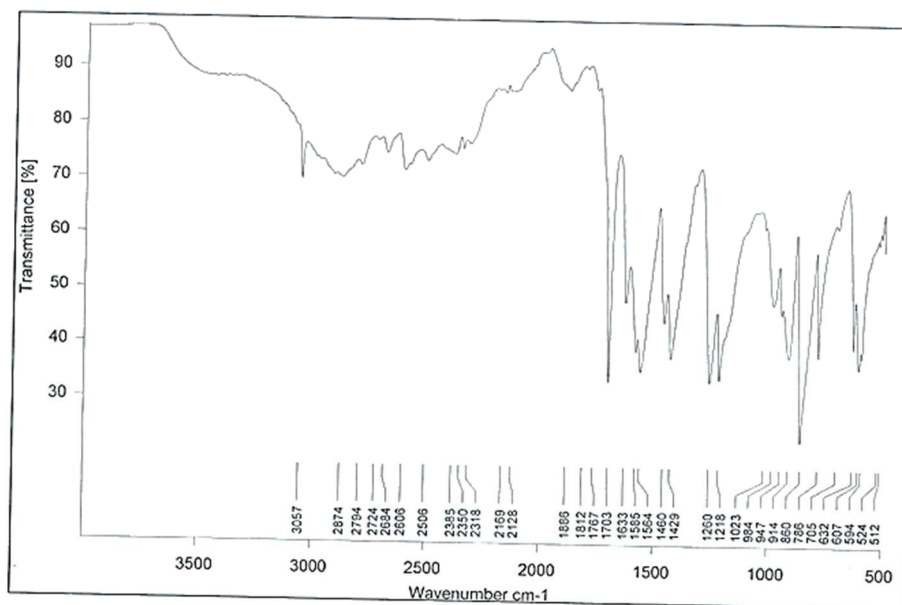
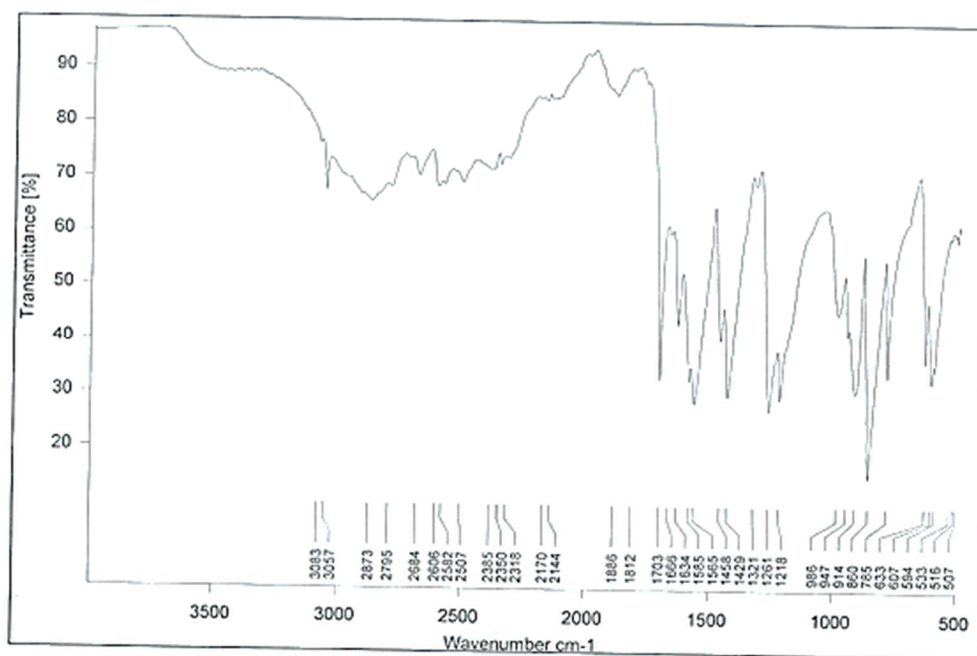


Supplementary Data

A. FT-IR



(A)



(B)

Fig. S1: (A) and (B) shows the FTIR spectra of TCDA derivative (6) and (6').

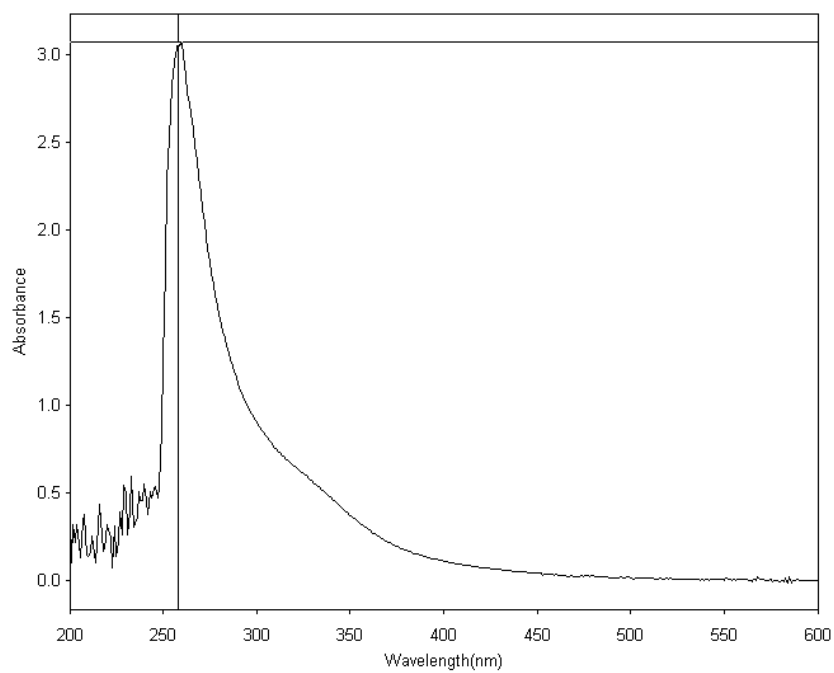
(6)

FT-IR (KBr, ν_{max} , cm^{-1}): 1886, 1767 (C=O, asym. and sym. stretch of anhydride), 1634, 1585 (C=C aromatic), 1218, 1260 (C-O-C anhydride), 3057 (C-H aromatic), 2874 (C-H aliphatic).

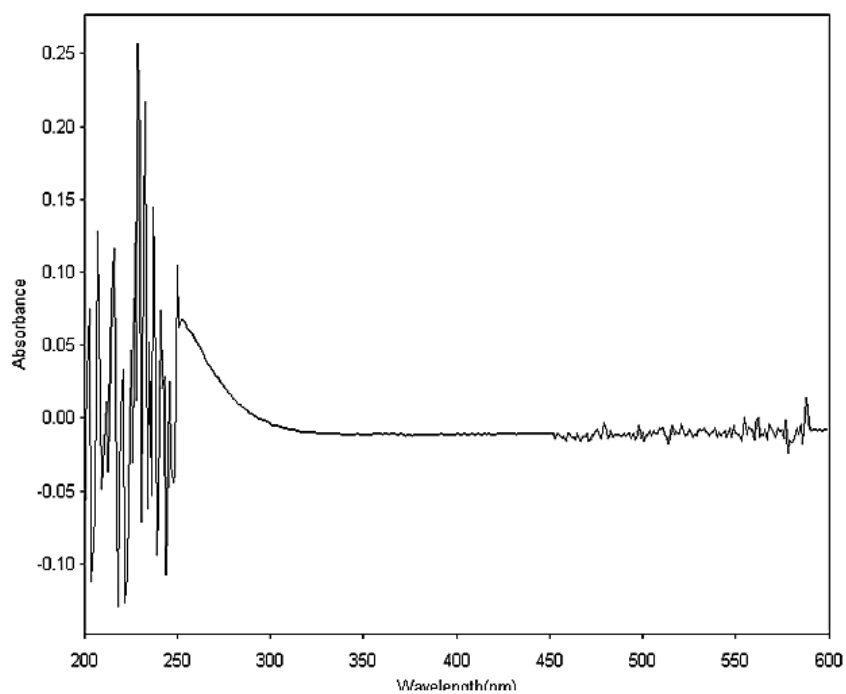
(6')

FT-IR (KBr, ν_{max} , cm^{-1}): 1886, 1767 (C=O, asym. and sym. stretch of anhydride), 1218, 1261 (C-O-C anhydride), 2873 (C-H aliphatic).

B. UV-Vis



(A)



(B)

Fig. S2: shows the UV-Vis spectra of TCDA (6) in (A) and TCDA (6') in (B)

(6)

$\lambda_{\text{max}} = 258.00 \text{ nm}$

$A = 3.073$

$\epsilon_{\text{max}} = 7682.5 \text{ L mol}^{-1} \text{ cm}^{-1}$

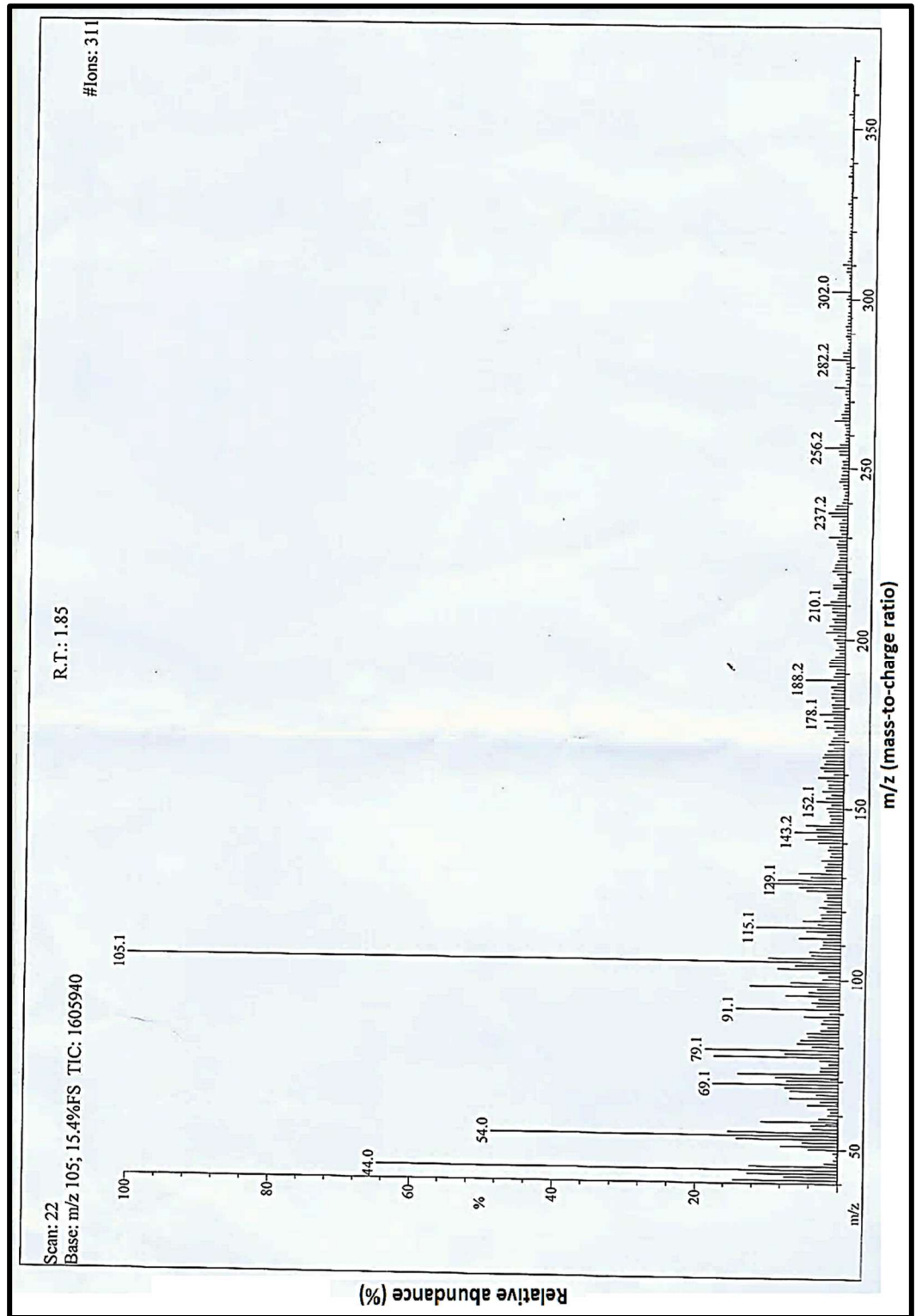
(6')

