

Theoretical study of a derivative of chlorophosphine with aliphatic and aromatic Grignard reagents: $S_N2@P$ or the novel $S_N2@Cl$ followed by $S_N2@C$?

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Supplementary Information

S.1 Computational details

S.1.1 Distortion/interaction-activation strain model

Equation S1 shows how the D/I-ASM relates the relative electronic energy of a reaction (ΔE) to the relative strain (ΔE_{strain}) and relative interaction (ΔE_{int}) energies of the deformed reactant fragments along the reaction coordinate (ζ).

$$\Delta E(\zeta) = \Delta E_{\text{strain}}(\zeta) + \Delta E_{\text{int}}(\zeta) \quad \text{Equation S1}$$

The $\Delta E_{\text{strain}}(\zeta)$ corresponds to the relative electronic energy necessary to distort the reactant fragments throughout the reaction while the $\Delta E_{\text{int}}(\zeta)$ corresponds to the interactions between the deforming reactant fragments. We also investigated the effect of solvation along the PES using the D/I-ASM. The solvent-phase PES is described in terms of its components, solute energy and solvation energy, as in equation S2. The solvation energy englobes the solute-solvent interaction, as well as the formation of the solvent cavity.

$$\Delta E_{\text{solvation}}(\zeta) = \Delta E_{\text{solute}}(\zeta) + \Delta E_{\text{solvation}}(\zeta) \quad \text{Equation S2}$$

We obtained the $\Delta E_{\text{solute}}(\zeta)$ from the SP energy values of the reactant fragments in gas phase, computed using their geometry from solvent-phase computations. Equation S3 shows a further breakdown of the ΔE_{solute} into ΔE_{strain} and ΔE_{int} .

$$\Delta E_{\text{solute}}(\zeta) = \Delta E_{\text{strain}}(\zeta) + \Delta E_{\text{int}}(\zeta) \quad \text{Equation S3}$$

S.1.2 Diastereomeric ratio and relative Gibbs free energy barrier

Equation S4 shows how stereoselectivity of the diastereomers A and B is related to the temperature-dependent equilibrium constant K and hence to the standard-state Gibbs free energy of reaction (ΔG) at a particular temperature T.^[1]

$$\frac{[A]}{[B]} = K = e^{-\frac{\Delta G}{RT}} \quad \text{Equation S4}$$

The extent of diastereoselectivity depends on the relative stability of the diastereomers A and B which can be calculated from the difference between the computed Gibbs free activation energies ($\Delta\Delta G^\ddagger$) at a particular temperature.^[2]

S.2 Steric effect

The effect of steric congestion around the P atom in an organophosphorus reactant is a well-investigated aspect of the $S_N2@P$ reaction:^[3-5] An increase in the bulkiness of the substituents of the organophosphorus reactant changes the PES from a single-well to a triple-well and back to the archetypal double-well PES (Figure 1 in manuscript). However, this consensus was reached upon investigation of anionic $S_N2@P$ reactions. In this section, we built on this consensus and showed that TCs, and hence single- and triple-well PESs, are not located in ion-pair $S_N2@P$ reactions of trivalent organophosphorus reactants. Figure S1 shows the TSs of the $S_N2@P$ -b and $S_N2@P$ -f reactions in the gas phase and in THF. The ΔG of the RCs, TSs, PCs and Ps are listed in Table S1.

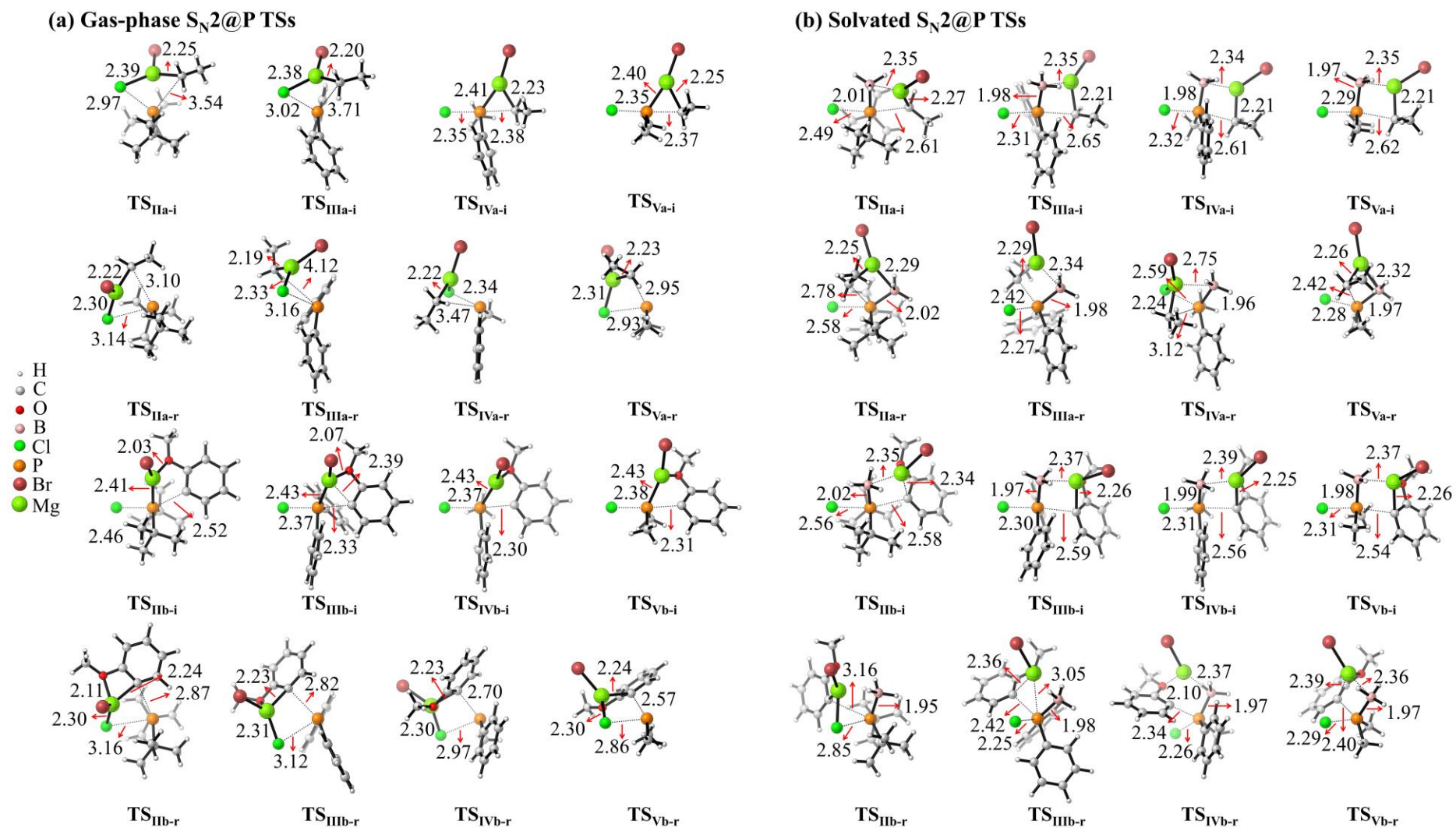


Figure S1: Geometries of the TSs of the $S_N2@P$ -b and $S_N2@P$ -f pathways of the $R1_n + a$ and $R1_n + b$ reactions in the (a) gas phase and (b) bulk-solvated with THF. The bond lengths/distances are in Å. The atom symbols are shown on the left-hand side.

Table S1: ΔG , in kcal mol⁻¹, of the RCs, TSs, PCs and Ps along the S_N2@P-b and S_N2@P-f pathways of the reactions of **R1_n** with nucleophiles **a** and **b** in the gas phase and in THF. The values corresponding to the bulk-solvated phase are in brackets.

Inversion pathway									
Pathway	RC	TS	PC	P	Pathway	RC	TS	PC	P
Ia-i	-1.5 (+10.0)	+21.7 (+41.7)	-48.7 (-11.0)	-33.4 (-47.3)	Ib-i	+1.9 (+8.1)	+27.7 (+53.9)	-43.2 (+14.4)	-17.5 (-33.7)
IIa-i	-0.8 (+8.8)	+32.2 (+56.0)	-48.5 (-15.1)	-30.9 (-43.7)	IIb-i	-1.7 (+8.0)	+33.9 (+57.8)	-43.3 (-1.0)	-14.2 (-20.2)
IIIa-i	-0.6 (+8.8)	+22.2 (+34.9)	-50.4 (-19.4)	-37.7 (-50.8)	IIIb-i	-0.7 (+9.2)	+21.0 (+30.1)	-46.5 (-39.2)	-22.3 (-37.0)
IVa-i	-0.1 (+9.8)	+23.0 (+30.8)	-51.3 (-17.0)	-37.2 (-50.8)	IVb-i	-0.7 (+9.6)	+18.5 (+27.6)	-45.4 (-11.5)	-21.4 (-36.5)
Va-i	+1.7 (+10.0)	+22.6 (+30.6)	-51.2 (-17.8)	-36.7 (-49.9)	Vb-i	-0.6 (+8.8)	+18.8 (+28.6)	-44.8 (-11.5)	-20.4 (-35.9)
Retention pathway									
Ia-r	+0.2 (+8.3)	+21.7 (+44.3)	-33.9 (-49.0)	-33.4 (-47.3)	Ib-r	-0.8 (+6.9)	+25.9 (+59.1)	-28.0 (+5.5)	-18.1 (-33.7)
IIa-r	+1.0 (+8.3)	+28.3 (+63.7)	-28.4 (-12.3)	-30.9 (-44.5)	IIb-r	+2.4 (+7.4)	+31.8 (+63.7)	-22.7 (-28.6)	-14.2 (-20.2)
IIIa-r	+0.2 (+8.9)	+23.3 (+48.0)	-51.5 (-48.7)	-37.6 (-50.8)	IIIb-r	+3.4 (+9.9)	+25.6 (+50.7)	-35.5 (-39.1)	-20.0 (-37.0)
IVa-r	+0.7 (+10.3)	+24.3 (+44.5)	-50.8 (-49.2)	-37.1 (-50.8)	IVb-r	+3.2 (+9.4)	+27.4 (+46.8)	-31.1 (-11.6)	-20.3 (-36.5)
Va-r	-0.4 (+9.2)	+26.8 (+47.5)	-32.3 (-48.3)	-36.7 (-49.9)	Vb-r	+3.6 (+8.8)	+28.8 (+47.9)	-29.7 (-36.5)	-20.4 (-35.9)

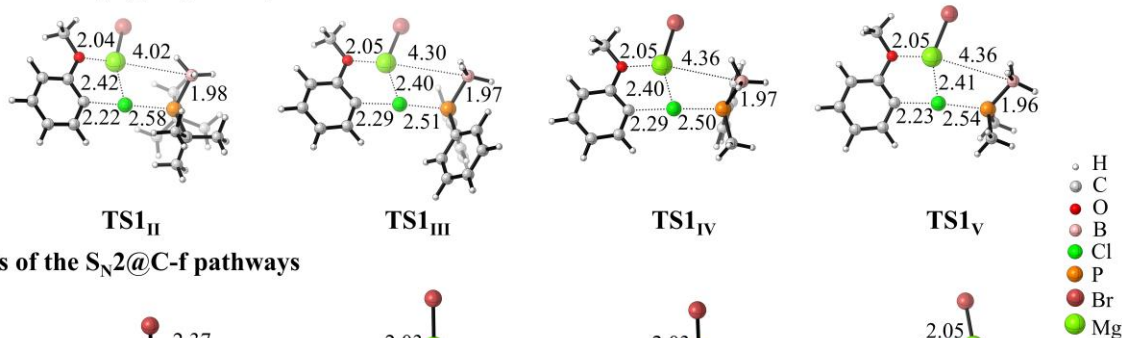
An increase in the substituent size in the **R1_n** organophosphorus reactants causes the Cl–P–C bond angle of the TSs of the S_N2@P-b pathways to bend (Figure S1), allowing for more interaction between the Mg²⁺ cation and the Cl leaving group. In the S_N2@P-f pathways, the Mg²⁺ cation interacts with both the C atom of the nucleophile and the Cl atom of **R1_n** on the same side of the P atom. An analysis of Table S1 shows that gas-phase ion-pair S_N2 reactions occur mostly through unimodal PESs or through hill-and-well PESs with the PC as the minimum point, contrary to anionic S_N2 reactions.^[3-5] The preference of the pathway depends on the steric hindrance around the P atom of the organophosphorus reactants. On increasing the bulkiness of the substituents of **R1_n**, we observed that (i) the PESs of the S_N2@P-b pathways (**R1_I** + **a** and **R1_{II}** + **b**) shift back to the typical double-well shape; (ii) there is a general decrease in exergonicity in the reactions and; (iii) there is a general decrease in the $\Delta\Delta G^\ddagger$ of the pathways. In line with the third observation, **R1_{II}** prefers the S_N2@P-f with both nucleophiles **a** and **b**. The trend in the PESs is explained through the D/I-ASM in the SI.

In the THF-solvated S_N2@P-b pathways, the Mg²⁺ cation is attracted to the high electron density of the B atom of the BH₃ moiety. The TSs of the S_N2@P-b pathways have near-linear Cl–P–C bond angles. The combined effect of bulk solvation by THF and the ion-pair nucleophile renders the PESs of the S_N2@P-b and S_N2@P-f pathways (mostly) unimodal with only the TS as the stationary point. The reactions also become more exergonic than in the gas phase. As the bulkiness of the substituents increases, the Gibbs free energy barrier that reactants must overcome to reach the TS increases and the general decrease in exergonicity persists (Table S1). The S_N2@P-b pathways have a lower Gibbs free energy barrier than the S_N2@P-f pathways with both nucleophiles **a** and **b** in THF.

Next, we compared the S_N2@P-b and S_N2@Cl pathways of the **R1_n** + **b** reactions in THF to investigate how the presence of less bulky substituents affects the preference of the pathway. Figure S2 illustrates

the bulk-solvated TSs of the $S_N2@Cl$ and the consequent $S_N2@C-f$ pathways of the $R1_n + b$ reactions. Table 2 lists the ΔG of the RCs, TSs, INTs and PCs of the $S_N2@Cl$ and $S_N2@C-f$ pathways.

(a) TSs of the $S_N2@Cl$ pathways



(b) TSs of the $S_N2@C-f$ pathways

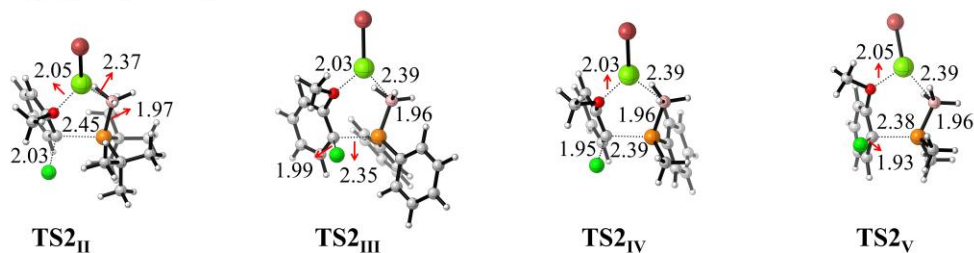


Figure S2: Geometries of the TSs of the (a) $S_N2@Cl$ and (b) $S_N2@C-f$ pathways of the $R1_n + b$ bulk-solvated with THF. The bond lengths/distances are in Å. The atom symbols are shown on the right-hand side.

Table S2: ΔG of the RCs, TSs, INTs, PCs and Ps of the THF-solvated $S_N2@Cl$ and $S_N2@C-f$ pathways in kcal mol⁻¹.

$S_N2@Cl$ pathway					
	R1_I	R1_{II}	R1_{III}	R1_{IV}	R1_V
RC	+6.3	+8.0	+8.2	+6.8	+8.4
TS1	+43.9	+48.5	+42.2	+43.4	+46.7
INT1	+12.7	+12.6	+8.9	+9.6	+12.4
$S_N2@C-f$ pathway					
INT2	+9.7	+15.2	+9.3	+14.3	+17.5
TS2	+54.2	+53.6	+43.7	+43.4	+46.5
PC	-4.2	-5.0	-12.2	-12.1	-12.2
P	-33.7	-20.2	-37.0	-36.5	-35.9

A comparison of Tables S1 and S2 shows that, similar to the $R1_I + b$ reaction, the Gibbs free energy barrier of the $S_N2@P-b$ pathway of the $R1_{II} + b$ reaction is higher (+57.8 kcal mol⁻¹) than that of the $S_N2@Cl$ pathway (+48.5 kcal mol⁻¹). The reactions of $R1_{III}$, $R1_{IV}$ and $R1_V$ investigated occur through the $S_N2@P-b$ pathway in THF. This shows that the nucleophile b may approach the reactive backside of the P atom better when the P atom is less crowded by the presence of small substituents. As the bulkiness of the substituent increases, competing mechanisms, such as the $S_N2@Cl$ mechanism, become more favourable.

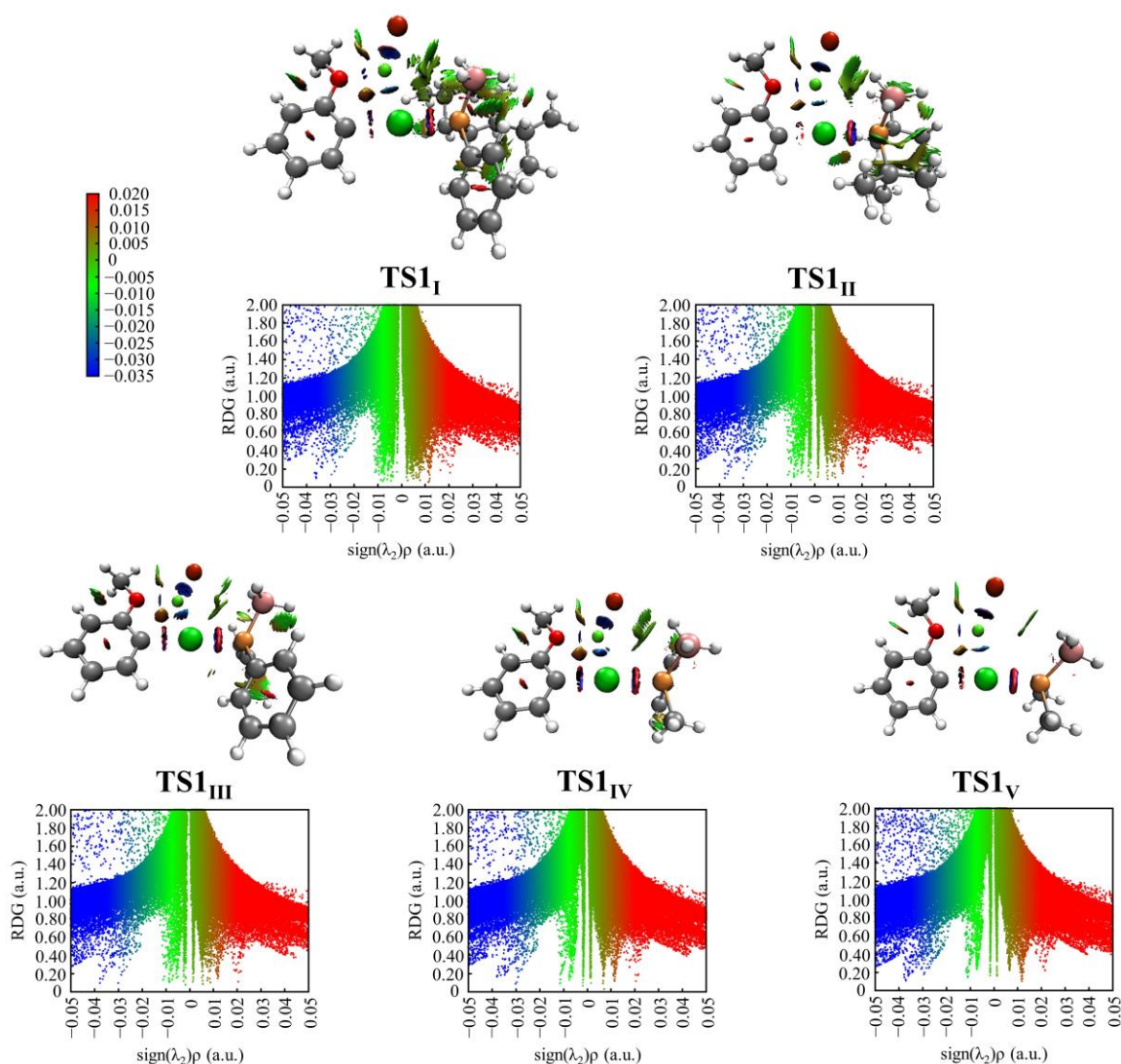


Figure S3: 2D and 3D plots of the **TS1_n** of the $S_N2@Cl$ pathways. The NCI isosurfaces correspond to an isovalue of $s = 0.5$ a.u.

We also performed NCI analysis of the **TS1_n** of the $S_N2@Cl$ pathways and the 2D and 3D NCI plots are displayed in Figure S3. In the plot for the **TS1_V**, a blue patch between the Mg^{2+} cation and the O atom shows attractive interaction which spreads over a broad intermolecular space from a value of $sign(\lambda_2)\rho$ of -0.05 to -0.04 a.u. A trough at approximately $sign(\lambda_2)\rho = -0.04$ a.u. shows the $Mg\cdots Br$ interaction which is also depicted by a blue isosurface. The $Mg\cdots Cl$ interaction is less attractive and represented by a pale blue isosurface and a trough at approximately $sign(\lambda_2)\rho = -0.03$ a.u. The green isosurfaces ($-0.03 > sign(\lambda_2)\rho > 0$) represent three types of van der Waals interactions: $O-C\cdots H-C$, $Br\cdots H-C$ and $B-H\cdots Br$. In the $0 > sign(\lambda_2)\rho > 0.01$ region, the repulsive interactions depicted by three brown isosurfaces occur at three positions due to *pseudo*-ring enclosures. These include the $C-O-C-C-H$ of the phenyl ring of the nucleophile **b** and the $O-Mg-Cl-C-C$ and $O-Mg-Br-H-C$ *pseudo*-rings formed at the TS. Between the C and Cl atoms and the Cl and P atoms, an attractive isosurface is observed enclosed by a repulsive wall at $sign(\lambda_2)\rho = 0.02$ a.u. Finally, the non-bonded overlap between the C atoms of the phenyl ring causes a steric repulsion shown by the red region at $sign(\lambda_2)\rho = 0.04$ a.u. Similar isosurfaces were observed in all the **TS1_n**. In the **TS1_I** and **TS1_{II}**, areas of van der Waals interaction and steric repulsion were also observed between the B atom and surrounding H atoms of the substituents, and between the B atom and surrounding C atoms, respectively.

Figure S4 shows the changes in strain, interaction and solvation which are responsible for the trends in the PESs of the $\mathbf{R1}_n + \mathbf{a}$ and $\mathbf{R1}_n + \mathbf{b}$ reactions. A comparison of $\Delta E_{\text{solvation}}$ along the $\text{S}_{\text{N}}2@P\text{-b}$ and $\text{S}_{\text{N}}2@P\text{-f}$ pathways in Figures S4 (a) shows that THF stabilises all points on the PES of the $\text{S}_{\text{N}}2@P\text{-b}$ pathways to a greater extent than those of the $\text{S}_{\text{N}}2@P\text{-f}$ pathways. This happens because of the charge separation along the PESs. The reactants along the inversion pathways deform to generate TSs with linear Cl–P–C bond angles, whereas along the retention pathways, the reactants deform and lead to TSs with a cyclic geometry. There is more charge separation, and hence more stabilisation by THF, along the pathways forming the TSs with linear Cl–P–C bond angles than along pathways featuring TSs with cyclic geometries.

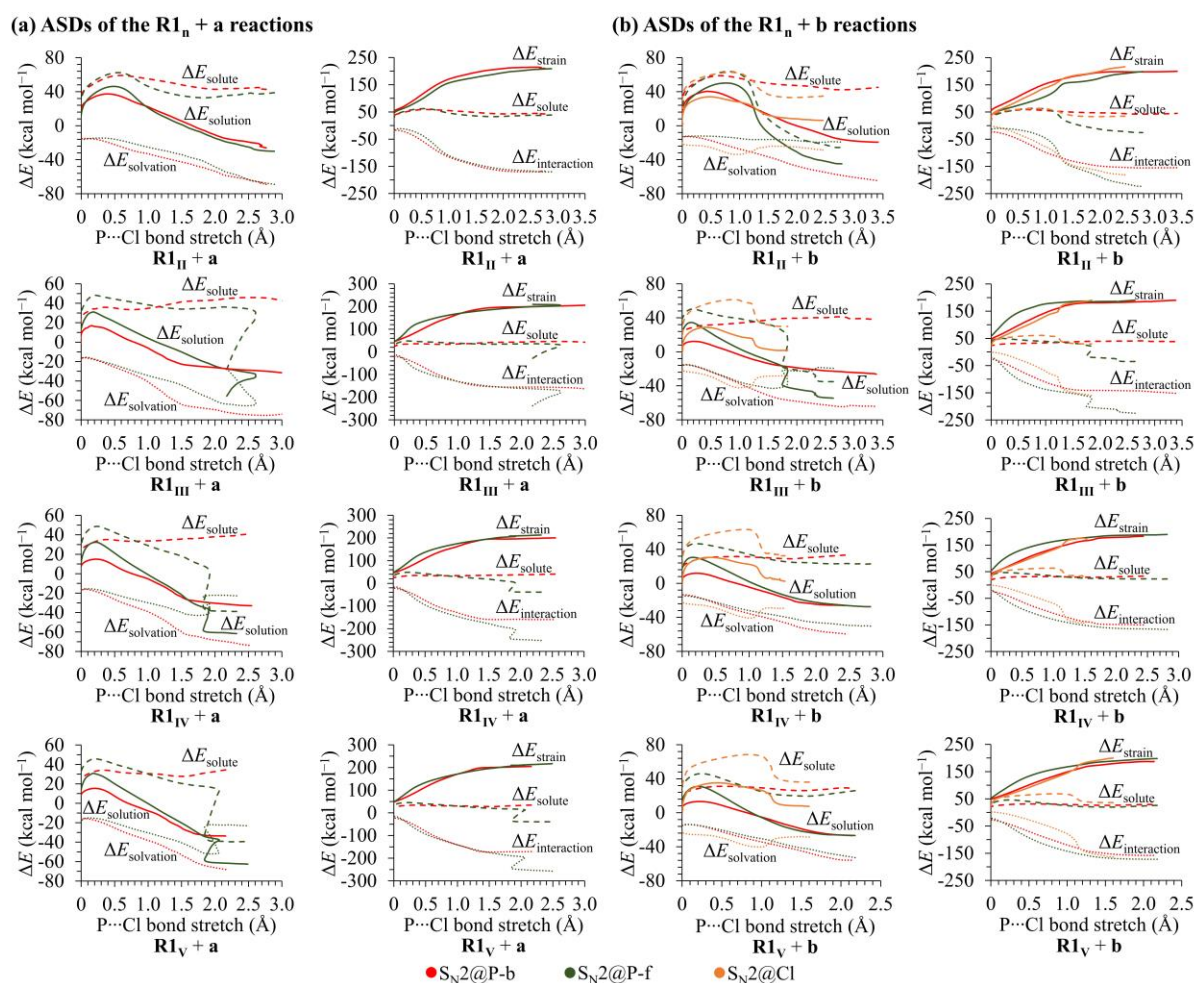


Figure S4: ASDs of the (a) $\mathbf{R1}_n + \mathbf{a}$ and (b) $\mathbf{R1}_n + \mathbf{b}$ reactions.

At the start of the reactions, in the presence of small substituents ($\mathbf{R1}_{\text{III}}$, $\mathbf{R1}_{\text{IV}}$ and $\mathbf{R1}_{\text{V}}$), the deforming reactant fragments experience more ΔE_{strain} and less stabilising $\Delta E_{\text{interaction}}$ in the $\text{S}_{\text{N}}2@P\text{-f}$ pathway than in the $\text{S}_{\text{N}}2@P\text{-b}$ pathway. As the reactions progress, the ΔE_{strain} becomes comparable along both pathways and ΔE_{int} becomes more stabilising along the $\text{S}_{\text{N}}2@P\text{-f}$ pathway. The $\text{S}_{\text{N}}2@P\text{-b}$ pathways are preferred to the $\text{S}_{\text{N}}2@P\text{-f}$ pathways due to more stabilisation by THF and due to lower deformational strain in the initial stages of the reaction. As the substituents of the organophosphorus reactant increase in size in $\mathbf{R1}_{\text{II}}$ [Figure S4 (a)] and $\mathbf{R1}_{\text{I}}$ [Figure 5 (a) in manuscript], the ΔE_{strain} is higher throughout the inversion pathway. However, the lower Gibbs free energy barrier (Table S1) of the $\text{S}_{\text{N}}2@P\text{-b}$ pathway is due to more stabilising $\Delta E_{\text{interaction}}$ between deforming reactants and more stabilising $\Delta E_{\text{solvation}}$ along the pathway. Hence, the $\mathbf{R1}_n + \mathbf{a}$ reactions proceed through the $\text{S}_{\text{N}}2@P\text{-b}$ pathway.

When comparing the ASDs for the $\mathbf{R1}_n + \mathbf{b}$ reactions [Figure S4 (b)], the same trends in strain, interaction and solvation as in the $\mathbf{R1}_n + \mathbf{a}$ reactions were observed for the $\text{S}_{\text{N}}2@P$ pathways. The

$S_N2@Cl$ pathways experience the most stabilisation by solvent before the TS is formed, at the TS and even after the formation of the TS. This is because of higher charge separation caused by the linearity of the $C\cdots Cl\cdots P$ backbone. The $\Delta E_{solvation}$ becomes less stabilising than the $S_N2@P$ pathways as the geometry becomes increasingly non-linear while the PESs progress towards the **INT1_n**.

The deformed reactants along the $S_N2@P$ -f pathway of the **R1_{II}** + **b** reaction experience the least strain throughout the PES. However, the $\Delta E_{interaction}$ and $\Delta E_{solvation}$ have the least stabilising effect on the PES of the $S_N2@P$ -f pathway. Similar to the **R1_I** + **b** reaction, the $S_N2@Cl$ pathway is favoured due to lower strain and better stabilisation by THF. As the size of the substituents decreases, the $\Delta E_{interaction}$ of the $S_N2@P$ -f pathways of the **R1_n** + **b** reactions becomes the most stabilising. However, the $S_N2@P$ -f pathways have the highest energy barrier due to the highest ΔE_{strain} and the least stabilisation by THF. The ΔE_{strain} along the $S_N2@Cl$ pathways is lower to or comparable to the $S_N2@P$ -b pathway in the initial stages. As the reactions progress, the strain component becomes higher than that of the $S_N2@P$ -b pathway. The $\Delta E_{interaction}$ remains less stabilising than that of the $S_N2@P$ -b pathway. Although THF stabilises the $S_N2@Cl$ pathways the most, the interplay between the ΔE_{strain} and $\Delta E_{interaction}$ makes the $S_N2@P$ -b pathways preferred as the size of the substituents decreases.

S.2.1 Use of dispersion-corrected M06-2X functional

The reactions were also investigated using the M06-2X-D3/6-31++G(d,p) method. Tables S3 and S4 list the ΔG values along the PESs of the $S_N2@C$ -b and $S_N2@C$ -f pathways of the reactions of **R1_I** to **R1_V** with **a** and **b**. Table S5 lists the ΔG values along the two-step S_N2 reactions ($S_N2@Cl$ and $S_N2@C$ -f pathways). From tables S3 to S5, it is observed that the ΔG values are lower than the values computed with the B3LYP/6-31++G(d,p) method.

Table S3: ΔG , in kcal mol⁻¹, of the RCs, TSs, PCs and Ps of the S_N2@C-b and S_N2@C-f pathways of the reactions of **R1_I** to **R1_V** with **a**.

S_N2@P-b pathways				
Pathways	RC	TS	PC	P
Ia-i	+1.9	+29.3	-48.7	-50.3
IIa-i	+2.1	+44.5	-20.5	-46.9
IIIa-i	+4.1	+20.3	-58.6	-54.6
IVa-i	+3.4	+18.2	-54.1	-53.4
Va-i	+4.3	+19.4	-25.8	-52.6
S_N2@P-f pathways				
Ia-r	+1.9	+41.6	-59.0	-50.3
IIa-r	+2.5	+50.9	-22.0	-48.0
IIIa-r	+3.5	+32.2	-57.3	-54.6
IVa-r	+4.4	+36.6	-56.6	-53.0
Va-r	+2.6	+35.1	-57.0	-52.6

Table S4: ΔG , in kcal mol⁻¹, of the RCs, TSs, PCs and Ps of the S_N2@C-b and S_N2@C-f pathways of the reactions of **R1_I** to **R1_V** with **b**. ΔE values are in parentheses.

S_N2@P-b pathways				
Pathways	RC	TS	PC	P
Ib-i	-2.7	+31.5	-2.9	-34.3
IIb-i	-1.5	+40.5	-14.1	-30.0
IIIb-i	+0.9	+10.3	-56.7	-41.3
IVb-i	+0.4	+12.6	-20.2	-39.5
Vb-i	+3.6	+14.9	-21.2	-38.4
S_N2@P-f pathways				
Ib-r	-1.7	+47.6	-7.6	-37.2
IIb-r	-1.3	+50.1	-13.1	-30.0
IIIb-r	+2.1	+32.6	-54.2	-41.3
IVb-r	+1.9	+30.0	-22.0	-39.5
Vb-r	+1.5	+32.8	-51.1	-38.4

S.3 Gas-phase S_N2@P reactions

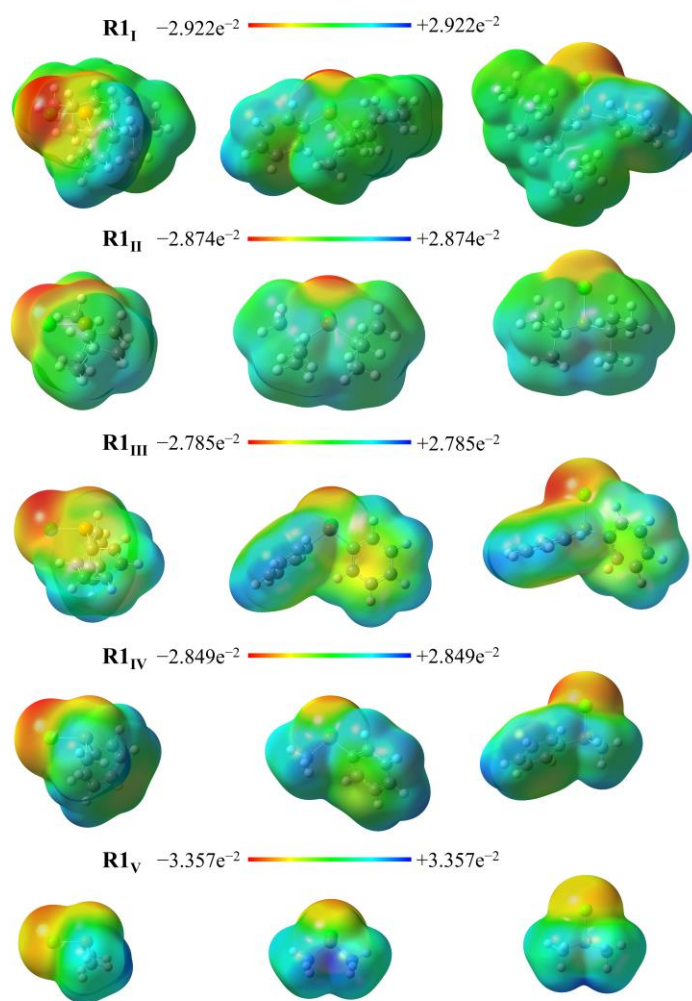


Figure S5: ESP maps (electrostatic potentials in au) in the gas phase.

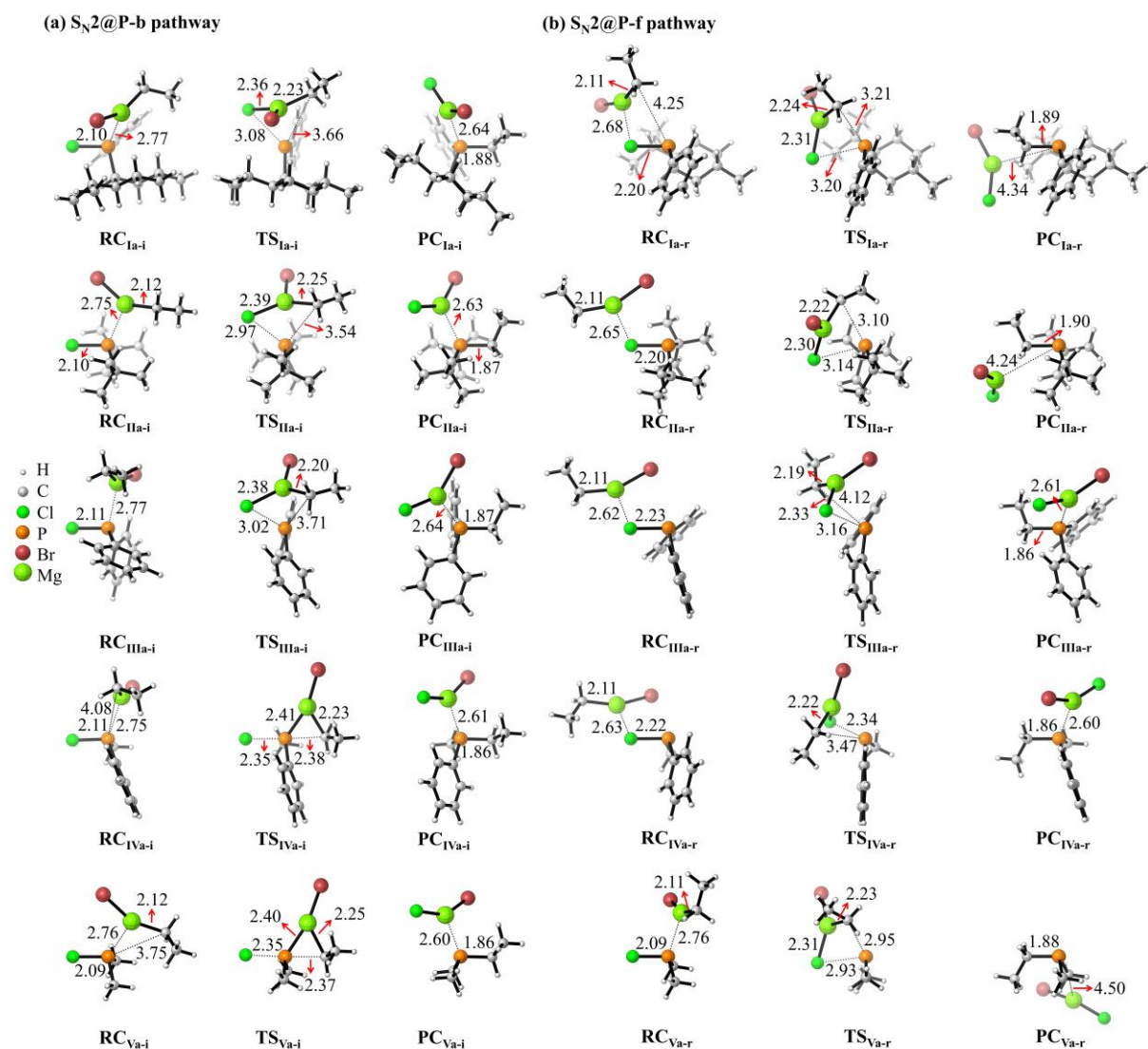


Figure S6: Gas-phase geometries of the RCs, TSs and PCs of the inversion and retention pathways of the $S_N2@P$ reactions. Bond lengths/distances are in Å.

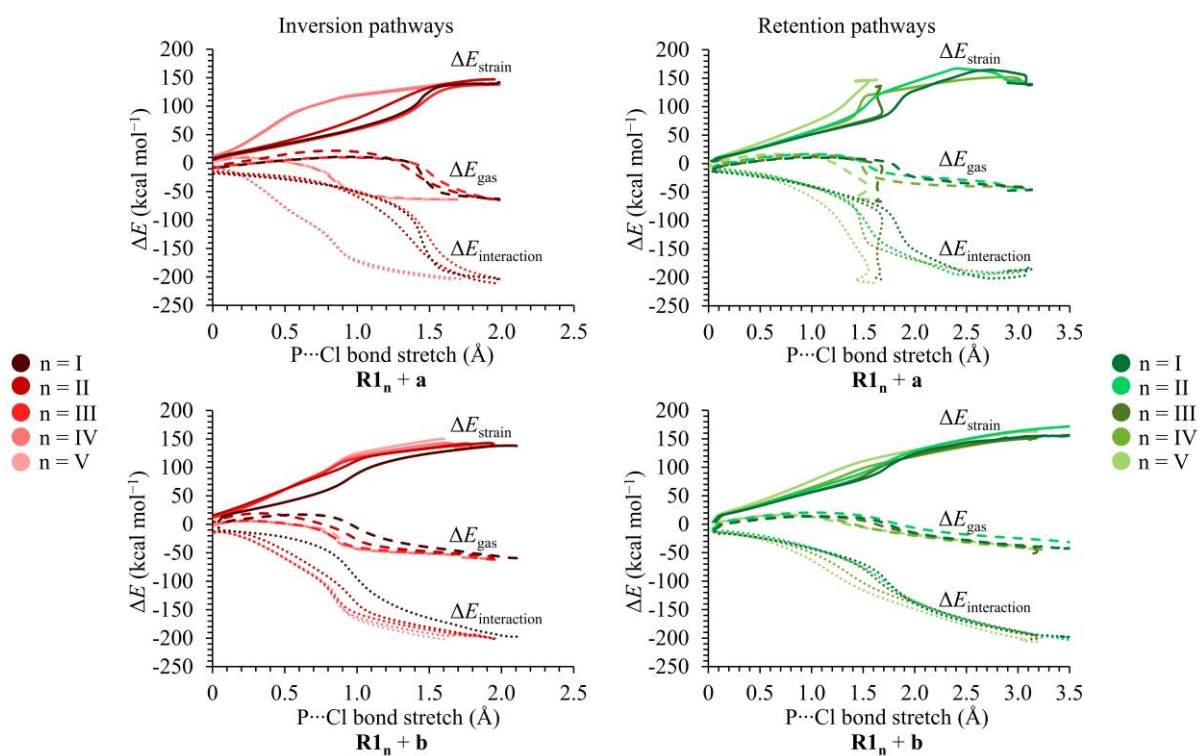


Figure S7: ASDs of the inversion and retention pathways of the $\mathbf{R1}_n + \mathbf{a}$ and $\mathbf{R1}_n + \mathbf{b}$ $\text{S}_{\text{N}}2@P$ reactions in the gas phase.

S.4 THF-solvated $S_N2@P$ reactions

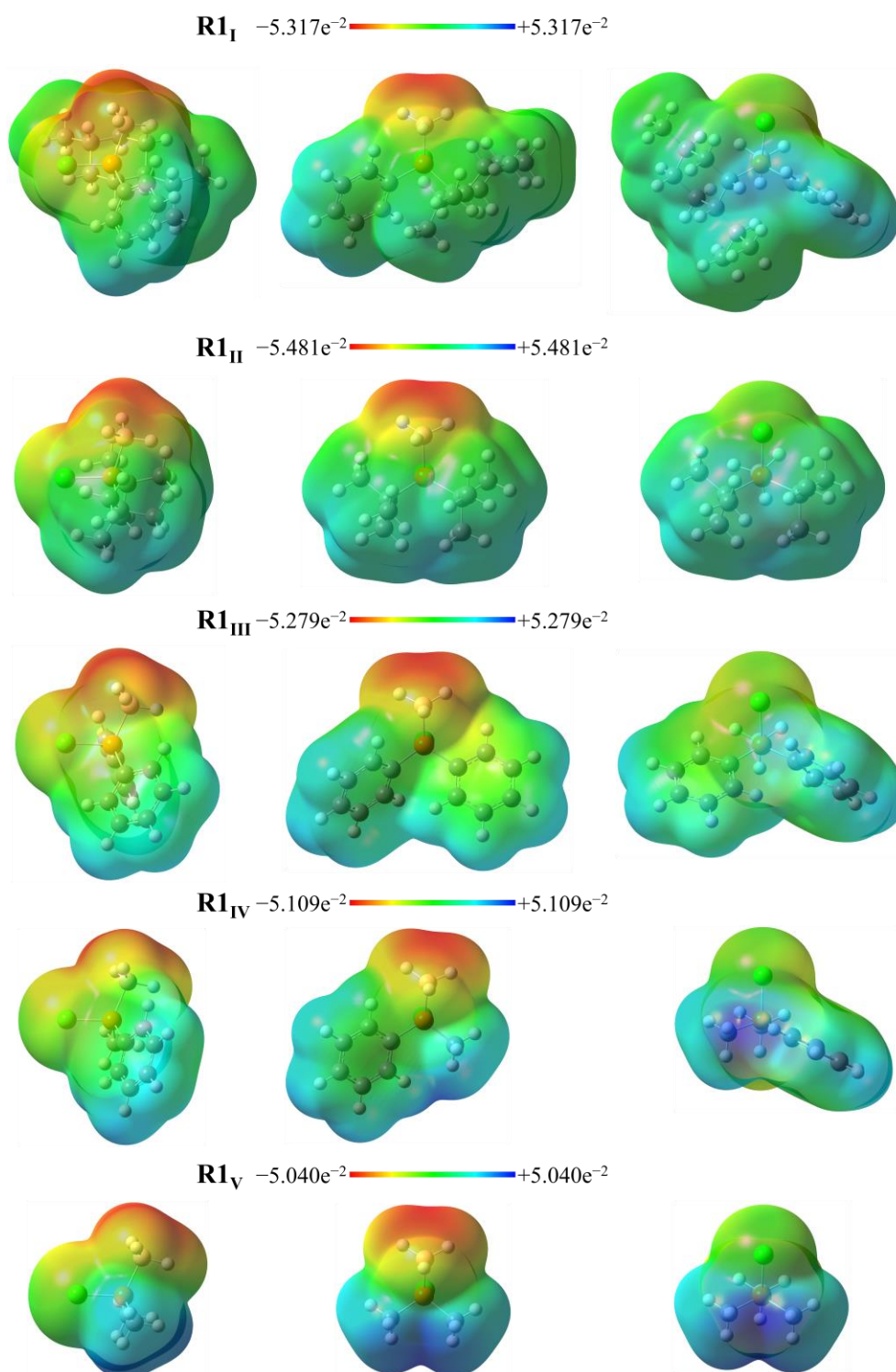


Figure S8: ESP maps (electrostatic potential in au) in THF.

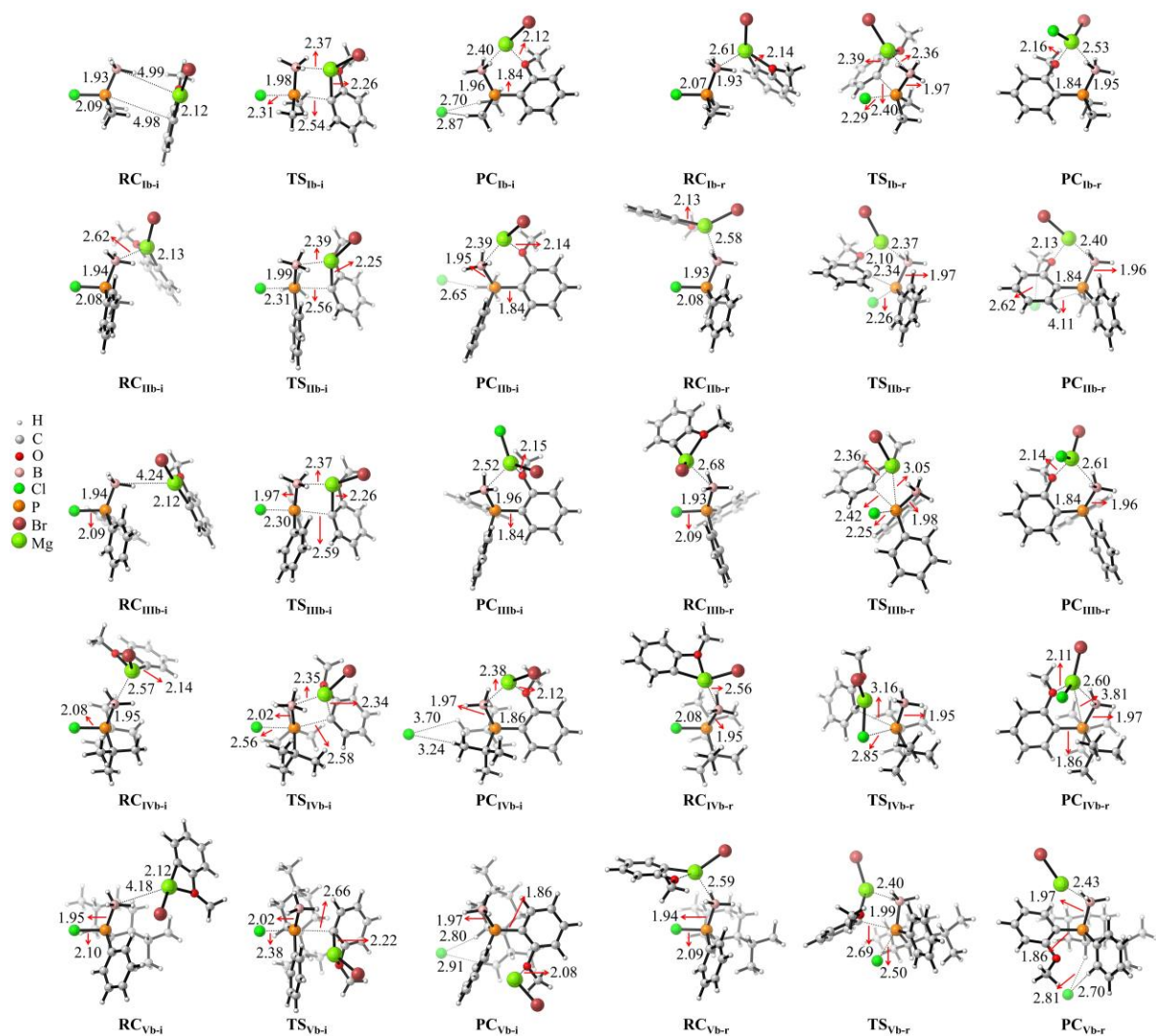


Figure S9: THF-based geometries of the RCs, TSs and PCs of the inversion and retention pathways of the $S_N2@P$ reactions. Bond lengths/distances are in Å.

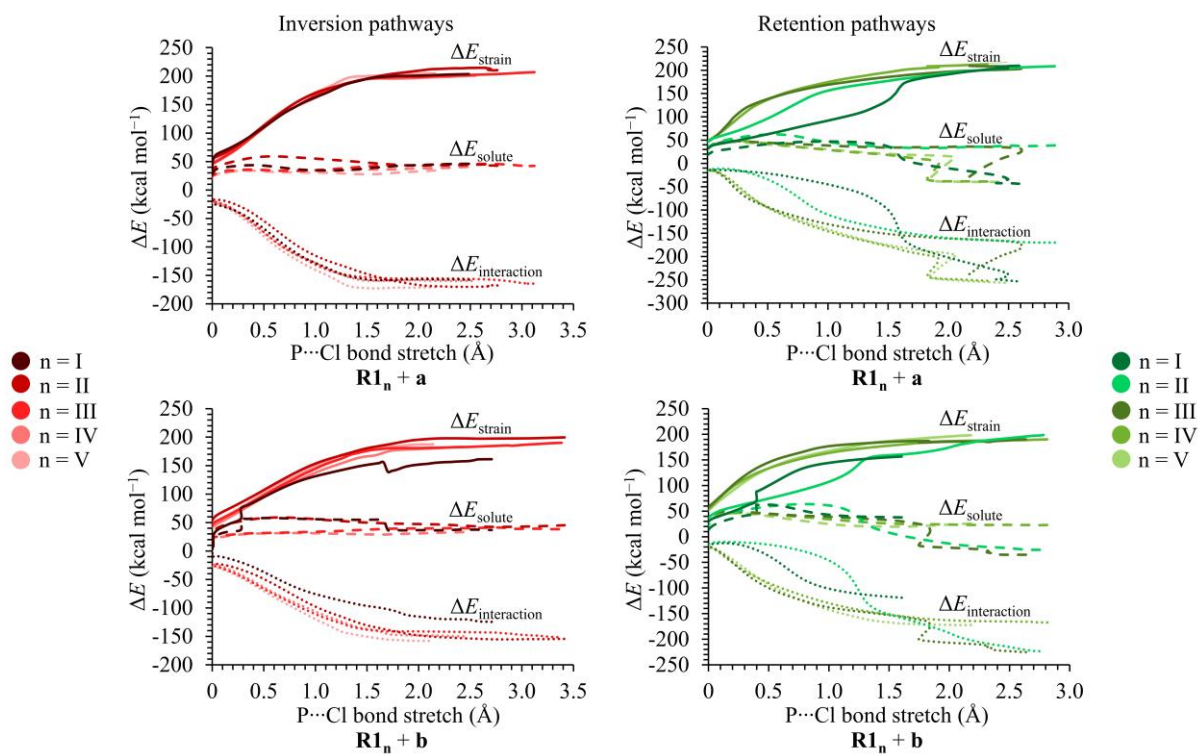


Figure S10: ASDs of the inversion and retention pathways of the $\mathbf{R1}_n + \mathbf{a}$ and $\mathbf{R1}_n + \mathbf{b}$ $S_N2@P$ reactions in THF.

S.5 THF-solvated $R1_n + b$ $S_N2@Cl$ reactions

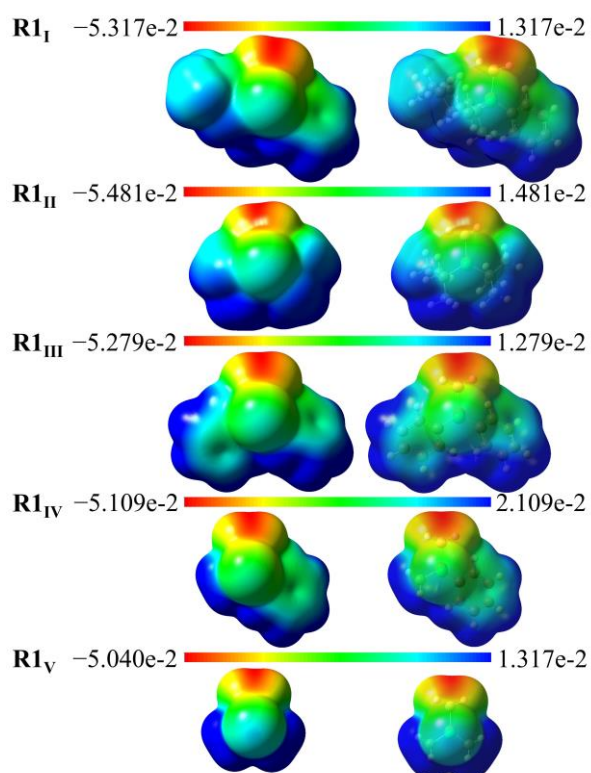


Figure S11: ESP maps (electrostatic potential in au) in THF showing the σ -hole at the extremity of the Cl atom.

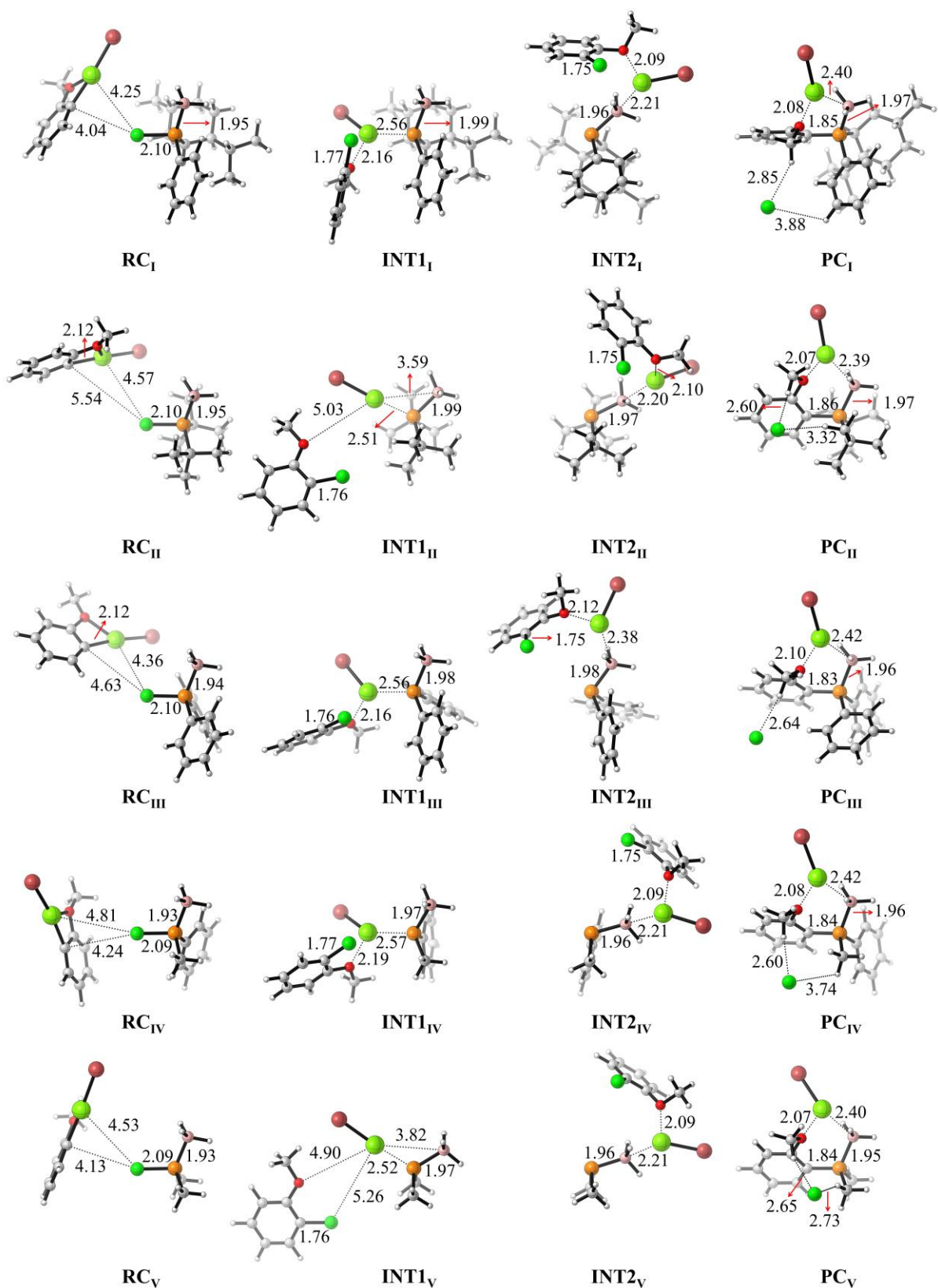


Figure S12 RCs, INTs and PCs of the $S_N2@Cl$, $S_N2@C-f$ mechanisms in THF.

S.6 Gas-phase $R1_n + b$ $S_{N2}@Cl$ reactions

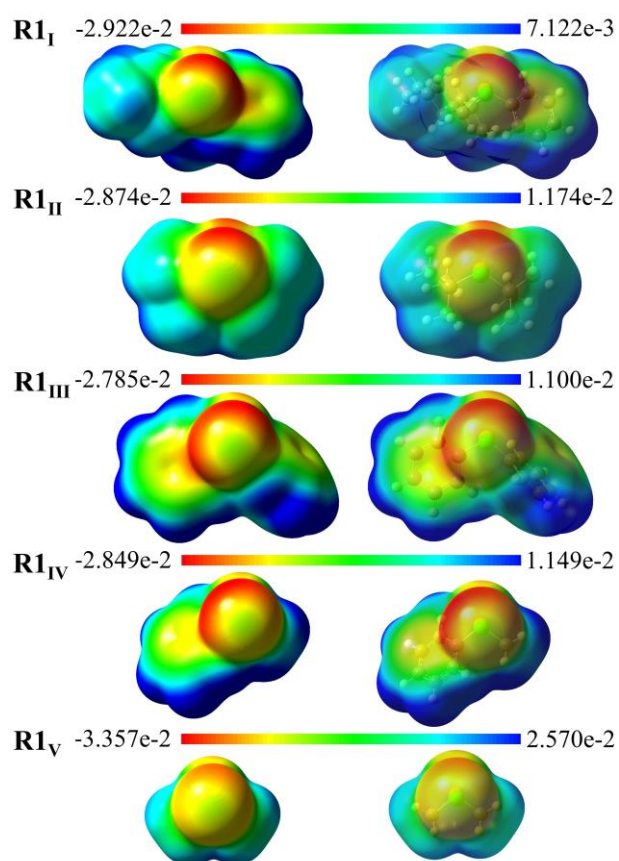


Figure S13: ESP maps (electrostatic potential in au) in the gas phase showing the σ -hole at the extremity of the Cl atom.

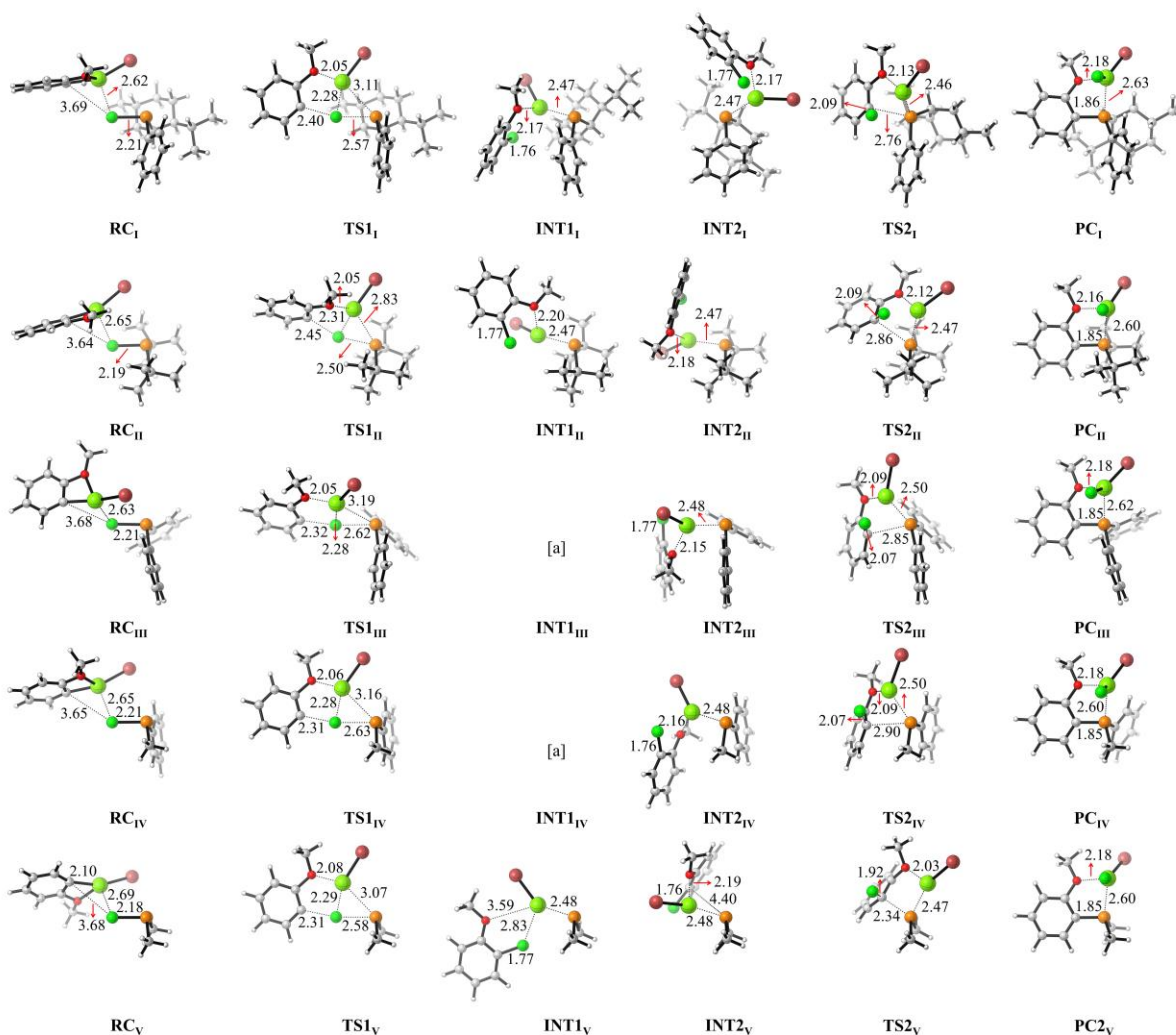


Figure S14: Geometries of the RCs, TSs, INTs, PCs and Ps of the gas-phase $S_N2@Cl$ and $S_N2@C-f$ pathways of the $R1 + b$ reaction. Bond lengths/distances are in Å.

Table S3: ΔG of the RCs, TSs, INTs, PCs and Ps of the gas-phase $S_N2@Cl$ and $S_N2@C-f$ pathways in kcal mol⁻¹.

$S_N2@Cl$ pathway					
	R1_I	R1_{II}	R1_{III}	R1_{IV}	R1_V
RC	-1.0	+1.7	+1.1	+1.6	+2.5
TS1	+43.1	+47.1	+44.6	+46.5	+50.9
INT1	+8.8	+14.6	[a]	[a]	+27.4
$S_N2@C-f$ pathway					
INT2	+11.4	+13.7	+9.9	+12.2	+17.7
TS2	+38.7	+42.1	+33.8	+35.3	+45.0
PC	-38.7	-43.1	-45.9	-44.4	-44.3
P	-18.1	-14.2	-20.0	-20.3	-20.4

[a] INT1_n converged to INT2_n (n = III and IV).

A comparison of the Table S3 with Table S1 shows that the $S_N2@Cl$ mechanisms are accompanied by higher Gibbs free activation energies than the $S_N2@P$ mechanisms. Hence, the $R1_n + b$ reactions occur *via* an $S_N2@P$ mechanism in the gas phase.

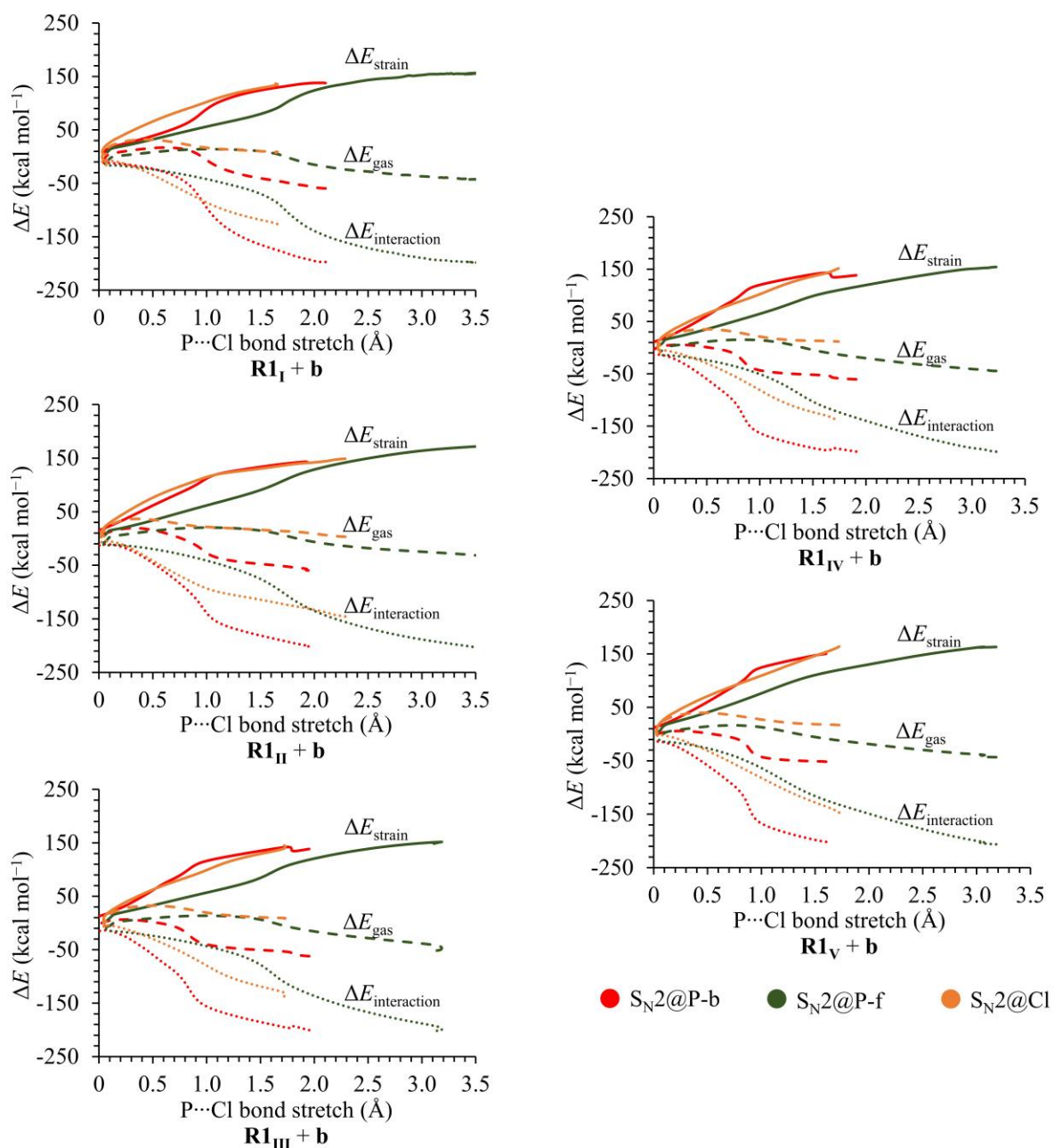


Figure S15: ASDs of the $S_N2@P-b$, $S_N2@P-f$ and $S_N2@Cl$ pathways of the $R1_n + b$ reactions in the gas phase.

