

CBS extrapolation of Hartree-Fock energy: Pople and Dunning basis sets hand-to-hand on the endeavour

Supplementary Information

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Table 1 Relative HF-GE/CBS(bs₁,bs₂) energies (in kJ mol⁻¹) for the conformers of ACE-ALA- \mathcal{G} -ALA-NME with respect to the β_a one.^{a)}

| Method, (bs ₁ ,bs ₂) | \mathcal{G} = GLY | | | | | SER | | | | |
|---|---------------------|------------|--------|------------|---------|----------------|------------|--------|------------|---------|
| | $\beta_a^{b)}$ | α_R | PP-II | α_L | β | $\beta_a^{b)}$ | α_R | PP-II | α_L | β |
| MINI | 0 | 10.98 | 4.62 | 6.37 | 15.93 | 0 | 7.73 | 9.89 | -2.93 | 15.79 |
| MINI-s | 0 | 13.54 | 4.60 | 6.93 | 6.98 | 0 | 15.33 | 11.47 | -3.81 | 9.79 |
| MIDI | 0 | 8.57 | 29.92 | 3.59 | 19.10 | 0 | 14.58 | 37.47 | -2.88 | 15.49 |
| MIDI! | 0 | -12.63 | -4.03 | -14.82 | 16.27 | 0 | -5.33 | 3.97 | -16.70 | 12.56 |
| 3-21G | 0 | 4.90 | 27.68 | 0.69 | 20.16 | 0 | 8.47 | 35.77 | -5.67 | 18.24 |
| 3-21++G | 0 | 16.43 | 32.30 | 22.42 | 15.49 | 0 | 17.20 | 40.56 | 14.49 | 13.50 |
| STO-6G | 0 | -7.33 | -21.84 | -8.29 | 2.95 | 0 | -8.52 | -22.34 | -11.58 | 2.63 |
| 3-21GSP | 0 | 6.61 | 17.46 | 5.31 | 9.18 | 0 | 13.03 | 27.41 | 4.26 | 19.71 |
| 4-22GSP | 0 | 15.95 | 6.82 | 14.49 | 16.56 | 0 | 12.54 | 12.52 | 4.42 | 17.58 |
| 4-31G | 0 | 29.79 | 28.73 | 35.17 | 15.84 | 0 | 32.18 | 37.07 | 30.51 | 16.29 |
| (STO-2G,VDZ) | 0 | 17.63 | 1.78 | 21.39 | 11.32 | 0 | 19.41 | 7.73 | 19.11 | 11.38 |
| (STO-2G,AVDZ) | 0 | 28.78 | 3.39 | 37.44 | 11.38 | 0 | 29.24 | 10.56 | 35.53 | 10.93 |
| (STO-2G,VTZ) | 0 | 30.17 | 5.45 | 38.63 | 11.62 | 0 | 31.01 | 12.15 | 37.57 | 11.41 |
| (STO-2G,AVTZ) | 0 | 33.39 | 6.50 | 42.75 | 11.79 | 0 | 33.62 | 13.53 | 41.23 | 11.09 |
| (STO-2G,VQZ) | 0 | 33.53 | 6.45 | 42.70 | 11.69 | 0 | 33.90 | 13.31 | 41.42 | 11.07 |
| (STO-2G,AVQZ) | 0 | 34.52 | 6.83 | 43.86 | 11.75 | 0 | 34.77 | 13.86 | 42.40 | 11.06 |
| (STO-2G,V5Z) | 0 | 34.64 | 6.80 | 43.96 | 11.72 | 0 | 34.90 | 13.84 | 42.54 | 11.04 |
| (VDZ,VTZ) | 0 | 25.96 | 4.17 | 32.84 | 11.51 | 0 | 27.12 | 10.62 | 31.38 | 11.40 |
| (AVDZ,AVTZ) | 0 | 31.70 | 5.26 | 40.83 | 11.62 | 0 | 32.02 | 12.36 | 39.18 | 11.02 |
| (VTZ,VQZ) | 0 | 31.94 | 5.96 | 40.78 | 11.66 | 0 | 32.54 | 12.74 | 39.62 | 11.24 |
| (AVTZ,AVQZ) | 0 | 34.01 | 6.67 | 43.38 | 11.76 | 0 | 34.25 | 13.70 | 41.90 | 11.08 |
| (VQZ,V5Z) | 0 | 34.11 | 6.63 | 43.37 | 11.70 | 0 | 34.42 | 13.57 | 42.01 | 11.06 |
| 3-param ^{c)} | 0 | 34.63 | 6.76 | 43.93 | 11.70 | 0 | 34.90 | 13.79 | 42.52 | 11.04 |
| other ^{d)} | 0 | 34.6 | 6.8 | 44.0 | 11.7 | 0 | 34.8 | 13.7 | 42.6 | 11.0 |