$\lambda_{\text{max}} = 253.00 \text{ nm}$

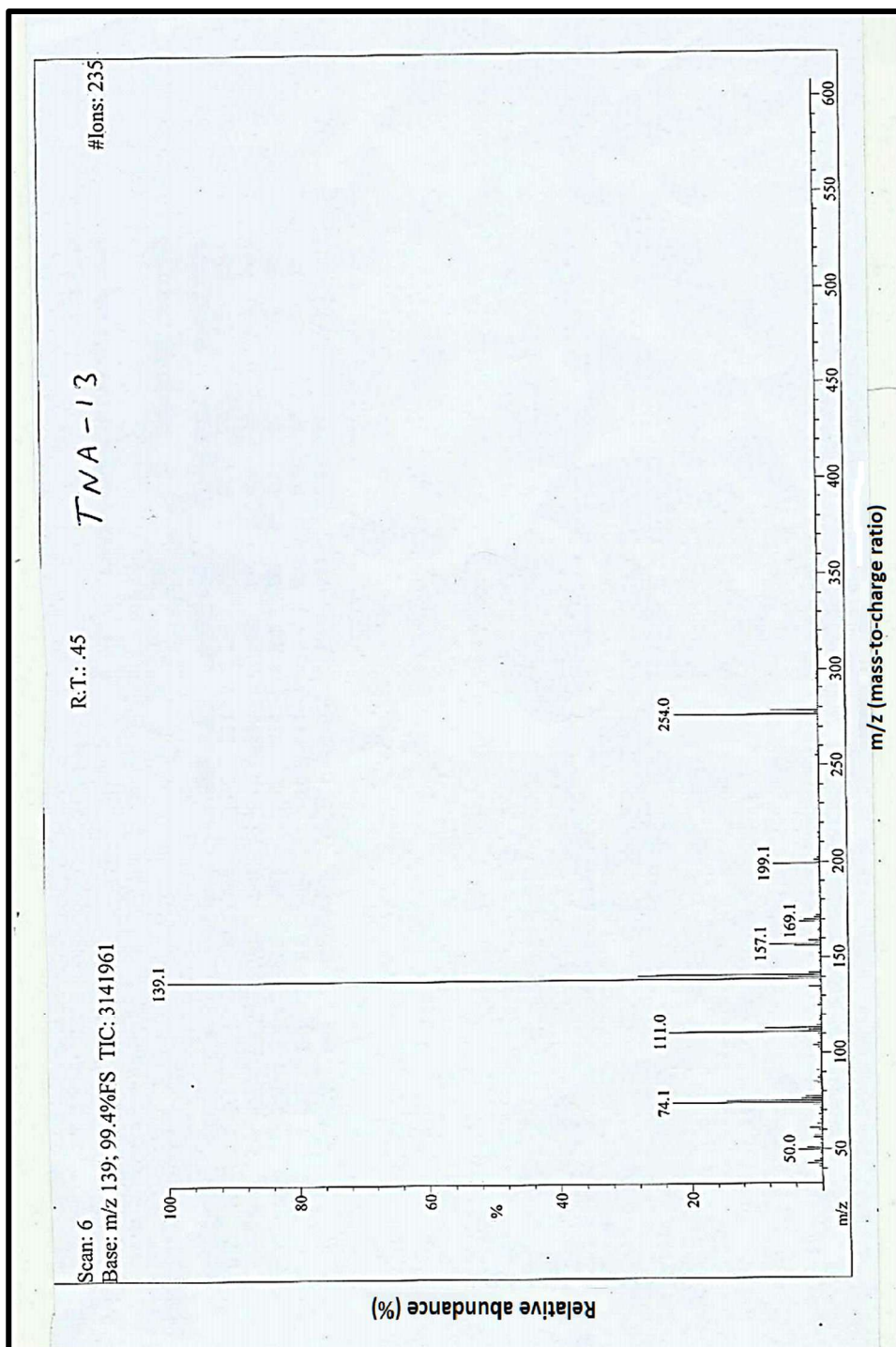
$A = 0.067$

$\epsilon_{\text{max}} = 167.5 \text{ L mol}^{-1} \text{ cm}^{-1}$

C. EI-MS

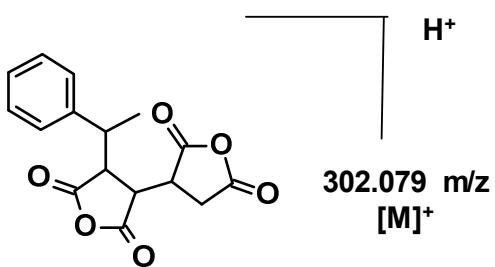


(A)

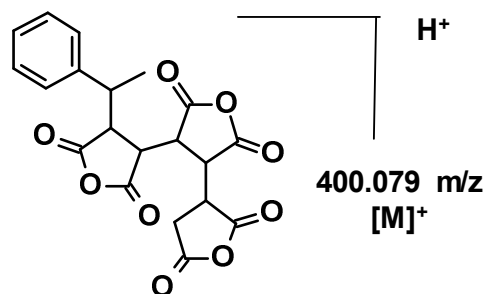


(B)

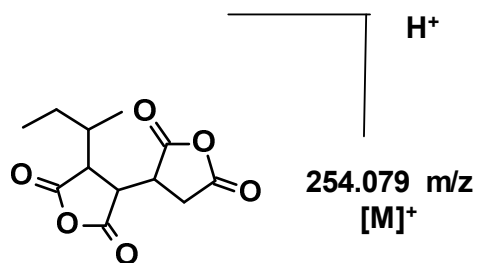
Fig. S3: (A) shows the EI MS spectra of (6) 302.079 m/z $[M]^+$, while (B) shows the EI MS spectra of (6') 254.079 $[M]$.



TCDA (6)



Hexacarboxylic tryanhydride peak was also shown in TCDA (6) MS



TCDA (6')

Fig. S4: $[M]^+$ of TCDA (6) (left), hexacarboxylic acid anhydride (right) and TCDA (6') at bottom.

D. RELAXED POTENTIAL ENERGY SURFACE SCANS

6a(RRRR)

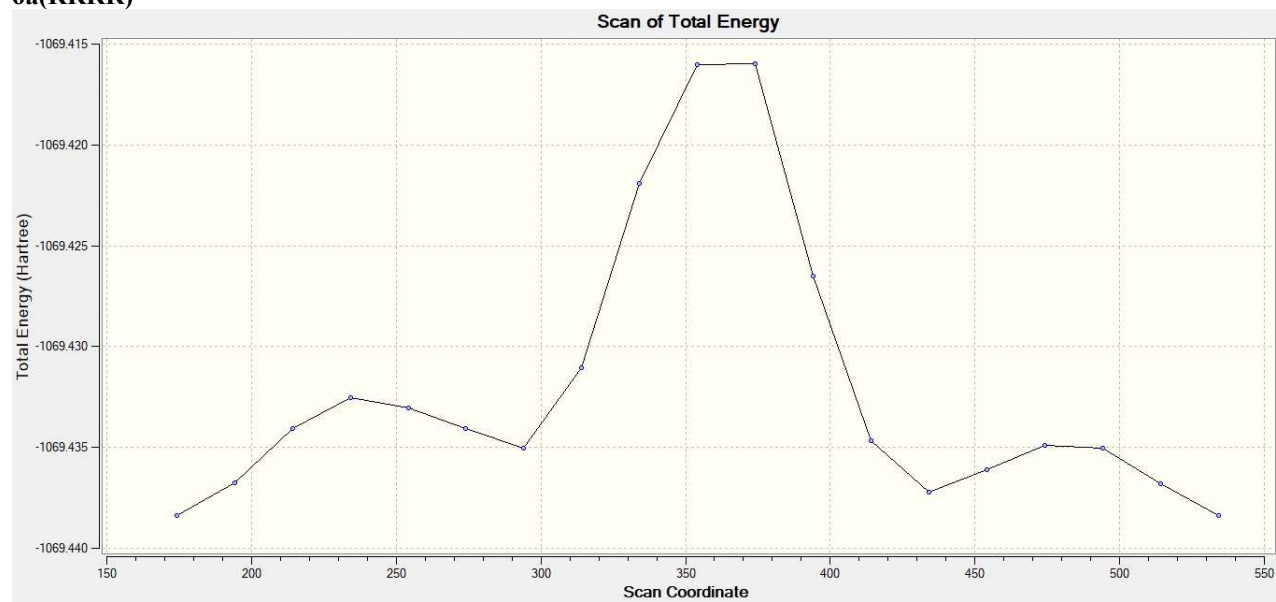


Fig. S5: Relaxed potential energy surface scan (PESS) of 6a(RRRR).

6b(SSSS)

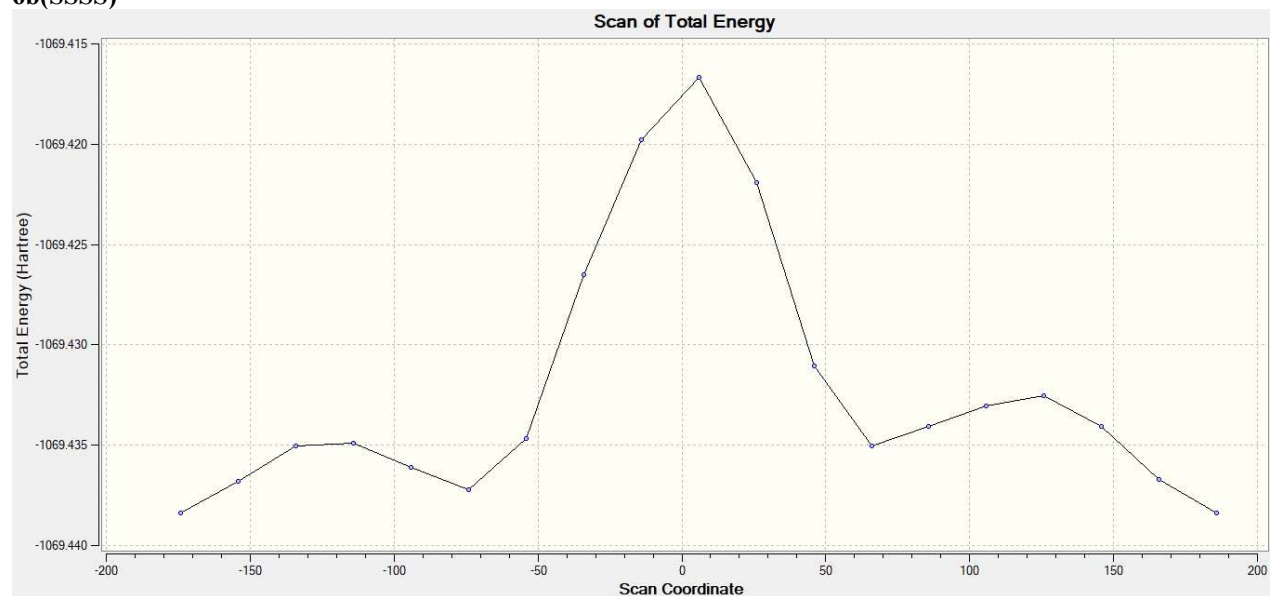


Fig. S6: Relaxed potential energy surface scan (PESS) of 6b(SSSS).