S.7 $\mathbf{R1}_n + \mathbf{a}$ $\text{S}_{\text{N}2@}\text{Cl}$ reaction

We also attempted to locate the TS of the $\text{S}_{\text{N}2@}\text{Cl}$ mechanism of the $\mathbf{R1}_n + \mathbf{a}$ reaction to compare with the $\text{S}_{\text{N}2@}\text{P}$ pathways. However, the guess TS fails to converge. We attributed this to the fact that the σ -hole on the Cl atom is not attracted to the electron density on nucleophile **a**, which is lower than that of **b**.

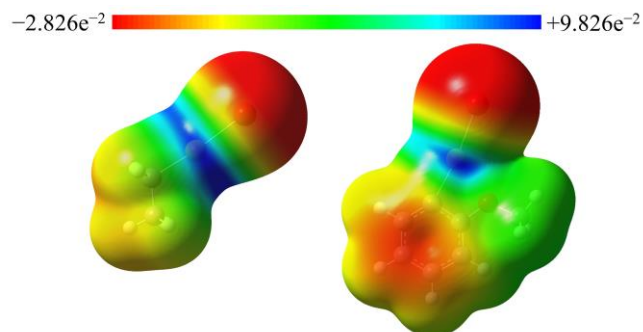


Figure S16: ESP maps of the nucleophiles **a** and **b**.

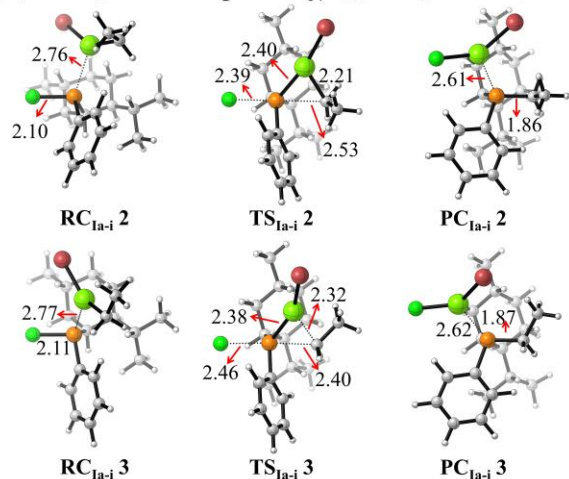
S.8 Alternative gas-phase S_N2@P reactions

Tables S4 and S5 list the gas-phase ΔG , in kcal mol⁻¹, of the RCs, TSs, PCs and Ps along the PES of alternative inversion and retention pathways of the S_N2@P reactions of reactants **R1_n** with the aliphatic and aromatic ion-pair nucleophiles **a** and **b**, respectively. The relative electronic energies (ΔE) are in parentheses in kcal mol⁻¹. The alternative pathways are labelled as 2, 3 and so on. Figures S13–S16 show the RCs, TSs and PCs of the alternative gas-phase S_N2@P reactions.

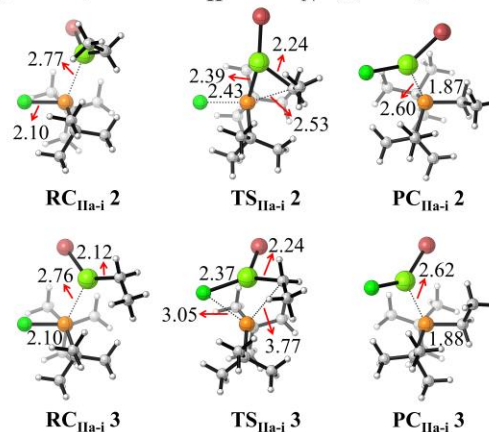
Table S4: ΔG , in kcal mol⁻¹, of the RCs, TSs, PCs and Ps along the PES of the alternative S_N2@P reactions of **R1_n** with nucleophile **a** in the gas phase. ΔE are in parentheses in kcal mol⁻¹.

Inversion pathway				
Pathways	RC	TS	PC	P
Ia-i 2	-1.9 (-13.4)	+31.6 (+18.1)	-49.8 (-62.3)	-33.4 (-35.5)
Ia-i 3	-2.4 (-13.5)	+34.6 (+21.0)	-46.3 (-59.1)	-33.4 (-35.5)
IIa-i 2	-0.8 (-12.2)	+32.3 (+19.2)	-48.6 (-61.3)	-30.9 (-33.3)
IIa-i 3	+0.6 (-11.1)	+32.8 (+21.4)	-48.7 (-61.0)	-30.9 (-33.3)
IIIa-i 2	+0.7 (-11.2)	+26.1 (+12.5)	-52.2 (-63.9)	-37.8 (-39.6)
IVa-i 2	-0.5 (-10.6)	+23.1 (+10.5)	-51.5 (-63.3)	-37.1 (-38.5)
IVa-i 3	+0.3 (-10.3)	+27.4 (+16.7)	-51.0 (-62.2)	-37.1 (-38.5)
Va-i 2	-0.1 (-9.7)	+31.8 (+21.2)	-50.8 (-61.4)	-36.7 (-38.3)
Retention pathway				
Ia-r 2	+2.6 (-8.4)	+25.4 (+13.8)	-54.2 (-66.7)	-33.4 (-35.5)
IIa-r 2	+3.6 (-6.2)	+37.4 (+25.6)	-48.5 (-61.3)	-30.9 (-33.3)
IIIa-r 2	+2.7 (-9.4)	+24.8 (+13.1)	-50.4 (-62.9)	-37.6 (-39.5)
IIIa-r 3	+2.8 (-7.1)	+24.1 (+12.6)	-40.8 (-53.3)	-37.6 (-39.5)
IVa-r 2	+2.2 (-6.9)	+25.9 (+15.0)	-32.9 (-42.9)	-37.2 (-38.8)
IVa-r 3	+2.8 (-6.5)	+26.1 (+15.1)	-40.3 (-51.5)	-37.1 (-38.5)
Va-r 2	-0.5 (-9.8)	+27.8 (+16.5)	-50.7 (-61.6)	-36.7 (-38.3)

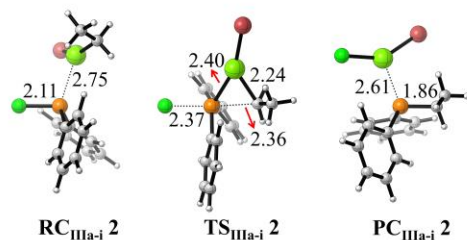
(a) Gas-phase $\mathbf{R1}_I + \mathbf{a}$ $S_N2@P$ -b pathways



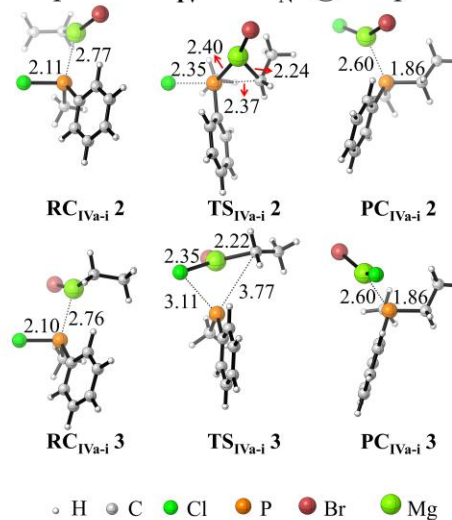
(b) Gas-phase $\mathbf{R1}_{II} + \mathbf{a}$ $S_N2@P$ -b pathways



(c) Gas-phase $\mathbf{R1}_{III} + \mathbf{a}$ $S_N2@P$ -b pathways



(d) Gas-phase $\mathbf{R1}_{IV} + \mathbf{a}$ $S_N2@P$ -b pathways



(e) Gas-phase $\mathbf{R1}_V + \mathbf{a}$ $S_N2@P$ -b pathways

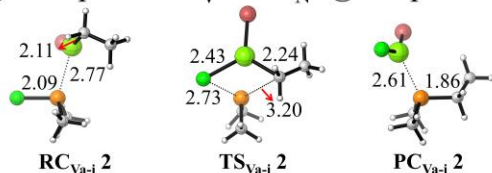


Figure S17: Alternative gas-phase $S_N2@P$ -b pathways of the $\mathbf{R1}_n + \mathbf{a}$ reactions. Bond lengths/distances are in Å.

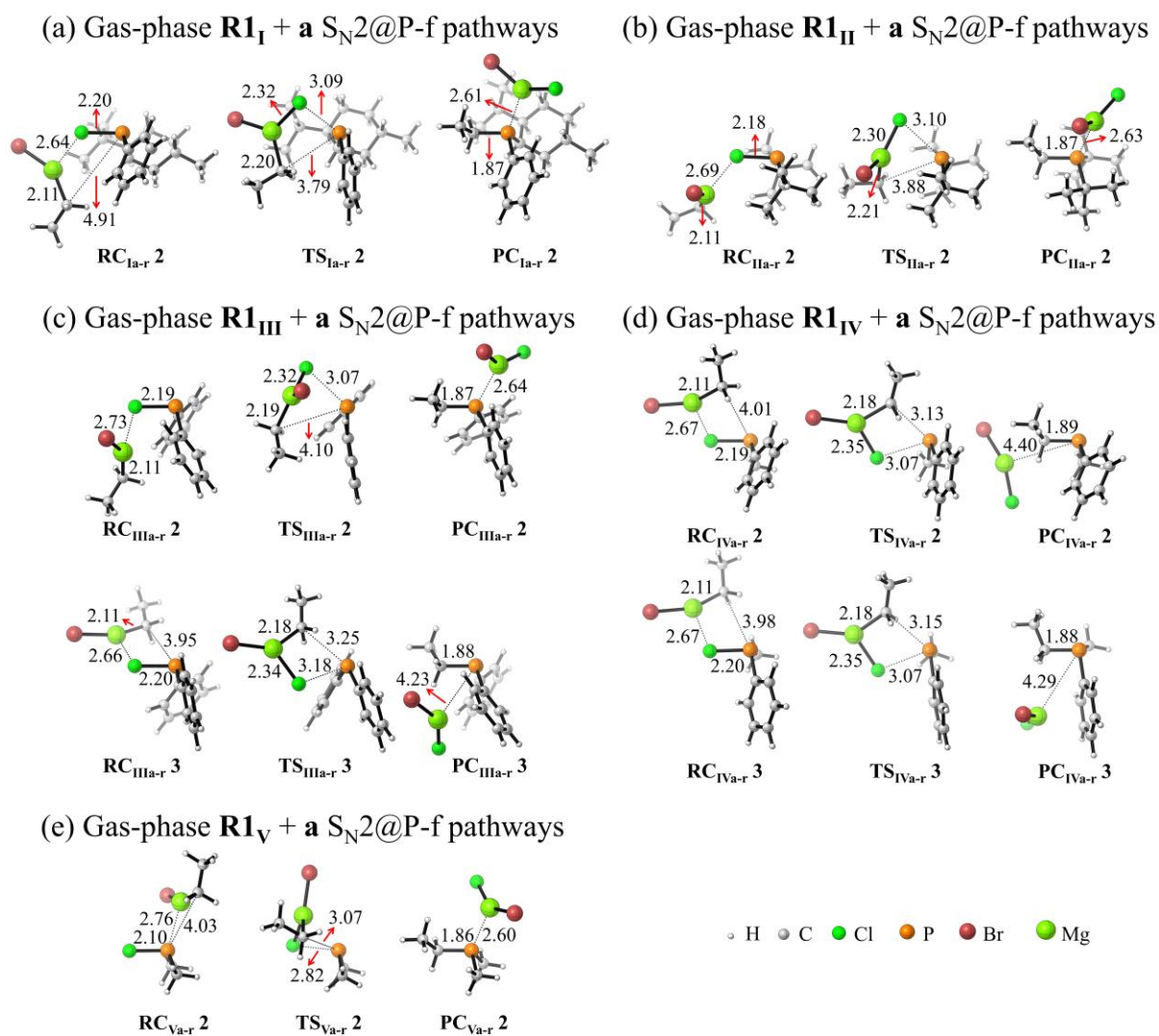
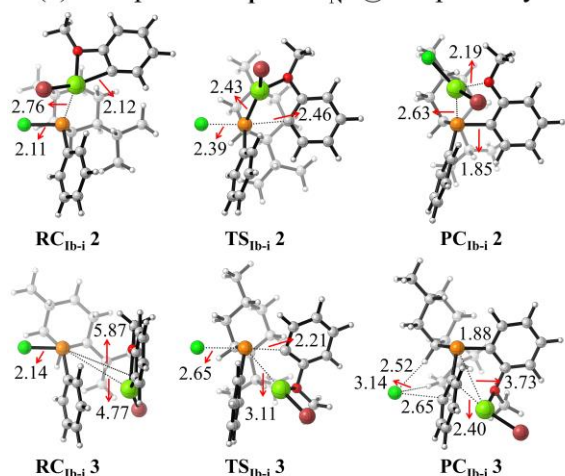


Figure S18: Alternative gas-phase $S_N2@P$ -f pathways of the $\mathbf{R1}_n + \mathbf{a}$ reactions. Bond lengths/distances are in Å.

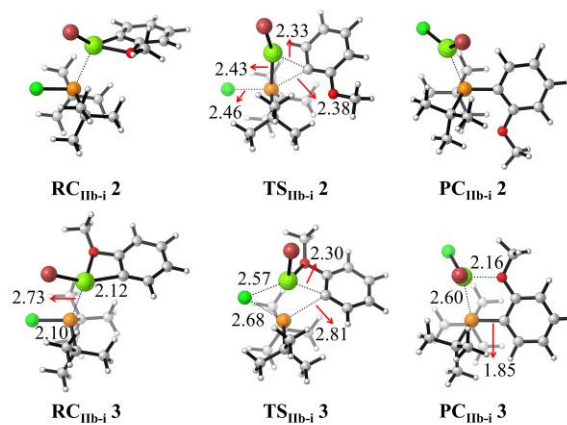
Table S5: ΔG , in kcal mol⁻¹, of the RCs, TSs, PCs and Ps along the PES of the alternative **R1_n + b** **S_N2@P** reactions in the gas phase. ΔE are in parentheses in kcal mol⁻¹.

Inversion pathway				
Pathways	RC	TS	PC	P
Ib-i 2	+0.4 (-11.4)	+30.4 (+16.0)	-37.1 (-51.8)	-17.5 (-19.3)
Ib-i 3	+5.7 (-5.8)	+37.6 (+23.0)	+27.5 (+14.1)	-18.8 (-20.3)
IIb-i 2	-1.3 (-12.8)	+42.6 (+28.7)	-31.4 (-44.9)	-14.2 (-16.7)
IIb-i 3	-1.7 (-12.6)	+34.8 (+22.9)	-43.3 (-57.4)	-14.2 (-16.7)
IIIb-i 2	+2.3 (-8.2)	+27.6 (+15.1)	-46.5 (-60.1)	-22.3 (-24.5)
IVb-i 2	-0.8 (-11.3)	+20.1 (+7.8)	-44.9 (-57.5)	-21.2 (-22.9)
IVb-i 3	+2.4 (-10.0)	+27.1 (+14.5)	-44.9 (-57.5)	-21.2 (-22.9)
Vb-i 2	+3.5 (-6.4)	+31.1 (+19.1)	-44.8 (-56.8)	-20.4 (-22.1)
Retention pathway				
Ib-r 2	+2.4 (-8.6)	+31.6 (+19.0)	-43.6 (-57.6)	-18.1 (-20.3)
IVb-r 2	+2.9 (-6.9)	+28.8 (+16.3)	-35.0 (-48.8)	-21.4 (-22.8)
IVb-r 3	+3.0 (-6.8)	+32.4 (+20.8)	-26.3 (-38.7)	-21.4 (-22.8)
IVb-r 4	+0.6 (-10.3)	+30.5 (+18.6)	-27.9 (-40.8)	-21.2 (-22.9)
IVb-r 5	+2.6 (-7.1)	+32.4 (+21.4)	-24.8 (-36.9)	-21.2 (-22.9)
IVb-r 6	+3.0 (-6.8)	+30.9 (+19.8)	-28.4 (-40.3)	-21.4 (-22.8)
Vb-r 2	+3.5 (-6.4)	+30.3 (+18.3)	-29.7 (-41.8)	-20.4 (-22.1)

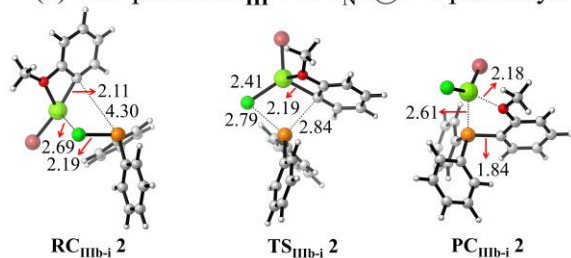
(a) Gas-phase $\mathbf{R1}_I + \mathbf{b}$ $S_N2@P$ -b pathways



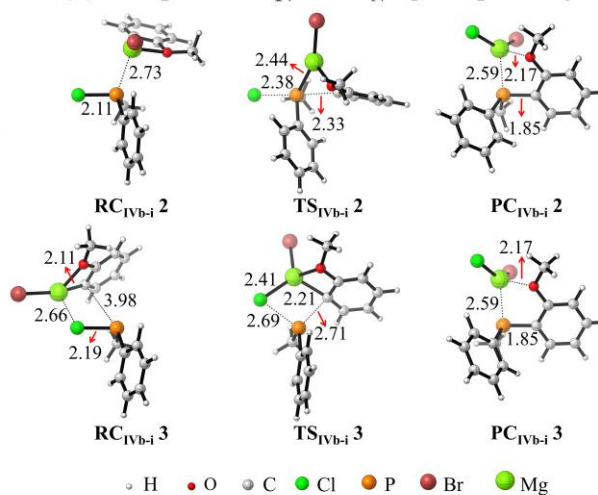
(b) Gas-phase $\mathbf{R1}_{II} + \mathbf{b}$ $S_N2@P$ -b pathways



(c) Gas-phase $\mathbf{R1}_{III} + \mathbf{b}$ $S_N2@P$ -b pathways



(d) Gas-phase $\mathbf{R1}_{IV} + \mathbf{b}$ $S_N2@P$ -b pathways



(e) Gas-phase $\mathbf{R1}_V + \mathbf{b}$ $S_N2@P$ -b pathways

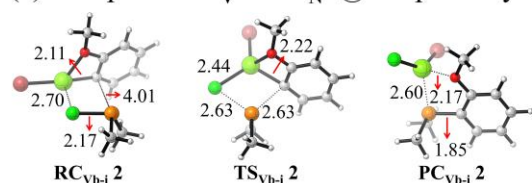
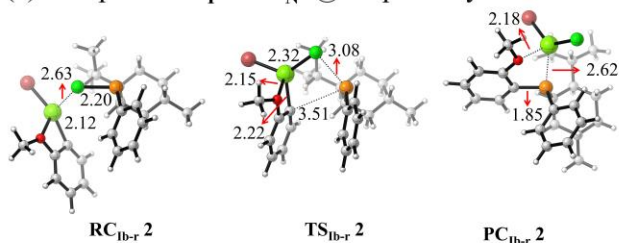
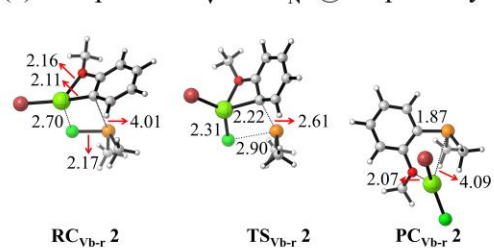


Figure S19: Alternative gas-phase $S_N2@P$ -b pathways of the $\mathbf{R1}_n + \mathbf{b}$ reactions. Bond lengths/distances are in Å.

(a) Gas-phase $\mathbf{R1}_I + \mathbf{b}$ $\text{S}_N2@P$ -f pathways



(c) Gas-phase $\mathbf{R1}_V + \mathbf{b}$ $\text{S}_N2@P$ -f pathways



(b) Gas-phase $\mathbf{R1}_{IV} + \mathbf{b}$ $\text{S}_N2@P$ -f pathways

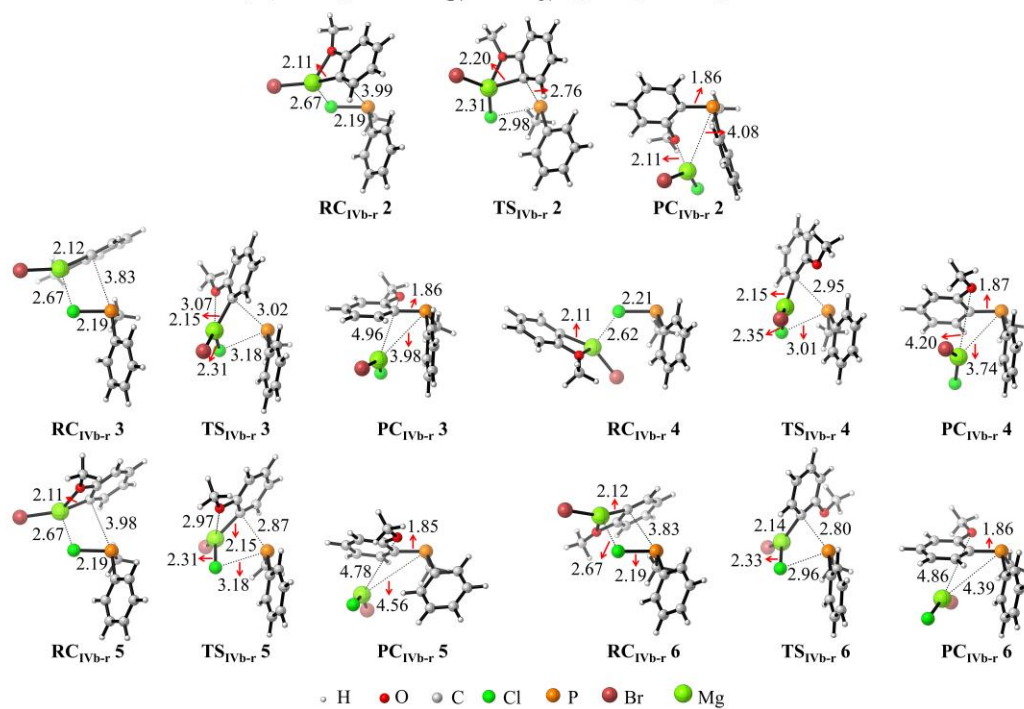


Figure S20: Alternative gas-phase $\text{S}_N2@P$ -f pathways of the $\mathbf{R1}_n + \mathbf{b}$ reactions. Bond lengths/distances are in Å.

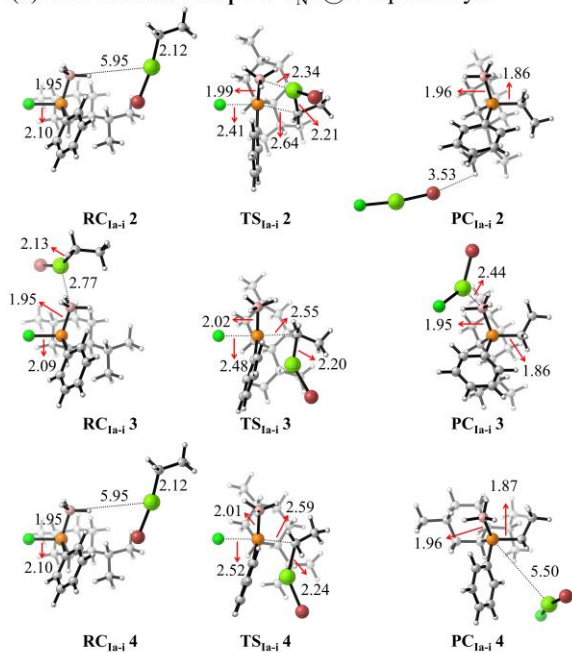
S.9 Alternative THF-solvated S_N2@P reactions

Tables S6 and S7 list the THF-solvated ΔG , in kcal mol⁻¹, of the RCs, TSs, PCs and Ps along the PES of alternative inversion and retention pathways of the S_N2@P reactions of **R1_n** with the aliphatic and aromatic ion-pair nucleophiles **a** and **b**, respectively. The relative electronic energies (ΔE) are in parentheses in kcal mol⁻¹. The alternative pathways are labelled as 2, 3 and so on. Figures S21–S24 show the RCs, TSs and PCs of the alternative THF-solvated S_N2@P reactions.

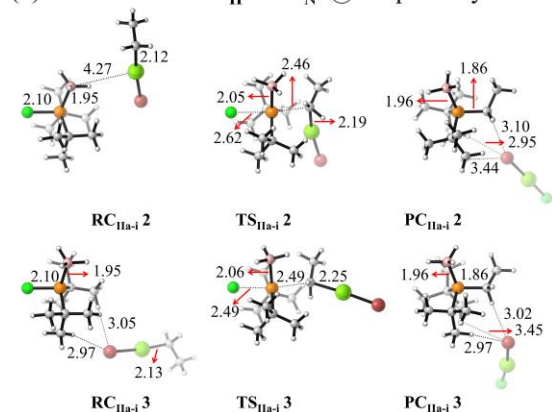
Table S6: ΔG , in kcal mol⁻¹, of the RCs, TSs, PCs and Ps along the alternative inversion and retention pathways of the **R1_n** + **a** S_N2@P reactions in THF. ΔE are in parentheses in kcal mol⁻¹.

Inversion pathway				
Pathways	RC	TS	PC	P
Ia-i 2	+5.1 (-4.4)	+57.5 (+41.9)	-37.6 (-48.5)	-42.6 (-45.8)
Ia-i 3	+8.7 (-2.6)	+45.4 (+30.8)	-44.8 (-57.1)	-47.3 (-50.3)
Ia-i 4	+5.1 (-4.4)	+61.7 (+46.2)	-36.2 (-48.6)	-47.3 (-50.3)
IIa-i 2	+7.0 (-2.6)	+73.5 (+58.4)	-41.8 (-53.3)	-43.7 (-47.0)
IIa-i 3	+6.4 (-3.0)	+58.0 (+44.5)	-40.4 (-51.4)	-43.7 (-47.0)
IIIa-i 2	+7.7 (-0.6)	+36.1 (+22.7)	+2.7 (-8.6)	-50.8 (-53.6)
IVa-i 2	+9.7 (-0.7)	+31.8 (+17.9)	-48.9 (-60.5)	-50.4 (-52.9)
IVa-i 3	+7.1 (-1.1)	+34.9 (+22.8)	-48.7 (-60.7)	-50.4 (-52.9)
IVa-i 4	+7.9 (-1.0)	+43.1 (+28.9)	-46.4 (-57.5)	-50.8 (-53.3)
Va-i 2	+8.3 (+0.1)	+51.0 (+37.2)	-44.4 (-53.4)	-49.9 (-52.6)
Retention pathway				
IVa-r 2	+10.3 (+0.1)	+44.5 (+31.2)	-49.2 (-60.8)	-50.8 (-53.3)

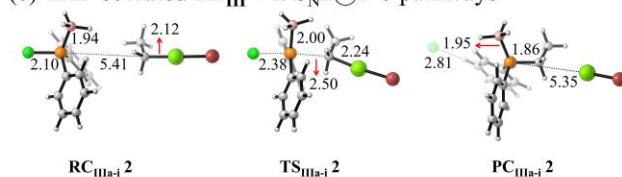
(a) THF-solvated $\mathbf{R1}_I + \mathbf{a}$ $S_N2@P$ -b pathways



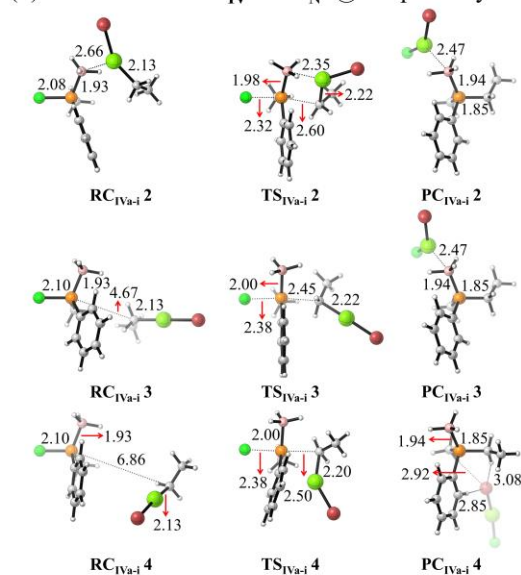
(b) THF-solvated $\mathbf{R1}_{II} + \mathbf{a}$ $S_N2@P$ -b pathways



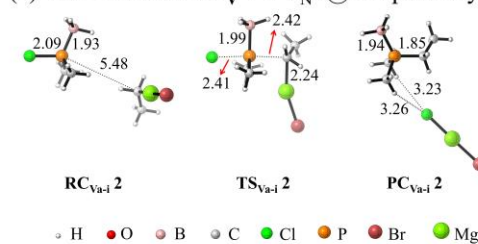
(c) THF-solvated $\mathbf{R1}_{III} + \mathbf{a}$ $S_N2@P$ -b pathways



(d) THF-solvated $\mathbf{R1}_{IV} + \mathbf{a}$ $S_N2@P$ -b pathways



(e) THF-solvated $\mathbf{R1}_V + \mathbf{a}$ $S_N2@P$ -b pathways



○ H ● O ● B ● C ● Cl ● P ● Br ● Mg

Figure S21: Alternative THF-solvated $S_N2@P$ -b pathways of $\mathbf{R1}_n + \mathbf{a}$ reactions. Bond lengths/distances are in Å.

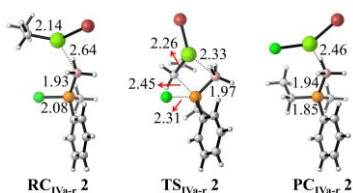
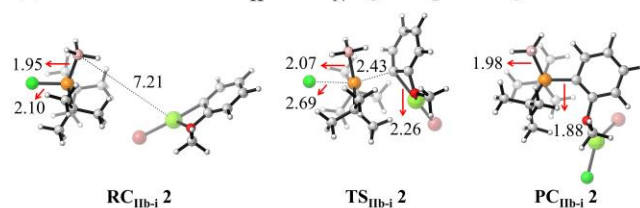


Figure S22: Alternative THF-solvated $S_N2@P$ -f pathways of $\mathbf{R1}_{IV} + \mathbf{a}$ reaction. Bond lengths/distances are in Å.

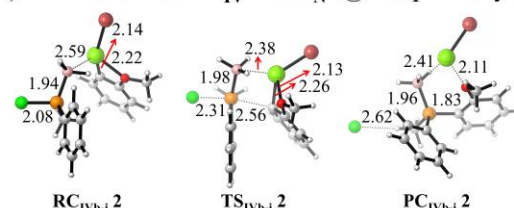
Table S7: ΔG , in kcal mol⁻¹, of the RCs, TSs, PCs and Ps along the alternative inversion and retention pathways of the **R1_n** + **b** S_N2@P reactions in THF. ΔE are in parentheses in kcal mol⁻¹

Inversion pathway				
Pathways	RC	TS	PC	P
Iib-i 2	+7.1 (-2.5)	+73.1 (+57.8)	-17.3 (-32.6)	-29.4 (-33.3)
IIIb-i 2	+7.6 (-4.2)	+41.6 (+24.9)	-33.5 (-46.0)	-37.0 (-40.4)
IVb-i 2	+8.7 (-2.1)	+28.9 (+14.5)	-10.9 (-24.0)	-36.9 (-39.9)
Vb-i 2	+7.7 (-0.4)	+43.5 (+29.0)	+3.0 (-8.6)	-37.6 (-40.7)
Retention pathway				
Iib-r 2	+5.9 (-6.0)	+77.9 (+62.6)	+14.9 (+0.2)	-33.7 (-37.2)
Iib-r 3	+8.6 (-3.2)	+59.3 (+43.7)	-5.5 (-20.7)	-29.8 (-33.3)
Iib-r 4	+5.0 (-5.4)	+78.4 (+63.3)	-20.7 (-33.7)	-33.7 (-37.2)
IIIb-r 2	+9.8 (-1.1)	+51.4 (+37.2)	-34.0 (-47.7)	-36.6 (-40.3)
IIIb-r 3	+11.2 (-0.2)	+51.2 (+37.0)	-32.5 (-46.3)	-36.6 (-40.3)
IVb-r 2	+9.3 (-2.1)	+48.9 (+34.3)	-37.2 (-50.4)	-36.5 (-39.5)
IVb-r 3	+9.4 (-1.3)	+46.8 (+32.2)	-11.6 (-24.6)	-36.5 (-39.5)
IVb-r 4	+9.5 (-1.0)	+49.6 (+36.1)	-38.3 (-52.0)	-36.5 (-39.5)
Vb-r 2	+8.1 (-1.0)	+48.4 (+34.9)	-36.2 (-48.4)	-37.6 (-40.7)

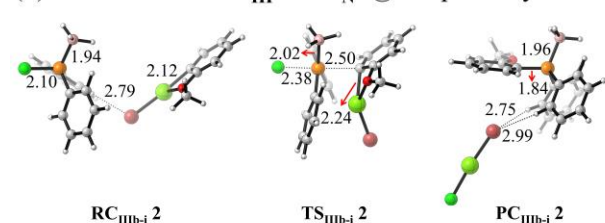
(a) THF-solvated **R1_{II}** + **b** S_N2@P-b pathways



(c) THF-solvated **R1_{IV}** + **b** S_N2@P-b pathways



(b) THF-solvated **R1_{III}** + **b** S_N2@P-b pathways



(d) THF-solvated **R1_V** + **b** S_N2@P-b pathways

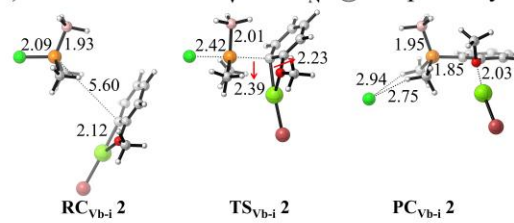
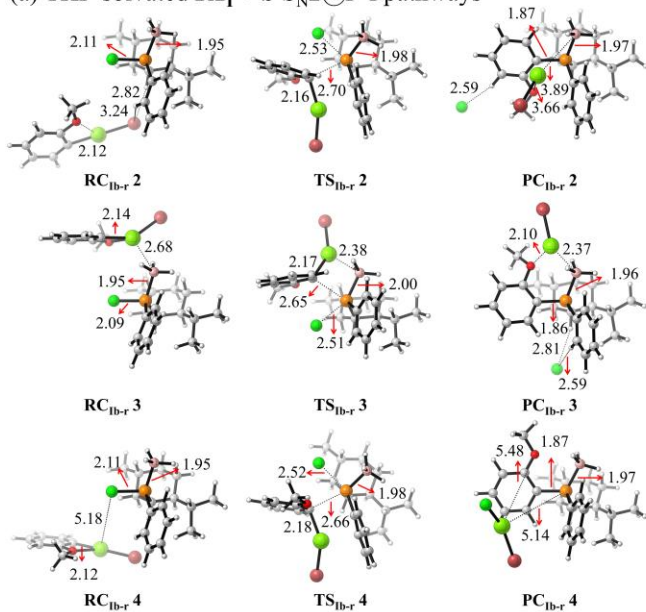
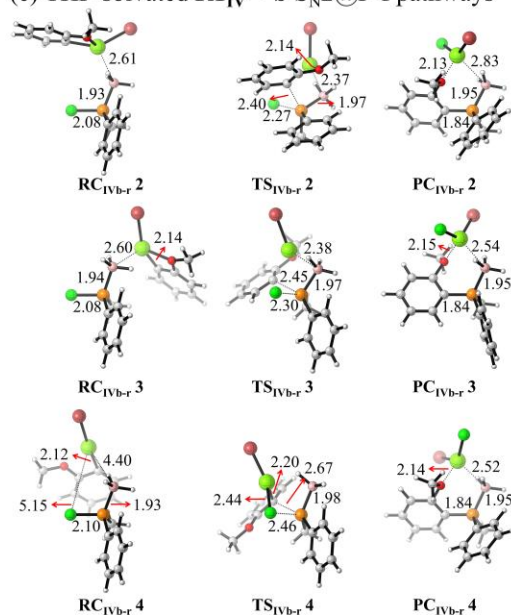


Figure S23: Alternative THF-solvated S_N2@P-b pathways of **R1_n** + **b** reactions. Bond lengths/distances are in Å.

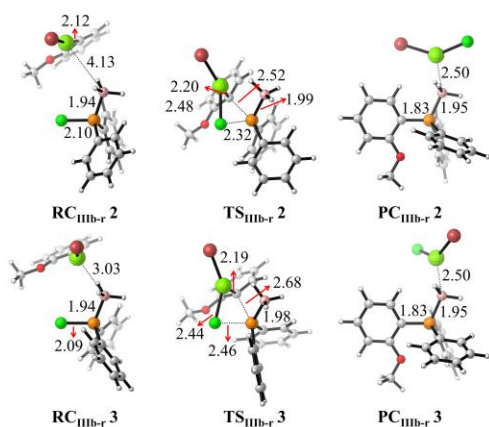
(a) THF-solvated $\mathbf{R1}_I + \mathbf{b}$ $S_N2@P$ -f pathways



(c) THF-solvated $\mathbf{R1}_{IV} + \mathbf{b}$ $S_N2@P$ -f pathways



(b) THF-solvated $\mathbf{R1}_{III} + \mathbf{b}$ $S_N2@P$ -f pathways



(d) THF-solvated $\mathbf{R1}_V + \mathbf{b}$ $S_N2@P$ -f pathways

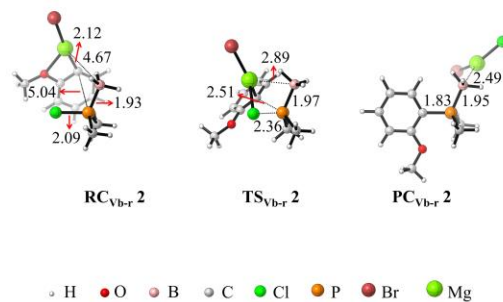


Figure S24: Alternative THF-solvated $S_N2@P$ -f pathways of $\mathbf{R1}_n + \mathbf{b}$ reactions. Bond lengths/distances are in Å.

S.9 Noncovalent interactions

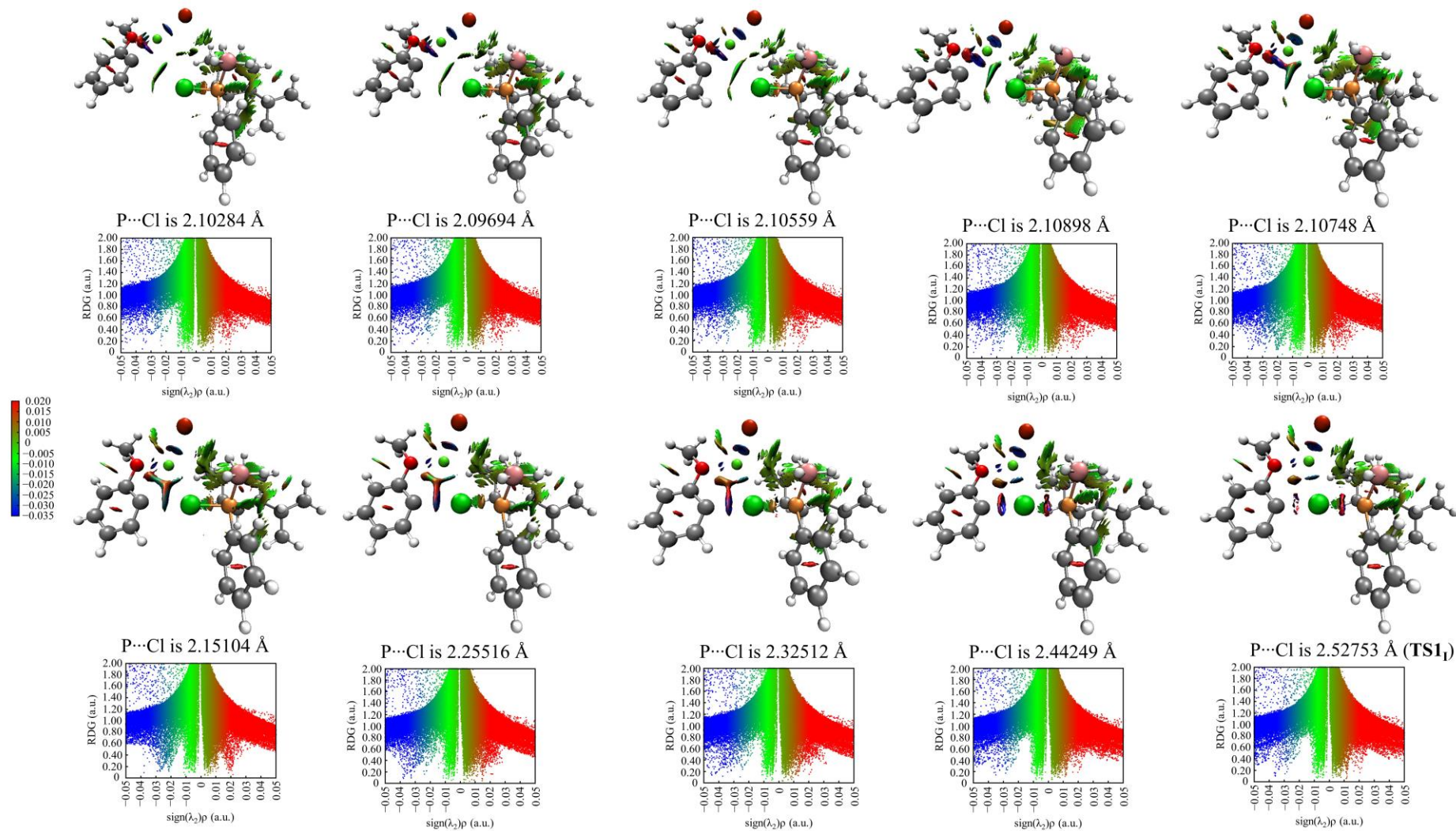


Figure S25: 2D and 3D plots of the NCI isosurfaces of along the first part of the PES of the $\mathbf{R1I} + \mathbf{b} \text{ S}_{\text{N}}2@Cl$ mechanism in THF.

The isosurfaces in Figure S25 show the evolution of the interaction between the Cl atom and the nucleophile **b** along the first part of the PES of the **R1_I** + **b** S_N2@Cl mechanism in THF. At the start of the reaction, there are van der Waals forces of attraction between the Cl atom of **R1_I** and phenyl ring of **b**, shown by the green isosurface. As the reaction proceeds towards the TS, the green isosurface becomes blue, which depicts attraction between the Cl atom of **R1_I** and the C atom of **b**.

S.11 Effect of temperature

We investigated the effect of temperature on the **RI**₁ + **a** and **RI**₁ + **b** reactions with a frequency computation of the optimised geometries at 193.15 K (−80 °C) both in the gas phase and in THF. Tables S8–S9 list the ΔG of the RCs, TSs and PCs of the inversion and retention pathways in kcal mol^{−1}. Table S10 shows the ΔG of the RC, TSs, INTs and PC of the halogen bond-assisted mechanism of the **RI**₁ + **b** reaction. The temperature of 193.15 K causes a decrease in the ΔG along the PESs in both the gas phase and in THF. The trend in the preference of pathways remains similar to the trend observed at room temperature: the S_N2@P-b inversion pathway is preferred by the **RI**₁ + **a** reaction and the halogen bond-assisted S_N2@Cl, followed by S_N2@C-f, is preferred by the **RI**₁ + **b** reaction.

Table S8: ΔG , in kcal mol^{−1}, of the RCs, TSs and PCs of the inversion and retention pathways of the **RI**₁ + **a** reaction in the gas phase at 193.15 K. The ΔG at room temperature is in parentheses.

Inversion pathway	
RC _{Ia-i}	−5.6 (−1.5)
TS _{Ia-i}	+17.8 (+21.7)
PC _{Ia-i}	−53.0 (−48.7)
Retention pathway	
RC _{Ia-r}	−3.0 (+0.2)
TS _{Ia-r}	+17.7 (+21.7)
PC _{Ia-r}	−38.1 (−33.9)

Table S9: ΔG , in kcal mol^{−1}, of the RCs, TSs and PCs of the inversion and retention pathways of the **RI**₁ + **b** reaction in the gas phase at 193.15 K. The ΔG at room temperature is in parentheses.

Inversion pathway	
RC _{Ib-i}	−1.6 (+1.9)
TS _{Ib-i}	+23.7 (+27.7)
PC _{Ib-i}	−48.1 (−43.2)
Retention pathway	
RC _{Ib-r}	−4.2 (−0.8)
TS _{Ib-r}	+21.7 (+25.9)
PC _{Ib-r}	−32.6 (−28.0)

Table S10: ΔG , in kcal mol^{−1}, of the RCs, TSs and PCs of the inversion and retention pathways of the **RI**₁ + **a** reaction in THF at 193.15 K. The ΔG at room temperature is in parentheses.

Inversion pathway	
RC _{Ia-i}	+5.9 (+10.0)
TS _{Ia-i}	+36.6 (+41.7)
PC _{Ia-i}	−15.4 (−11.0)
Retention pathway	
RC _{Ia-r}	+4.5 (+8.3)
TS _{Ia-r}	+40.2 (+44.3)
PC _{Ia-r}	−53.3 (−49.0)

Table S11: ΔG , in kcal mol⁻¹, of the RCs, TSs and PCs of the inversion and retention pathways of the **R1_I + b** reaction in THF at 193.15 K. The ΔG at room temperature is in parentheses.

Inversion pathway	
RC_{Ib-i}	+4.3 (+8.1)
TS_{Ib-i}	+48.2 (+53.9)
PC_{Ib-i}	+8.9 (+14.4)
Retention pathway	
RC_{Ib-r}	+3.1 (+6.9)
TS_{Ib-r}	+54.0 (+59.1)
PC_{Ib-r}	+0.8 (+5.5)

Table S10: ΔG , in kcal mol⁻¹, of the RCs, TSs, INTs and PCs of halogen bond-assisted reaction mechanism for the **R1_I + b** reaction in THF at 193.15 K. The ΔG at room temperature is in parentheses.

RC_I	+3.7 (+6.3)
TS1_I	+38.9 (+43.9)
INT1_I	+7.3 (+12.7)
INT2_I	+6.0 (+9.7)
TS2_I	+48.7 (+54.2)
PC_I	-9.1 (-4.2)

S.12 Coordinates

S.12.1 Gas-phase reactions in manuscript

R1r

E = -1425.796240 ZPVE = 0.365813 NIMAG = 0.

6	0.81644	0.000516	0.649576
6	2.331227	1.479196	-0.77703
6	3.182969	-0.80932	-0.003498
6	2.073524	-0.797421	1.06085
6	3.551436	0.633535	-0.3795
6	0.037296	2.42615	0.000227
6	4.403533	-1.605971	0.472841
6	-0.898725	2.572395	1.213441
6	0.498544	3.826928	-0.443976
1	0.13361	0.008471	1.504751
1	2.66441	2.50522	-0.9577
1	1.921104	1.113249	-1.728232
1	2.790154	-1.306114	-0.903303
1	1.801244	-1.820437	1.33489
1	2.470803	-0.3263	1.973339
1	4.283991	0.633914	-1.19704
1	4.048738	1.105035	0.482436
1	-0.545978	2.002416	-0.831068
1	4.136329	-2.64383	0.700833
1	5.188923	-1.621914	-0.291503
1	4.831651	-1.162252	1.380921
1	-0.356225	3.001417	2.065907
1	-1.730288	3.24531	0.978206
1	-1.333462	1.622552	1.532429
1	1.173749	4.273071	0.297879

1	-0.365086	4.493183	-0.54496
1	1.015919	3.815407	-1.406917
6	-1.900014	-0.567731	-0.29572
6	-2.771045	0.023491	-1.223499
6	-2.414488	-0.99029	0.941575
6	-4.1217	0.214746	-0.914283
1	-2.392107	0.333254	-2.194246
6	-3.76314	-0.809902	1.24743
1	-1.764467	-1.47896	1.661819
6	-4.618871	-0.200925	0.321892
1	-4.782215	0.677836	-1.64168
1	-4.148819	-1.145912	2.205857
1	-5.668799	-0.060821	0.562478
17	0.068324	-2.864932	-0.408871
6	1.227868	1.472244	0.304659
1	1.692582	1.856124	1.229316
15	-0.135758	-0.774794	-0.820901

R1_{II}

E = -1117.304696 ZPVE = 0.246396 NIMAG = 0.

15	0.005074	0.249873	0.779851
17	-0.036045	2.21376	-0.061814
6	-1.585101	-0.468776	-0.029252
6	-1.607223	-1.987712	0.243622
1	-2.613091	-2.373901	0.036581
1	-0.911105	-2.532286	-0.400233
1	-1.37478	-2.227574	1.287857
6	-1.80404	-0.199618	-1.52719

1	-2.797359	-0.56904	-1.814153
1	-1.768162	0.868519	-1.756002
1	-1.07093	-0.708597	-2.155532
6	-2.733965	0.190524	0.771037
1	-3.693602	-0.217665	0.429677
1	-2.64687	-0.00609	1.844857
1	-2.760503	1.274273	0.623618
6	1.597963	-0.443785	-0.03679
6	1.611457	-0.555637	-1.568423
1	2.622579	-0.819527	-1.905576
1	0.936095	-1.336166	-1.92898
1	1.338229	0.389721	-2.046594
6	1.847854	-1.828242	0.605823
1	2.838478	-2.188306	0.301208
1	1.838069	-1.77684	1.700236
1	1.118267	-2.578466	0.292356
6	2.736141	0.499632	0.417539
1	2.737363	0.644111	1.503739
1	3.699786	0.055863	0.137886
1	2.665668	1.48164	-0.056068

R1m

E = -1264.903251 ZPVE = 0.183825 NIMAG = 0.

6	-1.435307	0.074489	-0.252112
6	-2.559494	-0.046305	-1.083687
6	-1.454881	-0.526841	1.018029
6	-3.682702	-0.764012	-0.659639
1	-2.556213	0.422097	-2.064645

6	-2.576986	-1.236621	1.442501
1	-0.593071	-0.435998	1.672273
6	-3.691561	-1.358205	0.603239
1	-4.545678	-0.854226	-1.312847
1	-2.584905	-1.696029	2.426799
1	-4.563468	-1.913564	0.936859
17	0.052023	2.659106	0.483335
15	-0.014099	1.048723	-0.913601
6	1.420442	0.025862	-0.340151
6	1.443138	-1.329684	-0.717084
6	2.546768	0.568947	0.295128
6	2.559003	-2.123689	-0.448244
1	0.584301	-1.77475	-1.212596
6	3.661836	-0.229962	0.565255
1	2.55078	1.611804	0.593768
6	3.672818	-1.576373	0.195444
1	2.555039	-3.170543	-0.738199
1	4.521438	0.204619	1.067557
1	4.540424	-2.194676	0.406288

R1_{IV}

E = -1073.161639 ZPVE = 0.130411 NIMAG = 0.

17	-2.316313	0.944074	0.783211
15	-1.330677	-0.838458	0.150293
6	-1.801574	-0.777838	-1.646383
1	-2.877373	-0.949787	-1.739038
1	-1.544758	0.170821	-2.125351
1	-1.273174	-1.591348	-2.156349

6	0.423655	-0.266575	0.057391
6	1.385391	-1.096233	0.654621
6	0.843999	0.912178	-0.581155
6	2.743988	-0.767848	0.597484
1	1.071029	-2.001311	1.168349
6	2.197184	1.245276	-0.629343
1	0.11218	1.581544	-1.024227
6	3.150277	0.402919	-0.04412
1	3.477903	-1.420622	1.061025
1	2.510473	2.16216	-1.120494
1	4.203673	0.664895	-0.083867

R1v

E = -881.418727 ZPVE = 0.076697 NIMAG = 0.

17	0.257024	-1.562552	0
15	-0.666418	0.354126	0
6	0.257024	1.124877	1.415731
1	-0.040673	0.643652	2.350987
1	1.342791	1.051145	1.301561
1	-0.030832	2.181681	1.470135
6	0.257024	1.124877	-1.415731
1	1.342791	1.051145	-1.301561
1	-0.040673	0.643652	-2.350987
1	-0.030832	2.181681	-1.470135

Nucleophile a

E = -2851.112773 ZPVE = 0.064954 NIMAG = 0.

6	-2.642586	0.612788	0.000154
1	-2.856774	1.245181	-0.873056
1	-2.856718	1.244993	0.873514
6	-3.581909	-0.610838	0.000052
1	-3.432404	-1.245463	0.881453
1	-4.639538	-0.312239	0.000117
1	-3.432459	-1.245275	-0.881493
12	-0.577227	0.243663	0.000048
35	1.756902	-0.074938	-0.000067

Nucleophile b

E = -3118.095888 ZPVE = 0.123724 NIMAG = 0.

12	0.786393	-0.416458	-0.000001
35	3.134896	-0.266011	0.000039
6	-1.24189	-0.917329	-0.000053
6	-1.64387	0.422494	-0.000001
6	-2.275054	-1.859943	-0.000109
6	-2.959663	0.871689	-0.000001
6	-3.623428	-1.467246	-0.000113
1	-2.04137	-2.922511	-0.000152
6	-3.960084	-0.112436	-0.000059
1	-3.224129	1.923977	0.000041
1	-4.409161	-2.2176	-0.000158
1	-5.002948	0.191332	-0.000062
8	-0.508691	1.286191	0.000057
6	-0.678544	2.705792	0.000058
1	-1.219568	3.024799	0.896944

1	0.323383	3.135428	0.000073
1	-1.219545	3.024803	-0.89684

MgClBr

E = -3232.161622 ZPVE = 0.002541 NIMAG = 0.

17	0	0	-2.884437
12	0	0	-0.689014
35	0	0	1.637246

R11 + a S_N2@P-b pathway

RC_{1a-i}

E = -4276.931440 ZPVE = 0.431783 NIMAG = 0.

6	0.216286	-1.795286	0.258675
6	-1.477242	-0.96584	1.971127
6	1.019958	-0.903811	2.550722
6	1.249247	-1.907781	1.408026
6	-0.416315	-1.037796	3.078846
6	-2.35593	-2.040968	-0.234128
6	2.06052	-1.078812	3.663017
6	-2.199683	-3.27515	-1.140531
6	-3.760322	-2.058888	0.395725
1	0.427584	-2.588982	-0.466628
1	-2.459955	-1.14773	2.413075
1	-1.533659	0.053269	1.562131
1	1.138936	0.115034	2.146126
1	2.270013	-1.820556	1.024313

1	1.159687	-2.925666	1.815135
1	-0.612463	-0.266068	3.833853
1	-0.50667	-2.005212	3.595946
1	-2.307791	-1.142925	-0.859398
1	3.078874	-0.939896	3.283309
1	1.900981	-0.35557	4.470208
1	1.999374	-2.083895	4.098756
1	-2.29842	-4.199648	-0.556244
1	-2.979817	-3.284375	-1.90872
1	-1.238792	-3.306802	-1.661389
1	-3.857624	-2.862964	1.137576
1	-4.511468	-2.236107	-0.381162
1	-4.011368	-1.109606	0.874631
6	2.302668	-0.110548	-0.944461
6	2.995865	0.962553	-0.364058
6	3.017948	-1.083983	-1.662875
6	4.386746	1.0504	-0.482927
1	2.456606	1.734075	0.176496
6	4.403285	-0.98878	-1.785309
1	2.493061	-1.906775	-2.138578
6	5.090722	0.077398	-1.193183
1	4.911894	1.886249	-0.030582
1	4.946977	-1.743345	-2.346137
1	6.169652	0.150269	-1.293269
17	-0.137482	-0.691863	-2.656352
6	-1.225349	-1.976077	0.831336
1	-1.198616	-2.972265	1.306109
6	0.517128	3.75085	0.530827
1	1.352963	3.818449	-0.183183
1	-0.06014	4.674332	0.367792

6	1.07092	3.76361	1.971319
1	1.714297	4.633065	2.173291
1	0.265111	3.789434	2.715629
1	1.671873	2.871288	2.196432
15	0.480288	-0.182951	-0.712933
12	-0.783494	2.198668	-0.080549
35	-3.063572	1.743094	-0.675995

TS_{1a-i}

E = -4276.891567 ZPVE = 0.429453 NIMAG = 1.

6	-0.615291	1.923192	-0.308242
6	1.769558	2.192843	0.565356
6	-0.185817	2.373973	2.201738
6	-1.118966	2.602616	1.001763
6	1.230089	2.848862	1.843535
6	1.386203	1.740872	-1.961496
6	-0.726587	3.057773	3.462203
6	0.497895	2.060223	-3.17768
6	2.83282	2.17572	-2.253327
1	-1.276548	2.241183	-1.122047
1	2.747115	2.625983	0.336045
1	1.959192	1.127345	0.743087
1	-0.137311	1.289896	2.399486
1	-2.136646	2.275912	1.241423
1	-1.176863	3.682654	0.79945
1	1.91378	2.64442	2.676443
1	1.207461	3.942916	1.719293
1	1.407192	0.648514	-1.835725

1	-1.722917	2.68518	3.726779
1	-0.065105	2.882748	4.317518
1	-0.802419	4.142871	3.317416
1	0.424497	3.144353	-3.336533
1	0.924893	1.618581	-4.083301
1	-0.518193	1.66226	-3.08723
1	2.918741	3.270119	-2.289827
1	3.151921	1.785496	-3.225145
1	3.533866	1.795999	-1.506981
6	-2.559045	-0.223505	-0.23889
6	-3.000487	-1.531021	0.094304
6	-3.532439	0.734481	-0.620274
6	-4.351885	-1.857262	0.059592
1	-2.275016	-2.284785	0.375919
6	-4.880157	0.398886	-0.659882
1	-3.236577	1.738398	-0.900911
6	-5.294582	-0.895202	-0.316483
1	-4.669608	-2.861806	0.320138
1	-5.611715	1.142102	-0.961776
1	-6.34933	-1.15176	-0.348565
17	-0.165853	-2.270365	-2.108188
6	0.836775	2.373769	-0.650883
1	0.750897	3.458624	-0.835999
6	-0.087454	-2.902817	1.831692
1	-0.796708	-2.213218	2.296688
1	-0.639197	-3.750272	1.399141
6	1.020648	-3.329844	2.787215
1	0.611049	-3.822508	3.686349
1	1.718852	-4.038886	2.328438
1	1.614787	-2.476852	3.131995

15	-0.789449	0.062675	-0.201095
12	0.884175	-2.089928	-0.006655
35	3.178668	-1.340903	0.162642

PC_{1a-i}

E = -4277.010399 ZPVE = 0.434871 NIMAG = 0.

6	0.153962	1.612257	0.716185
6	-2.380503	1.37698	1.012341
6	-1.48969	3.146594	-0.593225
6	-0.11543	2.996939	0.081359
6	-2.596289	2.767629	0.400878
6	-0.819984	-0.089537	2.474302
6	-1.678961	4.561638	-1.153981
6	0.552286	-0.192387	3.162343
6	-1.93018	-0.312896	3.517735
1	1.060468	1.715565	1.319381
1	-3.174553	1.189356	1.740482
1	-2.493549	0.606226	0.240458
1	-1.548405	2.440649	-1.432958
1	0.682192	3.268858	-0.620023
1	-0.054666	3.735773	0.894956
1	-3.572794	2.804163	-0.097671
1	-2.626635	3.5215	1.202809
1	-0.910407	-0.923285	1.756461
1	-0.905945	4.81105	-1.890479
1	-2.652979	4.662918	-1.645043
1	-1.630502	5.310264	-0.353394
1	0.690358	0.637719	3.866754

1	0.624438	-1.12452	3.731434
1	1.392165	-0.178336	2.462317
1	-1.97824	0.529858	4.218994
1	-1.72402	-1.217031	4.099479
1	-2.914519	-0.436099	3.061129
6	2.553122	0.274948	-0.269509
6	3.249054	-0.917102	-0.017817
6	3.279271	1.477356	-0.365078
6	4.639489	-0.904959	0.14058
1	2.716488	-1.860343	0.057266
6	4.665398	1.485349	-0.208193
1	2.769807	2.415611	-0.56375
6	5.349679	0.291899	0.046547
1	5.160149	-1.837493	0.336936
1	5.210269	2.421875	-0.285711
1	6.428734	0.298819	0.169692
17	0.997343	-3.833671	0.034565
6	-1.005517	1.242565	1.695447
1	-0.955003	2.034588	2.463303
6	0.568484	0.832459	-2.286657
1	0.530155	1.924812	-2.313795
1	1.520188	0.543616	-2.74429
6	-0.59156	0.221385	-3.083731
1	-0.573619	0.608176	-4.108663
1	-0.515408	-0.86893	-3.142468
1	-1.569178	0.450205	-2.652797
15	0.71866	0.242038	-0.505511
12	-0.428665	-2.12798	-0.301639
35	-2.742615	-1.989562	-0.879235

P_{1a-i}

E = -1044.805304 ZPVE = 0.430489 NIMAG = 0.

6	-0.527808	0.181855	-0.564428
6	-2.976914	0.050756	0.140007
6	-1.836123	-2.069127	-0.720518
6	-0.707348	-1.179409	-1.274603
6	-3.14515	-1.271975	-0.62216
6	-1.814351	2.367703	0.121595
6	-2.004987	-3.337898	-1.566815
6	-0.796429	3.256343	-0.615681
6	-3.182662	3.075671	0.122866
1	0.130461	0.775627	-1.208192
1	-3.937953	0.5733	0.147598
1	-2.726959	-0.147146	1.192167
1	-1.569317	-2.382747	0.296255
1	0.23952	-1.732994	-1.279945
1	-0.934642	-0.972628	-2.332891
1	-3.919872	-1.886975	-0.145389
1	-3.506694	-1.051983	-1.638627
1	-1.483534	2.273511	1.164416
1	-1.07723	-3.920935	-1.604862
1	-2.790337	-3.98514	-1.159478
1	-2.282208	-3.08685	-2.598437
1	-1.051067	3.34233	-1.680449
1	-0.794076	4.267577	-0.194047
1	0.225733	2.875509	-0.546616
1	-3.611139	3.112313	-0.887644
1	-3.073667	4.108718	0.471194

1	-3.910012	2.589378	0.778624
6	2.209709	0.123497	0.293387
6	2.909093	1.333496	0.136184
6	2.844809	-1.060219	-0.121899
6	4.183765	1.366518	-0.435576
1	2.453585	2.259373	0.478147
6	4.123911	-1.033181	-0.685109
1	2.34776	-2.018263	-0.005956
6	4.796142	0.180821	-0.848906
1	4.70119	2.315587	-0.545781
1	4.593624	-1.962069	-0.99758
1	5.790085	0.200921	-1.286691
6	-1.889852	0.941238	-0.491651
1	-2.186469	1.08389	-1.546818
6	0.436433	-1.47948	1.878692
1	0.376636	-2.300008	1.155709
1	1.411119	-1.571965	2.372553
6	-0.66686	-1.610467	2.938089
1	-0.583434	-2.56942	3.46223
1	-0.593134	-0.811918	3.68355
1	-1.669171	-1.562911	2.501751
15	0.513263	0.211272	1.056958

R1_{II} + a S_N2@P-b pathway

RC_{IIa-i}

E = -3968.437426 ZPVE = 0.312509 NIMAG = 0.

15	1.007718000	-0.112117000	-0.502983000
17	0.903218000	0.033368000	-2.592425000
6	2.570061000	-1.190992000	-0.288438000

6	2.126866000	-2.606468000	-0.731213000
1	2.969527000	-3.296854000	-0.605489000
1	1.300585000	-2.986421000	-0.121762000
1	1.829368000	-2.633253000	-1.783390000
6	2.928593000	-1.225469000	1.212579000
1	3.679242000	-2.007965000	1.375430000
1	3.363880000	-0.281987000	1.552847000
1	2.067188000	-1.465063000	1.844660000
6	3.792831000	-0.764694000	-1.118557000
1	4.585377000	-1.510316000	-0.979940000
1	3.564796000	-0.717738000	-2.186205000
1	4.193538000	0.201946000	-0.808771000
6	-0.736379000	-1.836421000	3.563709000
1	-0.564169000	-2.568140000	4.367286000
1	-1.622621000	-1.256963000	3.851894000
1	0.114484000	-1.141370000	3.589188000
6	-0.908877000	-2.498547000	2.179171000
1	-1.751472000	-3.205419000	2.226891000
1	-0.028856000	-3.127023000	1.970162000
12	-1.284965000	-1.225057000	0.528577000
35	-2.942441000	-0.253032000	-0.906614000
6	1.218677000	1.708103000	0.032400000
6	2.533655000	2.368462000	-0.409352000
1	2.485837000	3.440620000	-0.182283000
1	3.399481000	1.961883000	0.120235000
1	2.699416000	2.265769000	-1.485668000
6	1.091105000	1.744819000	1.573227000
1	1.109404000	2.792095000	1.896803000
1	0.144991000	1.318265000	1.924158000
1	1.908062000	1.230237000	2.083706000

6	0.021808000	2.478051000	-0.574495000
1	-0.936599000	1.985896000	-0.381101000
1	-0.012152000	3.477452000	-0.125021000
1	0.122277000	2.595800000	-1.655790000

TS_{IIa-i}

E = -3968.383025 ZPVE = 0.310230 NIMAG = 1.

15	1.031667	0.083297	0.044743
17	-0.221052	-0.90394	-2.457152
6	2.620892	-0.946047	0.031729
6	2.274741	-2.366936	-0.465975
1	3.186328	-2.975651	-0.42967
1	1.525615	-2.851653	0.164893
1	1.903355	-2.360424	-1.492007
6	3.156547	-1.054325	1.483644
1	4.005461	-1.74961	1.480153
1	3.509626	-0.103222	1.882821
1	2.404473	-1.463853	2.166316
6	3.685869	-0.341441	-0.910202
1	4.560828	-1.003273	-0.911877
1	3.317322	-0.277656	-1.938245
1	4.024375	0.648154	-0.597796
6	-1.856388	-1.856818	2.58647
1	-2.139467	-2.691912	3.250052
1	-2.766792	-1.283241	2.383693
1	-1.184668	-1.209436	3.161433
6	-1.197438	-2.359809	1.312771
1	-1.831953	-3.066949	0.752232

1	-0.223403	-2.824089	1.472192
12	-1.377116	-0.872815	-0.365407
35	-3.234694	0.654313	-0.153236
6	1.370491	1.912178	0.412437
6	1.5156	2.579516	-0.986069
1	1.54127	3.667026	-0.840636
1	2.438671	2.285398	-1.492976
1	0.672897	2.351511	-1.645092
6	2.567229	2.287619	1.303963
1	2.581106	3.379031	1.41518
1	2.477404	1.861949	2.307684
1	3.530672	1.993244	0.88307
6	0.069929	2.422661	1.081881
1	-0.054221	2.006917	2.087652
1	0.128694	3.513726	1.178509
1	-0.829868	2.184774	0.507117

PCIIa-i

E = -3968.519922 ZPVE = 0.316043 NIMAG = 0.

15	-0.929995	-0.234159	0.284675
17	1.030953	3.255471	-0.516317
6	-2.488135	0.867912	0.129908
6	-2.241159	2.082792	1.056848
1	-3.106995	2.753062	0.993213
1	-2.137437	1.794864	2.10845
1	-1.358078	2.65505	0.760926
6	-3.797028	0.176153	0.562934
1	-4.608272	0.914003	0.535222

1	-4.081022	-0.645331	-0.095956
1	-3.748166	-0.207817	1.586509
6	-2.620028	1.382088	-1.318171
1	-3.438028	2.111129	-1.363538
1	-1.712188	1.892671	-1.654665
1	-2.859498	0.581916	-2.024203
6	0.277402	-1.054027	2.759245
1	0.111902	-1.455294	3.765217
1	0.749007	-0.071952	2.873284
1	0.993125	-1.701434	2.248378
6	-1.061363	-0.947839	2.012242
1	-1.734155	-0.292956	2.572891
1	-1.55594	-1.923559	1.959525
12	1.320105	1.062571	-0.117008
35	3.153152	-0.469986	0.005217
6	-0.94305	-1.737163	-0.908964
6	-0.381045	-1.265932	-2.269384
1	-0.377172	-2.108348	-2.971588
1	-0.973815	-0.465638	-2.720141
1	0.65677	-0.925568	-2.177297
6	-2.326348	-2.381745	-1.109386
1	-2.2078	-3.290691	-1.712108
1	-2.787758	-2.678078	-0.161896
1	-3.019579	-1.726819	-1.643042
6	0.019947	-2.801948	-0.334963
1	-0.363245	-3.255989	0.583668
1	0.126628	-3.605358	-1.073917
1	1.018737	-2.401584	-0.142003

P11a-i

E = -736.311758 ZPVE = 0.311601 NIMAG = 0.

