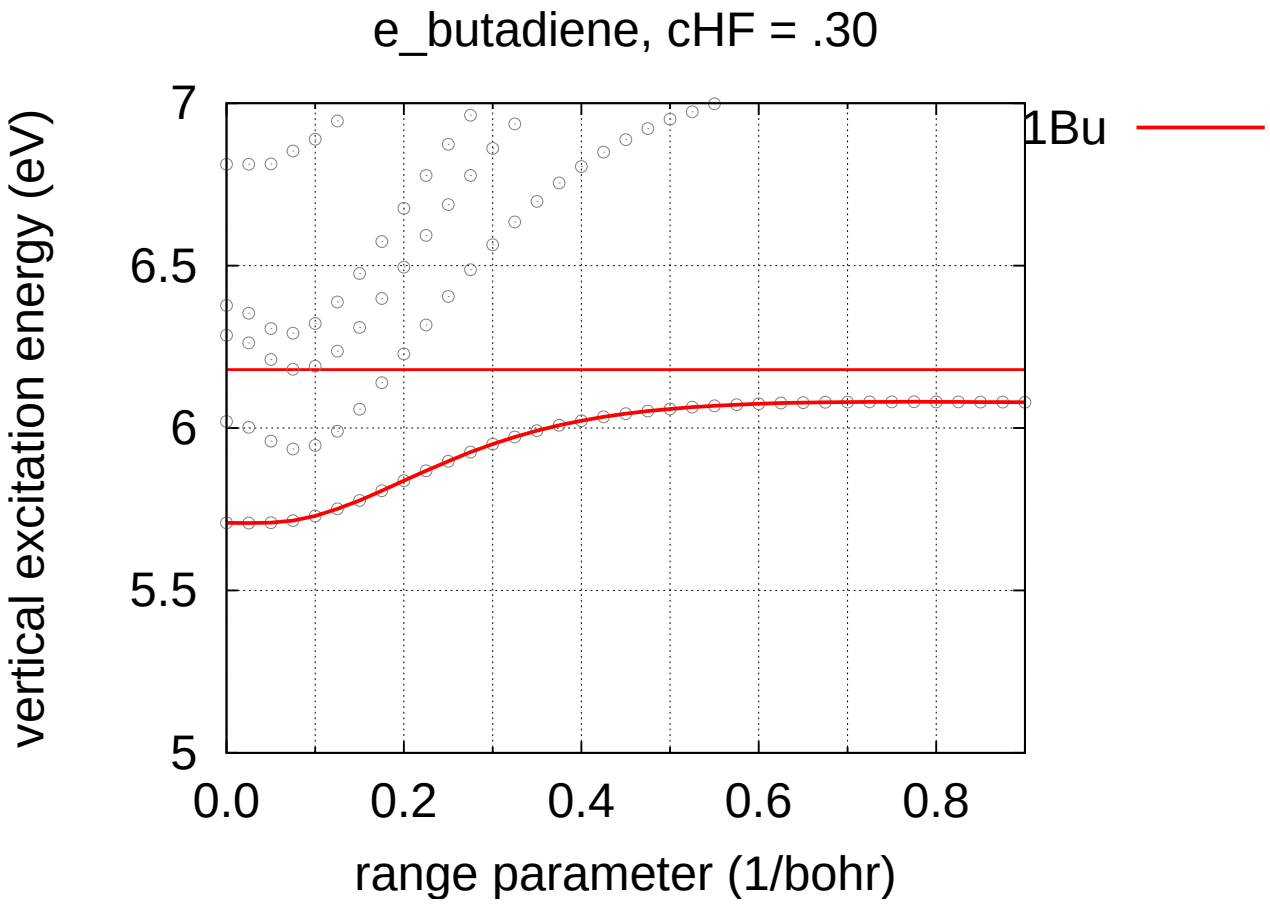

cytosine, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
2Ap
1APP
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8

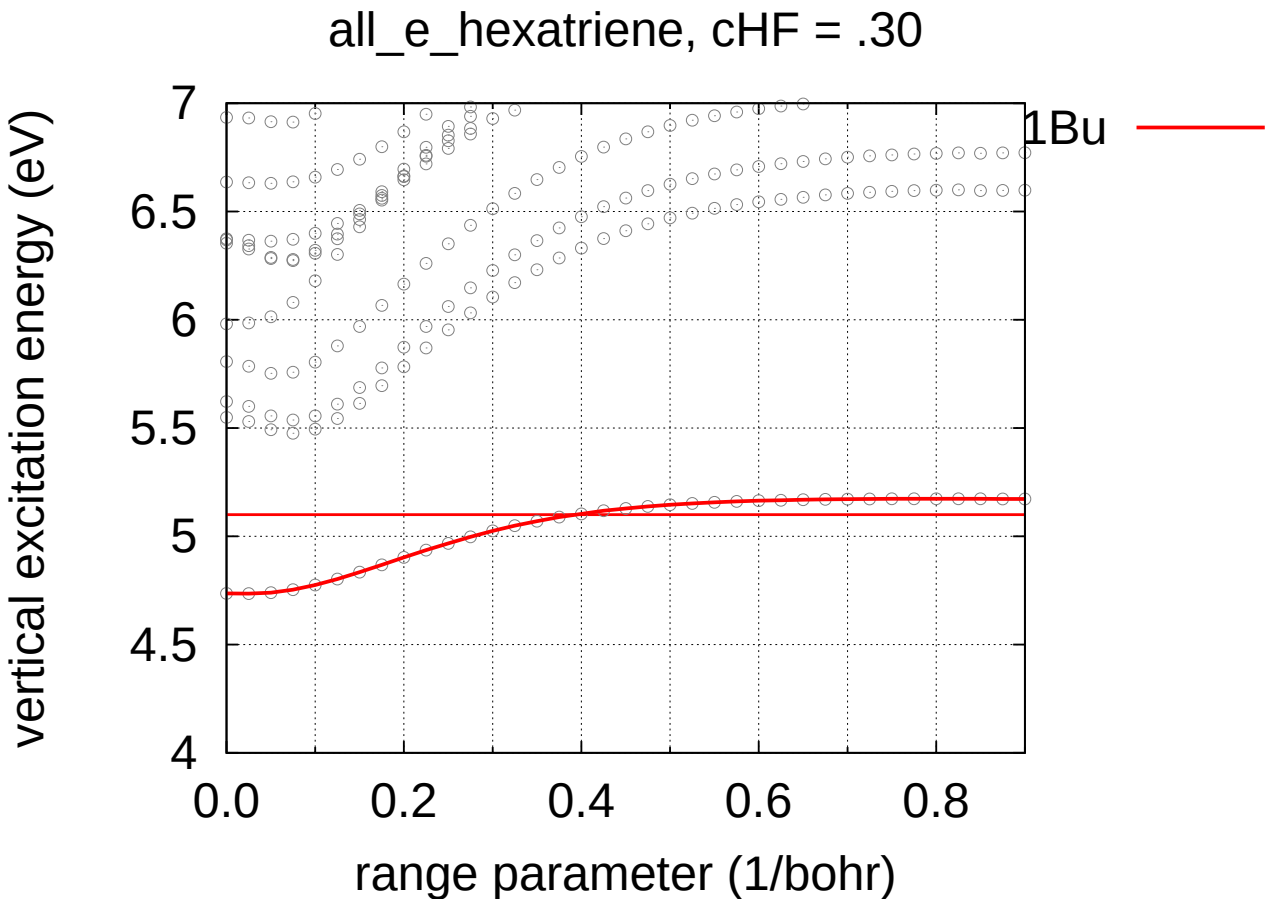

thymine, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8

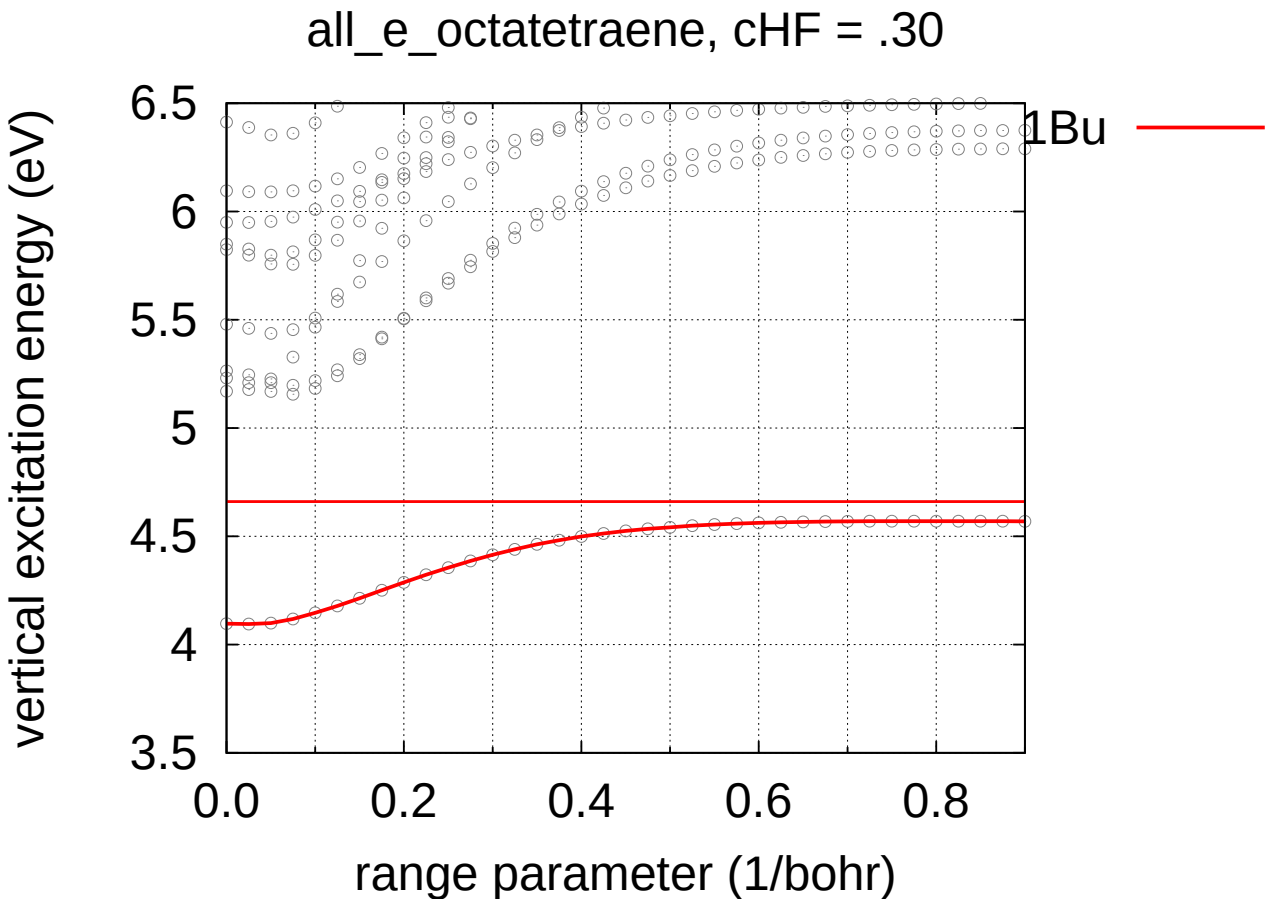

uracil, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8

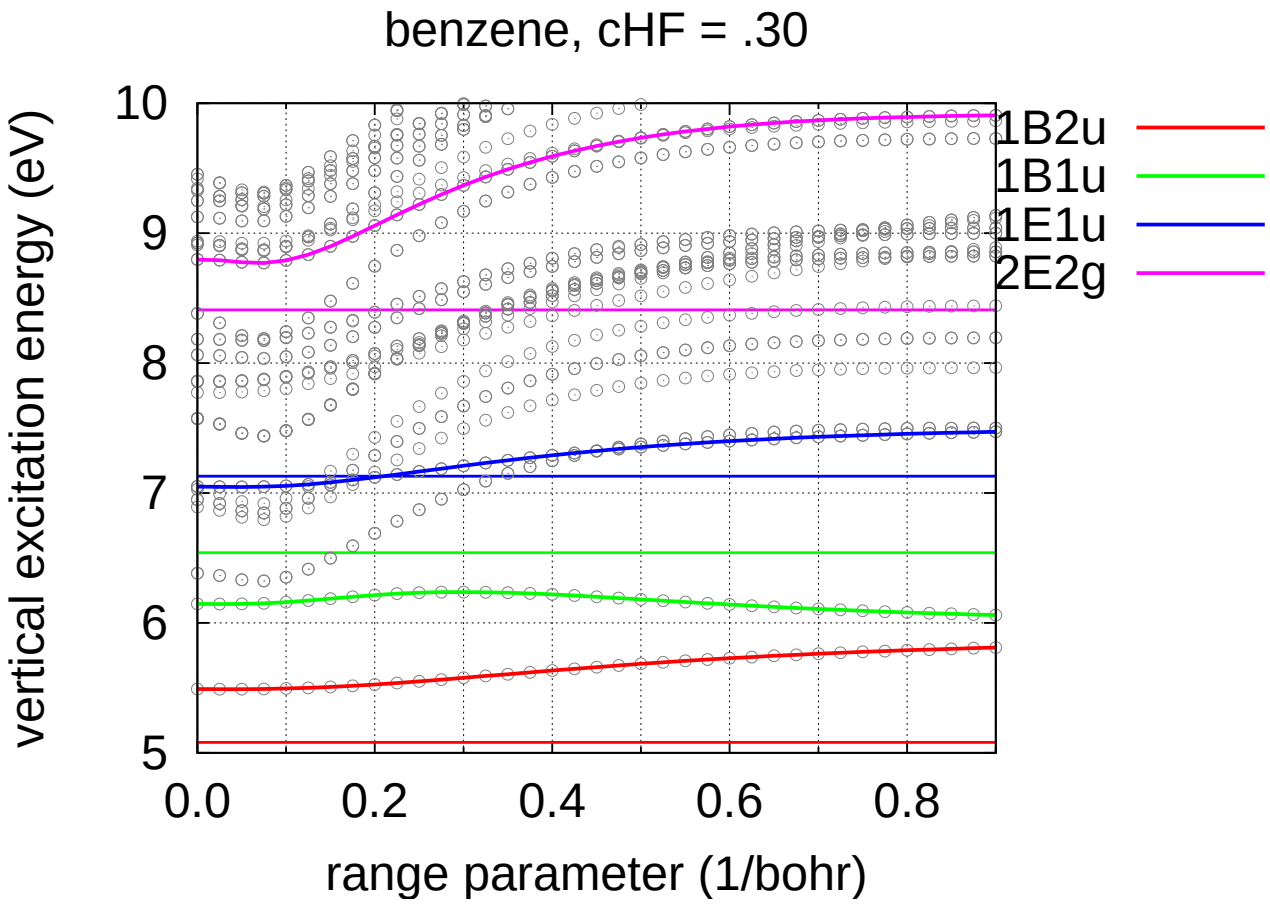

adenine, cHF = .20
vertical excitation energy (eV)
range parameter (1/bohr)
2Ap
3Ap
1APP
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8