6c(RRRS)

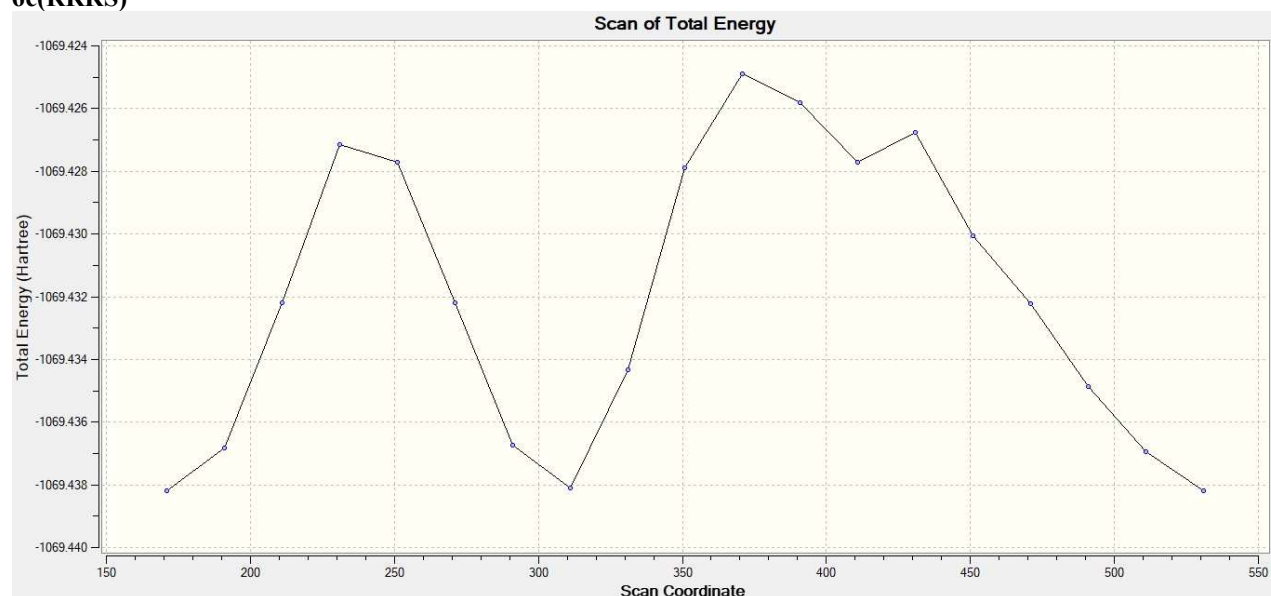


Fig. S7: Relaxed potential energy surface scan (PESS) of 6c(RRRS).

6d(SSSR)

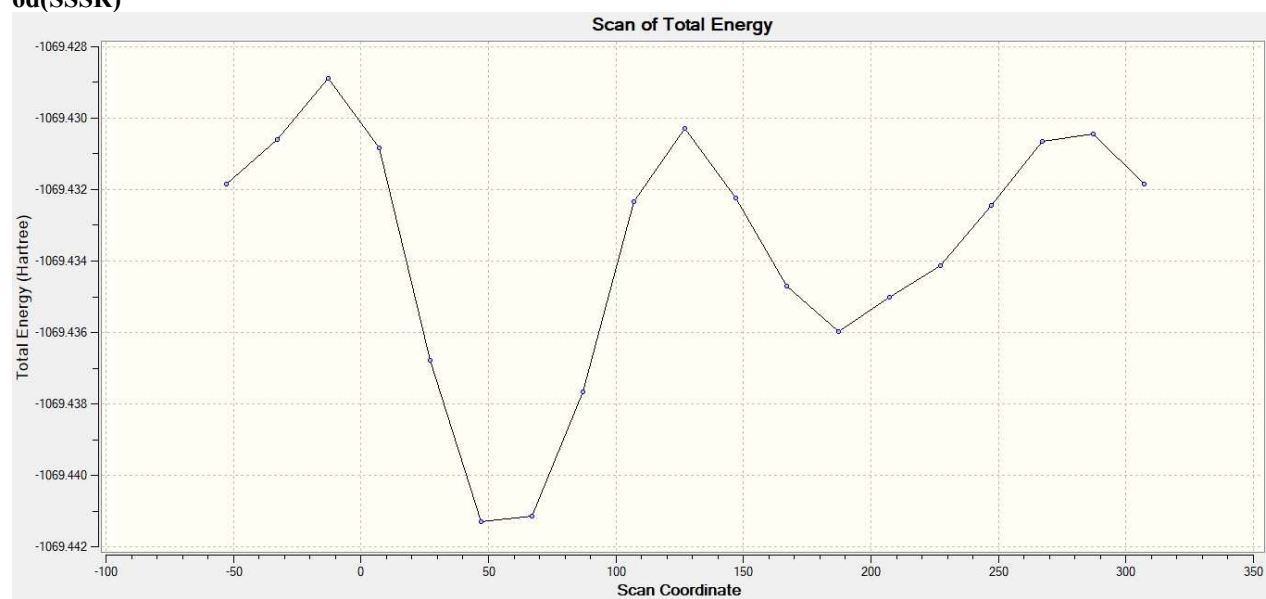


Fig. S8: Relaxed potential energy surface scan (PESS) of 6d(SSSR).

6e(RSSS)

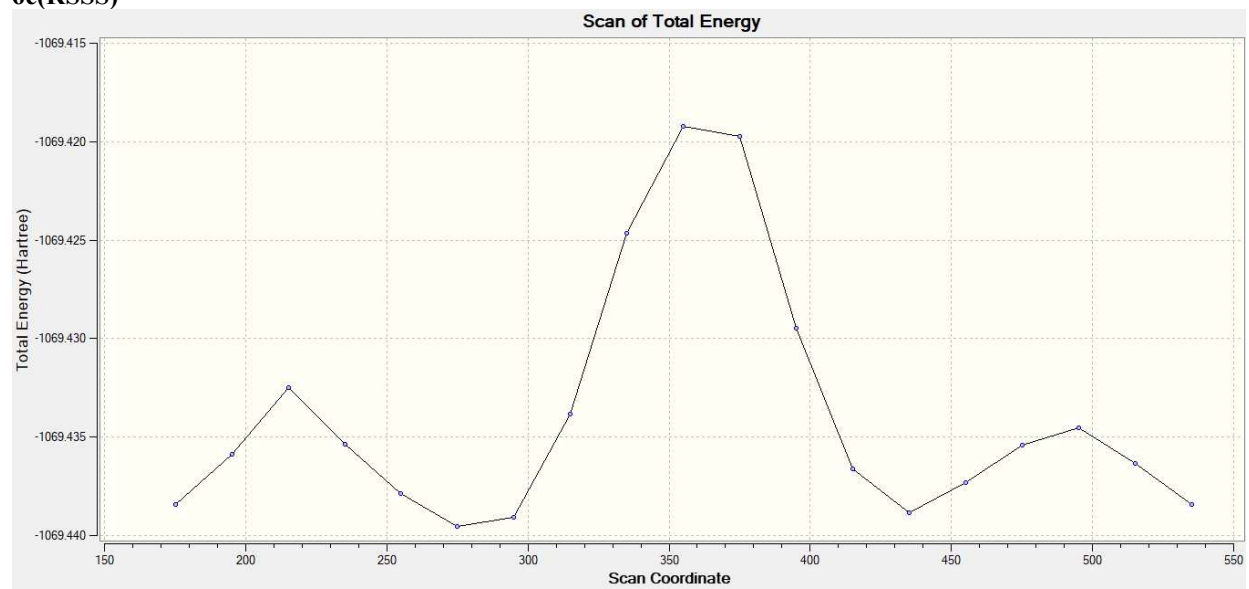


Fig. S9: Relaxed potential energy surface scan (PESS) of 6e(RSSS).

6f(SRRR)

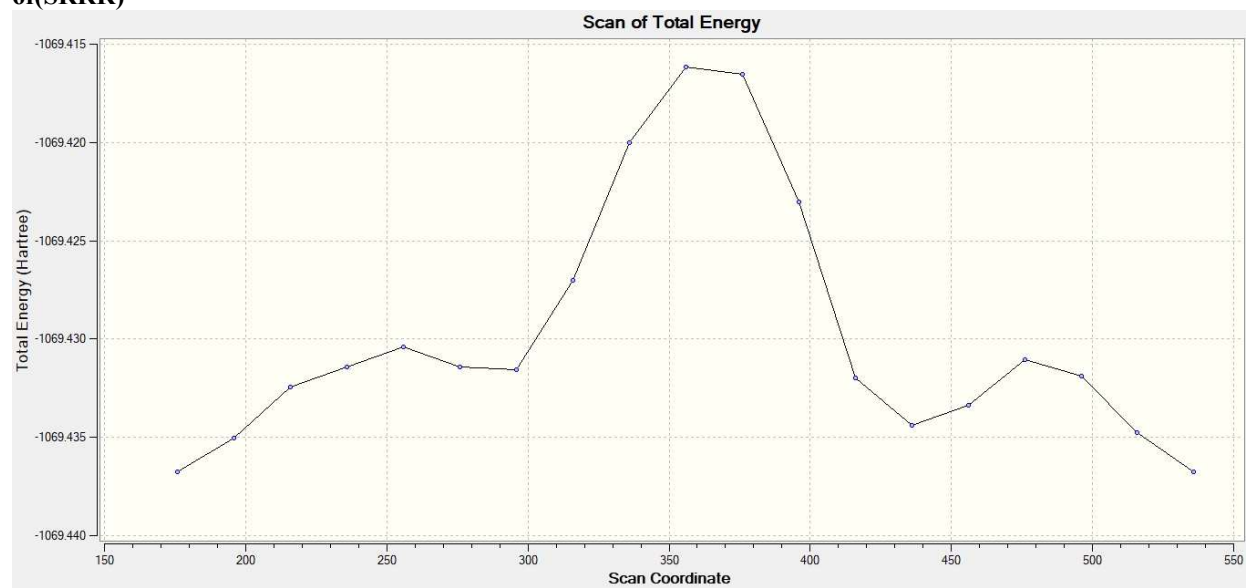


Fig. S10: Relaxed potential energy surface scan (PESS) of 6f(SRRR).