^{a)}The convergence threshold criterion for all SCF steps was rather strict warranting a convergence up to $10^{-8} E_h$ for all systems but β_a and β GLY-conformers where it is only $10^{-7} E_h$ after 60 iterations. ^{b)}Assumed as reference. ^{c)}This work CBS extrapolation with three adjustable parameters, (STO-2G,VQZ,V5Z): see text. ^{d)}CBS extrapolation¹ from (VQZ,V5Z) using CBS scheme of Halkier *et al.*^{2,3}

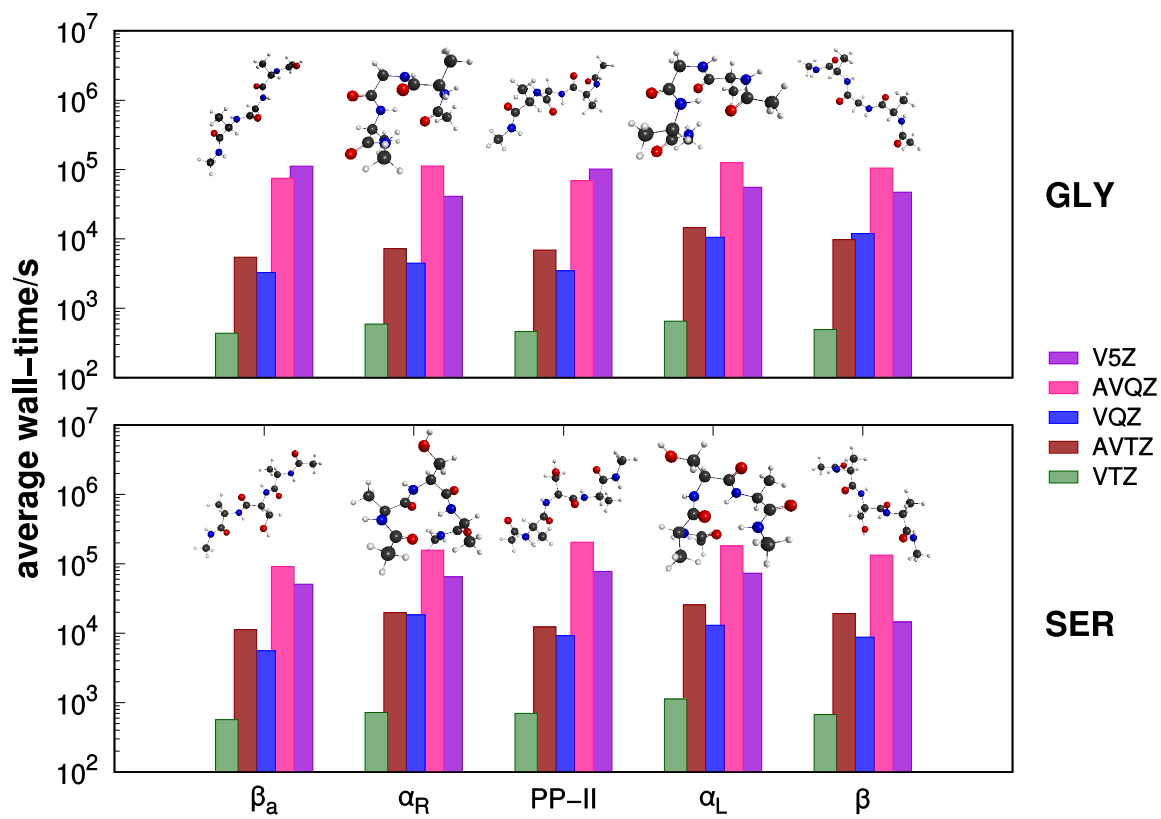


Figure 1 Wall times (in logarithmic scale) for all conformers of TS-10 with TZ, QZ and 5Z basis sets.

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Notes and references

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