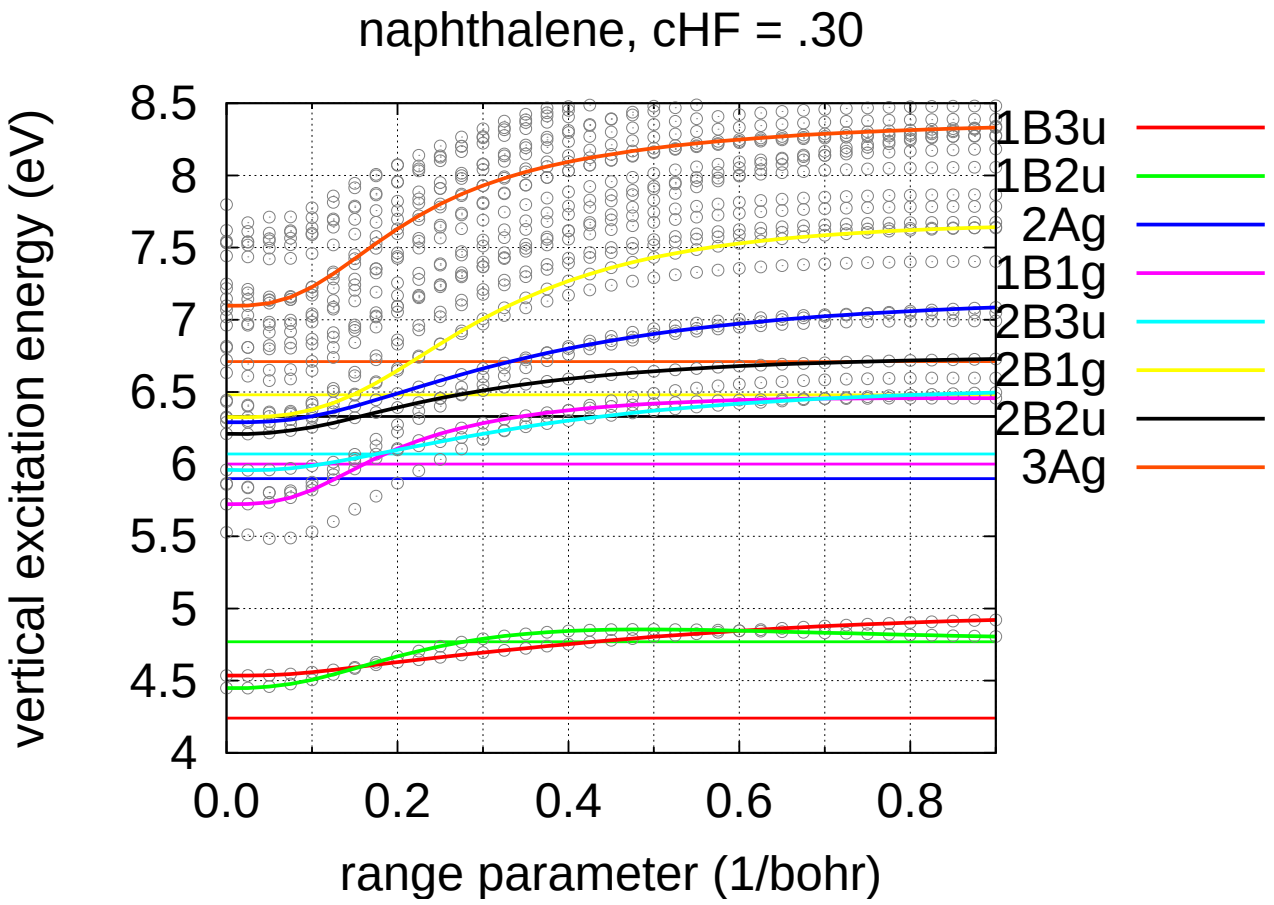

ethene, cHF = .30
vertical excitation energy (eV)
8.5
8
7.5
7
6.5
6
0.0
0.2
0.4
0.6
0.8
range parameter (1/bohr)
1B1u

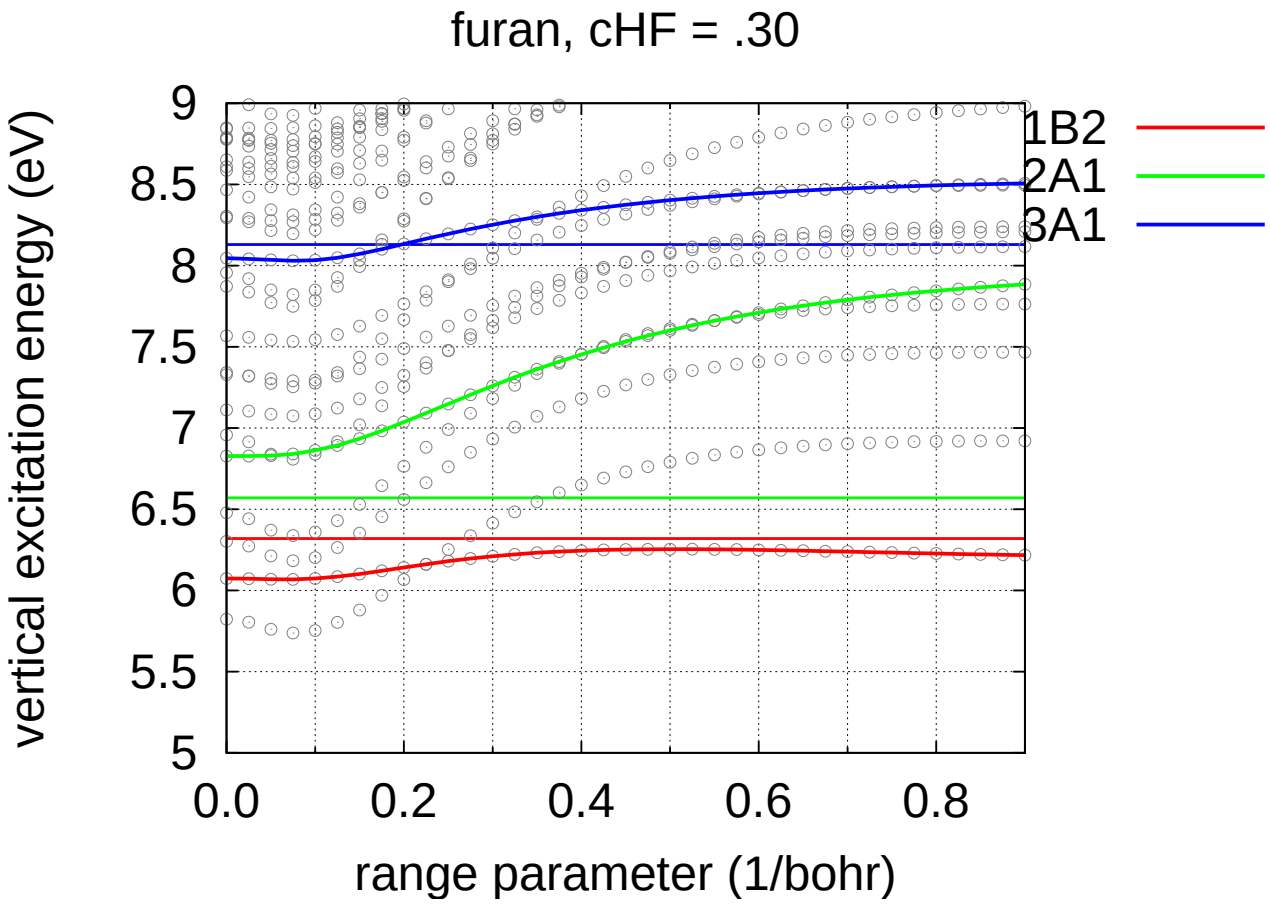

e_butadiene, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
1Bu
7
6.5
6
5.5
5
0.0
0.2
0.4
0.6
0.8

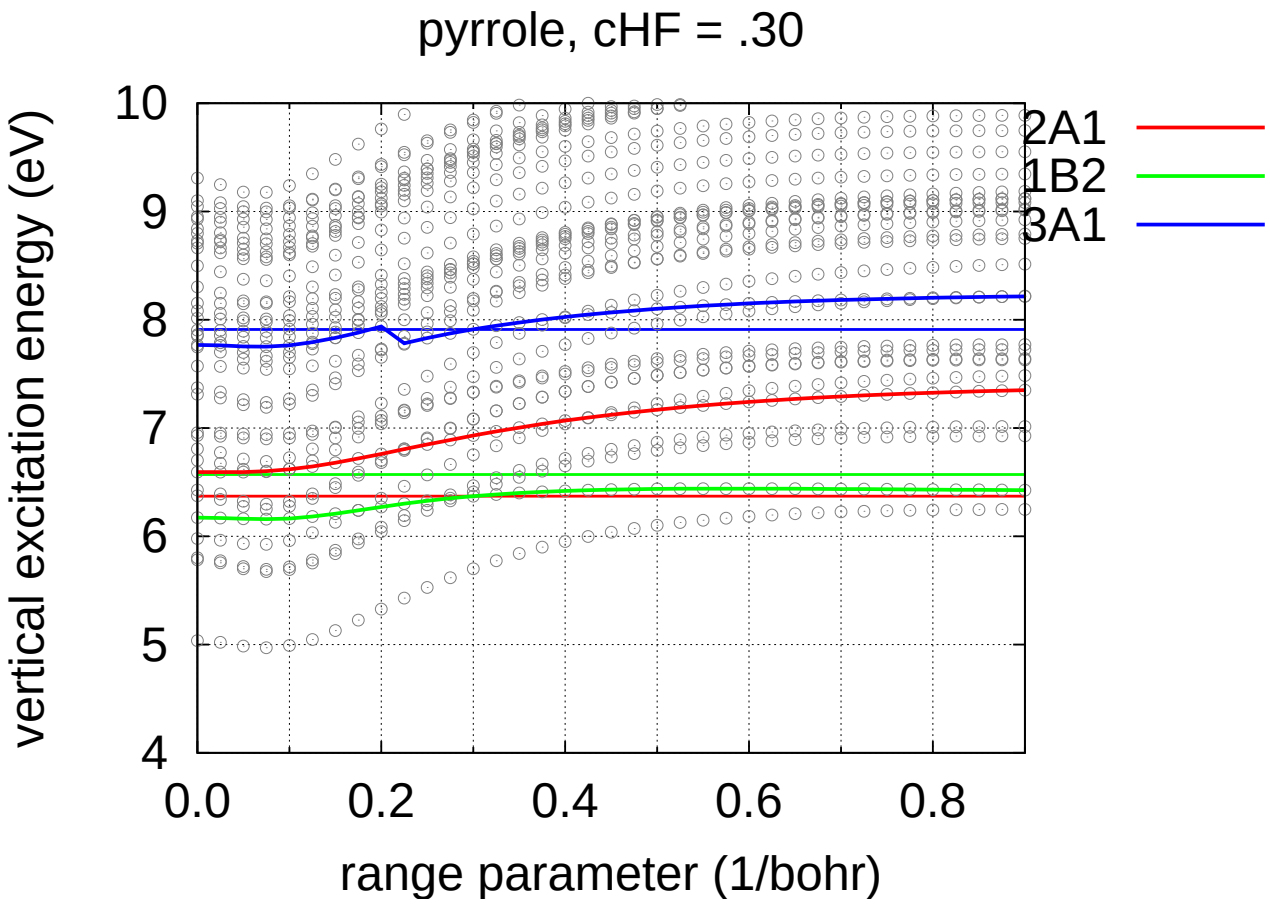

all_e_hexatriene, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
1Bu
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8

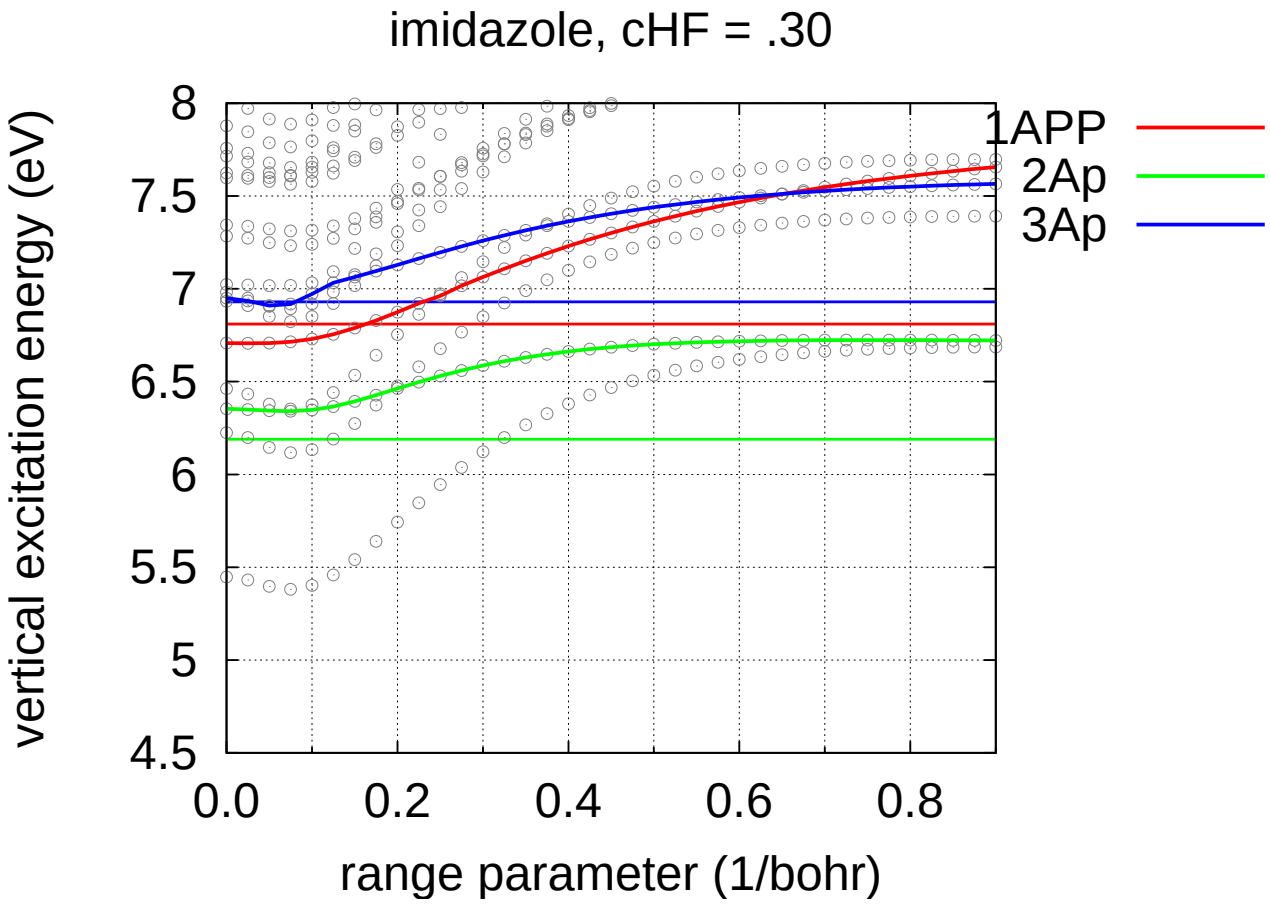

all_e_octatetraene, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
1Bu
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8