6g(RRSS)

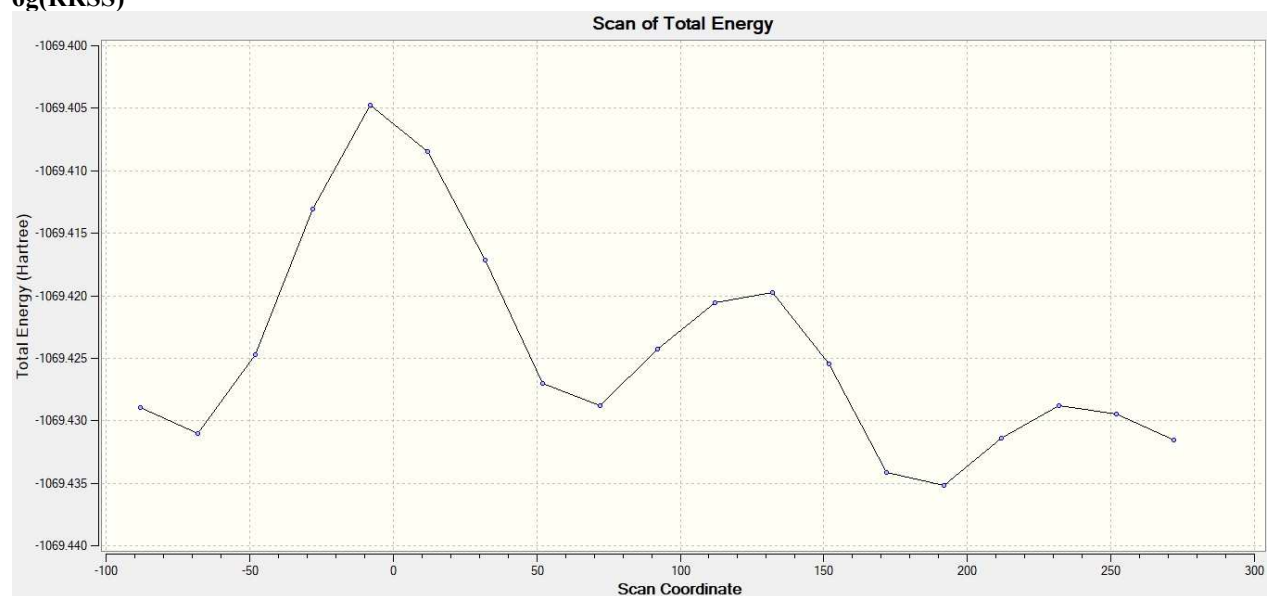


Fig. S11: Relaxed potential energy surface scan (PESS) of 6g(RRSS).

6h(SSRR)

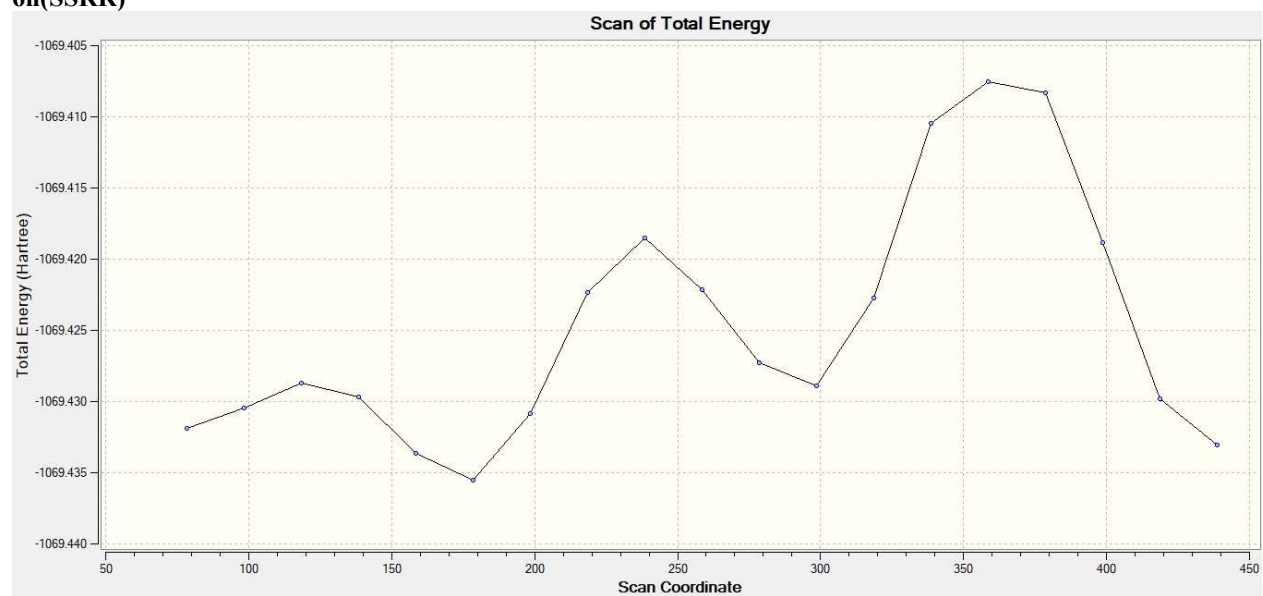


Fig. S12: Relaxed potential energy surface scan (PESS) of 6h(SSRR).

6i(RSRR)

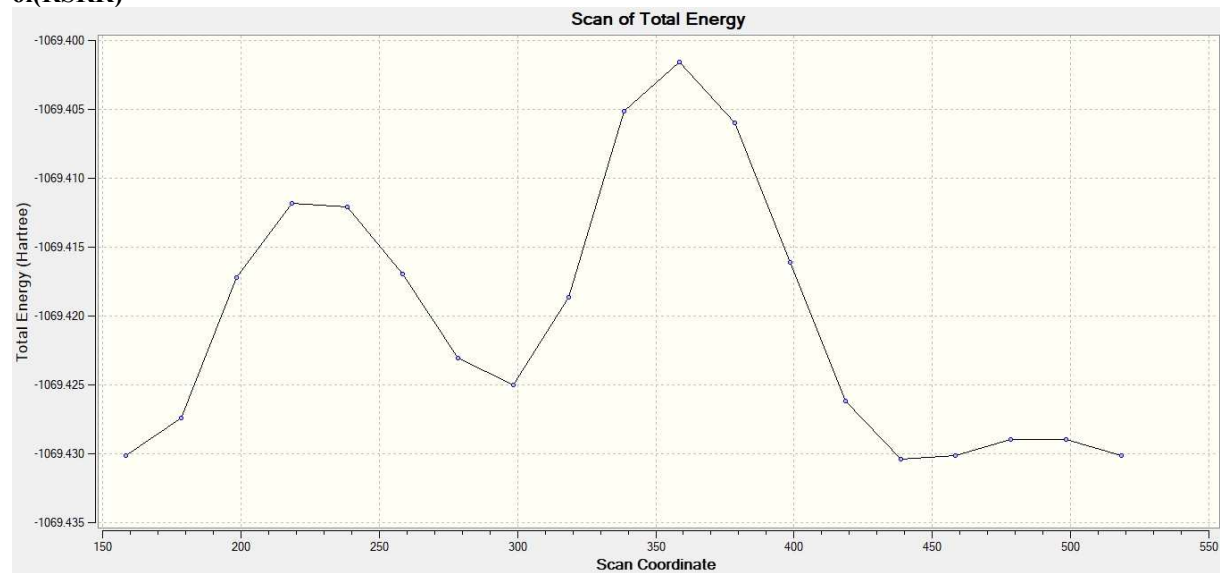


Fig. S13: Relaxed potential energy surface scan (PESS) of 6i(RSRR).

6j(SRSS)

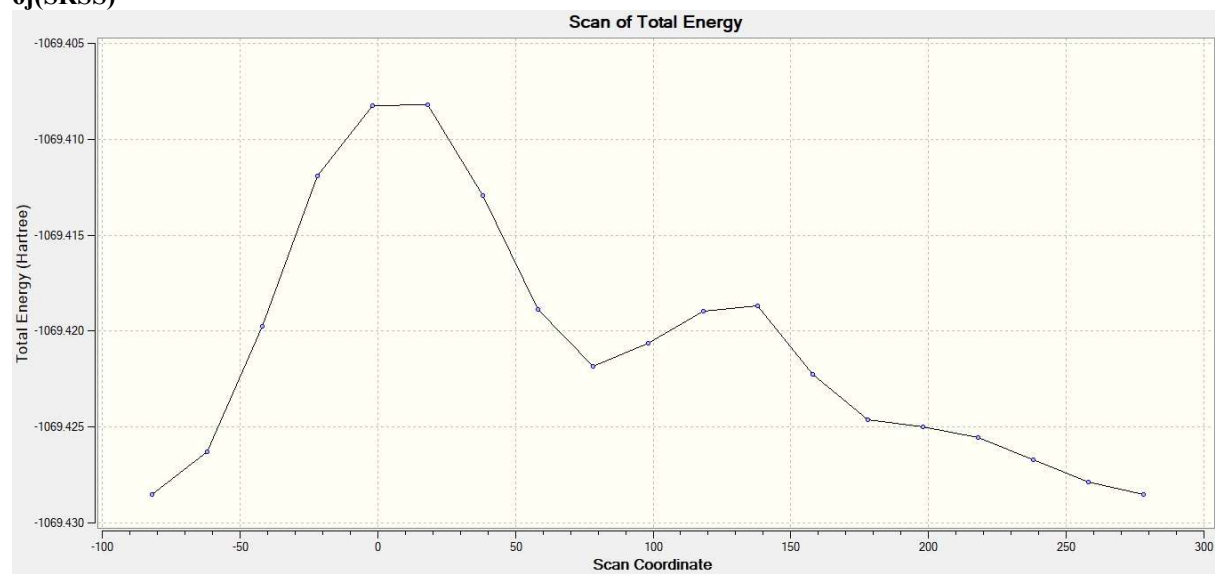


Fig. S14: Relaxed potential energy surface scan (PESS) of 6j(SRSS).

6k(RSSR)

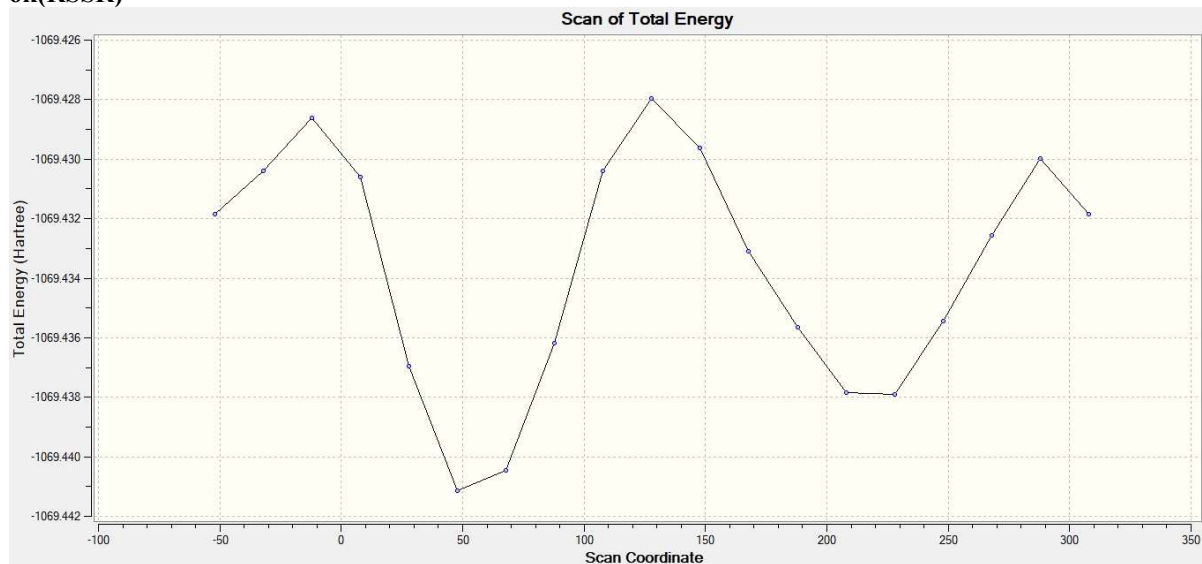


Fig. S15: Relaxed potential energy surface scan (PESS) of 6k(RSSR).