15	-0.011095	0.350312	-0.678037
6	-1.303284	-0.911162	0.019635
6	-1.7013	-0.70631	1.493512
1	-2.449445	-1.458173	1.779823
1	-0.852197	-0.813636	2.173524
1	-2.150595	0.275781	1.668031
6	-0.813876	-2.360204	-0.175187
1	-1.641599	-3.051324	0.032267
1	-0.48349	-2.544155	-1.203102
1	0.00326	-2.621861	0.502052
6	-2.557803	-0.735482	-0.871056
1	-3.337597	-1.439588	-0.55059
1	-2.979334	0.271129	-0.811692
1	-2.329269	-0.938177	-1.922199
6	-1.687625	2.646712	-0.106338
1	-2.581703	2.11164	0.225577
1	-1.758394	2.773929	-1.192017
1	-1.7198	3.642873	0.350135
6	-0.389791	1.924593	0.288759
1	0.445283	2.594363	0.064676
1	-0.368939	1.75145	1.37146
6	1.749595	-0.070484	0.002464
6	2.324733	-1.233266	-0.837414
1	3.374565	-1.400048	-0.561859
1	1.793482	-2.173632	-0.680185
1	2.291653	-1.002205	-1.907469
6	1.844966	-0.411837	1.500658

1	2.898366	-0.541893	1.785201
1	1.43437	0.384	2.130861
1	1.326917	-1.342461	1.747633
6	2.636529	1.166127	-0.279122
1	2.426482	1.996049	0.401326
1	3.690444	0.893212	-0.140245
1	2.521091	1.525916	-1.308123

R1_{III} + a S_N2@P-b pathway

RC_{IIIa-i}

E = -4116.035688 ZPVE = 0.250003 NIMAG = 0.

6	-0.181422	1.910258	0.169016
6	1.058108	2.401673	-0.270925
6	-1.261406	2.792712	0.353767
6	1.208345	3.766635	-0.53579
1	1.89755	1.725229	-0.404052
6	-1.100659	4.151054	0.092649
1	-2.218859	2.418026	0.702516
6	0.133991	4.638568	-0.355196
1	2.167059	4.142048	-0.880265
1	-1.934958	4.830976	0.237618
1	0.254714	5.698578	-0.559158
17	-0.591356	0.070115	2.612567
6	0.788595	-3.676173	0.59151
1	1.613345	-4.341493	0.888121
1	0.175664	-3.560652	1.498552
6	-0.050866	-4.363772	-0.507001
1	-0.446874	-5.339291	-0.186413
1	-0.915956	-3.757077	-0.804294

1	0.535576	-4.546975	-1.416393
15	-0.323313	0.123152	0.520046
12	1.632885	-1.798354	0.126649
35	3.525445	-0.47853	-0.557614
6	-1.987318	-0.326647	-0.121805
6	-2.286797	0.024491	-1.450819
6	-2.891417	-1.119097	0.599552
6	-3.480354	-0.398253	-2.037455
1	-1.598304	0.635678	-2.027671
6	-4.08734	-1.533864	0.007974
1	-2.672513	-1.40393	1.622821
6	-4.38436	-1.176657	-1.308975
1	-3.70369	-0.114769	-3.061629
1	-4.784142	-2.139405	0.579738
1	-5.31365	-1.502963	-1.766141

TSIIIa-i

E = -4116.000107 ZPVE = 0.248280 NIMAG = 1.

6	-0.635272	-1.858503	0.000185
6	0.583673	-2.522102	0.305025
6	-1.786549	-2.635169	-0.290425
6	0.621256	-3.910874	0.390473
1	1.490581	-1.940368	0.458229
6	-1.729436	-4.020947	-0.221921
1	-2.709494	-2.149017	-0.585981
6	-0.530804	-4.659962	0.130514
1	1.553096	-4.407798	0.640506
1	-2.611439	-4.610592	-0.45266

1	-0.494888	-5.74416	0.18483
17	0.567933	1.516189	-2.446862
6	1.140883	2.980914	1.157288
1	1.696101	3.833049	0.734373
1	0.069521	3.195529	1.075387
6	1.586118	2.654685	2.577067
1	1.498445	3.524453	3.250719
1	0.984034	1.851723	3.018409
1	2.631325	2.327222	2.615655
15	-0.517373	-0.079343	-0.125712
12	1.694215	1.481522	-0.349753
35	3.500808	-0.084499	0.111261
6	-2.204305	0.552438	0.011222
6	-3.135267	0.007334	0.927661
6	-2.554247	1.721431	-0.703307
6	-4.376968	0.610789	1.112695
1	-2.874724	-0.864729	1.517764
6	-3.808122	2.301796	-0.52778
1	-1.847437	2.148526	-1.407402
6	-4.720457	1.751023	0.378526
1	-5.076055	0.19242	1.830532
1	-4.072192	3.187474	-1.097325
1	-5.693046	2.213288	0.518861

PCIIIa-i

E = -4116.120878 ZPVE = 0.253275 NIMAG = 0.

6	0.360963	1.671789	-0.309372
6	-0.896203	2.175849	-0.688845

6	1.516578	2.404257	-0.625801
6	-0.988993	3.396727	-1.361539
1	-1.805148	1.62244	-0.466733
6	1.415544	3.625453	-1.295763
1	2.496317	2.020281	-0.361219
6	0.163462	4.12622	-1.662363
1	-1.965396	3.773491	-1.651337
1	2.317317	4.181038	-1.536479
1	0.087795	5.073334	-2.188328
17	-0.689532	-3.246544	-1.590187
6	0.247918	0.486674	2.388453
1	0.391968	-0.454923	2.932028
1	1.071049	1.152477	2.667168
6	-1.093723	1.126403	2.770031
1	-1.134836	1.26666	3.855044
1	-1.213252	2.10837	2.302905
1	-1.943327	0.508183	2.46937
15	0.422921	0.054981	0.579464
12	-1.466918	-1.515519	-0.398127
35	-3.547846	-0.5621	0.306339
6	2.153307	-0.548497	0.412068
6	3.195701	-0.12205	1.254143
6	2.441278	-1.468671	-0.610399
6	4.495712	-0.597707	1.070104
1	3.007807	0.583563	2.056527
6	3.744448	-1.935987	-0.796277
1	1.649136	-1.841111	-1.252788
6	4.773265	-1.504434	0.043403
1	5.28931	-0.259843	1.73024
1	3.947055	-2.649096	-1.589558

1	5.78452	-1.874757	-0.097022
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P_{IIIa-i}

E = -883.919984 ZPVE = 0.248631 NIMAG = 0.

6	-1.330334	-0.149017	0.240533
6	-2.491655	-0.309155	1.012948
6	-1.210047	-0.886128	-0.950046
6	-3.51401	-1.171401	0.602415
1	-2.593312	0.241693	1.944596
6	-2.226517	-1.751018	-1.359692
1	-0.312357	-0.79309	-1.555207
6	-3.382882	-1.894123	-0.585007
1	-4.405811	-1.281569	1.213149
1	-2.115806	-2.31568	-2.281491
1	-4.172358	-2.568859	-0.903743
6	-0.2032	2.403669	-0.450375
1	0.657283	3.070304	-0.31668
1	-0.140969	1.981621	-1.460847
6	-1.502874	3.204105	-0.288585
1	-1.550017	4.011985	-1.027007
1	-2.383924	2.570641	-0.43281
1	-1.572601	3.654999	0.707149
15	-0.043417	1.052035	0.841666
6	1.52135	0.194425	0.33618
6	2.394565	0.654326	-0.662454
6	1.892895	-0.951663	1.064662
6	3.594414	-0.014777	-0.931298
1	2.150274	1.537241	-1.243762

6	3.081375	-1.627175	0.789277
1	1.242342	-1.319322	1.854691
6	3.94045	-1.158568	-0.210845
1	4.254643	0.360471	-1.708588
1	3.341948	-2.513795	1.360646
1	4.870751	-1.678156	-0.421367

R1_{IV} + a S_N2@P-b pathway

RC_{IVa-i}

E = -3924.291525 ZPVE = 0.196575 NIMAG = 0.

17	-0.841690000	1.068443000	1.305630000
6	-0.260255000	-3.246936000	-0.835032000
1	-0.883313000	-2.426481000	-1.225442000
1	-0.951466000	-4.095840000	-0.725040000
6	0.819557000	-3.607970000	-1.878426000
1	1.418528000	-4.471234000	-1.562468000
1	0.390953000	-3.863770000	-2.859158000
1	1.524214000	-2.783089000	-2.049386000
15	0.967601000	-0.016077000	1.335474000
12	0.395098000	-2.694989000	1.093480000
35	0.913107000	-3.211536000	3.384816000
6	1.652271000	0.498791000	2.959529000
1	1.750264000	1.583661000	3.044240000
1	0.976895000	0.129440000	3.733951000
1	2.622121000	0.012822000	3.104241000
6	1.987391000	0.829760000	0.073774000
6	1.672221000	0.596884000	-1.277501000
6	3.082933000	1.648791000	0.390951000
6	2.431724000	1.182142000	-2.289725000

1	0.834019000	-0.043625000	-1.538665000
6	3.846285000	2.226138000	-0.626398000
1	3.349945000	1.842071000	1.424198000
6	3.520593000	1.997375000	-1.965269000
1	2.177129000	0.998029000	-3.328928000
1	4.692779000	2.856371000	-0.370683000
1	4.114916000	2.449277000	-2.753775000

TSIVa-i

E = -3924.258873 ZPVE = 0.196301 NIMAG = 1.

17	1.195023	2.792083	-0.823913
6	-0.297412	-0.97677	1.610633
1	-1.195285	-0.81606	2.244698
1	0.52926	-1.047894	2.314123
6	-0.419691	-2.282472	0.799468
1	0.55174	-2.563763	0.385039
1	-0.802389	-3.121515	1.392778
1	-1.104165	-2.236916	-0.076381
15	0.504492	0.91505	0.402816
12	-1.670538	-0.066304	0.102161
35	-3.933029	-0.32328	-0.418497
6	0.820845	1.800377	1.998671
1	1.840318	2.190812	1.980464
1	0.144206	2.657029	2.041817
1	0.670744	1.16342	2.871253
6	1.976415	-0.08848	-0.03943
6	2.132279	-0.487359	-1.375077
6	2.944492	-0.460462	0.903436

6	3.228479	-1.263132	-1.757223
1	1.416275	-0.163813	-2.125183
6	4.048023	-1.224878	0.516617
1	2.850228	-0.15482	1.940954
6	4.189509	-1.632655	-0.812502
1	3.33818	-1.564112	-2.794812
1	4.795735	-1.500237	1.25469
1	5.047242	-2.227847	-1.111262

PC_{IVa-i}

E = -3924.378831 ZPVE = 0.199352 NIMAG = 0.

17	-0.876211	3.176042	-0.176871
6	0.107057	-2.110515	-0.892145
1	-0.834813	-2.589567	-0.602553
1	0.907846	-2.846382	-0.754905
6	0.034401	-1.640508	-2.349925
1	0.943886	-1.113275	-2.655645
1	-0.095158	-2.497075	-3.018978
1	-0.821105	-0.974475	-2.506086
15	0.35417	-0.718762	0.316095
12	-1.540903	1.045917	0.016312
35	-3.407052	-0.443129	0.143645
6	0.193868	-1.571786	1.950154
1	0.404096	-0.865153	2.757662
1	-0.834907	-1.927758	2.054918
1	0.88221	-2.417898	2.034499
6	2.124099	-0.245244	0.183997
6	2.454779	1.105847	-0.008003

6	3.156329	-1.195044	0.282178
6	3.794014	1.497394	-0.102988
1	1.671448	1.855267	-0.082635
6	4.491179	-0.801225	0.186185
1	2.926023	-2.2464	0.43349
6	4.811651	0.547098	-0.007136
1	4.035608	2.545384	-0.252379
1	5.280028	-1.543887	0.262542
1	5.851269	0.85232	-0.081798

P_{IVa-i}

E = -692.176821 ZPVE = 0.195001 NIMAG = 0.

6	2.25932	0.686397	0.540459
1	3.323543	0.419995	0.503621
1	1.914294	0.472844	1.560486
6	2.08052	2.174389	0.214471
1	1.026774	2.468606	0.262563
1	2.632536	2.798566	0.9261
1	2.44696	2.407814	-0.791073
15	1.405649	-0.447517	-0.689098
6	1.755744	-2.089705	0.129997
1	1.497794	-2.109279	1.194578
1	1.193253	-2.876159	-0.381584
1	2.822007	-2.315266	0.024428
6	-0.382364	-0.196535	-0.23977
6	-1.27533	0.146479	-1.267398
6	-0.889846	-0.328394	1.064368
6	-2.633917	0.352347	-1.004595

1	-0.900694	0.251788	-2.282343
6	-2.244919	-0.124372	1.332223
1	-0.227154	-0.592669	1.884536
6	-3.121422	0.216998	0.296573
1	-3.307346	0.616975	-1.815091
1	-2.617663	-0.231504	2.347379
1	-4.175765	0.375421	0.504889

R1_v + a S_N2@P-b pathway

RC_{Va-i}

E = -3732.545114 ZPVE = 0.142563 NIMAG = 0.

17	-1.923239	-2.203023	-0.236867
6	0.554199	2.884216	0.586853
1	1.411869	3.307466	1.131151
1	-0.286402	2.952302	1.296082
6	0.253666	3.76964	-0.642051
1	-0.60635	3.404572	-1.220728
1	0.025416	4.81083	-0.369665
1	1.103051	3.804741	-1.335336
15	-1.5693	-0.165096	0.057371
12	0.992115	0.842326	0.224527
35	2.44587	-1.025679	-0.042536
6	-2.605273	0.585366	-1.271562
1	-2.195145	0.324291	-2.250278
1	-3.643181	0.246298	-1.212424
1	-2.568373	1.674373	-1.15788
6	-2.573465	0.169303	1.56833
1	-3.613166	-0.143197	1.438041
1	-2.142055	-0.359467	2.421972

1	-2.536688	1.245336	1.770269
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TS_{Va-i}

E = -3732.515826 ZPVE = 0.143017 NIMAG = 1.

17	-2.851143	-1.85672	-0.459507
6	-0.253332	1.929923	0.586475
1	0.474806	1.832077	1.419492
1	-1.046363	2.557492	0.991977
6	0.408401	2.608285	-0.631043
1	-0.342613	2.914563	-1.365343
1	0.999212	3.492527	-0.363909
1	1.118971	1.967246	-1.19547
15	-1.59758	0.046934	0.092182
12	0.799805	0.038957	-0.01366
35	3.04632	-0.606472	-0.009246
6	-2.65203	1.130498	-0.980918
1	-2.40457	0.950642	-2.029618
1	-3.688987	0.826821	-0.82773
1	-2.531965	2.188569	-0.744779
6	-2.322612	0.10113	1.798605
1	-3.410338	0.14185	1.705797
1	-2.07069	-0.828357	2.313824
1	-1.96576	0.956834	2.373462

PC_{Va-i}

E = -3732.634254 ZPVE = 0.145595 NIMAG = 0.

17	-0.696739	3.119922	-0.314029
6	1.832756	-1.653125	-0.651826
1	1.175947	-2.418255	-0.222912
1	2.86725	-1.992956	-0.516438
6	1.499641	-1.45976	-2.137516
1	2.122173	-0.688927	-2.604272
1	1.664124	-2.391496	-2.687801
1	0.448413	-1.183933	-2.270601
15	1.571398	-0.124111	0.369133
12	-0.785656	0.901713	-0.037622
35	-2.154913	-1.048615	0.145244
6	3.057401	0.924356	0.052837
1	3.069916	1.243489	-0.992745
1	3.003109	1.823841	0.672147
1	3.983202	0.384198	0.276209
6	1.814788	-0.730816	2.096938
1	2.776744	-1.241737	2.208118
1	1.777198	0.10997	2.79566
1	1.007833	-1.424153	2.349469

P_{Va-i}

E = -500.432930 ZPVE = 0.141195 NIMAG = 0.

6	1.013989	-0.690442	0.359012
1	1.049471	-1.764342	0.135607
1	0.83543	-0.595286	1.439352
6	2.35109	-0.041163	-0.023342
1	2.368163	1.026179	0.222943
1	3.1825	-0.512744	0.512527

1	2.546741	-0.137864	-1.096746
15	-0.450298	-0.001472	-0.589938
6	-0.672597	1.633554	0.284503
1	0.140011	2.314918	0.014886
1	-1.609351	2.094831	-0.044555
1	-0.697523	1.526656	1.376238
6	-1.816752	-0.970037	0.234022
1	-1.772253	-0.9151	1.328767
1	-2.787093	-0.586222	-0.096835
1	-1.75601	-2.020434	-0.068274

RI + a SN2@P-f pathway

RC_{Ia-r}

E = -4276.923179 ZPVE = 0.431496 NIMAG = 0.

6	-1.228107	-0.880731	0.486262
6	-2.023716	-3.128124	-0.406313
6	-3.757516	-1.431814	0.430239
6	-2.612243	-0.716854	1.169115
6	-3.404425	-2.914375	0.234408
6	0.534578	-2.730006	-0.143466
6	-5.090387	-1.25278	1.166569
6	1.604231	-2.256075	0.858535
6	0.758215	-4.229244	-0.413847
1	-0.488185	-0.379631	1.118805
1	-1.818766	-4.201591	-0.438648
1	-2.038946	-2.785825	-1.45052
1	-3.865121	-0.976817	-0.567945
1	-2.852077	0.341312	1.3077

1	-2.524399	-1.147371	2.177692
1	-4.175736	-3.405842	-0.371997
1	-3.421866	-3.408796	1.217733
1	0.696318	-2.207925	-1.094332
1	-5.351775	-0.193554	1.26807
1	-5.90722	-1.751338	0.632905
1	-5.039507	-1.683107	2.174625
1	1.615428	-2.902975	1.744586
1	2.603768	-2.281725	0.413163
1	1.408951	-1.243275	1.235331
1	0.497469	-4.835112	0.463482
1	1.814147	-4.412658	-0.638993
1	0.175573	-4.593158	-1.26427
6	-1.87054	1.692831	-0.742329
6	-2.929968	2.185604	-1.521919
6	-1.358865	2.488849	0.297502
6	-3.488441	3.438949	-1.250741
1	-3.317619	1.59057	-2.344843
6	-1.913101	3.739791	0.562577
1	-0.526613	2.13975	0.899783
6	-2.980565	4.215929	-0.20872
1	-4.309047	3.807363	-1.859108
1	-1.509141	4.34551	1.368407
1	-3.407465	5.192543	-0.000043
17	0.871646	0.521898	-1.464387
6	-0.898191	-2.405443	0.365736
1	-0.941847	-2.7797	1.403134
6	1.835925	1.674198	2.241228
1	1.58724	2.718255	1.99104
1	0.876364	1.213662	2.525484

6	2.78163	1.664359	3.462267
1	2.353948	2.176403	4.337187
1	3.026803	0.643247	3.781344
1	3.735468	2.15871	3.240567
15	-1.251684	0.019216	-1.192971
12	2.624438	0.770359	0.500783
35	4.566194	0.157939	-0.743234

TS_{1a-r}

E = -4276.885950 ZPVE = 0.429632 NIMAG = 1.

6	-1.548703	0.926228	-0.698527
6	-1.496737	3.089133	0.636007
6	-3.758029	1.929098	0.238943
6	-3.090186	1.122285	-0.892285
6	-3.014912	3.257827	0.46024
6	0.680447	2.253734	-0.564875
6	-5.247076	2.150384	-0.051605
6	1.201452	1.88053	-1.965103
6	1.370049	3.54755	-0.103127
1	-1.152871	0.426288	-1.587326
1	-1.041754	4.080242	0.714391
1	-1.278476	2.57832	1.584139
1	-3.68255	1.345906	1.17065
1	-3.596081	0.158244	-1.0155
1	-3.218552	1.66515	-1.840748
1	-3.437758	3.774782	1.330514
1	-3.200776	3.909068	-0.407602
1	0.988324	1.472093	0.149518

1	-5.779439	1.199496	-0.167701
1	-5.727942	2.706658	0.760374
1	-5.38392	2.725987	-0.97577
1	0.985771	2.693042	-2.670479
1	2.283821	1.727853	-1.943065
1	0.749388	0.967195	-2.364417
1	1.063299	4.400784	-0.721849
1	2.454256	3.435049	-0.195054
1	1.154146	3.785582	0.941985
6	-1.719279	-1.817871	0.2052
6	-1.810871	-2.808999	1.221685
6	-1.985401	-2.204187	-1.133301
6	-2.190387	-4.109514	0.916611
1	-1.567755	-2.539	2.245315
6	-2.379588	-3.505924	-1.429268
1	-1.904191	-1.483578	-1.938174
6	-2.484349	-4.457733	-0.409063
1	-2.256078	-4.853816	1.70388
1	-2.592463	-3.784003	-2.456858
1	-2.785445	-5.473633	-0.647503
17	1.158709	-0.861761	2.494393
6	-0.871467	2.322074	-0.546911
1	-1.159411	2.874674	-1.4572
6	1.36816	-1.969461	-1.161124
1	0.779413	-2.735189	-0.643544
1	0.700417	-1.34505	-1.763089
6	2.511995	-2.547022	-1.993118
1	2.13936	-3.122431	-2.858029
1	3.170104	-1.766767	-2.391358
1	3.140451	-3.23306	-1.412295

15	-1.335323	-0.179756	0.808218
12	2.272629	-0.784062	0.46222
35	4.285892	0.480467	0.06857

PC_{1a-r}

E = -4277.019369 ZPVE = 0.434798 NIMAG = 0.

6	-0.22648	1.725563	-0.689197
6	1.473286	1.956864	1.201894
6	-1.030366	2.159659	1.730943
6	-1.262622	2.415639	0.231927
6	0.400172	2.56809	2.114377
6	2.35739	1.735905	-1.231158
6	-2.076376	2.882243	2.588262
6	2.157736	2.236239	-2.673528
6	3.744299	2.184752	-0.734018
1	-0.436552	2.036728	-1.719343
1	2.447732	2.366201	1.479724
1	1.564062	0.874771	1.390405
1	-1.138898	1.081493	1.922967
1	-2.280097	2.124732	-0.046084
1	-1.190771	3.497705	0.045757
1	0.601676	2.295913	3.157565
1	0.47837	3.664513	2.058427
1	2.377042	0.639525	-1.236381
1	-3.091414	2.556362	2.335555
1	-1.916687	2.68311	3.65345
1	-2.024663	3.968171	2.438245
1	2.17766	3.333201	-2.707705

1	2.962646	1.872243	-3.320732
1	1.21312	1.909532	-3.117948
1	3.777111	3.268454	-0.560647
1	4.504205	1.946976	-1.485669
1	4.038044	1.677955	0.188318
6	-2.292859	-0.407198	-0.774326
6	-2.945986	-1.099509	0.257539
6	-3.050171	0.063967	-1.861913
6	-4.328136	-1.308841	0.205323
1	-2.384201	-1.469355	1.110826
6	-4.427951	-0.149358	-1.913739
1	-2.570346	0.601726	-2.675172
6	-5.070207	-0.83766	-0.878529
1	-4.817257	-1.84501	1.013064
1	-4.999307	0.220255	-2.760392
1	-6.14268	-1.004019	-0.91965
17	-0.398903	-2.005199	2.983248
6	1.208416	2.20978	-0.29724
1	1.16039	3.306159	-0.414042
6	0.097267	-0.770431	-2.361412
1	-0.424229	-0.20953	-3.14526
1	1.162228	-0.544257	-2.446865
6	-0.118907	-2.281566	-2.526407
1	0.219954	-2.600204	-3.517623
1	0.464675	-2.841726	-1.788828
1	-1.172792	-2.558519	-2.427071
15	-0.46698	-0.162022	-0.690441
12	0.797742	-1.506523	1.148946
35	2.914374	-1.998884	0.143325

P_{Ia-r}

E = -1044.804084 ZPVE = 0.430657 NIMAG = 0.

6	-0.876857	0.020668	-0.874721
6	-2.416462	1.137814	0.841876
6	-3.250944	-0.905888	-0.473623
6	-2.136011	-0.63414	-1.495248
6	-3.625232	0.40533	0.234697
6	-0.08975	2.203759	0.355139
6	-4.470309	-1.565956	-1.129149
6	0.844872	2.648813	-0.784524
6	-0.547653	3.449839	1.136526
1	-0.211135	0.26603	-1.711303
1	-2.759978	2.104419	1.222932
1	-2.042807	0.584132	1.710696
1	-2.859041	-1.606901	0.279987
1	-1.859036	-1.563976	-2.005452
1	-2.533462	0.04362	-2.267159
1	-4.372573	0.213147	1.01599
1	-4.110084	1.067607	-0.49919
1	0.494788	1.58146	1.044038
1	-4.201481	-2.517011	-1.602752
1	-5.257335	-1.767806	-0.393203
1	-4.897719	-0.916102	-1.903406
1	0.302737	3.278629	-1.502123
1	1.678524	3.239592	-0.389666
1	1.277686	1.807113	-1.329413
1	-1.215832	4.074712	0.529428
1	0.318328	4.063701	1.407918

1	-1.072345	3.198618	2.062654
6	1.899738	-0.754305	-0.211836
6	2.49473	-0.938052	-1.474365
6	2.691163	-0.204988	0.809939
6	3.814183	-0.552801	-1.718915
1	1.918619	-1.398168	-2.274197
6	4.018702	0.165328	0.57498
1	2.278601	-0.053048	1.802398
6	4.584154	0.000085	-0.691522
1	4.244626	-0.699015	-2.705801
1	4.608805	0.588224	1.383718
1	5.61491	0.290152	-0.873596
6	-1.279329	1.359113	-0.180214
1	-1.725669	1.962937	-0.991723
6	-0.119471	-1.29373	1.834399
1	-1.198498	-1.399524	1.983286
1	0.162639	-0.331045	2.275344
6	0.596719	-2.451613	2.549864
1	0.378398	-2.433492	3.623752
1	0.268177	-3.418526	2.155022
1	1.683095	-2.399236	2.429933
15	0.152906	-1.359727	-0.019863

R1_{II} + a SN2@P-f pathway

RC_{IIa-r}

E = -3968.432239 ZPVE = 0.311808 NIMAG = 0.

15	-1.379714	-0.1098	0.374098
17	0.061863	1.16497	-0.689442
6	-1.993312	-1.201238	-1.073249

6	-0.7358	-1.85768	-1.690431
1	-1.052512	-2.695361	-2.323668
1	-0.186166	-1.155618	-2.323281
1	-0.048787	-2.243997	-0.931313
6	-2.814084	-0.52696	-2.181782
1	-2.998281	-1.253453	-2.983678
1	-3.789033	-0.182245	-1.826462
1	-2.282968	0.321909	-2.622856
6	-2.823788	-2.316588	-0.388541
1	-3.111824	-3.052705	-1.148823
1	-2.245189	-2.843241	0.377422
1	-3.74379	-1.943892	0.068892
6	5.23456	1.894203	-0.745791
1	5.617851	1.010726	-1.27149
1	5.548997	1.797048	0.300862
1	5.767967	2.76425	-1.157488
6	3.703132	2.023258	-0.87778
1	3.366693	2.945036	-0.378732
1	3.434982	2.162296	-1.936318
12	2.543078	0.43466	-0.121062
35	2.237428	-1.683572	0.966136
6	-2.643442	1.258873	0.831302
6	-3.036482	2.282099	-0.24714
1	-3.57	1.828729	-1.083714
1	-3.70173	3.030823	0.201853
1	-2.165682	2.811919	-0.641748
6	-1.971352	2.001899	2.011126
1	-2.672388	2.739628	2.420494
1	-1.6914	1.317638	2.81875
1	-1.073206	2.539906	1.692854

6	-3.901765	0.533748	1.359708
1	-4.488937	0.085206	0.55378
1	-3.65936	-0.246672	2.090495
1	-4.544125	1.264004	1.866662

TS_{IIa-r}

E = -3968.390977 ZPVE = 0.310744 NIMAG = 1.

15	-1.320897	-0.096309	0.633886
17	0.029645	-0.44288	-2.176533
6	-2.885797	-0.791324	-0.196709
6	-2.581391	-2.261737	-0.567285
1	-3.516441	-2.746965	-0.87287
1	-1.872747	-2.325732	-1.395127
1	-2.181479	-2.825711	0.281919
6	-3.478514	-0.063039	-1.41054
1	-4.336317	-0.637708	-1.782668
1	-3.845579	0.933976	-1.153406
1	-2.753465	0.024621	-2.222123
6	-3.922996	-0.801341	0.96687
1	-4.82227	-1.318943	0.609844
1	-3.558611	-1.341126	1.846875
1	-4.22277	0.202878	1.276987
6	1.1536	-1.659089	2.556058
1	0.34689	-0.98024	2.867353
1	2.107997	-1.132857	2.661751
1	1.151527	-2.488854	3.281483
6	0.936159	-2.153299	1.145959
1	1.79117	-2.740907	0.766649

1	0.017178	-2.718052	0.996222
12	1.521395	-0.72137	-0.447824
35	3.679579	0.266962	-0.171266
6	-1.173589	1.796525	0.449937
6	-1.294659	2.47499	-0.923686
1	-2.27346	2.328958	-1.380945
1	-1.14916	3.554451	-0.78886
1	-0.537388	2.113797	-1.620381
6	0.198306	2.148264	1.071982
1	0.273472	3.236324	1.186106
1	0.332924	1.701473	2.062916
1	1.039194	1.842408	0.439961
6	-2.290821	2.330962	1.393147
1	-3.28619	2.219287	0.955648
1	-2.28412	1.856951	2.381282
1	-2.114646	3.402857	1.547964

PCIIa-r

E = -3968.484826 ZPVE = 0.314715 NIMAG = 0.

15	1.788919	-0.710364	0.795021
17	-1.341586	2.787274	-1.372616
6	2.913672	0.783891	0.336603
6	2.813652	1.777658	1.516372
1	3.574819	2.5581	1.394
1	1.842976	2.281367	1.556674
1	2.993318	1.289741	2.480858
6	2.592433	1.533802	-0.968284
1	3.264942	2.396492	-1.064959

1	2.746065	0.909342	-1.852687
1	1.570376	1.924428	-0.994969
6	4.36721	0.260295	0.291337
1	5.054767	1.10489	0.155775
1	4.638766	-0.247941	1.222404
1	4.537847	-0.435018	-0.534044
6	-0.183849	0.316631	2.657914
1	0.511134	1.02147	3.119726
1	-0.103351	-0.633285	3.193836
1	-1.202179	0.694783	2.805653
6	0.119585	0.109273	1.16432
1	-0.625774	-0.598277	0.774478
1	0.072431	1.072401	0.623815
12	-1.954125	0.895488	-0.391068
35	-3.58107	-0.651409	0.315975
6	1.324715	-1.714933	-0.786425
6	0.389246	-1.026048	-1.802548
1	0.744769	-0.050197	-2.136695
1	0.273253	-1.661092	-2.689955
1	-0.631315	-0.925022	-1.401192
6	0.61612	-2.983108	-0.25286
1	0.326744	-3.625911	-1.094092
1	1.272237	-3.559739	0.405939
1	-0.299199	-2.751275	0.303573
6	2.612976	-2.156397	-1.50957
1	3.108861	-1.326756	-2.020376
1	3.328674	-2.61141	-0.816571
1	2.365372	-2.90822	-2.269505

R1_{III} + a S_N2@P-f pathway

R1Ma-r

E = -1264.903326 ZPVE = 0.183787 NIMAG = 0.

6	1.442039	0.136966	0.352929
6	1.919716	-0.810519	1.275506
6	2.136792	0.32231	-0.850461
6	3.05091	-1.576256	0.987908
1	1.408928	-0.950219	2.225817
6	3.276577	-0.437128	-1.131279
1	1.795743	1.065366	-1.563623
6	3.733223	-1.390293	-0.217885
1	3.404826	-2.306895	1.709486
1	3.807084	-0.28069	-2.066321
1	4.619936	-1.977268	-0.43888
17	-0.123189	2.645065	-0.53999
15	-0.063684	1.068332	0.893035
6	-1.424043	-0.01073	0.260058
6	-2.642989	0.055546	0.955429
6	-1.313802	-0.87425	-0.842108
6	-3.733914	-0.719721	0.553757
1	-2.737705	0.716013	1.813725
6	-2.402731	-1.649774	-1.241207
1	-0.376662	-0.94378	-1.385322
6	-3.614277	-1.572952	-0.545437
1	-4.671195	-0.658669	1.099107
1	-2.306887	-2.31498	-2.094657
1	-4.459594	-2.179156	-0.858291

RCMa-r

E = -4116.031804 ZPVE = 0.249112 NIMAG = 0.

6	-0.828991000	1.411407000	0.133864000
6	-0.633634000	2.540412000	-0.677895000
6	-0.945588000	1.574884000	1.525327000
6	-0.550933000	3.813757000	-0.107962000
1	-0.506893000	2.420258000	-1.750147000
6	-0.855046000	2.846436000	2.090517000
1	-1.083703000	0.709894000	2.166893000
6	-0.664150000	3.968017000	1.274522000
1	-0.384999000	4.678046000	-0.743770000
1	-0.932334000	2.964125000	3.167518000
1	-0.588957000	4.955764000	1.719702000
17	0.208247000	-1.468177000	0.637182000
6	3.771500000	-1.940638000	1.844955000
1	3.662875000	-1.338306000	2.760594000
1	3.221538000	-2.870844000	2.053102000
6	5.263383000	-2.259438000	1.616572000
1	5.721123000	-2.775361000	2.474117000
1	5.414740000	-2.905344000	0.742480000
1	5.853993000	-1.351454000	1.441851000
15	-0.944744000	-0.181928000	-0.770200000
12	2.751930000	-0.921673000	0.307065000
35	2.647961000	0.543108000	-1.597306000
6	-2.621803000	-0.814204000	-0.352268000
6	-2.966699000	-2.049884000	-0.934688000
6	-3.594056000	-0.117280000	0.384271000
6	-4.236494000	-2.593631000	-0.750165000
1	-2.232920000	-2.591229000	-1.526717000
6	-4.872024000	-0.656451000	0.552556000

1	-3.361087000	0.847715000	0.820002000
6	-5.193539000	-1.895515000	-0.006185000
1	-4.483354000	-3.552707000	-1.195792000
1	-5.615617000	-0.105636000	1.121178000
1	-6.186794000	-2.312950000	0.130326000

TS_{IIIa-r}

E = -4115.996535 ZPVE = 0.247938 NIMAG = 1.

6	-0.475176	-1.490386	0.302309
6	0.633272	-2.009824	1.023586
6	-1.150082	-2.337175	-0.612545
6	0.989542	-3.348478	0.896641
1	1.20838	-1.352931	1.671783
6	-0.769825	-3.667888	-0.749263
1	-1.95492	-1.941409	-1.222561
6	0.286144	-4.179884	0.017208
1	1.824716	-3.740095	1.468589
1	-1.286856	-4.307434	-1.458149
1	0.576137	-5.220819	-0.09137
17	0.072601	2.602435	-1.29471
6	2.153203	-0.488113	-2.150533
1	1.485761	-1.260603	-1.74815
1	1.784807	-0.176276	-3.134924
6	3.610686	-0.935756	-2.172233
1	3.747082	-1.869294	-2.746031
1	4.261846	-0.187031	-2.639666
1	4.000374	-1.121503	-1.164491
15	-0.816461	0.245945	0.608546

12	1.857238	1.19638	-0.785091
35	3.051552	1.182864	1.326183
6	-2.58023	0.432224	0.260691
6	-3.071865	1.708538	-0.107056
6	-3.514785	-0.587551	0.572773
6	-4.440996	1.938434	-0.197048
1	-2.369807	2.497662	-0.353218
6	-4.883321	-0.341229	0.496757
1	-3.169971	-1.55896	0.908187
6	-5.350107	0.917295	0.103852
1	-4.800951	2.916187	-0.501852
1	-5.585792	-1.12957	0.750024
1	-6.418027	1.103467	0.037549

PCIIIa-r

E = -4116.122655 ZPVE = 0.253125 NIMAG = 0.

6	-0.968528	1.616089	0.33528
6	-0.112551	2.466959	-0.382117
6	-2.187738	2.121014	0.822758
6	-0.473751	3.799022	-0.608702
1	0.835941	2.096356	-0.760148
6	-2.541913	3.451065	0.596869
1	-2.867527	1.47894	1.375267
6	-1.684505	4.292547	-0.120627
1	0.19759	4.447158	-1.163833
1	-3.485701	3.82979	0.97824
1	-1.960927	5.328349	-0.294863
17	2.1135	-2.857975	1.190363

6	-0.871968	-0.463542	2.414499
1	-1.931549	-0.245371	2.584738
1	-0.734877	-1.540558	2.553463
6	0.022743	0.314583	3.387506
1	-0.256481	0.083639	4.420444
1	1.076407	0.041731	3.266015
1	-0.070447	1.396364	3.25058
15	-0.460216	-0.123138	0.629676
12	1.982858	-0.888657	0.11064
35	3.224138	0.670165	-1.190435
6	-1.645268	-1.177935	-0.310666
6	-1.576319	-2.572867	-0.137208
6	-2.556258	-0.649549	-1.238222
6	-2.423866	-3.415202	-0.858466
1	-0.850512	-3.008006	0.544586
6	-3.399575	-1.498854	-1.960061
1	-2.611606	0.421458	-1.401519
6	-3.338874	-2.880874	-1.770255
1	-2.360515	-4.48946	-0.712758
1	-4.100197	-1.076129	-2.674294
1	-3.994758	-3.538268	-2.333229

PIIIa-r

E = -883.919780 ZPVE = 0.248603 NIMAG = 0.

6	-1.382185	-0.012555	-0.322886
6	-1.867393	-0.873026	-1.32411
6	-2.036573	-0.008105	0.91984
6	-2.953203	-1.717921	-1.086023

1	-1.389181	-0.87719	-2.300612
6	-3.133758	-0.842179	1.157088
1	-1.696957	0.646401	1.716545
6	-3.592613	-1.702711	0.157
1	-3.306205	-2.378177	-1.873266
1	-3.626803	-0.819719	2.125203
1	-4.444409	-2.35081	0.342259
6	0.081965	2.361031	0.580276
1	0.044241	1.896672	1.573147
1	1.069933	2.829868	0.500785
6	-1.014816	3.422163	0.419214
1	-0.922083	4.194499	1.19109
1	-0.947801	3.913668	-0.557222
1	-2.016229	2.987584	0.502453
15	0.060689	1.062719	-0.775613
6	1.51277	0.030844	-0.240921
6	2.753824	0.318298	-0.835128
6	1.450356	-1.00054	0.710012
6	3.904694	-0.386719	-0.473269
1	2.817412	1.094885	-1.593855
6	2.598196	-1.714611	1.06475
1	0.501076	-1.255686	1.171148
6	3.829095	-1.407284	0.478238
1	4.854863	-0.146962	-0.942542
1	2.529608	-2.512031	1.799833
1	4.720042	-1.963892	0.754737

R1_{IV} + a S_N2@P-f pathway

RC_{IVa-r}

E = -3924.285141 ZPVE = 0.195705 NIMAG = 0.

17	-0.006099	-0.507502	0.209086
6	2.33493	2.452909	0.014049
1	1.475732	2.725303	-0.619659
1	2.040236	2.748437	1.034646
6	3.564644	3.281758	-0.410747
1	4.431284	3.081738	0.23136
1	3.876987	3.052462	-1.437129
1	3.381516	4.365772	-0.369139
15	-1.400784	1.106796	-0.30776
12	2.510951	0.351055	-0.004632
35	3.652565	-1.738391	-0.063192
6	-1.33122	2.024534	1.298122
1	-1.508876	1.398025	2.17554
1	-0.356517	2.511196	1.382433
1	-2.102984	2.802049	1.254196
6	-2.981843	0.184461	-0.1567
6	-3.428983	-0.464033	1.007967
6	-3.790317	0.159403	-1.305762
6	-4.66232	-1.112776	1.022599
1	-2.809737	-0.47922	1.899793
6	-5.031503	-0.483416	-1.286815
1	-3.448064	0.643889	-2.216572
6	-5.466929	-1.119447	-0.123415
1	-4.996801	-1.616013	1.924938
1	-5.649536	-0.491944	-2.17948
1	-6.427749	-1.625441	-0.107452

TSIVa-r

E = -3924.249447 ZPVE = 0.194469 NIMAG = 1.

17	-0.085592	-0.874266	-0.552354
6	-1.284231	1.960545	0.481157
1	-0.567837	1.511058	1.183059
1	-0.842029	2.004126	-0.525867
6	-1.860974	3.275791	0.95096
1	-2.6061	3.663277	0.246577
1	-2.35318	3.17108	1.924641
1	-1.094298	4.061232	1.06755
15	1.766833	1.548547	-0.203283
12	-2.175874	0.02103	0.053231
35	-4.290425	-1.064738	0.079248
6	1.66473	1.687634	-2.043499
1	1.330834	0.763148	-2.52114
1	0.963117	2.487196	-2.292786
1	2.654829	1.958018	-2.431299
6	2.941856	0.212554	0.053739
6	3.439272	-0.666338	-0.93495
6	3.44034	0.099959	1.37367
6	4.413617	-1.605178	-0.61578
1	3.052026	-0.6243	-1.94669
6	4.411738	-0.846016	1.691001
1	3.060704	0.763947	2.146184
6	4.900227	-1.69798	0.695657
1	4.788996	-2.27644	-1.382147
1	4.78569	-0.921375	2.707292
1	5.655733	-2.439006	0.939712

PCIVa-r

E = -3924.359612 ZPVE = 0.198487 NIMAG = 0.

17	1.340835	2.100884	2.362669
6	-2.000574	1.196044	-0.890267
1	-1.174958	1.046214	-1.595597
1	-1.588923	1.671508	0.013051
6	-3.061963	2.109064	-1.519692
1	-3.891849	2.30563	-0.832679
1	-2.62331	3.075412	-1.789482
1	-3.476304	1.663106	-2.429768
15	-2.666515	-0.510554	-0.462848
12	1.276815	0.742517	0.589968
35	2.039479	0.374818	-1.619662
6	-3.598227	-0.125581	1.106469
1	-3.05787	0.530775	1.797191
1	-4.537678	0.364791	0.834572
1	-3.850069	-1.057959	1.620418
6	-1.101067	-1.27646	0.203785
6	-0.475573	-0.895515	1.410191
6	-0.499007	-2.294465	-0.554018
6	0.72797	-1.500643	1.825445
1	-0.932951	-0.154931	2.061441
6	0.695116	-2.896175	-0.146921
1	-0.969829	-2.613028	-1.479797
6	1.319477	-2.496024	1.035812
1	1.171451	-1.211711	2.775154
1	1.145372	-3.668254	-0.763005
1	2.249989	-2.958577	1.349562

P1V_{a-r}

E = -692.176347 ZPVE = 0.194948 NIMAG = 0.

6	2.019389	0.045661	1.061529
1	1.588125	-0.539499	1.88238
1	1.740254	1.092799	1.236408
6	3.546728	-0.108237	1.05692
1	4.013958	0.496565	0.27206
1	3.972389	0.214211	2.013767
1	3.841208	-1.150611	0.893716
15	1.215933	-0.590661	-0.51373
6	1.662514	0.786128	-1.695587
1	2.729154	0.721949	-1.931838
1	1.106324	0.651643	-2.627993
1	1.451322	1.786323	-1.301071
6	-0.567382	-0.200147	-0.161597
6	-1.490351	-1.257306	-0.209564
6	-1.044006	1.083566	0.155944
6	-2.847395	-1.043456	0.053726
1	-1.140596	-2.256167	-0.457737
6	-2.397973	1.302673	0.417951
1	-0.358298	1.925549	0.200529
6	-3.303965	0.238029	0.367811
1	-3.544235	-1.875919	0.010665
1	-2.746589	2.302814	0.661112
1	-4.357371	0.408789	0.571146

R1_v + a S_{N2}@P-f pathway

RC_{V_{a-r}}

E = -3732.547871 ZPVE = 0.142471 NIMAG = 0.

17	2.301598	0.058876	1.560863
6	-1.975448	2.424008	-0.124193
1	-1.349594	3.043624	0.53772
1	-1.794325	2.824221	-1.134984
6	-3.461155	2.61823	0.242551
1	-4.123135	2.048615	-0.421405
1	-3.676483	2.281531	1.264227
1	-3.778852	3.669851	0.181615
15	1.551748	0.480337	-0.350093
12	-1.195575	0.464385	-0.080313
35	-1.298166	-1.937765	-0.02959
6	2.55651	1.955933	-0.812921
1	2.286414	2.797723	-0.17089
1	3.628599	1.758622	-0.727048
1	2.316674	2.221058	-1.848904
6	2.305484	-0.865208	-1.351706
1	2.091042	-0.669264	-2.408525
1	3.387609	-0.917358	-1.203459
1	1.839025	-1.813169	-1.07462

TS_{Va-r}

E = -3732.505125 ZPVE = 0.141593 NIMAG = 1.

17	-1.067232	-0.739896	-1.834915
6	-0.289592	2.158572	0.108958
1	-1.271211	2.429679	-0.277878
1	-0.226016	2.349831	1.184703

6	0.832488	2.84667	-0.680673
1	1.835985	2.565022	-0.339277
1	0.768151	2.646544	-1.758436
1	0.765031	3.941851	-0.571408
15	-1.885477	-0.361676	0.833363
12	0.521158	0.1329	-0.349727
35	2.631969	-0.638338	0.428676
6	-3.04066	1.036896	1.158935
1	-2.532821	1.863523	1.653671
1	-3.502724	1.398305	0.232807
1	-3.8425	0.660521	1.806217
6	-3.13231	-1.619674	0.295725
1	-3.713133	-1.866752	1.196006
1	-3.816721	-1.253909	-0.474351
1	-2.63133	-2.518984	-0.063554

PC_{Va-r}

E = -3732.633660 ZPVE = 0.145712 NIMAG = 0.

17	0.134381	2.997406	-0.162877
6	-2.830139	-0.081672	0.736509
1	-3.142341	0.927341	0.443663
1	-3.678051	-0.752784	0.549637
6	-2.433608	-0.097321	2.21943
1	-2.096071	-1.086314	2.54614
1	-1.634259	0.622096	2.42596
1	-3.290009	0.179118	2.842367
15	-1.449137	-0.546793	-0.414317
12	0.731266	0.837705	-0.089784

35	2.502259	-0.738352	0.142814
6	-1.239858	-2.366567	-0.204154
1	-0.845415	-2.584947	0.791429
1	-2.186876	-2.898069	-0.344653
1	-0.508329	-2.731453	-0.930204
6	-2.227148	-0.386958	-2.082601
1	-1.537361	-0.751487	-2.849211
1	-3.158764	-0.959071	-2.142882
1	-2.439672	0.666545	-2.284765

P_{Va-r}

E = -500.432930 ZPVE = 0.141195 NIMAG = 0.

6	1.013989	-0.690442	0.359012
1	1.049471	-1.764342	0.135607
1	0.83543	-0.595286	1.439352
6	2.35109	-0.041163	-0.023342
1	2.368163	1.026179	0.222943
1	3.1825	-0.512744	0.512527
1	2.546741	-0.137864	-1.096746
15	-0.450298	-0.001472	-0.589938
6	-0.672597	1.633554	0.284503
1	0.140011	2.314918	0.014886
1	-1.609351	2.094831	-0.044555
1	-0.697523	1.526656	1.376238
6	-1.816752	-0.970037	0.234022
1	-1.772253	-0.9151	1.328767
1	-2.787093	-0.586222	-0.096835
1	-1.75601	-2.020434	-0.068274

R1 + b S_N2@P-b pathway

RC_{1b-i}

E = -4543.905902 ZPVE = 0.489525 NIMAG = 0.

6	3.796945	-1.233337	-0.385231
6	3.095968	0.163332	-0.419111
6	3.179032	-2.122346	0.717229
6	2.491154	-0.07083	2.093676
6	3.094537	0.805618	0.983727
6	3.180273	-1.443256	2.095901
6	3.92527	-1.94183	-1.763974
6	2.59619	0.624439	3.456068
6	4.668283	-1.071179	-2.794167
6	4.639944	-3.30175	-1.650693
1	4.829107	-1.011183	-0.062755
1	3.709963	0.821614	-1.060073
1	3.747021	-3.054457	0.790303
1	2.155684	-2.401928	0.440795
1	1.425841	-0.221769	1.884204
1	2.607177	1.784572	0.95826
1	4.14807	1.002809	1.238456
1	2.697954	-2.100189	2.830698
1	4.221878	-1.316181	2.430633
1	2.91465	-2.135695	-2.152051
1	2.057689	1.578196	3.456193
1	2.159048	0.003689	4.245456
1	3.643675	0.821151	3.719603
1	5.670839	-0.809416	-2.431538

1	4.789436	-1.614039	-3.73754
1	4.140892	-0.141883	-3.027609
1	5.621277	-3.193311	-1.170619
1	4.805564	-3.725547	-2.646945
1	4.063744	-4.03295	-1.078178
15	1.572618	0.253718	-1.53683
6	0.937722	1.960311	-1.258841
6	0.330518	2.4275	-0.081393
6	1.066658	2.836219	-2.350863
6	-0.147812	3.735254	-0.002099
1	0.214262	1.780412	0.781342
6	0.624859	4.159566	-2.254792
1	1.499739	2.482	-3.283144
6	0.021242	4.611262	-1.079331
1	-0.629303	4.070456	0.911794
1	0.739582	4.828081	-3.102939
1	-0.337384	5.63419	-1.010839
17	0.018441	-0.923657	-0.531589
6	-4.979267	-2.125263	-1.115137
6	-4.002802	-1.365161	-0.479707
6	-3.715638	-0.021126	-0.742366
6	-4.50511	0.578221	-1.729322
6	-5.50557	-0.136867	-2.409046
6	-5.738403	-1.478733	-2.102862
1	-5.162914	-3.168138	-0.877166
1	-6.102689	0.353051	-3.173749
1	-6.512055	-2.033391	-2.626421
12	-2.187406	0.049791	0.699538
35	-1.297004	0.759357	2.822314
1	-4.346949	1.623524	-1.988756

8	-3.145956	-1.872557	0.539829
6	-3.341588	-3.186736	1.060685
1	-2.610759	-3.312948	1.860071
1	-4.354021	-3.290345	1.465801
1	-3.172586	-3.938332	0.281996

TS_{1b-i}

E = -4543.865002 ZPVE = 0.487912 NIMAG = 1.

6	2.810329000	-1.832020000	-1.373476000
6	2.308040000	-0.773520000	-0.353559000
6	3.043129000	-3.175685000	-0.649703000
6	3.559226000	-1.982364000	1.559524000
6	3.290862000	-0.647159000	0.844869000
6	4.008190000	-3.040427000	0.538934000
6	1.929988000	-1.949049000	-2.649540000
6	4.580999000	-1.808435000	2.689399000
6	1.743188000	-0.592543000	-3.354932000
6	2.504587000	-2.963209000	-3.655666000
1	3.797448000	-1.469999000	-1.709733000
1	2.274729000	0.211278000	-0.836372000
1	3.446300000	-3.915024000	-1.347766000
1	2.079677000	-3.574385000	-0.299271000
1	2.616391000	-2.328371000	2.008475000
1	2.927126000	0.102232000	1.555893000
1	4.241337000	-0.263682000	0.443884000
1	4.119929000	-4.011483000	1.036972000
1	5.006076000	-2.767424000	0.162016000
1	0.935312000	-2.310564000	-2.349003000

1	4.237489000	-1.076577000	3.429159000
1	4.753988000	-2.755470000	3.212328000
1	5.545965000	-1.462204000	2.297750000
1	2.713373000	-0.146823000	-3.610697000
1	1.180389000	-0.720861000	-4.284791000
1	1.186345000	0.131008000	-2.752041000
1	3.529856000	-2.694544000	-3.941713000
1	1.900319000	-2.975380000	-4.569008000
1	2.521673000	-3.983246000	-3.263035000
15	0.526033000	-1.118312000	0.202454000
6	0.228489000	0.471781000	1.084962000
6	-0.365183000	0.518159000	2.362278000
6	0.495712000	1.694519000	0.429478000
6	-0.655212000	1.741381000	2.968243000
1	-0.575221000	-0.402437000	2.893111000
6	0.182792000	2.912999000	1.031066000
1	0.922771000	1.707936000	-0.567762000
6	-0.387347000	2.941839000	2.306439000
1	-1.094983000	1.751422000	3.961068000
1	0.385868000	3.838805000	0.500736000
1	-0.621903000	3.891193000	2.778591000
17	-0.326265000	-2.843654000	2.170103000
6	-2.365166000	-1.997087000	-3.265718000
6	-2.078025000	-2.163660000	-1.914901000
6	-2.057175000	-1.127802000	-0.960715000
6	-2.301011000	0.159949000	-1.467408000
6	-2.567766000	0.386691000	-2.825332000
6	-2.603044000	-0.689089000	-3.716143000
1	-2.410199000	-2.830383000	-3.959611000
1	-2.764741000	1.393251000	-3.184632000

1	-2.819909000	-0.521069000	-4.767273000
12	-2.215914000	-2.586434000	0.666624000
35	-4.355040000	-3.477213000	1.273018000
1	-2.293167000	1.012597000	-0.790614000
8	-1.825232000	-3.415194000	-1.317835000
6	-2.247915000	-4.615654000	-1.980190000
1	-2.074358000	-5.428160000	-1.274836000
1	-3.313153000	-4.559583000	-2.223646000
1	-1.655399000	-4.781100000	-2.885363000

PC_{1b-i}

E = -4543.986825 ZPVE = 0.492955 NIMAG = 0.

6	-2.98512	-0.089522	0.553374
6	-1.951238	1.071612	0.416604
6	-3.134148	-0.846339	-0.780626
6	-2.564666	1.281252	-2.094052
6	-2.390983	2.003432	-0.746207
6	-3.518152	0.087175	-1.939328
6	-2.821153	-1.000975	1.801718
6	-3.03681	2.250452	-3.184644
6	-2.858923	-0.191939	3.111112
6	-3.906777	-2.092683	1.864303
1	-3.938892	0.444443	0.712762
1	-1.976101	1.649725	1.345325
1	-3.907413	-1.613817	-0.687486
1	-2.207102	-1.37625	-1.029937
1	-1.58941	0.883516	-2.406157
1	-1.695283	2.841621	-0.859913

1	-3.35543	2.445786	-0.454365
1	-3.544815	-0.484256	-2.873882
1	-4.537307	0.468579	-1.768892
1	-1.852232	-1.510069	1.744538
1	-2.335064	3.082651	-3.313086
1	-3.126823	1.737454	-4.148061
1	-4.018551	2.674657	-2.937373
1	-3.809818	0.3488	3.204225
1	-2.771558	-0.85739	3.976504
1	-2.047736	0.536499	3.18626
1	-4.911986	-1.653931	1.817959
1	-3.832232	-2.644988	2.807412
1	-3.820409	-2.81972	1.052819
15	-0.118383	0.6416	0.150309
6	0.740429	2.26822	0.356788
6	2.010277	2.408835	-0.229207
6	0.203414	3.353582	1.070373
6	2.72249	3.603352	-0.099828
1	2.462578	1.578314	-0.763596
6	0.916597	4.548368	1.193433
1	-0.776125	3.286754	1.531912
6	2.178925	4.676792	0.608596
1	3.703708	3.688255	-0.557064
1	0.482802	5.376807	1.746182
1	2.731899	5.606825	0.702942
17	-0.434627	-1.890772	-3.242208
6	1.391762	-2.447653	2.448419
6	0.8256	-1.695276	1.419415
6	0.517112	-0.329458	1.596418
6	0.822257	0.254163	2.832558

6	1.380866	-0.488346	3.87404
6	1.663294	-1.838922	3.676599
1	1.638991	-3.491619	2.305244
1	1.604263	-0.011359	4.822914
1	2.108137	-2.428932	4.472076
12	0.877059	-1.069064	-1.594564
35	3.280313	-0.928217	-1.484671
1	0.633226	1.313139	2.976952
8	0.525384	-2.2508	0.178262
6	0.771726	-3.660197	-0.039465
1	0.402304	-3.864088	-1.045031
1	1.842543	-3.870328	0.024071
1	0.208847	-4.250778	0.68746

P_{1b-i}

E = -1311.761951 ZPVE = 0.487694 NIMAG = 0.

6	1.233504	1.890763	-0.815051
6	-0.191713	1.257734	-0.752752
6	1.526605	2.659718	0.49151
6	-0.959419	3.24318	0.73198
6	-1.215458	2.406206	-0.536033
6	0.486594	3.763774	0.744235
6	2.38372	0.955641	-1.280471
6	-1.975138	4.38587	0.856009
6	2.063246	0.271858	-2.621843
6	3.716388	1.717482	-1.421088
1	1.150269	2.654287	-1.609964
1	-0.401463	0.796492	-1.723342

1	2.517169	3.121869	0.444948
1	1.545033	1.957642	1.335056
1	-1.084601	2.584362	1.602465
1	-2.239048	2.017501	-0.516027
1	-1.157877	3.070685	-1.412352
1	0.693524	4.2626	1.700377
1	0.591072	4.53442	-0.035769
1	2.530544	0.176057	-0.526049
1	-3.002566	4.005127	0.887941
1	-1.80578	4.968696	1.768961
1	-1.899963	5.073776	0.003793
1	1.858174	1.018674	-3.400677
1	2.914712	-0.329931	-2.958126
1	1.203179	-0.398213	-2.557158
1	3.611538	2.573306	-2.101263
1	4.4871	1.059314	-1.837555
1	4.092502	2.093323	-0.465674
15	-0.500998	-0.051716	0.611742
6	-2.205118	-0.655856	0.154664
6	-2.95016	-1.226293	1.201982
6	-2.805261	-0.585305	-1.114393
6	-4.23739	-1.726175	0.989303
1	-2.514257	-1.274648	2.19683
6	-4.097792	-1.072329	-1.329534
1	-2.270337	-0.146053	-1.951029
6	-4.81748	-1.64839	-0.279315
1	-4.789063	-2.165175	1.816025
1	-4.5402	-1.002863	-2.319785
1	-5.821683	-2.026995	-0.447453
6	2.402777	-3.018726	0.640843

6	1.67636	-1.843337	0.873189
6	0.499185	-1.557963	0.138841
6	0.093506	-2.495458	-0.820048
6	0.814553	-3.668101	-1.065576
6	1.969302	-3.92611	-0.330014
1	3.301946	-3.233531	1.205811
1	0.469237	-4.371212	-1.817425
1	2.540088	-4.834381	-0.501531
1	-0.818606	-2.316454	-1.379575
8	2.057185	-0.903818	1.791891
6	3.175579	-1.165493	2.629791
1	3.247746	-0.308979	3.30139
1	3.027939	-2.078897	3.219273
1	4.102851	-1.250663	2.049252

R1_{II} + b SN2@P-b pathway

RC_{III-i}

E = -4235.421442 ZPVE = 0.370813 NIMAG = 0.

15	-1.514504	-0.415323	-0.176374
17	-2.721924	0.593811	-1.566678
6	-2.631727	-0.475283	1.370137
6	-1.767967	-1.026321	2.529122
1	-2.350985	-0.961813	3.455456
1	-1.485703	-2.072186	2.390955
1	-0.852625	-0.444269	2.680426
6	-3.914723	-1.30709	1.218706
1	-4.547655	-1.145421	2.100015
1	-4.491799	-1.010807	0.33795
1	-3.707681	-2.378714	1.159086

6	-3.004522	0.990832	1.694679
1	-3.492459	1.014191	2.676339
1	-2.13195	1.650334	1.735496
1	-3.699542	1.405033	0.960768
12	0.797561	0.953368	0.34684
35	0.053205	3.229734	0.195762
6	2.298985	-0.394373	1.009024
6	2.997566	-0.315149	-0.201714
6	2.896855	-1.2	1.98743
6	4.206724	-0.943598	-0.486008
6	4.110711	-1.868268	1.757574
1	2.42386	-1.310089	2.962328
6	4.762241	-1.736177	0.529047
1	4.710861	-0.840277	-1.441966
1	4.552989	-2.481327	2.538712
1	5.705378	-2.245399	0.352086
8	2.295238	0.490707	-1.143387
6	2.995612	1.09717	-2.234235
1	2.296827	1.79483	-2.696769
1	3.872885	1.640175	-1.867085
1	3.302003	0.340504	-2.963976
6	-1.283685	-2.099242	-1.049008
6	-2.56799	-2.763165	-1.574031
1	-2.28854	-3.653864	-2.150302
1	-3.231221	-3.088017	-0.770723
1	-3.128273	-2.100808	-2.238888
6	-0.351838	-1.791885	-2.24597
1	0.595406	-1.346191	-1.928969
1	-0.121345	-2.732135	-2.761417
1	-0.82634	-1.123872	-2.970592

6	-0.550326	-3.045853	-0.073888
1	0.333259	-2.5826	0.377137
1	-1.207646	-3.402634	0.723769
1	-0.209724	-3.925931	-0.632532

TS_{nb-i}

E = -4235.369831 ZPVE = 0.371658 NIMAG = 1.

15	1.248303	-0.233166	-0.144713
17	2.077345	-2.108194	-1.511383
6	2.018903	-0.870428	1.519004
6	1.755553	0.06102	2.714698
1	2.230221	-0.379964	3.600214
1	2.184192	1.056381	2.575866
1	0.689753	0.159157	2.926816
6	3.537586	-1.104613	1.405312
1	3.870384	-1.618991	2.315573
1	3.797082	-1.729442	0.549009
1	4.09166	-0.163511	1.346025
6	1.313661	-2.217439	1.796661
1	1.696404	-2.627516	2.739414
1	0.230086	-2.10005	1.925958
1	1.497564	-2.946775	1.00573
12	-1.05286	-0.901938	-0.378602
35	-2.806702	-2.337917	0.26947
6	-0.508494	1.413996	0.604006
6	-1.566352	1.673544	-0.286671
6	-0.460087	2.296279	1.699175
6	-2.503037	2.69871	-0.142622

6	-1.363275	3.350588	1.879241
1	0.322933	2.188555	2.440757
6	-2.386843	3.553623	0.95498
1	-3.309211	2.841911	-0.852853
1	-1.265929	4.006301	2.740103
1	-3.098889	4.363377	1.082133
8	-1.672977	0.752682	-1.37515
6	-2.717917	0.901059	-2.351264
1	-2.558587	0.110463	-3.084936
1	-3.701258	0.784374	-1.887152
1	-2.632519	1.875644	-2.838688
6	2.288383	1.161268	-1.01499
6	3.640736	0.646893	-1.556273
1	4.14399	1.500516	-2.027349
1	4.296703	0.270109	-0.771099
1	3.517891	-0.137826	-2.301074
6	1.447744	1.636211	-2.217476
1	0.513269	2.107335	-1.908554
1	2.028734	2.379598	-2.776951
1	1.22587	0.808431	-2.898202
6	2.576368	2.342927	-0.067924
1	1.668232	2.808268	0.31321
1	3.202698	2.045592	0.778349
1	3.13446	3.101919	-0.630268

PC_{nb-i}

E = -4235.495754 ZPVE = 0.373819 NIMAG = 0.

15	0.935835	-0.567454	0.06969
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17	-2.110607	-1.892075	-2.347634
6	1.378403	-1.12073	1.85381
6	2.876366	-1.302686	2.159468
1	2.984167	-1.590807	3.212513
1	3.33172	-2.094488	1.55897
1	3.45335	-0.385031	2.015414
6	0.651191	-2.47247	2.059121
1	0.856822	-2.838166	3.072427
1	-0.433282	-2.361239	1.963307
1	0.985	-3.242342	1.357639
6	0.772346	-0.094937	2.836471
1	0.84488	-0.504978	3.851273
1	1.306192	0.858361	2.822584
1	-0.285395	0.09666	2.633781
12	-1.594362	-0.690985	-0.493933
35	-2.941377	-0.114598	1.424213
6	1.078846	1.274592	-0.012801
6	0.018898	2.009433	-0.593762
6	2.159806	2.002892	0.506947
6	0.037723	3.406152	-0.619725
6	2.199546	3.397397	0.469649
1	2.988882	1.468602	0.956782
6	1.13124	4.09485	-0.09137
1	-0.784404	3.965197	-1.047359
1	3.051454	3.929048	0.881242
1	1.137522	5.180133	-0.119952
8	-1.031413	1.289901	-1.14698
6	-2.123989	1.997672	-1.775638
1	-2.767094	1.224904	-2.197834
1	-2.672332	2.58331	-1.033716

1	-1.744326	2.630555	-2.581453
6	2.136856	-1.21356	-1.274727
6	2.09643	-2.755815	-1.262107
1	2.675916	-3.132515	-2.113593
1	2.539731	-3.177818	-0.355399
1	1.075638	-3.13669	-1.365916
6	1.566939	-0.713812	-2.622223
1	1.56903	0.379234	-2.684041
1	2.20545	-1.088905	-3.431514
1	0.551467	-1.076358	-2.803997
6	3.587973	-0.715668	-1.144049
1	3.647772	0.375682	-1.183427
1	4.077315	-1.058562	-0.230809
1	4.167704	-1.103002	-1.991279

P11b-i

E = -1003.265709 ZPVE = 0.368314 NIMAG = 0.

15	0.72486	0.296371	-0.594634
6	1.877597	-1.254702	-0.719027
6	2.595759	-1.775398	0.540281
1	3.205986	-2.649179	0.272409
1	3.272432	-1.029983	0.967167
1	1.905612	-2.096483	1.324244
6	2.953678	-0.868419	-1.763506
1	3.590238	-1.738282	-1.973684
1	2.497558	-0.545804	-2.704516
1	3.604352	-0.062131	-1.413519
6	1.025981	-2.389477	-1.328909

1	1.684088	-3.212944	-1.636118
1	0.296067	-2.788595	-0.620283
1	0.481466	-2.05083	-2.217769
6	-0.847893	-0.327435	0.199906
6	-2.085754	0.108853	-0.339928
6	-0.906487	-1.223976	1.277663
6	-3.304031	-0.352104	0.182767
6	-2.113582	-1.691372	1.80559
1	0.01683	-1.573326	1.723125
6	-3.313498	-1.250709	1.251352
1	-4.24519	-0.016442	-0.235516
1	-2.110543	-2.387223	2.639123
1	-4.263767	-1.599573	1.64574
8	-2.02234	0.994847	-1.377403
6	-3.225164	1.437895	-1.989927
1	-2.915365	2.107077	-2.793825
1	-3.793212	0.599979	-2.413614
1	-3.85914	1.988586	-1.283267
6	1.373253	1.527454	0.744838
6	2.786394	1.991134	0.336796
1	3.088023	2.840833	0.963411
1	3.536138	1.205967	0.472842
1	2.819496	2.319658	-0.707712
6	0.418322	2.739259	0.642779
1	-0.606967	2.47163	0.917517
1	0.752439	3.527765	1.330251
1	0.399547	3.154509	-0.369725
6	1.391023	1.046541	2.206779
1	0.391884	0.770274	2.553942
1	2.056049	0.193703	2.361747

1 1.748219 1.861207 2.852053

R1_{III} + b S_N2@P-b pathway

RC_{IIIb-i}

E = -4383.020022 ZPVE = 0.308471 NIMAG = 0.

6	-2.509622	-0.170958	0.509293
6	-2.921772	1.111583	0.916869
6	-3.217996	-1.300787	0.950072
6	-4.036269	1.25333	1.7445
1	-2.381373	1.993173	0.582214
6	-4.332158	-1.148427	1.777033
1	-2.903051	-2.294878	0.652096
6	-4.744051	0.12698	2.173375
1	-4.349705	2.245764	2.054152
1	-4.875367	-2.026839	2.11307
1	-5.609887	0.241802	2.819023
17	-1.721121	0.092874	-2.469119
15	-0.99957	-0.277487	-0.526229
12	0.943533	1.540403	0.15372
35	-0.240045	3.554345	-0.39678
6	2.410189	0.523454	1.2869
6	2.931294	0.085916	2.510231
6	3.200088	0.243308	0.165388
6	4.153146	-0.604045	2.589246
1	2.382628	0.276496	3.431192
6	4.419121	-0.427679	0.1796
6	4.889807	-0.856942	1.430503
1	4.533412	-0.933433	3.552772
1	4.997088	-0.620329	-0.718596

1	5.837814	-1.384269	1.488991
8	2.587621	0.74456	-1.017067
6	3.263068	0.655957	-2.272385
1	2.609935	1.125605	-3.008369
1	4.219122	1.188909	-2.230894
1	3.430991	-0.391706	-2.544159
6	-0.584753	-2.065147	-0.578258
6	-1.181373	-2.985246	-1.454222
6	0.388405	-2.507855	0.333777
6	-0.818651	-4.33251	-1.406195
1	-1.920565	-2.650665	-2.174454
6	0.741061	-3.858997	0.381508
1	0.881853	-1.802663	0.997079
6	0.140897	-4.771879	-0.488613
1	-1.283709	-5.037509	-2.08917
1	1.496066	-4.189488	1.088305
1	0.422986	-5.820244	-0.457312

TS_{nb-i}

E = -4382.988880 ZPVE = 0.308352 NIMAG = 1.