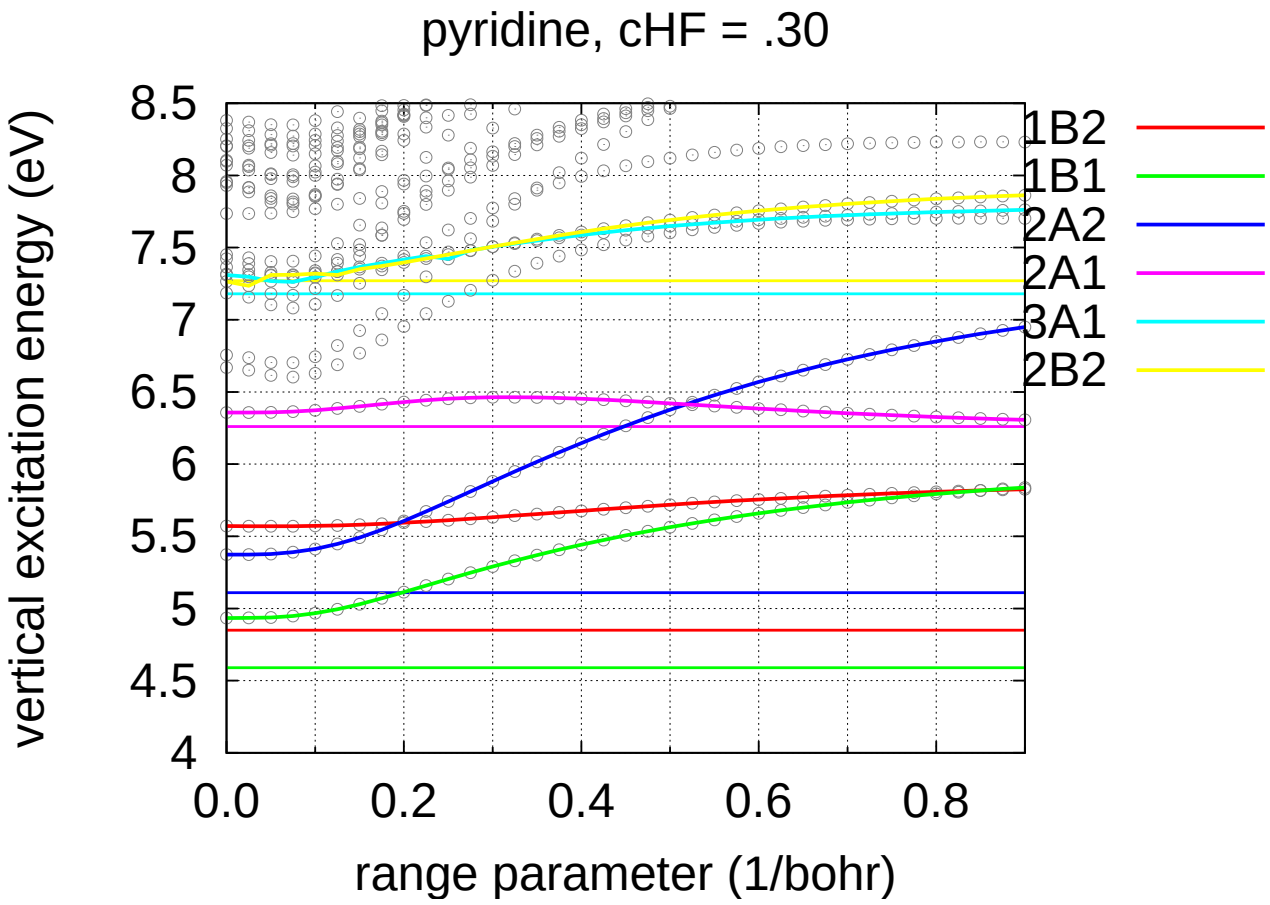

benzene, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
10
9
8
7
6
5
0.0
0.2
0.4
0.6
0.8
1B2u
1B1u
1E1u
2E2g

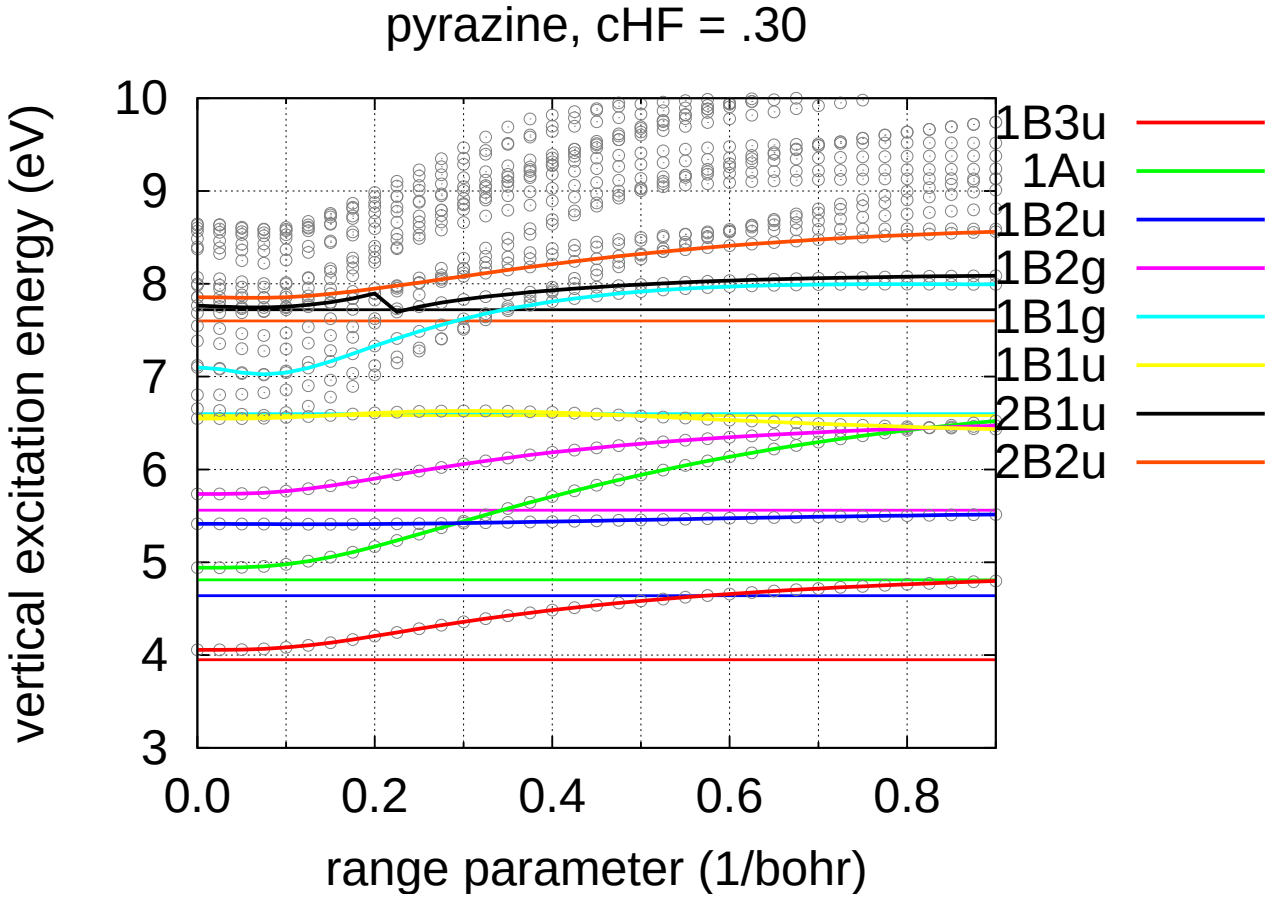

naphthalene, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8
1B3u
1B2u
2Ag
1B1g
2B3u
2B1g
2B2u
3Ag

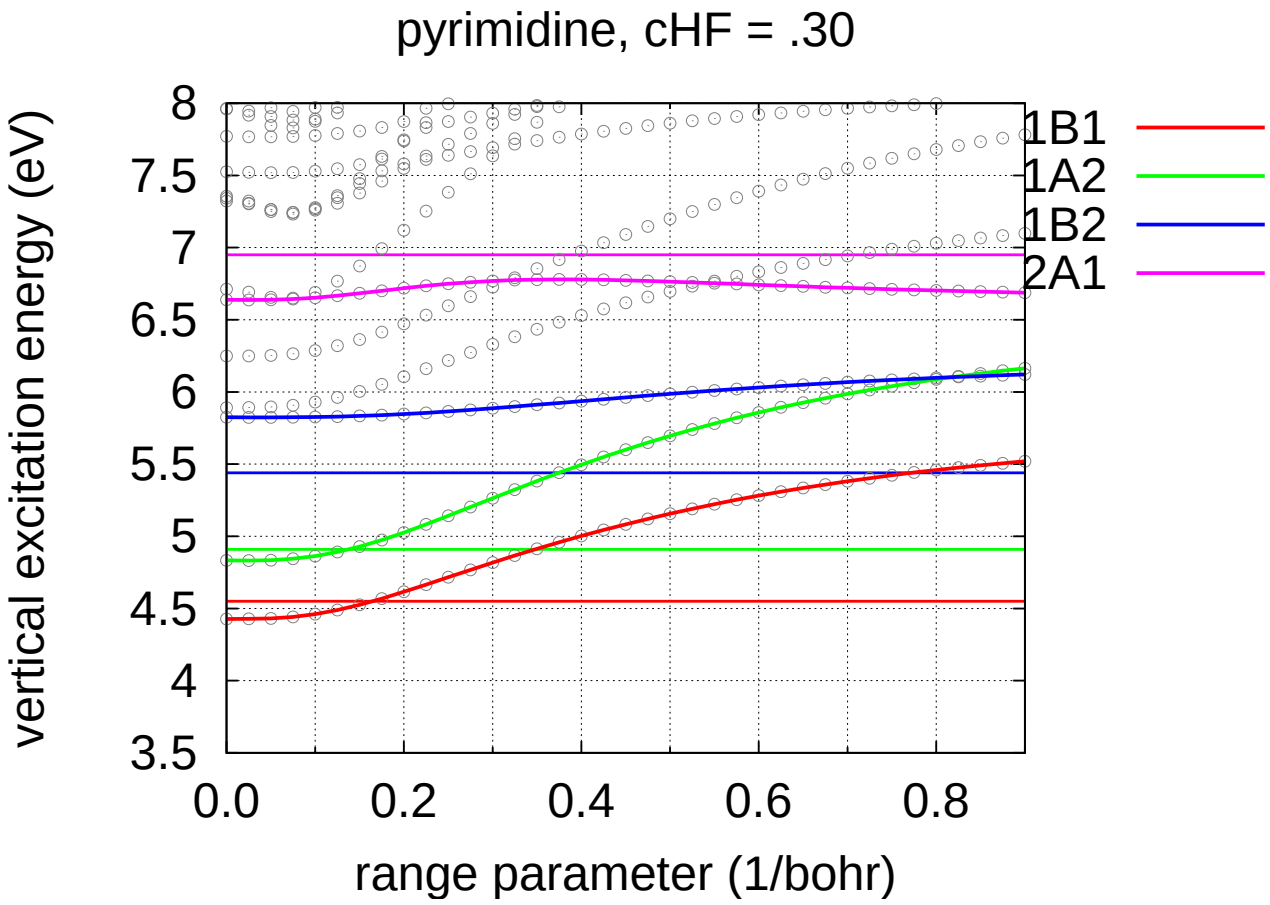

furan, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
9
8.5
8
7.5
7
6.5
6
5.5
5
0.0
0.2
0.4
0.6
0.8
1B2
2A1
3A1

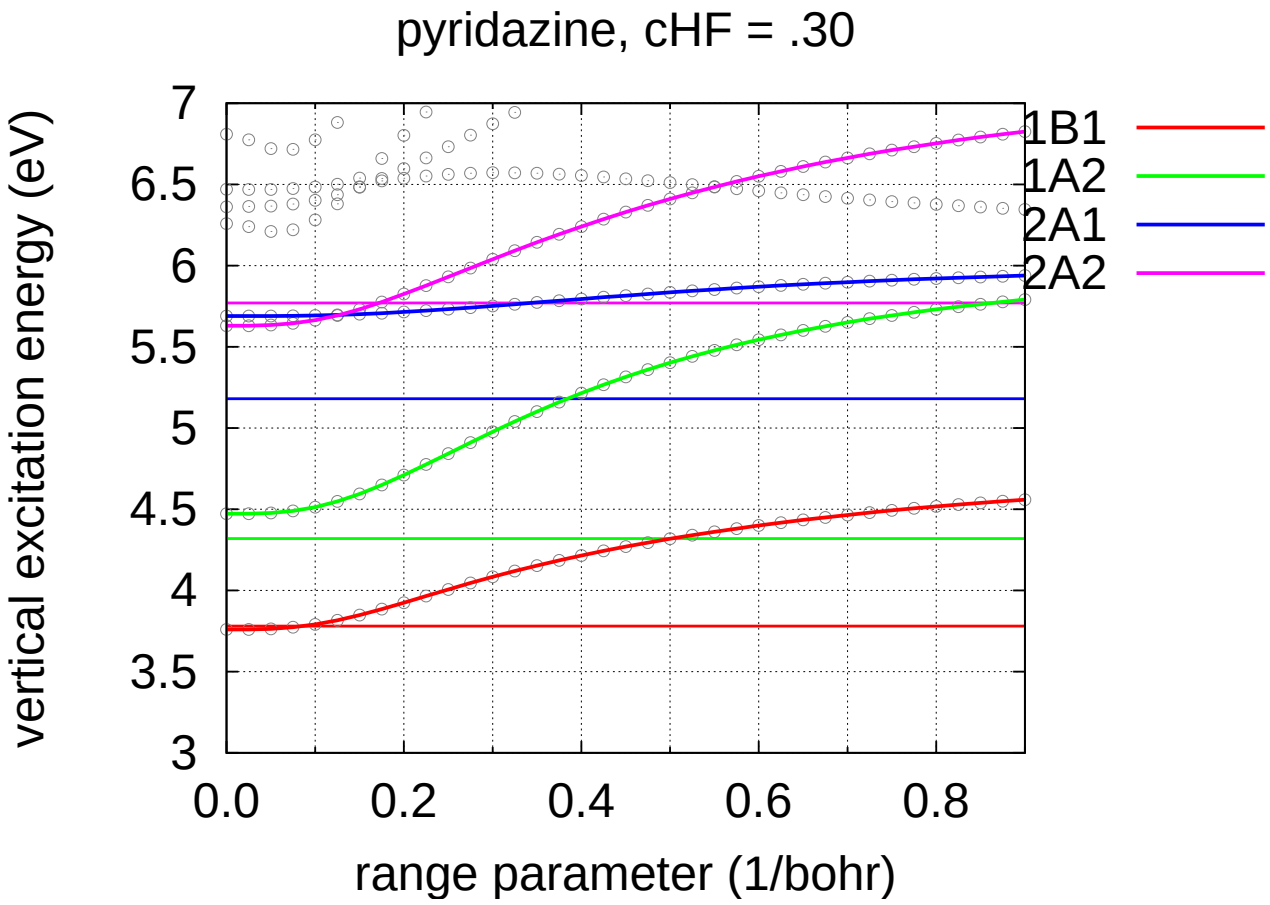

pyrrole, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
10
9
8
7
6
5
4
0.0
0.2
0.4
0.6
0.8
2A1
1B2
3A1

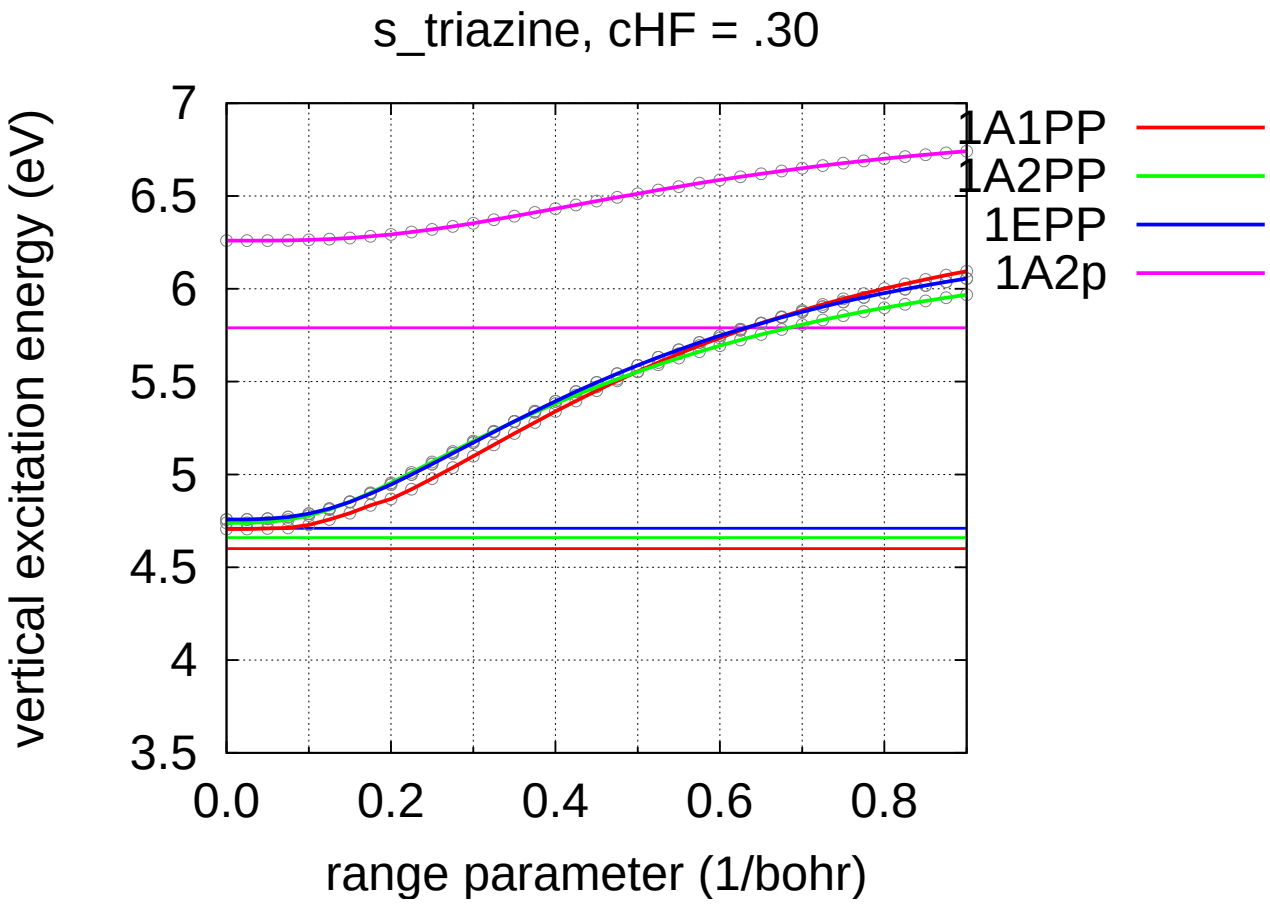

imidazole, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
8
7.5
7
6.5
6
5.5
5
4.5
0.0
0.2
0.4
0.6
0.8
1APP
2Ap
3Ap