6l(SRRS)

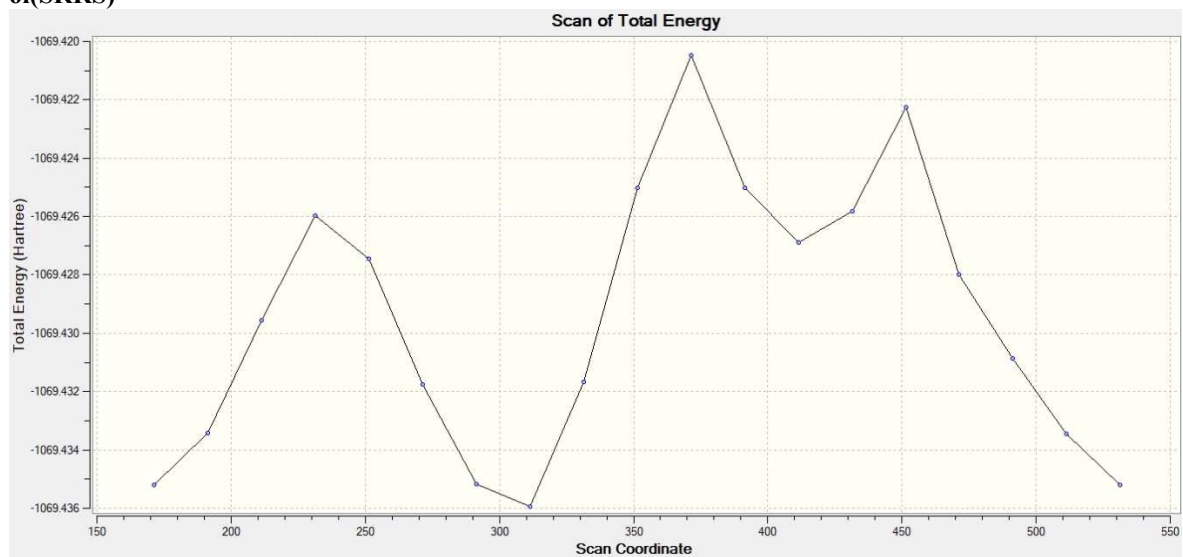


Fig. S16: Relaxed potential energy surface scan (PESS) of 6l(SRRS).

6m(RRSR)

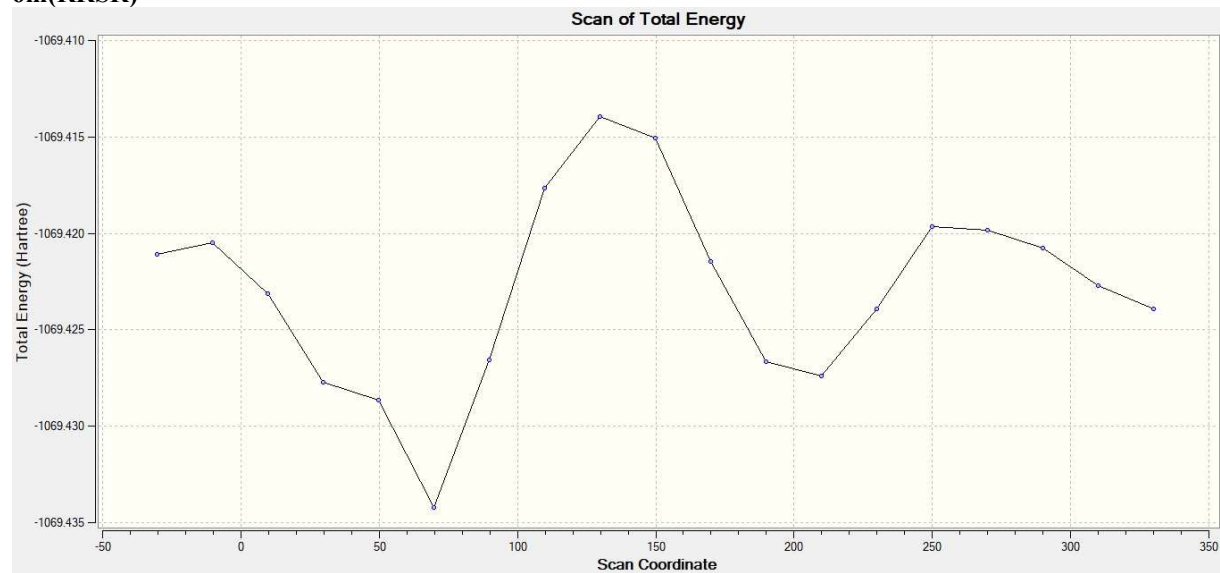


Fig. S17: Relaxed potential energy surface scan (PESS) of 6m(RRSR).

6n(SSRS)

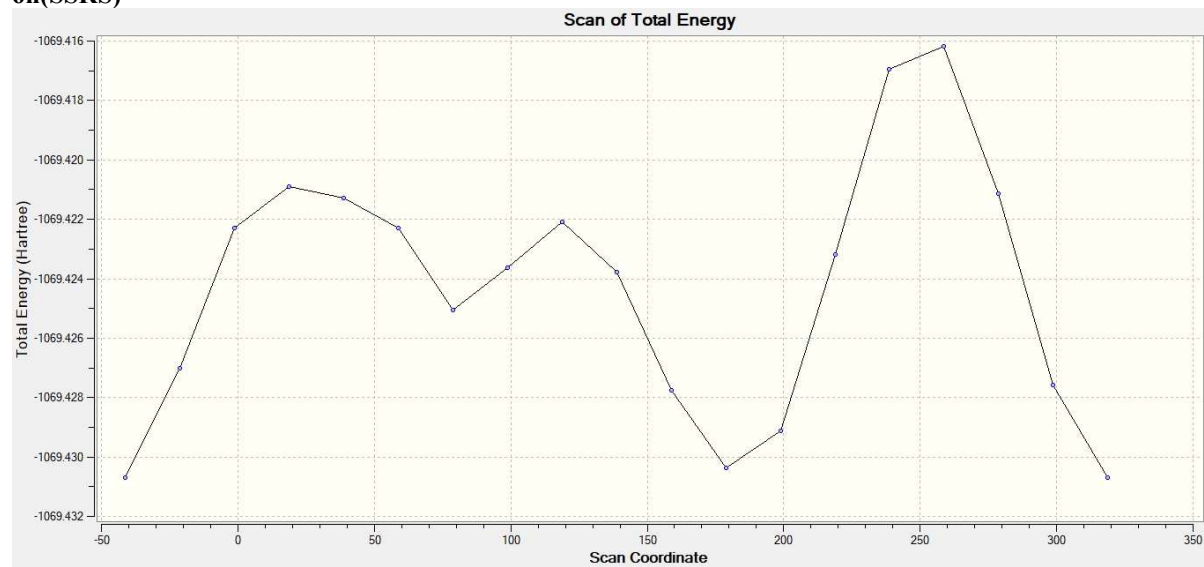


Fig. S18: Relaxed potential energy surface scan (PESS) of 6n(SSRS).

6o(RSRS)

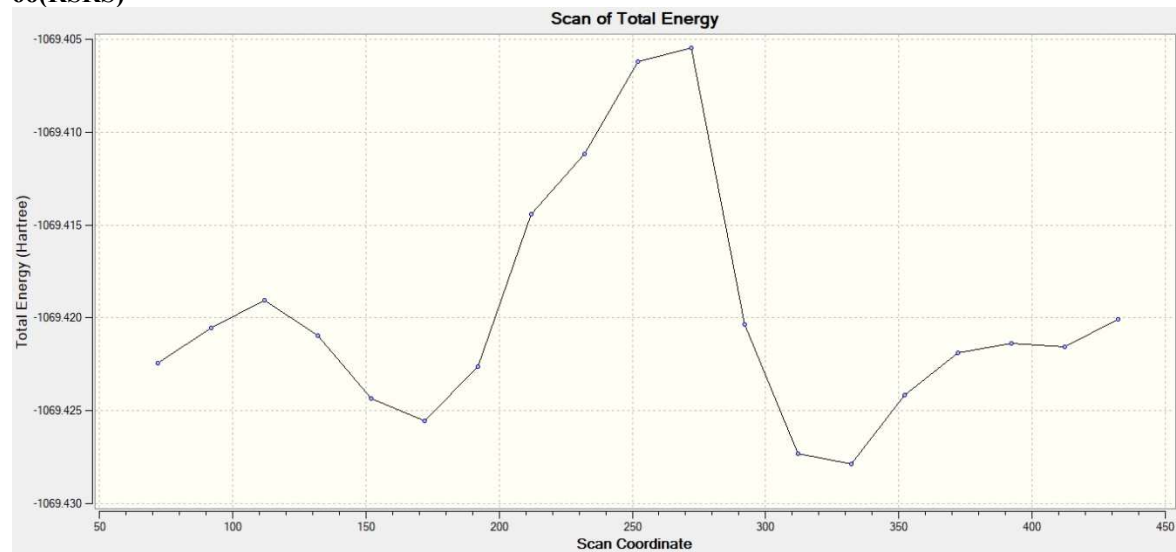


Fig. S19: Relaxed potential energy surface scan (PESS) of 6o(RSRS).

6p(SRSR)

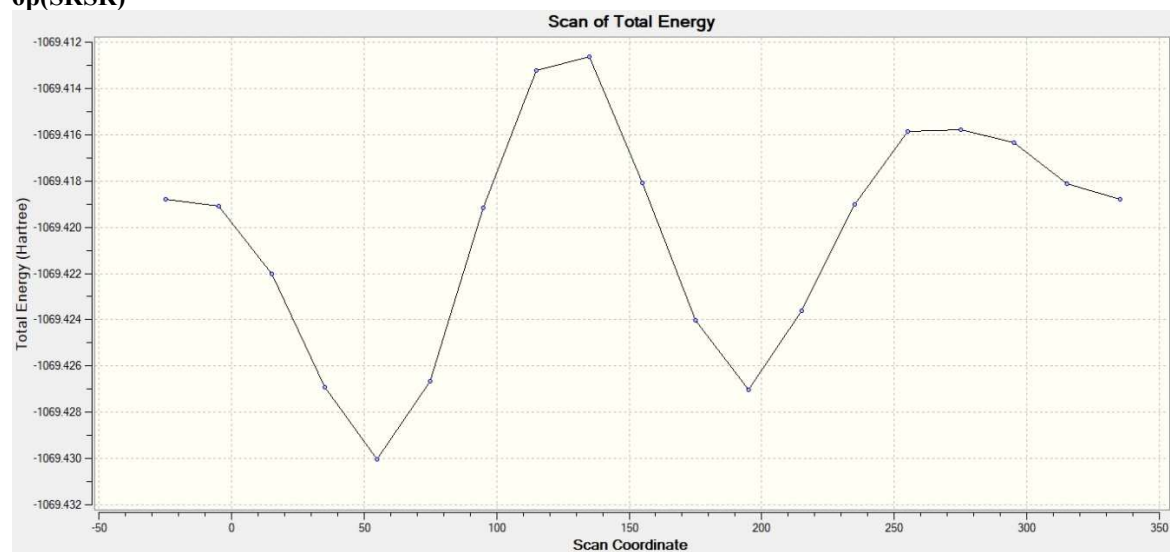


Fig. S20: Relaxed potential energy surface scan (PESS) of 6p(SRSR).