6	-1.55375	1.691839	0.109174
6	-0.775812	2.765423	0.566483
6	-2.946902	1.747116	0.251432
6	-1.378465	3.873291	1.165576
1	0.30618	2.749541	0.459685
6	-3.547137	2.851274	0.860025
1	-3.564896	0.944376	-0.136007
6	-2.766595	3.916241	1.318066

1	-0.762622	4.699155	1.508948
1	-4.627892	2.883425	0.962749
1	-3.237167	4.777484	1.78302
17	-1.692801	0.919475	-2.856897
15	-0.722664	0.319168	-0.77937
12	1.71019	0.258974	-0.750305
35	3.86087	1.198039	-0.884207
6	0.393761	-0.310899	1.165456
6	0.026332	0.119918	2.449083
6	1.268534	-1.408729	1.12815
6	0.46934	-0.527811	3.608183
1	-0.640572	0.971896	2.552981
6	1.743706	-2.079519	2.253068
6	1.316782	-1.632465	3.507591
1	0.152252	-0.17309	4.58474
1	2.425056	-2.919442	2.17846
1	1.663286	-2.143452	4.40084
8	1.702173	-1.732771	-0.186777
6	2.635613	-2.805924	-0.391987
1	2.79792	-2.86133	-1.468372
1	3.581537	-2.599534	0.11705
1	2.200978	-3.743805	-0.03685
6	-1.696596	-1.245642	-0.638643
6	-1.704094	-2.124158	-1.732781
6	-2.389882	-1.602975	0.527163
6	-2.383051	-3.342105	-1.656545
1	-1.206835	-1.842087	-2.654492
6	-3.086576	-2.811469	0.592609
1	-2.383667	-0.946429	1.389694
6	-3.080268	-3.687262	-0.496147

1	-2.37932	-4.011329	-2.511986
1	-3.628048	-3.068505	1.498468
1	-3.618381	-4.629231	-0.44176

PC_{IIIb-i}

E = -4383.098363 ZPVE = 0.310816 NIMAG = 0.

6	-1.344497	1.738599	-0.463719
6	-0.465408	2.783598	-0.801384
6	-2.72151	1.993375	-0.378016
6	-0.963972	4.068144	-1.023096
1	0.602125	2.594328	-0.883185
6	-3.213709	3.280669	-0.610999
1	-3.412251	1.190854	-0.139707
6	-2.336006	4.320171	-0.927623
1	-0.277296	4.869633	-1.278459
1	-4.28173	3.467399	-0.545806
1	-2.719406	5.320179	-1.108733
17	1.575732	-2.471226	-2.60691
15	-0.620942	0.070403	-0.205849
12	1.661648	-0.707285	-1.199625
35	3.097531	1.198242	-0.875433
6	0.005748	0.083077	1.528673
6	-0.486294	0.92423	2.533291
6	1.084561	-0.769207	1.841692
6	0.049616	0.899015	3.823293
1	-1.292422	1.612609	2.298202
6	1.627847	-0.805437	3.124472
6	1.099415	0.028968	4.114318

1	-0.347824	1.556744	4.589623
1	2.460477	-1.456399	3.359996
1	1.52783	0.002423	5.111554
8	1.570793	-1.556018	0.802543
6	2.481976	-2.637106	1.101265
1	2.614926	-3.168834	0.158748
1	3.439342	-2.245551	1.455878
1	2.032904	-3.299633	1.845673
6	-2.016246	-1.125111	-0.212607
6	-2.264465	-1.818786	-1.408691
6	-2.821436	-1.379798	0.909309
6	-3.318125	-2.73218	-1.487386
1	-1.623173	-1.664273	-2.271651
6	-3.869844	-2.298905	0.828561
1	-2.62681	-0.870388	1.848082
6	-4.12257	-2.97211	-0.370664
1	-3.497644	-3.265235	-2.416103
1	-4.485845	-2.490621	1.702454
1	-4.936713	-3.688558	-0.430182

R_{int}-i

E = -1150.877424 ZPVE = 0.305833 NIMAG = 0.

6	1.911533	-0.457264	-0.485859
6	2.593018	-1.405175	-1.26943
6	2.572948	0.091102	0.624794
6	3.888033	-1.812603	-0.940351
1	2.105187	-1.823742	-2.14649
6	3.874044	-0.305261	0.947927

1	2.074097	0.834356	1.238709
6	4.533537	-1.26072	0.169906
1	4.395312	-2.549865	-1.556444
1	4.371204	0.13314	1.809026
1	5.544623	-1.56743	0.422433
15	0.203951	0.017404	-1.044333
6	-0.853066	-1.136607	-0.046948
6	-0.352853	-2.112957	0.822248
6	-2.251667	-1.0958	-0.262598
6	-1.197939	-3.025465	1.465075
1	0.71608	-2.165083	1.000118
6	-3.105071	-2.001139	0.377718
6	-2.571275	-2.965163	1.240318
1	-0.780647	-3.771758	2.134149
1	-4.175399	-1.965038	0.212731
1	-3.23987	-3.665787	1.732425
8	-2.683212	-0.120189	-1.115493
6	-4.069443	-0.019812	-1.414099
1	-4.160567	0.807934	-2.118284
1	-4.445039	-0.939132	-1.880443
1	-4.656206	0.201759	-0.513936
6	-0.04836	1.6435	-0.18589
6	0.334459	2.800523	-0.885196
6	-0.609479	1.788389	1.092314
6	0.181064	4.066714	-0.315749
1	0.752707	2.708646	-1.884681
6	-0.77561	3.05561	1.658943
1	-0.920832	0.90876	1.647843
6	-0.377523	4.197809	0.958984
1	0.487433	4.949054	-0.870856

1	-1.213882	3.148666	2.649059
1	-0.505865	5.181867	1.400943

R1_{IV} + b S_{N2}@P-b pathway

RC_{IVb-i}

E = -4191.277044 ZPVE = 0.255200 NIMAG = 0.

17	0.620879	-1.799958	1.935766
15	0.855694	-1.025584	-0.020009
12	-0.926762	1.080242	-0.35379
35	0.406171	3.057538	-0.11047
6	0.426373	-2.521874	-1.00628
1	0.998125	-3.4017	-0.703042
1	-0.641607	-2.719059	-0.888573
1	0.625901	-2.300332	-2.060137
6	2.668061	-0.864201	-0.191858
6	3.187535	0.438233	-0.281719
6	3.541926	-1.965052	-0.238033
6	4.564209	0.632625	-0.424894
1	2.522439	1.295984	-0.230855
6	4.913207	-1.763845	-0.382985
1	3.15962	-2.97725	-0.149381
6	5.425312	-0.464051	-0.479463
1	4.95742	1.642276	-0.493389
1	5.583353	-2.617739	-0.41755
1	6.494776	-0.31098	-0.591834
6	-2.590139	-0.002038	-1.082445
6	-3.126515	-0.173164	0.200064
6	-3.336291	-0.570514	-2.12143
6	-4.301868	-0.853161	0.504225

6	-4.52791	-1.274658	-1.877974
1	-2.993993	-0.472521	-3.150501
6	-5.004639	-1.414238	-0.573319
1	-4.677146	-0.957426	1.517143
1	-5.085043	-1.707542	-2.704805
1	-5.927503	-1.954637	-0.382514
8	-2.302959	0.454235	1.176284
6	-2.654449	0.404467	2.559561
1	-2.685451	-0.632704	2.909114
1	-1.876979	0.948902	3.095714
1	-3.624339	0.886013	2.723699

TS_{IVb-i}

E = -4191.248568 ZPVE = 0.254950 NIMAG = 1.

17	-1.905462	-2.129951	2.281334
15	-0.910507	-0.349693	1.065628
12	1.282637	-0.8315	0.137929
35	2.784057	-2.04537	-1.204349
6	-1.168364	0.85142	2.455235
1	-1.932432	0.455899	3.124349
1	-0.227658	0.933385	3.005504
1	-1.445417	1.836852	2.078393
6	-2.301331	-0.208572	-0.117055
6	-2.172865	-0.806139	-1.37905
6	-3.501345	0.433954	0.21514
6	-3.222349	-0.75608	-2.297929
1	-1.257207	-1.325584	-1.652825
6	-4.55174	0.483419	-0.704523

1	-3.630788	0.882139	1.194805
6	-4.415123	-0.109723	-1.96222
1	-3.108663	-1.22627	-3.270113
1	-5.478814	0.980148	-0.433528
1	-5.23483	-0.074802	-2.673664
6	0.220821	1.348392	0.001999
6	1.507603	1.71854	0.422541
6	-0.422056	2.265632	-0.843423
6	2.14167	2.910027	0.074061
6	0.168696	3.480019	-1.211515
1	-1.418611	2.037582	-1.212684
6	1.444344	3.80337	-0.745446
1	3.1421	3.152921	0.41389
1	-0.36447	4.170648	-1.858561
1	1.910494	4.743338	-1.025026
8	2.155836	0.715543	1.200963
6	3.517167	0.905912	1.626334
1	3.581454	1.783814	2.274315
1	3.784201	0.011931	2.189525
1	4.17998	1.013155	0.763003

PC_{IVb-i}

E = -4191.353844 ZPVE = 0.257403 NIMAG = 0.

17	2.704003	-2.010298	2.184811
15	-0.644844	0.036718	1.100342
12	1.556121	-1.178434	0.427437
35	1.326782	-1.62907	-1.928255
6	-0.883613	0.540629	2.861981

1	-1.23153	-0.318976	3.441394
1	0.089325	0.843731	3.257245
1	-1.584932	1.372298	2.969939
6	-2.301747	-0.422497	0.463955
6	-2.361841	-1.121765	-0.755196
6	-3.491763	-0.138386	1.152392
6	-3.596684	-1.501604	-1.282898
1	-1.44674	-1.361703	-1.291084
6	-4.724374	-0.531826	0.623794
1	-3.470265	0.386481	2.102154
6	-4.778872	-1.209746	-0.59617
1	-3.63093	-2.03688	-2.227005
1	-5.638194	-0.308679	1.166828
1	-5.736928	-1.514994	-1.006707
6	-0.219981	1.618123	0.245057
6	1.134011	1.883055	-0.045072
6	-1.180254	2.547374	-0.172068
6	1.511747	3.042533	-0.722746
6	-0.815183	3.715818	-0.843776
1	-2.229632	2.344488	0.019962
6	0.530733	3.956992	-1.116468
1	2.550102	3.238892	-0.957824
1	-1.575867	4.422762	-1.158946
1	0.829711	4.856595	-1.645671
8	2.059409	0.937989	0.384619
6	3.470155	1.214751	0.23861
1	3.716885	2.154943	0.738184
1	3.979368	0.389912	0.738185
1	3.744154	1.24949	-0.819222

Pivb-i

E = -959.133098 ZPVE = 0.252524 NIMAG = 0.

15	-0.156963	-1.203751	-0.382265
6	0.064834	-2.165977	1.203448
1	-0.673995	-2.972669	1.233588
1	1.063136	-2.608578	1.184879
1	-0.028094	-1.555431	2.106576
6	0.929561	0.26952	-0.056099
6	2.331421	0.080572	-0.088334
6	0.453324	1.574683	0.115973
6	3.209867	1.159455	0.055926
6	1.323086	2.662575	0.257531
1	-0.617303	1.748988	0.135766
6	2.699163	2.450822	0.228802
1	4.282589	1.007742	0.035216
1	0.921749	3.662791	0.389625
1	3.386971	3.284346	0.338779
8	2.74687	-1.213958	-0.262934
6	4.135307	-1.480725	-0.412295
1	4.693308	-1.221349	0.496205
1	4.213913	-2.553986	-0.590748
1	4.555547	-0.937454	-1.267611
6	-1.85314	-0.48085	-0.165688
6	-2.570328	-0.180855	-1.336789
6	-2.479559	-0.254819	1.071542
6	-3.863987	0.344489	-1.277155
1	-2.109782	-0.366816	-2.303952
6	-3.777985	0.258258	1.13558

1	-1.956341	-0.474553	1.996971
6	-4.472776	0.562591	-0.038636
1	-4.397833	0.572062	-2.195642
1	-4.245212	0.422738	2.102821
1	-5.481888	0.961648	0.012133

R1_v + b S_{N2}@P-b pathway

RC_{v_b-i}

E = -3999.532798 ZPVE = 0.201327 NIMAG = 0.

17	-0.923657	2.79407	1.102911
15	-1.433425	1.449822	-0.431891
12	-0.142915	-0.962961	-0.236076
35	-2.161606	-2.245668	-0.040007
6	-3.269955	1.469628	-0.338167
1	-3.589413	1.013231	0.601221
1	-3.668973	2.484452	-0.418286
1	-3.652248	0.850078	-1.156374
6	-1.091908	2.463428	-1.93213
1	-1.603312	3.429271	-1.898804
1	-0.014215	2.617191	-2.026048
1	-1.437301	1.897731	-2.805124
6	1.838499	-0.613968	-0.868088
6	2.28245	-0.343066	0.431552
6	2.815687	-0.516982	-1.865307
6	3.578184	0.017697	0.787644
6	4.140819	-0.154964	-1.569994
1	2.553994	-0.723231	-2.901924
6	4.516067	0.111969	-0.252211
1	3.874309	0.219843	1.811906

1	4.878252	-0.085359	-2.365403
1	5.540164	0.390546	-0.020353
8	1.218968	-0.491775	1.368151
6	1.440311	-0.227036	2.753779
1	1.760735	0.810063	2.898456
1	0.487065	-0.390057	3.257345
1	2.193025	-0.912396	3.157745

TS_{vb-i}

E = -3999.505169 ZPVE = 0.201791 NIMAG = 1.

17	-3.212673	-2.261091	0.516373
15	-1.850027	-0.398319	-0.045121
12	0.540716	-0.84937	-0.061077
35	2.505106	-2.024036	-0.59964
6	-2.730172	-0.03733	-1.63273
1	-2.022184	-0.062054	-2.464955
1	-3.489519	-0.804316	-1.780791
1	-3.206126	0.946024	-1.597101
6	-2.663438	0.631579	1.268337
1	-3.727301	0.389181	1.267858
1	-2.252345	0.352436	2.241136
1	-2.510931	1.696479	1.091478
6	-0.398095	1.359666	-0.417695
6	0.576999	1.659734	0.548833
6	-0.626919	2.3719	-1.363726
6	1.271234	2.865859	0.627841
6	0.03941	3.60261	-1.322985
1	-1.357256	2.215332	-2.153446

6	0.979639	3.850273	-0.321765
1	2.020587	3.050872	1.389049
1	-0.174178	4.36296	-2.068699
1	1.500417	4.802044	-0.279168
8	0.849965	0.571969	1.422815
6	1.907481	0.67501	2.393192
1	1.682657	1.476779	3.101322
1	1.930785	-0.281771	2.914128
1	2.867408	0.851489	1.899652

PC_{v_b-i}

E = -3999.608408 ZPVE = 0.203708 NIMAG = 0.

17	-2.86573	0.428132	2.180147
15	0.451089	1.692481	0.050147
12	-1.572035	0.095618	0.359846
35	-1.843459	-0.712956	-1.89317
6	0.674516	2.55323	-1.564935
1	0.433279	1.85308	-2.368497
1	-0.034172	3.385709	-1.612954
1	1.686191	2.945382	-1.703012
6	1.066581	2.910313	1.29959
1	0.395829	3.774692	1.309235
1	1.044736	2.451337	2.291168
1	2.085043	3.242464	1.076525
6	1.728541	0.360051	0.053369
6	1.390425	-0.910737	0.564764
6	3.019615	0.538182	-0.460137
6	2.316505	-1.955105	0.569124

6	3.957248	-0.496008	-0.457784
1	3.301131	1.503478	-0.870715
6	3.599098	-1.740508	0.058799
1	2.052785	-2.931914	0.954087
1	4.952098	-0.331236	-0.858754
1	4.313233	-2.558195	0.062777
8	0.109277	-1.063515	1.080301
6	-0.221376	-2.267547	1.808373
1	0.4948	-2.417441	2.620205
1	-1.214196	-2.090745	2.223153
1	-0.235345	-3.129163	1.135489

P_{Vb-i}

E = -767.389453 ZPVE = 0.199123 NIMAG = 0.

15	-1.754158	-0.424508	-0.494451
6	-2.994777	0.950737	-0.277769
1	-2.923655	1.666515	-1.102113
1	-3.991014	0.498764	-0.322898
1	-2.899128	1.48535	0.674286
6	-2.046314	-1.326702	1.117261
1	-3.037168	-1.791728	1.083106
1	-1.299751	-2.116073	1.226732
1	-1.994225	-0.659192	1.984286
6	-0.158834	0.448007	-0.127923
6	1.029348	-0.318937	-0.065414
6	-0.036287	1.838271	-0.012723
6	2.275824	0.289126	0.115097
6	1.206241	2.459674	0.163513

1	-0.923805	2.460009	-0.06369
6	2.358823	1.681511	0.229048
1	3.180276	-0.305272	0.167544
1	1.264753	3.540504	0.249318
1	3.330399	2.147051	0.367405
8	0.860899	-1.672979	-0.188551
6	2.007732	-2.511605	-0.23753
1	2.573649	-2.472182	0.701753
1	1.629236	-3.523312	-0.389381
1	2.665074	-2.239479	-1.072536

R1 + b S_N2@P-f pathway

RC_{1b-r}

E = -4543.910143 ZPVE = 0.489618 NIMAG = 0.

6	1.867636	-2.064269	-1.139063
6	2.349251	-0.578051	-1.119903
6	2.334574	-2.78208	0.14692
6	4.404306	-1.26893	0.292686
6	3.895387	-0.556301	-0.97405
6	3.858258	-2.704783	0.33703
6	0.366126	-2.277048	-1.482258
6	5.934938	-1.23382	0.372782
6	0.024859	-1.741123	-2.884475
6	-0.048162	-3.758002	-1.398181
1	2.428744	-2.520187	-1.973746
1	2.092304	-0.088433	-2.065273
1	2.046724	-3.836034	0.107774
1	1.819478	-2.357127	1.018432

1	4.012809	-0.734732	1.173477
1	4.275066	0.469493	-1.010472
1	4.309083	-1.069763	-1.854817
1	4.138702	-3.18095	1.285073
1	4.348408	-3.286354	-0.45923
1	-0.238802	-1.73604	-0.745283
1	6.311723	-0.204712	0.381433
1	6.294494	-1.731047	1.280586
1	6.382561	-1.747087	-0.487742
1	0.595574	-2.279729	-3.652323
1	-1.038969	-1.884174	-3.102229
1	0.232362	-0.674028	-2.996097
1	0.601556	-4.389502	-2.018458
1	-1.07248	-3.881479	-1.767031
1	-0.022304	-4.140657	-0.374967
15	1.609364	0.458227	0.292709
6	2.457829	2.076592	0.04252
6	3.013314	2.658286	1.193432
6	2.562439	2.759331	-1.182155
6	3.696107	3.876764	1.116897
1	2.911806	2.157156	2.15252
6	3.232769	3.978822	-1.256544
1	2.115307	2.341832	-2.079531
6	3.803426	4.538853	-0.106567
1	4.128845	4.31011	2.013747
1	3.305154	4.49781	-2.207994
1	4.324492	5.489864	-0.167457
17	-0.310284	1.056202	-0.617524
6	-5.744068	0.289344	-1.037763
6	-4.519068	0.276174	-0.377123

6	-3.942198	1.355144	0.300408
6	-4.682597	2.544705	0.265056
6	-5.923853	2.621833	-0.385726
6	-6.452111	1.499071	-1.029287
1	-6.144422	-0.582771	-1.545827
1	-6.481669	3.554843	-0.387836
1	-7.414147	1.558167	-1.53057
12	-2.267135	0.209256	0.874273
35	-1.101472	-1.264658	2.380796
1	-4.302352	3.433963	0.76499
8	-3.670244	-0.873034	-0.336913
6	-4.250094	-2.182741	-0.328902
1	-3.446258	-2.87056	-0.063799
1	-5.048711	-2.239836	0.418759
1	-4.646025	-2.437285	-1.317037

TS_{1b-r}

E = -4543.869499 ZPVE = 0.488189 NIMAG = 1.

6	-2.342753000	-2.200059000	-0.080873000
6	-2.448582000	-0.785402000	0.578659000
6	-2.818702000	-2.140692000	-1.549071000
6	-4.414898000	-0.207067000	-1.013938000
6	-3.911858000	-0.265239000	0.439669000
6	-4.243064000	-1.580889000	-1.680697000
6	-0.963048000	-2.884236000	0.134586000
6	-5.864694000	0.286022000	-1.079994000
6	-0.796743000	-3.354262000	1.590037000
6	-0.691295000	-4.068006000	-0.808922000

1	-3.080628000	-2.817762000	0.457760000
1	-2.200421000	-0.849534000	1.640745000
1	-2.794624000	-3.144096000	-1.982738000
1	-2.124136000	-1.535110000	-2.148765000
1	-3.790563000	0.514970000	-1.567689000
1	-4.026397000	0.712441000	0.915829000
1	-4.548360000	-0.963508000	1.003658000
1	-4.524902000	-1.520187000	-2.739560000
1	-4.948573000	-2.283853000	-1.211533000
1	-0.179006000	-2.140192000	-0.079635000
1	-5.968984000	1.284515000	-0.640581000
1	-6.218914000	0.335787000	-2.115643000
1	-6.531707000	-0.391861000	-0.532492000
1	-1.495604000	-4.174854000	1.798595000
1	0.219531000	-3.724352000	1.755343000
1	-0.971828000	-2.557678000	2.316904000
1	-1.463585000	-4.841649000	-0.707551000
1	0.272209000	-4.519298000	-0.554302000
1	-0.642636000	-3.767981000	-1.859506000
15	-1.264315000	0.428008000	-0.257052000
6	-1.564497000	2.018453000	0.537998000
6	-1.231930000	3.139775000	-0.257605000
6	-2.108181000	2.234939000	1.824054000
6	-1.480768000	4.433661000	0.197992000
1	-0.773435000	2.988025000	-1.230707000
6	-2.344445000	3.526704000	2.278367000
1	-2.309714000	1.391869000	2.474496000
6	-2.038493000	4.627238000	1.464280000
1	-1.227890000	5.285398000	-0.425761000
1	-2.754604000	3.683388000	3.271407000

1	-2.221995000	5.634376000	1.827489000
17	0.383594000	-0.045140000	2.434291000
6	3.484959000	2.227611000	-1.692767000
6	2.758943000	1.437183000	-0.802337000
6	1.565947000	0.781743000	-1.138493000
6	1.098789000	0.967919000	-2.435708000
6	1.792236000	1.759760000	-3.365050000
6	2.976914000	2.393780000	-2.986901000
1	4.409477000	2.715762000	-1.401596000
1	1.409678000	1.875539000	-4.375547000
1	3.517785000	3.013337000	-3.696364000
12	1.844332000	-0.464296000	0.696613000
35	3.145419000	-2.458022000	0.326749000
1	0.167334000	0.495083000	-2.747268000
8	3.181403000	1.173026000	0.514332000
6	4.550047000	1.393233000	0.880334000
1	4.666059000	0.972813000	1.879106000
1	5.219482000	0.882530000	0.181573000
1	4.767518000	2.465312000	0.906877000

PC_{1b-r}

E = -4543.960401 ZPVE = 0.491933 NIMAG = 0.

6	1.504566	-2.308516	-0.567667
6	1.769388	-0.770094	-0.643986
6	2.626348	-3.007088	0.228325
6	4.321935	-1.265058	-0.59614
6	3.157831	-0.550633	-1.309823
6	4.003285	-2.757042	-0.409184

6	0.061513	-2.715063	-0.157866
6	5.640528	-1.058498	-1.352262
6	-0.959072	-2.225994	-1.204144
6	-0.120137	-4.233535	0.016829
1	1.616801	-2.653765	-1.610865
1	1.021048	-0.310857	-1.295918
1	2.448429	-4.085906	0.260195
1	2.625608	-2.658108	1.269771
1	4.432528	-0.819696	0.402051
1	3.382143	0.517948	-1.395909
1	3.087985	-0.929439	-2.34061
1	4.786855	-3.231082	0.195821
1	4.030256	-3.251355	-1.392722
1	-0.179817	-2.247875	0.801192
1	5.881964	0.006023	-1.450215
1	6.474277	-1.544183	-0.832398
1	5.585681	-1.482965	-2.362854
1	-0.922773	-2.840045	-2.111468
1	-1.984114	-2.277588	-0.817741
1	-0.705251	-1.212347	-1.551065
1	0.228562	-4.780025	-0.86877
1	-1.180088	-4.472792	0.15594
1	0.418805	-4.618374	0.886546
15	1.807043	0.179971	1.011081
6	1.783259	1.958807	0.47177
6	2.147211	2.893693	1.459362
6	1.49486	2.434797	-0.817679
6	2.193591	4.26117	1.178272
1	2.402338	2.544977	2.457306
6	1.559017	3.801328	-1.105821

1	1.191703	1.757999	-1.608809
6	1.902553	4.719565	-0.110161
1	2.470657	4.963323	1.959562
1	1.326503	4.143696	-2.11015
1	1.950045	5.78064	-0.337471
17	-1.44312	1.204986	-3.142266
6	-2.245374	0.221206	2.323467
6	-1.126075	0.426016	1.516472
6	0.158947	-0.013017	1.87974
6	0.257366	-0.667737	3.125506
6	-0.849003	-0.886732	3.946924
6	-2.107675	-0.439605	3.544164
1	-3.220469	0.543801	1.974248
1	-0.724835	-1.39857	4.896408
1	-2.981301	-0.605557	4.166776
12	-2.339642	0.216799	-1.328387
35	-4.481526	-0.536745	-0.599951
1	1.23753	-1.006363	3.448831
8	-1.333097	1.081267	0.279729
6	-1.616079	2.511138	0.403174
1	-1.719752	2.888983	-0.61492
1	-2.538858	2.657587	0.96956
1	-0.773886	2.997273	0.895453

P_{lb-r}

E = -1311.763713 ZPVE = 0.487806 NIMAG = 0.

6	-0.757526	0.934362	0.606455
6	-2.252491	2.46333	-0.790741

6	0.112167	3.24104	-0.186397
6	0.116686	2.171919	0.919783
6	-1.332971	3.658937	-0.495844
6	-3.254574	0.256647	0.162253
6	0.983974	4.443416	0.19602
6	-3.439528	-0.530793	1.472136
6	-4.634367	0.743271	-0.318662
1	-0.742802	0.293213	1.491725
1	-3.271947	2.836804	-0.925709
1	-1.959809	1.995353	-1.739693
1	0.537868	2.79441	-1.097096
1	1.142651	1.868437	1.143954
1	-0.276854	2.629336	1.841577
1	-1.348859	4.358314	-1.342313
1	-1.730456	4.21174	0.370068
1	-2.873576	-0.435775	-0.600598
1	2.022098	4.141637	0.376634
1	0.988008	5.199445	-0.597871
1	0.610487	4.923292	1.110021
1	-3.871273	0.115006	2.248153
1	-4.121964	-1.374937	1.324287
1	-2.501423	-0.937651	1.856031
1	-5.039282	1.514525	0.34984
1	-5.344909	-0.090891	-0.3259
1	-4.605254	1.155745	-1.330898
6	-0.486524	-1.843162	-0.51386
6	-0.867643	-2.606634	-1.631549
6	-0.447987	-2.480011	0.737883
6	-1.192822	-3.960719	-1.508619
1	-0.912037	-2.130779	-2.607851

6	-0.777779	-3.831403	0.865823
1	-0.144885	-1.921538	1.615129
6	-1.149925	-4.577452	-0.256559
1	-1.483302	-4.528377	-2.388395
1	-0.742463	-4.303343	1.844387
1	-1.405609	-5.628408	-0.154323
6	-2.225236	1.410174	0.33904
1	-2.52395	1.940325	1.261034
15	-0.05886	-0.061807	-0.866438
6	2.518566	0.185868	-1.821522
6	3.916599	0.17241	-1.858364
6	4.620282	-0.094735	-0.68742
6	3.935489	-0.341552	0.506614
6	2.534595	-0.327053	0.53068
6	1.793607	-0.0643	-0.646565
1	1.961928	0.39364	-2.731373
1	4.440897	0.368728	-2.788382
1	5.706528	-0.111449	-0.688643
1	4.501972	-0.544144	1.407587
8	1.81606	-0.548025	1.674719
6	2.510329	-0.81677	2.887127
1	3.114165	-1.729037	2.808836
1	3.151841	0.024673	3.176359
1	1.739126	-0.957735	3.645978

R1_{II} + b SN2@P-f pathway

RC_{IIb-r}

E = -4235.413002 ZPVE = 0.370297 NIMAG = 0.

15	1.949744	-0.575732	-0.437989
17	0.656501	0.258798	1.104604
6	3.38667	0.687719	-0.316687
6	2.85516	1.926201	-1.077906
1	2.589235	1.683003	-2.11206
1	1.979264	2.372312	-0.597334
1	3.640912	2.691245	-1.106464
6	4.5782	0.097611	-1.103106
1	5.312291	0.89347	-1.277742
1	5.0846	-0.699629	-0.551939
1	4.282371	-0.289462	-2.085275
6	3.842888	1.115433	1.088119
1	4.620672	1.882775	0.985787
1	3.024913	1.552943	1.665351
1	4.267776	0.290588	1.662944
12	-1.470408	1.046923	-0.316151
35	-1.008512	3.389478	-0.320289
6	-2.372149	-0.737507	-0.97944
6	-3.155626	-0.865753	0.173365
6	-2.548027	-1.742818	-1.936601
6	-4.058527	-1.892929	0.430395
6	-3.441267	-2.808779	-1.733919
1	-1.982938	-1.709278	-2.86661
6	-4.189844	-2.88102	-0.55778
1	-4.644929	-1.948118	1.342062
1	-3.557597	-3.576028	-2.495063
1	-4.884048	-3.70172	-0.400213
8	-2.90869	0.210671	1.070439
6	-3.699137	0.364113	2.24851
1	-3.545697	-0.481154	2.928409

1	-3.365286	1.286028	2.725611
1	-4.760503	0.444956	1.98956
6	2.375353	-2.253937	0.376053
6	3.181948	-2.218376	1.682343
1	3.253902	-3.235194	2.089418
1	4.20223	-1.85711	1.528172
1	2.701829	-1.592576	2.44062
6	1.02391	-2.964712	0.620671
1	0.379154	-2.946456	-0.264107
1	1.218798	-4.014098	0.873381
1	0.471132	-2.516619	1.449416
6	3.141068	-3.050809	-0.708913
1	3.284795	-4.078121	-0.352689
1	2.579324	-3.104166	-1.647751
1	4.129756	-2.637954	-0.922108

TS_{nb-r}

E = -4235.368161 ZPVE = 0.369030 NIMAG = 1.

15	1.810327	0.327049	0.530982
17	0.623095	-1.119152	-2.010541
6	2.557933	-1.379372	0.930457
6	1.457305	-2.119726	1.725328
1	1.009548	-1.493175	2.50411
1	0.655855	-2.4808	1.073828
1	1.895858	-2.997928	2.214531
6	3.686561	-0.956728	1.922784
1	4.032282	-1.864629	2.432628
1	4.546306	-0.519018	1.407804

1	3.347272	-0.26167	2.699282
6	3.142736	-2.319562	-0.131047
1	3.512311	-3.221459	0.374019
1	2.387064	-2.619684	-0.856683
1	3.981666	-1.877762	-0.669541
12	-1.130337	-0.761307	-0.565163
35	-2.670084	-2.315114	0.411948
6	-0.938556	1.157357	0.584
6	-2.021621	1.610473	-0.186123
6	-0.698971	1.831968	1.7763
6	-2.850746	2.664416	0.196846
6	-1.513363	2.890097	2.205191
1	0.15178	1.542224	2.392975
6	-2.577145	3.312011	1.406725
1	-3.683807	2.986797	-0.418891
1	-1.307875	3.387211	3.149035
1	-3.203303	4.142153	1.72019
8	-2.238302	0.849637	-1.351309
6	-3.505671	0.9197	-2.021598
1	-3.637023	1.904487	-2.479213
1	-3.474471	0.157792	-2.800262
1	-4.319923	0.707001	-1.322579
6	2.82339	1.322962	-0.733409
6	3.731112	0.588326	-1.728253
1	4.176162	1.325873	-2.408544
1	4.555454	0.071962	-1.228847
1	3.172974	-0.131769	-2.328842
6	1.826902	2.227859	-1.497453
1	1.164112	2.773721	-0.819895
1	2.398859	2.961963	-2.078644

1	1.213186	1.642826	-2.185171
6	3.689176	2.23568	0.187873
1	4.228709	2.943104	-0.454303
1	3.082566	2.81923	0.887499
1	4.43608	1.676189	0.758512

PC_{IIb-r}

E = -4235.462125 ZPVE = 0.372972 NIMAG = 0.

15	2.310423	0.616027	0.519085
17	-1.596685	-3.36235	-0.890453
6	1.489972	-0.290736	2.006003
6	1.200973	0.821411	3.041162
1	2.119658	1.337524	3.335908
1	0.498604	1.567603	2.656825
1	0.755561	0.379868	3.941626
6	2.514579	-1.267198	2.618943
1	2.137246	-1.628729	3.583635
1	2.688559	-2.143321	1.988814
1	3.476306	-0.777269	2.802628
6	0.17239	-1.039835	1.734637
1	-0.610177	-0.3029	1.500943
1	0.289036	-1.802085	0.955049
1	-0.164634	-1.555737	2.642336
12	-1.789357	-1.260852	-0.121388
35	-3.483248	0.139404	0.795296
6	0.892768	1.597782	-0.235463
6	-0.258297	1.247274	-0.966784
6	1.031626	2.977428	0.042782

6	-1.214349	2.185431	-1.359483
6	0.096388	3.932406	-0.353538
1	1.915049	3.29623	0.587451
6	-1.037299	3.533728	-1.059889
1	-2.112519	1.855338	-1.868664
1	0.255923	4.978328	-0.110187
1	-1.789517	4.256024	-1.360756
8	-0.513666	-0.106948	-1.307796
6	-0.649523	-0.373549	-2.737786
1	0.22553	0.015632	-3.259121
1	-0.70953	-1.457729	-2.835443
1	-1.557728	0.091479	-3.127805
6	3.001743	-0.624781	-0.779304
6	2.25402	-1.945229	-1.025032
1	2.774587	-2.519369	-1.803098
1	2.228883	-2.576468	-0.132431
1	1.227549	-1.79729	-1.356608
6	3.131334	0.170937	-2.095677
1	3.688031	1.103384	-1.950329
1	3.676565	-0.430924	-2.833455
1	2.161195	0.429475	-2.525423
6	4.438488	-0.952398	-0.300356
1	4.94262	-1.558296	-1.06399
1	5.028519	-0.044162	-0.143753
1	4.448391	-1.526417	0.62964

P_{11b-r}

E = -1003.266468 ZPVE = 0.368521 NIMAG = 0.

15	-0.8664	-0.460742	-0.807631
6	-1.438206	-1.514591	0.701279
6	-0.854382	-2.922407	0.440557
1	-1.174158	-3.32004	-0.528315
1	0.239898	-2.919885	0.462882
1	-1.201906	-3.611942	1.221204
6	-2.977042	-1.61908	0.648147
1	-3.317193	-2.36355	1.379904
1	-3.467778	-0.673325	0.895097
1	-3.327338	-1.939479	-0.339164
6	-0.996362	-1.058525	2.102964
1	0.092381	-1.029091	2.189894
1	-1.381221	-0.070892	2.362334
1	-1.372003	-1.772123	2.849989
6	0.986461	-0.338189	-0.592198
6	1.752576	0.395478	0.346614
6	1.699001	-1.12125	-1.517278
6	3.15279	0.318389	0.351039
6	3.094159	-1.211019	-1.519609
1	1.12948	-1.674796	-2.258482
6	3.818517	-0.4862	-0.577654
1	3.7331	0.881268	1.072143
1	3.600237	-1.832949	-2.251423
1	4.903738	-0.533192	-0.558569
8	1.065874	1.183218	1.229486
6	1.785626	1.924604	2.206733
1	2.465445	2.649309	1.741979
1	1.032153	2.459189	2.787359
1	2.354276	1.263964	2.87278
6	-1.619334	1.317185	-0.754614

6	-1.955767	1.945723	0.609311
1	-2.359433	2.955517	0.449516
1	-2.720969	1.377551	1.146086
1	-1.074208	2.027881	1.244305
6	-0.642045	2.236753	-1.516637
1	-0.356232	1.812972	-2.485976
1	-1.127395	3.202967	-1.708266
1	0.268997	2.424916	-0.943713
6	-2.923054	1.218765	-1.584827
1	-3.376083	2.215086	-1.674425
1	-2.729193	0.840562	-2.593313
1	-3.663224	0.561659	-1.118209

R1_{III} + b_{S_N2@P-f} pathway

RC_{IIIb-r}

E = -4383.010526 ZPVE = 0.307548 NIMAG = 0.

15	1.547483	0.021599	0.75982
6	1.641604	1.468981	-0.366375
6	0.984129	2.634025	0.063768
6	2.30018	1.46708	-1.609655
6	1.00315	3.78644	-0.727918
1	0.446739	2.637182	1.008232
6	2.310943	2.615445	-2.398618
1	2.801871	0.569032	-1.956688
6	1.666473	3.777962	-1.955913
1	0.494511	4.682334	-0.385302
1	2.820301	2.606935	-3.357905
1	1.680175	4.672319	-2.572369
17	0.353924	-1.347481	-0.474606

6	-3.02875	2.723756	0.320176
6	-2.718742	1.367048	0.315253
6	-2.238026	0.633944	1.407787
6	-2.066607	1.366374	2.588108
6	-2.356501	2.740343	2.655317
6	-2.835995	3.411727	1.528345
1	-3.403837	3.244713	-0.555053
1	-2.217262	3.282598	3.58714
1	-3.070293	4.471404	1.581013
12	-2.185225	-1.172928	0.311718
35	-2.88261	-3.316477	-0.458809
1	-1.70174	0.869555	3.485345
8	-2.850838	0.531828	-0.825225
6	-3.460872	1.016955	-2.020885
1	-3.49853	0.17048	-2.707022
1	-4.476242	1.372816	-1.814897
1	-2.8628	1.823854	-2.457812
6	3.201971	-0.767505	0.5295
6	3.364006	-2.163219	0.517527
6	4.348069	0.047249	0.582178
6	4.641191	-2.72715	0.532291
1	2.496733	-2.814082	0.479448
6	5.622951	-0.522269	0.610811
1	4.252294	1.128726	0.598366
6	5.774076	-1.910449	0.580002
1	4.748145	-3.807604	0.506303
1	6.496393	0.12231	0.647002
1	6.765817	-2.352573	0.594519

TS_{mb-r}

E = -4382.977540 ZPVE = 0.306926 NIMAG = 1.

15	-1.441918	-0.091921	0.95509
6	-1.671525	-1.593588	-0.042821
6	-1.470849	-2.812578	0.638106
6	-1.999934	-1.620193	-1.413185
6	-1.652855	-4.02824	-0.020821
1	-1.168448	-2.807278	1.681464
6	-2.155021	-2.838756	-2.07172
1	-2.088417	-0.689042	-1.96224
6	-1.995183	-4.042714	-1.375868
1	-1.509731	-4.959897	0.517951
1	-2.393976	-2.849711	-3.131092
1	-2.119772	-4.989234	-1.893899
17	-0.524388	1.630261	-1.473016
6	2.945141	-2.363974	0.477976
6	2.171458	-1.265146	0.104685
6	1.343247	-0.560325	0.98968
6	1.31398	-1.008248	2.309524
6	2.08397	-2.101084	2.733009
6	2.886309	-2.78108	1.812962
1	3.57897	-2.887113	-0.23062
1	2.060025	-2.41644	3.77263
1	3.476366	-3.636357	2.129484
12	1.473535	1.163826	-0.413239
35	3.443758	2.507785	-0.144242
1	0.677206	-0.503563	3.036176
8	2.187638	-0.707883	-1.186683
6	3.276279	-1.008528	-2.072131

1	3.139052	-0.368594	-2.94366
1	4.232823	-0.782596	-1.591473
1	3.236589	-2.057763	-2.379962
6	-2.88532	0.93912	0.575124
6	-2.883606	2.206829	1.204137
6	-4.050631	0.528238	-0.108436
6	-3.988771	3.046454	1.122221
1	-1.999519	2.535881	1.743816
6	-5.163687	1.364109	-0.169248
1	-4.094356	-0.449274	-0.572976
6	-5.132572	2.626107	0.433354
1	-3.963495	4.023226	1.595214
1	-6.057518	1.031569	-0.688705
1	-6.00009	3.276814	0.374311

PC_{IIIb-r}

E = -4383.082369 ZPVE = 0.310265 NIMAG = 0.

15	1.593112	0.459386	1.638663
6	2.813335	-0.007415	0.32045
6	4.017223	0.720429	0.332221
6	2.657289	-1.033685	-0.625201
6	5.026973	0.452225	-0.594448
1	4.16763	1.499402	1.075846
6	3.677164	-1.315115	-1.538687
1	1.743893	-1.617185	-0.670399
6	4.860539	-0.57163	-1.531101
1	5.946382	1.030282	-0.572674
1	3.536839	-2.114427	-2.260839

1	5.649275	-0.793149	-2.24427
17	-0.692747	-2.592	-1.948127
6	-0.844361	2.928915	-0.759411
6	-0.104702	1.831135	-0.32413
6	0.595855	1.839204	0.893726
6	0.532205	3.019633	1.65761
6	-0.187464	4.135751	1.227828
6	-0.877909	4.088468	0.016082
1	-1.419934	2.859598	-1.675777
1	-0.214906	5.031428	1.840544
1	-1.461731	4.940104	-0.318878
12	-1.526075	-0.850249	-0.770859
35	-3.646295	0.273517	-0.596365
1	1.059687	3.051402	2.606601
8	-0.101812	0.663517	-1.10845
6	0.493554	0.804895	-2.432684
1	0.489239	-0.19345	-2.868582
1	-0.10226	1.490819	-3.03922
1	1.515064	1.171727	-2.320786
6	0.394023	-0.947155	1.690368
6	-1.001887	-0.739954	1.722695
6	0.872086	-2.255825	1.88562
6	-1.886392	-1.815478	1.920946
1	-1.414383	0.263916	1.649315
6	-0.00865	-3.321875	2.071029
1	1.94108	-2.447308	1.88477
6	-1.390315	-3.110162	2.082328
1	-2.954748	-1.623574	1.937568
1	0.387228	-4.32518	2.196957
1	-2.072031	-3.943631	2.217254

P_{11b-r}

E = -1150.873876 ZPVE = 0.305799 NIMAG = 0.

15	0.195897	-0.016729	-1.36989
6	0.607782	-1.629979	-0.543361
6	0.162668	-2.79128	-1.197402
6	1.360548	-1.772012	0.632611
6	0.435456	-4.059399	-0.677656
1	-0.399072	-2.702367	-2.124248
6	1.653138	-3.039356	1.141935
1	1.716295	-0.889807	1.153497
6	1.186621	-4.18696	0.493258
1	0.075663	-4.944036	-1.19575
1	2.24189	-3.130246	2.051056
1	1.413364	-5.171258	0.893278
6	-3.20051	0.709439	1.005793
6	-1.877212	0.410592	0.651742
6	-1.480277	0.415769	-0.708195
6	-2.447577	0.73593	-1.671924
6	-3.767297	1.043893	-1.327231
6	-4.136531	1.024324	0.015845
1	-3.509094	0.702351	2.044373
1	-4.49142	1.288984	-2.097713
1	-5.157438	1.254534	0.307629
1	-2.150749	0.738489	-2.717271
8	-0.911304	0.11513	1.564259
6	-1.251804	0.052926	2.943548
1	-0.331835	-0.219694	3.461828

1	-1.603434	1.024081	3.313516
1	-2.015443	-0.71142	3.132132
6	1.346973	1.198827	-0.582846
6	0.91214	2.387845	0.022449
6	2.731063	1.00233	-0.745248
6	1.831372	3.342397	0.468155
1	-0.149535	2.573663	0.149195
6	3.64967	1.949113	-0.28961
1	3.096029	0.100661	-1.230814
6	3.202992	3.126013	0.319573
1	1.471358	4.255316	0.935055
1	4.713776	1.770989	-0.418501
1	3.916312	3.867189	0.668392

R1_{iv} + b S_{N2}@P-f pathway

RC_{ivb-r}

E = -4191.268247 ZPVE = 0.254090 NIMAG = 0.

17	0.451254	-2.012866	-0.212493
15	-1.357068	-1.667803	-1.400243
12	1.988057	0.167024	-0.286908
35	4.005432	-0.901924	0.394749
6	-1.823525	-3.45453	-1.567712
1	-1.096737	-3.945064	-2.220435
1	-1.873924	-3.997702	-0.621069
1	-2.805461	-3.491249	-2.053268
6	-2.516577	-1.084298	-0.100061
6	-2.990816	-1.862633	0.97091
6	-2.970093	0.239365	-0.236503
6	-3.908448	-1.3318	1.875893

1	-2.63998	-2.880549	1.109312
6	-3.892781	0.768527	0.670668
1	-2.592199	0.86024	-1.044274
6	-4.36359	-0.016098	1.724479
1	-4.268175	-1.940806	2.700192
1	-4.234885	1.792259	0.55362
1	-5.080866	0.393353	2.430022
6	0.71494	1.633163	-1.123805
6	0.387996	2.169203	0.128376
6	0.13255	2.28046	-2.219617
6	-0.444314	3.261767	0.352501
6	-0.722612	3.384558	-2.058388
1	0.341022	1.929897	-3.228897
6	-1.006353	3.870952	-0.780307
1	-0.661771	3.641846	1.345651
1	-1.158514	3.868941	-2.928463
1	-1.658706	4.730665	-0.654235
8	1.029117	1.440052	1.164125
6	0.953429	1.875149	2.521267
1	1.347643	2.892475	2.619759
1	-0.080953	1.838153	2.879616
1	1.569617	1.183233	3.095964

TS_{IVb-r}

E = -4191.233239 ZPVE = 0.253660 NIMAG = 1.

17	0.23656	-2.725417	0.223409
15	-1.541007	-1.091011	-1.508028
12	1.523318	-0.820646	0.063603

35	3.892566	-0.507628	0.21413
6	-2.16868	-2.833005	-1.644069
1	-1.443226	-3.432962	-2.196498
1	-2.438168	-3.348763	-0.723535
1	-3.068421	-2.716233	-2.270557
6	-2.616854	-0.42702	-0.201806
6	-3.14081	-1.177323	0.869399
6	-2.994053	0.927755	-0.331852
6	-4.032007	-0.596399	1.769252
1	-2.826981	-2.204401	1.018385
6	-3.903112	1.498757	0.556946
1	-2.571246	1.530222	-1.13042
6	-4.422217	0.73807	1.609272
1	-4.420533	-1.181876	2.59718
1	-4.197412	2.536735	0.435086
1	-5.12091	1.186217	2.309871
6	0.337109	0.768271	-0.954238
6	0.486799	1.51117	0.227005
6	0.184031	1.497619	-2.135781
6	0.468402	2.904942	0.27276
6	0.184217	2.898592	-2.140204
1	0.04553	0.968711	-3.077974
6	0.308527	3.59516	-0.934455
1	0.586744	3.451325	1.202505
1	0.080943	3.442327	-3.075084
1	0.291241	4.681148	-0.927221
8	0.72038	0.700031	1.351279
6	1.260865	1.287394	2.545756
1	2.197158	1.807868	2.324115
1	0.532614	1.969599	2.99397

1	1.450268	0.457902	3.226717
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PC_{IVb-r}

E = -4191.328936 ZPVE = 0.256178 NIMAG = 0.

17	-1.237096	-3.55442	-0.858791
15	1.195669	0.764769	1.689818
12	-1.751149	-1.462618	-0.247324
35	-3.478596	-0.087103	0.622249
6	0.154353	-0.74361	2.040132
1	-0.883231	-0.42146	2.180279
1	0.230255	-1.526673	1.275008
1	0.480876	-1.186146	2.985623
6	2.641814	0.057251	0.772584
6	3.053115	-1.277075	0.924092
6	3.44508	0.918506	0.001363
6	4.218012	-1.742328	0.304437
1	2.468861	-1.971545	1.51961
6	4.603205	0.452565	-0.622082
1	3.161339	1.960947	-0.118672
6	4.993794	-0.882824	-0.47517
1	4.511857	-2.780531	0.429847
1	5.202206	1.133293	-1.220486
1	5.896648	-1.24543	-0.957376
6	0.274696	1.665235	0.34298
6	-0.313514	1.136541	-0.816065
6	0.149264	3.054301	0.531521
6	-0.993698	1.928379	-1.736879
6	-0.504516	3.870497	-0.393877

1	0.578418	3.494812	1.426895
6	-1.080364	3.30582	-1.532136
1	-1.46155	1.465759	-2.600579
1	-0.577698	4.938802	-0.215378
1	-1.609708	3.925211	-2.249217
8	-0.285669	-0.25751	-1.052085
6	0.630489	-0.699089	-2.102221
1	0.360639	-0.215665	-3.043938
1	1.650046	-0.443533	-1.811496
1	0.506248	-1.779158	-2.174161

PIVb-r

E = -959.132021 ZPVE = 0.252569 NIMAG = 0.

15	0.161073	1.716692	0.338681
6	0.198703	1.621624	2.199985
1	-0.724323	2.076993	2.57134
1	0.27411	0.600063	2.578526
1	1.033944	2.221245	2.57442
6	1.562724	0.612198	-0.158757
6	2.654901	0.346554	0.682222
6	1.605916	0.122714	-1.4766
6	3.748751	-0.396265	0.225821
1	2.660003	0.709437	1.705272
6	2.691859	-0.626941	-1.930215
1	0.779338	0.323401	-2.153716
6	3.771198	-0.889616	-1.080115
1	4.581747	-0.59091	0.896241
1	2.697536	-1.002132	-2.950105

1	4.620007	-1.46775	-1.433879
6	-1.329706	0.701146	-0.09264
6	-1.5647	-0.636872	0.308927
6	-2.300486	1.326033	-0.887393
6	-2.731203	-1.303774	-0.088943
6	-3.47042	0.670272	-1.285938
1	-2.126034	2.351901	-1.201087
6	-3.677189	-0.64663	-0.88271
1	-2.914117	-2.32741	0.215596
1	-4.202366	1.182379	-1.902592
1	-4.577075	-1.177205	-1.181179
8	-0.60652	-1.214768	1.089431
6	-0.732697	-2.586842	1.44236
1	-1.618239	-2.761437	2.066321
1	-0.779826	-3.224149	0.551074
1	0.165457	-2.828267	2.012061

R1_v + b S_{N2}@P-f pathway

RC_{v_{b-r}}

E = -3999.524470 ZPVE = 0.200439 NIMAG = 0.

17	-0.414143	2.000534	0.407607
15	1.527339	2.573957	-0.380112
12	-1.079995	-0.459962	-0.471653
35	-3.440812	-0.184189	-0.3741
6	1.551815	4.288677	0.328741
1	0.786487	4.899774	-0.156539
1	1.398397	4.305817	1.411692
1	2.531325	4.724803	0.097878
6	2.612813	1.713639	0.847991

1	2.338559	1.930176	1.884632
1	2.584436	0.636448	0.668981
1	3.638346	2.060099	0.668463
6	0.834911	-1.210592	-0.958922
6	0.975807	-1.854497	0.277647
6	1.913667	-1.364871	-1.837538
6	2.075232	-2.606086	0.68194
6	3.052891	-2.109919	-1.486616
1	1.880108	-0.902092	-2.82218
6	3.130724	-2.725746	-0.235943
1	2.133108	-3.08992	1.651851
1	3.874092	-2.214906	-2.190847
1	4.007818	-3.306845	0.034574
8	-0.168598	-1.631837	1.088725
6	-0.335648	-2.324972	2.325581
1	0.441919	-2.032299	3.039469
1	-1.31503	-2.034485	2.70642
1	-0.30536	-3.407934	2.164205

TS_{Vb-r}

E = -3999.488267 ZPVE = 0.200370 NIMAG = 1.

17	-1.056616	-2.490272	0.37648
15	-2.708297	-0.364209	-0.58369
12	0.585155	-0.93437	-0.035693
35	2.892756	-1.121643	-0.618608
6	-3.893228	-1.769119	-0.257618
1	-3.680066	-2.617199	-0.9095
1	-3.956339	-2.106403	0.779024

1	-4.864223	-1.338289	-0.555428
6	-3.148753	0.609084	0.928565
1	-2.718025	0.142431	1.821196
1	-2.779634	1.632572	0.853314
1	-4.238845	0.604509	1.043253
6	-0.505495	0.965192	-0.486852
6	0.202397	1.492403	0.605119
6	-0.802134	1.853268	-1.52412
6	0.58636	2.829982	0.706317
6	-0.412589	3.196939	-1.477265
1	-1.370628	1.497736	-2.383374
6	0.265157	3.68254	-0.355178
1	1.128801	3.20829	1.565939
1	-0.642142	3.862186	-2.304595
1	0.55346	4.728231	-0.301991
8	0.547144	0.512192	1.554331
6	1.558326	0.804575	2.534951
1	1.204993	1.57911	3.221585
1	1.717583	-0.12372	3.083121
1	2.486247	1.111516	2.044094

PC_{Vb-r}

E = -3999.583583 ZPVE = 0.202731 NIMAG = 0.

17	-3.276346	1.621628	0.789661
15	1.641813	1.54479	-1.52847
12	-1.785704	0.073049	0.147022
35	-1.542738	-2.09066	-0.793647
6	-0.19052	1.47435	-1.894386

1	-0.481294	0.446807	-2.142428
1	-0.814993	1.898584	-1.095996
1	-0.383308	2.07887	-2.786159
6	1.705571	3.102829	-0.503283
1	0.964656	3.132315	0.300588
1	2.70725	3.216324	-0.078726
1	1.527364	3.954116	-1.168528
6	1.927044	0.206853	-0.259215
6	1.159111	-0.135906	0.863917
6	3.082615	-0.566682	-0.482789
6	1.503601	-1.180742	1.717853
6	3.459539	-1.603327	0.372147
1	3.693849	-0.339298	-1.351503
6	2.660043	-1.920444	1.470703
1	0.857769	-1.431995	2.553352
1	4.359228	-2.174674	0.165863
1	2.92626	-2.739904	2.130794
8	-0.035866	0.574918	1.133887
6	-0.042837	1.343872	2.371519
1	0.801836	2.035851	2.36274
1	-0.989693	1.883426	2.386241
1	0.027978	0.672408	3.230047

P_{Vb-r}

E = -767.388711 ZPVE = 0.199059 NIMAG = 0.

15	1.725268	-1.051852	-0.000008
6	2.342391	-0.027071	-1.433598
1	1.945081	-0.439962	-2.365882

1	2.063682	1.026494	-1.358121
1	3.433774	-0.11361	-1.468924
6	2.342381	-0.027114	1.433617
1	2.063623	1.026443	1.358198
1	1.945112	-0.440067	2.365891
1	3.43377	-0.113605	1.468912
6	-0.102436	-0.71128	-0.000007
6	-0.731691	0.557709	0.000021
6	-0.930857	-1.842923	-0.000031
6	-2.12896	0.663653	0.000035
6	-2.32674	-1.750041	-0.000025
1	-0.459148	-2.822041	-0.000055
6	-2.919453	-0.490331	0.000012
1	-2.610984	1.633937	0.000071
1	-2.935315	-2.648959	-0.000044
1	-4.001324	-0.390877	0.000024
8	0.091501	1.652672	0.000045
6	-0.486082	2.952348	-0.000043
1	-1.096847	3.119829	0.895721
1	0.353133	3.649446	-0.000128
1	-1.096911	3.119679	-0.895791

S.12.2 Solvent-phase reactions in manuscript

R1r

E = -1452.461417 ZPVE = 0.397479 NIMAG = 0.

6	-0.837876	0.029861	-0.736168
6	-2.359499	1.527852	0.680459
6	-3.236176	-0.740759	-0.13149

6	-2.105449	-0.743035	-1.171363
6	-3.58404	0.707348	0.24414
6	-0.02304	2.440081	-0.04472
6	-4.460584	-1.507019	-0.647302
6	0.891175	2.624968	-1.269912
6	-0.472696	3.826905	0.451417
1	-0.160335	0.052303	-1.595751
1	-2.678211	2.561625	0.839731
1	-1.990318	1.162908	1.644914
1	-2.876632	-1.250996	0.773377
1	-1.852347	-1.765803	-1.462015
1	-2.466405	-0.245927	-2.083562
1	-4.335412	0.715905	1.043806
1	-4.050379	1.192036	-0.62746
1	0.570698	1.991734	0.763168
1	-4.210478	-2.548442	-0.879759
1	-5.263104	-1.512759	0.09887
1	-4.856346	-1.044459	-1.560477
1	0.339987	3.105629	-2.088186
1	1.741398	3.268181	-1.019227
1	1.298771	1.68369	-1.64641
1	-1.156086	4.300488	-0.265182
1	0.397392	4.48297	0.561898
1	-0.975268	3.782725	1.421093
6	1.941365	-0.550256	0.162463
6	2.792791	-0.012452	1.139928
6	2.456096	-0.862251	-1.107718
6	4.137741	0.22682	0.842853
1	2.409866	0.218424	2.127871
6	3.800356	-0.629548	-1.396567

1	1.817782	-1.300532	-1.869188
6	4.642399	-0.080346	-0.422651
1	4.788269	0.64686	1.603805
1	4.190297	-0.877699	-2.378963
1	5.688584	0.101166	-0.649934
17	-0.007716	-2.881796	0.085132
6	-1.22433	1.503906	-0.365947
1	-1.658849	1.889969	-1.303205
15	0.187343	-0.852915	0.589013
5	-0.174648	-0.685254	2.496669
1	0.634737	-1.426299	3.006241
1	0.01754	0.482004	2.756096
1	-1.320276	-1.027622	2.658131

R1u

E = -1143.972958 ZPVE = 0.278142 NIMAG = 0.

15	0.003364	0.313694	0.45966
17	-0.031072	2.14398	-0.562527
6	-1.600321	-0.518228	-0.144581
6	-1.570964	-2.006402	0.270863
1	-2.563358	-2.431269	0.081787
1	-0.852395	-2.586689	-0.313364
1	-1.352406	-2.138103	1.334293
6	-1.838252	-0.402276	-1.662408
1	-2.79889	-0.87808	-1.890964
1	-1.898363	0.638716	-1.988194
1	-1.072787	-0.906552	-2.253425
6	-2.757616	0.1893	0.597758

1	-3.701301	-0.257662	0.264974
1	-2.684921	0.067588	1.680394
1	-2.79615	1.258913	0.371563
6	1.607971	-0.501133	-0.159229
6	1.550272	-0.950503	-1.629436
1	2.545955	-1.302697	-1.922917
1	0.854374	-1.778274	-1.784696
1	1.279268	-0.130017	-2.300191
6	2.753017	0.523926	0.011827
1	2.805282	0.918129	1.029679
1	3.698502	0.012836	-0.201797
1	2.65998	1.361382	-0.683278
6	1.893802	-1.711426	0.762385
1	1.987963	-1.410698	1.808536
1	1.130551	-2.489175	0.69282
1	2.845998	-2.155989	0.451162
5	0.020453	0.649275	2.380094
1	-0.847273	1.461477	2.59406
1	1.130473	1.044627	2.649564
1	-0.22245	-0.437448	2.86451

R1m

E = -1291.571049 ZPVE = 0.215171 NIMAG = 0.

6	-1.486432	0.070549	0.120339
6	-2.316933	-0.065502	1.245007
6	-1.858001	-0.526376	-1.096697
6	-3.499045	-0.805444	1.153998
1	-2.044723	0.403167	2.184376

6	-3.042533	-1.258075	-1.181324
1	-1.234907	-0.412536	-1.97794
6	-3.862538	-1.400656	-0.05621
1	-4.136368	-0.90704	2.026848
1	-3.326056	-1.713687	-2.125013
1	-4.784647	-1.969668	-0.126442
17	0.151756	2.146437	-1.461632
15	0.051538	1.027774	0.311143
6	1.456569	-0.125513	0.154072
6	2.755412	0.39818	0.288957
6	1.281562	-1.504401	-0.04117
6	3.861541	-0.447587	0.213953
1	2.902873	1.461206	0.450841
6	2.394619	-2.347045	-0.107023
1	0.28735	-1.926138	-0.134866
6	3.68281	-1.8214	0.016614
1	4.86078	-0.03554	0.314905
1	2.251017	-3.412924	-0.25493
1	4.545386	-2.478692	-0.037216
5	0.133189	2.196235	1.853204
1	-0.837878	2.912195	1.787513
1	1.18929	2.776444	1.760916
1	0.106824	1.41561	2.782479

R1v

E = -1099.830918 ZPVE = 0.161713 NIMAG = 0.

17	-1.999513	-0.906393	1.263111
15	-1.217332	0.295874	-0.26514

6	-1.724146	-0.616948	-1.762847
1	-1.299789	-0.098288	-2.62775
1	-1.376789	-1.651405	-1.750423
1	-2.813988	-0.596237	-1.832163
5	-1.894905	2.102052	-0.171928
1	-3.093099	1.985178	-0.287482
1	-1.372117	2.615488	-1.141787
1	-1.541182	2.58265	0.87819
6	0.584538	0.096685	-0.109334
6	1.348773	1.214098	0.2644
6	1.222154	-1.131293	-0.358067
6	2.736879	1.104188	0.38061
1	0.862904	2.163957	0.460039
6	2.607651	-1.235199	-0.237618
1	0.646948	-2.00867	-0.636501
6	3.366046	-0.117642	0.130063
1	3.322436	1.972272	0.66687
1	3.094821	-2.18604	-0.430157
1	4.444713	-0.201921	0.221761

R1v

E = -908.089378 ZPVE = 0.107757 NIMAG = 0.

17	1.718488	-0.136987	0
15	-0.352936	0.125499	0
6	-0.879213	-0.841665	-1.455906
1	-0.4853	-0.377393	-2.362536
1	-0.533963	-1.87544	-1.385905
1	-1.972852	-0.821829	-1.494608

6	-0.879213	-0.841665	1.455906
1	-0.533963	-1.87544	1.385905
1	-0.4853	-0.377393	2.362536
1	-1.972852	-0.821829	1.494608
5	-0.879213	1.979121	0
1	-0.44888	2.467586	1.018923
1	-2.091645	1.864802	0
1	-0.44888	2.467586	-1.018923

Nucleophile a

E = -2851.146200 ZPVE = 0.064205 NIMAG = 0.

6	-2.711903	-0.615568	0.000121
1	-2.9213	-1.251697	-0.873882
1	-2.9204	-1.250732	0.875066
6	-3.674219	0.589763	0.000033
1	-3.528611	1.229698	0.879833
1	-3.530466	1.227995	-0.881304
1	-4.734477	0.289905	0.001444
12	-0.630616	-0.200615	-0.000312
35	1.814839	0.066201	0.000047

Nucleophile b

E = -3118.124328 ZPVE = 0.123227 NIMAG = 0.

12	-0.79966	-0.447012	0.000299
35	-3.228796	-0.244675	-0.000124
6	1.277319	-0.913849	0.00026

6	1.697436	0.423333	0.000169
6	2.304543	-1.86552	0.000086
6	3.02282	0.852363	-0.000106
6	3.661505	-1.492494	-0.000176
1	2.062846	-2.927585	0.000136
6	4.014661	-0.141554	-0.000283
1	3.298816	1.901666	-0.000196
1	4.437642	-2.253558	-0.000319
1	5.060815	0.151855	-0.000514
8	0.589837	1.297015	0.000369
6	0.78446	2.715102	-0.000077
1	1.329122	3.027247	-0.896928
1	-0.210343	3.160018	0.000146
1	1.329731	3.027734	0.896232

MgClBr

E = -3232.208677 ZPVE = 0.001644 NIMAG = 0.

17	0.02211	-3.00732	0
12	0	-0.723316	0
35	-0.010739	1.708692	0

R11 + a S_N2@P-b pathways in THF

RC_{1a-i}

E = -4303.612900 ZPVE = 0.464086 NIMAG = 0.

6	-2.485353	-0.551386	0.015199
6	-1.538608	-1.92649	1.960197

6	-2.333236	-3.135012	-0.153727
6	-3.102997	-1.860301	-0.531451
6	-2.16357	-3.200873	1.371425
6	-1.831761	0.653501	2.266481
6	-3.035037	-4.382634	-0.704468
6	-2.843822	1.799896	2.085723
6	-1.568299	0.455836	3.770722
1	-3.186908	0.258727	-0.209628
1	-1.524454	-2.019417	3.049323
1	-0.493946	-1.847393	1.641466
1	-1.332684	-3.085131	-0.606902
1	-3.2404	-1.799697	-1.614127
1	-4.11215	-1.918132	-0.09891
1	-1.550357	-4.06933	1.641925
1	-3.15199	-3.361459	1.828317
1	-0.877921	0.96365	1.818078
1	-3.122234	-4.342312	-1.796089
1	-2.479987	-5.290882	-0.444912
1	-4.046339	-4.47816	-0.289345
1	-3.80228	1.539254	2.551972
1	-2.476975	2.712413	2.567002
1	-3.035266	2.042785	1.037587
1	-2.455321	0.05421	4.276963
1	-1.328575	1.417846	4.235709
1	-0.73129	-0.219541	3.965424
6	-1.010098	1.830551	-1.025094
6	0.0185	2.605067	-0.467927
6	-2.082393	2.463116	-1.67822
6	-0.030983	3.999056	-0.55557
1	0.851567	2.134654	0.04314

6	-2.121937	3.853813	-1.768738
1	-2.877919	1.877657	-2.129594
6	-1.098124	4.623587	-1.204415
1	0.766918	4.591178	-0.118771
1	-2.949404	4.335558	-2.280108
1	-1.131535	5.706398	-1.276175
17	-1.226861	-0.582074	-2.867849
6	-2.318129	-0.651384	1.57126
1	-3.352879	-0.804654	1.919539
6	3.131138	1.725946	1.807052
1	3.568141	1.376182	2.757458
1	2.084598	1.965666	2.055288
6	3.860229	3.013658	1.368425
1	3.822318	3.818041	2.121075
1	4.922727	2.826951	1.164218
1	3.436399	3.429812	0.444466
15	-0.926773	0.012658	-0.893786
12	3.155882	0.057807	0.480548
35	4.52851	-1.744078	-0.506128
5	0.823538	-0.66605	-0.396697
1	1.601962	-0.114193	-1.151748
1	0.995849	-0.353615	0.764052
1	0.809304	-1.858078	-0.536325

TS_{1a-i}

E = -4303.567878 ZPVE = 0.465795 NIMAG = 1.

6	0.769469	1.788535	-0.358329
6	-1.096712	2.233409	1.371869

6	-1.602704	2.654773	-1.083282
6	-0.092069	2.591611	-1.379873
6	-1.86175	3.098989	0.3614
6	1.37941	1.770827	2.211769
6	-2.307034	3.559812	-2.102691
6	2.724089	2.520678	2.135261
6	0.802991	1.918941	3.629959
1	1.811767	2.058273	-0.540158
1	-1.287849	2.613943	2.378487
1	-1.484803	1.212175	1.345475
1	-2.02678	1.647925	-1.191913
1	0.07642	2.233534	-2.398731
1	0.303915	3.616794	-1.358901
1	-2.937557	3.0613	0.573402
1	-1.554779	4.149407	0.478092
1	1.585696	0.705857	2.07028
1	-2.151078	3.203578	-3.127269
1	-3.386524	3.591732	-1.918205
1	-1.925493	4.586783	-2.04303
1	2.586689	3.575999	2.400801
1	3.450446	2.092638	2.834487
1	3.172066	2.494153	1.135998
1	0.537395	2.960396	3.848694
1	1.551998	1.608748	4.366679
1	-0.086915	1.301656	3.782465
6	2.157608	-1.163328	-0.3953
6	2.142199	-2.493324	-0.844894
6	3.223088	-0.723193	0.402787
6	3.165241	-3.37198	-0.48095
1	1.343241	-2.85103	-1.484039

6	4.236592	-1.609064	0.774022
1	3.287616	0.308176	0.723676
6	4.211274	-2.935964	0.335435
1	3.138893	-4.397234	-0.837442
1	5.05243	-1.254378	1.396495
1	5.003146	-3.621276	0.621745
17	2.295094	0.686993	-2.702694
6	0.418165	2.266203	1.086281
1	0.645947	3.342507	0.999198
6	-0.446737	-1.147689	1.146795
1	-1.322724	-0.716168	1.658856
1	0.390978	-0.605156	1.568944
6	-0.319521	-2.638146	1.523643
1	-0.219172	-2.759553	2.611699
1	-1.195214	-3.236909	1.237467
1	0.556516	-3.104072	1.064985
15	0.840088	-0.039899	-0.994113
12	-1.893918	-1.380954	-0.494676
35	-4.113684	-1.87698	0.38374
5	-0.503293	-0.768338	-2.273853
1	-0.610477	-1.955114	-2.014361
1	-1.531661	-0.153032	-2.042237
1	-0.191227	-0.611157	-3.413071

PC_{1a-i}

E = -4303.652421 ZPVE = 0.469047 NIMAG = 0.