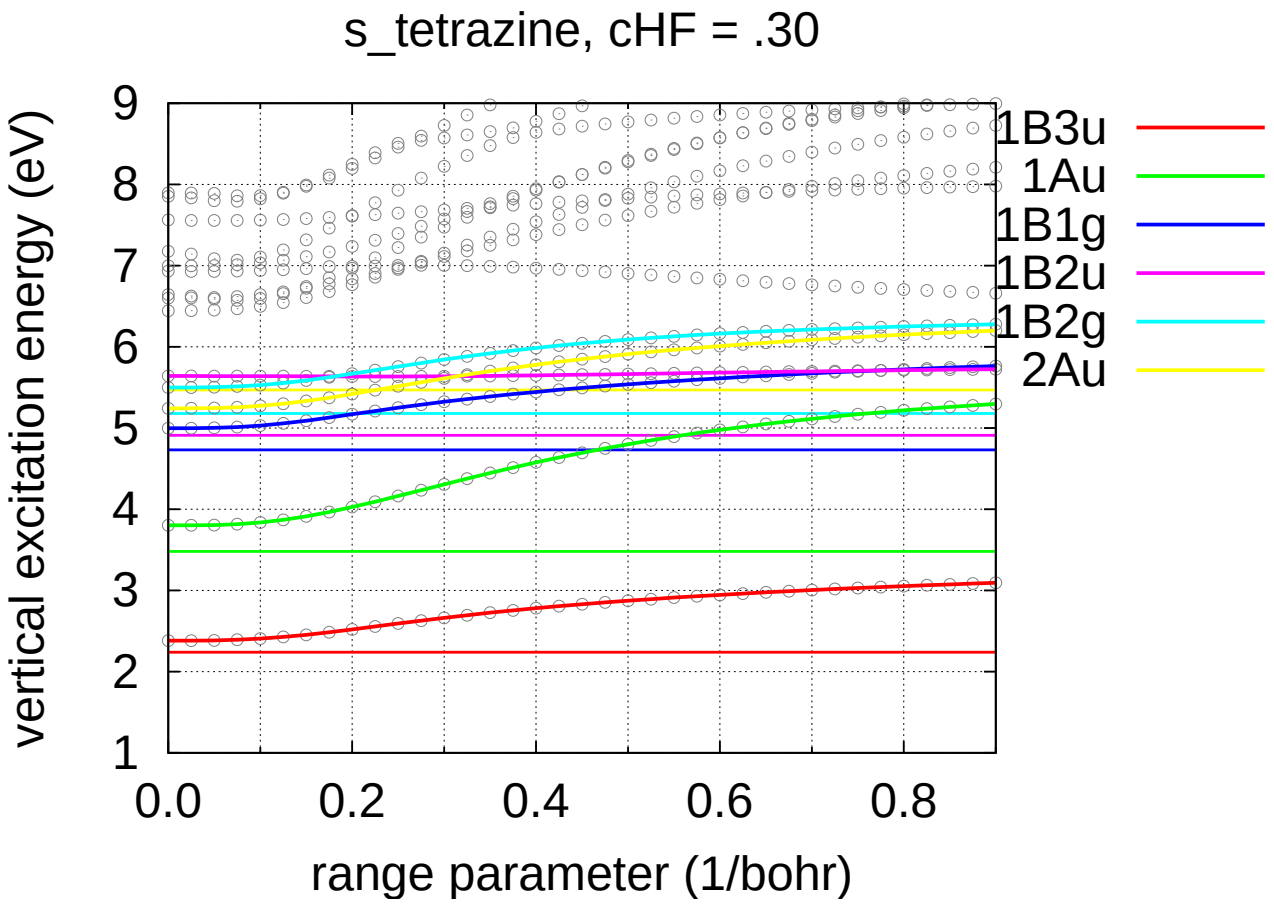

pyridine, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8
1B2
1B1
2A2
2A1
3A1
2B2

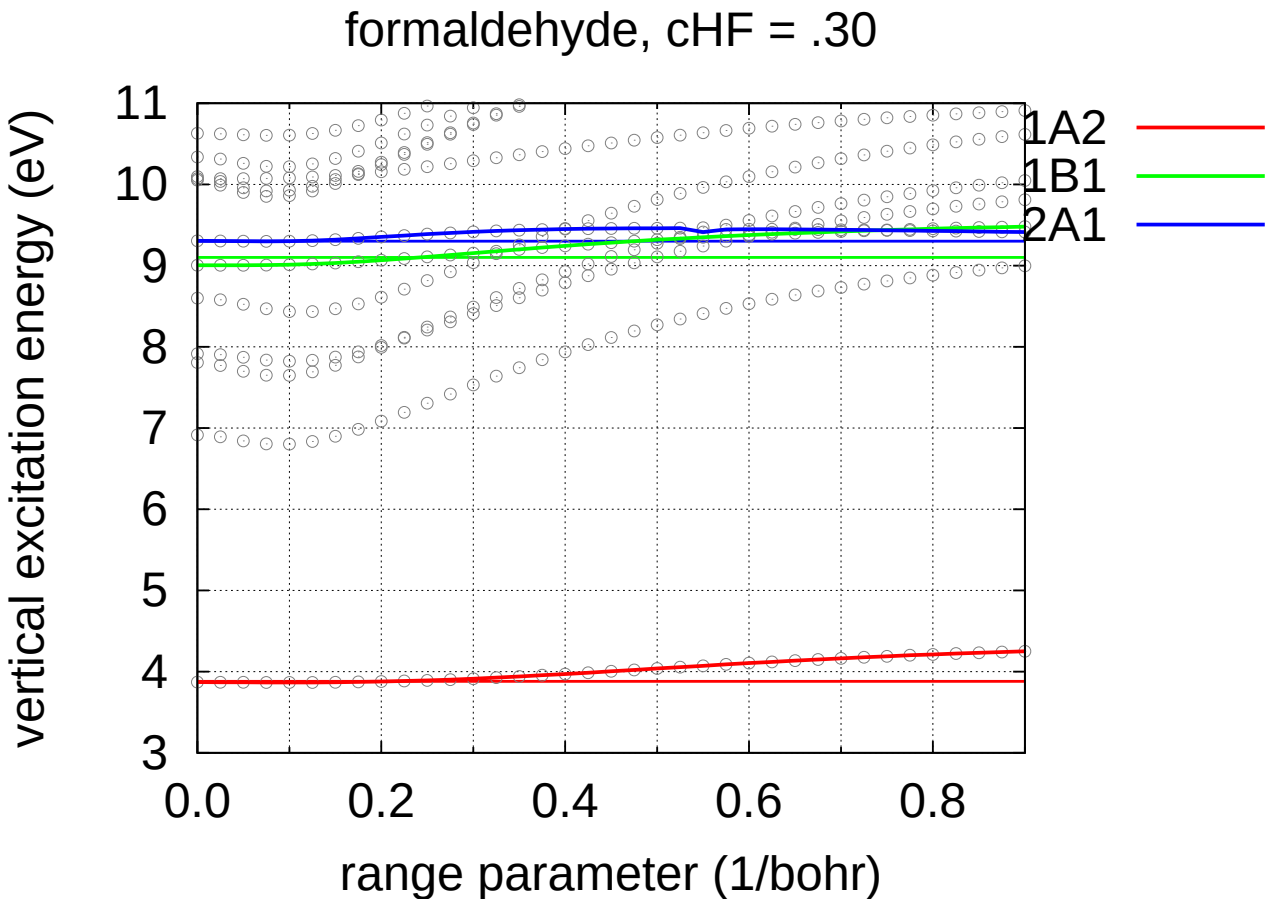

pyrazine, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
10
9
8
7
6
5
4
3
0.0
0.2
0.4
0.6
0.8
1B3u
1Au
1B2u
1B2g
1B1g
1B1u
2B1u
2B2u

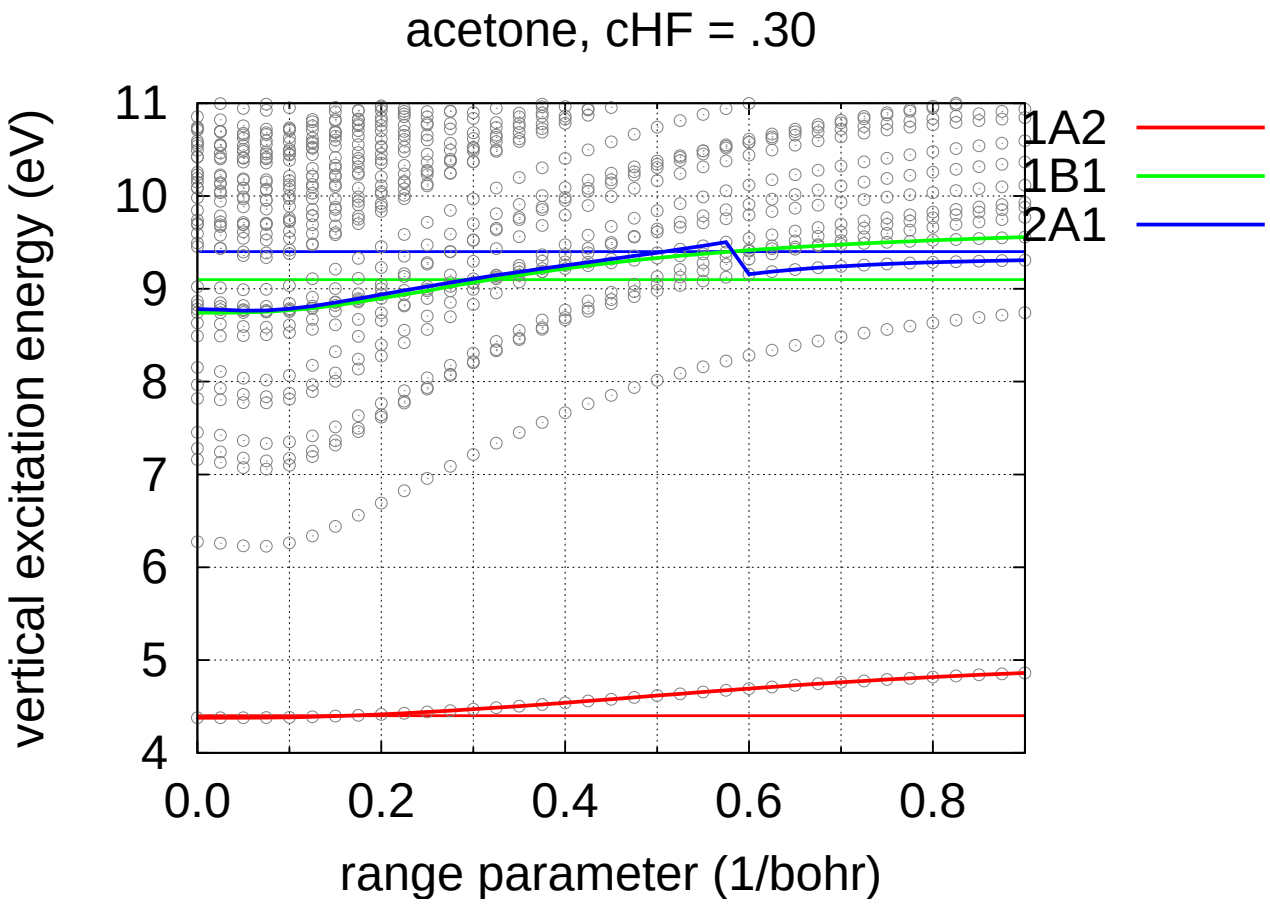

pyrimidine, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8
1B1
1A2
1B2
2A1

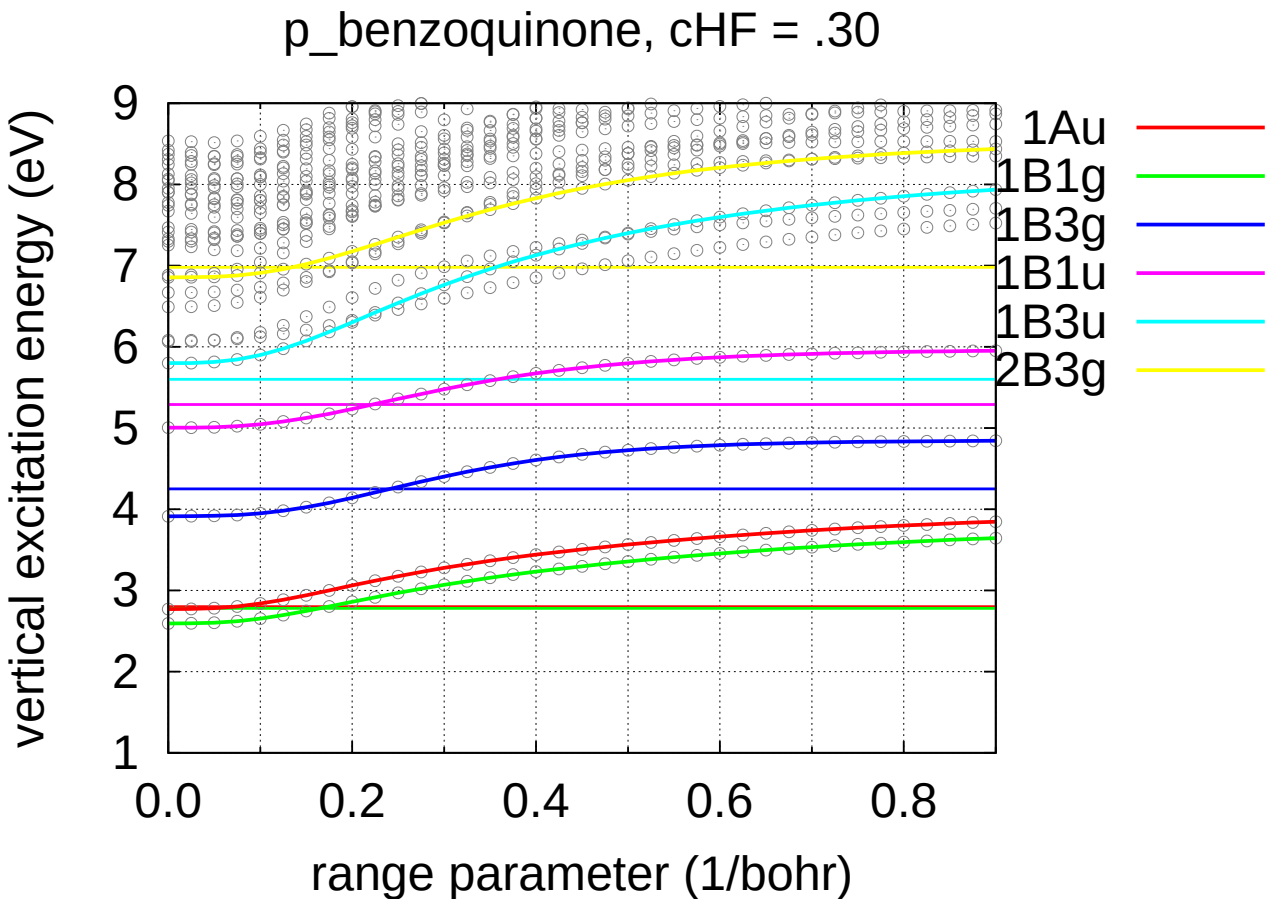

pyridazine, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
7
6.5
6
5.5
5
4.5
4
3.5
3
0.0
0.2
0.4
0.6
0.8
1B1
1A2
2A1
2A2