E. DIHEDRAL ANGLES (θ_a)

6a(RRRR)

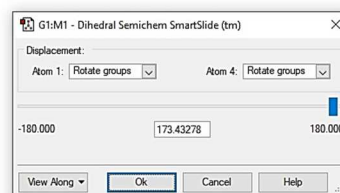
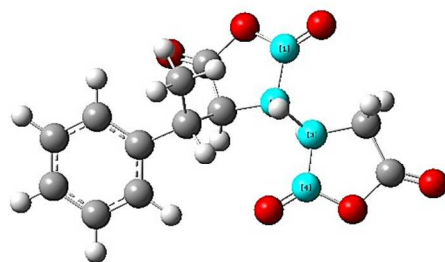


Fig. S21: Dihedral angle of (θ_a) of 6a(RRRR).

6b(SSSS)

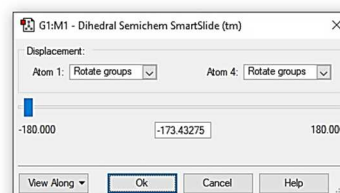
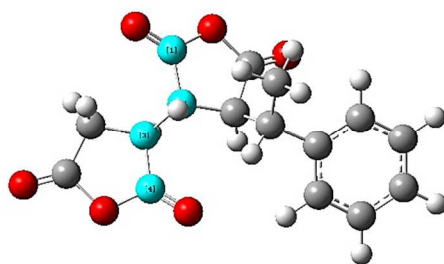


Fig. S22: Dihedral angle of (θ_a) of 6b(SSSS).

6c(RRRS)

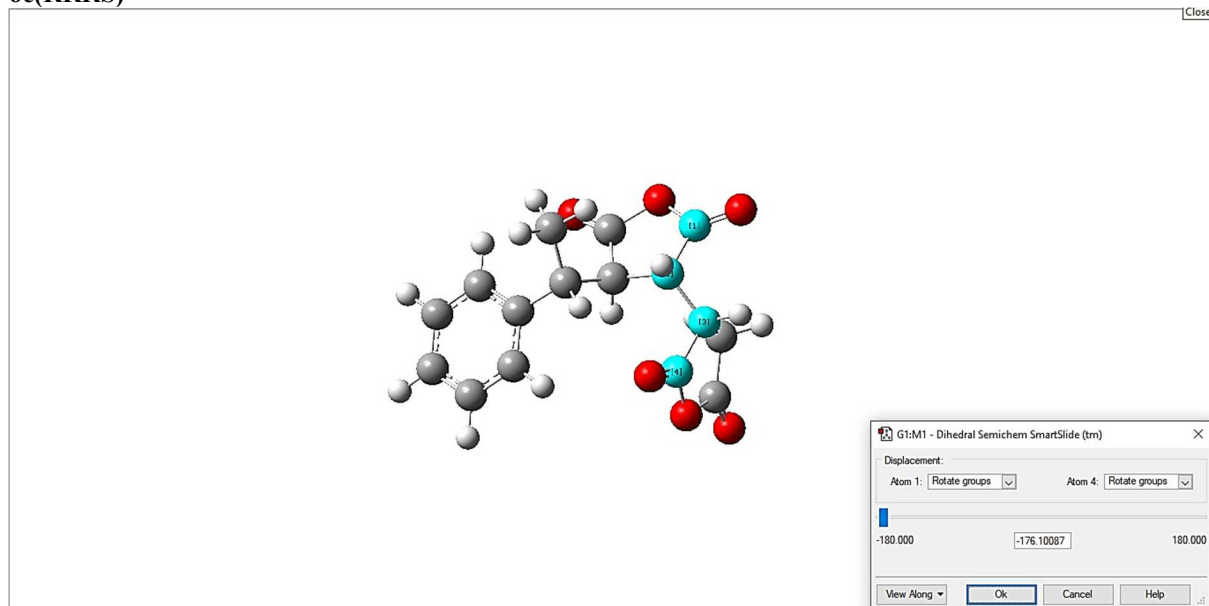


Fig. S23: Dihedral angle of (θ_a) of 6c(RRRS).

6d(SSSR)

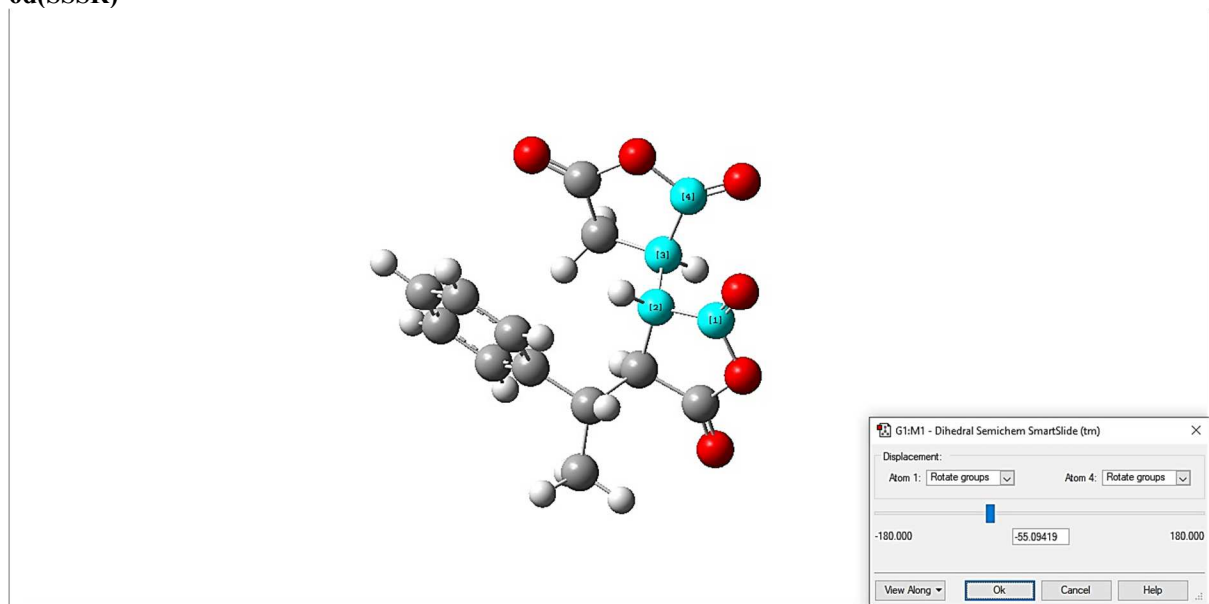


Fig. S24: Dihedral angle of (θ_a) of 6d(SSSR).

6e(RSSS)

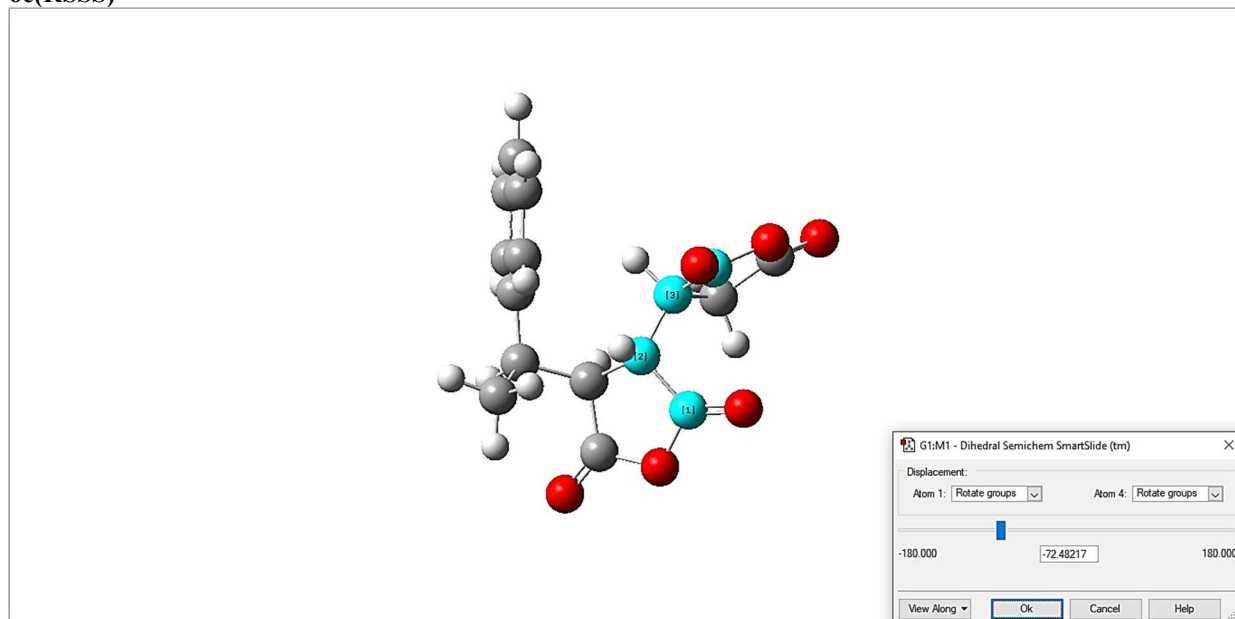


Fig. S25: Dihedral angle of (θ_a) of 6e(RSSS).

6f(SRRR)

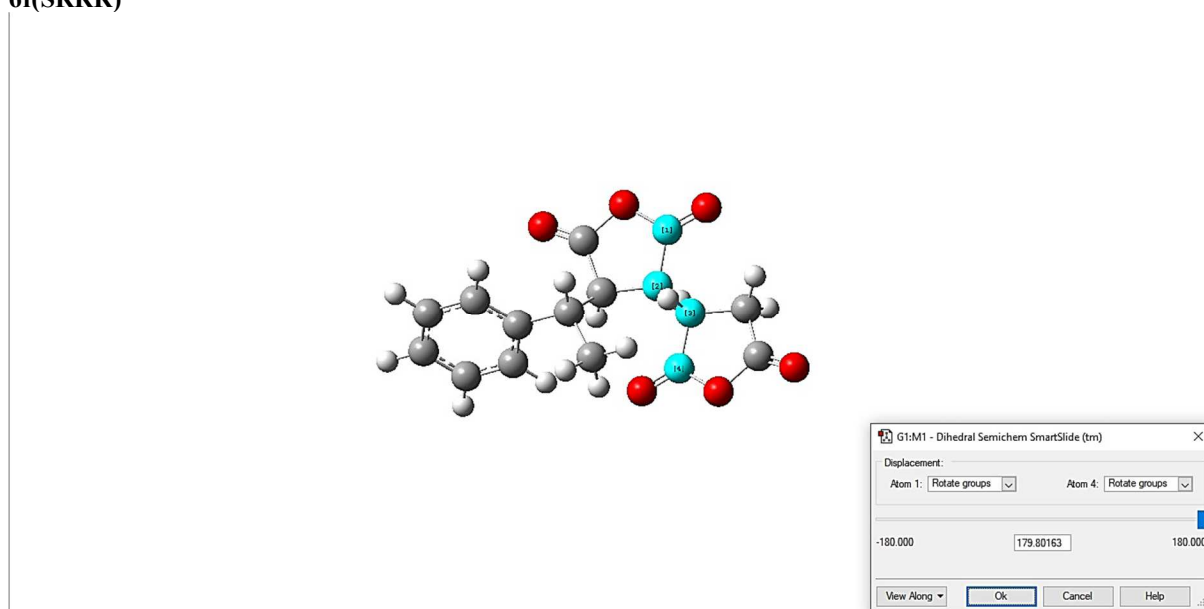


Fig. S26: Dihedral angle of (θ_a) of 6f(SRRR).

