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Estimating relative disulfide energies: an accurate ab initio PES

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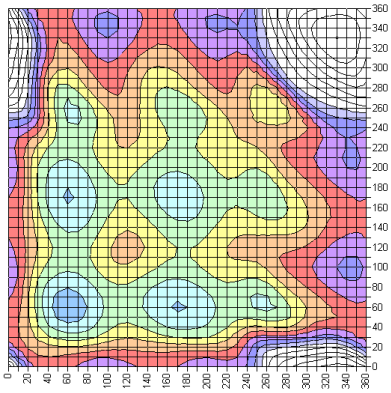
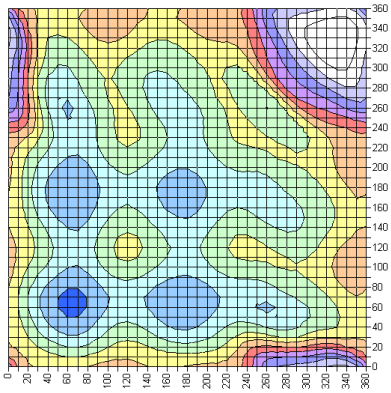
Appendix 1: Contour plots of slices through the M05-2X/6-31G(d) 3D-PES for diethyl disulfide. χ_3 values are: (a) 60º, (b) 70º, (c) 80º, (d) 90º, (e) 100º, (f) 110º, (g) 120º. The horizontal and vertical axes show χ_2 and χ_2'. Due to the symmetry of the system, any specific labelling would be arbitrary. Energies, in kJ mol^{-1}, are relative to the absolute minimum.

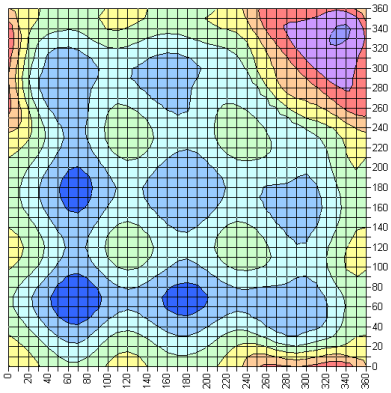
(a)



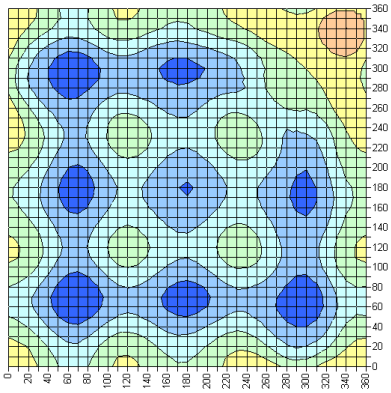
(b)



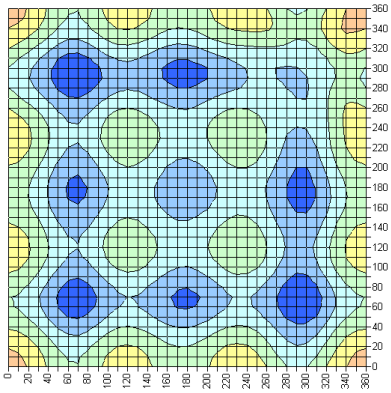
(c)



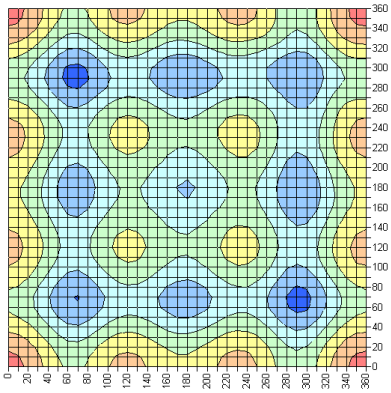
(d)



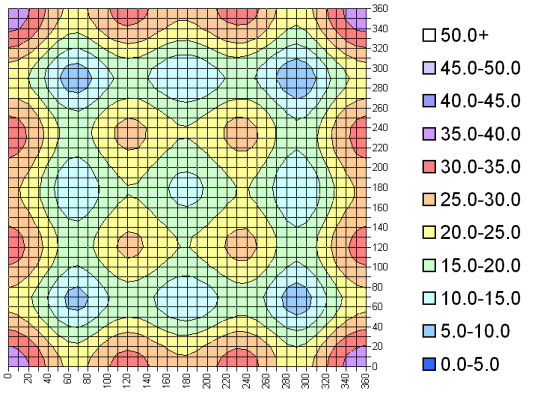
(e)



(f)



(g)



Appendix 2: Contour plots of slices through the M06-2X/6-31G(d) 3D-PES for diethyl disulfide. χ_3 values are: (a) 70º, (b) 80º, (c) 90º, (d) 100º. The horizontal and vertical axes show χ_2 and χ_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.