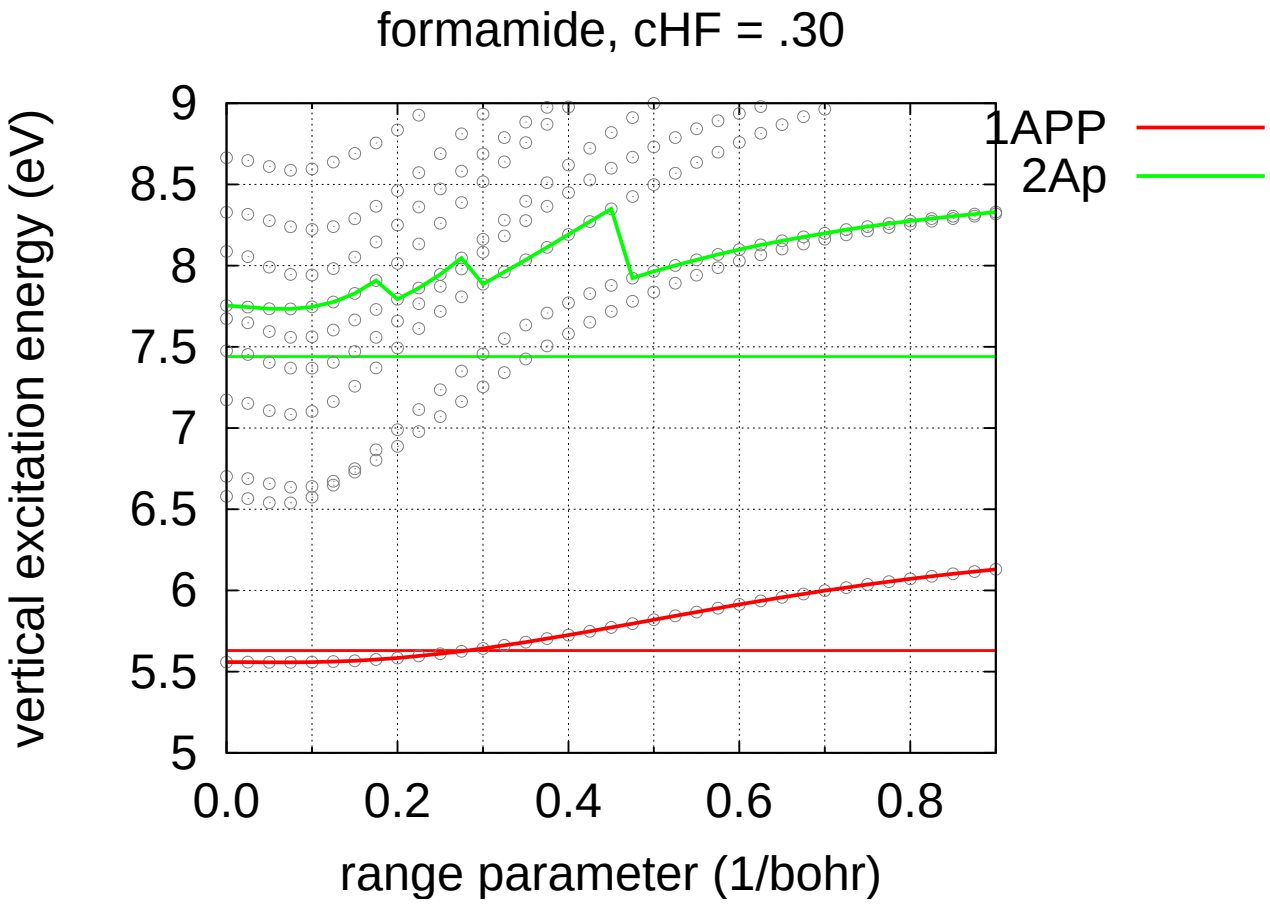

s_triazine, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8
1A1PP
1A2PP
1EPP
1A2p

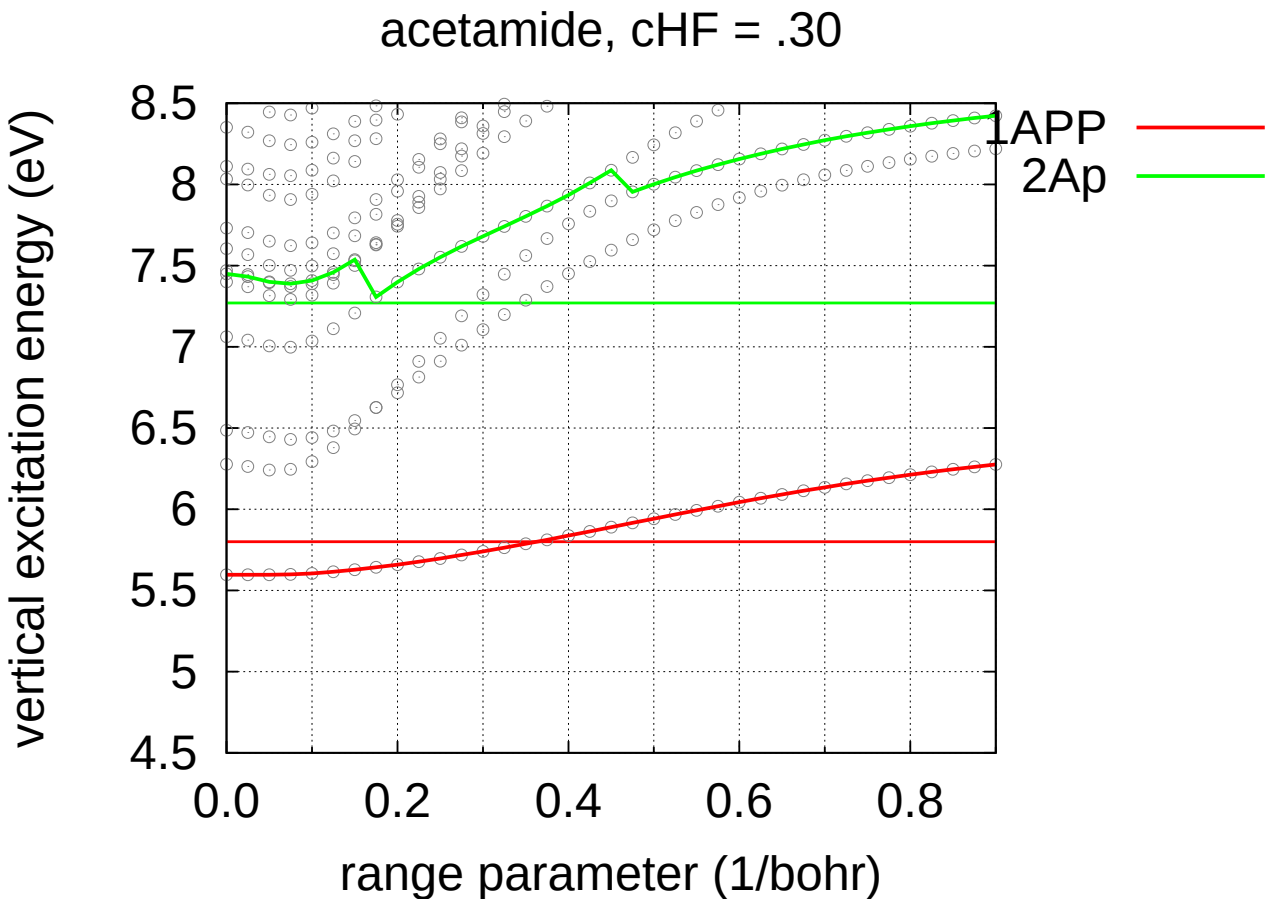

s_tetrazine, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
1
2
3
4
5
6
7
8
9
0.0
0.2
0.4
0.6
0.8
1B3u
1Au
1B1g
1B2u
1B2g
2Au

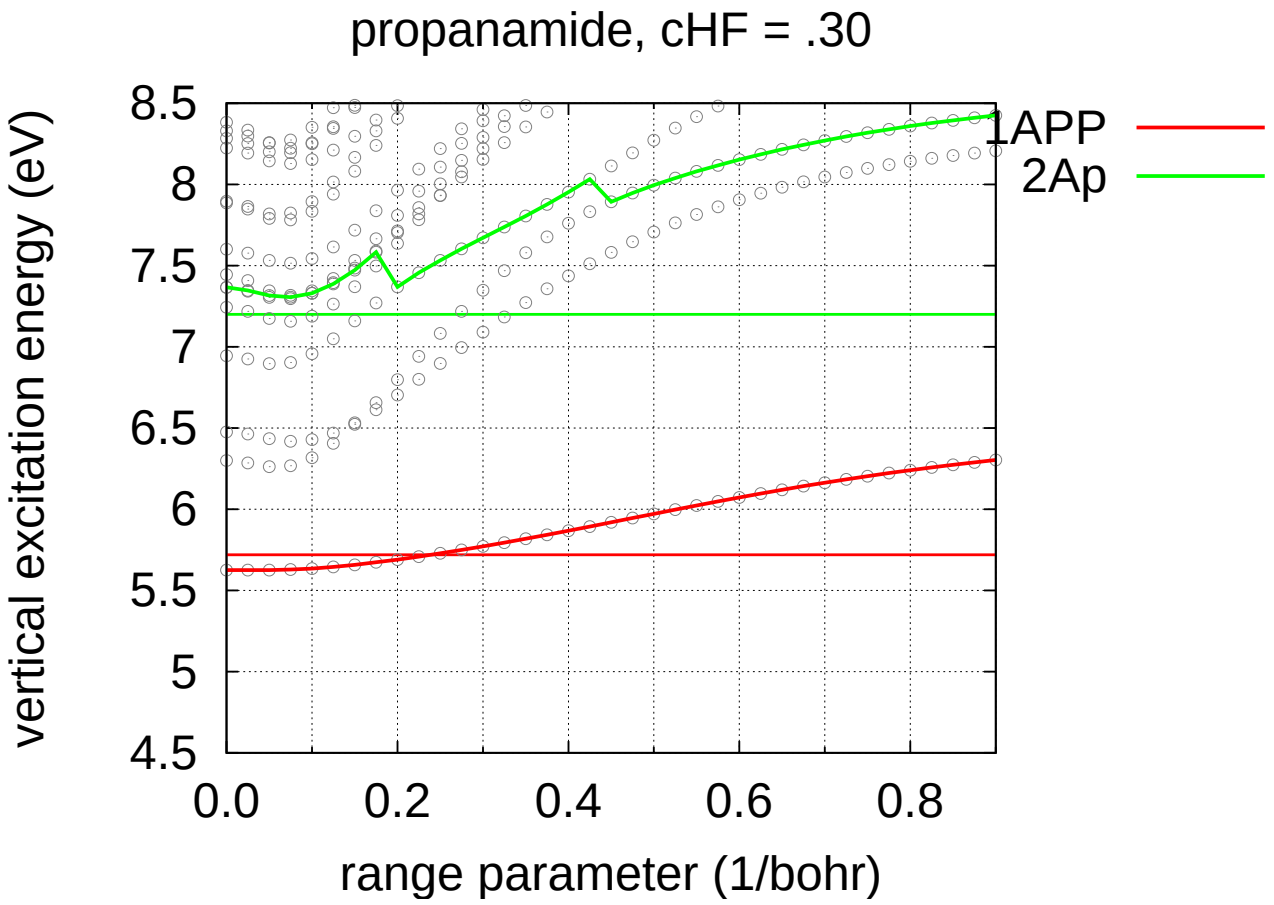

formaldehyde, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
11
10
9
8
7
6
5
4
3
0.0
0.2
0.4
0.6
0.8
1A2
1B1
2A1

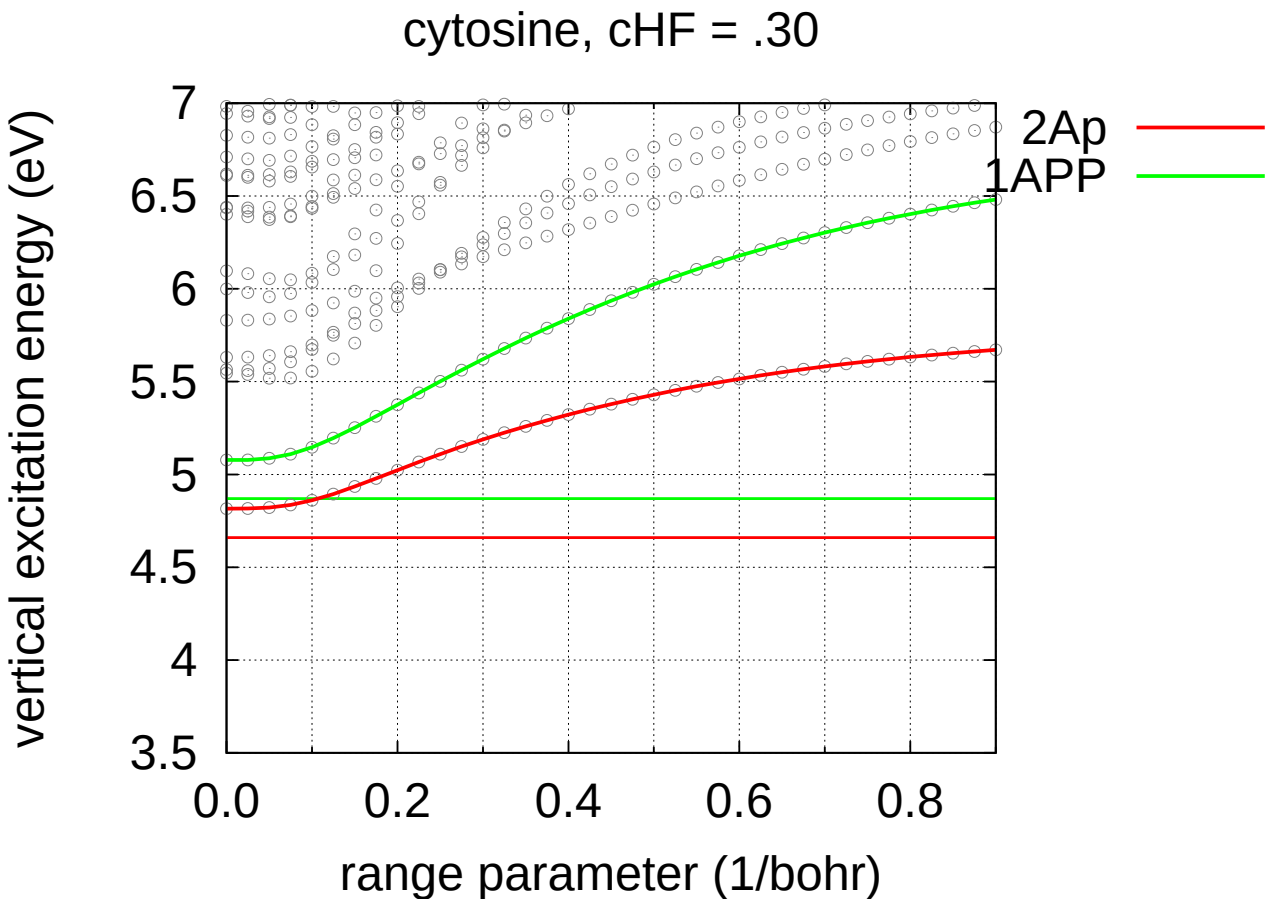

acetone, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
11
10
9
8
7
6
5
4
0.0
0.2
0.4
0.6
0.8
1A2
1B1
2A1