6	1.457873	-0.956461	0.378345
6	1.777024	-2.759416	-1.445778

6	0.027732	-3.12537	0.384208
6	0.726413	-2.037463	1.215837
6	1.040338	-3.780992	-0.565898
6	3.378239	-0.66139	-1.397144
6	-0.654765	-4.158047	1.290205
6	4.616416	-0.307249	-0.551205
6	3.840131	-1.166448	-2.775667
1	2.039995	-0.367786	1.099474
1	2.544207	-3.286069	-2.021169
1	1.083557	-2.341796	-2.182747
1	-0.755247	-2.653149	-0.229231
1	0.025079	-1.573054	1.914112
1	1.495645	-2.513772	1.838338
1	0.535011	-4.520061	-1.200509
1	1.776095	-4.334974	0.03574
1	2.823718	0.268527	-1.578564
1	-1.399144	-3.687471	1.94287
1	-1.163061	-4.927911	0.698728
1	0.080262	-4.658951	1.931957
1	5.28569	-1.174231	-0.488142
1	5.179157	0.517932	-1.001562
1	4.360376	-0.025426	0.474704
1	4.429344	-2.086827	-2.68943
1	4.479233	-0.411539	-3.246689
1	3.004983	-1.363096	-3.455175
6	0.920632	2.023241	-0.127341
6	0.081283	3.114453	-0.426321
6	2.226848	2.278572	0.314494
6	0.555099	4.42299	-0.325902
1	-0.95046	2.956094	-0.717495

6	2.694201	3.591692	0.423815
1	2.883825	1.472126	0.609335
6	1.866328	4.665684	0.094522
1	-0.105199	5.250544	-0.567121
1	3.70546	3.766457	0.777433
1	2.232726	5.684344	0.17859
17	3.348575	0.202903	3.497008
6	2.455501	-1.650597	-0.610294
1	3.123902	-2.192309	0.076459
6	-0.139978	0.017768	-2.082142
1	-0.580073	-0.983556	-2.109023
1	0.812348	-0.033281	-2.615634
6	-1.079743	1.011559	-2.777686
1	-1.28565	0.647504	-3.788982
1	-2.038091	1.108136	-2.260031
1	-0.630595	2.002786	-2.869161
15	0.234395	0.323707	-0.288436
12	-3.651438	0.135708	1.168436
35	-5.773039	0.112826	-0.006402
5	-1.41152	0.306112	0.73506
1	-2.111182	1.203224	0.286086
1	-1.944506	-0.788145	0.561084
1	-1.185311	0.497668	1.904408

P1a-i

E = -1071.481311 ZPVE = 0.462313 NIMAG = 0.

6	-0.903051	0.105643	-0.855895
6	-2.371276	1.362078	0.831449

6	-3.300809	-0.72709	-0.335161
6	-2.193976	-0.566327	-1.388694
6	-3.617086	0.636602	0.29686
6	-0.046174	2.362006	0.204397
6	-4.551615	-1.376843	-0.94035
6	0.860356	2.706663	-0.991655
6	-0.473417	3.671582	0.894275
1	-0.263719	0.281995	-1.729537
1	-2.673541	2.359064	1.164049
1	-1.992102	0.847823	1.722168
1	-2.930907	-1.397614	0.454582
1	-1.958868	-1.532946	-1.841651
1	-2.577135	0.074319	-2.197002
1	-4.35009	0.516358	1.10499
1	-4.096042	1.269813	-0.465513
1	0.550724	1.795868	0.930529
1	-4.324067	-2.364617	-1.356556
1	-5.336517	-1.501668	-0.185529
1	-4.960692	-0.757619	-1.748829
1	0.304648	3.292402	-1.735158
1	1.71396	3.309826	-0.664341
1	1.262003	1.821716	-1.490709
1	-1.157213	4.248205	0.258032
1	0.405219	4.297062	1.086095
1	-0.968679	3.500783	1.854007
6	1.918491	-0.608347	-0.137034
6	2.540392	-0.875607	-1.369406
6	2.66568	0.019736	0.871398
6	3.867926	-0.504148	-1.593798
1	1.98936	-1.384005	-2.154519

6	3.997481	0.382101	0.650418
1	2.222445	0.234022	1.838066
6	4.600905	0.125638	-0.583539
1	4.330077	-0.715509	-2.55357
1	4.560177	0.865034	1.443953
1	5.63527	0.408855	-0.75446
6	-1.259257	1.494033	-0.232869
1	-1.718984	2.040302	-1.074604
6	-0.159767	-1.126468	1.903468
1	-1.236505	-1.286501	2.010185
1	0.050819	-0.132006	2.307771
6	0.597503	-2.210225	2.687658
1	0.34159	-2.13595	3.749592
1	0.326947	-3.2099	2.340251
1	1.681993	-2.104592	2.595819
15	0.170726	-1.151319	0.079658
5	-0.041129	-2.956448	-0.649945
1	0.847659	-3.610174	-0.146726
1	-1.14606	-3.33588	-0.320962
1	0.079135	-2.868599	-1.854706

R1_{II} + a S_N2@P-b pathways in THF

RC_{IIa-i}

E = -3995.124880 ZPVE = 0.344370 NIMAG = 0.

17	-2.24199	-1.118657	-2.008506
6	-2.037175	1.572017	-0.408203
6	-1.317696	2.343431	0.723079
1	-1.53323	3.409531	0.59142
1	-1.664157	2.060608	1.718774

1	-0.233125	2.218367	0.682906
6	-3.554169	1.822328	-0.346843
1	-3.736541	2.87976	-0.568548
1	-4.100859	1.230379	-1.08638
1	-3.96792	1.622177	0.644189
6	-1.492195	2.065783	-1.768417
1	-1.643861	3.149562	-1.81643
1	-0.422531	1.87315	-1.883104
1	-2.020958	1.615095	-2.611007
6	2.696043	3.67352	0.155988
1	1.769547	3.666724	-0.433815
1	3.52287	3.612924	-0.563949
1	2.760583	4.669196	0.624597
6	2.739211	2.513651	1.173554
1	3.670024	2.586089	1.759396
1	1.930869	2.648533	1.910572
12	2.636491	0.528462	0.398437
35	3.988401	-1.445891	-0.271049
6	-2.522339	-1.233737	1.098375
6	-4.020129	-1.405515	0.779915
1	-4.468052	-1.999654	1.584249
1	-4.557515	-0.457692	0.732414
1	-4.179524	-1.94362	-0.157287
6	-2.347005	-0.513094	2.45373
1	-2.739634	-1.169526	3.237965
1	-1.297992	-0.312582	2.690109
1	-2.907428	0.423608	2.501813
6	-1.862345	-2.629966	1.176876
1	-0.817481	-2.576312	1.489413
1	-2.410193	-3.220641	1.919366

1	-1.912185	-3.163086	0.223245
15	-1.574851	-0.261014	-0.233385
5	0.343825	-0.58828	-0.142376
1	0.869334	0.148189	-0.952747
1	0.666458	-0.339537	1.006614
1	0.515845	-1.743345	-0.409371

TS_{IIa-i}

E = -3995.059658 ZPVE = 0.349108 NIMAG = 1.

17	2.561321	-1.823087	-1.426435
6	1.241104	-1.161077	1.352936
6	0.5135	-0.481562	2.523016
1	0.66867	-1.101469	3.413774
1	0.904688	0.512392	2.74159
1	-0.5616	-0.410161	2.358272
6	2.709807	-1.375007	1.779113
1	2.702254	-2.014094	2.669719
1	3.300151	-1.870275	1.01019
1	3.197582	-0.438988	2.060703
6	0.573009	-2.527958	1.100188
1	0.648064	-3.111581	2.025169
1	-0.490513	-2.434362	0.866809
1	1.05888	-3.085723	0.30024
6	-1.146769	2.159332	1.793812
1	-0.342032	2.246992	2.52773
1	-1.908534	1.508865	2.237409
1	-1.599063	3.155776	1.693032
6	-0.620882	1.67412	0.429997

1	-1.349738	1.976198	-0.356422
1	0.189653	2.321674	0.124216
12	-1.96462	0.040937	-0.385452
35	-4.378464	-0.189353	-0.326849
6	2.463784	1.339641	-0.469262
6	3.894886	0.835328	-0.764945
1	4.544407	1.718732	-0.770572
1	4.269594	0.14843	-0.005644
1	3.969821	0.347787	-1.734764
6	2.570215	2.192131	0.818057
1	3.26201	3.016155	0.610756
1	1.637159	2.636685	1.158544
1	2.994529	1.618101	1.645017
6	2.020928	2.186056	-1.684104
1	1.050492	2.670023	-1.561523
1	2.765125	2.975843	-1.838195
1	1.988082	1.580331	-2.594291
15	1.145177	-0.106743	-0.30341
5	-0.161173	-0.500098	-1.783272
1	-0.856873	-1.379765	-1.280805
1	-0.790064	0.515561	-2.012353
1	0.337209	-0.918907	-2.779395

PCIIa-i

E = -3995.168846 ZPVE = 0.349229 NIMAG = 0.

17	-5.287615	-2.801619	0.115187
6	-1.656023	0.206017	-1.634367
6	-3.007346	0.90572	-1.890229

1	-3.474989	0.43284	-2.760682
1	-3.704062	0.810894	-1.056379
1	-2.877313	1.964651	-2.126465
6	-1.867962	-1.319488	-1.542657
1	-2.196055	-1.675754	-2.525617
1	-0.944949	-1.851408	-1.293075
1	-2.647312	-1.594484	-0.828066
6	-0.7142	0.508713	-2.823244
1	-1.226009	0.208918	-3.744425
1	-0.475546	1.572661	-2.916016
1	0.219891	-0.054636	-2.763529
6	-1.98576	3.547757	0.188292
1	-2.352105	3.410579	1.20766
1	-2.809014	3.342039	-0.496817
1	-1.718887	4.603594	0.077535
6	-0.738537	2.700082	-0.103408
1	-0.342586	2.937173	-1.096841
1	0.05844	2.960904	0.60097
12	3.222303	-0.202468	-0.115237
35	5.565924	-0.715446	0.043622
6	-1.564652	0.25993	1.582559
6	-1.157308	-1.20568	1.85218
1	-1.572435	-1.500488	2.822173
1	-1.55264	-1.896719	1.106718
1	-0.07218	-1.326968	1.903852
6	-3.103155	0.37187	1.589506
1	-3.456707	0.133262	2.599013
1	-3.455663	1.377813	1.349327
1	-3.575556	-0.343202	0.911685
6	-0.970795	1.141949	2.706595

1	-1.283301	2.186132	2.63679
1	-1.33349	0.755907	3.665457
1	0.122087	1.106144	2.731327
15	-0.799828	0.841319	-0.058845
5	1.063034	0.311733	-0.094688
1	1.616255	0.935841	-0.987291
1	1.564835	0.607941	0.977874
1	1.180471	-0.885556	-0.292525

P11a-i

E = -762.988034 ZPVE = 0.343366 NIMAG = 0.

6	1.643607	-0.333273	-0.305577
6	1.879038	0.498254	-1.583426
1	2.800657	0.145583	-2.062564
1	1.072672	0.403075	-2.31322
1	2.019963	1.558198	-1.357482
6	1.685483	-1.835946	-0.655826
1	2.691548	-2.082713	-1.015694
1	1.479444	-2.465414	0.214383
1	0.983403	-2.097116	-1.451759
6	2.79726	-0.037125	0.681998
1	3.748046	-0.246263	0.177039
1	2.817719	1.010579	0.997915
1	2.738537	-0.661926	1.575381
6	-0.448323	2.839522	-0.443416
1	-1.461524	2.660972	-0.81056
1	0.237059	2.728024	-1.285187
1	-0.402592	3.88455	-0.118034

6	-0.089251	1.935173	0.745704
1	0.882843	2.228781	1.1573
1	-0.804698	2.09653	1.559499
6	-1.542078	-0.552456	-0.289885
6	-1.713739	-2.061762	-0.003011
1	-2.655413	-2.39681	-0.454672
1	-0.911054	-2.665832	-0.430389
1	-1.760898	-2.264261	1.06955
6	-1.53282	-0.323042	-1.814543
1	-2.500256	-0.64099	-2.222492
1	-1.3924	0.726686	-2.08299
1	-0.76166	-0.913123	-2.316262
6	-2.75516	0.182675	0.329731
1	-2.764769	1.250679	0.100248
1	-3.672123	-0.249882	-0.087701
1	-2.792661	0.060593	1.415404
15	0.018689	0.078848	0.610563
5	0.070771	-0.600069	2.451955
1	0.849762	0.118615	3.04453
1	-1.058969	-0.487007	2.883028
1	0.439062	-1.756024	2.426015

R1_{III} + a S_N2@P-b pathways in THF

RC_{IIIa-i}

E = -4142.721673 ZPVE = 0.280763 NIMAG = 0.

6	-2.8332	0.500058	-0.32912
6	-2.700379	1.895298	-0.422146
6	-3.997745	-0.053905	0.229848
6	-3.717427	2.726312	0.055372

1	-1.810472	2.331062	-0.863099
6	-5.011358	0.781983	0.698229
1	-4.120169	-1.130556	0.290416
6	-4.871235	2.172014	0.614369
1	-3.608471	3.803759	-0.019091
1	-5.910041	0.348531	1.125955
1	-5.662964	2.81924	0.979345
17	-2.428357	-2.089096	-1.953574
6	2.393845	3.2901	1.065841
1	2.90442	3.344109	2.040251
1	1.323131	3.202226	1.305906
6	2.638232	4.597425	0.284691
1	2.11246	4.601741	-0.678811
1	2.300763	5.492601	0.831434
1	3.702532	4.748244	0.062686
15	-1.462261	-0.528164	-0.944042
12	3.021491	1.48154	0.133608
35	4.170034	-0.573325	-0.59458
6	-0.699285	-1.360925	0.48876
6	0.385369	-2.224259	0.247945
6	-1.121643	-1.127106	1.80737
6	1.031789	-2.847384	1.314967
1	0.729794	-2.404992	-0.765141
6	-0.465089	-1.751873	2.871259
1	-1.949603	-0.457605	2.010863
6	0.607445	-2.613291	2.627411
1	1.870561	-3.508084	1.121042
1	-0.794685	-1.563051	3.88833
1	1.114213	-3.098306	3.456195
5	-0.207721	0.354777	-2.126435

1	-0.860136	0.814009	-3.033973
1	0.57648	-0.500418	-2.459444
1	0.291748	1.201892	-1.411081

TS_{IIIa-i}

E = -4142.691552 ZPVE = 0.284670 NIMAG = 1.

6	-2.309083	-0.687658	0.057119
6	-2.45931	-2.055723	0.332158
6	-3.330258	-0.000156	-0.618271
6	-3.606446	-2.733226	-0.088614
1	-1.695706	-2.594143	0.882318
6	-4.467347	-0.686417	-1.046175
1	-3.261967	1.068308	-0.786462
6	-4.607168	-2.053661	-0.786385
1	-3.713635	-3.790597	0.132869
1	-5.250372	-0.14722	-1.57027
1	-5.496833	-2.581986	-1.115134
17	-2.057627	1.348097	2.278064
6	0.41585	-0.984975	-1.308609
1	1.276033	-0.495118	-1.806266
1	-0.436415	-0.505724	-1.780755
6	0.363149	-2.491513	-1.636891
1	-0.576325	-2.933184	-1.293064
1	0.426221	-2.664636	-2.720308
1	1.168964	-3.091988	-1.191866
15	-0.83917	0.154308	0.727176
12	1.885329	-1.065595	0.344288
35	4.299558	-1.081348	0.006667

6	-0.27692	1.687996	-0.110569
6	0.629889	2.504527	0.587093
6	-0.702072	2.072483	-1.390947
6	1.105943	3.681762	0.008466
1	0.95539	2.237961	1.587201
6	-0.232632	3.26026	-1.957791
1	-1.392291	1.461242	-1.959629
6	0.672358	4.066348	-1.26364
1	1.807757	4.300708	0.558791
1	-0.576028	3.548563	-2.946604
1	1.036579	4.986758	-1.709395
5	0.288139	-0.797767	2.047515
1	-0.223723	-0.838324	3.124055
1	1.312714	-0.134283	2.094169
1	0.481946	-1.915729	1.601573

PCIIIa-i

E = -4142.775149 ZPVE = 0.286463 NIMAG = 0.

6	1.66125	-1.397485	-0.71944
6	1.415547	-2.206925	-1.839901
6	2.815991	-1.608302	0.054852
6	2.323028	-3.210471	-2.190325
1	0.52255	-2.06121	-2.438543
6	3.715438	-2.614897	-0.301313
1	3.019925	-1.005651	0.937387
6	3.473667	-3.413521	-1.423936
1	2.128148	-3.831266	-3.059547
1	4.603872	-2.773688	0.302105

1	4.177881	-4.19377	-1.697128
17	3.417153	0.254634	3.382261
6	0.187334	-0.169968	1.533332
1	-0.486998	0.661466	1.770756
1	1.129754	0.016672	2.062415
6	-0.413438	-1.51208	1.975312
1	0.275177	-2.33977	1.784911
1	-0.607437	-1.482405	3.051269
1	-1.357645	-1.735028	1.467862
15	0.49695	-0.059254	-0.279493
12	-3.428258	-0.087007	-0.465671
35	-5.686058	-0.042225	0.363117
6	1.305682	1.550661	-0.598525
6	0.934318	2.300267	-1.727801
6	2.308348	2.035614	0.259204
6	1.561564	3.518632	-1.998626
1	0.159158	1.941301	-2.396374
6	2.926186	3.257657	-0.017454
1	2.617184	1.479959	1.142056
6	2.557269	3.999266	-1.143673
1	1.26893	4.090102	-2.874325
1	3.696971	3.626934	0.652071
1	3.042178	4.948125	-1.353096
5	-1.152859	-0.178457	-1.301045
1	-0.97801	-0.184437	-2.486039
1	-1.75241	0.853601	-0.997045
1	-1.722764	-1.207345	-0.960842

E = -910.596380 ZPVE = 0.280050 NIMAG = 0.

6	1.350871	-0.219109	0.078893
6	2.409796	-0.353074	0.989095
6	1.341589	-1.005406	-1.086152
6	3.44653	-1.257571	0.736442
1	2.423416	0.247145	1.89284
6	2.377579	-1.906637	-1.336331
1	0.523148	-0.924538	-1.796137
6	3.4324	-2.033488	-0.424986
1	4.260826	-1.354759	1.448318
1	2.360471	-2.510804	-2.238564
1	4.236713	-2.736713	-0.619947
6	0.130398	2.239326	-0.947826
1	-0.717628	2.920906	-0.820365
1	0.001329	1.72397	-1.905406
6	1.44743	3.028711	-0.936098
1	2.311293	2.372086	-1.076629
1	1.444396	3.757859	-1.752211
1	1.580575	3.571316	0.003489
15	0.015284	0.995215	0.416198
6	-1.548295	0.072983	0.138437
6	-1.817928	-1.037156	0.958478
6	-2.499017	0.459291	-0.818253
6	-3.008906	-1.749953	0.81651
1	-1.097064	-1.346549	1.70975
6	-3.694347	-0.254845	-0.955855
1	-2.323803	1.314234	-1.462135
6	-3.951101	-1.359777	-0.141678
1	-3.202209	-2.606494	1.455407

1	-4.421041	0.05584	-1.700662
1	-4.879146	-1.913148	-0.250101
5	0.095044	1.792548	2.192609
1	-0.031683	0.881688	2.98317
1	-0.842137	2.564346	2.212564
1	1.166074	2.352902	2.286546

R1_{IV} + a S_N2@P-b pathways in THF

RC_{IVa-i}

E = -3950.980038 ZPVE = 0.228001 NIMAG = 0.

17	2.061628000	2.398806000	-1.722525000
15	1.614735000	1.471655000	0.088551000
6	2.225246000	2.665067000	1.319950000
1	2.113304000	2.225488000	2.315211000
1	3.268010000	2.933987000	1.144512000
1	1.603994000	3.561072000	1.255076000
5	-0.297933000	1.202622000	0.206629000
1	-0.796606000	2.273305000	-0.009901000
1	-0.457086000	0.848498000	1.360995000
1	-0.614511000	0.365749000	-0.614346000
6	2.665906000	-0.004794000	0.130323000
6	2.207683000	-1.168391000	-0.512700000
6	3.917869000	-0.008162000	0.768295000
6	2.993370000	-2.320794000	-0.513360000
1	1.243397000	-1.177349000	-1.009794000
6	4.696573000	-1.166574000	0.766770000
1	4.291782000	0.878941000	1.267344000
6	4.237499000	-2.320556000	0.124800000
1	2.634031000	-3.216232000	-1.010331000

1	5.660905000	-1.165261000	1.264817000
1	4.847151000	-3.218860000	0.123906000
6	-1.089656000	-2.470357000	1.822260000
1	0.007593000	-2.421907000	1.736092000
1	-1.297803000	-2.321973000	2.894930000
6	-1.574390000	-3.874550000	1.404386000
1	-1.118844000	-4.688084000	1.992465000
1	-2.661676000	-3.978840000	1.516209000
1	-1.349820000	-4.087012000	0.350480000
12	-1.910722000	-0.793293000	0.797300000
35	-3.986294000	0.400097000	0.138759000

TS_{IVa-i}

E = -3950.953176 ZPVE = 0.229664 NIMAG = 1.

17	2.71119	2.466475	-0.717653
15	1.01993	1.153683	0.183923
6	1.223918	2.015101	1.796591
1	0.469385	1.713121	2.520371
1	2.223885	1.827543	2.191771
1	1.136006	3.082919	1.588813
5	-0.383891	1.704403	-1.093521
1	0.024764	2.421251	-1.954569
1	-1.192842	2.292643	-0.389802
1	-0.830203	0.673123	-1.571232
6	1.980688	-0.372408	-0.06544
6	1.853657	-1.04134	-1.291974
6	2.862076	-0.863972	0.907621
6	2.600704	-2.195439	-1.538786

1	1.184436	-0.66565	-2.059246
6	3.606599	-2.017663	0.653705
1	2.979715	-0.35815	1.860535
6	3.477982	-2.68581	-0.567969
1	2.4966	-2.70615	-2.49113
1	4.2879	-2.39178	1.411695
1	4.059502	-3.58177	-0.762207
6	-0.510603	-0.453592	1.557265
1	0.411836	-0.399902	2.129199
1	-1.264226	-0.075271	2.281018
6	-0.779275	-1.935391	1.217391
1	-0.723631	-2.56604	2.115166
1	-1.770319	-2.115559	0.780161
1	-0.03935	-2.315806	0.505889
12	-1.93467	0.432938	0.116121
35	-4.217189	-0.299544	-0.304327

PC_{IVa-i}

E = -3951.030348 ZPVE = 0.233133 NIMAG = 0.

17	3.018813000	4.371145000	-0.866151000
15	1.037225000	0.357971000	0.881927000
6	2.031832000	1.679662000	1.656172000
1	1.363039000	2.326941000	2.230312000
1	2.781463000	1.254607000	2.327662000
1	2.515556000	2.281310000	0.879311000
5	-0.123232000	1.117567000	-0.474562000
1	0.524064000	1.659585000	-1.323124000
1	-0.792687000	1.960258000	0.120099000

1	-0.786703000	0.214258000	-0.973084000
6	2.182829000	-0.882729000	0.189383000
6	2.101652000	-1.256560000	-1.160495000
6	3.155096000	-1.477076000	1.012917000
6	2.981229000	-2.211313000	-1.678836000
1	1.360300000	-0.805489000	-1.810957000
6	4.030148000	-2.430565000	0.491620000
1	3.240066000	-1.200965000	2.059908000
6	3.943982000	-2.799023000	-0.855168000
1	2.912837000	-2.491650000	-2.725335000
1	4.778774000	-2.882074000	1.135240000
1	4.627544000	-3.539211000	-1.259828000
6	0.138414000	-0.454289000	2.275669000
1	0.896509000	-0.756265000	3.006666000
1	-0.459065000	0.333022000	2.750520000
6	-0.741208000	-1.649832000	1.887126000
1	-1.163066000	-2.100248000	2.790588000
1	-1.578179000	-1.355478000	1.247056000
1	-0.167401000	-2.421836000	1.366169000
12	-2.533527000	1.145540000	-0.597040000
35	-4.506794000	-0.263667000	-0.578487000

PrVa-i

E = -718.855556 ZPVE = 0.226499 NIMAG = 0.

15	1.2632	-0.394934	0.215603
6	1.596169	-0.771685	1.982312
1	2.676613	-0.859789	2.126195
1	1.20755	0.008305	2.641854

1	1.129619	-1.726177	2.238226
5	1.987941	-1.754499	-0.968349
1	1.47522	-2.8043	-0.637285
1	3.182905	-1.731828	-0.745522
1	1.721814	-1.441456	-2.109177
6	-0.553575	-0.169111	0.097063
6	-1.285187	-0.928904	-0.828612
6	-1.232463	0.750788	0.91519
6	-2.671101	-0.773303	-0.933355
1	-0.771632	-1.641007	-1.466141
6	-2.61604	0.905134	0.809288
1	-0.689212	1.352312	1.638781
6	-3.337754	0.142333	-0.11559
1	-3.226168	-1.367484	-1.653178
1	-3.129276	1.618648	1.44711
1	-4.414018	0.262735	-0.196842
6	1.99938	1.283809	-0.030726
1	1.592643	1.952705	0.73602
1	3.06989	1.17079	0.176815
6	1.782743	1.866914	-1.433101
1	2.260493	2.849068	-1.505831
1	2.214274	1.222531	-2.204026
1	0.718542	1.995585	-1.654112

R1v + a S_N2@P-b pathways in THF

RC_{Va-i}

E = -3759.239634 ZPVE = 0.174944 NIMAG = 0.

17 3.582869000 -0.966159000 -1.234855000

15 2.549802000 -0.012327000 0.284078000

6	3.541455000	-0.354798000	1.771311000
1	3.535817000	-1.428384000	1.970609000
1	4.567119000	-0.003039000	1.642114000
1	3.076420000	0.166952000	2.613591000
6	2.746851000	1.757877000	-0.096197000
1	3.804382000	2.024331000	-0.155921000
1	2.250101000	1.987385000	-1.041200000
1	2.269310000	2.329858000	0.705567000
5	0.739975000	-0.681871000	0.379138000
1	0.251017000	-0.479645000	-0.715411000
1	0.235619000	-0.029632000	1.274705000
1	0.795313000	-1.851893000	0.641961000
6	-1.498754000	2.629589000	-0.510312000
1	-0.561145000	3.063156000	-0.125989000
1	-1.445097000	2.761237000	-1.603617000
6	-2.695961000	3.436362000	0.037189000
1	-3.650913000	3.060743000	-0.353368000
1	-2.763804000	3.372976000	1.131575000
1	-2.654907000	4.509219000	-0.212995000
12	-1.521442000	0.539172000	-0.092506000
35	-3.055569000	-1.376526000	0.294024000

TS_{Va-i}

E = -3759.211066 ZPVE = 0.176090 NIMAG = 1.

17	-3.944411	-1.064178	-0.21375
15	-1.930519	0.000413	0.033808
6	-2.561695	1.469682	-0.872278
1	-3.000298	1.115502	-1.806495

1	-3.344584	1.940827	-0.27354
1	-1.772937	2.187156	-1.084119
6	-2.158815	0.022969	1.862058
1	-3.05378	0.602545	2.097877
1	-2.320961	-1.009303	2.178656
1	-1.295927	0.440727	2.376902
5	-0.8292	-1.367594	-0.867345
1	-0.177535	-1.886757	0.033311
1	-0.141419	-0.754195	-1.665883
1	-1.487822	-2.195234	-1.420779
6	0.09975	1.571971	0.57374
1	-0.775794	2.091284	0.962038
1	0.71567	1.439651	1.484626
6	0.822994	2.512951	-0.419993
1	1.778439	2.115772	-0.7904
1	0.211671	2.714966	-1.306868
1	1.055378	3.483205	0.039618
12	1.099203	-0.295169	-0.053075
35	3.52471	-0.493907	0.011833

PC_{Va-i}

E = -3759.289733 ZPVE = 0.178857 NIMAG = 0.

17	-5.212900000	-1.520887000	-0.349756000
15	-1.678235000	0.793285000	0.262652000
6	-2.930203000	1.507356000	-0.855192000
1	-3.707376000	0.751244000	-1.008599000
1	-3.372589000	2.399804000	-0.403956000
1	-2.477517000	1.768960000	-1.814281000

6	-2.563050000	0.262545000	1.767566000
1	-3.066874000	1.117988000	2.225694000
1	-3.308506000	-0.486557000	1.482267000
1	-1.853710000	-0.166266000	2.480309000
5	-0.758944000	-0.703715000	-0.569422000
1	-0.238922000	-1.325549000	0.359172000
1	0.053816000	-0.237054000	-1.363218000
1	-1.528564000	-1.421714000	-1.140809000
6	-0.532153000	2.140952000	0.782786000
1	-1.097252000	2.804554000	1.447100000
1	0.246157000	1.667353000	1.392887000
6	0.091135000	2.940680000	-0.370458000
1	0.635863000	2.299652000	-1.069878000
1	-0.668519000	3.489008000	-0.934769000
1	0.799773000	3.671492000	0.030104000
12	1.572209000	-1.262149000	-0.465742000
35	3.753451000	-0.315193000	0.015126000

P_{Va-i}

E = -527.113057 ZPVE = 0.172680 NIMAG = 0.

15	-0.413988	0.084126	-0.001734
6	-0.508194	-0.638628	1.683087
1	-1.481049	-0.396068	2.119228
1	-0.386813	-1.725366	1.654884
1	0.269153	-0.203697	2.316247
6	-1.712377	-0.791489	-0.957944
1	-1.567331	-1.874874	-0.921904
1	-2.693307	-0.545236	-0.542648

1	-1.682996	-0.45739	-1.9986
5	-0.62903	2.013473	-0.031599
1	-1.73647	2.223584	0.424964
1	-0.536382	2.342291	-1.19886
1	0.252716	2.483537	0.658464
6	1.171014	-0.52909	-0.726222
1	1.149795	-1.625165	-0.705182
1	1.157205	-0.22717	-1.779938
6	2.435758	0.004172	-0.038505
1	2.472906	1.096812	-0.062828
1	2.494313	-0.314224	1.007087
1	3.326035	-0.376072	-0.549406

R11 + a S_N2@P-f pathways in THF

RC_{1a-r}

E = -4303.614385 ZPVE = 0.463926 NIMAG = 0.

6	1.425353	-1.218611	1.074084
6	0.045606	-2.820083	-0.387271
6	-0.859317	-2.12876	1.907425
6	0.563755	-1.679915	2.275889
6	-0.789331	-3.227523	0.837437
6	2.401496	-2.066348	-1.224219
6	-1.631658	-2.583241	3.15202
6	3.876264	-1.983701	-0.789574
6	2.270976	-3.125187	-2.334673
1	2.442063	-1.055279	1.447135
1	0.121633	-3.68444	-1.052144
1	-0.477017	-2.042121	-0.95372

1	-1.399313	-1.27428	1.477525
1	0.538181	-0.910575	3.051477
1	1.096015	-2.536114	2.714394
1	-1.801967	-3.499066	0.515361
1	-0.350107	-4.129702	1.289811
1	2.119938	-1.103583	-1.672086
1	-1.713845	-1.773933	3.886632
1	-2.645913	-2.90304	2.88883
1	-1.128947	-3.428592	3.638494
1	4.208671	-2.949293	-0.388066
1	4.515198	-1.741289	-1.645218
1	4.056855	-1.223281	-0.026057
1	2.446662	-4.134439	-1.941068
1	3.017706	-2.939409	-3.114012
1	1.287909	-3.112881	-2.812232
6	2.47326	1.323555	-0.150154
6	2.502088	1.882305	-1.437817
6	3.594163	1.450061	0.688521
6	3.648021	2.544913	-1.885523
1	1.638973	1.803822	-2.089454
6	4.731833	2.118053	0.237992
1	3.580777	1.044435	1.69563
6	4.761522	2.663119	-1.050811
1	3.664688	2.970753	-2.883821
1	5.592745	2.214631	0.892092
1	5.649143	3.182269	-1.399294
17	0.488494	1.569726	2.141306
6	1.467993	-2.351278	-0.011641
1	1.933367	-3.190261	0.531596
15	0.954535	0.488123	0.415974

5	-0.516637	0.684305	-0.840579
1	-0.739211	1.87109	-0.935037
1	-0.169043	0.182097	-1.87694
1	-1.419005	0.041739	-0.351036
12	-3.066953	1.337146	-0.24961
35	-4.174161	-0.457976	-1.5918
6	-3.311675	2.965744	1.09811
1	-2.527395	2.882693	1.866823
1	-4.262182	2.82851	1.638376
6	-3.274718	4.382559	0.487605
1	-4.07727	4.530804	-0.247104
1	-3.383244	5.18404	1.236654
1	-2.330033	4.575406	-0.038519

TS_{1a-r}

E = -4303.555010 ZPVE = 0.460691 NIMAG = 1.

6	2.084606	-0.713508	0.675554
6	2.560273	-2.292406	-1.304592
6	1.323429	-3.189458	0.747761
6	1.838604	-1.975137	1.533161
6	2.28682	-3.506585	-0.404563
6	3.499695	0.142627	-1.392471
6	1.123151	-4.39635	1.672609
6	4.294082	1.177248	-0.574355
6	4.344883	-0.282502	-2.60746
1	2.577624	0.026489	1.310852
1	3.314752	-2.572584	-2.044719
1	1.6567	-2.036108	-1.868871

1	0.344674	-2.932152	0.31959
1	1.1667	-1.738478	2.35979
1	2.813268	-2.230352	1.973999
1	1.887076	-4.328662	-1.011106
1	3.238222	-3.863721	0.018054
1	2.598952	0.633485	-1.789574
1	0.401952	-4.172139	2.465737
1	0.749832	-5.260476	1.111675
1	2.068864	-4.688408	2.146644
1	5.221391	0.729883	-0.194895
1	4.569203	2.030988	-1.202235
1	3.739474	1.570836	0.280902
1	5.220219	-0.865964	-2.294957
1	4.710311	0.605727	-3.133459
1	3.777185	-0.879364	-3.32571
6	0.856229	1.954194	0.326496
6	0.517007	2.883902	-0.686872
6	1.3816	2.433045	1.551559
6	0.74782	4.242818	-0.492687
1	0.114646	2.53567	-1.63128
6	1.582221	3.796157	1.742544
1	1.613484	1.743941	2.357049
6	1.272568	4.703006	0.720697
1	0.512385	4.944694	-1.286264
1	1.975901	4.15347	2.688554
1	1.438349	5.765113	0.871111
17	-1.352516	-1.12049	2.133698
6	3.06621	-1.067691	-0.516535
1	3.971378	-1.392465	0.023066
15	0.572418	0.213769	0.056613

5	-0.549248	-0.323341	-1.463384
1	-1.324437	0.593484	-1.593496
1	0.14199	-0.516895	-2.432065
1	-1.081777	-1.357332	-1.110495
12	-2.512377	-0.297014	0.236166
35	-4.538117	-0.867619	-1.042403
6	-2.562964	1.923482	0.862707
1	-1.607302	2.179057	1.31612
1	-3.320992	1.681206	1.616159
6	-3.031903	2.807777	-0.258155
1	-4.002691	2.492355	-0.652359
1	-3.138743	3.855764	0.077554
1	-2.319188	2.838572	-1.092771

PC_{1a-r}

E = -4303.711172 ZPVE = 0.467743 NIMAG = 0.

6	1.948833	1.379302	-0.339004
6	0.74012	2.502877	1.621593
6	0.289034	3.328023	-0.764735
6	1.584837	2.620426	-1.193374
6	0.376426	3.696642	0.723949
6	2.520792	0.662533	2.124513
6	0.012545	4.554206	-1.643682
6	3.978454	0.266192	1.825237
6	2.410068	1.052411	3.61021
1	2.943848	1.051816	-0.661094
1	0.872872	2.870348	2.642801
1	-0.092554	1.792608	1.65641

1	-0.551957	2.631516	-0.892976
1	1.552922	2.372226	-2.258328
1	2.418551	3.328213	-1.079084
1	-0.574224	4.131656	1.057053
1	1.138291	4.481862	0.84395
1	1.887281	-0.221963	1.979276
1	-0.09164	4.273999	-2.698118
1	-0.911915	5.056228	-1.33745
1	0.830029	5.28219	-1.568171
1	4.649359	1.11519	2.00837
1	4.294649	-0.554232	2.478208
1	4.129528	-0.064753	0.794858
1	2.942559	1.990168	3.814567
1	2.861831	0.273248	4.233608
1	1.373564	1.17224	3.936214
6	1.944121	-1.616724	-0.539319
6	1.544365	-2.653324	0.317569
6	3.139231	-1.752431	-1.266987
6	2.332898	-3.799756	0.453181
1	0.620026	-2.573518	0.879353
6	3.922848	-2.899461	-1.131998
1	3.466493	-0.970027	-1.946167
6	3.521866	-3.924775	-0.26908
1	2.012877	-4.593933	1.120824
1	4.843445	-2.991686	-1.700212
1	4.132065	-4.816724	-0.163883
17	-3.802708	0.11598	-2.443727
6	2.032058	1.788768	1.16837
1	2.824504	2.556116	1.181902
15	0.889534	-0.131403	-0.760434

5	-0.791855	-0.359082	0.197244
1	-1.312279	-1.353285	-0.288073
1	-0.623408	-0.502638	1.375175
1	-1.433754	0.655249	-0.023684
12	-3.180367	-0.422437	-0.294178
35	-4.268051	-1.100582	1.787334
6	0.606677	-0.04931	-2.590813
1	1.563401	0.189055	-3.067525
1	-0.063342	0.797149	-2.769426
6	0.014275	-1.330492	-3.193866
1	-0.960282	-1.567465	-2.761139
1	-0.127127	-1.188217	-4.269522
1	0.676216	-2.188857	-3.051204

R1_{II} + a S_N2@P-f pathways in THF

RC_{IIa-r}

E = -3995.124825 ZPVE = 0.344369 NIMAG = 0.

17	1.41312	1.080727	1.764278
6	-2.641417	2.703335	0.992619
1	-3.525978	2.792857	1.642756
1	-1.774758	2.778004	1.668938
6	-2.614047	3.887758	0.002532
1	-1.738551	3.844434	-0.659568
1	-3.498428	3.894597	-0.648394
1	-2.582158	4.871779	0.498464
15	1.501724	-0.001456	-0.017053
12	-2.606112	0.765012	0.106814
35	-3.878493	-1.32042	-0.428531

5	-0.174221	0.213172	-0.98398
1	-0.961017	-0.513181	-0.414168
1	-0.475035	1.382912	-0.963027
1	0.024734	-0.196478	-2.100908
6	1.75204	-1.796036	0.556344
6	0.667268	-2.111948	1.612538
1	-0.342812	-1.918147	1.242956
1	0.733782	-3.178944	1.851164
1	0.81762	-1.551272	2.537738
6	3.142402	-2.047131	1.165949
1	3.940548	-1.975028	0.423442
1	3.361947	-1.36247	1.990238
1	3.162441	-3.066218	1.567965
6	1.526509	-2.714395	-0.668823
1	0.527853	-2.591521	-1.094477
1	2.263763	-2.559307	-1.458752
1	1.620428	-3.752182	-0.330244
6	2.966784	0.79518	-0.928969
6	3.337915	-0.093474	-2.137419
1	4.053197	0.459793	-2.75594
1	3.821598	-1.025103	-1.833817
1	2.473951	-0.329289	-2.765064
6	4.202343	1.016107	-0.035817
1	4.628707	0.083941	0.337095
1	4.970121	1.512404	-0.639821
1	3.981194	1.662994	0.816185
6	2.460122	2.163793	-1.440087
1	1.629854	2.058529	-2.141912
1	2.144105	2.817157	-0.621723
1	3.286186	2.658777	-1.962545

TS_{IIa-r}

E = -3995.045548 ZPVE = 0.347165 NIMAG = 1.

17	0.914226	-0.200089	2.372733
6	-0.856129	1.692827	0.832919
1	-1.399833	1.159607	1.620142
1	0.084482	2.015668	1.255841
6	-1.61949	2.856231	0.19154
1	-1.103957	3.268041	-0.682296
1	-2.650357	2.617709	-0.105262
1	-1.713047	3.676654	0.920151
15	1.070679	-0.017899	-0.19961
12	-1.806885	0.276141	-0.639917
35	-4.051513	-0.434379	-0.065553
5	0.058468	0.04195	-1.94111
1	-0.762891	-0.871663	-1.895892
1	-0.49313	1.12896	-1.983648
1	0.76068	-0.132414	-2.894315
6	1.690508	-1.874782	-0.150916
6	0.538451	-2.754321	0.387454
1	-0.388874	-2.624326	-0.180187
1	0.83472	-3.804576	0.279635
1	0.335695	-2.560631	1.440302
6	2.952678	-2.100525	0.701964
1	3.831414	-1.603444	0.283632
1	2.817897	-1.773343	1.731695
1	3.165653	-3.176445	0.71155
6	1.987281	-2.340117	-1.599755

1	1.093644	-2.36169	-2.223892
1	2.746675	-1.741442	-2.103654
1	2.368323	-3.36619	-1.533576
6	2.49554	1.27467	-0.356784
6	3.449006	0.777026	-1.472126
1	4.196066	1.562125	-1.636334
1	3.988595	-0.129172	-1.194244
1	2.933976	0.610507	-2.420907
6	3.293942	1.483747	0.9403
1	3.746733	0.561249	1.306923
1	4.099462	2.197036	0.72836
1	2.674032	1.8948	1.738374
6	1.91051	2.628274	-0.813158
1	1.323884	2.54262	-1.730502
1	1.297658	3.099921	-0.044523
1	2.749933	3.302081	-1.019361

PCIIa-r

E = -3995.168082 ZPVE = 0.350517 NIMAG = 0.

17	2.625666	3.827708	-0.205091
6	0.172297	0.974059	-0.403027
1	-0.560698	1.198191	0.377978
1	0.985407	1.703293	-0.293532
6	-0.501253	1.146635	-1.773021
1	0.213708	1.100323	-2.596801
1	-1.287806	0.409181	-1.957448
1	-0.968899	2.135021	-1.80302
15	0.823507	-0.700387	0.054972

12	-3.002599	-1.475444	0.050249
35	-4.205292	0.631701	0.04057
5	-0.659694	-1.96001	0.249129
1	-1.326517	-1.543146	1.193835
1	-1.27052	-1.937036	-0.819201
1	-0.304988	-3.084322	0.465018
6	1.651726	-0.466867	1.758729
6	0.693902	0.365034	2.645152
1	-0.302202	-0.080963	2.721749
1	1.115582	0.398814	3.655909
1	0.595452	1.396117	2.299089
6	2.993564	0.28617	1.651282
1	3.760567	-0.301404	1.141263
1	2.895121	1.253085	1.148038
1	3.35813	0.479846	2.667006
6	1.863156	-1.838481	2.437233
1	0.919853	-2.369613	2.590656
1	2.536227	-2.490973	1.878896
1	2.31326	-1.666697	3.421652
6	2.014253	-1.306118	-1.303761
6	2.8978	-2.463521	-0.792008
1	3.468733	-2.85708	-1.640844
1	3.618985	-2.140821	-0.0385
1	2.305219	-3.287533	-0.383567
6	2.907738	-0.15544	-1.814024
1	3.545006	0.262924	-1.033721
1	3.560621	-0.549777	-2.601348
1	2.329115	0.663465	-2.246104
6	1.161156	-1.851946	-2.474616
1	0.598988	-2.743407	-2.183833

1	0.461318	-1.116534	-2.875371
1	1.840282	-2.137503	-3.286059

P_{IIa-r}

E = -762.989835 ZPVE = 0.343658 NIMAG = 0.

6	-0.389394	1.864445	-0.640703
1	0.386669	2.579662	-0.354389
1	-0.230325	1.633558	-1.699447
6	-1.75865	2.531405	-0.438408
1	-2.57818	1.938537	-0.851605
1	-1.965718	2.711799	0.619724
1	-1.765408	3.498519	-0.952124
15	-0.011285	0.350923	0.376026
5	-0.062073	0.764738	2.291002
1	0.900968	1.472639	2.506315
1	-1.105826	1.347571	2.495111
1	-0.002622	-0.287218	2.89394
6	1.765048	-0.116131	-0.167786
6	2.62983	1.167633	-0.120215
1	2.546179	1.687402	0.838133
1	3.67925	0.879891	-0.253914
1	2.381048	1.866868	-0.922947
6	1.844914	-0.696656	-1.593684
1	1.359074	-1.671225	-1.679332
1	1.409936	-0.02577	-2.341102
1	2.900509	-0.836224	-1.857104
6	2.361949	-1.120637	0.843006
1	2.367535	-0.711484	1.856345
1	1.827074	-2.071723	0.862416

1	3.399298	-1.330951	0.555786
6	-1.290521	-0.987446	-0.099202
6	-0.789087	-2.391582	0.301446
1	-1.607456	-3.106775	0.155262
1	0.050418	-2.730742	-0.309527
1	-0.496733	-2.434951	1.354618
6	-1.635914	-0.972338	-1.602769
1	-0.770713	-1.176556	-2.236742
1	-2.38012	-1.753522	-1.80007
1	-2.073385	-0.021295	-1.918415
6	-2.576163	-0.708495	0.717067
1	-2.392213	-0.779044	1.791425
1	-3.005141	0.274176	0.511775
1	-3.326559	-1.461863	0.447955

R1_{III} + a S_N2@P-f pathways in THF

RC_{IIIa-r}

E = -4142.721865 ZPVE = 0.281148 NIMAG = 0.

17	0.860557	0.497991	2.303978
6	-3.326122	1.644411	2.123115
1	-4.374378	1.655419	2.462133
1	-2.755095	1.228682	2.969032
6	-2.861317	3.093698	1.864532
1	-1.811476	3.133401	1.544419
1	-3.448643	3.574217	1.070639
1	-2.941747	3.743161	2.751651
15	1.000697	0.028883	0.277768
12	-3.163701	0.312655	0.469746

35	-4.419991	-0.925491	-1.279621
5	-0.762521	-0.088404	-0.510984
1	-1.322501	-0.955399	0.126382
1	-1.275107	1.008915	-0.428378
1	-0.57726	-0.427515	-1.651375
6	1.890111	-1.559912	0.249666
6	2.880672	-1.797106	-0.716938
6	1.492964	-2.595313	1.113027
6	3.473615	-3.058924	-0.809044
1	3.190306	-1.011233	-1.397127
6	2.094612	-3.849876	1.017235
1	0.725504	-2.426595	1.861605
6	3.084572	-4.083514	0.056733
1	4.240122	-3.235704	-1.556995
1	1.788087	-4.644127	1.690495
1	3.549704	-5.061786	-0.015941
6	2.076881	1.308365	-0.420215
6	3.393446	1.485598	0.04175
6	1.564478	2.148613	-1.421995
6	4.189196	2.491497	-0.503118
1	3.794009	0.847426	0.82325
6	2.371666	3.150229	-1.967161
1	0.545585	2.026917	-1.77361
6	3.679798	3.322213	-1.508694
1	5.204327	2.627935	-0.14404
1	1.974485	3.795267	-2.744294
1	4.303444	4.104395	-1.930639

TSIIIa-r

E = -4142.667876 ZPVE = 0.282924 NIMAG = 1.

17	0.209214	-0.999985	2.120445
6	-1.207154	1.321454	0.877894
1	-2.088565	0.987153	1.468308
1	-0.531525	1.600248	1.681993
6	-1.550242	2.550098	0.020659
1	-0.643538	2.995798	-0.395949
1	-2.210417	2.346399	-0.833592
1	-2.05176	3.320792	0.621862
15	0.51653	-0.155719	0.031879
12	-2.462621	-0.239525	-0.227144
35	-4.876899	-0.424962	-0.201328
5	-0.574908	-0.636155	-1.544545
1	-1.283601	-1.573389	-1.185757
1	-1.229682	0.359693	-1.803941
1	0.072841	-1.004032	-2.482069
6	1.939074	-1.397561	-0.123068
6	3.2682	-1.080492	0.19648
6	1.655069	-2.69561	-0.580736
6	4.285499	-2.030036	0.054411
1	3.525838	-0.090709	0.556439
6	2.669474	-3.645331	-0.722165
1	0.637603	-2.977688	-0.830927
6	3.99092	-3.315653	-0.405405
1	5.307763	-1.759985	0.304239
1	2.426167	-4.640763	-1.082762
1	4.781067	-4.052433	-0.516715
6	1.493779	1.392751	-0.104997
6	2.001403	2.046318	1.027031

6	1.778531	1.896938	-1.382777
6	2.779229	3.197406	0.882616
1	1.797358	1.66061	2.021544
6	2.557145	3.05041	-1.521081
1	1.399676	1.398655	-2.269561
6	3.057162	3.702934	-0.391261
1	3.167456	3.695838	1.765768
1	2.767741	3.437018	-2.513692
1	3.659878	4.599323	-0.501601

PC_{IIIa-r}

E = -4142.820021 ZPVE = 0.285242 NIMAG = 0.

17	3.944662000	1.030085000	0.807053000
6	-0.310284000	0.214763000	1.872979000
1	0.276277000	1.139310000	1.879844000
1	-1.178140000	0.380410000	2.519350000
6	0.536194000	-0.961422000	2.377701000
1	-0.038762000	-1.891446000	2.399373000
1	1.422904000	-1.116455000	1.757941000
1	0.875696000	-0.751009000	3.396140000
15	-0.933093000	0.010935000	0.142779000
12	2.926202000	0.357503000	-1.152055000
35	3.659784000	-0.166250000	-3.427314000
5	0.484035000	-0.039503000	-1.188422000
1	0.966817000	1.082622000	-1.178496000
1	1.265966000	-0.912491000	-0.843010000
1	0.017259000	-0.276864000	-2.267912000
6	-2.050049000	1.433112000	-0.153509000

6	-3.362545000	1.258520000	-0.617037000
6	-1.559598000	2.734576000	0.053514000
6	-4.175999000	2.369615000	-0.857766000
1	-3.755369000	0.262609000	-0.790688000
6	-2.377663000	3.840310000	-0.183846000
1	-0.541546000	2.895801000	0.395145000
6	-3.687765000	3.659874000	-0.639002000
1	-5.190359000	2.222538000	-1.215921000
1	-1.989775000	4.840347000	-0.016214000
1	-4.322561000	4.521113000	-0.823865000
6	-1.942772000	-1.509909000	0.123834000
6	-2.916720000	-1.733352000	1.113575000
6	-1.730725000	-2.482180000	-0.865818000
6	-3.669191000	-2.908194000	1.106199000
1	-3.096188000	-0.994764000	1.889143000
6	-2.489677000	-3.656263000	-0.871142000
1	-0.981473000	-2.325473000	-1.633852000
6	-3.456845000	-3.871027000	0.113226000
1	-4.419263000	-3.071188000	1.873932000
1	-2.318956000	-4.401404000	-1.641989000
1	-4.043446000	-4.784723000	0.109238000

R1_{IV} + a S_N2@P-f pathways in THF

RC_{IVa-r}

E = -3950.978076 ZPVE = 0.227082 NIMAG = 0.

17	-1.063521	-1.661521	1.832572
6	1.427587	2.405967	1.274893
1	0.414825	2.063549	1.539028
1	1.93029	2.592814	2.237009

6	1.330421	3.729526	0.48666
1	2.322585	4.134722	0.24825
1	0.808908	3.598164	-0.470912
1	0.790207	4.52093	1.031164
15	-1.390995	-1.404329	-0.213819
12	2.425221	0.805361	0.294961
35	4.444463	-0.45146	-0.385785
6	-2.150337	-2.990147	-0.697639
1	-1.422557	-3.790902	-0.548859
1	-3.051874	-3.198269	-0.118978
1	-2.40388	-2.925226	-1.760004
5	0.26956	-1.022425	-1.131464
1	0.640048	0.056722	-0.706249
1	1.0027	-1.942403	-0.875784
1	-0.042087	-0.950086	-2.297653
6	-2.681519	-0.129346	-0.309965
6	-3.954477	-0.325539	0.254109
6	-2.390043	1.074229	-0.972099
6	-4.922642	0.672415	0.151855
1	-4.192345	-1.243939	0.781802
6	-3.366468	2.068482	-1.073804
1	-1.410486	1.235272	-1.408494
6	-4.629717	1.86929	-0.51248
1	-5.902858	0.518373	0.591908
1	-3.136134	2.99626	-1.587882
1	-5.386047	2.644442	-0.589698

TS_{IVa-r}

E = -3950.928881 ZPVE = 0.227419 NIMAG = 1.

17	0.61994	2.305283	-1.13537
6	0.219391	-1.019119	-1.365629
1	-0.7796	-0.73405	-1.685412
1	0.903651	-0.811997	-2.206525
6	0.320137	-2.451331	-0.867389
1	1.352959	-2.738485	-0.643749
1	-0.272048	-2.614179	0.040911
1	-0.06469	-3.166792	-1.613306
15	-0.962003	1.136255	0.553257
12	1.668216	0.2725	-0.237955
35	3.880043	-0.703104	0.200716
6	-1.766008	2.779187	0.676972
1	-1.009077	3.522405	0.925973
1	-2.27448	3.071055	-0.242842
1	-2.500511	2.703646	1.486627
5	0.263464	0.822552	2.056175
1	1.111214	0.004559	1.755557
1	0.720616	1.913561	2.277714
1	-0.44752	0.38051	2.926693
6	-2.337459	0.014529	0.248448
6	-3.37355	0.349046	-0.647173
6	-2.397015	-1.202936	0.958625
6	-4.4578	-0.510351	-0.811608
1	-3.334709	1.270433	-1.218227
6	-3.496349	-2.045603	0.800955
1	-1.610193	-1.468106	1.655694
6	-4.52284	-1.705823	-0.0866
1	-5.251684	-0.247042	-1.503236
1	-3.549292	-2.968693	1.369475

1 -5.372044 -2.370165 -0.212989

PCIVa-r

E = -3951.079225 ZPVE = 0.231117 NIMAG = 0.

17 -3.041387 2.602732 0.383175
6 1.455757 2.260856 0.551341
1 2.416233 2.774889 0.436445
1 0.676769 2.955332 0.2175
6 1.229064 1.851533 2.012658
1 0.26072 1.362374 2.148851
1 2.009587 1.171261 2.365736
1 1.244567 2.741583 2.648476
15 1.427934 0.857305 -0.64597
12 -2.609438 0.368015 -0.007755
35 -3.810631 -1.772332 -0.021536
6 1.894834 1.580152 -2.263375
1 1.155292 2.334834 -2.544155
1 2.883296 2.042906 -2.216315
1 1.90151 0.790418 -3.018445
5 -0.286186 -0.03835 -0.782167
1 -1.014742 0.791146 -1.304799
1 -0.174031 -1.006479 -1.485143
1 -0.641769 -0.352153 0.342563
6 2.776065 -0.281766 -0.17141
6 4.099375 0.183739 -0.074397
6 2.499699 -1.630134 0.10196
6 5.127643 -0.689017 0.284256
1 4.337847 1.224131 -0.276878

6	3.532351	-2.500901	0.462424
1	1.48472	-2.004925	0.027149
6	4.845206	-2.032834	0.552856
1	6.14657	-0.320604	0.353433
1	3.307692	-3.542569	0.6702
1	5.646618	-2.710729	0.830733

P_{IVa-r}

E = -718.854970 ZPVE = 0.226515 NIMAG = 0.

15	-1.086775	0.316224	0.24488
6	-1.5186	-0.422676	1.870741
1	-2.597779	-0.343615	2.024305
1	-1.222338	-1.472695	1.933295
1	-1.014008	0.14172	2.65896
5	-1.657291	2.168054	0.098082
1	-1.063881	2.77809	0.964196
1	-2.85558	2.145519	0.29102
1	-1.373565	2.54145	-1.021966
6	0.7229	0.073963	0.063632
6	1.535317	1.166819	-0.276445
6	1.316179	-1.187184	0.248207
6	2.915286	1.001416	-0.430953
1	1.089461	2.145554	-0.418729
6	2.69444	-1.350218	0.094933
1	0.710892	-2.049415	0.5136
6	3.496425	-0.255429	-0.245456
1	3.532951	1.855041	-0.693896
1	3.140856	-2.329288	0.241518
1	4.568367	-0.383199	-0.364087

6	-1.829261	-0.803069	-1.029294
1	-1.465817	-0.43411	-1.994908
1	-1.409405	-1.805504	-0.890741
6	-3.363655	-0.850736	-1.018066
1	-3.717991	-1.50306	-1.822581
1	-3.751967	-1.248858	-0.075424
1	-3.796302	0.141426	-1.171969

R1v + a S_N2@P-f pathways in THF

RC_{Va-r}

E = -3759.239761 ZPVE = 0.174271 NIMAG = 0.

17	-3.037822	1.194974	-0.17046
6	1.134819	2.761103	-0.601423
1	1.988089	3.19436	-1.147499
1	0.286781	2.815472	-1.303301
6	0.825305	3.637565	0.631948
1	-0.046546	3.26548	1.186771
1	1.663361	3.652833	1.341535
1	0.6092	4.688671	0.379655
15	-2.392538	-0.763421	0.040221
12	1.5482	0.701805	-0.22929
35	3.256859	-1.085399	0.047987
6	-3.1978	-1.327587	1.572267
1	-2.801824	-0.768463	2.422668
1	-4.28034	-1.198418	1.511114
1	-2.960593	-2.388069	1.701256
6	-3.202444	-1.639058	-1.334742

1	-2.946816	-2.699913	-1.252623
1	-4.286462	-1.517357	-1.286082
1	-2.825678	-1.254229	-2.284767
5	-0.471638	-0.937635	0.057875
1	-0.071233	-0.635656	-1.045384
1	-0.055649	-0.242739	0.962173
1	-0.310795	-2.111885	0.283249

TS_{Va-r}

E = -3759.186368 ZPVE = 0.176492 NIMAG = 1.

17	-1.736217	-1.516868	-1.298635
6	-0.284191	1.061589	-1.035577
1	0.437804	0.437073	-1.596483
1	-1.065737	1.218811	-1.776346
6	0.344652	2.407232	-0.625818
1	-0.337247	3.015016	-0.022662
1	1.266695	2.307111	-0.033548
1	0.624141	3.002454	-1.505594
15	-2.02026	0.054738	0.322512
12	0.888639	-0.091031	0.510152
35	3.262599	-0.3083	0.059562
6	-2.966809	1.583961	-0.08022
1	-2.334203	2.466485	-0.137302
1	-3.469405	1.438074	-1.041073
1	-3.72867	1.718573	0.692182
6	-3.494117	-0.961916	0.885109
1	-3.924109	-0.457841	1.757602
1	-4.252519	-1.052027	0.103486

1	-3.167347	-1.96102	1.181136
5	-0.922729	0.033358	1.957446
1	-0.271118	-1.00724	1.888114
1	-0.205801	1.021828	1.923453
1	-1.591084	-0.010724	2.951486

PC_{Va-r}

E = -3759.337496 ZPVE = 0.178328 NIMAG = 0.

17	-1.089051	2.849077	0.246799
6	3.102934	0.94899	0.44416
1	2.62219	1.252357	1.381136
1	4.177278	0.867018	0.64562
6	2.833044	1.982061	-0.6592
1	3.331006	1.714897	-1.59607
1	1.763174	2.096654	-0.852705
1	3.218093	2.957293	-0.346691
15	2.491899	-0.750383	0.079693
12	-1.379464	0.553925	0.064873
35	-3.300031	-0.958495	-0.095275
6	3.345729	-1.322707	-1.433669
1	3.015503	-0.735037	-2.293451
1	4.429322	-1.22712	-1.323262
1	3.091434	-2.370852	-1.610297
6	3.11454	-1.802523	1.440462
1	2.816497	-2.838453	1.260368
1	4.204266	-1.74452	1.504608
1	2.678167	-1.471745	2.386437
5	0.569044	-0.936571	-0.083871

1	0.098053	-0.555793	0.978902
1	0.203404	-0.275264	-1.043799
1	0.318965	-2.09985	-0.256785

R1 + b S_N2@P-b pathways in THF

RC_{1b-i}

E = -4570.591517 ZPVE = 0.521561 NIMAG = 0.

6	2.901318	1.301643	0.548407
6	0.807641	2.767339	0.729101
6	2.755343	3.537883	-0.749729
6	3.648989	2.540904	0.00334
6	1.586177	3.960761	0.152273
6	0.964642	0.61588	2.199414
6	3.566657	4.744636	-1.237416
6	1.886899	-0.136326	3.176382
6	-0.26792	1.119879	2.972998
1	3.613185	0.733724	1.155772
1	0.057161	3.15154	1.425379
1	0.259745	2.258647	-0.071107
1	2.339622	3.032501	-1.632927
1	4.4955	2.237633	-0.618018
1	4.07846	3.047327	0.880076
1	0.900296	4.61128	-0.404845
1	1.98538	4.564934	0.981561
1	0.599822	-0.100566	1.451039
1	4.376757	4.435621	-1.907822
1	2.930676	5.451311	-1.782348
1	4.016128	5.281941	-0.392544

1	1.343134	-0.953558	3.662128
1	2.760509	-0.575377	2.688812
1	2.243568	0.540925	3.962854
1	0.006175	1.916293	3.67682
1	-0.702285	0.300059	3.555189
1	-1.04943	1.50589	2.31336
6	2.66598	-1.601478	-0.056249
6	3.908413	-1.973184	0.487233
6	1.606555	-2.521203	-0.057628
6	4.083399	-3.246373	1.028171
1	4.745596	-1.281424	0.477276
6	1.786608	-3.793648	0.49291
1	0.644617	-2.260005	-0.484508
6	3.020592	-4.157778	1.035248
1	5.047286	-3.527493	1.441428
1	0.959341	-4.496782	0.486963
1	3.15848	-5.148294	1.45843
17	3.962129	0.152293	-2.174928
6	1.719375	1.764498	1.468951
1	2.229708	2.336288	2.262064
15	2.393611	0.05398	-0.783305
12	-3.164855	-1.098466	-1.003478
35	-2.014324	-3.258511	-1.002341
6	-4.269377	0.714434	-1.070206
6	-4.499507	0.741554	0.312333
6	-4.79935	1.792266	-1.78936
6	-5.205184	1.731333	0.992742
6	-5.518474	2.822988	-1.156784
1	-4.660141	1.846806	-2.868297
6	-5.719662	2.788689	0.224691

1	-5.360771	1.708122	2.066361
1	-5.919318	3.64767	-1.740824
1	-6.275822	3.581635	0.716988
8	-3.906191	-0.377092	0.942381
6	-4.112917	-0.615493	2.338737
1	-5.181156	-0.721012	2.55411
1	-3.595052	-1.546057	2.569785
1	-3.690476	0.199775	2.934194
5	0.728569	0.202862	-1.786738
1	-0.158173	0.068259	-0.971155
1	0.790347	-0.706259	-2.581368
1	0.739887	1.296625	-2.296549

TS_{lb-i}

E = -4570.527586 ZPVE = 0.522893 NIMAG = 1.

6	-2.425475	0.935913	0.342109
6	-3.050715	-1.562585	0.67153
6	-3.994535	-0.285414	-1.332145
6	-3.638476	1.031436	-0.624841
6	-4.228839	-1.395454	-0.298933
6	-1.653093	-0.324794	2.522201
6	-5.20847	-0.096967	-2.250904
6	-1.873022	0.832496	3.51879
6	-1.72727	-1.648111	3.305584
1	-2.406158	1.853383	0.931056
1	-3.339764	-2.283213	1.442075
1	-2.196058	-1.990991	0.148998
1	-3.142491	-0.577627	-1.959699

1	-3.492593	1.827712	-1.357987
1	-4.494524	1.342731	-0.008367
1	-4.424435	-2.347111	-0.809649
1	-5.138307	-1.15637	0.273998
1	-0.64017	-0.254439	2.111678
1	-5.017467	0.668406	-3.011465
1	-5.45833	-1.030707	-2.767586
1	-6.090678	0.2131	-1.676258
1	-1.073254	0.865959	4.267066
1	-1.922529	1.816254	3.040805
1	-2.820371	0.690663	4.05315
1	-2.731578	-1.813519	3.71452
1	-1.031294	-1.616553	4.151539
1	-1.465587	-2.513369	2.691312
6	0.68432	1.852024	0.106698
6	0.802337	2.054577	1.489047
6	1.783905	2.180827	-0.718572
6	1.994218	2.535369	2.036086
1	-0.031302	1.855526	2.14578
6	2.98422	2.643411	-0.159301
1	1.681096	2.136227	-1.800879
6	3.096539	2.810118	1.221212
1	2.061824	2.684721	3.109366
1	3.818809	2.876471	-0.811936
1	4.024199	3.169115	1.654245
17	-1.52103	3.576303	-0.712897
6	-2.67139	-0.233972	1.34836
1	-3.608202	0.112095	1.820043
15	-0.852612	1.295149	-0.763749
12	2.11102	-0.253803	-0.707522

35	4.480105	-0.754441	-0.914748
6	0.102948	-1.185309	-0.807813
6	0.592139	-1.969136	0.258558
6	-0.581732	-1.90889	-1.803358
6	0.392111	-3.343145	0.397302
6	-0.798266	-3.288986	-1.715943
1	-0.958393	-1.378719	-2.6719
6	-0.328579	-3.998244	-0.607184
1	0.799164	-3.903332	1.231499
1	-1.332577	-3.807853	-2.506463
1	-0.498642	-5.067852	-0.527264
8	1.452981	-1.234703	1.097982
6	2.170232	-1.896122	2.1579
1	2.844572	-2.654509	1.750954
1	2.742074	-1.11769	2.661071
1	1.465784	-2.347191	2.860211
5	-0.726714	1.294685	-2.780951
1	0.002486	0.397732	-3.110828
1	-0.277844	2.386651	-3.017924
1	-1.865605	1.160939	-3.156653

PC_{1b-i}

E = -4570.591642 ZPVE = 0.525111 NIMAG = 0.

6	-2.46433	0.441823	-0.044541
6	-3.140404	-1.674439	1.233879
6	-4.310373	-1.137971	-0.978633
6	-3.771152	0.297176	-0.868578
6	-4.43596	-1.774268	0.413445

6	-1.514201	0.06424	2.37145
6	-5.642183	-1.163589	-1.739623
6	-1.68554	1.45446	3.015541
6	-1.393961	-0.985066	3.490767
1	-2.324969	1.521837	0.092079
1	-3.329042	-2.082003	2.231251
1	-2.36239	-2.303282	0.786271
1	-3.589532	-1.731947	-1.557279
1	-3.647728	0.732658	-1.863321
1	-4.518514	0.916605	-0.353433
1	-4.73656	-2.825538	0.316934
1	-5.243628	-1.267673	0.963168
1	-0.566309	0.061435	1.818407
1	-5.531715	-0.749472	-2.748065
1	-6.022508	-2.187207	-1.834758
1	-6.402487	-0.571103	-1.215455
1	-0.787629	1.743811	3.573716
1	-1.907425	2.242231	2.289222
1	-2.523045	1.433924	3.723884
1	-2.322475	-1.051855	4.069588
1	-0.6004	-0.697148	4.189688
1	-1.163629	-1.985652	3.111741
6	0.300554	1.341749	-0.950683
6	0.189262	2.392537	-0.034711
6	1.356642	1.387614	-1.896137
6	1.107389	3.452483	-0.037781
1	-0.627048	2.435491	0.67198
6	2.263456	2.464193	-1.908356
1	1.395179	0.656708	-2.700224
6	2.146815	3.495933	-0.965404

1	0.984472	4.255704	0.681078
1	3.031218	2.50623	-2.675814
1	2.842636	4.327898	-0.978946
17	-2.936473	4.235773	0.436759
6	-2.666561	-0.211607	1.35841
1	-3.537143	0.335325	1.753613
15	-0.963852	-0.001556	-1.139462
12	3.059011	0.332158	-0.480883
35	5.302281	-0.208537	0.177289
6	-0.126351	-1.598061	-0.69015
6	1.006141	-1.798916	0.118568
6	-0.677186	-2.745761	-1.296041
6	1.548855	-3.067775	0.331042
6	-0.163169	-4.020974	-1.073981
1	-1.526558	-2.630325	-1.959281
6	0.950812	-4.185016	-0.249057
1	2.433696	-3.182283	0.946951
1	-0.628207	-4.878275	-1.549324
1	1.369603	-5.170281	-0.072228
8	1.664356	-0.683538	0.686731
6	2.0275 -0.79807	2.105587	
1	2.982045	-1.31488	2.208434
1	2.105924	0.22358	2.477645
1	1.236055	-1.330343	2.629321
5	-1.373104	-0.052374	-3.068053
1	-0.318448	-0.348272	-3.58725
1	-1.730915	1.071681	-3.336195
1	-2.228344	-0.883465	-3.254559

P1b-i

E = -1338.437486 ZPVE = 0.520185 NIMAG = 0.

