Isomerization of bicyclo[1.1.0]butane by means of the diffusion quantum Monte Carlo method: Supporting information

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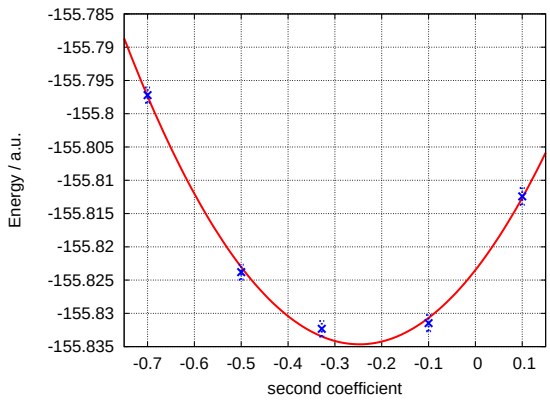

Figure 1: DMC energy optimization for con_TS.

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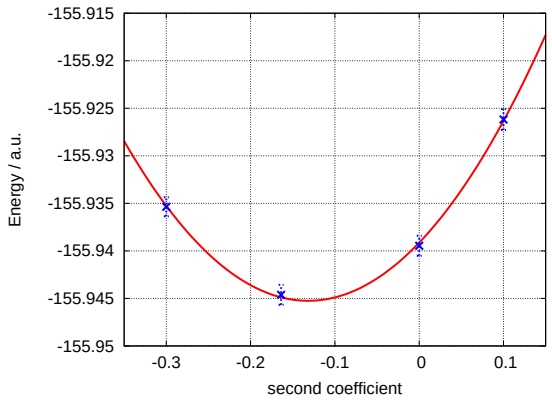

Figure 2: DMC energy optimization for *g*-but.

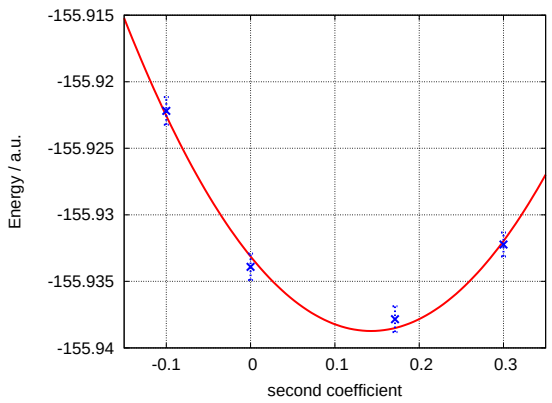

Figure 3: DMC energy optimization for *gt*-TS.

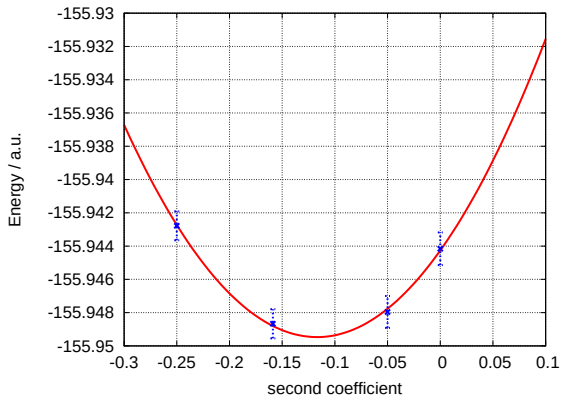

Figure 4: DMC energy optimization for *t*-but.

Table 1: Comparison of the coefficients before and after the optimization. OMR2-DMC refers to the DMC energy obtained by using the CASSCF(10,10) coefficients, OMR3-DMC refers to the DMC energy obtained by using the optimized coefficients. The last column shows the percental changing of the coefficients.

Molecule	$c^{(CASSCF)}$	OMR2-DMC	$c^{(opt)}$	OMR3-DMC	$c_{\%}$
con_TS	-0.328	-155.8331(8)	-0.248	-155.8365(8)	24
dis_TS	-0.573 -0.513	-155.8045(7)	-0.645 -0.592	-155.8041(7)	13 16
g-but	-0.164	-155.9421(7)	-0.132	-155.9437(7)	20
gt-TS	0.171	-155.9384(6)	0.143	-155.9382(6)	18
t-but	-0.159	-155.9474(7)	-0.117	-155.9480(7)	26