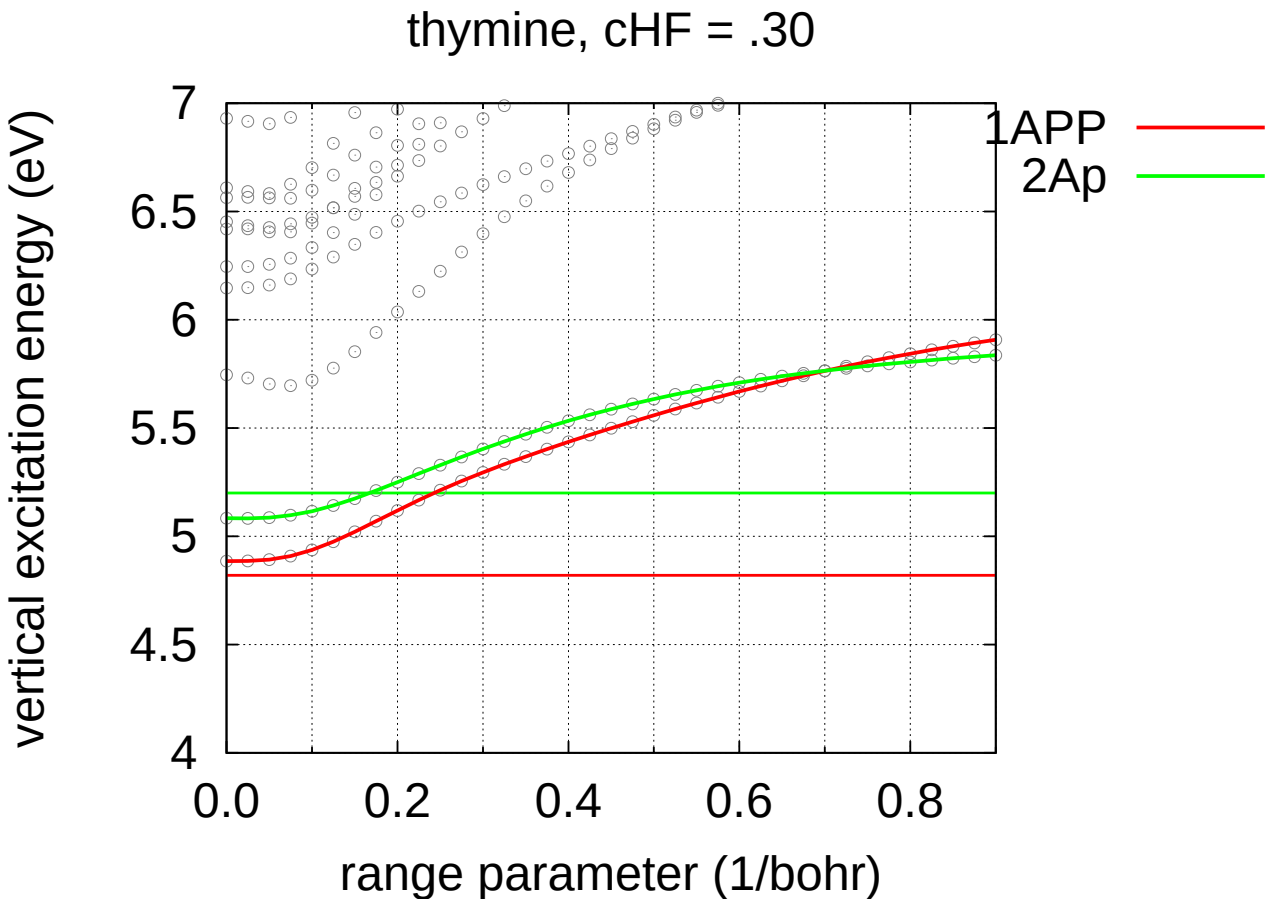

p_benzoquinone, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
1
2
3
4
5
6
7
8
9
0.0
0.2
0.4
0.6
0.8
1Au
1B1g
1B3g
1B1u
1B3u
2B3g

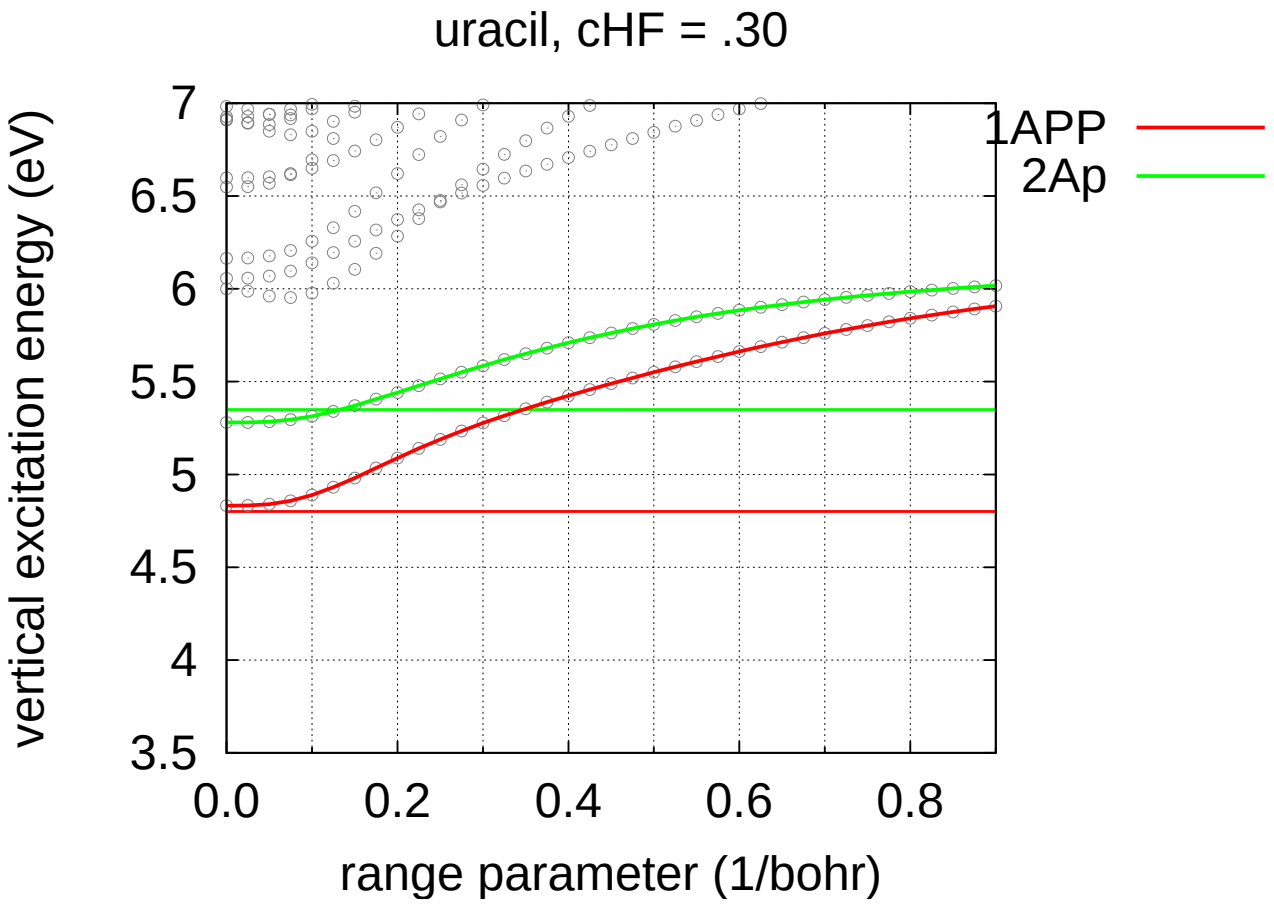

formamide, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
9
8.5
8
7.5
7
6.5
6
5.5
5
0.0
0.2
0.4
0.6
0.8

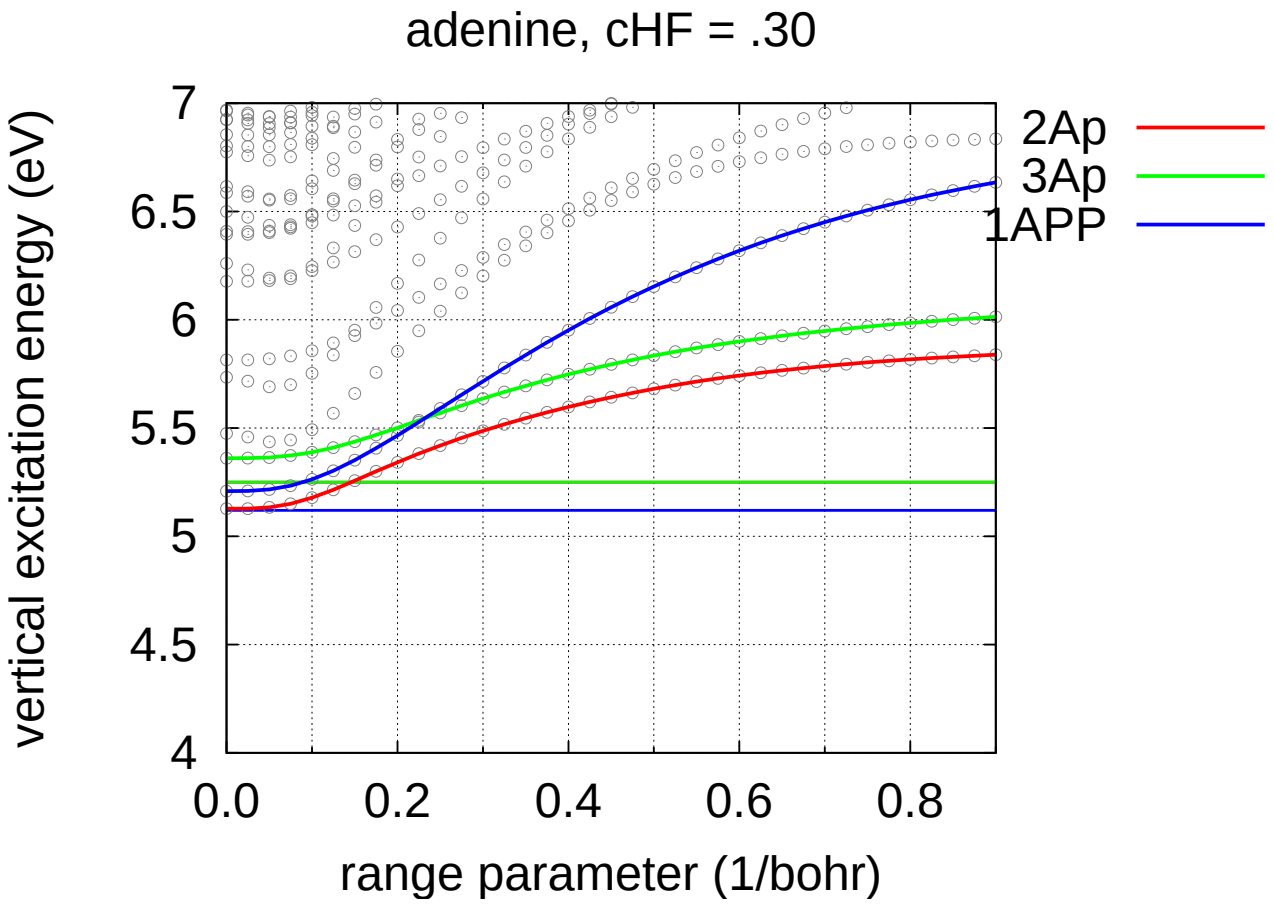

acetamide, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
8.5
8
7.5
7
6.5
6
5.5
5
4.5
0.0
0.2
0.4
0.6
0.8
1APP
2Ap

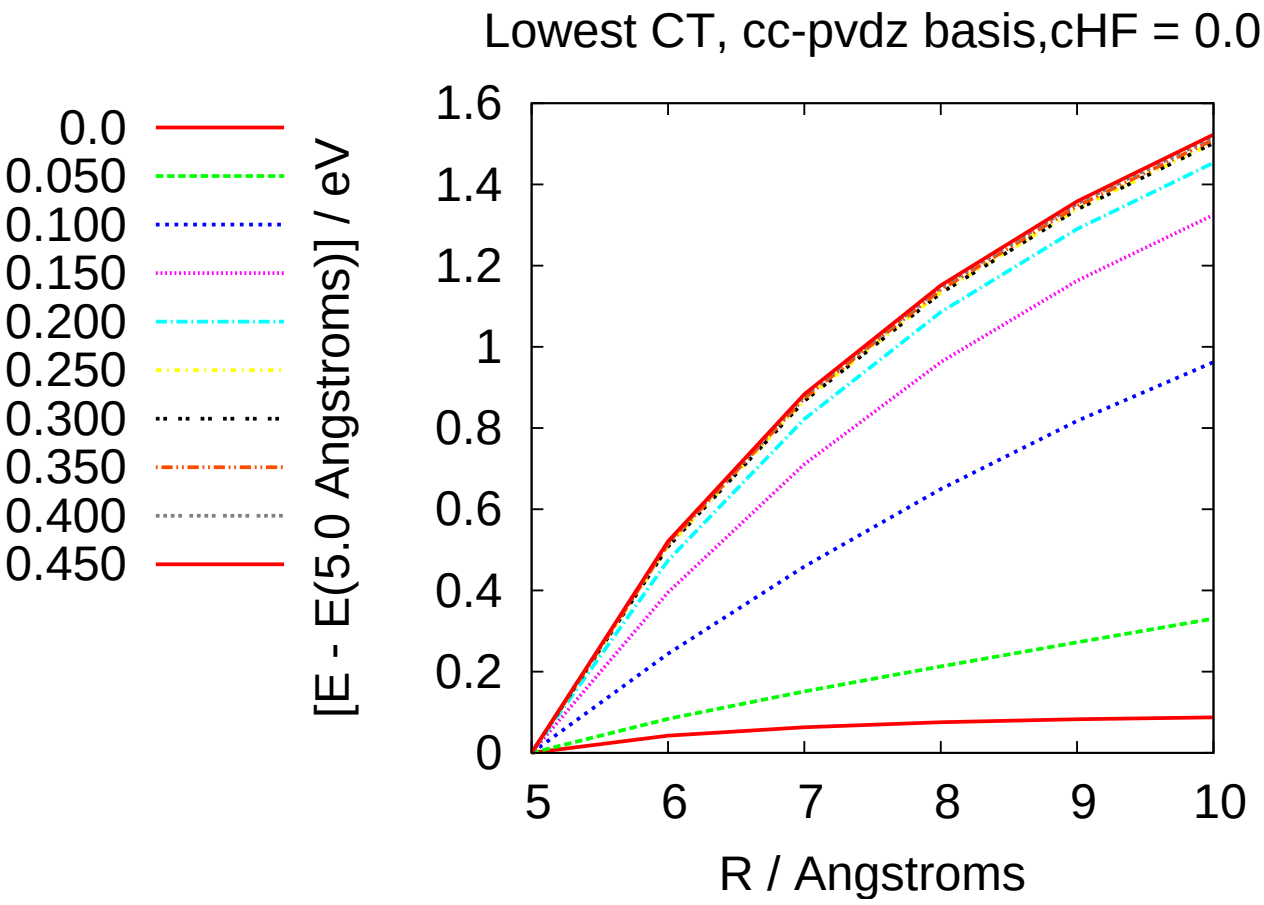

propanamide, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
8.5
8
7.5
7
6.5
6
5.5
5
4.5
0.0
0.2
0.4
0.6
0.8