6	-0.654312	-0.950892	-0.617537
6	-2.246688	-2.587895	0.561648
6	0.168734	-3.306588	0.11535
6	0.263604	-2.165628	-0.909488
6	-1.293174	-3.753249	0.25595
6	-3.189614	-0.31365	-0.318214
6	1.0863	-4.472758	-0.273739
6	-3.315727	0.505321	-1.616241
6	-4.584954	-0.834947	0.071627
1	-0.595667	-0.297192	-1.491372
1	-3.270506	-2.973318	0.560579
1	-2.054569	-2.204105	1.567956
1	0.502485	-2.925133	1.089931
1	1.302598	-1.848331	-1.022305
1	-0.042803	-2.557135	-1.891421
1	-1.378216	-4.515901	1.040965
1	-1.60324	-4.237035	-0.683777
1	-2.866887	0.360977	0.484147
1	2.13277	-4.152844	-0.339323
1	1.028475	-5.282147	0.46314
1	0.800618	-4.888268	-1.248847
1	-3.709498	-0.123384	-2.425418
1	-4.007268	1.343923	-1.479396
1	-2.362402	0.922482	-1.949297
1	-4.944851	-1.584401	-0.645232
1	-5.303759	-0.007929	0.072665
1	-4.600133	-1.284441	1.068152

6	-0.536979	1.880999	0.447321
6	-1.106619	2.610413	1.50511
6	-0.393526	2.509225	-0.801847
6	-1.522496	3.931877	1.318253
1	-1.227168	2.145891	2.476509
6	-0.808268	3.830321	-0.98593
1	0.053745	1.974273	-1.62952
6	-1.374478	4.54658	0.072651
1	-1.961755	4.477066	2.148651
1	-0.688238	4.298138	-1.958963
1	-1.69708	5.573472	-0.072775
6	-2.132793	-1.447045	-0.472753
1	-2.339908	-1.910666	-1.453092
15	0.019083	0.145044	0.78098
5	-0.455864	-0.339144	2.627145
1	0.077338	0.483258	3.340774
1	-1.662564	-0.27426	2.693098
1	-0.037555	-1.456992	2.824188
6	2.617695	0.017295	1.776125
6	4.014086	0.070121	1.769822
6	4.681921	0.297075	0.56821
6	3.963317	0.463879	-0.618431
6	2.563025	0.40925	-0.60759
6	1.863338	0.188338	0.60506
1	2.098252	-0.157505	2.710476
1	4.565679	-0.065487	2.694511
1	5.766675	0.343392	0.54115
1	4.499029	0.633028	-1.544109
8	1.812992	0.545092	-1.738874
6	2.467669	0.737346	-2.996796

1	3.050345	1.66454	-3.001054
1	3.116016	-0.111941	-3.236451
1	1.668801	0.804967	-3.735335

R1_{II} + b S_N2@P-b pathways in THF

RC_{IIb-i}

E = -4262.103979 ZPVE = 0.403442 NIMAG = 0.

15	2.367853	-0.064366	0.224308
17	3.01703	0.209893	2.181969
6	3.805687	0.569379	-0.845219
6	3.259037	0.757718	-2.281074
1	4.073931	1.146421	-2.901659
1	2.920077	-0.176712	-2.733684
1	2.439356	1.479194	-2.315179
6	5.019106	-0.376766	-0.856121
1	5.831545	0.116026	-1.401691
1	5.383284	-0.593689	0.15209
1	4.808386	-1.318105	-1.368597
6	4.241749	1.946496	-0.294215
1	4.956584	2.378469	-1.003028
1	3.404254	2.641127	-0.196682
1	4.7393	1.859932	0.674202
12	-1.734895	0.954135	-0.426317
35	-2.21633	3.374543	-0.230801
6	-2.683121	-0.884597	-0.982225
6	-3.163991	-1.160586	0.306135
6	-3.051711	-1.810911	-1.966743
6	-3.963235	-2.247953	0.65484
6	-3.848323	-2.933599	-1.674157

1	-2.722463	-1.66836	-2.995766
6	-4.301874	-3.146122	-0.370346
1	-4.31841	-2.413631	1.666913
1	-4.118774	-3.633378	-2.461239
1	-4.923686	-4.006825	-0.139595
8	-2.723335	-0.184772	1.226361
6	-3.26516	-0.142208	2.549861
1	-2.804534	0.714286	3.041982
1	-4.351752	-0.010204	2.514441
1	-3.017598	-1.05645	3.098604
6	2.035211	-1.933797	0.144156
6	3.185505	-2.785117	0.716217
1	2.877658	-3.835656	0.672487
1	4.110865	-2.69029	0.147889
1	3.391564	-2.544186	1.761772
6	0.761866	-2.190709	0.982251
1	-0.120628	-1.711467	0.55479
1	0.577764	-3.270619	0.993612
1	0.876122	-1.860665	2.018738
6	1.764549	-2.320348	-1.327179
1	0.984663	-1.705709	-1.785436
1	2.665724	-2.269901	-1.943426
1	1.414016	-3.358162	-1.344121
5	0.795615	1.058775	-0.019337
1	1.165173	2.199764	-0.015371
1	0.038329	0.821886	0.89826
1	0.339093	0.74461	-1.105837

E = -4262.032959 ZPVE = 0.405402 NIMAG = 1.

15	1.60179	-0.399169	-0.141746
17	3.364212	-1.485907	-1.648422
6	2.520555	-1.072221	1.461902
6	1.782589	-0.754286	2.772556
1	2.276986	-1.317261	3.572611
1	1.854286	0.301444	3.037276
1	0.735072	-1.062938	2.755584
6	3.946632	-0.503059	1.572808
1	4.432676	-0.985709	2.429269
1	4.544698	-0.706612	0.684426
1	3.941536	0.572136	1.768285
6	2.585802	-2.613579	1.343157
1	3.15701	-2.979341	2.204599
1	1.594578	-3.06998	1.387206
1	3.086236	-2.943616	0.43438
12	-1.661051	-1.059528	-0.15722
35	-4.032593	-1.584122	0.036884
6	-0.515308	0.778312	0.732927
6	-1.415752	1.403242	-0.170493
6	-0.509085	1.373206	2.0132
6	-2.170757	2.5433	0.113663
6	-1.256727	2.508239	2.343456
1	0.110067	0.962398	2.7942
6	-2.067222	3.112911	1.383279
1	-2.843569	2.970942	-0.619928
1	-1.196387	2.918871	3.346969
1	-2.641628	4.002943	1.621086
8	-1.598142	0.695326	-1.369224

6	-2.512459	1.177093	-2.374594
1	-2.438857	0.467522	-3.198029
1	-3.534165	1.200013	-1.987251
1	-2.203724	2.16905	-2.712763
6	2.191578	1.375046	-0.882517
6	3.724749	1.534284	-1.004753
1	3.887701	2.453903	-1.579384
1	4.201623	1.674046	-0.033914
1	4.20805	0.716508	-1.529205
6	1.561998	1.434276	-2.28662
1	0.476999	1.326858	-2.261173
1	1.794142	2.413397	-2.72315
1	1.977925	0.663563	-2.939736
6	1.732404	2.572158	-0.024509
1	0.664339	2.760034	-0.068721
1	2.030012	2.473544	1.022532
1	2.238305	3.459009	-0.422831
5	0.424905	-1.873437	-0.875043
1	1.034148	-2.799452	-1.300941
1	-0.308412	-1.394956	-1.709927
1	-0.158125	-2.24872	0.141814

PC_{11b-i}

E = -4262.128108 ZPVE = 0.408152 NIMAG = 0.

15	1.272277000	0.303241000	0.266117000
17	5.862812000	-2.992596000	-1.357291000
6	2.178893000	-0.465166000	1.786568000
6	1.112515000	-0.905881000	2.815825000

1	1.612609000	-1.512563000	3.578741000
1	0.632980000	-0.066016000	3.321157000
1	0.332979000	-1.526367000	2.364350000
6	3.213043000	0.460405000	2.463634000
1	3.616378000	-0.073975000	3.330839000
1	4.055612000	0.685783000	1.806703000
1	2.802560000	1.401411000	2.833167000
6	2.932188000	-1.730856000	1.307727000
1	3.507852000	-2.111358000	2.158415000
1	2.249525000	-2.519907000	0.990336000
1	3.636989000	-1.543264000	0.495302000
12	-1.726845000	-1.286513000	-0.981300000
35	-3.890168000	-1.749755000	0.006510000
6	-0.103226000	1.381832000	0.898543000
6	-1.366635000	1.521478000	0.284076000
6	0.112024000	2.151667000	2.058789000
6	-2.362992000	2.334162000	0.828754000
6	-0.864813000	2.984259000	2.599855000
1	1.071339000	2.111718000	2.553837000
6	-2.114468000	3.065899000	1.987734000
1	-3.332232000	2.396579000	0.349495000
1	-0.646449000	3.558196000	3.494079000
1	-2.895550000	3.694580000	2.402496000
8	-1.635192000	0.828411000	-0.902695000
6	-2.428050000	1.528994000	-1.911095000
1	-2.204689000	1.036752000	-2.858431000
1	-3.491494000	1.444694000	-1.682636000
1	-2.115901000	2.572494000	-1.953006000
6	2.362474000	1.444146000	-0.807197000
6	3.626907000	0.680257000	-1.251545000

1	4.171934000	1.307259000	-1.965946000
1	4.304798000	0.470473000	-0.421715000
1	3.393892000	-0.263215000	-1.751141000
6	1.532296000	1.816256000	-2.056128000
1	0.617934000	2.357520000	-1.796608000
1	2.139082000	2.479440000	-2.682358000
1	1.268899000	0.942317000	-2.656101000
6	2.751985000	2.744981000	-0.077429000
1	1.876170000	3.331001000	0.213644000
1	3.365363000	2.570148000	0.807474000
1	3.342674000	3.357094000	-0.768289000
5	0.643867000	-1.232049000	-0.794994000
1	1.567954000	-1.909996000	-1.125185000
1	0.068597000	-0.851326000	-1.798694000
1	-0.066348000	-1.887561000	-0.036624000

P11b-i

E = -1029.936084 ZPVE = 0.401078 NIMAG = 0.

15	0.726051	0.358605	0.309968
5	0.712831	1.81289	1.653131
1	0.031737	2.718779	1.244577
1	0.293489	1.332007	2.684709
1	1.880392	2.128977	1.747567
6	-0.917407	-0.351504	-0.197239
6	-2.163647	0.199727	0.205348
6	-0.960144	-1.497784	-1.010794
6	-3.370158	-0.395622	-0.204172
6	-2.154515	-2.092863	-1.418346

1	-0.035323	-1.948469	-1.341715
6	-3.364215	-1.53326	-1.009233
1	-4.316538	0.028597	0.106435
1	-2.132923	-2.978284	-2.045421
1	-4.308236	-1.976583	-1.312463
8	-2.135738	1.305459	0.986667
6	-3.357514	1.893672	1.431569
1	-3.936071	1.193891	2.045099
1	-3.061254	2.750046	2.03745
1	-3.965725	2.23631	0.586792
6	1.496088	1.02504	-1.318874
6	1.438793	0.062448	-2.521572
1	1.961116	-0.87995	-2.34465
1	0.412005	-0.15756	-2.822024
1	1.929269	0.551767	-3.371922
6	2.964708	1.427756	-1.064955
1	3.064834	2.096609	-0.207144
1	3.610335	0.559278	-0.907332
1	3.339146	1.955563	-1.950333
6	0.68437	2.290088	-1.683522
1	1.071517	2.694332	-2.626674
1	-0.377054	2.063673	-1.829735
1	0.767332	3.063441	-0.917736
6	1.717701	-1.116092	1.069641
6	2.865974	-0.542674	1.933323
1	3.579345	0.04343	1.349108
1	2.491805	0.086347	2.74158
1	3.410887	-1.384847	2.376666
6	2.339032	-2.109547	0.066335
1	1.602199	-2.616122	-0.559303

1	3.081591	-1.637238	-0.581394
1	2.858411	-2.888707	0.637573
6	0.75002	-1.875405	2.005799
1	-0.029453	-2.406341	1.454245
1	1.324509	-2.616464	2.574541
1	0.269134	-1.203551	2.723135

R1_{III} + b S_N2@P-b pathways in THF

RC_{IIIb-i}

E = -4409.698841 ZPVE = 0.339478 NIMAG = 0.

15	2.224745	-0.904461	-0.776875
6	1.985244	-1.457733	0.939152
6	0.855058	-2.23466	1.240646
6	2.914894	-1.153563	1.94909
6	0.650844	-2.690877	2.545591
1	0.143926	-2.488152	0.461937
6	2.708245	-1.617695	3.247415
1	3.795619	-0.559959	1.724515
6	1.575132	-2.38351	3.546925
1	-0.224748	-3.289962	2.775192
1	3.428055	-1.380966	4.02478
1	1.416675	-2.741631	4.559713
17	3.907874	-1.976637	-1.412952
6	-2.452492	3.530399	0.166312
6	-2.644969	2.155096	0.056369
6	-2.72205	1.260061	1.132362
6	-2.600512	1.833571	2.403434
6	-2.406049	3.216408	2.577312
6	-2.331345	4.055404	1.463426

1	-2.39503	4.185657	-0.696663
1	-2.312286	3.634435	3.576453
1	-2.180464	5.123792	1.591442
12	-2.998841	-0.441669	-0.10652
35	-3.564661	-2.653183	-0.97249
1	-2.650201	1.204061	3.291047
8	-2.787898	1.47543	-1.173784
6	-2.674608	2.187127	-2.411628
1	-2.794819	1.447769	-3.20286
1	-3.460264	2.945223	-2.490311
1	-1.689634	2.657347	-2.492047
6	2.816814	0.822572	-0.704626
6	2.247486	1.700624	0.233254
6	3.717329	1.317826	-1.660899
6	2.587763	3.055323	0.218039
1	1.542922	1.338038	0.974649
6	4.056125	2.672165	-1.666699
1	4.161082	0.652862	-2.39411
6	3.493187	3.542435	-0.728367
1	2.14553	3.72539	0.948658
1	4.759775	3.044725	-2.404718
1	3.758597	4.595241	-0.735322
5	0.734411	-1.17375	-1.982747
1	-0.109413	-0.453595	-1.485013
1	1.1296	-0.762274	-3.048693
1	0.453823	-2.347321	-1.968588

TS_{imb-i}

E = -4409.675785 ZPVE = 0.341971 NIMAG = 1.

15	1.255779	-0.246111	-1.004591
6	1.864317	-1.661515	-0.021068
6	1.100202	-2.837472	0.012249
6	3.110181	-1.629251	0.624891
6	1.572531	-3.963873	0.689715
1	0.136517	-2.884592	-0.48074
6	3.569783	-2.752518	1.314122
1	3.735326	-0.74531	0.57287
6	2.804998	-3.922942	1.345932
1	0.972673	-4.868483	0.703093
1	4.533139	-2.715322	1.813271
1	3.170172	-4.797963	1.874895
17	3.101532	-0.268415	-2.381119
6	-1.71883	1.851023	2.033502
6	-1.369635	1.203954	0.849979
6	-0.604645	0.021025	0.772827
6	-0.241338	-0.524571	2.016574
6	-0.577827	0.081847	3.233479
6	-1.295427	1.279516	3.238802
1	-2.311798	2.758433	2.039367
1	-0.275141	-0.376083	4.170875
1	-1.549397	1.764773	4.17659
12	-1.935331	-0.428707	-1.003078
35	-4.180105	-1.258853	-0.525604
1	0.332931	-1.445042	2.051339
8	-1.850048	1.614161	-0.407856
6	-2.776473	2.711236	-0.50579
1	-3.016754	2.803434	-1.564371
1	-3.682925	2.502251	0.068909

1	-2.303747	3.631504	-0.154358
6	1.667858	1.431416	-0.395938
6	2.18006	1.674817	0.885629
6	1.46624	2.502201	-1.279899
6	2.49823	2.977994	1.272441
1	2.311509	0.864598	1.592888
6	1.768449	3.805228	-0.879192
1	1.078559	2.327079	-2.278323
6	2.290716	4.046161	0.394723
1	2.897807	3.156245	2.266159
1	1.603592	4.628164	-1.568012
1	2.532796	5.058975	0.70221
5	-0.060844	-0.583417	-2.45281
1	-0.769914	0.402146	-2.500889
1	0.476534	-0.780838	-3.498104
1	-0.6587	-1.586773	-2.097681

PC_{IIIb-i}

E = -4409.786016 ZPVE = 0.343290 NIMAG = 0.

15	1.071145	-0.012053	-0.402716
6	2.283143	-1.343485	-0.733365
6	1.83843	-2.507241	-1.383902
6	3.633549	-1.224524	-0.371999
6	2.734987	-3.541572	-1.65709
1	0.799046	-2.608665	-1.679875
6	4.527343	-2.26186	-0.651588
1	3.993407	-0.326745	0.119629
6	4.07978	-3.420104	-1.292367

1	2.383524	-4.437107	-2.160061
1	5.571305	-2.160622	-0.371191
1	4.776119	-4.224164	-1.510643
17	-3.616337	2.339018	-1.877435
6	-1.543546	-0.171778	2.800775
6	-0.91962	0.164529	1.601835
6	0.272719	-0.456313	1.193744
6	0.823829	-1.438504	2.033334
6	0.21752	-1.770094	3.245435
6	-0.966276	-1.136128	3.628176
1	-2.47515	0.306075	3.081111
1	0.664052	-2.527896	3.880749
1	-1.451662	-1.397827	4.562846
12	-2.510568	0.475279	-1.041129
35	-3.615253	-1.62719	-0.368995
1	1.735243	-1.946104	1.738089
8	-1.497236	1.107747	0.744255
6	-1.800809	2.411846	1.329514
1	-2.075438	3.053289	0.494136
1	-2.637168	2.327501	2.025216
1	-0.909137	2.787952	1.833213
6	2.019403	1.523398	-0.111245
6	2.457262	1.893689	1.16984
6	2.328556	2.337503	-1.21387
6	3.198646	3.065231	1.343928
1	2.220163	1.277347	2.031215
6	3.073392	3.504625	-1.034062
1	1.988036	2.0657	-2.208033
6	3.508053	3.870193	0.243876
1	3.531514	3.346926	2.338248

1	3.307199	4.129346	-1.890525
1	4.082672	4.781047	0.382039
5	-0.170794	0.161873	-1.908612
1	-0.666416	1.265581	-1.838499
1	0.445231	0.029011	-2.930279
1	-0.977622	-0.742655	-1.788646

P_{imag}-i

E = -1177.551727 ZPVE = 0.337342 NIMAG = 0.

15	-0.246931	0.026772	0.839106
6	-1.976833	-0.310208	0.303153
6	-2.810115	-1.065671	1.144619
6	-2.488815	0.169315	-0.913547
6	-4.127626	-1.343678	0.770287
1	-2.431526	-1.432355	2.09257
6	-3.807044	-0.107817	-1.283994
1	-1.86597	0.764892	-1.572844
6	-4.628567	-0.86568	-0.443797
1	-4.761375	-1.928151	1.430644
1	-4.191351	0.272054	-2.22602
1	-5.653988	-1.077892	-0.731796
6	2.954326	-2.234763	-0.472778
6	2.177334	-1.222853	0.106834
6	0.765886	-1.254079	-0.006199
6	0.173341	-2.314633	-0.704166
6	0.945184	-3.327509	-1.280994
6	2.333796	-3.281202	-1.160967
1	4.034074	-2.214111	-0.391281

1	0.462463	-4.139339	-1.815232
1	2.94766	-4.06046	-1.603072
1	-0.906215	-2.353919	-0.797766
8	2.697782	-0.16676	0.784899
6	4.112672	-0.082298	0.97295
1	4.276399	0.825389	1.553144
1	4.48734	-0.94752	1.530366
1	4.633502	-0.003249	0.012495
6	0.185526	1.632225	0.05914
6	0.714975	1.715011	-1.237712
6	-0.042036	2.811998	0.785083
6	1.005665	2.959549	-1.802397
1	0.9096	0.810914	-1.806726
6	0.246961	4.05553	0.216736
1	-0.439145	2.759985	1.79374
6	0.770549	4.131788	-1.077257
1	1.417328	3.011377	-2.806102
1	0.068171	4.961814	0.787722
1	0.99824	5.098491	-1.516721
5	-0.1157	0.026433	2.795568
1	1.009183	0.365744	3.073824
1	-0.962963	0.810144	3.170488
1	-0.362296	-1.113627	3.12899

R1_{IV} + b S_N2@P-b pathways in THF

RC_{IVb-i}

E = -4217.960106 ZPVE = 0.287008 NIMAG = 0.

17 -2.477381000 -1.499586000 2.431688000

15 -1.925317000 -0.502476000 0.689744000

12	1.859925000	0.373992000	-0.531104000
35	3.101719000	-1.266324000	-1.884099000
6	-1.996474000	1.249293000	1.181995000
1	-2.989394000	1.527562000	1.538899000
1	-1.261169000	1.421961000	1.970547000
1	-1.728553000	1.854086000	0.310837000
6	-3.268476000	-0.808792000	-0.490326000
6	-3.025413000	-1.655252000	-1.585250000
6	-4.531433000	-0.209894000	-0.336890000
6	-4.036483000	-1.894177000	-2.518702000
1	-2.055640000	-2.123777000	-1.711695000
6	-5.535597000	-0.453866000	-1.272932000
1	-4.740618000	0.439227000	0.507068000
6	-5.288790000	-1.294497000	-2.364239000
1	-3.842249000	-2.545744000	-3.364689000
1	-6.508730000	0.011169000	-1.150855000
1	-6.072657000	-1.480185000	-3.092177000
6	1.480145000	2.427759000	-0.091488000
6	2.064557000	2.384672000	1.182277000
6	0.949344000	3.669644000	-0.462294000
6	2.136816000	3.452275000	2.075370000
6	0.987307000	4.783822000	0.396949000
1	0.483441000	3.790566000	-1.440041000
6	1.578529000	4.671800000	1.657282000
1	2.600058000	3.369964000	3.053379000
1	0.563102000	5.733910000	0.081352000
1	1.614354000	5.528916000	2.324200000
8	2.578895000	1.097814000	1.451865000
6	3.211100000	0.819210000	2.704709000
1	2.515200000	0.987872000	3.533185000

1	3.499823000	-0.231313000	2.675593000
1	4.101106000	1.443867000	2.832911000
5	-0.191477000	-1.130095000	0.101918000
1	0.594399000	-0.779329000	0.956754000
1	-0.049164000	-0.568619000	-0.967893000
1	-0.233307000	-2.321990000	-0.031732000

TS_{IVb-i}

E = -4217.936224 ZPVE = 0.287331 NIMAG = 1.

17	-2.829238	-2.220301	1.933839
15	-1.320885	-0.806055	0.892757
12	1.675545	-0.743124	-0.285877
35	3.856603	-1.193152	-1.291152
6	-1.252677	0.303863	2.365747
1	-2.05976	0.054962	3.052778
1	-0.290521	0.133831	2.853465
1	-1.315244	1.346797	2.059167
6	-2.5354	-0.2714	-0.350955
6	-2.511219	-0.857047	-1.624697
6	-3.521179	0.676767	-0.038437
6	-3.462348	-0.489406	-2.580299
1	-1.76026	-1.598354	-1.876504
6	-4.466818	1.04118	-0.997601
1	-3.560071	1.131172	0.946155
6	-4.439081	0.46036	-2.270127
1	-3.437341	-0.947462	-3.564281
1	-5.226244	1.7763	-0.749406
1	-5.177265	0.744703	-3.013805

6	0.25899	0.986692	-0.023865
6	1.271878	1.511544	0.805556
6	-0.380945	1.932617	-0.845573
6	1.603663	2.862715	0.8994
6	-0.077073	3.298632	-0.795528
1	-1.155663	1.605749	-1.533046
6	0.896037	3.762128	0.093638
1	2.388659	3.219356	1.55644
1	-0.600655	3.997431	-1.441514
1	1.127339	4.821704	0.149889
8	1.992486	0.497054	1.461299
6	3.140886	0.829145	2.264485
1	2.841702	1.47446	3.09409
1	3.51647	-0.117252	2.650945
1	3.906997	1.317807	1.656328
5	-0.026195	-2.247972	0.458157
1	0.925288	-2.028058	1.184472
1	0.226239	-2.113227	-0.728089
1	-0.484219	-3.32949	0.665483

PC_{IVb-i}

E = -4217.998041 ZPVE = 0.289852 NIMAG = 0.

17	-2.477381000	-1.499586000	2.431688000
15	-1.925317000	-0.502476000	0.689744000
12	1.859925000	0.373992000	-0.531104000
35	3.101719000	-1.266324000	-1.884099000
6	-1.996474000	1.249293000	1.181995000
1	-2.989394000	1.527562000	1.538899000

1	-1.261169000	1.421961000	1.970547000
1	-1.728553000	1.854086000	0.310837000
6	-3.268476000	-0.808792000	-0.490326000
6	-3.025413000	-1.655252000	-1.585250000
6	-4.531433000	-0.209894000	-0.336890000
6	-4.036483000	-1.894177000	-2.518702000
1	-2.055640000	-2.123777000	-1.711695000
6	-5.535597000	-0.453866000	-1.272932000
1	-4.740618000	0.439227000	0.507068000
6	-5.288790000	-1.294497000	-2.364239000
1	-3.842249000	-2.545744000	-3.364689000
1	-6.508730000	0.011169000	-1.150855000
1	-6.072657000	-1.480185000	-3.092177000
6	1.480145000	2.427759000	-0.091488000
6	2.064557000	2.384672000	1.182277000
6	0.949344000	3.669644000	-0.462294000
6	2.136816000	3.452275000	2.075370000
6	0.987307000	4.783822000	0.396949000
1	0.483441000	3.790566000	-1.440041000
6	1.578529000	4.671800000	1.657282000
1	2.600058000	3.369964000	3.053379000
1	0.563102000	5.733910000	0.081352000
1	1.614354000	5.528916000	2.324200000
8	2.578895000	1.097814000	1.451865000
6	3.211100000	0.819210000	2.704709000
1	2.515200000	0.987872000	3.533185000
1	3.499823000	-0.231313000	2.675593000
1	4.101106000	1.443867000	2.832911000
5	-0.191477000	-1.130095000	0.101918000
1	0.594399000	-0.779329000	0.956754000

1	-0.049164000	-0.568619000	-0.967893000
1	-0.233307000	-2.321990000	-0.031732000

Pivb-i

E = -985.810215 ZPVE = 0.283964 NIMAG = 0.

15	0.199066	-1.044043	0.17508
6	-0.049095	-1.99987	-1.376419
1	0.755263	-2.73667	-1.447748
1	-1.009928	-2.51176	-1.325318
1	-0.029978	-1.354327	-2.257235
6	1.873806	-0.314056	-0.017791
6	2.790043	-0.402945	1.041249
6	2.270704	0.308469	-1.214418
6	4.079105	0.123273	0.907762
1	2.497166	-0.884959	1.967671
6	3.558272	0.831171	-1.346605
1	1.577931	0.395246	-2.046126
6	4.465171	0.739426	-0.284818
1	4.77863	0.047619	1.734941
1	3.85258	1.309417	-2.27612
1	5.466845	1.14594	-0.389105
6	-0.953845	0.390348	0.134912
6	-0.491091	1.691126	0.376702
6	-2.344166	0.194441	-0.046749
6	-1.365741	2.780291	0.427584
6	-3.223923	1.284185	-0.002756
6	-2.730414	2.570197	0.233755
1	-0.980001	3.776938	0.615953

1	-4.287134	1.138772	-0.148077
1	-3.423989	3.405245	0.26722
5	0.048006	-2.154451	1.772995
1	-1.079833	-2.593352	1.762674
1	0.262993	-1.432637	2.724104
1	0.891421	-3.018396	1.634965
1	0.569366	1.859111	0.529375
8	-2.749406	-1.088268	-0.26217
6	-4.144987	-1.367282	-0.402605
1	-4.562955	-0.859816	-1.278867
1	-4.215372	-2.446401	-0.537619
1	-4.69682	-1.073567	0.496683

R1v + b S_N2@P-b pathways in THF

RC_vb-i

E = -4026.216104 ZPVE = 0.231745 NIMAG = 0.

17	-4.767232	-2.035648	-0.292667
15	-2.992613	-1.015294	0.11729
12	2.319446	-0.004104	-0.45353
35	3.856207	-1.883999	-0.266684
6	-2.256727	-0.795235	-1.537646
1	-1.962662	-1.76894	-1.935852
1	-2.960195	-0.311667	-2.219063
1	-1.365866	-0.167716	-1.427666
6	-3.578377	0.635994	0.626647
1	-4.118957	0.554007	1.572091
1	-2.697358	1.269829	0.771704
1	-4.224392	1.077325	-0.135254
6	1.08514	1.662139	-0.902423

6	0.791909	1.945499	0.439019
6	0.494698	2.514656	-1.842872
6	-0.024104	2.985456	0.880379
6	-0.335963	3.582657	-1.456487
1	0.675028	2.359685	-2.905888
6	-0.592884	3.81175	-0.103198
1	-0.223674	3.169106	1.930969
1	-0.779747	4.230031	-2.208584
1	-1.23341	4.635094	0.20059
8	1.435599	1.028701	1.296617
6	1.28979	1.141079	2.717079
1	0.241414	1.01573	3.004443
1	1.887346	0.339723	3.150369
1	1.661261	2.110756	3.063634
5	-1.886756	-1.93186	1.40231
1	-2.525577	-2.008176	2.426203
1	-1.583404	-2.994635	0.911609
1	-0.950158	-1.159791	1.485519

TS_{vb-i}

E = -4026.192882 ZPVE = 0.234348 NIMAG = 1.

17	-1.665987000	-0.658878000	2.755794000
15	-0.874791000	0.118358000	0.728180000
12	1.645884000	0.383504000	-1.118046000
35	3.311195000	0.038784000	-2.865978000
6	-1.919539000	-1.086236000	-0.186406000
1	-1.945447000	-2.005081000	0.399157000
1	-2.936252000	-0.704890000	-0.297874000

1	-1.481764000	-1.289446000	-1.162564000
6	-1.581229000	1.800191000	1.034162000
1	-0.776844000	2.530542000	0.939401000
1	-2.347506000	2.015344000	0.288717000
1	-2.006223000	1.841609000	2.035544000
6	-0.417647000	1.224701000	-1.514150000
6	0.258225000	2.462352000	-1.585158000
6	-1.502796000	1.104805000	-2.403049000
6	-0.101310000	3.524637000	-2.412642000
6	-1.902387000	2.142151000	-3.255198000
1	-2.078408000	0.185445000	-2.440440000
6	-1.212859000	3.355901000	-3.244898000
1	0.458910000	4.452329000	-2.431230000
1	-2.750362000	2.002851000	-3.919254000
1	-1.520584000	4.169352000	-3.895038000
8	1.416133000	2.482519000	-0.787846000
6	2.317301000	3.604151000	-0.843540000
1	1.807035000	4.510738000	-0.509617000
1	3.128624000	3.365929000	-0.156821000
1	2.706159000	3.734521000	-1.857020000
5	1.013308000	-0.406296000	1.026694000
1	1.691330000	0.598972000	0.966696000
1	1.155970000	-0.959468000	2.073824000
1	1.234705000	-1.193198000	0.116508000

PC_{v_b-i}

E = -4026.257864 ZPVE = 0.236424 NIMAG = 0.

17 -5.564807 -1.690366 0.098108

15	-1.793192	0.224095	-0.235685
12	1.167181	-1.701765	-0.033643
35	3.530976	-1.497801	-0.543539
6	-3.051626	0.810098	-1.415748
1	-3.862136	0.073877	-1.384296
1	-3.449685	1.784806	-1.125495
1	-2.636194	0.857484	-2.424769
6	-2.610757	0.177883	1.396299
1	-1.919883	-0.203187	2.150644
1	-2.946342	1.1799	1.674774
1	-3.476877	-0.488163	1.306221
6	-0.466081	1.490736	-0.163084
6	0.720951	1.246329	0.548991
6	-0.589172	2.723798	-0.822246
6	1.744094	2.187384	0.620673
6	0.425406	3.680894	-0.755674
1	-1.487632	2.948961	-1.385178
6	1.589364	3.410919	-0.035531
1	2.654882	1.970947	1.165783
1	0.304213	4.630151	-1.266662
1	2.384884	4.147075	0.017909
8	0.842441	-0.00103	1.186022
6	1.438811	0.007687	2.521319
1	1.0111	0.832578	3.092051
1	1.167654	-0.944534	2.978081
1	2.523253	0.098913	2.44991
5	-1.090834	-1.508316	-0.808351
1	-0.787977	-2.151173	0.192138
1	-1.919111	-2.119178	-1.41729
1	-0.142191	-1.263982	-1.545232

P_{Vb-i}

E = -794.068414 ZPVE = 0.230450 NIMAG = 0.

15	1.637988	-0.00221	-0.065753
6	2.633168	-1.51599	0.22941
1	3.678576	-1.205141	0.306836
1	2.342817	-2.025847	1.151519
1	2.546268	-2.201046	-0.617015
6	1.933716	0.999324	1.446626
1	1.350369	1.919011	1.394924
1	1.657294	0.439569	2.344095
1	2.997549	1.249805	1.48777
6	-0.113852	-0.549113	-0.004739
6	-1.158049	0.406741	0.010551
6	-0.457272	-1.907679	-0.032301
6	-2.497065	-0.004682	0.001325
6	-1.792099	-2.324143	-0.043577
1	0.322114	-2.661167	-0.049743
6	-2.806279	-1.367617	-0.026248
1	-3.297464	0.724667	0.015329
1	-2.02973	-3.382702	-0.066355
1	-3.848202	-1.673749	-0.034768
8	-0.772126	1.712745	0.041421
6	-1.767659	2.737988	-0.013883
1	-2.42633	2.696498	0.860491
1	-1.218727	3.679387	-0.013122
1	-2.360921	2.659832	-0.931156
5	2.211718	0.857659	-1.719554

1	1.573469	1.874562	-1.8695
1	3.397473	1.064239	-1.536069
1	2.016394	0.036004	-2.593521

R1 + b SN2@P-f pathways in THF

RC_{1b-r}

E = -4570.593992 ZPVE = 0.522060 NIMAG = 0.

6	-2.730996	-0.561886	-1.218264
6	-2.715665	-2.661891	0.25734
6	-1.520147	-2.711209	-2.009208
6	-2.333107	-1.469547	-2.406677
6	-2.294747	-3.511972	-0.952061
6	-4.080044	-0.577908	1.046318
6	-1.179626	-3.562306	-3.23862
6	-5.142035	0.432646	0.575177
6	-4.695832	-1.471387	2.138789
1	-3.398128	0.213602	-1.608619
1	-3.33728	-3.279117	0.91136
1	-1.833611	-2.384895	0.844301
1	-0.572627	-2.38056	-1.560146
1	-1.809826	-0.893943	-3.174325
1	-3.277484	-1.799219	-2.862839
1	-1.69118	-4.361626	-0.60976
1	-3.193525	-3.936531	-1.424655
1	-3.260056	-0.020612	1.519448
1	-0.592198	-2.9922	-3.967187
1	-0.597326	-4.445799	-2.954585
1	-2.092167	-3.909306	-3.739531

1	-5.999509	-0.092969	0.136411
1	-5.510723	1.022574	1.420827
1	-4.764026	1.137643	-0.169159
1	-5.465637	-2.132687	1.721132
1	-5.173576	-0.848312	2.902307
1	-3.950231	-2.092244	2.641944
6	-1.941038	2.079827	-0.029217
6	-1.668158	2.562411	1.260935
6	-2.676565	2.873443	-0.926864
6	-2.148229	3.814336	1.654418
1	-1.083031	1.972052	1.957044
6	-3.143005	4.126331	-0.531431
1	-2.87715	2.527979	-1.936654
6	-2.885671	4.595304	0.761928
1	-1.939113	4.176935	2.655979
1	-3.70708	4.734877	-1.231243
1	-3.254004	5.56966	1.068173
17	-0.130468	0.908955	-2.18577
6	-3.510568	-1.401007	-0.146158
1	-4.389316	-1.758136	-0.708083
15	-1.295954	0.445854	-0.519862
5	-0.116266	-0.297278	0.834963
1	0.685514	0.595952	1.033842
1	-0.767298	-0.529604	1.816443
1	0.37082	-1.302215	0.364183
6	4.405198	-0.893167	-1.891788
6	5.283949	-0.12389	-2.677029
6	5.550928	1.201711	-2.328005
6	4.942224	1.77676	-1.199901
6	4.078506	0.96685	-0.464739

6	3.76967	-0.368242	-0.759803
1	4.220069	-1.925319	-2.188156
1	5.761088	-0.559387	-3.551658
1	6.231765	1.799958	-2.927471
1	5.15353	2.806484	-0.930247
12	2.451583	-0.632291	0.897739
35	2.445568	-1.870476	3.046413
8	3.390842	1.396826	0.691655
6	3.548567	2.735895	1.168291
1	4.588151	2.92219	1.457524
1	3.240301	3.455762	0.402814
1	2.901177	2.82828	2.040643

TS_{lb-r}

E = -4570.516666 ZPVE = 0.522858 NIMAG = 1.

6	1.983781	-1.033407	0.958998
6	2.058354	-3.130029	-0.570793
6	0.475632	-3.104356	1.442586
6	1.279762	-1.925579	2.014503
6	1.363671	-3.954215	0.523107
6	3.739078	-1.158356	-1.007743
6	-0.136122	-3.947049	2.569739
6	4.935186	-0.508215	-0.287404
6	4.268887	-2.025597	-2.163489
1	2.661191	-0.3771	1.50933
1	2.753684	-3.785644	-1.103173
1	1.327328	-2.793487	-1.310256
1	-0.348632	-2.703794	0.836342

1	0.656013	-1.312594	2.668943
1	2.077843	-2.335431	2.651012
1	0.768713	-4.75325	0.062399
1	2.127989	-4.450738	1.140478
1	3.141763	-0.36179	-1.464482
1	-0.794055	-3.348894	3.210629
1	-0.725148	-4.777602	2.164328
1	0.649292	-4.373447	3.206235
1	5.622821	-1.282228	0.076833
1	5.494187	0.143624	-0.96733
1	4.634137	0.096601	0.572014
1	4.850514	-2.879058	-1.793129
1	4.931965	-1.427053	-2.7981
1	3.465145	-2.410833	-2.797323
6	1.743467	1.692009	-0.450598
6	1.392609	2.246834	-1.69493
6	2.829349	2.251965	0.249629
6	2.117984	3.313485	-2.23214
1	0.551493	1.856412	-2.25197
6	3.560779	3.305366	-0.294765
1	3.096269	1.87741	1.22937
6	3.206608	3.843105	-1.537457
1	1.827277	3.725742	-3.193677
1	4.401595	3.713807	0.2578
1	3.771298	4.671724	-1.954427
17	0.73942	1.33024	2.404589
6	2.847894	-1.937415	0.008976
1	3.554425	-2.39034	0.726402
15	0.790491	0.236039	0.161237
5	-0.003792	-0.547346	-1.488232

1	-0.743829	0.293492	-1.97244
1	0.87396	-0.801332	-2.272032
1	-0.589748	-1.550111	-1.118453
6	-2.17857	-0.333226	1.998505
6	-2.96189	0.161119	3.044886
6	-3.344239	1.505926	3.028065
6	-2.960899	2.349731	1.981032
6	-2.176218	1.831528	0.940953
6	-1.776826	0.470937	0.912064
1	-1.880653	-1.378702	2.029049
1	-3.270518	-0.488983	3.858315
1	-3.944904	1.910383	3.838033
1	-3.269184	3.388757	1.993955
12	-2.350441	-0.434545	-0.995823
35	-4.116325	-1.335679	-2.419835
8	-1.762484	2.580107	-0.126547
6	-2.119784	3.963023	-0.192109
1	-3.207605	4.089858	-0.230101
1	-1.711872	4.515578	0.660986
1	-1.675726	4.338056	-1.114193

PC_{1b-r}

E = -4570.602641 ZPVE = 0.525318 NIMAG = 0.

6	-1.493174	1.2117	0.624281
6	-1.158725	3.520252	-0.44859
6	0.184402	2.941684	1.642472
6	-0.779642	1.766022	1.882997
6	-0.514142	4.048039	0.840953

6	-3.058693	1.959538	-1.366403
6	0.753403	3.461896	2.968453
6	-4.374634	1.335545	-0.865481
6	-3.393166	3.112179	-2.330455
1	-2.269797	0.534803	0.999827
1	-1.675284	4.34859	-0.940543
1	-0.383603	3.182708	-1.14674
1	1.031992	2.595796	1.033674
1	-0.282396	0.960975	2.431857
1	-1.584476	2.114141	2.544288
1	0.203428	4.84376	0.603876
1	-1.292379	4.50504	1.470131
1	-2.52294	1.206121	-1.956309
1	1.289513	2.674478	3.510219
1	1.450047	4.290662	2.798831
1	-0.050178	3.827178	3.619322
1	-5.000586	2.10731	-0.400144
1	-4.94122	0.900282	-1.695672
1	-4.21799	0.550047	-0.122752
1	-3.881816	3.943378	-1.806908
1	-4.086536	2.756386	-3.100575
1	-2.508344	3.504212	-2.840237
6	-1.52838	-1.136108	-1.275364
6	-1.259456	-1.473689	-2.612373
6	-2.666061	-1.6695	-0.646353
6	-2.115644	-2.330981	-3.309569
1	-0.398376	-1.063791	-3.126202
6	-3.515707	-2.524226	-1.348549
1	-2.889143	-1.446065	0.39361
6	-3.244416	-2.858782	-2.679337

1	-1.898083	-2.579781	-4.34389
1	-4.391513	-2.928532	-0.849993
1	-3.911216	-3.522898	-3.221421
17	-3.548417	-1.003227	2.973567
6	-2.168451	2.389365	-0.160802
1	-2.866776	2.804365	0.584162
15	-0.416871	0.035528	-0.402669
5	0.817213	0.808878	-1.725254
1	1.36871	-0.185528	-2.202618
1	0.270453	1.386497	-2.618558
1	1.589615	1.556742	-1.14878
6	1.897847	-0.178078	1.131669
6	2.895427	-0.756547	1.921849
6	2.7381	-2.07981	2.338299
6	1.590603	-2.788527	1.996286
6	0.575385	-2.202587	1.213096
6	0.731981	-0.87699	0.73771
1	1.973928	0.883187	0.910697
1	3.763805	-0.17576	2.211835
1	3.499188	-2.557728	2.946344
1	1.476355	-3.80648	2.346535
12	3.045519	0.004137	-1.176219
35	5.442726	0.207106	-1.151288
8	-0.557249	-2.850824	0.887797
6	-0.80924	-4.163617	1.406492
1	-0.067248	-4.879003	1.037327
1	-0.819635	-4.154355	2.500183
1	-1.796745	-4.431617	1.033945

P_{lb-r}

E = -1338.430919 ZPVE = 0.519871 NIMAG = 0.

6	1.315111	0.721434	-0.564539
6	3.338924	-0.121597	0.74685
6	2.707847	2.351318	0.945784
6	1.803756	2.175668	-0.291003
6	3.840066	1.3137	0.971882
6	2.363607	-1.656463	-1.142063
6	3.252287	3.784771	1.010809
6	1.769511	-1.630074	-2.56277
6	3.689482	-2.441973	-1.182399
1	0.899469	0.699709	-1.575143
1	4.201087	-0.79344	0.733746
1	2.705256	-0.438142	1.584731
1	2.091584	2.187024	1.834293
1	0.957261	2.866149	-0.206514
1	2.364382	2.487904	-1.18502
1	4.374622	1.38256	1.92814
1	4.573464	1.554952	0.186622
1	1.678302	-2.20931	-0.49315
1	2.439231	4.519601	1.041332
1	3.867414	3.930268	1.90632
1	3.876457	4.010853	0.136396
1	2.430669	-1.082164	-3.247195
1	1.660994	-2.648643	-2.95044
1	0.782326	-1.163348	-2.606364
1	4.4628	-1.886969	-1.729807
1	3.542365	-3.398125	-1.696395
1	4.077457	-2.666492	-0.185352

6	-0.574884	-1.472026	0.41005
6	-0.232134	-2.302846	1.488065
6	-1.21876	-2.030004	-0.704567
6	-0.504715	-3.672774	1.439444
1	0.243401	-1.880253	2.366911
6	-1.49424	-3.398153	-0.750578
1	-1.515705	-1.398757	-1.536507
6	-1.133171	-4.224046	0.319193
1	-0.231831	-4.30535	2.279109
1	-1.993418	-3.817421	-1.619414
1	-1.348189	-5.288037	0.282642
6	2.565915	-0.219083	-0.583002
1	3.212255	0.270207	-1.333233
15	-0.196071	0.32656	0.524311
5	-0.105524	0.910811	2.405443
1	-1.111713	0.488588	2.921413
1	0.901088	0.428056	2.876487
1	-0.068959	2.12164	2.370848
6	-1.40677	1.983036	-1.483294
6	-2.474451	2.624877	-2.1181
6	-3.770585	2.422915	-1.648645
6	-4.000211	1.582709	-0.557339
6	-2.926728	0.940838	0.07657
6	-1.596652	1.136244	-0.381411
1	-0.411341	2.163263	-1.868047
1	-2.285735	3.274575	-2.966535
1	-4.612256	2.914692	-2.127404
1	-5.012944	1.430235	-0.20562
8	-3.086187	0.099733	1.129667
6	-4.390109	-0.112419	1.673303

1	-4.825862	0.826544	2.031709
1	-5.055911	-0.574413	0.935889
1	-4.248425	-0.792601	2.512907

R1_{II} + b S_N2@P-f pathways in THF

RC_{IIb-r}

E = -4262.105329 ZPVE = 0.403173 NIMAG = 0.

17	1.711737	-1.923555	-1.061412
15	2.27756	-0.196397	-0.048176
12	-1.712468	0.873262	-0.501406
35	-2.231699	3.275237	-0.135557
5	0.797191	1.070177	-0.055199
1	0.337872	1.045203	-1.179019
1	0.019169	0.707466	0.803012
1	1.25624	2.15136	0.201171
6	-2.692688	-0.957915	-1.035587
6	-3.189722	-1.186951	0.255801
6	-3.041026	-1.925131	-1.987481
6	-3.995762	-2.259089	0.634465
6	-3.848795	-3.03162	-1.665345
1	-2.693009	-1.824352	-3.015232
6	-4.324628	-3.192557	-0.361901
1	-4.361075	-2.387815	1.648483
1	-4.108284	-3.760758	-2.429139
1	-4.952551	-4.042481	-0.108656
8	-2.751797	-0.183189	1.148619
6	-3.364349	-0.037415	2.433152
1	-3.146451	-0.902813	3.067122
1	-2.932692	0.859914	2.876406

1	-4.447525	0.085747	2.32879
6	3.743538	0.446643	-1.071677
6	4.761412	-0.64979	-1.439665
1	5.254651	-1.082064	-0.568087
1	4.303927	-1.456201	-2.017411
1	5.536048	-0.191799	-2.064558
6	4.441392	1.575989	-0.280607
1	3.744214	2.354547	0.040903
1	4.982066	1.200495	0.591606
1	5.176816	2.045643	-0.943167
6	3.140968	1.032	-2.370038
1	3.965344	1.401533	-2.989723
1	2.601236	0.277257	-2.949417
1	2.46699	1.868103	-2.171457
6	2.682208	-0.794688	1.707349
6	2.766486	0.456473	2.614456
1	3.580674	1.129008	2.337658
1	1.832546	1.023996	2.616471
1	2.95417	0.115453	3.638511
6	3.988606	-1.603999	1.784355
1	3.987531	-2.455271	1.097585
1	4.870472	-0.990263	1.586871
1	4.087603	-1.99991	2.801274
6	1.506355	-1.676526	2.187154
1	1.462615	-2.627603	1.652258
1	1.661887	-1.892962	3.249583
1	0.540134	-1.175379	2.086613

TSlib-r

E = -4262.017403 ZPVE = 0.401733 NIMAG = 1.

17	0.297728	-1.316318	1.889687
15	1.689472	-0.230405	-0.353212
12	-1.320566	-0.750635	0.115464
35	-3.053444	-2.494243	-0.133021
5	0.590232	-1.037077	-1.744726
1	-0.158155	-1.844605	-1.230439
1	0.029577	-0.143008	-2.31556
1	1.395003	-1.64622	-2.416488
6	-0.853074	1.34856	0.674268
6	-1.904189	1.826892	-0.120592
6	-0.458767	2.130936	1.761486
6	-2.560227	3.034822	0.120573
6	-1.086869	3.356838	2.033545
1	0.339157	1.787177	2.415383
6	-2.11918	3.80764	1.204874
1	-3.388222	3.375012	-0.492637
1	-0.774035	3.954085	2.885601
1	-2.603733	4.758273	1.408202
8	-2.27077	0.905759	-1.102216
6	-3.43043	1.14101	-1.913897
1	-3.291114	2.040024	-2.521374
1	-3.525496	0.267805	-2.557619
1	-4.322893	1.241965	-1.288533
6	3.106091	-1.400583	0.284321
6	3.588707	-1.063597	1.707835
1	3.982146	-0.048523	1.78973
1	2.795812	-1.192213	2.443986
1	4.401515	-1.754543	1.959006

6	4.315168	-1.306356	-0.685328
1	4.045273	-1.528495	-1.720342
1	4.840033	-0.352426	-0.635837
1	5.022391	-2.078709	-0.363298
6	2.599537	-2.8574	0.210043
1	3.421876	-3.504559	0.535983
1	1.748165	-3.041713	0.861833
1	2.333675	-3.142485	-0.810652
6	2.378737	1.497251	-0.88587
6	3.065838	1.22892	-2.264724
1	3.900002	0.53564	-2.231922
1	2.346174	0.884786	-3.010455
1	3.45917	2.196321	-2.597836
6	3.367855	2.092567	0.129218
1	2.901923	2.237737	1.107594
1	4.269148	1.491364	0.255881
1	3.682177	3.076521	-0.236814
6	1.266142	2.518598	-1.169376
1	0.841353	2.926717	-0.25579
1	1.721572	3.343452	-1.72899
1	0.464377	2.102929	-1.78183

PC_{11b-r}

E = -4262.171132 ZPVE = 0.406946 NIMAG = 0.

17	-2.170921	1.440147	2.495007
15	1.454708	-0.663819	0.078139
12	-2.255723	-0.019179	0.683495
35	-4.18496	-1.165101	-0.327961

5	-0.227094	-1.621608	0.438987
1	-0.734496	-1.032078	1.381395
1	-0.903509	-1.658656	-0.555295
1	0.063963	-2.720663	0.831157
6	1.214492	1.128927	-0.36128
6	-0.024617	1.707805	-0.714714
6	2.324716	1.999414	-0.360544
6	-0.155875	3.077521	-0.949744
6	2.210969	3.361919	-0.630612
1	3.309416	1.608784	-0.153767
6	0.958492	3.910907	-0.904406
1	-1.136156	3.484064	-1.171971
1	3.097995	3.98673	-0.617516
1	0.846015	4.974445	-1.088319
8	-1.173645	0.919149	-0.869769
6	-1.762183	0.948115	-2.208854
1	-0.990756	0.712565	-2.942834
1	-2.542235	0.188484	-2.206573
1	-2.197835	1.92823	-2.40744
6	2.489868	-0.750163	1.704152
6	3.773786	0.105079	1.766149
1	4.446854	-0.049121	0.920375
1	3.555132	1.17002	1.861295
1	4.318862	-0.188814	2.670503
6	2.882504	-2.225698	1.948451
1	2.038451	-2.910587	1.845204
1	3.687526	-2.55193	1.284818
1	3.254138	-2.308989	2.976022
6	1.558585	-0.28197	2.846418
1	2.148825	-0.235479	3.76868

1	1.144659	0.714677	2.666445
1	0.731224	-0.97283	3.01474
6	2.313259	-1.458838	-1.439587
6	2.217614	-2.998174	-1.341429
1	2.799444	-3.404327	-0.512521
1	1.186201	-3.341358	-1.236389
1	2.622883	-3.422801	-2.267029
6	3.788444	-1.046064	-1.596935
1	3.914528	0.036412	-1.683971
1	4.411139	-1.41041	-0.776421
1	4.175016	-1.491827	-2.520862
6	1.524582	-1.004038	-2.687472
1	1.605442	0.072984	-2.856841
1	1.9439	-1.510722	-3.563891
1	0.467514	-1.276938	-2.623838

R1_{III} + b S_N2@P-f pathways in THF

RC_{IIIb-r}

E = -4409.699316 ZPVE = 0.340209 NIMAG = 0.

17	-1.221776	0.171112	-2.172316
15	-1.721012	0.159033	-0.147701
12	2.234984	-1.006601	-0.071908
35	2.311174	-3.481343	0.074994
5	-0.173449	-0.33903	0.899227
1	0.129448	-1.450711	0.527303
1	0.660217	0.506859	0.674108
1	-0.531379	-0.351472	2.050351
6	3.310733	0.645316	-0.890358
6	3.798018	1.090931	0.346501

6	3.694982	1.414545	-1.995798
6	4.606542	2.209489	0.540222
6	4.505928	2.557225	-1.863743
1	3.360911	1.133866	-2.994299
6	4.955313	2.950217	-0.601274
1	4.961707	2.514861	1.519177
1	4.78479	3.135399	-2.741339
1	5.583123	3.830437	-0.492362
8	3.364655	0.245825	1.391236
6	3.705256	0.544549	2.747768
1	3.313114	1.525737	3.035379
1	3.242208	-0.230156	3.358897
1	4.791279	0.522579	2.885092
6	-2.341737	1.8374	0.178636
6	-3.011668	2.601439	-0.790583
6	-2.153359	2.355425	1.471617
6	-3.495346	3.869074	-0.463495
1	-3.145577	2.220032	-1.797246
6	-2.64684	3.622146	1.79118
1	-1.621742	1.780837	2.222335
6	-3.316663	4.379128	0.826382
1	-4.007729	4.457695	-1.217969
1	-2.499569	4.016575	2.791605
1	-3.69291	5.366473	1.075969
6	-3.111196	-1.00642	-0.028305
6	-4.446717	-0.572677	-0.063541
6	-2.823408	-2.376308	0.110091
6	-5.482703	-1.503035	0.034805
1	-4.681877	0.481613	-0.158107
6	-3.865239	-3.299462	0.202522

1	-1.796102	-2.72371	0.142962
6	-5.193917	-2.864523	0.16599
1	-6.513172	-1.162629	0.011469
1	-3.637856	-4.355396	0.308965
1	-6.002284	-3.585271	0.242971

TS_{mb-r}

E = -4409.640469 ZPVE = 0.340324 NIMAG = 1.

17	0.533293	-2.160746	1.458962
15	1.003753	-0.646741	-0.140948
12	-1.955309	-0.986194	-0.794685
35	-4.207669	-1.752818	-0.284611
5	0.165683	-1.469733	-1.734875
1	-0.552383	-2.345642	-1.267501
1	-0.464239	-0.622566	-2.330859
1	0.974592	-1.993424	-2.441839
6	-0.952063	0.400102	0.823282
6	-1.755479	1.366945	0.181478
6	-0.81631	0.568191	2.211179
6	-2.364905	2.438346	0.831158
6	-1.412161	1.628969	2.902619
1	-0.21644	-0.137812	2.774914
6	-2.171221	2.57274	2.209727
1	-2.993783	3.142596	0.299114
1	-1.275726	1.719032	3.976241
1	-2.631696	3.404246	2.734537
8	-1.990651	1.080174	-1.174104
6	-2.86737	1.914242	-1.955988

1	-2.47404	2.932536	-1.994608
1	-2.870747	1.481543	-2.955813
1	-3.878038	1.907744	-1.539454
6	1.466837	1.152787	-0.309335
6	2.160888	1.818168	0.712986
6	1.181537	1.832951	-1.502519
6	2.550097	3.148153	0.550792
1	2.401389	1.306387	1.639749
6	1.592003	3.160626	-1.667097
1	0.651365	1.337854	-2.307693
6	2.268336	3.824445	-0.641451
1	3.079045	3.652982	1.353855
1	1.378067	3.672171	-2.601246
1	2.578811	4.85701	-0.769789
6	2.816554	-1.190916	-0.087288
6	3.533717	-1.468284	1.084757
6	3.506607	-1.187055	-1.311074
6	4.902375	-1.751632	1.034149
1	3.031511	-1.476494	2.045033
6	4.872058	-1.481782	-1.362541
1	2.986266	-0.961579	-2.236103
6	5.576381	-1.764452	-0.189247
1	5.43709	-1.965595	1.955202
1	5.380805	-1.489928	-2.322254
1	6.637495	-1.992267	-0.228312

PC_{IIIb-r}

E = -4409.783904 ZPVE = 0.342671 NIMAG = 0.

17	-2.831932	-3.050278	-0.896987
15	1.0941	0.077369	-0.384567
12	-2.525745	-0.756409	-0.7272
35	-4.190507	1.034005	-1.05325
5	-0.237073	-0.123643	-1.803906
1	-0.500759	-1.304393	-1.862475
1	-1.19291	0.567639	-1.518145
1	0.25121	0.284979	-2.824393
6	0.776187	-0.98938	1.080638
6	-0.505415	-1.059313	1.650744
6	1.783519	-1.798275	1.632335
6	-0.786326	-1.902276	2.722678
6	1.518696	-2.634756	2.71788
1	2.781309	-1.775934	1.208741
6	0.233546	-2.688654	3.261379
1	-1.794127	-1.950591	3.120652
1	2.31369	-3.247876	3.129521
1	0.017424	-3.349614	4.094517
8	-1.532604	-0.277555	1.101328
6	-2.061751	0.761657	1.98745
1	-1.250343	1.438756	2.259342
1	-2.825424	1.280082	1.410288
1	-2.500978	0.302498	2.874308
6	1.231359	1.793888	0.228579
6	1.646155	2.083832	1.538428
6	0.929804	2.845091	-0.653279
6	1.759368	3.41127	1.959025
1	1.877224	1.281234	2.232032
6	1.049427	4.169948	-0.228424
1	0.606922	2.633697	-1.667738

6	1.460927	4.454349	1.077265
1	2.078234	3.62769	2.974058
1	0.812372	4.976902	-0.914659
1	1.547068	5.485214	1.407111
6	2.744102	-0.417262	-1.005203
6	2.826381	-1.510614	-1.884907
6	3.913074	0.267335	-0.6402
6	4.06558	-1.916358	-2.382992
1	1.928735	-2.041699	-2.185296
6	5.150255	-0.139549	-1.147511
1	3.86447	1.120456	0.028212
6	5.228509	-1.231389	-2.016024
1	4.11996	-2.76163	-3.062052
1	6.049249	0.39934	-0.864376
1	6.190515	-1.544433	-2.410451

R1_{IV} + b S_N2@P-f pathways in THF

RC_{IVb-r}

E = -4217.959327 ZPVE = 0.286950 NIMAG = 0.

17	1.447039	2.404268	-0.032883
15	2.073754	0.602052	0.794495
12	-1.702944	-0.970327	-0.217335
35	-1.79967	-3.442375	-0.088881
6	2.391056	1.038368	2.535129
1	2.766623	0.143357	3.039954
1	3.125594	1.840798	2.6197
1	1.452615	1.348876	2.999611
5	0.74632	-0.78326	0.579735
1	-0.202596	-0.41411	1.243503

1	0.521763	-0.90037	-0.60662
1	1.25242	-1.772003	1.045616
6	-2.753223	0.66881	-1.082312
6	-3.100063	1.403931	-2.222723
6	-3.32876	1.112916	0.116198
6	-3.960982	2.515276	-2.159405
6	-4.190657	2.201536	0.240846
6	-4.503002	2.906791	-0.93336
1	-4.21049	3.067411	-3.062259
1	-4.616329	2.507641	1.190991
1	-5.171979	3.761322	-0.8779
6	3.671161	0.243141	0.014572
6	4.789634	1.066913	0.232859
6	3.785277	-0.887185	-0.81133
6	6.009503	0.755834	-0.3659
1	4.715014	1.951509	0.857257
6	5.01217	-1.193644	-1.404792
1	2.928657	-1.528904	-0.986036
6	6.122091	-0.375145	-1.182827
1	6.870592	1.394172	-0.195242
1	5.096862	-2.070889	-2.038215
1	7.074377	-0.615548	-1.645573
8	-2.914384	0.309522	1.200603
6	-3.434257	0.548942	2.510879
1	-2.963073	-0.182942	3.167222
1	-3.181273	1.559951	2.847242
1	-4.521028	0.414219	2.524941
1	-2.696168	1.120472	-3.194288

TSIVb-r

E = -4217.906595 ZPVE = 0.287640 NIMAG = 1.

17	-1.260267	2.735658	0.018469
15	-1.439285	0.751106	-1.041976
12	1.660843	-0.383555	-1.148235
35	3.696179	-1.581134	-0.529275
6	-2.692751	1.62185	-2.158577
1	-3.091935	0.861167	-2.837862
1	-3.511182	2.083183	-1.60364
1	-2.182172	2.389895	-2.745867
5	-0.270711	0.029289	-2.451348
1	0.67669	0.790963	-2.540482
1	0.048009	-1.088906	-2.056634
1	-0.828111	-0.057417	-3.508751
6	0.054864	0.236191	0.684505
6	-0.472515	-0.443085	1.797229
6	1.235636	0.959316	0.943899
6	0.101746	-0.36919	3.07198
6	1.839423	1.063581	2.19689
6	1.247181	0.401417	3.275608
1	-0.350702	-0.90587	3.901025
1	2.7542	1.626321	2.341836
1	1.695463	0.477134	4.261617
6	-2.637521	-0.454011	-0.336525
6	-3.73259	0.001295	0.41335
6	-2.50731	-1.826299	-0.598143
6	-4.683314	-0.902089	0.893698
1	-3.841705	1.058704	0.635001
6	-3.469355	-2.725999	-0.128668

1	-1.663115	-2.201373	-1.166009
6	-4.556588	-2.267725	0.620016
1	-5.522208	-0.537929	1.479269
1	-3.36121	-3.784696	-0.344973
1	-5.298967	-2.969103	0.988856
8	1.840983	1.485482	-0.217233
6	3.000461	2.335105	-0.105547
1	3.221351	2.665798	-1.119945
1	2.764778	3.19725	0.522404
1	3.848799	1.779776	0.302924
1	-1.37903	-1.02776	1.686692

PC_{IVb-r}

E = -4217.999720 ZPVE = 0.290182 NIMAG = 0.

17	1.173274	4.942222	-0.651989
15	-1.342394	0.088515	-0.857047
12	1.848509	-1.381032	-1.336296
35	3.549547	-2.341961	0.099612
6	-1.556134	1.675362	-1.738221
1	-2.148911	1.505061	-2.640459
1	-2.04143	2.418337	-1.103369
1	-0.570964	2.053206	-2.019152
5	-0.458771	-1.240937	-1.986688
1	0.417433	-0.660303	-2.608835
1	-0.035106	-2.115431	-1.240095
1	-1.24434	-1.720148	-2.751973
6	-0.439738	0.453772	0.701206
6	-1.128561	0.534427	1.922302

6	0.946414	0.691982	0.707786
6	-0.461063	0.854002	3.10469
6	1.624323	1.005243	1.883448
6	0.913967	1.090472	3.082049
1	-1.014931	0.919168	4.035179
1	2.692994	1.179684	1.870882
1	1.443203	1.338083	3.996462
6	-2.991527	-0.521289	-0.372516
6	-4.093911	0.3404	-0.257945
6	-3.157063	-1.894184	-0.120302
6	-5.344816	-0.166883	0.103553
1	-3.991747	1.403272	-0.448083
6	-4.408296	-2.39466	0.241934
1	-2.316265	-2.574844	-0.207435
6	-5.503476	-1.532304	0.353731
1	-6.191951	0.506619	0.187124
1	-4.5268	-3.456622	0.433188
1	-6.477109	-1.924211	0.631582
8	1.633436	0.567745	-0.507379
6	2.6769	1.570951	-0.778933
1	2.913697	1.460687	-1.837365
1	2.268146	2.566503	-0.585939
1	3.559841	1.360268	-0.174295
1	-2.197492	0.355184	1.94701

R1v + b S_N2@P-f pathways in THF

RC_vb-r

E = -4026.218110 ZPVE = 0.232766 NIMAG = 0.

17	-4.584569	-0.278476	-0.732745
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15	-2.871504	0.2056	0.32556
12	0.962169	-0.825315	-0.525139
35	1.707698	-3.173008	-0.35773
6	-2.436798	1.864566	-0.284654
1	-2.196953	1.809976	-1.348292
1	-3.25983	2.563534	-0.121108
1	-1.548263	2.202784	0.256814
6	-3.458378	0.404212	2.038075
1	-2.610919	0.736979	2.645989
1	-4.260089	1.143685	2.09109
1	-3.810203	-0.558237	2.415624
5	-1.543039	-1.181452	0.102291
1	-1.22268	-1.170011	-1.067665
1	-0.661005	-0.842051	0.871016
1	-2.03884	-2.220589	0.443616
6	1.393609	1.226938	-0.936962
6	1.912247	1.505575	0.336662
6	1.394504	2.306281	-1.830236
6	2.414241	2.738199	0.751941
6	1.884444	3.574878	-1.467829
1	1.011851	2.173133	-2.841871
6	2.39258	3.785265	-0.183956
1	2.811604	2.903003	1.748376
1	1.874835	4.391126	-2.186064
1	2.777829	4.760793	0.100025
8	1.852694	0.364916	1.163596
6	2.47611	0.368357	2.450722
1	2.005868	1.107693	3.107573
1	2.3335	-0.631642	2.8599
1	3.546323	0.581279	2.357653

TS_{vb-r}

E = -4026.164249 ZPVE = 0.234226 NIMAG = 1.

17	-2.22919	-1.250397	-1.703594
15	-2.224417	-0.573954	0.486419
12	0.76213	-1.025234	0.401712
35	2.982342	-1.376442	-0.545339
6	-2.614768	0.97412	1.445813
1	-1.713298	1.368865	1.912478
1	-3.034056	1.732988	0.780578
1	-3.359624	0.722845	2.206643
6	-3.977864	-1.23575	0.549173
1	-4.282104	-1.253599	1.600851
1	-4.662976	-0.593449	-0.011098
1	-4.018867	-2.245753	0.141589
5	-1.151736	-1.901935	1.46721
1	-0.562101	-2.573463	0.629862
1	-0.391507	-1.303514	2.200658
1	-1.881481	-2.625511	2.084927
6	-0.495221	0.866441	-0.352026
6	0.457626	1.530638	0.450473
6	-0.904167	1.577964	-1.492593
6	0.983658	2.790857	0.167707
6	-0.415072	2.852304	-1.803365
1	-1.641602	1.137149	-2.153671
6	0.521363	3.462019	-0.967879
1	1.739136	3.244437	0.79846
1	-0.77047	3.365488	-2.692016

1	0.907303	4.450464	-1.198028
8	0.918988	0.752986	1.525828
6	1.969582	1.242513	2.382156
1	1.651814	2.166828	2.869993
1	2.123992	0.466373	3.1308
1	2.88675	1.403324	1.809702

PC_v-r

E = -4026.298634 ZPVE = 0.236070 NIMAG = 0.

17	1.476656000	-1.657980000	-1.804634000
15	-2.279782000	0.156956000	1.079046000
12	0.960970000	-1.482979000	0.455996000
35	2.318903000	-2.406003000	2.316730000
6	-2.340097000	0.791593000	2.797297000
1	-1.329267000	0.855875000	3.204713000
1	-2.811516000	1.776735000	2.826859000
1	-2.917105000	0.089548000	3.406007000
6	-4.015149000	0.166491000	0.505186000
1	-4.554496000	-0.579691000	1.094311000
1	-4.485201000	1.141461000	0.651903000
1	-4.066985000	-0.120121000	-0.547679000
5	-1.517703000	-1.633452000	0.957701000
1	-1.136352000	-1.777159000	-0.187570000
1	-0.624884000	-1.708217000	1.777176000
1	-2.384898000	-2.422513000	1.230408000
6	-1.390945000	1.405716000	0.069661000
6	0.010191000	1.492458000	0.116541000
6	-2.070257000	2.267422000	-0.807965000

6	0.717497000	2.394018000	-0.674793000
6	-1.374869000	3.186026000	-1.595690000
1	-3.150657000	2.226038000	-0.883579000
6	0.018385000	3.249255000	-1.528127000
1	1.800785000	2.417084000	-0.636877000
1	-1.921313000	3.842323000	-2.264914000
1	0.566325000	3.950278000	-2.149377000
8	0.700364000	0.604824000	0.958357000
6	1.542406000	1.229361000	1.977812000
1	0.928485000	1.901468000	2.580638000
1	1.933316000	0.409013000	2.577380000
1	2.361839000	1.775100000	1.507826000

R1₁ + b S_{N2}@Cl pathway, followed by S_{N2}@C-f pathway in THF

RC₁

E = -4570.588985 ZPVE = 0.520893 NIMAG = 0.

