Estimating relative disulfide energies: an accurate ab initio PES

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Appendix 1: Contour plots of slices through the M05-2X/6-31G(d) 3D-PES for diethyl disulfide. $\chi_3$ values are: (a) 60°, (b) 70°, (c) 80°, (d) 90°, (e) 100°, (f) 110°, (g) 120°. The horizontal and vertical axes show $\chi_2$ and $\chi_2'$. Due to the symmetry of the system, any specific labelling would be arbitrary. Energies, in kJ mol$^{-1}$, are relative to the absolute minimum.
Appendix 2: Contour plots of slices through the M06-2X/6-31G(d) 3D-PES for diethyl disulfide. \( \chi_3 \) values are: (a) 70º, (b) 80º, (c) 90º, (d) 100º. The horizontal and vertical axes show \( \chi_2 \) and \( \chi_2' \). Due to the symmetry of the system, any specific labelling would be arbitrary. Energies, in kJ mol\(^{-1} \), are relative to the absolute minimum.