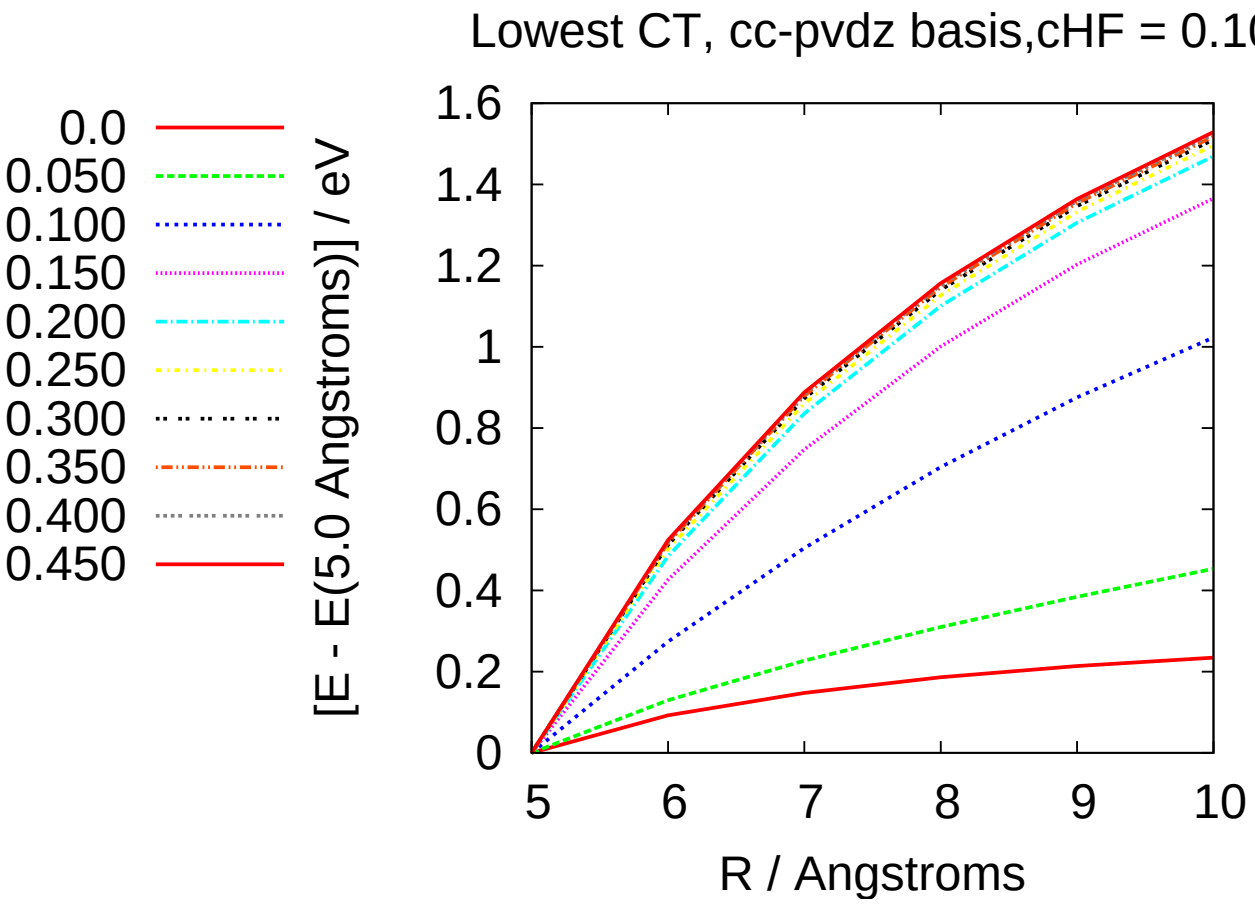

cytosine, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
2Ap
1APP
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8

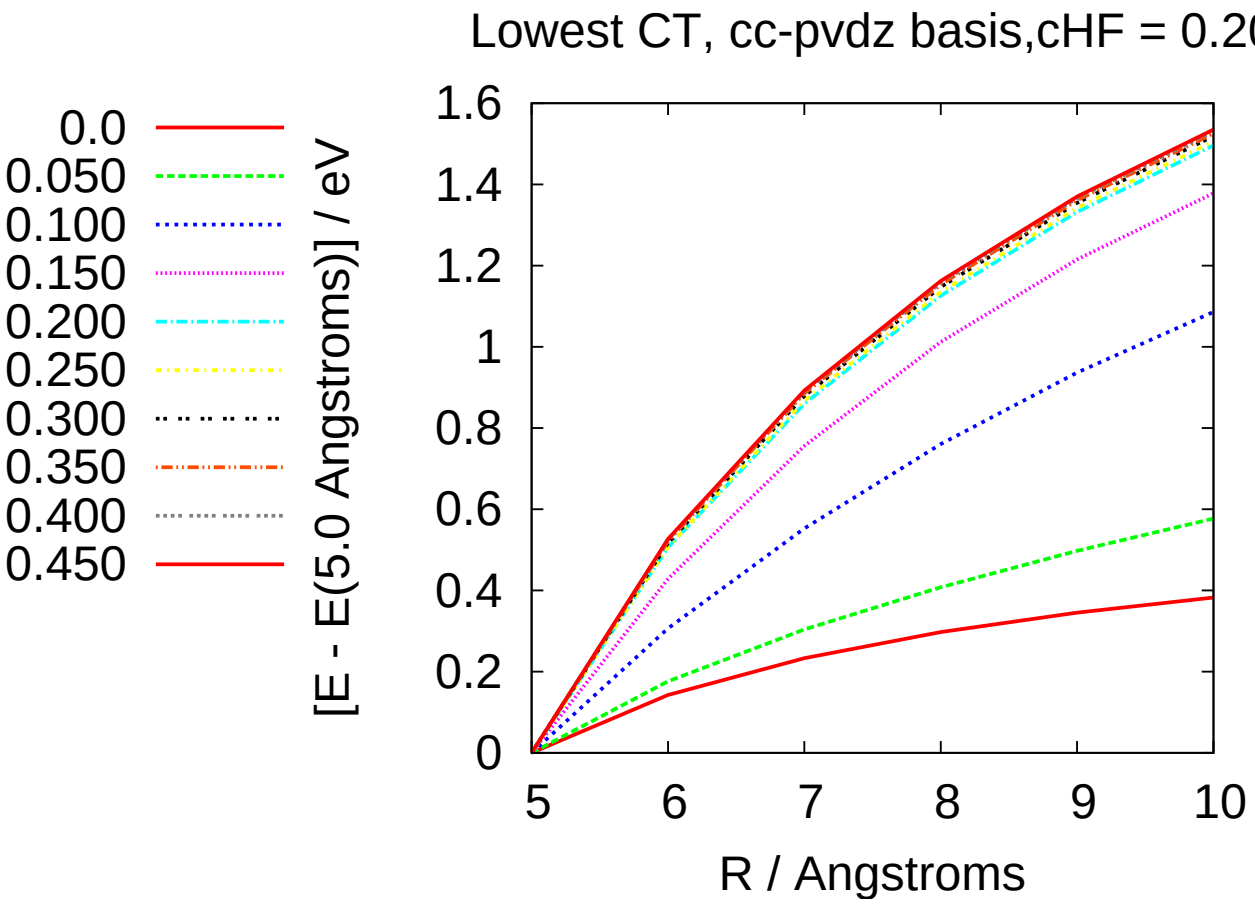

thymine, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8

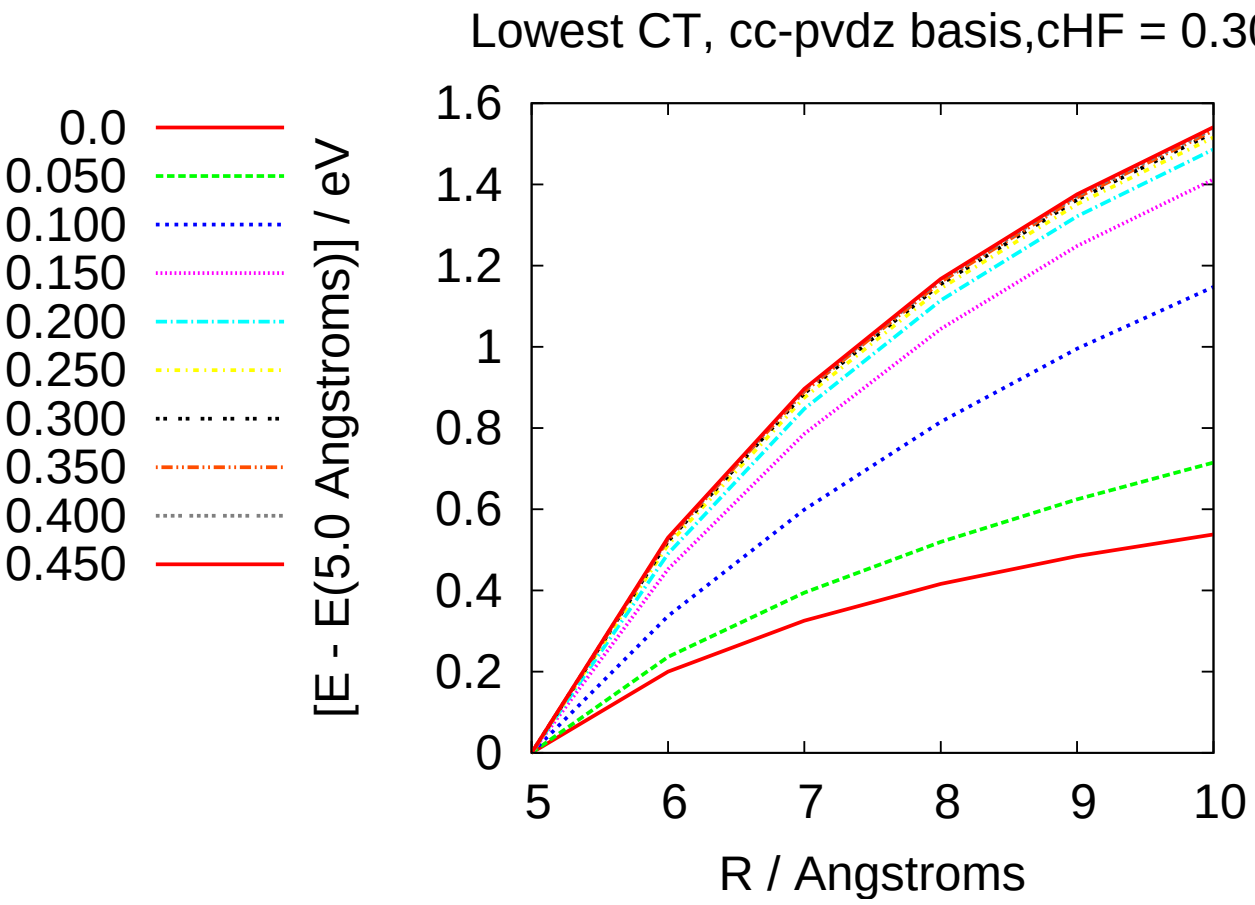

uracil, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
1APP
2Ap
7
6.5
6
5.5
5
4.5
4
3.5
0.0
0.2
0.4
0.6
0.8

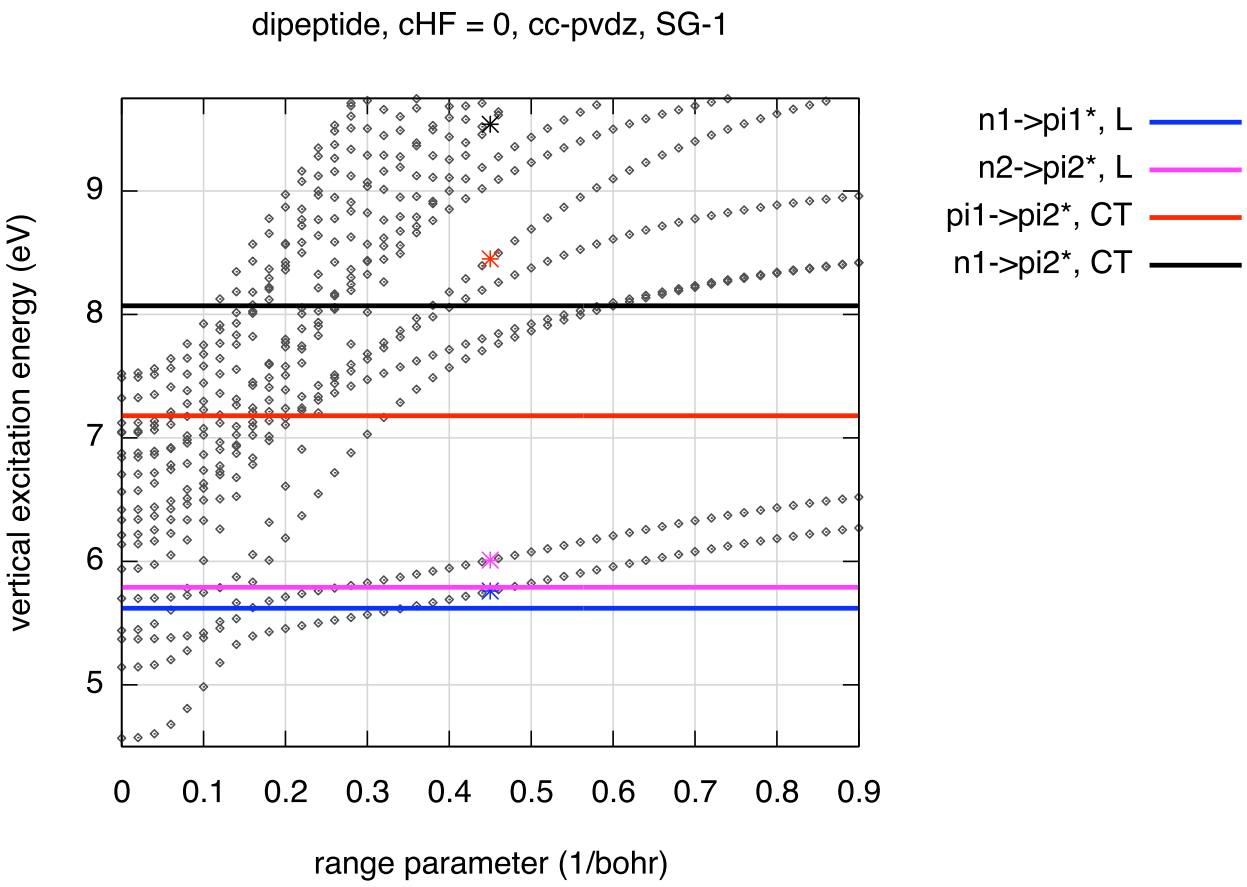

adenine, cHF = .30
vertical excitation energy (eV)
range parameter (1/bohr)
7
6.5
6
5.5
5
4.5
4
0.0
0.2
0.4
0.6
0.8
2Ap
3Ap
1APP