6	-2.430889	-0.549444	-1.194511
6	-2.916212	-2.984389	-0.562052
6	-0.591217	-2.355995	-1.443035
6	-1.211355	-1.063735	-1.996268
6	-1.673118	-3.441684	-1.342498
6	-4.863615	-1.247645	-0.460524
6	0.595895	-2.811048	-2.301131
6	-5.565773	-0.149907	-1.280867
6	-5.834819	-2.428977	-0.279928
1	-2.846866	0.301019	-1.744275
1	-3.667297	-3.777046	-0.618566
1	-2.667989	-2.864671	0.49796

1	-0.216379	-2.155547	-0.429431
1	-0.453546	-0.281521	-2.089279
1	-1.577079	-1.258064	-3.015055
1	-1.256377	-4.34199	-0.873886
1	-1.973831	-3.730222	-2.361534
1	-4.658603	-0.850002	0.542642
1	1.380366	-2.046157	-2.335865
1	1.039837	-3.729887	-1.901858
1	0.279376	-3.012887	-3.33235
1	-5.821889	-0.525434	-2.27979
1	-6.496704	0.156907	-0.79237
1	-4.955818	0.748	-1.405815
1	-6.013121	-2.943312	-1.233022
1	-6.801056	-2.064112	0.08472
1	-5.469616	-3.165781	0.440156
6	-3.10624	1.630268	0.727532
6	-3.849279	1.708459	1.915671
6	-3.220011	2.654085	-0.228691
6	-4.709674	2.788328	2.134123
1	-3.757587	0.931827	2.666869
6	-4.073525	3.733433	-0.002371
1	-2.635454	2.622526	-1.143436
6	-4.822508	3.800289	1.178177
1	-5.283818	2.838587	3.054183
1	-4.151877	4.521999	-0.744476
1	-5.486898	4.641362	1.352204
17	-0.16805	1.189864	0.097063
6	-3.518929	-1.675777	-1.117211
1	-3.754383	-1.868298	-2.177343
15	-1.983083	0.206439	0.482569

5	-1.741996	-0.859023	2.096684
1	-1.382981	-0.048294	2.920434
1	-2.832628	-1.329453	2.333167
1	-0.909889	-1.692833	1.837579
6	3.5096	3.09059	0.374831
6	3.907013	4.043331	-0.581105
6	4.640034	3.644548	-1.700856
6	4.986807	2.295579	-1.881794
6	4.568229	1.397643	-0.901964
6	3.831125	1.734866	0.241179
1	2.935804	3.430108	1.236046
1	3.644169	5.090181	-0.451534
1	4.949014	4.376293	-2.442213
1	5.556678	1.98994	-2.753133
8	4.837162	0.011369	-0.936646
6	5.616326	-0.545219	-2.000455
1	5.699188	-1.612385	-1.795838
1	5.117297	-0.391099	-2.962684
1	6.613712	-0.094241	-2.021876
12	3.733536	-0.249463	0.990357
35	3.716068	-2.388505	2.182829

TS1r

E = -4570.538474 ZPVE = 0.520932 NIMAG = 1.

6	2.246512	-0.458082	1.131858
6	2.913036	-2.798616	0.3607
6	0.63996	-2.452306	1.489924
6	1.166702	-1.112285	2.025652

6	1.814488	-3.411581	1.244359
6	4.640141	-0.856519	0.14516
6	-0.405965	-3.061089	2.431992
6	5.286904	0.305553	0.921782
6	5.722108	-1.905888	-0.171009
1	2.625006	0.411933	1.676631
1	3.739706	-3.512214	0.294082
1	2.535115	-2.657275	-0.657964
1	0.155286	-2.271136	0.519791
1	0.337116	-0.415812	2.188784
1	1.622471	-1.288036	3.012195
1	1.44957	-4.341835	0.79019
1	2.248593	-3.689267	2.217681
1	4.275473	-0.466645	-0.814095
1	-1.227395	-2.361577	2.629176
1	-0.837344	-3.973404	2.005701
1	0.043407	-3.319881	3.399241
1	5.670266	-0.044194	1.889447
1	6.132291	0.718354	0.360125
1	4.592535	1.128003	1.110843
1	6.063945	-2.4106	0.742329
1	6.593206	-1.421116	-0.625785
1	5.372308	-2.671185	-0.86909
6	2.320678	1.954613	-0.588559
6	2.88515	2.363207	-1.810277
6	2.320801	2.863763	0.487525
6	3.451994	3.63424	-1.944361
1	2.884986	1.682349	-2.654879
6	2.889781	4.131331	0.353399
1	1.870818	2.586317	1.437097

6	3.459304	4.521244	-0.864086
1	3.891226	3.928169	-2.893583
1	2.882252	4.816245	1.196682
1	3.900494	5.508121	-0.969131
17	-0.848172	1.103361	-0.017397
6	3.431101	-1.455693	0.917645
1	3.797364	-1.663824	1.938965
15	1.51538	0.316019	-0.444156
5	1.445022	-0.641396	-2.160322
1	0.928821	0.168734	-2.909244
1	2.554957	-0.967359	-2.527241
1	0.718762	-1.595897	-1.977874
6	-2.889004	3.334442	0.663379
6	-4.076646	3.973739	1.055078
6	-5.269701	3.249767	1.090787
6	-5.293374	1.89525	0.731589
6	-4.094371	1.292394	0.34319
6	-2.89737	1.99381	0.300606
1	-1.956313	3.896083	0.648111
1	-4.065588	5.023608	1.334932
1	-6.193836	3.730327	1.397232
1	-6.229814	1.349261	0.76171
8	-4.025667	-0.062298	-0.055435
6	-5.208345	-0.891425	0.060475
1	-4.905474	-1.883287	-0.270252
1	-5.534103	-0.919272	1.102639
1	-5.999595	-0.503336	-0.584606
12	-2.234425	-0.688489	-0.857758
35	-2.479379	-3.050279	-1.390412

INT1

E = -4570.594581 ZPVE = 0.525857 NIMAG = 0.

6	2.325025	-0.177494	-0.780942
6	4.576651	0.250826	0.334256
6	3.146916	2.244367	-0.427543
6	2.376511	1.266864	-1.328722
6	4.562641	1.700552	-0.177436
6	3.881577	-2.205385	-0.206334
6	3.180732	3.655928	-1.026262
6	3.364616	-3.105569	-1.344121
6	5.315796	-2.637724	0.150852
1	1.84429	-0.789757	-1.551055
1	5.617771	-0.080432	0.398406
1	4.166912	0.210647	1.348434
1	2.626959	2.300388	0.539772
1	1.36424	1.640622	-1.517272
1	2.876338	1.232221	-2.309623
1	5.088822	2.349587	0.534953
1	5.127107	1.753741	-1.121937
1	3.258109	-2.378011	0.679376
1	2.169264	4.057016	-1.151758
1	3.735483	4.344739	-0.378256
1	3.672128	3.652626	-2.008086
1	3.97597	-2.97316	-2.246852
1	3.422795	-4.161416	-1.056609
1	2.324497	-2.898926	-1.607404
1	6.015634	-2.400373	-0.661575
1	5.352799	-3.72112	0.311834

1	5.682665	-2.158604	1.0626
6	0.331834	-2.002657	0.425663
6	0.33482	-2.974841	1.439297
6	-0.335531	-2.301831	-0.776457
6	-0.287166	-4.213817	1.248589
1	0.839482	-2.765895	2.37636
6	-0.956713	-3.537661	-0.970438
1	-0.372362	-1.564356	-1.575118
6	-0.934002	-4.501446	0.043809
1	-0.263519	-4.953696	2.044173
1	-1.461766	-3.745585	-1.909843
1	-1.417109	-5.462997	-0.104159
17	-3.047984	0.322595	1.92449
6	3.782301	-0.7011	-0.584919
1	4.241709	-0.614667	-1.58674
15	1.117424	-0.342975	0.698908
5	1.840466	-0.281672	2.547068
1	0.85039	-0.442146	3.245236
1	2.667807	-1.150489	2.739501
1	2.29979	0.833301	2.701227
6	-4.962101	-1.150022	0.664319
6	-5.639485	-1.630295	-0.458625
6	-5.225726	-1.242445	-1.73293
6	-4.138185	-0.380825	-1.89925
6	-3.457339	0.107694	-0.781539
6	-3.882976	-0.289947	0.492729
1	-5.265531	-1.436033	1.665219
1	-6.482921	-2.29994	-0.330466
1	-5.744149	-1.610535	-2.612036
1	-3.829397	-0.098179	-2.89748

8	-2.365666	0.955152	-0.87184
6	-2.11008	1.594709	-2.155356
1	-1.355458	2.353928	-1.956818
1	-1.743711	0.85676	-2.871511
1	-3.024869	2.071941	-2.510084
12	-0.844728	1.297702	0.625919
35	-0.709908	3.751336	0.484404

INT2_t

E = -4570.588302 ZPVE = 0.521492 NIMAG = 0.

17	3.733669	0.391084	2.435665
15	-1.350592	0.537688	0.287151
12	2.29841	-1.087503	-0.854363
35	3.462255	-3.092691	-1.626683
5	0.290439	-0.30573	-0.371264
1	0.742986	0.359228	-1.304335
1	1.108104	-0.273039	0.551497
1	0.18303	-1.469141	-0.752916
6	3.42203	1.768237	1.397086
6	3.467737	1.623946	0.006166
6	3.118369	3.008761	1.959734
6	3.215278	2.714227	-0.824047
6	2.869855	4.101381	1.12645
1	3.075789	3.110517	3.038382
6	2.918375	3.957366	-0.262988
1	3.249345	2.575477	-1.899923
1	2.633246	5.06374	1.568414
1	2.719195	4.805806	-0.909118

8	3.7576	0.378365	-0.564656
6	5.180133	0.159846	-0.836598
1	5.739521	0.245147	0.096567
1	5.256612	-0.848744	-1.239224
1	5.518445	0.898915	-1.564826
6	-3.673014	1.284163	-1.384764
6	-2.492752	0.275928	-1.240539
6	-4.861165	0.85464	-0.50131
6	-4.214815	-1.605844	-0.710169
6	-2.981155	-1.164287	-1.518388
6	-5.337534	-0.566018	-0.838272
6	-3.28683	2.779556	-1.214591
6	-4.683539	-3.003053	-1.136914
6	-2.086488	3.175224	-2.093062
6	-4.465609	3.722177	-1.524162
1	-4.009766	1.178626	-2.432742
1	-1.774954	0.512869	-2.034571
1	-5.699957	1.546577	-0.626277
1	-4.568754	0.907051	0.556612
1	-3.931092	-1.655982	0.347367
1	-2.160673	-1.874841	-1.361309
1	-3.240247	-1.228626	-2.588613
1	-6.178568	-0.845626	-0.189587
1	-5.723004	-0.577435	-1.870172
1	-2.996918	2.935511	-0.166691
1	-3.887951	-3.746777	-1.009428
1	-5.545944	-3.330078	-0.543817
1	-4.982416	-3.01163	-2.193395
1	-2.289357	2.966095	-3.152082
1	-1.880877	4.247772	-1.999877

1	-1.173679	2.642962	-1.811437
1	-4.841949	3.560237	-2.543161
1	-4.144764	4.767764	-1.453064
1	-5.303517	3.592688	-0.8336
6	-1.906042	-0.626225	1.63501
6	-2.752327	-0.122199	2.641094
6	-1.475814	-1.960064	1.754832
6	-3.176966	-0.921432	3.706282
1	-3.078239	0.913844	2.591631
6	-1.889817	-2.762831	2.823052
1	-0.813396	-2.381739	1.006134
6	-2.747984	-2.24951	3.800272
1	-3.833956	-0.50529	4.465478
1	-1.542013	-3.790635	2.889693
1	-3.070162	-2.872996	4.629585

TS2_t

E = -4570.525859 ZPVE = 0.522896 NIMAG = 1.

17	-0.488545	-1.982888	2.390261
15	0.547138	0.180418	0.300882
12	-3.091149	0.75557	0.085883
35	-5.204526	1.836558	-0.397931
5	-0.886206	1.48703	0.638016
1	-1.448851	1.591675	-0.454899
1	-1.617752	1.060195	1.516564
1	-0.497037	2.5897	0.911955
6	-0.477134	-1.981669	0.346435
6	-1.799427	-1.994708	-0.170588

6	0.379038	-2.995048	-0.166343
6	-2.180385	-2.812554	-1.2336
6	-0.013173	-3.831821	-1.202111
1	1.360285	-3.117864	0.277784
6	-1.288449	-3.733805	-1.780563
1	-3.20098	-2.737324	-1.600038
1	0.691906	-4.576229	-1.561704
1	-1.5864	-4.374645	-2.602947
8	-2.812994	-1.211649	0.445831
6	-3.734196	-1.9882	1.276271
1	-3.1527	-2.565816	1.993596
1	-4.37711	-1.276781	1.796697
1	-4.334654	-2.63844	0.63771
6	2.668426	0.274466	-1.895496
6	1.249401	0.714773	-1.417848
6	3.778579	1.074295	-1.178255
6	2.196641	3.073682	-0.928205
6	1.125458	2.244238	-1.652844
6	3.593601	2.591405	-1.346505
6	2.876531	-1.263116	-1.983994
6	2.007821	4.573388	-1.188869
6	2.087677	-1.840948	-3.17333
6	4.350934	-1.684908	-2.108442
1	2.699687	0.624069	-2.94181
1	0.508748	0.230493	-2.068918
1	4.751458	0.797464	-1.595465
1	3.8134	0.823397	-0.114284
1	2.086574	2.904567	0.151983
1	0.131177	2.607941	-1.390653
1	1.233405	2.406524	-2.736766

1	4.362949	3.124397	-0.772829
1	3.752214	2.857127	-2.403307
1	2.480875	-1.722189	-1.07029
1	1.025827	4.91535	-0.842284
1	2.771725	5.163704	-0.66967
1	2.083186	4.798447	-2.260542
1	2.481104	-1.441735	-4.117048
1	2.175584	-2.93149	-3.208465
1	1.021178	-1.604727	-3.124052
1	4.825478	-1.220939	-2.98244
1	4.418732	-2.771124	-2.235732
1	4.93895	-1.41853	-1.2254
6	1.790419	0.321251	1.652464
6	2.834859	-0.61422	1.772501
6	1.656297	1.299852	2.65302
6	3.72814	-0.560057	2.84295
1	2.956299	-1.395397	1.03024
6	2.550645	1.354803	3.725771
1	0.85244	2.025055	2.597343
6	3.590824	0.426973	3.824638
1	4.527342	-1.292423	2.912635
1	2.430557	2.123467	4.484058
1	4.284599	0.468144	4.659213

PC₁

E = -4570.620148 ZPVE = 0.526352 NIMAG = 0.

17	-1.915222	5.394766	-1.284623
15	0.570024	-0.547632	0.164743

12	-2.981391	-1.233491	-0.144478
35	-5.087881	-2.432339	-0.151423
5	-0.702354	-1.895141	-0.511748
1	-1.332447	-2.289926	0.460774
1	-1.374278	-1.324725	-1.354775
1	-0.161649	-2.824784	-1.026718
6	-0.2471	0.473179	1.478551
6	-1.535681	1.009347	1.279854
6	0.367774	0.752249	2.709933
6	-2.169455	1.793776	2.239446
6	-0.253473	1.539188	3.680934
1	1.351518	0.363377	2.925966
6	-1.520707	2.069327	3.443407
1	-3.162496	2.183797	2.047026
1	0.25997	1.737479	4.615773
1	-2.011651	2.684629	4.189958
8	-2.222275	0.692927	0.096064
6	-2.712874	1.831909	-0.699714
1	-1.940627	2.598422	-0.756414
1	-2.928488	1.428061	-1.688315
1	-3.619604	2.233794	-0.247254
6	3.521474	-0.75295	0.76103
6	2.102524	-1.387006	0.946468
6	4.042869	-0.959095	-0.675932
6	2.708094	-3.136112	-0.870045
6	2.169236	-2.884373	0.548208
6	4.069619	-2.448691	-1.053978
6	3.683969	0.6743	1.372465
6	2.777029	-4.63837	-1.171119
6	3.988722	0.569562	2.88038

6	4.766895	1.537774	0.703872
1	4.153142	-1.406819	1.383399
1	1.848037	-1.362578	2.011258
1	5.059477	-0.563017	-0.749087
1	3.441012	-0.397609	-1.39758
1	2.009515	-2.687521	-1.590021
1	1.196935	-3.367292	0.677787
1	2.846715	-3.362681	1.269502
1	4.403221	-2.562417	-2.092918
1	4.813991	-2.963689	-0.428134
1	2.740138	1.21833	1.253394
1	1.788294	-5.104691	-1.093954
1	3.155989	-4.819147	-2.183144
1	3.446156	-5.148556	-0.467122
1	5.006017	0.188523	3.031331
1	3.921054	1.547799	3.368004
1	3.313418	-0.114797	3.406395
1	5.755168	1.06848	0.775115
1	4.826817	2.508028	1.208731
1	4.553749	1.726221	-0.351922
6	0.96381	0.624635	-1.189573
6	1.192997	1.987761	-0.948724
6	1.000513	0.141748	-2.509351
6	1.469276	2.852256	-2.010539
1	1.140654	2.38941	0.057473
6	1.286588	1.007606	-3.565704
1	0.80574	-0.905049	-2.719448
6	1.522795	2.363507	-3.317986
1	1.627534	3.907188	-1.812812
1	1.314598	0.623632	-4.580787

1	1.733937	3.038481	-4.141565
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R1_{II} + b S_N2@Cl pathway, followed by S_N2@C-f pathway in THF

RC_{II}

E = -4262.101166 ZPVE = 0.402015 NIMAG = 0.

17	1.221442	-0.838992	-0.870202
15	2.907215	-0.432591	0.311312
12	-2.829924	1.17315	-0.246609
35	-1.139626	2.879741	0.215447
6	3.925585	-2.03439	0.170876
6	3.66854	1.075237	-0.56905
5	2.34107	-0.05938	2.139093
1	1.43431	0.733122	2.060506
1	2.02049	-1.120087	2.622869
1	3.334361	0.410685	2.656036
6	-4.284683	-0.216623	-0.928838
6	-4.474011	-0.793506	0.33478
6	-5.060362	-0.758638	-1.960507
6	-5.353477	-1.8353	0.620765
6	-5.965772	-1.811309	-1.731981
1	-4.970743	-0.365815	-2.972528
6	-6.106778	-2.345119	-0.449326
1	-5.466405	-2.250911	1.61672
1	-6.554418	-2.21388	-2.552502
1	-6.803437	-3.158973	-0.268277
8	-3.648009	-0.173099	1.298307
6	-3.652438	-0.623977	2.657234
1	-3.346598	-1.67353	2.712561
1	-2.932254	-0.00168	3.187529

1	-4.646442	-0.500156	3.098712
6	2.991011	-3.219398	0.507774
1	3.60427	-4.125237	0.5728
1	2.484905	-3.085324	1.466987
1	2.237153	-3.379331	-0.266331
6	4.541316	-2.259599	-1.220943
1	5.313836	-1.524611	-1.45887
1	5.016392	-3.247389	-1.233319
1	3.785395	-2.246268	-2.011514
6	5.036947	-1.969668	1.246399
1	4.622645	-1.854349	2.250794
1	5.592189	-2.914096	1.215461
1	5.751775	-1.163077	1.071808
6	2.798135	2.290967	-0.177856
1	2.796053	2.465145	0.900216
1	3.216052	3.178821	-0.666527
1	1.761601	2.184231	-0.507721
6	5.101736	1.287358	-0.03117
1	5.795845	0.517759	-0.377977
1	5.466035	2.249436	-0.409003
1	5.134747	1.328781	1.061281
6	3.696605	0.957481	-2.105001
1	4.317841	0.133521	-2.458687
1	2.694008	0.840823	-2.522514
1	4.118227	1.885991	-2.506931

TS1_{II}

E = -4262.043062 ZPVE = 0.402482 NIMAG = 1.

17	0.044857	-0.943974	0.101622
15	-2.329074	-0.05514	-0.371031
12	1.364616	1.063685	-0.189569
35	1.643723	3.475123	-0.189559
6	-3.326522	-1.64595	-0.75218
6	-2.995736	0.878208	1.165243
5	-2.238178	1.111901	-1.963151
1	-1.232867	1.790579	-1.840251
1	-2.145297	0.372117	-2.922027
1	-3.238235	1.803721	-2.015206
6	2.055515	-1.866068	0.299027
6	3.264251	-1.231117	0.051734
6	2.052228	-3.224995	0.585658
6	4.479146	-1.920266	0.085694
6	3.256345	-3.944929	0.640366
1	1.111182	-3.738462	0.774411
6	4.461735	-3.288637	0.387076
1	5.425364	-1.429234	-0.111636
1	3.248957	-5.00608	0.8732
1	5.400659	-3.832797	0.420017
8	3.193619	0.152356	-0.230155
6	4.42222	0.874621	-0.501658
1	4.88969	0.478313	-1.40554
1	4.129455	1.913092	-0.646878
1	5.095078	0.792718	0.354363
6	-2.468592	-2.487027	-1.72614
1	-3.048892	-3.363829	-2.040417
1	-2.199771	-1.922982	-2.62335
1	-1.549316	-2.84679	-1.256314
6	-3.605551	-2.493696	0.503064

1	-4.297866	-2.003793	1.192609
1	-4.065837	-3.443011	0.200083
1	-2.685779	-2.730192	1.047786
6	-4.654279	-1.297384	-1.460904
1	-4.479777	-0.712392	-2.367939
1	-5.160708	-2.228469	-1.749566
1	-5.336494	-0.736111	-0.81886
6	-2.343628	2.277006	1.144685
1	-2.594598	2.833695	0.238943
1	-2.702175	2.848575	2.010183
1	-1.253638	2.224676	1.221402
6	-4.526936	1.060956	1.107556
1	-5.064221	0.116269	1.222869
1	-4.838538	1.716421	1.931803
1	-4.843434	1.529808	0.170978
6	-2.596909	0.180176	2.481513
1	-3.040458	-0.812193	2.584616
1	-1.510817	0.076881	2.565403
1	-2.9416	0.786856	3.32918

INT1_{II}

E = -4262.093608 ZPVE = 0.402915 NIMAG = 0.

17	2.733442	-1.886581	-0.683184
15	-3.288751	-0.380167	-0.330708
12	-1.54368	1.411202	-0.556511
35	-0.104035	3.374397	-0.539623
6	-2.578257	-2.14381	-0.591733
6	-4.132939	-0.16592	1.378796

5	-4.602873	-0.006385	-1.776626
1	-4.788539	1.198335	-1.77729
1	-4.064461	-0.354092	-2.813164
1	-5.635216	-0.61908	-1.574933
6	4.300305	-1.34742	-0.08887
6	4.479896	0.006544	0.258149
6	5.337494	-2.267692	0.027653
6	5.73855	0.408997	0.729077
6	6.587704	-1.853362	0.49842
1	5.163409	-3.301787	-0.250018
6	6.780212	-0.516348	0.846616
1	5.908388	1.442109	1.005919
1	7.395373	-2.572288	0.588174
1	7.745196	-0.180518	1.213728
8	3.41242	0.833468	0.111411
6	3.571122	2.223118	0.424351
1	4.344632	2.679228	-0.202854
1	2.605377	2.679208	0.210071
1	3.822022	2.360576	1.48188
6	-1.5917	-2.042928	-1.776743
1	-1.258362	-3.050349	-2.056537
1	-2.055735	-1.589022	-2.657291
1	-0.695913	-1.46841	-1.514724
6	-1.81265	-2.680815	0.631094
1	-2.472323	-2.880297	1.479618
1	-1.330239	-3.630227	0.364783
1	-1.026166	-1.992972	0.959731
6	-3.696909	-3.134431	-0.97791
1	-4.226491	-2.807424	-1.876119
1	-3.252481	-4.117499	-1.181838

1	-4.431727	-3.262324	-0.179518
6	-4.867425	1.191785	1.321244
1	-5.64266	1.205547	0.552233
1	-5.339174	1.386058	2.292826
1	-4.175315	2.020376	1.124009
6	-5.164835	-1.276226	1.656473
1	-4.689642	-2.247473	1.820587
1	-5.727067	-1.030328	2.566785
1	-5.880479	-1.375058	0.835184
6	-3.111399	-0.098691	2.531436
1	-2.527898	-1.014915	2.638396
1	-2.415594	0.736654	2.395054
1	-3.640776	0.069413	3.478503

INT2_{II}

E = -4262.092932 ZPVE = 0.403416 NIMAG = 0.

17	2.252833	-2.890224	-1.404456
15	-2.678932	-0.696666	0.513039
12	0.836768	1.32465	-0.420436
35	1.950285	3.50231	-0.445081
6	-3.371777	-1.228096	-1.211092
6	-3.832578	0.613193	1.339924
5	-1.083244	0.34549	0.030113
1	-0.357808	0.448729	1.024153
1	-0.447127	-0.275668	-0.81795
1	-1.296897	1.478935	-0.407446
6	2.793971	-2.242634	0.131077
6	2.85409	-0.858982	0.333384

6	3.155999	-3.112555	1.161101
6	3.263639	-0.345671	1.563472
6	3.577166	-2.59565	2.388468
1	3.102138	-4.183244	0.998573
6	3.631784	-1.214499	2.592002
1	3.301518	0.730601	1.699512
1	3.857516	-3.27756	3.184626
1	3.95292	-0.811466	3.546647
8	2.472371	0.026222	-0.682288
6	3.55036	0.371457	-1.610875
1	3.928725	-0.542923	-2.069311
1	3.112908	1.023424	-2.364515
1	4.336912	0.898182	-1.067913
6	-5.013596	-0.111913	2.021071
1	-5.617077	0.610637	2.587957
1	-5.675312	-0.599851	1.30093
1	-4.657731	-0.875601	2.720933
6	-2.985164	1.271231	2.451669
1	-2.18319	1.890325	2.040066
1	-3.625369	1.916411	3.068241
1	-2.53153	0.522823	3.112259
6	-4.374815	1.717927	0.416026
1	-4.912621	2.469352	1.011847
1	-3.57021	2.231838	-0.118976
1	-5.08109	1.325585	-0.321513
6	-4.818833	-1.741413	-1.07862
1	-5.527126	-0.931645	-0.879891
1	-5.128346	-2.222027	-2.016882
1	-4.913539	-2.482556	-0.277109
6	-2.481881	-2.418982	-1.636933

1	-2.809888	-2.794612	-2.615836
1	-1.430073	-2.129272	-1.727045
1	-2.545134	-3.244244	-0.919543
6	-3.310241	-0.15787	-2.317847
1	-3.937652	0.707863	-2.094523
1	-2.288406	0.198849	-2.47626
1	-3.663377	-0.586221	-3.267058

TS2_{II}

E = -4262.037434 ZPVE = 0.402641 NIMAG = 1.

17	-1.586976	1.488446	2.325043
15	-1.389438	-0.662235	-0.235501
12	2.269204	-0.428962	-0.31994
35	4.626055	-0.959623	-0.530429
6	-1.696552	-2.044705	1.087784
6	-2.805144	-0.604155	-1.542309
5	0.223871	-1.213569	-1.22824
1	0.782729	-0.193499	-1.634574
1	0.926565	-1.853809	-0.448963
1	0.000951	-1.924068	-2.171046
6	-0.895969	1.640702	0.421557
6	0.50705	1.803513	0.32023
6	-1.666786	2.628069	-0.25179
6	1.095241	2.797823	-0.458862
6	-1.079184	3.624185	-1.02294
1	-2.742833	2.618257	-0.134782
6	0.313627	3.725218	-1.147093
1	2.181005	2.838271	-0.511206

1	-1.725355	4.344271	-1.518016
1	0.773723	4.503616	-1.745408
8	1.364042	0.875506	0.969755
6	1.949603	1.341559	2.224198
1	1.14684	1.683075	2.876613
1	2.462212	0.487466	2.665963
1	2.65783	2.147526	2.019289
6	-4.081131	0.056579	-0.979453
1	-4.83337	0.109083	-1.776908
1	-4.515351	-0.513454	-0.15613
1	-3.904492	1.073654	-0.628238
6	-2.275681	0.237534	-2.727469
1	-1.425705	-0.245242	-3.216851
1	-3.076878	0.336722	-3.471
1	-1.974314	1.242177	-2.424548
6	-3.175046	-2.002029	-2.080072
1	-3.836824	-1.875909	-2.947191
1	-2.298632	-2.566117	-2.410315
1	-3.71916	-2.597119	-1.342723
6	-3.082506	-1.906273	1.74653
1	-3.892241	-2.144247	1.051814
1	-3.152233	-2.616805	2.580045
1	-3.246319	-0.902676	2.147505
6	-0.610682	-1.89753	2.178065
1	-0.782951	-2.66519	2.942946
1	0.394385	-2.0628	1.77955
1	-0.64119	-0.92143	2.662525
6	-1.555858	-3.462628	0.487034
1	-2.340674	-3.700195	-0.231098
1	-0.589069	-3.609396	-0.001156

1	-1.628417	-4.191246	1.305675
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PCII

E = -4262.132219 ZPVE = 0.407612 NIMAG = 0.

17	0.025169	4.929815	1.152477
15	-1.390844	-0.858841	0.327844
12	2.211449	-1.064227	0.195877
35	4.609817	-1.273907	0.193914
6	-2.410912	0.121778	1.607273
6	-2.350422	-2.313708	-0.508006
5	0.149814	-1.698456	1.214301
1	0.714973	-2.339253	0.330153
1	0.841601	-0.856881	1.745279
1	-0.232854	-2.476644	2.036646
6	-0.92899	0.348823	-1.005491
6	0.318254	0.999096	-1.125068
6	-1.896532	0.676331	-1.977802
6	0.587627	1.88305	-2.171894
6	-1.646213	1.570738	-3.014606
1	-2.879613	0.231442	-1.922376
6	-0.392246	2.17214	-3.117383
1	1.561121	2.353615	-2.239044
1	-2.428857	1.794718	-3.731536
1	-0.174268	2.867345	-3.921281
8	1.328462	0.770788	-0.178691
6	2.033793	1.969722	0.318022
1	1.315155	2.783195	0.446114
1	2.460487	1.691944	1.281927

1	2.829906	2.239024	-0.376682
6	-3.84334	-2.038071	-0.787979
1	-4.258734	-2.925149	-1.279173
1	-4.414065	-1.88104	0.129575
1	-4.024295	-1.194611	-1.4553
6	-1.628132	-2.671089	-1.826587
1	-0.566417	-2.881562	-1.66746
1	-2.084105	-3.582717	-2.228417
1	-1.717935	-1.891998	-2.585659
6	-2.273291	-3.548792	0.423838
1	-2.851723	-4.353421	-0.043151
1	-1.251109	-3.904571	0.557112
1	-2.701665	-3.364255	1.411128
6	-3.53691	0.952517	0.961819
1	-4.276873	0.340871	0.442617
1	-4.0588	1.490667	1.760797
1	-3.14673	1.700572	0.267939
6	-1.43178	1.085551	2.314229
1	-2.000852	1.67178	3.044048
1	-0.64744	0.552493	2.85682
1	-0.969493	1.798066	1.625458
6	-2.999322	-0.852705	2.649502
1	-3.767492	-1.505552	2.228182
1	-2.229176	-1.471302	3.118131
1	-3.473191	-0.259862	3.43969

R1_{III} + b S_N2@Cl pathway, followed by S_N2@C-f pathway in THF

RC_{III}

E = -4409.700337 ZPVE = 0.339551 NIMAG = 0.

17	0.953387	1.246158	0.230963
15	2.524587	0.203001	-0.699487
12	-3.016537	-0.506832	-0.210379
35	-2.003938	-2.6863	-0.67905
5	2.077096	-0.165905	-2.54685
1	1.072642	-0.836036	-2.496926
1	1.937226	0.906164	-3.086562
1	3.04319	-0.790385	-2.935268
6	-3.669817	1.441686	0.324712
6	-5.033583	1.147587	0.189996
6	-3.371866	2.754286	0.709506
6	-6.075607	2.04633	0.407744
6	-4.381887	3.705616	0.943466
1	-2.334627	3.062489	0.83359
6	-5.723778	3.350239	0.793011
1	-7.119324	1.773389	0.291364
1	-4.120606	4.71801	1.240978
1	-6.507504	4.081027	0.972248
8	-5.222965	-0.196619	-0.199466
6	-6.543439	-0.710548	-0.403942
1	-7.053439	-0.153196	-1.196218
1	-6.422926	-1.751049	-0.704628
1	-7.123742	-0.656922	0.522806
6	2.720354	-1.273189	0.352814
6	1.671291	-2.210182	0.373512
6	3.898574	-1.530644	1.071331
6	1.795837	-3.377504	1.125715
1	0.755329	-2.036679	-0.182351
6	4.01971	-2.70998	1.811709
1	4.721604	-0.82531	1.054052

6	2.970235	-3.631242	1.842876
1	0.977364	-4.090438	1.143449
1	4.935257	-2.904941	2.361731
1	3.066478	-4.545128	2.421423
6	3.959741	1.288141	-0.423485
6	4.236942	1.858278	0.831262
6	4.803219	1.557729	-1.513372
6	5.35104	2.681344	0.991915
1	3.581578	1.671976	1.676193
6	5.921968	2.378162	-1.343081
1	4.588728	1.131648	-2.487359
6	6.195917	2.93974	-0.093936
1	5.558386	3.121842	1.962225
1	6.571225	2.58202	-2.188825
1	7.062156	3.581685	0.03478

TS1_{III}

E = -4409.649319 ZPVE = 0.338393 NIMAG = 1.

17	-0.220241	0.713336	-0.000092
15	1.900038	-0.447617	-0.691013
12	-2.059516	-0.790611	-0.365892
35	-2.6162	-3.042656	-1.044883
5	1.705771	-1.542363	-2.312676
1	0.973034	-2.454445	-1.996114
1	1.209725	-0.815132	-3.149206
1	2.820437	-1.925451	-2.611836
6	-2.030676	2.001092	0.57133
6	-3.381416	1.695768	0.476618

6	-1.659755	3.267652	1.003818
6	-4.377857	2.616555	0.807698
6	-2.634343	4.218429	1.348783
1	-0.605901	3.530706	1.076755
6	-3.986634	3.887726	1.249209
1	-5.432349	2.375124	0.733095
1	-2.336453	5.206336	1.689274
1	-4.750111	4.614021	1.510522
8	-3.683573	0.390308	0.023974
6	-5.067168	-0.012589	-0.117706
1	-5.566417	0.630292	-0.845904
1	-5.04325	-1.040371	-0.477255
1	-5.567433	0.0353	0.851972
6	2.475772	-1.395116	0.763451
6	1.719478	-2.517707	1.156708
6	3.633565	-1.075905	1.495153
6	2.113126	-3.297179	2.244856
1	0.829755	-2.79577	0.599379
6	4.024952	-1.859412	2.584433
1	4.243218	-0.226128	1.208769
6	3.26651	-2.969267	2.966235
1	1.520472	-4.16254	2.527051
1	4.92741	-1.601185	3.131211
1	3.573069	-3.57674	3.812565
6	2.998879	0.997341	-0.882858
6	3.126199	1.966586	0.130879
6	3.670572	1.199377	-2.101798
6	3.924172	3.095324	-0.062401
1	2.599393	1.842129	1.072491
6	4.466934	2.332233	-2.293213

1	3.573341	0.467678	-2.896871
6	4.597696	3.280728	-1.275107
1	4.015796	3.831707	0.730763
1	4.984334	2.471205	-3.238068
1	5.216349	4.160649	-1.425148

INT1_{III}

E = -4409.707456 ZPVE = 0.341933 NIMAG = 0.

17	-2.024041	1.928969	-0.900542
15	1.947819	-0.094852	-0.941919
12	-0.570342	-0.52818	-0.821251
35	-1.841991	-2.433972	-1.717465
5	2.733918	-0.519965	-2.708031
1	2.513332	-1.707522	-2.856437
1	2.134619	0.1517	-3.529738
1	3.924477	-0.271243	-2.674482
6	-3.263598	1.293003	0.17999
6	-2.927853	0.271282	1.077556
6	-4.542097	1.839945	0.152032
6	-3.894708	-0.188932	1.972566
6	-5.509435	1.364555	1.040523
1	-4.769736	2.633807	-0.55063
6	-5.183155	0.35104	1.941976
1	-3.661405	-0.977843	2.675953
1	-6.508668	1.785862	1.020709
1	-5.927001	-0.022515	2.637743
8	-1.630655	-0.222597	1.04102
6	-1.167953	-0.967517	2.202889

1	-1.662562	-1.939133	2.25598
1	-0.09683	-1.100867	2.063356
1	-1.357416	-0.380557	3.103186
6	2.800215	-1.12603	0.337561
6	2.308491	-2.411234	0.630119
6	3.984048	-0.70555	0.967091
6	2.976707	-3.248641	1.527708
1	1.394243	-2.76792	0.160536
6	4.650071	-1.541084	1.868606
1	4.389071	0.27943	0.756062
6	4.152717	-2.81761	2.148702
1	2.579003	-4.237659	1.737136
1	5.563961	-1.196033	2.34424
1	4.672387	-3.466821	2.847379
6	2.323624	1.646398	-0.453426
6	1.916868	2.159602	0.792132
6	2.990137	2.501169	-1.345705
6	2.180523	3.485499	1.140259
1	1.396429	1.518462	1.499686
6	3.245757	3.833717	-1.001623
1	3.314278	2.121173	-2.30876
6	2.844508	4.328947	0.24122
1	1.864198	3.862395	2.108888
1	3.763589	4.479931	-1.704973
1	3.045693	5.362061	0.50941

INT2m

E = -4409.700553 ZPVE = 0.341174 NIMAG = 0.

17	-2.204858	3.390353	-0.102532
15	1.850355	0.231469	0.254845
12	-1.596739	-1.024665	-1.115127
35	-3.167525	-2.819151	-1.677668
5	0.770392	-0.896548	-0.95781
1	0.069019	-1.597757	-0.213603
1	0.075943	-0.117711	-1.633264
1	1.367473	-1.61974	-1.716664
6	-2.669014	2.260621	1.153547
6	-2.992452	0.937362	0.830019
6	-2.703531	2.678837	2.484781
6	-3.327074	0.029741	1.834593
6	-3.055961	1.772168	3.487397
1	-2.448119	3.704147	2.728233
6	-3.368661	0.449208	3.165375
1	-3.560913	-0.994583	1.560111
1	-3.081275	2.104759	4.519928
1	-3.63706	-0.257583	3.943446
8	-2.943492	0.49744	-0.499525
6	-4.180137	0.747048	-1.247677
1	-4.426724	1.80651	-1.174696
1	-3.982856	0.476175	-2.283502
1	-4.976054	0.124174	-0.83631
6	2.93327	-1.024888	1.099144
6	2.951192	-1.069961	2.502676
6	3.725372	-1.949584	0.394158
6	3.732562	-2.01048	3.185891
1	2.351726	-0.359463	3.066396
6	4.512822	-2.883537	1.070866
1	3.72697	-1.936666	-0.691919

6	4.517496	-2.918123	2.471051
1	3.731169	-2.027172	4.272441
1	5.119561	-3.587533	0.507458
1	5.128662	-3.646116	2.997148
6	3.059274	1.07106	-0.876305
6	4.316978	1.485361	-0.394628
6	2.710927	1.434272	-2.190256
6	5.194724	2.217907	-1.196601
1	4.616534	1.228068	0.617889
6	3.585385	2.175327	-2.992906
1	1.751849	1.132223	-2.599425
6	4.832797	2.569894	-2.502146
1	6.161595	2.516807	-0.800151
1	3.290525	2.437806	-4.005719
1	5.513607	3.141729	-3.126152

TS2_{III}

E = -4409.651567 ZPVE = 0.339901 NIMAG = 1.

17	-0.619214	-0.870209	2.766671
15	-1.055183	-0.229149	-0.348575
12	2.612011	-0.586593	-0.631763
35	4.898217	-0.709254	-1.454158
5	0.421485	-0.574057	-1.59388
1	1.12758	0.431335	-1.520856
1	1.003899	-1.594595	-1.238261
1	0.058302	-0.707796	-2.730456
6	-0.23533	0.719027	1.635493
6	1.156118	0.980875	1.505528

6	-1.034869	1.843191	1.997673
6	1.690468	2.261724	1.600653
6	-0.491977	3.116209	2.113935
1	-2.094805	1.691388	2.171984
6	0.874684	3.354576	1.90191
1	2.759885	2.387902	1.45262
1	-1.152857	3.93819	2.376256
1	1.293138	4.351439	1.984365
8	2.042863	-0.102495	1.260101
6	2.807898	-0.535683	2.430263
1	2.111466	-0.781718	3.230672
1	3.371717	-1.419787	2.127177
1	3.489487	0.262701	2.730539
6	-2.016727	1.124971	-1.126395
6	-1.393307	2.379887	-1.267382
6	-3.324909	0.966356	-1.616178
6	-2.057565	3.440568	-1.886909
1	-0.384131	2.534882	-0.89922
6	-3.987702	2.030578	-2.233458
1	-3.827447	0.009375	-1.531979
6	-3.357738	3.270784	-2.371743
1	-1.556737	4.39893	-1.989637
1	-4.995055	1.884464	-2.61284
1	-3.873334	4.095442	-2.854997
6	-2.167321	-1.676064	-0.233038
6	-3.354017	-1.601203	0.521863
6	-1.81048	-2.90945	-0.80602
6	-4.169666	-2.721546	0.679212
1	-3.641907	-0.665909	0.992056
6	-2.624325	-4.033778	-0.638506

1	-0.900485	-2.995982	-1.390021
6	-3.805162	-3.944014	0.103178
1	-5.083131	-2.643077	1.261524
1	-2.334341	-4.97764	-1.091008
1	-4.437358	-4.817562	0.232099

PC_{III}

E = -4409.742565 ZPVE = 0.343607 NIMAG = 0.

17	-0.623713	4.932376	0.929409
15	1.05508	-0.724713	-0.277413
12	-2.445478	-1.299881	-0.428677
35	-4.794993	-1.837491	-0.606991
5	-0.216387	-2.024163	-1.017043
1	-0.804454	-2.546403	-0.079055
1	-0.936767	-1.389486	-1.768647
1	0.354627	-2.861347	-1.652703
6	0.463097	-0.010219	1.305142
6	-0.831346	0.526464	1.410544
6	1.264234	-0.025898	2.458177
6	-1.316379	1.04018	2.609076
6	0.791821	0.491702	3.665051
1	2.26593	-0.437043	2.410102
6	-0.495421	1.025752	3.738584
1	-2.317773	1.451472	2.661322
1	1.43136	0.480177	4.541206
1	-0.868688	1.43148	4.673043
8	-1.642534	0.50974	0.263777
6	-2.323081	1.78099	-0.064735

1	-1.680247	2.617248	0.221129
1	-2.478745	1.763717	-1.142712
1	-3.279184	1.823455	0.458694
6	2.666978	-1.50465	0.079623
6	2.715068	-2.865765	0.421477
6	3.853648	-0.754591	0.035628
6	3.939728	-3.467244	0.719621
1	1.806816	-3.459098	0.450739
6	5.074791	-1.362552	0.333579
1	3.830226	0.295673	-0.236667
6	5.1188	-2.71705	0.677393
1	3.971398	-4.520619	0.979864
1	5.988558	-0.777885	0.294437
1	6.070116	-3.187909	0.905723
6	1.3673	0.638337	-1.447498
6	1.422028	1.976709	-1.035638
6	1.572618	0.310913	-2.800025
6	1.682361	2.982378	-1.971125
1	1.252096	2.250448	0.000406
6	1.84224	1.319426	-3.725119
1	1.52531	-0.721985	-3.132306
6	1.896764	2.655631	-3.311684
1	1.707463	4.016634	-1.644211
1	2.001642	1.063178	-4.767982
1	2.098428	3.439175	-4.035765

R1_{IV} + b S_N2@Cl pathway, followed by S_N2@C-f pathway in THF

RC_{IV}

E = -4217.956479 ZPVE = 0.285149 NIMAG = 0.

17	1.066171	-1.037249	-0.62429
15	2.979409	-1.880296	-0.507748
12	-3.600965	0.059291	-0.245589
35	-5.28473	-1.635242	0.253358
6	3.421203	-2.062284	-2.269886
1	2.750895	-2.793963	-2.726397
1	3.352834	-1.114988	-2.807287
1	4.447916	-2.437313	-2.317705
5	2.977856	-3.535934	0.486295
1	2.627058	-3.292835	1.616435
1	2.224734	-4.258887	-0.124365
1	4.139766	-3.882449	0.402414
6	-2.282893	1.532767	-1.020161
6	-1.835058	1.944646	0.24201
6	-1.727381	2.215902	-2.10846
6	-0.902798	2.952548	0.476816
6	-0.78389	3.244968	-1.933784
1	-2.024493	1.955387	-3.123538
6	-0.375278	3.606608	-0.648353
1	-0.583331	3.235841	1.474304
1	-0.369654	3.759136	-2.797463
1	0.354147	4.399578	-0.508028
8	-2.4604	1.196105	1.264329
6	-2.150173	1.450848	2.639031
1	-2.410328	2.48029	2.905319
1	-2.752168	0.755395	3.223228
1	-1.087537	1.272021	2.830686
6	4.011756	-0.536522	0.156197
6	4.197869	0.670016	-0.540884
6	4.641356	-0.72809	1.396563

6	5.008888	1.668582	-0.002633
1	3.706141	0.840915	-1.493458
6	5.455847	0.275137	1.928793
1	4.499146	-1.655393	1.941065
6	5.640116	1.47121	1.231148
1	5.147726	2.599156	-0.544145
1	5.942776	0.120098	2.886544
1	6.271977	2.250468	1.64659

TS1iv

E = -4217.906520 ZPVE = 0.284970 NIMAG = 1.

17	-0.35492	-1.34894	0.586214
15	2.06183	-1.460126	1.229059
12	-0.725312	1.014497	0.343285
35	0.135764	3.277641	0.453525
6	2.32247	-3.279822	1.340437
1	1.779858	-3.643031	2.217114
1	1.948179	-3.802552	0.457018
1	3.386858	-3.502362	1.467982
5	2.475793	-0.497816	2.885856
1	2.071185	0.639053	2.747701
1	1.861097	-1.097711	3.744995
1	3.680578	-0.548171	3.044862
6	-2.56343	-1.338862	-0.018664
6	-3.329003	-0.233143	-0.360587
6	-3.145372	-2.599078	-0.080315
6	-4.663915	-0.345584	-0.757363
6	-4.485438	-2.751431	-0.472484

1	-2.561633	-3.480702	0.179864
6	-5.236294	-1.623823	-0.808587
1	-5.26157	0.519249	-1.023113
1	-4.934231	-3.740149	-0.515107
1	-6.27315	-1.725553	-1.114328
8	-2.673035	1.020211	-0.282729
6	-3.411892	2.22284	-0.611212
1	-4.263918	2.329038	0.063754
1	-2.714529	3.047126	-0.469605
1	-3.742472	2.180436	-1.651238
6	2.976413	-0.893968	-0.2426
6	3.108926	-1.686823	-1.399806
6	3.512241	0.409081	-0.254563
6	3.76269	-1.192564	-2.530079
1	2.702796	-2.693238	-1.424901
6	4.156255	0.903846	-1.391208
1	3.43167	1.032668	0.630131
6	4.285743	0.105493	-2.531718
1	3.861456	-1.8208	-3.410752
1	4.564203	1.910397	-1.380386
1	4.790744	0.489201	-3.413249

INT1_{iv}

E = -4217.961121 ZPVE = 0.286690 NIMAG = 0.

17	-2.275142	1.952948	-0.79121
15	2.040575	1.600535	-0.367928
12	-0.1086	0.240155	-0.727885
35	-0.447911	-1.99232	-1.714745

6	1.802973	2.849367	0.986668
1	1.138401	3.629106	0.603811
1	1.348706	2.42121	1.883816
1	2.760605	3.309854	1.249861
5	2.7844	2.544345	-1.934745
1	2.92997	1.734396	-2.831614
1	1.933617	3.371117	-2.220898
1	3.834539	3.062728	-1.597668
6	-3.32157	0.827441	0.080704
6	-2.73702	-0.111948	0.939553
6	-4.699499	0.909525	-0.080423
6	-3.563945	-0.990515	1.641713
6	-5.521164	0.027694	0.626249
1	-5.11936	1.652311	-0.749492
6	-4.950483	-0.916832	1.479774
1	-3.140027	-1.735946	2.302309
1	-6.59733	0.083222	0.503836
1	-5.581124	-1.608241	2.028677
8	-1.355448	-0.113075	1.036263
6	-0.75676	-0.875925	2.119758
1	-0.865527	-1.946161	1.934205
1	0.298196	-0.605408	2.133946
1	-1.222845	-0.590134	3.064022
6	3.265181	0.402192	0.323453
6	3.379653	0.142675	1.701263
6	4.078408	-0.331652	-0.559847
6	4.275582	-0.818384	2.180201
1	2.773784	0.692946	2.415079
6	4.968595	-1.297128	-0.082152
1	4.019301	-0.140728	-1.62714

6	5.072477	-1.544476	1.290315
1	4.350956	-0.996008	3.249559
1	5.586584	-1.850546	-0.78379
1	5.76744	-2.291834	1.661909

INT2_{IV}

E = -4217.954376 ZPVE = 0.287933 NIMAG = 0.

17	-1.896045	-2.346211	2.341613
15	2.745701	0.600398	1.682816
12	-0.98431	1.448459	0.040112
35	-2.422196	3.180154	-0.903678
6	3.392529	2.337038	1.920615
1	2.739668	2.83128	2.647074
1	4.404007	2.325527	2.338025
1	3.391288	2.927454	0.997585
5	1.010977	0.948912	0.839507
1	0.470169	-0.094441	0.494038
1	0.28868	1.487741	1.681881
1	1.094039	1.692471	-0.141015
6	-2.020878	-2.462402	0.598508
6	-2.256665	-1.31772	-0.172167
6	-1.874493	-3.702292	-0.026085
6	-2.33065	-1.408271	-1.561547
6	-1.958491	-3.792176	-1.417605
1	-1.689361	-4.584252	0.576997
6	-2.188053	-2.648478	-2.186647
1	-2.514947	-0.506569	-2.138131
1	-1.84381	-4.759455	-1.895814

1	-2.251308	-2.716313	-3.267603
8	-2.379051	-0.063026	0.432251
6	-3.734429	0.260138	0.883107
1	-4.053369	-0.489717	1.60764
1	-3.677962	1.243319	1.345777
1	-4.400582	0.288552	0.019125
6	3.757055	-0.022133	0.260397
6	3.392739	-1.243174	-0.343624
6	4.923886	0.612135	-0.202225
6	4.154002	-1.79926	-1.372928
1	2.502601	-1.766215	-0.00227
6	5.692435	0.053148	-1.230768
1	5.245557	1.551286	0.236116
6	5.311851	-1.152929	-1.823496
1	3.846046	-2.740189	-1.821561
1	6.589563	0.566381	-1.567516
1	5.908042	-1.586226	-2.621372

TS2iv

E = -4217.909026 ZPVE = 0.285768 NIMAG = 1.

17	0.85564	2.659682	-1.626942
15	1.175566	-0.478403	-1.071234
12	-2.330344	-0.66747	-0.117844
35	-4.604567	-1.450242	0.205772
6	1.506745	-0.500873	-2.890331
1	0.583132	-0.219843	-3.402094
1	2.276662	0.224823	-3.15942
1	1.809142	-1.499823	-3.221152

5	-0.276656	-1.74662	-0.709461
1	-0.640599	-1.570731	0.455259
1	-1.15667	-1.484318	-1.529005
1	0.040804	-2.89904	-0.832452
6	0.743187	1.605256	0.01425
6	-0.553317	1.543452	0.590204
6	1.800582	1.899649	0.922805
6	-0.774754	1.646934	1.959964
6	1.573098	2.016618	2.288614
1	2.80568	2.011398	0.530446
6	0.286003	1.891615	2.834721
1	-1.792481	1.545815	2.330171
1	2.419996	2.223242	2.937671
1	0.113968	1.987603	3.900888
8	-1.661586	1.246577	-0.250005
6	-2.482975	2.393033	-0.633395
1	-1.844684	3.135442	-1.110743
1	-3.228708	2.019551	-1.336449
1	-2.968397	2.804087	0.254335
6	2.695492	-1.102138	-0.280122
6	2.624509	-1.660158	1.010971
6	3.960628	-0.971769	-0.883518
6	3.777912	-2.095736	1.66644
1	1.663076	-1.769049	1.503673
6	5.113244	-1.410727	-0.22702
1	4.05459	-0.536777	-1.873298
6	5.026986	-1.975366	1.049344
1	3.698946	-2.531793	2.658241
1	6.07863	-1.310955	-0.715026
1	5.923447	-2.318317	1.557364

PC_{IV}

E = -4218.000551 ZPVE = 0.289885 NIMAG = 0.

17	-0.026543	4.862777	-1.38651
15	1.254142	-0.167078	-0.74572
12	-2.239139	-0.965349	-0.645766
35	-4.42063	-1.89545	-0.148993
6	1.524273	1.273379	-1.835858
1	0.601669	1.85299	-1.91136
1	2.29936	1.930752	-1.440132
1	1.812026	0.912118	-2.826624
5	-0.031751	-1.419783	-1.526596
1	-0.512549	-2.081429	-0.613091
1	-0.849174	-0.749219	-2.141674
1	0.526492	-2.154626	-2.290011
6	0.718843	0.470328	0.895219
6	-0.595792	0.919	1.102632
6	1.599741	0.500437	1.988637
6	-1.026112	1.385844	2.34143
6	1.18577	0.979517	3.232266
1	2.618596	0.151223	1.866589
6	-0.126514	1.421183	3.408356
1	-2.050451	1.714893	2.474312
1	1.887231	1.002486	4.059549
1	-0.458149	1.788852	4.373878
8	-1.498504	0.8544	0.026087
6	-2.184102	2.114772	-0.309198
1	-1.439906	2.907341	-0.422859

1	-2.686945	1.938722	-1.258593
1	-2.917484	2.350029	0.46252
6	2.866104	-0.978408	-0.477775
6	2.899782	-2.358861	-0.218003
6	4.069139	-0.254125	-0.5197
6	4.118713	-3.001167	0.007579
1	1.98066	-2.935119	-0.190965
6	5.286127	-0.902884	-0.297979
1	4.070727	0.811648	-0.72054
6	5.312528	-2.274762	-0.032572
1	4.134464	-4.067979	0.207425
1	6.210049	-0.334184	-0.333029
1	6.259969	-2.776408	0.139089

R1v + b S_N2@Cl pathway, followed by S_N2@C-f pathway in THF

RCv

E = -4026.215350 ZPVE = 0.231775 NIMAG = 0.

17	2.2861	0.520704	-0.298995
15	4.003952	-0.582915	0.136748
6	5.116532	-0.162173	-1.247765
1	4.70744	-0.564871	-2.17683
1	5.245891	0.918681	-1.336019
1	6.085244	-0.633161	-1.053388
6	4.678376	0.275225	1.599883
1	5.639426	-0.187836	1.844808
1	4.824629	1.339323	1.40243
1	3.997212	0.143208	2.443289
5	3.643211	-2.461203	0.372476
1	2.90085	-2.55857	1.322199

1	3.186935	-2.865149	-0.671999
1	4.763671	-2.880257	0.598314
6	-1.865667	1.860485	0.39273
6	-1.376681	2.405811	-1.860526
6	-1.733548	3.180752	0.817979
6	-1.231167	3.755392	-1.489854
1	-1.230464	2.139748	-2.906639
6	-1.408901	4.136557	-0.158353
1	-1.870864	3.47973	1.851919
1	-0.979516	4.503486	-2.237387
1	-1.298212	5.177389	0.133178
8	-2.184395	0.786627	1.250269
6	-2.413606	1.019339	2.643652
1	-3.262292	1.696491	2.784851
1	-2.639658	0.048448	3.083906
1	-1.519034	1.438974	3.115038
6	-1.701423	1.415289	-0.926075
12	-2.092967	-0.627248	-0.485042
35	-2.613801	-3.002399	-0.281144

TS1v

E = -4026.157697 ZPVE = 0.230532 NIMAG = 1.

17	-0.427505	-1.320374	0.022991
15	-2.957465	-1.516805	-0.073412
12	-0.013162	1.049027	0.010516
35	-0.829298	3.329517	0.080086
6	-3.107056	-3.106708	-0.997948
1	-2.820012	-2.945563	-2.040708

1	-2.458808	-3.875739	-0.567228
1	-4.144573	-3.458594	-0.973659
6	-3.44412	-1.97022	1.649324
1	-4.480545	-2.326676	1.665324
1	-2.791501	-2.75253	2.047923
1	-3.372485	-1.087779	2.291088
5	-4.123523	-0.131354	-0.830804
1	-4.034319	0.847409	-0.115371
1	-3.730217	0.083153	-1.96248
1	-5.244482	-0.615725	-0.815102
6	1.804276	-1.383712	0.059909
6	2.654734	-0.29121	-0.035569
6	2.3512	-2.658931	0.121701
6	4.043969	-0.435914	-0.069528
6	3.743136	-2.84083	0.095683
1	1.697897	-3.527135	0.190376
6	4.580701	-1.728377	0.000219
1	4.709948	0.41609	-0.145896
1	4.16515	-3.840725	0.146927
1	5.658862	-1.853545	-0.024104
8	2.030782	0.977119	-0.099954
6	2.858025	2.163568	-0.203656
1	3.438635	2.128812	-1.127868
1	2.167639	3.005504	-0.221918
1	3.513909	2.233884	0.666671

INT1v

E = -4026.208317 ZPVE = 0.231856 NIMAG = 0.

17	-1.805613	-2.055109	0.006926
15	3.898654	-1.489017	-0.005412
12	2.673838	0.710532	-0.000432
35	1.668756	2.927353	0.000008
6	3.454166	-2.472941	1.505801
1	3.789317	-1.940488	2.400372
1	2.375941	-2.642181	1.577491
1	3.965001	-3.441233	1.47137
6	3.254309	-2.561445	-1.3787
1	3.768469	-3.528363	-1.357083
1	2.177082	-2.729635	-1.289814
1	3.459721	-2.085774	-2.341929
5	5.858772	-1.385389	-0.141231
1	6.112039	-0.805702	-1.184681
1	6.246504	-0.751725	0.826861
1	6.279958	-2.530993	-0.138222
6	-3.36533	-1.237571	0.001019
6	-3.408731	0.170916	0.00176
6	-4.530879	-1.997563	-0.004482
6	-4.665078	0.795091	-0.002486
6	-5.777039	-1.36252	-0.009032
1	-4.459204	-3.079941	-0.005169
6	-5.836105	0.031131	-0.007807
1	-4.733433	1.875886	-0.001642
1	-6.684867	-1.956667	-0.013339
1	-6.796351	0.537677	-0.011084
8	-2.221671	0.831191	0.006405
6	-2.233706	2.264716	0.00601
1	-2.73192	2.651789	0.90151
1	-1.186107	2.562823	0.007283

1	-2.72919	2.651426	-0.891151
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INT2v

E = -4026.206620 ZPVE = 0.233416 NIMAG = 0.

17	1.881235	-1.892014	-2.044413
15	-2.967218	-2.35045	0.0734
12	-0.727462	1.147316	-0.056631
35	-0.693813	3.58479	0.154173
6	-4.337473	-1.980954	-1.149631
1	-3.906443	-1.876059	-2.150709
1	-5.052223	-2.810526	-1.175415
1	-4.877384	-1.058398	-0.903952
6	-3.933357	-2.247399	1.675226
1	-4.500322	-1.312291	1.758352
1	-4.629802	-3.089632	1.748385
1	-3.239569	-2.310404	2.520051
5	-2.004627	-0.64514	0.083173
1	-1.085429	-0.681433	0.906189
1	-1.503239	-0.481188	-1.034602
1	-2.712735	0.329375	0.338531
6	2.308155	-1.512579	-0.388484
6	1.954351	-0.278785	0.170063
6	3.00382	-2.448246	0.379232
6	2.279689	0.013051	1.493599
6	3.335402	-2.150711	1.703069
1	3.270539	-3.403916	-0.058189
6	2.980683	-0.919504	2.260064
1	1.996454	0.976681	1.905543

1	3.87471	-2.883823	2.2939
1	3.236555	-0.686999	3.288433
8	1.240149	0.665396	-0.576435
6	2.075037	1.544117	-1.397787
1	2.655689	0.934431	-2.090637
1	1.392993	2.196931	-1.938574
1	2.724588	2.131368	-0.746234

TS2_v

E = -4026.163596 ZPVE = 0.232273 NIMAG = 1.

17	2.416223	-0.480757	2.054586
15	1.825486	1.562614	-0.3388
12	-1.722274	0.805822	-0.02342
35	-4.077972	0.2046	-0.195934
6	2.60521	2.868756	0.719017
1	2.036693	2.968007	1.647225
1	3.632451	2.589174	0.968359
1	2.610701	3.834474	0.200645
6	2.845241	1.581695	-1.87662
1	2.824601	2.575468	-2.335219
1	3.881885	1.311413	-1.653951
1	2.444781	0.856101	-2.589422
5	0.040608	2.192218	-0.840033
1	-0.48458	1.294933	-1.507664
1	-0.560546	2.414086	0.21543
1	0.042083	3.197911	-1.502547
6	1.822917	-0.744815	0.240042
6	0.481493	-1.202306	0.104271

6	2.784243	-1.43275	-0.559822
6	0.100423	-2.122443	-0.866166
6	2.399825	-2.3728	-1.50845
1	3.833186	-1.184675	-0.436557
6	1.05477	-2.731513	-1.68602
1	-0.952982	-2.375864	-0.954569
1	3.171908	-2.847045	-2.108946
1	0.759874	-3.466306	-2.426736
8	-0.525588	-0.58518	0.892815
6	-0.949845	-1.344956	2.066502
1	-0.070447	-1.596792	2.657938
1	-1.617539	-0.695441	2.634395
1	-1.477817	-2.24548	1.745505

PCv

E = -4026.259080 ZPVE = 0.236797 NIMAG = 0.

17	3.228735	3.45361	0.434881
15	1.571904	-0.912293	-1.42907
12	-1.708274	0.423464	-1.033282
35	-3.958345	0.257038	-0.14573
6	2.982231	0.242513	-1.520069
1	2.759401	1.184386	-1.008119
1	3.858364	-0.213861	-1.052473
1	3.195444	0.443801	-2.57391
6	2.173566	-2.501513	-2.105681
1	2.364656	-2.347601	-3.170679
1	3.100239	-2.822766	-1.626321
1	1.408917	-3.274081	-1.994932

5	0.032766	-0.354947	-2.487869
1	-0.900685	-1.068871	-2.128912
1	-0.163126	0.838956	-2.318392
1	0.254867	-0.567374	-3.646487
6	1.190058	-1.209955	0.342794
6	0.337653	-0.367406	1.079243
6	1.749217	-2.314292	1.009764
6	0.044871	-0.615485	2.418792
6	1.477366	-2.562787	2.354797
1	2.411691	-2.98839	0.479744
6	0.620918	-1.714117	3.057509
1	-0.633647	0.035428	2.957744
1	1.928324	-3.418692	2.84569
1	0.393841	-1.904016	4.101466
8	-0.268137	0.717542	0.42557
6	-0.106925	2.038127	1.057239
1	0.957927	2.27132	1.123586
1	-0.598778	2.745909	0.392253
1	-0.595582	2.044847	2.031192

S.11.3 Alternative gas-phase reactions in manuscript

R1_I + a S_N2@P-b pathways 2 and 3

RC_{Ia-i} 2

E = -4276.931533 ZPVE = 0.431862 NIMAG = 0.

6	-0.08348	-1.897886	-0.027026
6	1.600606	-1.264968	1.786515
6	2.453812	-2.035271	-0.503692
6	1.060596	-2.630015	-0.760338

6	2.720631	-1.97033	1.007312
6	-0.936313	-1.237641	2.367475
6	3.535934	-2.837261	-1.235866
6	-2.241226	-2.046465	2.255149
6	-0.553572	-1.104075	3.853149
1	-1.007149	-2.458088	-0.201072
1	1.821485	-1.326695	2.855505
1	1.621386	-0.193453	1.537944
1	2.475017	-1.009332	-0.893585
1	0.857613	-2.675702	-1.83437
1	1.045633	-3.669948	-0.39977
1	3.670343	-1.455558	1.193522
1	2.833786	-2.994735	1.394778
1	-1.138198	-0.218719	1.999555
1	3.3693	-2.83271	-2.318855
1	4.529171	-2.414346	-1.050233
1	3.548051	-3.882466	-0.90036
1	-2.092229	-3.067066	2.629899
1	-3.030631	-1.584792	2.857281
1	-2.615853	-2.113323	1.230771
1	-0.235823	-2.070126	4.26587
1	-1.417381	-0.765295	4.434384
1	0.252053	-0.383963	4.01775
6	-2.28403	-0.109375	-0.834585
6	-2.977594	0.938702	-0.211216
6	-3.004461	-1.072895	-1.561799
6	-4.372318	1.006748	-0.289457
1	-2.435681	1.698638	0.343188
6	-4.393457	-0.996053	-1.647193
1	-2.481356	-1.873873	-2.076146

6	-5.080641	0.041799	-1.006255
1	-4.898057	1.819439	0.202628
1	-4.94048	-1.742951	-2.215029
1	-6.1631	0.098539	-1.073092
17	0.088299	-0.240118	-2.721258
6	0.203963	-1.859369	1.510596
1	0.256783	-2.921917	1.801757
6	-0.536251	3.305952	1.57512
1	0.083785	3.701889	2.394302
1	-1.313264	2.709937	2.07828
6	-1.191979	4.490135	0.830195
1	-1.851868	4.15822	0.017076
1	-1.80225	5.124434	1.490698
1	-0.44144	5.14632	0.372243
15	-0.450864	-0.149917	-0.690503
12	0.742979	2.081359	0.413391
35	2.980719	1.892049	-0.43272

TS_{1a-i} 2

E = -4276.881227 ZPVE = 0.431846 NIMAG = 1.

6	-0.59349	1.581314	0.860281
6	0.438631	2.800437	-1.176039
6	1.941923	2.137961	0.786118
6	0.679146	2.001695	1.650677
6	1.695485	3.130358	-0.356804
6	-2.141698	2.495403	-1.089415
6	3.166641	2.512807	1.628184
6	-3.366191	2.503915	-0.155053

6	-2.302158	3.628693	-2.12209
1	-1.437106	1.65819	1.548474
1	0.266629	3.620587	-1.878434
1	0.612904	1.909876	-1.785271
1	2.169834	1.157495	0.318872
1	0.848969	1.320104	2.487655
1	0.469741	2.982774	2.100917
1	2.571334	3.173976	-1.016151
1	1.587198	4.133122	0.083082
1	-2.129175	1.555065	-1.655008
1	3.350457	1.77631	2.417503
1	4.067461	2.576203	1.008859
1	3.016991	3.487493	2.108199
1	-3.412094	3.448131	0.402147
1	-4.293023	2.419925	-0.732915
1	-3.362704	1.689868	0.573786
1	-2.20018	4.612764	-1.646887
1	-3.29797	3.585284	-2.575865
1	-1.572854	3.567926	-2.93396
6	-1.923607	-1.364793	0.281746
6	-1.937738	-2.660843	0.829393
6	-2.962859	-0.991153	-0.578328
6	-2.956589	-3.558958	0.510659
1	-1.166649	-2.960646	1.531501
6	-3.992763	-1.886127	-0.883267
1	-2.982991	-0.007029	-1.022826
6	-3.990994	-3.174276	-0.346501
1	-2.94597	-4.55467	0.943928
1	-4.793097	-1.570776	-1.546496
1	-4.789375	-3.869484	-0.588497

17	-0.972603	-0.513288	3.047077
6	-0.813809	2.60976	-0.294931
1	-0.917052	3.551604	0.273826
6	0.172502	-0.581597	-1.720589
1	1.054234	-0.071088	-2.149326
1	-0.688479	-0.020872	-2.074013
6	0.116058	-2.044115	-2.202331
1	-0.851432	-2.49815	-1.977318
1	0.291891	-2.127415	-3.282763
1	0.879238	-2.706133	-1.748955
15	-0.447016	-0.342752	0.723956
12	1.653428	-1.105786	-0.159967
35	3.876591	-1.701334	-0.618696

PC_{1a-i} 2

E = -4277.012524 ZPVE = 0.434948 NIMAG = 0.

6	0.621249	1.103251	-0.947177
6	0.636805	3.308998	0.354862
6	-1.553841	2.488213	-0.697641
6	-0.709694	1.566099	-1.591391
6	-0.706623	3.700414	-0.283538
6	2.884955	2.035444	0.003181
6	-2.856444	2.900173	-1.393342
6	3.743031	1.315155	-1.053005
6	3.631265	3.297871	0.474343
1	1.176258	0.559324	-1.721102
1	1.211152	4.222206	0.534653
1	0.463832	2.860002	1.340312

1	-1.83474	1.935001	0.210212
1	-1.301513	0.699968	-1.922184
1	-0.459852	2.107928	-2.515541
1	-1.274597	4.332972	0.41003
1	-0.51248	4.315832	-1.175243
1	2.790176	1.371086	0.872271
1	-3.478666	2.026115	-1.612783
1	-3.444562	3.570654	-0.75737
1	-2.653135	3.423368	-2.336272
1	3.868875	1.947479	-1.941178
1	4.740911	1.101812	-0.655793
1	3.315793	0.36206	-1.37305
1	3.67806	4.050065	-0.323577
1	4.661358	3.045492	0.747713
1	3.166705	3.762723	1.348158
6	1.749824	-1.428436	0.220954
6	1.84649	-2.331264	-0.853079
6	2.749048	-1.443928	1.207496
6	2.933125	-3.203392	-0.952271
1	1.062007	-2.374888	-1.603979
6	3.828248	-2.32504	1.112645
1	2.69865	-0.769863	2.056442
6	3.926839	-3.202377	0.029267
1	2.990036	-3.892979	-1.789088
1	4.591401	-2.323944	1.88562
1	4.76691	-3.88682	-0.043
17	-1.718573	-2.943947	-2.118501
6	1.461512	2.351495	-0.533507
1	1.618651	2.887754	-1.485944
6	0.140327	0.253949	2.039794

1	-0.641761	1.018194	2.048065
1	1.067864	0.734713	2.365832
6	-0.26467	-0.888613	2.985805
1	0.450444	-1.716305	2.968386
1	-0.318647	-0.515535	4.013954
1	-1.254945	-1.272535	2.725045
15	0.278157	-0.319389	0.274788
12	-1.953952	-1.467182	-0.445598
35	-3.629202	-0.517881	0.977969

RC_{Ia-i} 3

E = -4276.931474 ZPVE = 0.431791 NIMAG = 0.