6g(RRSS)

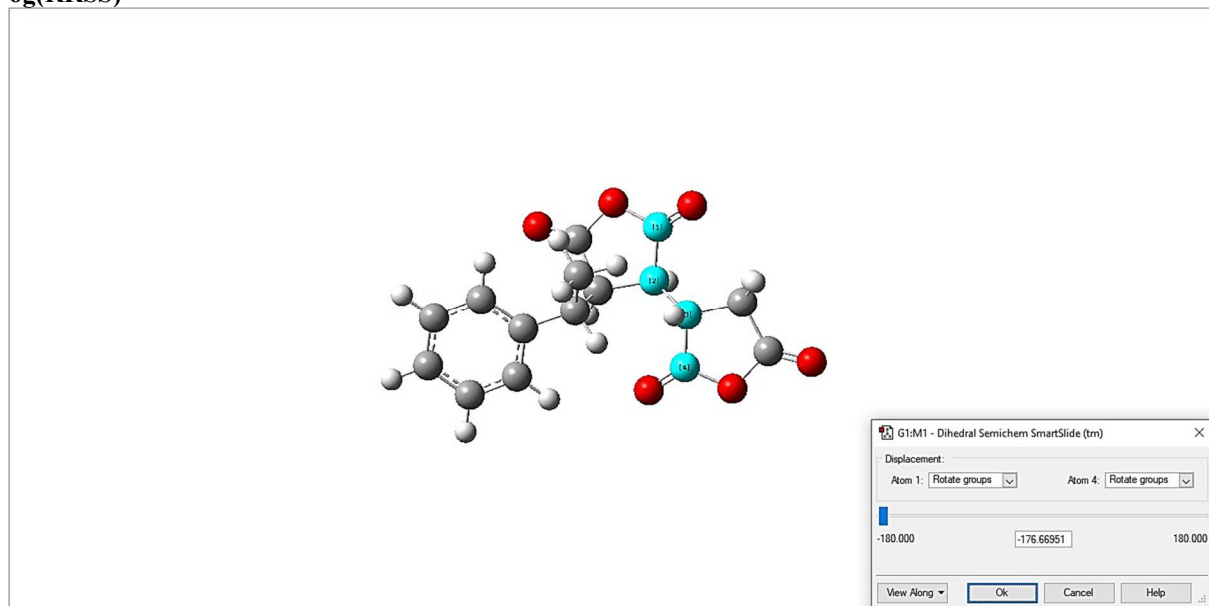


Fig. S27: Dihedral angle of (θ_a) of 6g(RRSS).

6h(SSRR)

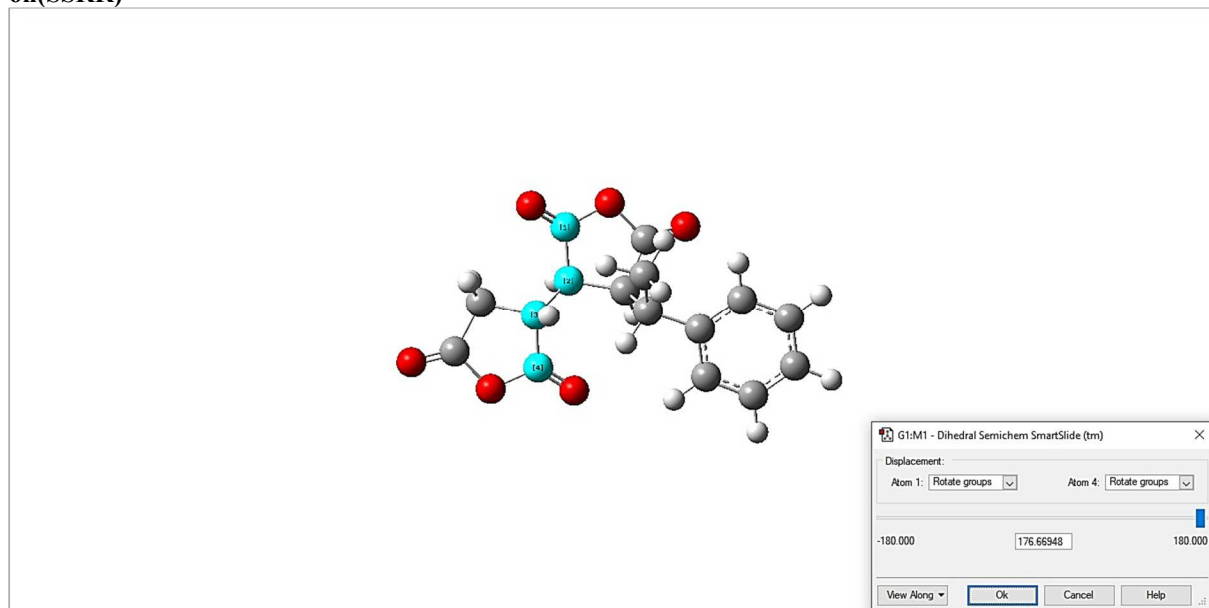


Fig. S28: Dihedral angle of (θ_a) of 6h(SSRR).

6i(RSRR)

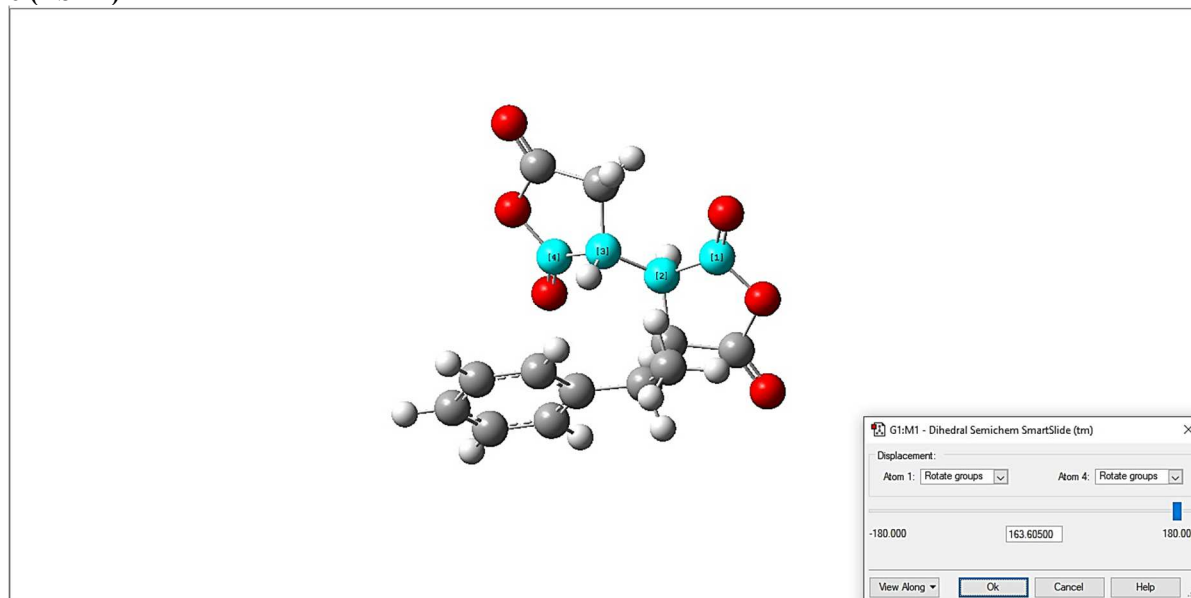


Fig. S29: Dihedral angle of (θ_a) of 6i(RSRR).

6j(SRSS)

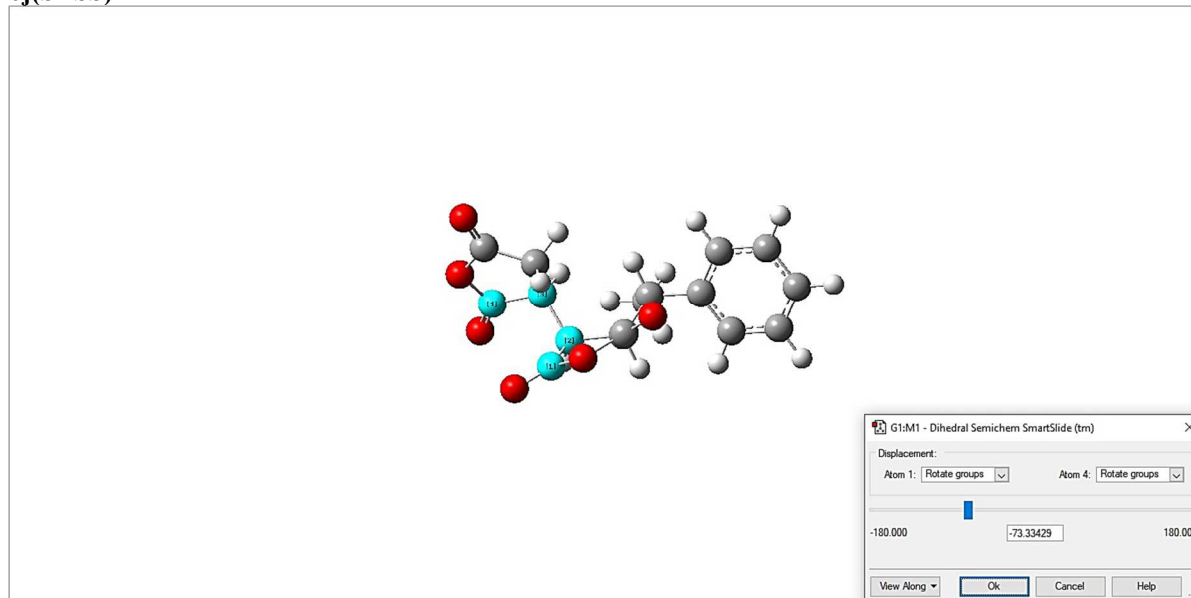


Fig. S30: Dihedral angle of (θ_a) of 6j(SRSS).