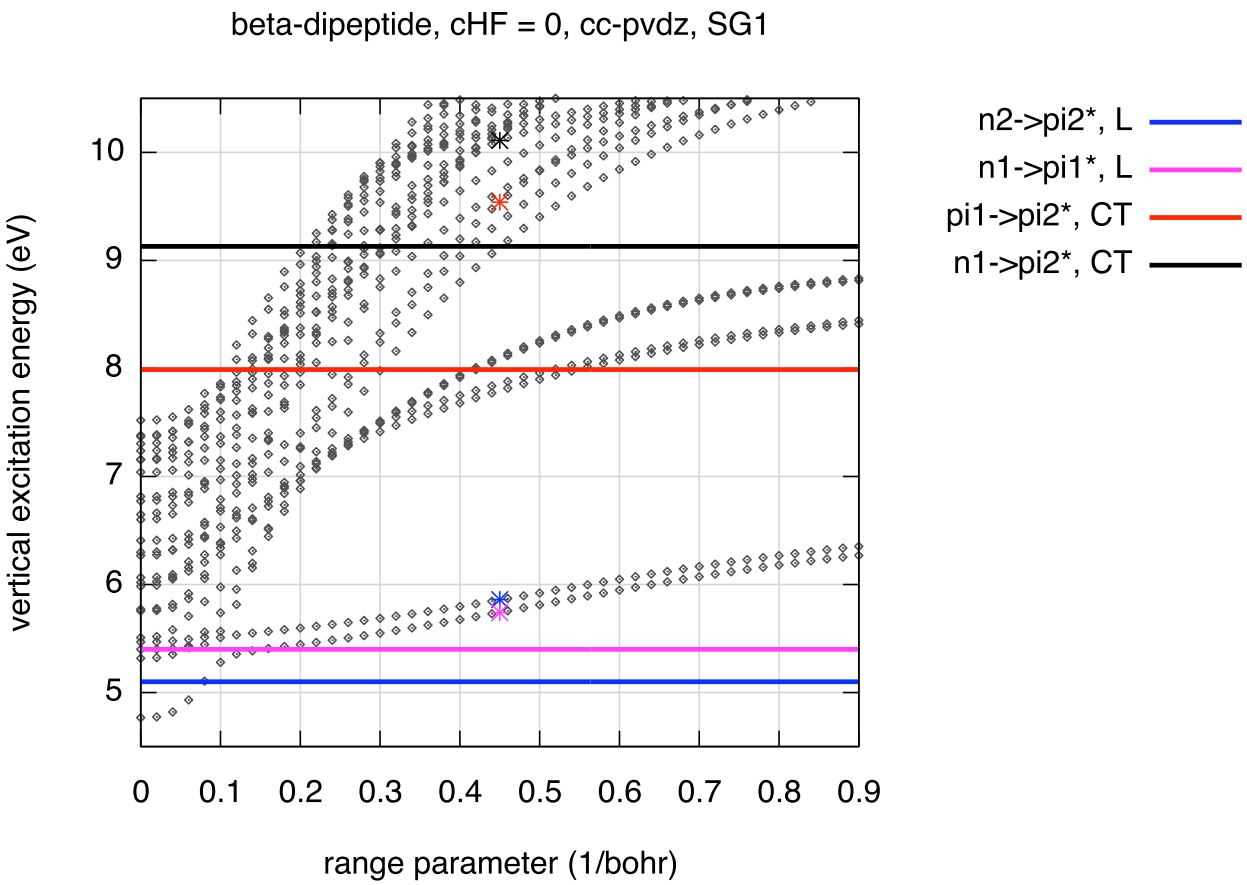

Lowest CT, cc-pvdz basis,cHF = 0.0
0.0
0.050
0.100
0.150
0.200
0.250
0.300
0.350
0.400
0.450
[E - E(5.0 Angstroms)] / eV
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
5
6
7
8
9
10
R / Angstroms

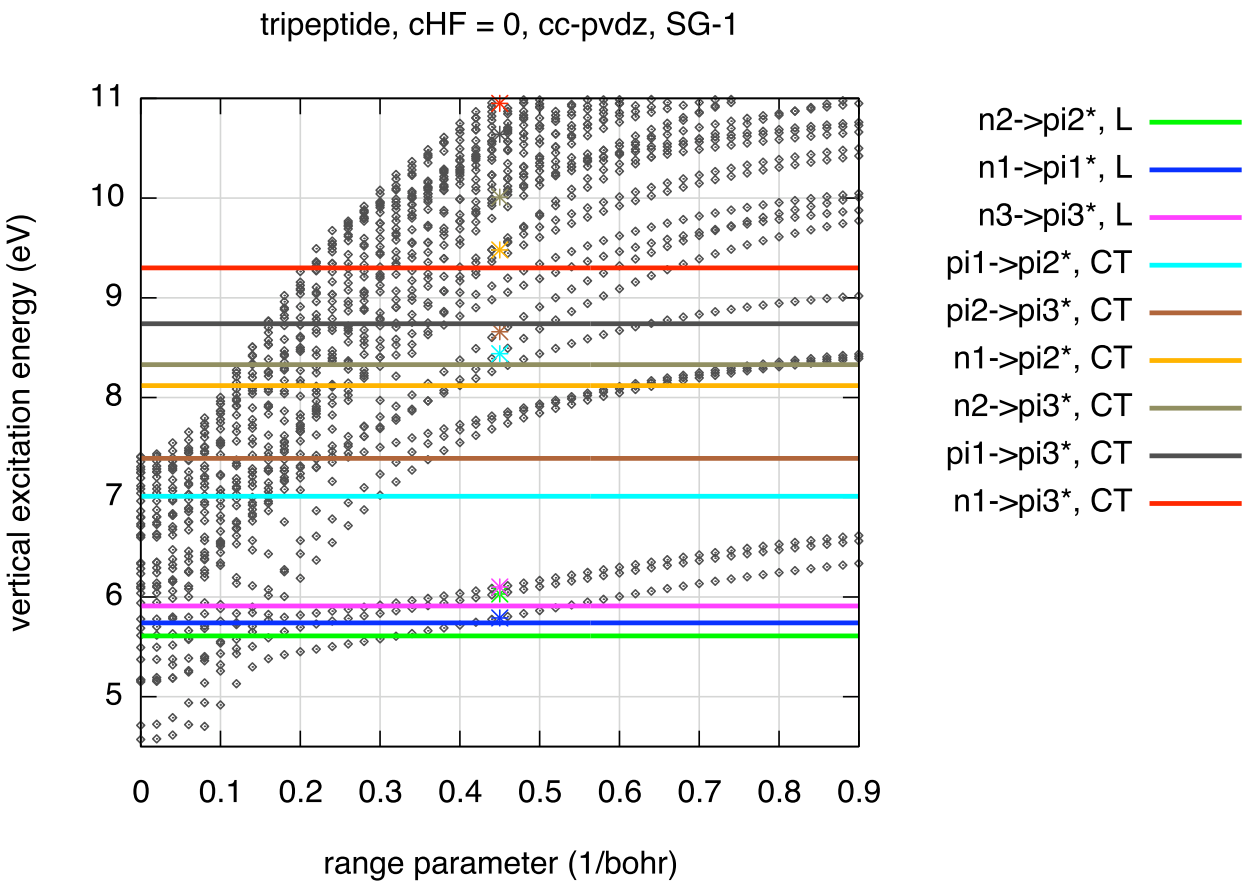

Lowest CT, cc-pvdz basis,cHF = 0.10
0.0
0.050
0.100
0.150
0.200
0.250
0.300
0.350
0.400
0.450
[E - E(5.0 Angstroms)] / eV
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
5
6
7
8
9
10
R / Angstroms

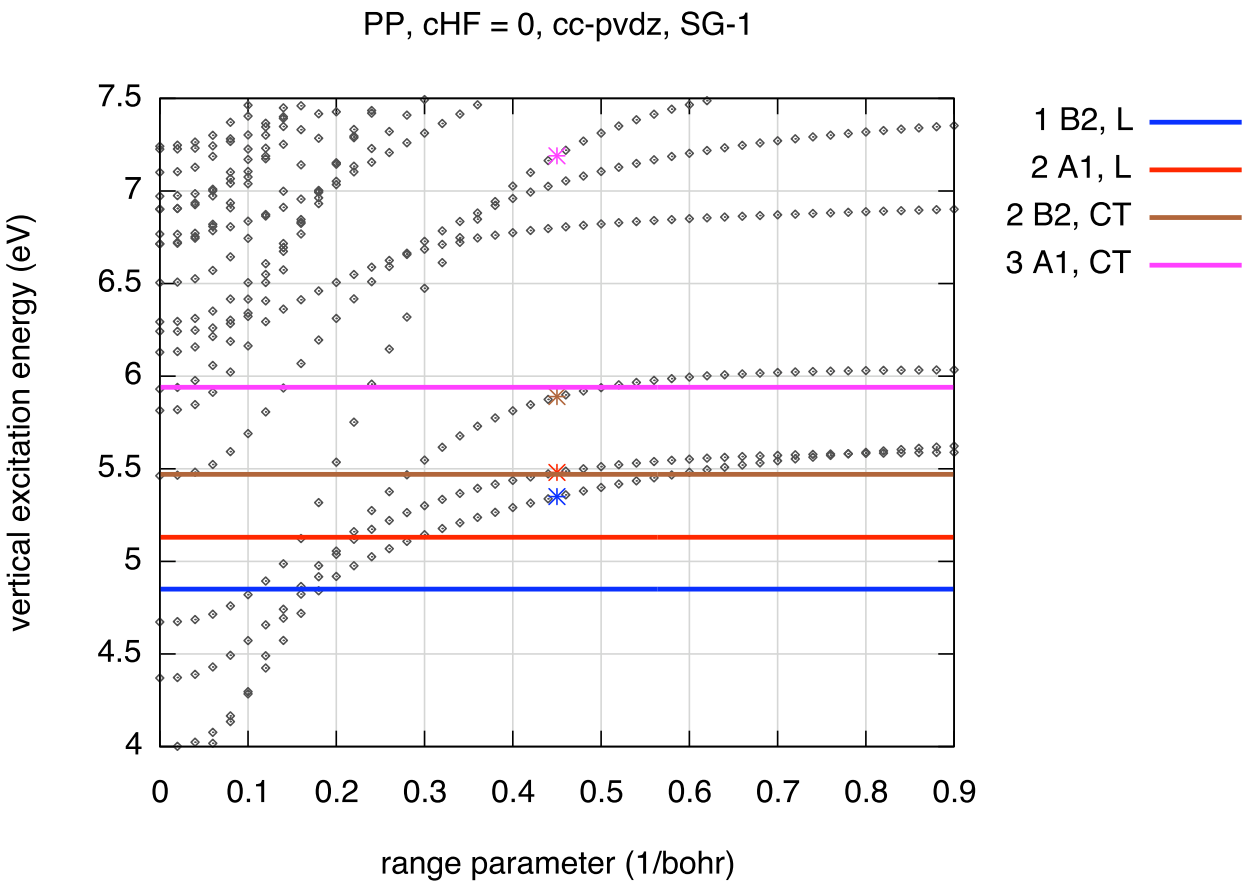

Lowest CT, cc-pvdz basis,cHF = 0.20
0.0
0.050
0.100
0.150
0.200
0.250
0.300
0.350
0.400
0.450
[E - E(5.0 Angstroms)] / eV
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
5
6
7
8
9
10
R / Angstroms

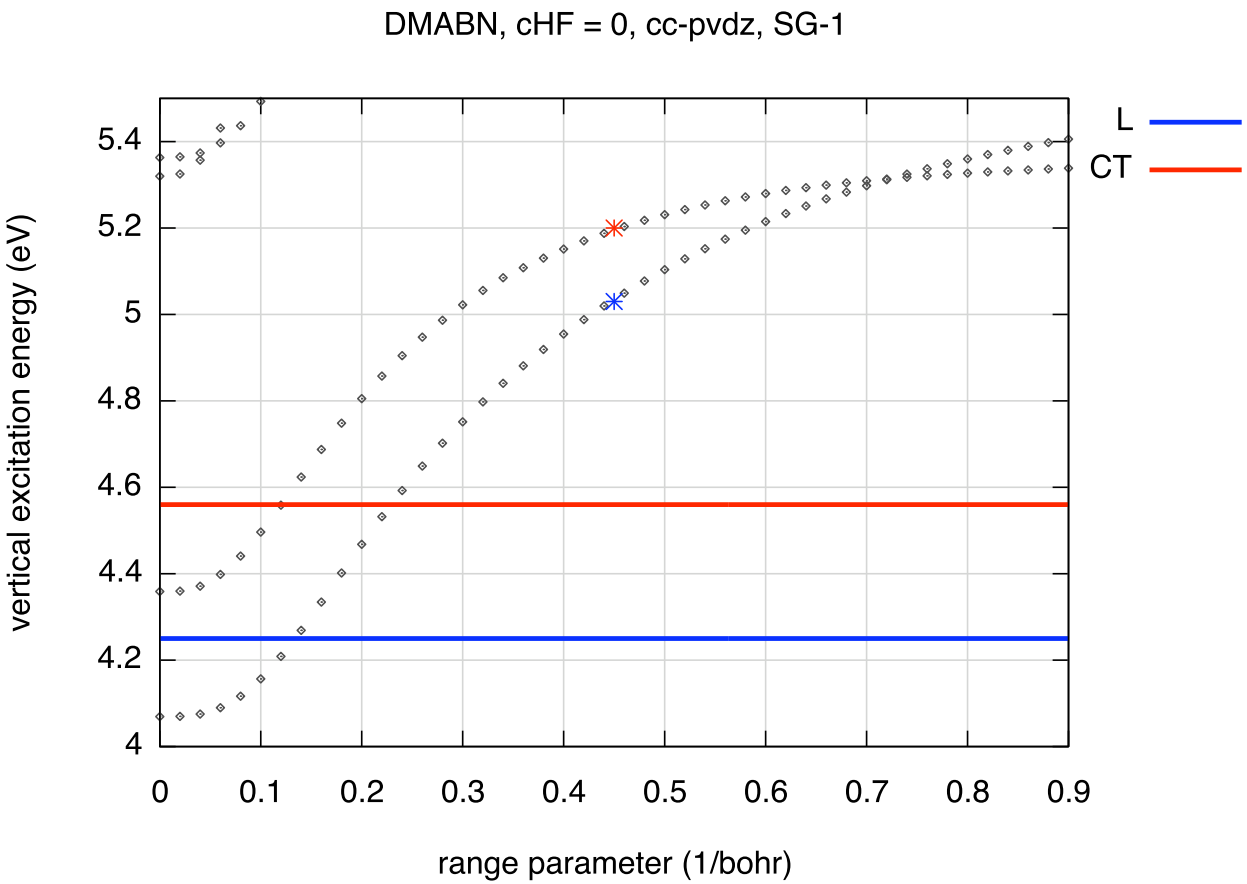

Lowest CT, cc-pvdz basis,cHF = 0.30
0.0
0.050
0.100
0.150
0.200
0.250
0.300
0.350
0.400
0.450
[E - E(5.0 Angstroms)] / eV
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
5
6
7
8
9
10
R / Angstroms


dipeptide, cHF = 0, cc-pvdz, SG-1
vertical excitation energy (eV)
range parameter (1/bohr)
5
6
7
8
9
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
n1->pi1*, L
n2->pi2*, L
pi1->pi2*, CT
n1->pi2*, CT


beta-dipeptide, cHF = 0, cc-pvdz, SG1
vertical excitation energy (eV)
range parameter (1/bohr)
10
9
8
7
6
5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
n2->pi2*, L
n1->pi1*, L
pi1->pi2*, CT
n1->pi2*, CT


tripeptide, cHF = 0, cc-pvdz, SG-1
vertical excitation energy (eV)
range parameter (1/bohr)
11
10
9
8
7
6
5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
n2->pi2*, L
n1->pi1*, L
n3->pi3*, L
pi1->pi2*, CT
pi2->pi3*, CT
n1->pi2*, CT
n2->pi3*, CT
pi1->pi3*, CT
n1->pi3*, CT


PP, cHF = 0, cc-pvdz, SG-1
vertical excitation energy (eV)
range parameter (1/bohr)
7.5
7
6.5
6
5.5
5
4.5
4
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1 B2, L
2 A1, L
2 B2, CT
3 A1, CT


DMABN, cHF = 0, cc-pvdz, SG-1
vertical excitation energy (eV)
range parameter (1/bohr)
L
CT
5.4
5.2
5
4.8
4.6
4.4
4.2
4
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9