6k(RSSR)

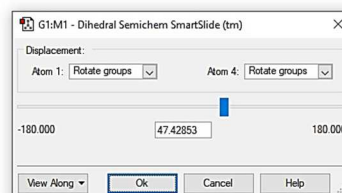
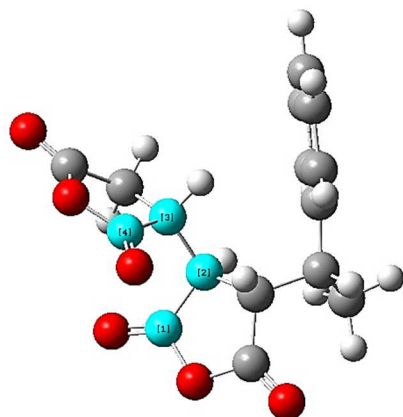


Fig. S31: Dihedral angle of (θ_a) of 6k(RSSR).

6l(SRRS)

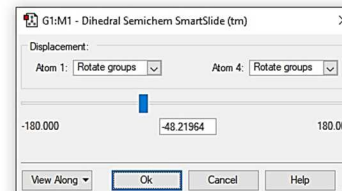
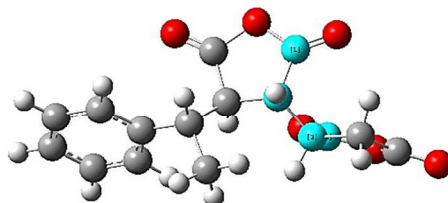


Fig. S32: Dihedral angle of (θ_a) of 6l(SRRS).

6m(RRSR)

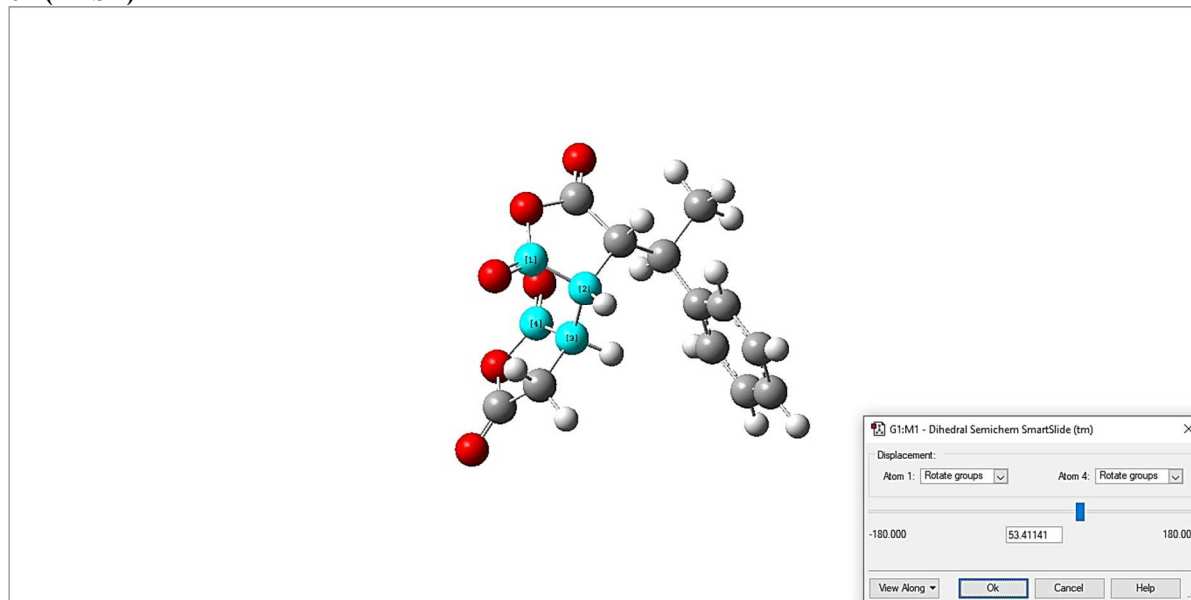


Fig. S33: Dihedral angle of (θ_a) of 6m(RRSR).

6n(SSRS)

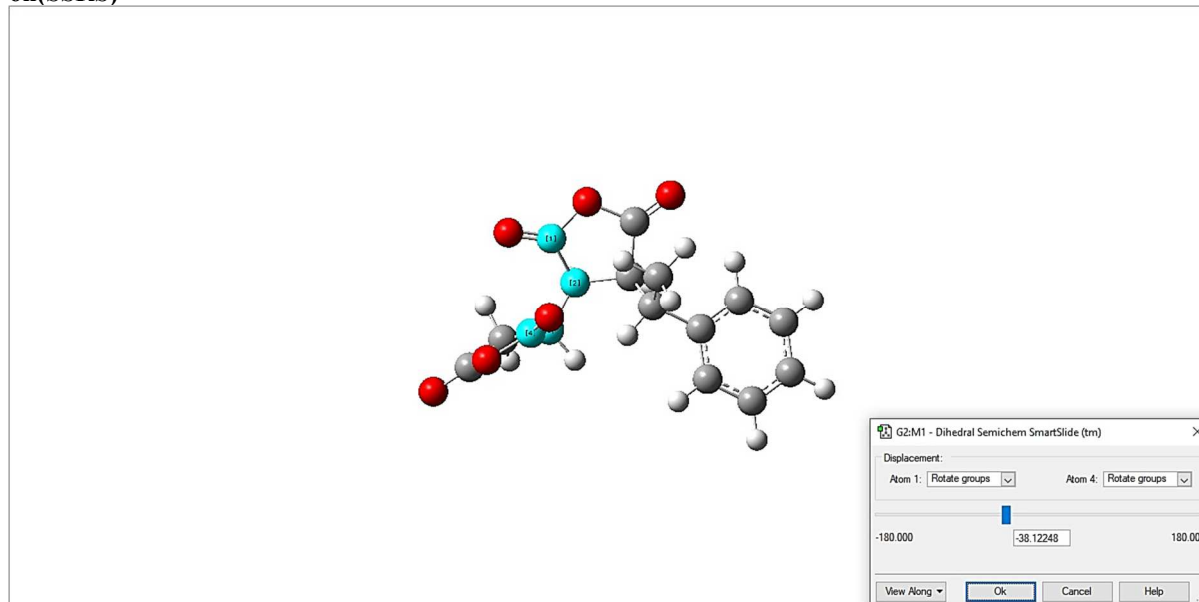


Fig. S34: Dihedral angle of (θ_a) of 6n(SSRS).

6o(RSRS)

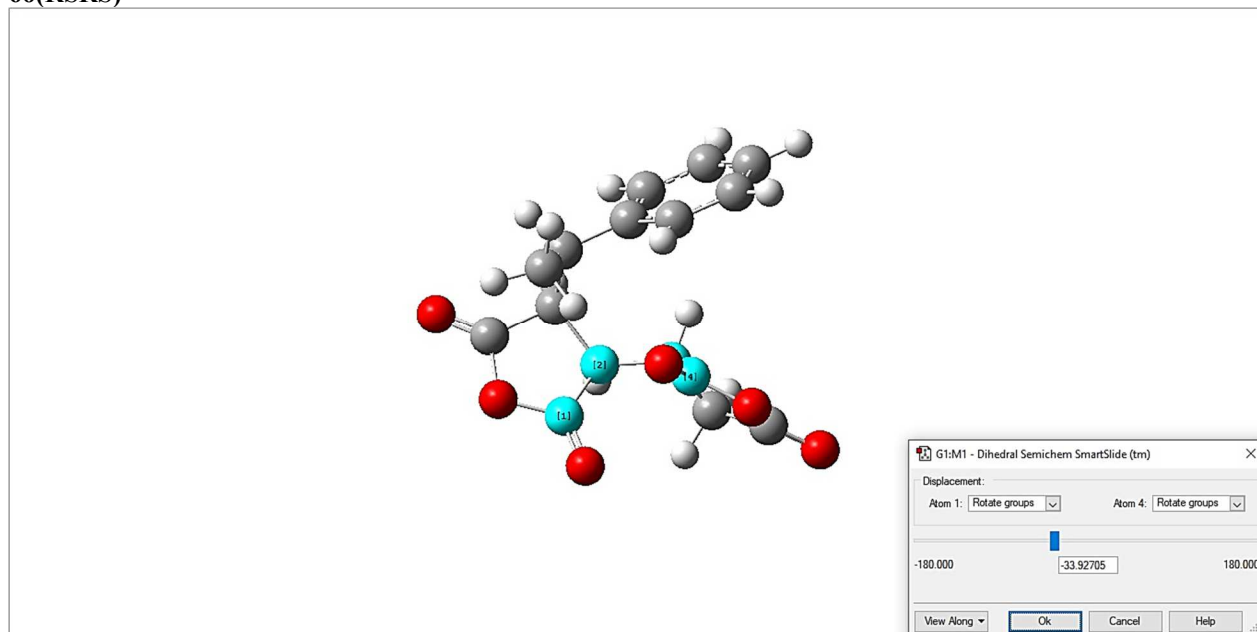


Fig. S35: Dihedral angle of (θ_a) of 6o(RSRS).

6p(SRSR)

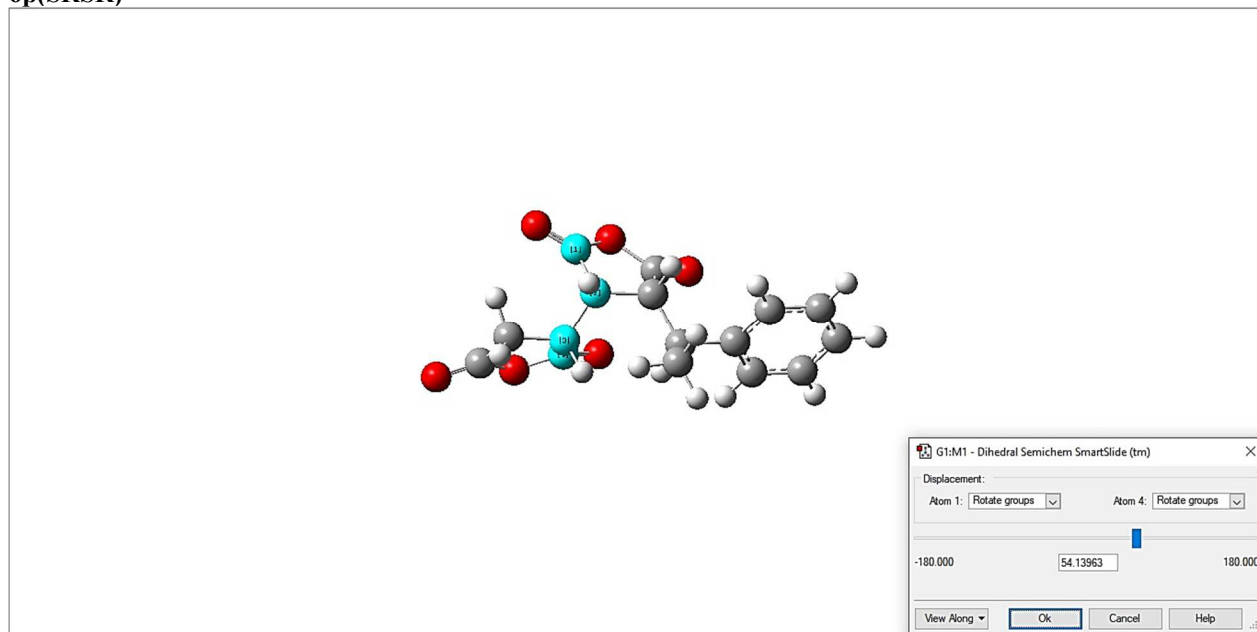


Fig. S36: Dihedral angle of (θ_a) of 6p(SRSR).