6	0.349374	1.877291	0.180989
6	-1.453396	1.230007	1.872776
6	-2.138785	2.362439	-0.322229
6	-0.68041	2.820412	-0.476
6	-2.461226	2.147179	1.163587
6	1.043967	0.8268	2.482531
6	-3.098838	3.365441	-0.972302
6	2.431445	1.492665	2.513942
6	0.595065	0.529406	3.925119
1	1.335167	2.344568	0.096076
1	-1.69978	1.195701	2.937581
1	-1.587517	0.204625	1.500144
1	-2.260922	1.40004	-0.83575
1	-0.437837	2.974725	-1.531551
1	-0.561415	3.79922	0.013371
1	-3.466913	1.723259	1.265575

1	-2.474771	3.12424	1.671186
1	1.148749	-0.147194	1.977187
1	-2.896486	3.471807	-2.043973
1	-4.138872	3.040384	-0.860514
1	-3.005959	4.357278	-0.510982
1	2.379719	2.45813	3.032958
1	3.146644	0.864167	3.054684
1	2.844889	1.666482	1.517386
1	0.370832	1.45702	4.466982
1	1.394608	0.015128	4.468534
1	-0.291083	-0.109205	3.96649
6	2.367634	-0.030846	-0.802594
6	3.213404	0.938807	-1.369077
6	2.922176	-1.22455	-0.316993
6	4.588759	0.722269	-1.432074
1	2.7984	1.856115	-1.776681
6	4.303823	-1.43422	-0.372073
1	2.283301	-1.993236	0.106226
6	5.137263	-0.463075	-0.92779
1	5.233087	1.475726	-1.875568
1	4.721034	-2.360133	0.012164
1	6.20939	-0.628926	-0.977077
17	0.088998	0.600832	-2.707775
6	0.01017	1.683894	1.696242
1	0.074726	2.700966	2.118163
6	0.266004	-3.673145	0.649764
1	0.950938	-3.331473	1.442097
1	0.921811	-3.991912	-0.176681
6	-0.529766	-4.893429	1.160929
1	-1.205038	-5.290956	0.393331

1	0.120971	-5.724047	1.473207
1	-1.155593	-4.638722	2.025395
15	0.545765	0.195281	-0.692722
12	-0.918643	-2.057898	-0.039349
35	-3.160794	-1.429326	-0.628092

TS_{1a-i} 3

E = -4276.876899 ZPVE = 0.432104 NIMAG = 1.

6	-0.905433	1.321628	0.946343
6	-0.480261	2.980532	-0.989484
6	1.396084	2.483464	0.698626
6	0.320736	1.955707	1.659357
6	0.779038	3.498065	-0.274637
6	-2.869216	2.008149	-0.688952
6	2.596981	3.06384	1.454461
6	-3.913035	1.551477	0.346984
6	-3.455556	3.179474	-1.501453
1	-1.64238	1.100082	1.71905
1	-0.929188	3.818884	-1.529724
1	-0.208068	2.244194	-1.749874
1	1.7832	1.634702	0.094777
1	0.742733	1.251693	2.381141
1	-0.050859	2.805324	2.250278
1	1.523819	3.820492	-1.0136
1	0.51636	4.394961	0.305735
1	-2.691931	1.18892	-1.398332
1	3.046496	2.320682	2.121109
1	3.372272	3.411233	0.763137

1	2.284805	3.918195	2.066886
1	-4.114798	2.356425	1.06496
1	-4.860707	1.306404	-0.144665
1	-3.603841	0.670706	0.914465
1	-3.558598	4.077224	-0.878506
1	-4.45345	2.91973	-1.870352
1	-2.84621	3.439987	-2.370961
6	-1.540906	-1.796872	0.098432
6	-1.193416	-3.091405	0.525833
6	-2.700623	-1.631669	-0.667954
6	-1.983808	-4.188866	0.184042
1	-0.326743	-3.23628	1.162204
6	-3.501347	-2.7307	-0.993759
1	-2.993562	-0.653381	-1.02192
6	-3.14328	-4.012909	-0.576175
1	-1.698699	-5.179159	0.526601
1	-4.403396	-2.577599	-1.579342
1	-3.764408	-4.865762	-0.833359
17	-0.61881	-0.997957	2.917712
6	-1.519042	2.379441	-0.020772
1	-1.773973	3.193629	0.681304
6	0.05546	-0.361541	-1.83791
1	-0.852983	0.187406	-2.075162
1	-0.129653	-1.403205	-2.12838
6	1.231673	0.21032	-2.682043
1	2.130821	-0.428129	-2.699229
1	0.946696	0.306384	-3.738038
1	1.555186	1.210345	-2.365436
15	-0.32396	-0.472795	0.533354
12	1.85344	-0.705243	-0.410146

35 4.145561 -1.189222 -0.440573

PC_{1a-i} 3

E = -4277.007867 ZPVE = 0.435362 NIMAG = 0.

6	1.111657	-0.879254	0.856546
6	1.881445	-2.895474	-0.507726
6	-0.366097	-2.988517	0.753089
6	0.137343	-1.817359	1.607216
6	0.83678	-3.7741	0.204559
6	3.480168	-0.844208	-0.274956
6	-1.324657	-3.893161	1.537792
6	4.078939	0.136244	0.750358
6	4.611739	-1.712495	-0.855948
1	1.46527	-0.141715	1.585719
1	2.745211	-3.521526	-0.749407
1	1.484774	-2.545499	-1.467449
1	-0.927255	-2.575539	-0.099293
1	-0.699031	-1.245678	2.027821
1	0.676865	-2.223927	2.475377
1	0.492171	-4.562299	-0.476928
1	1.322906	-4.28819	1.047458
1	3.067141	-0.25164	-1.101973
1	-2.197642	-3.337084	1.896952
1	-1.686227	-4.718191	0.914016
1	-0.824183	-4.328814	2.411342
1	4.51345	-0.410507	1.596903
1	4.879482	0.727112	0.293025
1	3.344406	0.842569	1.144139

1	5.014232	-2.395819	-0.097174
1	5.436811	-1.077528	-1.195865
1	4.287922	-2.312465	-1.710939
6	1.020757	1.890546	-0.221047
6	0.859445	2.646111	0.9553
6	1.807203	2.418234	-1.257724
6	1.4902	3.883788	1.096919
1	0.230781	2.278674	1.762513
6	2.42983	3.660938	-1.115944
1	1.952593	1.86665	-2.180173
6	2.276281	4.395958	0.061753
1	1.352742	4.450722	2.012888
1	3.03498	4.052113	-1.928745
1	2.760213	5.362176	0.16912
17	-2.192654	1.256388	2.734452
6	2.338229	-1.694979	0.349095
1	2.764637	-2.127693	1.271036
6	0.255295	-0.178636	-2.137507
1	1.287918	-0.431867	-2.394824
1	0.023822	0.765794	-2.643085
6	-0.719095	-1.248748	-2.650481
1	-1.755718	-0.977433	-2.436942
1	-0.612088	-1.337513	-3.736971
1	-0.52611	-2.235186	-2.222736
15	0.140642	0.267129	-0.325464
12	-2.291312	0.632512	0.572691
35	-3.928046	0.31758	-1.129988

R1_{II} + a S_N2@P-b pathways 2 and 3

RC_{IIa-i} 2

E = -3968.438569 ZPVE = 0.313020 NIMAG = 0.

15	-0.896603	-0.082657	-0.170367
17	-1.180826	-0.273649	-2.24684
6	-2.290087	1.145857	0.280769
6	-2.319345	1.271156	1.819485
1	-2.984848	2.098999	2.091232
1	-2.704804	0.369787	2.303666
1	-1.333048	1.500209	2.238033
6	-3.688937	0.794629	-0.256387
1	-4.362283	1.633605	-0.04235
1	-3.682379	0.645419	-1.339262
1	-4.112898	-0.093585	0.212707
6	-1.851431	2.499784	-0.324847
1	-2.58721	3.263807	-0.046907
1	-0.877212	2.824636	0.049914
1	-1.810389	2.461522	-1.417163
6	1.979292	3.944406	-0.288223
1	1.11751	3.96003	-0.968879
1	2.862315	3.738795	-0.90611
1	2.094475	4.96962	0.094507
6	1.816492	2.901498	0.839502
1	2.694577	2.95635	1.501713
1	0.96624	3.186304	1.47884
12	1.668329	0.872422	0.255686
35	3.026236	-1.089799	-0.059402
6	-1.185112	-1.851088	0.496048
6	-2.652173	-2.306228	0.538971
1	-2.680718	-3.361785	0.835803
1	-3.243923	-1.747703	1.268923

1	-3.133085	-2.227308	-0.440354
6	-0.573391	-1.85814	1.918571
1	-0.692064	-2.862351	2.34253
1	0.499528	-1.642178	1.897399
1	-1.06464	-1.158488	2.600801
6	-0.37586	-2.824103	-0.390461
1	0.666564	-2.515622	-0.501645
1	-0.383675	-3.809169	0.091598
1	-0.819848	-2.931722	-1.382926

TS_{IIa-i} 2

E = -3968.388369 ZPVE = 0.312768 NIMAG = 1.

15	-0.859973	-0.049709	-0.150004
17	-1.381584	-1.252665	-2.191037
6	-2.249874	1.294314	-0.344045
6	-2.52236	2.102987	0.939147
1	-3.346428	2.797032	0.732712
1	-2.83755	1.466594	1.770302
1	-1.670502	2.700121	1.262643
6	-3.594227	0.681067	-0.791989
1	-4.270664	1.509681	-1.035203
1	-3.4956	0.048038	-1.673011
1	-4.064224	0.102296	0.006153
6	-1.731317	2.230211	-1.457826
1	-2.4795	3.009585	-1.647971
1	-0.801774	2.735246	-1.175274
1	-1.566397	1.683811	-2.390241
6	1.104506	2.551712	1.089267

1	0.338165	3.289686	0.838099
1	1.734342	2.482502	0.173879
1	1.775986	2.998888	1.832694
6	0.474021	1.228367	1.574729
1	1.227584	0.620303	2.109487
1	-0.309258	1.418207	2.300792
12	1.499075	0.309571	-0.189547
35	3.790347	-0.169828	-0.326194
6	-1.255406	-1.526049	1.054794
6	-2.580032	-2.239565	0.71571
1	-2.61974	-3.169359	1.296543
1	-3.446066	-1.63986	1.006961
1	-2.663998	-2.492705	-0.341119
6	-1.305346	-1.127235	2.543309
1	-1.57432	-2.018446	3.123777
1	-0.345594	-0.771358	2.918799
1	-2.063309	-0.366423	2.747927
6	-0.07926	-2.503199	0.834006
1	0.889774	-2.058995	1.102642
1	-0.206637	-3.376141	1.485839
1	-0.033067	-2.854294	-0.199983

PCIIa-i 2

E = -3968.520073 ZPVE = 0.316235 NIMAG = 0.

15	0.817714	-0.294375	-0.132479
17	-1.178197	3.114131	0.81468
6	2.2299	0.783152	-0.848579
6	3.328362	-0.048824	-1.538873

1	4.094629	0.629827	-1.933451
1	3.824231	-0.738987	-0.851562
1	2.942577	-0.62669	-2.383416
6	2.857186	1.669292	0.247288
1	3.543317	2.37987	-0.229526
1	2.102769	2.253747	0.782568
1	3.439993	1.093202	0.970528
6	1.568194	1.728397	-1.882465
1	2.34768	2.341908	-2.351202
1	1.051776	1.192184	-2.682218
1	0.859053	2.411423	-1.404073
6	0.058214	-1.372764	-2.717827
1	0.799661	-0.85064	-3.327797
1	-0.84759	-0.76117	-2.66647
1	-0.205708	-2.295986	-3.244073
6	0.578611	-1.721693	-1.315202
1	-0.171254	-2.352046	-0.830199
1	1.50385	-2.305027	-1.379246
12	-1.428713	0.970116	0.20309
35	-3.114837	-0.671228	-0.237156
6	1.288954	-1.157068	1.516071
6	1.223972	-0.123772	2.662876
1	1.42381	-0.634296	3.612682
1	1.955685	0.678414	2.559934
1	0.23389	0.337797	2.746436
6	2.673952	-1.830004	1.492873
1	2.823341	-2.377338	2.432044
1	2.767463	-2.553872	0.677157
1	3.488184	-1.105935	1.406242
6	0.211821	-2.23457	1.792643

1	0.319797	-3.10578	1.140973
1	0.323491	-2.584004	2.825638
1	-0.808167	-1.852466	1.677198

RC_{IIa-i} 3

E = -3968.436864 ZPVE = 0.313051 NIMAG = 0.

15	-0.832619	-0.218261	0.194159
17	-1.013596	-1.033199	2.120731
6	-0.970566	-1.731111	-0.968171
6	-0.095585	-2.863658	-0.386264
1	-0.016579	-3.654587	-1.142008
1	0.91574	-2.526854	-0.145259
1	-0.542073	-3.298512	0.510988
6	-0.345188	-1.265337	-2.305656
1	-0.385039	-2.096143	-3.019962
1	-0.875462	-0.422125	-2.75845
1	0.709853	-0.99868	-2.182522
6	-2.395618	-2.259818	-1.195067
1	-2.335925	-3.168505	-1.806579
1	-2.884727	-2.529493	-0.254667
1	-3.029339	-1.548532	-1.731275
6	0.782188	4.203029	-0.42559
1	1.144207	5.184414	-0.766703
1	0.48471	4.329328	0.62337
1	-0.135497	3.997218	-0.991797
6	1.834217	3.093693	-0.59805
1	2.745941	3.379264	-0.048508
1	2.154399	3.066186	-1.652826

12	1.59831	1.057468	-0.068878
35	3.087374	-0.811483	0.23735
6	-2.349278	0.939042	0.136966
6	-2.008468	2.086353	1.116628
1	-2.794936	2.848109	1.058783
1	-1.960771	1.734809	2.151139
1	-1.061473	2.573355	0.868469
6	-3.690865	0.312404	0.555003
1	-4.444065	1.108015	0.608395
1	-4.050275	-0.431674	-0.156492
1	-3.631289	-0.152106	1.542765
6	-2.441367	1.509224	-1.295047
1	-2.748345	0.754799	-2.024625
1	-3.195838	2.30454	-1.308906
1	-1.497426	1.954831	-1.62737

TS_{IIa-i} 3

E = -3968.382213 ZPVE = 0.310171 NIMAG = 1.

15	-0.957386	-0.217321	0.054816
17	0.345884	1.153322	2.451828
6	-1.079156	-2.065882	-0.324243
6	-0.122277	-2.751929	0.687529
1	-0.036612	-3.811573	0.416332
1	0.883233	-2.322714	0.669459
1	-0.509928	-2.695068	1.709514
6	-0.464665	-2.171026	-1.752899
1	-0.35553	-3.236963	-1.992301
1	-1.108363	-1.720983	-2.515849

1	0.530558	-1.719854	-1.809898
6	-2.441148	-2.774377	-0.281852
1	-2.289579	-3.821453	-0.571381
1	-2.867915	-2.777554	0.724441
1	-3.1727	-2.350533	-0.973635
6	0.543972	3.536466	-1.695808
1	1.015291	4.203159	-2.43837
1	0.374208	4.145669	-0.799712
1	-0.436022	3.265125	-2.103592
6	1.402986	2.322348	-1.421624
1	2.424736	2.59144	-1.108971
1	1.46893	1.621102	-2.257081
12	1.390959	0.937426	0.335779
35	3.094108	-0.736175	-0.100265
6	-2.623969	0.669149	-0.009501
6	-2.369621	2.152445	0.337815
1	-3.31491	2.699534	0.236969
1	-2.008741	2.272196	1.361362
1	-1.643472	2.613333	-0.335054
6	-3.64304	0.094964	0.999834
1	-4.529764	0.741001	0.995002
1	-3.969606	-0.914264	0.750283
1	-3.242739	0.095286	2.018341
6	-3.163822	0.580852	-1.460843
1	-3.393826	-0.440642	-1.770985
1	-4.093271	1.161746	-1.515899
1	-2.464034	1.014336	-2.182811

E = -3968.519290 ZPVE = 0.315991 NIMAG = 0.

15	0.889696	-0.279396	0.276185
17	-1.003655	3.130847	-0.925905
6	0.991971	-1.744755	-0.962806
6	0.522527	-1.210652	-2.3365
1	0.58867	-2.014096	-3.079909
1	-0.527797	-0.897057	-2.302373
1	1.123715	-0.374031	-2.700656
6	-0.011654	-2.832867	-0.515422
1	-0.125396	-3.553885	-1.333888
1	0.340776	-3.391693	0.356346
1	-1.00311	-2.425837	-0.295769
6	2.386739	-2.381529	-1.097859
1	2.31114	-3.266444	-1.742107
1	3.11103	-1.705759	-1.559719
1	2.785182	-2.712532	-0.133483
6	-0.212272	-0.386247	2.917863
1	-0.174372	-0.849496	3.909933
1	-1.219254	-0.532817	2.515914
1	-0.053533	0.688706	3.05687
6	0.855609	-1.011257	2.003409
1	0.666635	-2.082704	1.909854
1	1.847786	-0.909262	2.452032
12	-1.324186	1.014842	-0.239345
35	-3.131835	-0.514439	0.135984
6	2.443286	0.840047	0.253773
6	2.127439	2.001412	1.227023
1	2.97383	2.698942	1.229684
1	1.241328	2.565558	0.921522

1	1.992506	1.654811	2.25682
6	2.64064	1.4251	-1.159903
1	3.443858	2.171162	-1.125725
1	2.938565	0.662593	-1.885467
1	1.741305	1.931404	-1.523417
6	3.745336	0.155493	0.716013
1	4.071464	-0.635839	0.040058
1	4.542049	0.908837	0.747265
1	3.667062	-0.265228	1.722948

R1III + a SN2@P-b pathway 2

R1IIIa-i 2

E = -1264.903326 ZPVE = 0.183787 NIMAG = 0.

6	1.424026	-0.01071	-0.260044
6	2.642955	0.055435	-0.955456
6	1.313778	-0.8741	0.842225
6	3.733857	-0.719834	-0.553726
1	2.737677	0.715804	-1.813828
6	2.402685	-1.649625	1.241383
1	0.376651	-0.943522	1.385475
6	3.614215	-1.572933	0.545569
1	4.671127	-0.658885	-1.099109
1	2.306837	-2.314727	2.094913
1	4.459515	-2.179137	0.85847
17	0.123198	2.645131	0.539862
15	0.063681	1.068334	-0.893082
6	-1.442029	0.136959	-0.352943
6	-2.136988	0.322537	0.85029
6	-1.919473	-0.810801	-1.27536

6	-3.276748	-0.43694	1.131115
1	-1.796109	1.065785	1.563331
6	-3.050638	-1.576572	-0.987751
1	-1.408523	-0.950694	-2.225556
6	-3.733163	-1.390372	0.217888
1	-3.807414	-0.280319	2.066037
1	-3.404369	-2.307427	-1.709201
1	-4.619856	-1.977375	0.438888

RCIIIa-i 2

E = -4116.035332 ZPVE = 0.250055 NIMAG = 0.

6	2.169182	-0.15103	-0.185394
6	2.646421	-1.344509	0.379239
6	3.082558	0.832061	-0.605319
6	4.021014	-1.545904	0.536978
1	1.950006	-2.116784	0.692876
6	4.451548	0.624641	-0.450356
1	2.721981	1.751806	-1.05577
6	4.921716	-0.563137	0.123781
1	4.382445	-2.469402	0.978871
1	5.152976	1.386092	-0.778131
1	5.989595	-0.720972	0.24317
17	0.133831	0.170382	-2.474504
6	-0.578425	-3.512374	1.470984
1	-1.342793	-3.920093	2.149686
1	0.221626	-3.153271	2.138193
6	-0.032247	-4.654825	0.586938
1	0.747597	-4.310204	-0.105836

1	0.408859	-5.473481	1.175148
1	-0.820807	-5.101946	-0.030908
15	0.360759	0.032749	-0.385803
12	-1.443973	-1.848288	0.497629
35	-3.366451	-0.565222	-0.136453
6	-0.005683	1.739166	0.176899
6	-1.057603	2.470512	-0.397445
6	0.66548	2.257895	1.297815
6	-1.410989	3.714094	0.126612
1	-1.594255	2.073955	-1.252047
6	0.29605	3.497218	1.825275
1	1.478478	1.705236	1.758565
6	-0.7378	4.229802	1.237491
1	-2.219971	4.275301	-0.33097
1	0.824349	3.890903	2.688599
1	-1.020462	5.195675	1.645496

TS_{IIIa-i} 2

E = -4115.997171 ZPVE = 0.249746 NIMAG = 1.

6	1.641104	-1.287461	-0.10883
6	1.232984	-2.628775	-0.071398
6	3.008387	-0.988512	-0.024868
6	2.170255	-3.651953	0.084437
1	0.184833	-2.888349	-0.193245
6	3.943006	-2.012485	0.139418
1	3.3499	0.036256	-0.118262
6	3.527908	-3.34528	0.201131
1	1.838623	-4.685929	0.104252

1	4.999035	-1.766801	0.202102
1	4.258259	-4.139921	0.320283
17	1.058973	0.271489	-2.673716
6	-0.44026	-0.247063	1.778944
1	-1.105474	0.598539	2.057626
1	0.4765	-0.05482	2.328876
6	-1.039639	-1.597302	2.228017
1	-0.273983	-2.376089	2.215452
1	-1.465057	-1.548628	3.237636
1	-1.86735	-1.993312	1.600697
15	0.380714	0.00756	-0.415453
12	-1.94054	-0.305821	0.110949
35	-4.25742	-0.384377	-0.150948
6	0.957594	1.689231	0.080839
6	0.447658	2.779541	-0.64321
6	1.815542	1.936308	1.163512
6	0.77651	4.087387	-0.281485
1	-0.177569	2.605472	-1.513063
6	2.160604	3.24502	1.509367
1	2.225391	1.115208	1.741579
6	1.636845	4.324002	0.793153
1	0.370675	4.918228	-0.850835
1	2.836112	3.417748	2.342197
1	1.902041	5.340777	1.067299

PCIIIa-i 2

E = -4116.122079 ZPVE = 0.252905 NIMAG = 0.

6	-1.963147	-0.755738	-0.346347
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6	-2.116216	-1.952438	0.37006
6	-3.084318	-0.174415	-0.964037
6	-3.371798	-2.563049	0.45861
1	-1.26629	-2.399201	0.878392
6	-4.333288	-0.788311	-0.876588
1	-2.986718	0.763637	-1.503828
6	-4.477794	-1.986312	-0.167044
1	-3.479579	-3.485928	1.020466
1	-5.19378	-0.331687	-1.35689
1	-5.451932	-2.461493	-0.09755
17	1.13081	-2.304638	2.540617
6	0.058524	0.137886	-2.278224
1	0.949968	0.764803	-2.38305
1	-0.774597	0.63897	-2.783638
6	0.330187	-1.242416	-2.892839
1	-0.525272	-1.91575	-2.779741
1	0.534964	-1.139882	-3.963118
1	1.208783	-1.709071	-2.436378
15	-0.301048	0.021795	-0.460315
12	1.727309	-1.054891	0.778952
35	3.565637	-0.241766	-0.506723
6	-0.550373	1.749075	0.125311
6	-0.993145	1.934674	1.447636
6	-0.259568	2.874971	-0.658631
6	-1.164178	3.218651	1.963676
1	-1.217318	1.074923	2.07412
6	-0.428585	4.161311	-0.136317
1	0.097617	2.764446	-1.676802
6	-0.880555	4.336541	1.172397
1	-1.512571	3.345369	2.98432

1	-0.20225	5.024123	-0.755887
1	-1.008543	5.336565	1.575715

PIIIa-i 2

E = -883.919984 ZPVE = 0.248631 NIMAG = 0.

6	-1.330384	-0.149029	-0.240486
6	-2.491825	-0.30889	-1.012787
6	-1.210003	-0.886447	0.949892
6	-3.514197	-1.171146	-0.602329
1	-2.593558	0.242179	-1.944296
6	-2.226491	-1.751357	1.359457
1	-0.312232	-0.793637	1.554964
6	-3.382973	-1.894174	0.584897
1	-4.406088	-1.281087	-1.212973
1	-2.1157	-2.316257	2.281101
1	-4.172462	-2.568922	0.903573
6	-0.203158	2.403673	0.450414
1	0.657347	3.070268	0.316663
1	-0.140899	1.98167	1.4609
6	-1.502804	3.204159	0.28865
1	-2.383876	2.570744	0.43295
1	-1.549872	4.012075	1.027037
1	-1.57256	3.655011	-0.707101
15	-0.043434	1.051996	-0.841599
6	1.521358	0.194401	-0.336149
6	1.893055	-0.951522	-1.06481
6	2.394465	0.654192	0.662635
6	3.081583	-1.626975	-0.789473

1	1.242582	-1.3191	-1.854941
6	3.594351	-0.014854	0.93144
1	2.150052	1.536973	1.244096
6	3.940544	-1.158478	0.210794
1	3.342274	-2.513466	-1.360989
1	4.254489	0.360305	1.708852
1	4.870877	-1.678021	0.421285

R1_{IV} + a S_N2@P-b pathways 2 and 3

RC_{IVa-i} 2

E = -3924.292355 ZPVE = 0.196468 NIMAG = 0.

17	0.229126	2.168687	1.645378
6	-3.519039	1.205192	-0.958878
1	-4.441366	0.68766	-1.261564
1	-3.124437	1.642187	-1.890707
6	-3.872218	2.342062	0.024524
1	-2.985107	2.897293	0.356617
1	-4.559991	3.080916	-0.413416
1	-4.357354	1.959542	0.931042
15	0.280371	1.084439	-0.16488
12	-2.141127	-0.257985	-0.306218
35	-1.556942	-2.53816	0.183454
6	0.418644	2.473585	-1.368742
1	-0.519856	3.033082	-1.363835
1	1.24356	3.150336	-1.134768
1	0.571635	2.048939	-2.366711
6	1.931302	0.304415	-0.16649
6	1.982067	-1.096255	-0.06668
6	3.126369	1.039035	-0.267396

6	3.216461	-1.751741	-0.086788
1	1.064266	-1.670138	0.027078
6	4.353012	0.378496	-0.283434
1	3.105655	2.123094	-0.322018
6	4.398589	-1.018395	-0.196619
1	3.248103	-2.834347	-0.012372
1	5.273012	0.950278	-0.360563
1	5.356541	-1.530061	-0.210243

TS_{iv-a}-i 2

E = -3924.258603 ZPVE = 0.196349 NIMAG = 1.

17	-1.438497	1.802917	-2.215682
6	0.320764	0.333179	1.908119
1	0.645302	-0.727735	1.964432
1	-0.589492	0.359486	2.503887
6	1.39813	1.267583	2.495668
1	1.007004	2.280145	2.634205
1	1.786938	0.921483	3.461088
1	2.303525	1.39099	1.864643
15	-0.62674	1.040926	-0.146016
12	1.585698	0.140507	0.074656
35	3.656403	-0.843958	-0.368019
6	-1.226643	2.577166	0.692348
1	-0.609671	3.411658	0.351616
1	-2.247596	2.764174	0.355494
1	-1.190663	2.507149	1.779973
6	-1.886837	-0.281366	0.04037
6	-1.780936	-1.41537	-0.778746

6	-2.935381	-0.203191	0.967217
6	-2.698136	-2.461422	-0.660662
1	-1.00375	-1.470803	-1.536915
6	-3.860762	-1.244053	1.073739
1	-3.044413	0.669218	1.604154
6	-3.740899	-2.377517	0.265425
1	-2.605694	-3.332306	-1.302651
1	-4.674071	-1.168075	1.789588
1	-4.460152	-3.186474	0.351257

PC_{IVa-i} 2

E = -3924.379341 ZPVE = 0.199445 NIMAG = 0.

17	2.405967	1.885919	-2.178541
6	-0.294112	0.527996	2.346806
1	-0.30933	-0.566618	2.362136
1	-1.187409	0.879379	2.87698
6	0.993215	1.039837	3.00688
1	1.056179	2.133085	3.003833
1	1.036856	0.711259	4.050113
1	1.877733	0.637235	2.502153
15	-0.43848	1.012624	0.554452
12	1.698644	0.311685	-0.757579
35	2.110892	-1.849997	0.195216
6	-0.872945	2.80434	0.586928
1	-0.01376	3.362865	0.967431
1	-1.071251	3.155201	-0.428992
1	-1.737776	3.009798	1.224773
6	-1.939864	0.13063	-0.035134

6	-1.825334	-1.241894	-0.325175
6	-3.177229	0.766224	-0.221147
6	-2.934296	-1.961172	-0.773307
1	-0.87257	-1.751482	-0.200112
6	-4.282469	0.042399	-0.6771
1	-3.291605	1.825647	-0.016417
6	-4.164566	-1.321899	-0.950556
1	-2.832981	-3.020273	-0.990439
1	-5.233531	0.547498	-0.818404
1	-5.024125	-1.882664	-1.305437

PIV_{a-i} 2

E = -692.176347 ZPVE = 0.194948 NIMAG = 0.

6	2.019389	0.045661	1.061529
1	1.588125	-0.539499	1.88238
1	1.740254	1.092799	1.236408
6	3.546728	-0.108237	1.05692
1	4.013958	0.496565	0.27206
1	3.972389	0.214211	2.013767
1	3.841208	-1.150611	0.893716
15	1.215933	-0.590661	-0.51373
6	1.662514	0.786128	-1.695587
1	2.729154	0.721949	-1.931838
1	1.106324	0.651643	-2.627993
1	1.451322	1.786323	-1.301071
6	-0.567382	-0.200147	-0.161597
6	-1.490351	-1.257306	-0.209564
6	-1.044006	1.083566	0.155944

6	-2.847395	-1.043456	0.053726
1	-1.140596	-2.256167	-0.457737
6	-2.397973	1.302673	0.417951
1	-0.358298	1.925549	0.200529
6	-3.303965	0.238029	0.367811
1	-3.544235	-1.875919	0.010665
1	-2.746589	2.302814	0.661112
1	-4.357371	0.408789	0.571146

RC_{va-i} 3

E = -3924.291804 ZPVE = 0.196384 NIMAG = 0.

17	0.179534	-2.043301	1.504836
6	-1.028469	3.036667	0.792327
1	-1.837497	3.521927	1.358337
1	-0.211027	2.91805	1.521415
6	-0.572658	3.983528	-0.339558
1	-0.211605	4.952641	0.03597
1	0.242475	3.55705	-0.940527
1	-1.390228	4.202886	-1.037535
15	0.327837	-0.726852	-0.128729
12	-1.698401	1.112015	0.236873
35	-3.403515	-0.499617	-0.267483
6	2.10195	-0.280203	-0.1487
6	3.133306	-1.217619	-0.331111
6	2.42642	1.073275	0.03858
6	4.464015	-0.803237	-0.336558
1	2.902045	-2.271394	-0.454028
6	3.76229	1.484711	0.033781

1	1.640178	1.805998	0.195054
6	4.779814	0.548933	-0.157111
1	5.255707	-1.533189	-0.476817
1	4.002922	2.53328	0.180016
1	5.817966	0.867692	-0.160126
6	0.120916	-1.897212	-1.533261
1	-0.905912	-2.269922	-1.516093
1	0.281324	-1.343373	-2.464677
1	0.822323	-2.733365	-1.483153

TS_{IVa-i} 3

E = -3924.246100 ZPVE = 0.193728 NIMAG = 1.

17	0.354043	0.649776	-2.479858
6	1.251634	2.565413	0.850181
1	1.812752	3.280865	0.229279
1	0.189668	2.829195	0.824482
6	1.81931	2.423396	2.251303
1	1.86574	3.395171	2.773204
1	1.208579	1.759227	2.872691
1	2.837155	2.017555	2.247721
15	-0.540362	-0.683724	0.18372
12	1.579747	0.819132	-0.478413
35	3.212164	-0.883844	0.107093
6	-2.294081	-0.362663	0.20295
6	-3.288065	-1.315327	0.539223
6	-2.701717	0.948586	-0.158953
6	-4.632479	-0.96466	0.522555
1	-3.005829	-2.325818	0.813426

6	-4.048842	1.290544	-0.173889
1	-1.952796	1.680104	-0.446016
6	-5.015046	0.336637	0.167196
1	-5.386896	-1.700389	0.783575
1	-4.348965	2.294456	-0.45654
1	-6.067457	0.604085	0.153428
6	-0.351707	-2.443525	0.677465
1	0.721674	-2.648724	0.670321
1	-0.747312	-2.624049	1.684526
1	-0.856352	-3.11747	-0.023813

PCIVa-i 3

E = -3924.377571 ZPVE = 0.199470 NIMAG = 0.

17	1.055798	2.946794	0.616647
6	-0.849988	-0.64747	2.501407
1	-1.292877	0.336562	2.688061
1	-1.630126	-1.395395	2.687012
6	0.361394	-0.865216	3.418037
1	0.050696	-0.826321	4.466926
1	0.835834	-1.837936	3.252811
1	1.118318	-0.087191	3.272206
15	-0.426895	-0.688281	0.687587
12	1.526494	0.860597	-0.064309
35	3.092589	-0.541797	-1.179727
6	-2.010438	-0.276231	-0.147577
6	-2.832483	-1.240279	-0.751843
6	-2.392862	1.076842	-0.196579
6	-4.022692	-0.860832	-1.378149

1	-2.554104	-2.289054	-0.742016
6	-3.584988	1.450434	-0.819308
1	-1.754108	1.84264	0.237401
6	-4.402715	0.482819	-1.409857
1	-4.649118	-1.616445	-1.843062
1	-3.867545	2.498398	-0.850632
1	-5.326753	0.775631	-1.89954
6	-0.099526	-2.464392	0.32601
1	0.841054	-2.750295	0.80344
1	-0.898933	-3.116852	0.690082
1	0.029752	-2.603321	-0.750211

R1_v + a S_N2@P-b pathway 2

RC_{v_a-i} 2

E = -3732.547898 ZPVE = 0.142552 NIMAG = 0.

17	-2.071213	-1.16036	-1.363667
6	1.107738	2.884042	-0.748098
1	2.087636	3.140065	-1.176128
1	0.389123	3.041678	-1.567775
6	0.78356	3.859132	0.404453
1	0.759003	4.909348	0.077235
1	-0.19589	3.654078	0.85892
1	1.524336	3.799007	1.211846
15	-1.481978	-0.035093	0.302277
12	1.082209	0.829448	-0.268291
35	2.03003	-1.345635	0.109856
6	-1.681163	-1.252164	1.667374
1	-0.91868	-2.027091	1.561506
1	-1.518404	-0.731885	2.618265

1	-2.678529	-1.700436	1.663735
6	-2.940199	1.073025	0.520452
1	-3.004266	1.761805	-0.325304
1	-3.871203	0.505333	0.601892
1	-2.790038	1.660228	1.433456

TS_{Va-i} 2

E = -3732.496341 ZPVE = 0.140276 NIMAG = 1.

17	-0.988259	-1.796428	-1.34932
6	-0.217227	2.076134	-1.104189
1	0.257456	1.965478	-2.095984
1	-1.269824	2.305366	-1.279083
6	0.490295	3.114625	-0.241246
1	0.504008	4.10476	-0.725381
1	-0.00374	3.241318	0.728843
1	1.531917	2.844269	-0.036778
15	-1.810535	-0.09672	0.616364
12	0.472328	0.002714	-0.602718
35	2.577514	-0.421692	0.438499
6	-2.650329	-0.287775	2.258222
1	-1.970063	-0.754531	2.973611
1	-2.920042	0.710355	2.633938
1	-3.571312	-0.875442	2.180958
6	-3.258096	0.384947	-0.409023
1	-2.954271	0.53304	-1.444538
1	-4.022523	-0.398111	-0.364894
1	-3.691951	1.312628	-0.015135

PC_{Va-i} 2

E = -3732.633204 ZPVE = 0.145534 NIMAG = 0.

17	-0.581638	3.103744	-0.422203
6	2.314409	-0.994954	-1.155652
1	2.504617	-0.237295	-1.925541
1	3.290522	-1.402849	-0.862977
6	1.406462	-2.100834	-1.71278
1	1.873651	-2.561865	-2.588793
1	1.230151	-2.891503	-0.977274
1	0.429627	-1.712413	-2.016489
15	1.612662	-0.083102	0.305294
12	-0.778198	0.90118	-0.066566
35	-2.258183	-0.954463	0.17858
6	1.681638	-1.305513	1.688746
1	0.911056	-2.066551	1.543356
1	2.665031	-1.783498	1.749168
1	1.477516	-0.796489	2.635406
6	2.943514	1.128865	0.713112
1	3.004084	1.879814	-0.079119
1	2.695826	1.646878	1.643742
1	3.914486	0.635341	0.8245

R1₁ + a S_{N2}@P-f pathway 2**RC_{Ia-r} 2**

E = -4276.924487 ZPVE = 0.431080 NIMAG = 0.

6	-1.384204	-1.313654	0.602018
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6	-0.820768	-2.773668	-1.40601
6	-3.205988	-1.866608	-1.149047
6	-2.882795	-1.606454	0.332934
6	-2.315439	-2.999206	-1.682586
6	0.989505	-2.428563	0.42746
6	-4.696374	-2.165623	-1.348996
6	1.237602	-2.447502	1.945853
6	1.819303	-3.553384	-0.217824
1	-1.250168	-1.196708	1.682659
1	-0.268653	-3.655327	-1.741934
1	-0.452534	-1.93286	-2.011009
1	-2.970027	-0.954168	-1.721299
1	-3.512442	-0.800962	0.722268
1	-3.141902	-2.506996	0.909515
1	-2.479464	-3.128193	-2.76
1	-2.629226	-3.940868	-1.206678
1	1.385615	-1.48461	0.031069
1	-5.320831	-1.333825	-1.004075
1	-4.926192	-2.343304	-2.405496
1	-4.992493	-3.061319	-0.788563
1	0.918075	-3.408053	2.370726
1	2.304079	-2.322401	2.153842
1	0.711017	-1.65114	2.477663
1	1.430889	-4.542486	0.058586
1	2.853824	-3.487757	0.132698
1	1.842801	-3.489285	-1.309239
6	-2.214822	1.488115	0.351745
6	-2.818372	2.270161	-0.645882
6	-2.638169	1.63473	1.684603
6	-3.843171	3.165864	-0.323185

1	-2.482115	2.185253	-1.675885
6	-3.65237	2.534605	2.006218
1	-2.167938	1.055333	2.4739
6	-4.260202	3.298275	1.001659
1	-4.302722	3.763949	-1.104327
1	-3.968426	2.644418	3.039497
1	-5.049792	3.999112	1.256342
17	0.664707	0.997611	1.192107
6	-0.523924	-2.514272	0.087444
1	-0.911429	-3.387326	0.640067
6	2.107646	2.884876	-1.817565
1	1.406263	2.432291	-2.535482
1	1.495766	3.591831	-1.235656
6	3.199819	3.656783	-2.585489
1	2.783253	4.431523	-3.24695
1	3.898086	4.162905	-1.907128
1	3.802542	2.991978	-3.216691
15	-0.891969	0.337349	-0.207811
12	2.722228	1.379074	-0.478349
35	4.309236	-0.136753	0.4838

TS_{1a-r} 2

E = -4276.892192 ZPVE = 0.429743 NIMAG = 1.

6	-1.220966	-1.294795	0.677986
6	-0.766195	-3.010446	-1.142786
6	-3.155005	-2.138595	-0.817598
6	-2.730871	-1.654223	0.580183
6	-2.267622	-3.313572	-1.256931

6	1.160083	-2.35322	0.486582
6	-4.644563	-2.497884	-0.85502
6	1.520811	-2.295144	1.980454
6	2.022846	-3.431277	-0.191318
1	-0.996953	-1.012427	1.711316
1	-0.205717	-3.911604	-1.405509
1	-0.481778	-2.249659	-1.884998
1	-2.99154	-1.311502	-1.529733
1	-3.353632	-0.810293	0.890088
1	-2.916055	-2.460877	1.305034
1	-2.513543	-3.602935	-2.286481
1	-2.505444	-4.183114	-0.625084
1	1.455487	-1.398152	0.023306
1	-5.270298	-1.640119	-0.583706
1	-4.946144	-2.831484	-1.854162
1	-4.867463	-3.310206	-0.151803
1	1.33938	-3.27221	2.446898
1	2.580987	-2.054211	2.102872
1	0.953469	-1.540669	2.530556
1	1.745565	-4.435183	0.155976
1	3.074025	-3.265704	0.062352
1	1.944574	-3.411855	-1.281736
6	-2.00359	1.456246	0.015063
6	-2.38824	2.322963	-1.035754
6	-2.570736	1.652798	1.295409
6	-3.332754	3.327498	-0.821548
1	-1.956117	2.193185	-2.023327
6	-3.497705	2.665657	1.506897
1	-2.2475	1.03842	2.128021
6	-3.886299	3.500713	0.448441

1	-3.627008	3.976148	-1.640846
1	-3.912545	2.818087	2.498672
1	-4.612386	4.289723	0.62118
17	0.8344	1.301763	2.078163
6	-0.366272	-2.540945	0.273064
1	-0.680813	-3.33731	0.968072
6	1.225998	2.35426	-1.630741
1	0.989885	1.598545	-2.384136
1	0.32594	2.872679	-1.292128
6	2.355578	3.291766	-2.034688
1	2.086883	3.854664	-2.946024
1	2.571744	4.041336	-1.26353
1	3.284427	2.755504	-2.25624
15	-0.806395	0.181221	-0.424787
12	2.060709	1.22979	0.12135
35	4.176806	0.135562	-0.208978

PC_{Ia-r} 2

E = -4276.985640 ZPVE = 0.434214 NIMAG = 0.

6	1.217004	0.979888	0.56711
6	1.434214	3.23465	-0.602364
6	3.55785	1.950919	0.039708
6	2.692665	1.133483	1.014354
6	2.913902	3.325427	-0.196707
6	-0.926252	2.455765	0.116895
6	4.999899	2.076693	0.545986
6	-1.732618	1.782754	1.244501
6	-1.46548	3.887432	-0.063605

1	0.696839	0.448001	1.373469
1	1.032766	4.249372	-0.675563
1	1.348547	2.789368	-1.602506
1	3.584588	1.421011	-0.924193
1	3.1436	0.151307	1.184007
1	2.691736	1.643315	1.990056
1	3.474236	3.876441	-0.962864
1	2.994943	3.914606	0.729918
1	-1.124321	1.926024	-0.824443
1	5.463693	1.092509	0.676461
1	5.617611	2.648709	-0.155747
1	5.031832	2.592383	1.514206
1	-1.685206	2.367191	2.170736
1	-2.796891	1.722856	0.97326
1	-1.334026	0.79768	1.528182
1	-1.193524	4.521482	0.789756
1	-2.558339	3.875307	-0.134542
1	-1.086869	4.360981	-0.972216
6	2.137549	-1.576556	-0.515715
6	3.190253	-1.945533	-1.367923
6	1.911988	-2.345442	0.64038
6	4.000659	-3.047639	-1.0749
1	3.373331	-1.367758	-2.270133
6	2.716817	-3.447607	0.933774
1	1.107783	-2.091324	1.326466
6	3.764868	-3.80065	0.076653
1	4.80995	-3.316967	-1.747639
1	2.524698	-4.030548	1.830054
1	4.389814	-4.658973	0.305747
17	-2.323883	-1.81958	2.590983

6	0.60091	2.40918	0.402433
1	0.733334	2.887561	1.388702
6	-0.603123	-0.908099	-0.840584
1	-0.689789	-1.338076	0.173313
1	-1.323093	-0.091459	-0.991343
6	-0.858005	-1.991158	-1.900893
1	-1.885963	-2.365766	-1.845459
1	-0.711955	-1.584235	-2.906082
1	-0.177172	-2.836244	-1.770621
15	1.105649	-0.111249	-1.007087
12	-2.825014	-0.73555	0.712237
35	-4.455695	-0.206217	-0.907796

R1_{II} + a S_N2@P-f pathway 2

RC_{IIa-r} 2

E = -3968.427810 ZPVE = 0.311814 NIMAG = 0.

15	-2.066321	-0.537941	-0.78856
17	-0.088338	0.09044	-1.46222
6	-1.566256	-1.691188	0.65787
6	-1.081575	-2.985447	-0.037724
1	-0.842508	-3.735621	0.725859
1	-1.848757	-3.40633	-0.69566
1	-0.175385	-2.814798	-0.626059
6	-2.861122	-2.000308	1.443049
1	-2.675919	-2.857959	2.10059
1	-3.171212	-1.163747	2.075011
1	-3.695945	-2.271	0.786231
6	-0.470694	-1.210165	1.62396
1	-0.364544	-1.942189	2.43434

1	0.504377	-1.172401	1.127934
1	-0.689826	-0.243523	2.080541
6	3.050562	3.591455	0.895642
1	3.634514	3.643862	-0.031763
1	3.706529	3.147658	1.654648
1	2.859018	4.628863	1.208196
6	1.750337	2.779516	0.713855
1	1.181019	2.792648	1.655934
1	1.101791	3.283796	-0.018809
12	2.002147	0.782808	0.082418
35	3.307546	-1.198451	-0.216571
6	-2.792283	1.125068	-0.1775
6	-4.295221	0.838446	0.068619
1	-4.469433	0.194455	0.933447
1	-4.804518	1.790221	0.261964
1	-4.773692	0.380801	-0.804053
6	-2.687167	2.098087	-1.374657
1	-3.281444	2.993256	-1.155748
1	-1.65769	2.414908	-1.555605
1	-3.077409	1.656809	-2.298518
6	-2.164204	1.77078	1.065424
1	-2.318786	1.171039	1.966525
1	-1.092585	1.949062	0.940047
1	-2.635179	2.74643	1.240844

TS_{IIa-r} 2

E = -3968.376027 ZPVE = 0.310731 NIMAG = 1.

15	1.626147	0.343327	-0.76502
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17	-0.437356	-1.427831	-2.244944
6	1.118738	1.885283	0.222429
6	0.100139	2.622881	-0.679646
1	-0.048109	3.637736	-0.291328
1	0.446521	2.706445	-1.715064
1	-0.879456	2.135412	-0.681172
6	2.446906	2.703689	0.242262
1	2.193373	3.728079	0.542816
1	3.166714	2.310607	0.963862
1	2.928664	2.772856	-0.740238
6	0.550798	1.771452	1.644486
1	0.370858	2.78267	2.030027
1	-0.408198	1.248591	1.648369
1	1.22642	1.266025	2.335272
6	-1.951264	-2.466851	1.990551
1	-2.203753	-3.255746	1.269174
1	-2.824651	-1.813843	2.093608
1	-1.8127	-2.974516	2.959844
6	-0.681581	-1.696665	1.597765
1	-0.427381	-0.935697	2.337817
1	0.166882	-2.365221	1.443375
12	-1.478161	-0.841477	-0.279801
35	-3.346366	0.651623	-0.027226
6	2.873423	-0.744331	0.157198
6	4.242058	-0.244707	-0.402047
1	4.505777	0.754874	-0.0482
1	5.016375	-0.937576	-0.048608
1	4.273538	-0.247733	-1.496475
6	2.658553	-2.185355	-0.368199
1	3.486878	-2.812435	-0.016574

1	1.723029	-2.615244	-0.007196
1	2.640399	-2.22533	-1.461144
6	2.904598	-0.731847	1.691816
1	3.178055	0.248423	2.091381
1	1.947714	-1.029384	2.123
1	3.662422	-1.446171	2.037625

PCIIa-r 2

E = -3968.519922 ZPVE = 0.316041 NIMAG = 0.

15	-0.929944	-0.23425	0.284686
17	1.030842	3.25546	-0.516097
6	-0.9432	-1.736673	-0.909697
6	-0.381306	-1.264809	-2.269939
1	-0.37762	-2.106858	-2.972584
1	-0.974013	-0.464197	-2.72021
1	0.65656	-0.924625	-2.177785
6	-2.326571	-2.381049	-1.110268
1	-2.208173	-3.289736	-1.71341
1	-2.787904	-2.677757	-0.16286
1	-3.0198	-1.725814	-1.64355
6	0.019791	-2.801786	-0.336301
1	0.126386	-3.604839	-1.075656
1	1.018614	-2.401556	-0.143218
1	-0.36335	-3.25625	0.582142
6	0.277244	-1.056312	2.758738
1	0.749432	-0.0746	2.87343
1	0.992572	-1.703791	2.247411
1	0.111532	-1.458191	3.764431

6	-1.061486	-0.948827	2.011863
1	-1.556716	-1.924191	1.958613
1	-1.733804	-0.293826	2.572943
12	1.320157	1.062567	-0.116859
35	3.153297	-0.469843	0.005433
6	-2.488007	0.868006	0.130485
6	-2.620055	1.382733	-1.317382
1	-2.85968	0.582835	-2.023672
1	-3.438015	2.111844	-1.362364
1	-1.712231	1.89338	-1.653817
6	-2.240811	2.082521	1.057851
1	-3.106576	2.752913	0.994548
1	-2.137011	1.794202	2.109339
1	-1.3577	2.654794	0.762041
6	-3.796907	0.176189	0.563413
1	-4.081083	-0.64498	-0.095794
1	-3.747937	-0.208228	1.586813
1	-4.608081	0.914134	0.536133

R1III + a S_N2@P-f pathways 2 and 3

RCIIIa-r 2

E = -4116.032137 ZPVE = 0.249792 NIMAG = 0.

6	2.790806	-0.234253	-0.614892
6	4.052581	-0.114421	-1.221526
6	2.700624	-0.739139	0.694762
6	5.210614	-0.463817	-0.520146
1	4.129865	0.251419	-2.242187
6	3.856475	-1.093593	1.387712
1	1.733873	-0.85477	1.173918

6	5.111979	-0.953957	0.78302
1	6.181529	-0.362412	-0.995526
1	3.778187	-1.483555	2.398173
1	6.009271	-1.233966	1.327179
17	0.038579	-1.450954	-1.392521
6	-0.78053	-1.095722	2.438826
1	-0.146926	-1.991793	2.336571
1	-0.081533	-0.268618	2.638108
6	-1.716378	-1.275316	3.653278
1	-1.169081	-1.466996	4.5887
1	-2.335448	-0.385803	3.825511
1	-2.408855	-2.114838	3.514374
15	1.36025	0.275521	-1.643967
12	-1.729599	-0.778439	0.578876
35	-3.73976	-0.726937	-0.729993
6	0.444148	1.448415	-0.547021
6	-0.906808	1.722138	-0.845851
6	1.074682	2.180393	0.472858
6	-1.622102	2.66473	-0.10253
1	-1.41288	1.198431	-1.652641
6	0.36041	3.138917	1.197522
1	2.115333	1.99611	0.716213
6	-0.98613	3.380052	0.917054
1	-2.668053	2.841242	-0.332597
1	0.858809	3.689506	1.989894
1	-1.539117	4.116963	1.491535

TSIIIa-r 2

E = -4115.994269 ZPVE = 0.247843 NIMAG = 1.

6	-2.497618	0.276364	-0.449533
6	-3.451072	0.852309	-1.316155
6	-2.876249	-0.034835	0.873692
6	-4.757078	1.074907	-0.883146
1	-3.163016	1.135607	-2.325014
6	-4.175485	0.214158	1.307909
1	-2.142677	-0.423282	1.57211
6	-5.121282	0.754026	0.4277
1	-5.484413	1.509551	-1.561794
1	-4.451538	-0.006337	2.334661
1	-6.133746	0.94421	0.771218
17	-0.16344	2.888577	-0.087068
6	0.973118	0.353075	2.528285
1	1.387445	1.057209	3.267241
1	-0.114274	0.333912	2.658174
6	1.620607	-1.018863	2.6272
1	1.445309	-1.494822	3.607635
1	1.226768	-1.713246	1.874764
1	2.70561	-0.968098	2.483938
15	-0.839192	0.08282	-1.145042
12	1.491191	1.495022	0.738834
35	3.520539	1.023647	-0.492108
6	-0.277047	-1.541624	-0.618475
6	1.046786	-1.864234	-1.026896
6	-1.071351	-2.56552	-0.039061
6	1.550007	-3.149755	-0.857968
1	1.683844	-1.094229	-1.455088
6	-0.563125	-3.850426	0.111066
1	-2.094936	-2.362181	0.250458

6	0.745872	-4.146146	-0.294887
1	2.566044	-3.372777	-1.16704
1	-1.188327	-4.6293	0.53709
1	1.134647	-5.152866	-0.173162

PC_{IIIa-r} 2

E = -4116.120878 ZPVE = 0.253275 NIMAG = 0.

6	2.153291	-0.548503	0.41209
6	2.441329	-1.468355	-0.610649
6	3.195631	-0.122329	1.254369
6	3.744508	-1.935619	-0.796588
1	1.649221	-1.840621	-1.253179
6	4.495653	-0.597934	1.070264
1	3.007693	0.583029	2.056965
6	4.773273	-1.504334	0.043295
1	3.947161	-2.648488	-1.590073
1	5.289207	-0.260281	1.730561
1	5.784535	-1.874619	-0.097179
17	-0.689512	-3.246682	-1.589996
6	0.247865	0.486662	2.388485
1	0.391977	-0.454914	2.93208
1	1.070936	1.152538	2.667199
6	-1.093825	1.126306	2.770042
1	-1.13498	1.266528	3.855057
1	-1.213388	2.10828	2.302941
1	-1.943389	0.508057	2.46933
15	0.422901	0.054961	0.579505
12	-1.466925	-1.515549	-0.398113

35	-3.547862	-0.562027	0.306201
6	0.360969	1.67177	-0.309327
6	-0.896182	2.175885	-0.688776
6	1.516613	2.404191	-0.62576
6	-0.988928	3.396768	-1.361467
1	-1.805146	1.622504	-0.466664
6	1.415622	3.625395	-1.295716
1	2.496339	2.02017	-0.361189
6	0.163556	4.126214	-1.6623
1	-1.965318	3.773573	-1.651255
1	2.317413	4.180945	-1.536439
1	0.087921	5.073333	-2.188261

RC_{Ma-r} 3

E = -4116.027977 ZPVE = 0.249321 NIMAG = 0.

6	1.359202	1.521061	-0.024496
6	1.649929	2.679742	0.715132
6	1.231087	1.612943	-1.420687
6	1.835162	3.904388	0.067957
1	1.717453	2.629887	1.798898
6	1.400153	2.840454	-2.06182
1	0.984637	0.731659	-2.004863
6	1.708568	3.986112	-1.319961
1	2.058742	4.793007	0.650428
1	1.289828	2.903212	-3.140456
1	1.836943	4.94005	-1.82279
17	-0.37391	-1.056433	-0.203127
6	-2.334092	1.734634	1.458218

1	-1.616536	1.440136	2.240899
1	-1.766492	2.418199	0.80742
6	-3.505195	2.503647	2.102433
1	-3.172065	3.387882	2.66662
1	-4.222411	2.858418	1.351726
1	-4.071345	1.876258	2.802209
15	1.171076	-0.011958	0.972156
12	-2.757002	0.011783	0.324433
35	-4.149825	-1.587572	-0.760897
6	2.608331	-1.048682	0.482923
6	2.799023	-2.220516	1.239988
6	3.539253	-0.725559	-0.518199
6	3.879281	-3.063962	0.982886
1	2.09651	-2.474435	2.02986
6	4.627286	-1.565352	-0.764515
1	3.422744	0.181809	-1.100171
6	4.79623	-2.736071	-0.0204
1	4.009612	-3.969095	1.568336
1	5.342694	-1.304112	-1.538758
1	5.64259	-3.387567	-0.217084

TS_{IIIa-r} 3

E = -4115.995460 ZPVE = 0.248131 NIMAG = 1.

6	1.860663	1.580852	0.145767
6	2.074025	2.812407	0.805192
6	1.828107	1.560623	-1.265722
6	2.30658	3.977341	0.076087
1	2.065501	2.850735	1.891668

6	2.041263	2.73239	-1.988137
1	1.590004	0.639277	-1.785136
6	2.290984	3.938211	-1.321727
1	2.485859	4.913859	0.59524
1	2.00056	2.709154	-3.073017
1	2.45576	4.848074	-1.891349
17	-0.57573	-1.002568	-0.806631
6	-1.580301	0.734345	1.810876
1	-1.072607	-0.203394	2.07977
1	-0.92412	1.332546	1.162826
6	-2.132276	1.495833	2.994056
1	-1.344937	1.832177	3.691542
1	-2.675902	2.393551	2.677168
1	-2.826677	0.882083	3.579436
15	1.568326	0.16024	1.231226
12	-2.575004	-0.202628	0.115698
35	-4.784548	-0.535343	-0.706126
6	2.440368	-1.225584	0.481473
6	2.161664	-2.496749	1.040337
6	3.461693	-1.126499	-0.490787
6	2.854078	-3.626761	0.6213
1	1.381853	-2.592479	1.790666
6	4.165925	-2.259192	-0.891962
1	3.721533	-0.162226	-0.911152
6	3.858652	-3.510448	-0.347092
1	2.61554	-4.596655	1.04646
1	4.955665	-2.167176	-1.631541
1	4.405147	-4.39152	-0.670172

PCIIIa-r 3

E = -4116.104598 ZPVE = 0.252312 NIMAG = 0.

6	2.84501	-0.37743	-0.334443
6	4.124382	-0.488399	-0.902496
6	2.732818	0.046795	1.002606
6	5.267983	-0.184028	-0.156629
1	4.224782	-0.816687	-1.933696
6	3.874048	0.350978	1.746554
1	1.757257	0.162462	1.467538
6	5.14353	0.234339	1.169406
1	6.250108	-0.275701	-0.611424
1	3.770282	0.67973	2.776568
1	6.029355	0.470431	1.752067
17	-0.904292	1.271652	2.418551
6	0.48603	-2.049345	-0.257844
1	-0.507501	-2.21447	-0.689492
1	0.352443	-1.598049	0.734085
6	1.216735	-3.392228	-0.128691
1	1.340145	-3.871447	-1.105518
1	2.209088	-3.266598	0.315186
1	0.647749	-4.073953	0.511801
15	1.402688	-0.856845	-1.390915
12	-2.04424	0.345178	0.739276
35	-3.884229	-1.057939	0.205798
6	0.293665	0.629135	-1.265448
6	-1.079509	0.489927	-1.572814
6	0.771516	1.923895	-0.992676
6	-1.945988	1.60194	-1.563954
1	-1.484715	-0.473385	-1.872617

6	-0.084148	3.027162	-0.994356
1	1.82013	2.070266	-0.757566
6	-1.447505	2.874373	-1.26242
1	-2.992102	1.461768	-1.822358
1	0.314067	4.010112	-0.761709
1	-2.11095	3.733191	-1.249519

R1_{IV} + a S_N2@P-f pathways 2 and 3

RC_{IVa-r} 2

E = -3924.285661 ZPVE = 0.195671 NIMAG = 0.

17	-0.271946	-1.492863	0.278646
6	-0.831515	2.238624	0.966601
1	-0.3158	1.88237	1.872337
1	-0.023859	2.481726	0.258608
6	-1.624583	3.520082	1.296619
1	-2.122736	3.931687	0.410016
1	-2.411444	3.334346	2.038274
1	-0.988512	4.320711	1.703533
15	1.52952	-0.972747	1.418974
12	-1.911379	0.614566	0.165847
35	-3.825479	-0.459474	-0.763113
6	2.236292	-2.684774	1.457884
1	1.605673	-3.315898	2.089316
1	2.336524	-3.147064	0.472952
1	3.227905	-2.61279	1.919394
6	2.541284	-0.165962	0.117446
6	2.962769	-0.777758	-1.076568
6	2.922182	1.161583	0.378051
6	3.759883	-0.078851	-1.981164

1	2.659184	-1.793652	-1.310787
6	3.73269	1.856279	-0.524362
1	2.583612	1.651608	1.286626
6	4.148634	1.237827	-1.704205
1	4.076324	-0.556805	-2.903547
1	4.0247	2.879803	-0.310194
1	4.771186	1.778338	-2.411139

TS_{IVa-r} 2

E = -3924.249623 ZPVE = 0.194494 NIMAG = 1.

17	-0.375372	-1.351196	0.896262
6	-0.77348	1.827206	0.414881
1	-0.652796	1.551042	1.472094
1	0.025783	1.371018	-0.185815
6	-0.958709	3.307911	0.184226
1	-1.132941	3.53151	-0.874578
1	-1.814966	3.69633	0.7473
1	-0.082079	3.902089	0.496206
15	1.884774	0.627313	1.549917
12	-2.048118	0.0912	0.084941
35	-4.229368	-0.46734	-0.672998
6	2.128884	-0.74634	2.756684
1	1.399997	-0.629364	3.562073
1	2.041747	-1.754331	2.350828
1	3.13319	-0.604399	3.182448
6	2.765133	0.08498	0.074451
6	3.201751	-1.22991	-0.198614
6	3.085973	1.109741	-0.848588

6	3.946056	-1.502516	-1.342495
1	2.944846	-2.040871	0.472678
6	3.829877	0.833156	-1.992065
1	2.747108	2.125097	-0.65875
6	4.261767	-0.474524	-2.239756
1	4.272805	-2.518174	-1.543835
1	4.07097	1.629832	-2.688949
1	4.837833	-0.694863	-3.133633

PC_{IVa-r} 2

E = -3924.345494 ZPVE = 0.198107 NIMAG = 0.

17	1.151617	2.818814	0.303095
6	0.109535	-0.926414	0.011544
1	0.984308	-1.245834	0.599063
1	0.057134	0.177176	-0.043244
6	0.15323	-1.544674	-1.393052
1	-0.711287	-1.228424	-1.983973
1	1.061568	-1.263099	-1.938054
1	0.141613	-2.636717	-1.328412
15	-1.388602	-1.46768	1.028936
12	2.179313	0.883686	-0.032926
35	3.980907	-0.583486	-0.34998
6	-1.074646	-0.452379	2.56295
1	-0.209257	-0.864897	3.092449
1	-0.899576	0.609831	2.362853
1	-1.940876	-0.542631	3.224792
6	-2.734445	-0.494068	0.201599
6	-2.694258	0.898096	0.00606

6	-3.860102	-1.202255	-0.249091
6	-3.749333	1.559155	-0.62563
1	-1.841267	1.482093	0.34248
6	-4.919086	-0.541499	-0.880148
1	-3.90685	-2.278374	-0.103406
6	-4.864391	0.840485	-1.069939
1	-3.700112	2.634542	-0.770834
1	-5.781889	-1.1063	-1.221508
1	-5.684488	1.357106	-1.560218

P_{IVa-r} 2

E = -692.176821 ZPVE = 0.195001 NIMAG = 0.

6	2.25932	0.686397	0.540459
1	3.323543	0.419995	0.503621
1	1.914294	0.472844	1.560486
6	2.08052	2.174389	0.214471
1	1.026774	2.468606	0.262563
1	2.632536	2.798566	0.9261
1	2.44696	2.407814	-0.791073
15	1.405649	-0.447517	-0.689098
6	1.755744	-2.089705	0.129997
1	1.497794	-2.109279	1.194578
1	1.193253	-2.876159	-0.381584
1	2.822007	-2.315266	0.024428
6	-0.382364	-0.196535	-0.23977
6	-1.27533	0.146479	-1.267398
6	-0.889846	-0.328394	1.064368
6	-2.633917	0.352347	-1.004595

1	-0.900694	0.251788	-2.282343
6	-2.244919	-0.124372	1.332223
1	-0.227154	-0.592669	1.884536
6	-3.121422	0.216998	0.296573
1	-3.307346	0.616975	-1.815091
1	-2.617663	-0.231504	2.347379
1	-4.175765	0.375421	0.504889

RC_{IVa-r} 3

E = -3924.289865 ZPVE = 0.195947 NIMAG = 0.

17	0.15644	1.070709	0.215899
6	3.701386	2.486251	-0.214083
1	4.178842	2.567948	-1.202522
1	4.537631	2.454195	0.500558
6	2.846917	3.742959	0.048031
1	2.393575	3.730067	1.047392
1	3.432433	4.671936	-0.021053
1	2.021967	3.835942	-0.66941
15	-0.906915	-0.846023	-0.118322
12	2.721216	0.622071	-0.139962
35	2.682407	-1.786914	-0.179368
6	-0.699172	-1.534515	1.585527
1	0.349085	-1.82184	1.696249
1	-0.98601	-0.849316	2.386721
1	-1.31876	-2.43718	1.644344
6	-2.632138	-0.214317	-0.088636
6	-3.295684	0.318141	1.030846
6	-3.32604	-0.313167	-1.307658

6	-4.623056	0.732484	0.932447
1	-2.778253	0.416812	1.979986
6	-4.658174	0.097054	-1.404343
1	-2.820435	-0.71691	-2.181358
6	-5.30639	0.620974	-0.284562
1	-5.12578	1.144902	1.802385
1	-5.183938	0.009686	-2.350319
1	-6.340841	0.943999	-0.356432

TS_{IVa-r} 3

E = -3924.254163 ZPVE = 0.195025 NIMAG = 1.

17	-1.005399	2.19183	1.175667
6	-0.28887	-1.408057	1.568645
1	0.076484	-2.09213	0.798078
1	-1.176246	-1.856388	2.045404
6	0.75343	-0.991942	2.583052
1	0.357054	-0.270313	3.305658
1	1.124321	-1.854102	3.16262
1	1.631018	-0.53491	2.111805
15	0.541728	0.893455	-0.895318
12	-1.654044	0.024109	0.572399
35	-3.541393	-0.795017	-0.644071
6	1.0323	2.653985	-1.163102
1	0.130782	3.229518	-1.37739
1	1.532456	3.109512	-0.305467
1	1.704229	2.682236	-2.029598
6	2.111711	0.087161	-0.559793
6	3.290186	0.744296	-0.136406

6	2.168322	-1.305853	-0.814321
6	4.479292	0.036977	0.011783
1	3.273501	1.805316	0.086415
6	3.366635	-2.002395	-0.690631
1	1.273179	-1.828374	-1.137153
6	4.521736	-1.334562	-0.269419
1	5.375237	0.551298	0.345758
1	3.399192	-3.064975	-0.910087
1	5.453489	-1.880976	-0.157769

PC_{IVa-r} 3

E = -3924.378363 ZPVE = 0.199564 NIMAG = 0.

17	-2.825915	2.041826	-1.690433
6	0.455206	0.660739	2.270229
1	0.168899	-0.392882	2.358332
1	-0.367417	1.236437	2.713584
6	1.770195	0.938859	3.004944
1	2.025682	2.003332	3.000707
1	1.685294	0.62718	4.051311
1	2.603441	0.386775	2.559708
15	0.407664	1.028623	0.443067
12	-1.933412	0.377232	-0.492983
35	-2.263163	-1.79961	0.449309
6	0.887216	2.802452	0.291329
1	0.105478	3.407605	0.759097
1	1.843261	3.029604	0.769854
1	0.932722	3.078102	-0.765271
6	1.78448	0.058201	-0.295156

6	3.022051	0.626526	-0.636623
6	1.570814	-1.310838	-0.541141
6	4.030202	-0.159376	-1.201294
1	3.211179	1.681708	-0.469018
6	2.585005	-2.093433	-1.095965
1	0.614933	-1.768887	-0.298157
6	3.815593	-1.520611	-1.428455
1	4.981692	0.294513	-1.462641
1	2.407325	-3.149369	-1.276411
1	4.600168	-2.130047	-1.866974

PIV_{a-r} 3

E = -692.175143 ZPVE = 0.195133 NIMAG = 0.

6	-2.141856	-1.170967	0.121008
1	-1.732956	-2.122467	-0.239964
1	-3.206328	-1.184627	-0.147773
6	-1.971225	-1.06675	1.640447
1	-2.440719	-0.16344	2.043068
1	-2.437529	-1.925126	2.138523
1	-0.913912	-1.05063	1.922955
15	-1.367192	0.15401	-0.971805
6	-2.033268	1.709596	-0.193023
1	-3.113541	1.73405	-0.369151
1	-1.854603	1.793682	0.883492
1	-1.600098	2.580999	-0.693064
6	0.391288	0.117111	-0.384866
6	0.994732	1.116247	0.395596
6	1.189965	-0.9622	-0.808193

6	2.345168	1.03318	0.75236
1	0.417447	1.970135	0.735358
6	2.532829	-1.055954	-0.440781
1	0.75794	-1.734396	-1.441098
6	3.117551	-0.054629	0.341419
1	2.790086	1.820082	1.35552
1	3.125717	-1.902904	-0.775074
1	4.165261	-0.119313	0.620478

R1v + a SN2@P-f pathway 2

RC_{va-r} 2

E = -3732.547882 ZPVE = 0.142484 NIMAG = 0.

17	2.333742	-0.007657	1.53493
6	-1.988862	2.420551	-0.064686
1	-1.409009	3.016391	0.658098
1	-1.753444	2.864889	-1.045372
6	-3.495243	2.587417	0.222809
1	-4.112038	2.04176	-0.502024
1	-3.765819	2.20547	1.214996
1	-3.819491	3.63824	0.188225
15	1.54987	0.502748	-0.338942
12	-1.197007	0.465306	-0.054714
35	-1.29153	-1.93758	-0.037089
6	2.546535	1.998362	-0.753219
1	2.293995	2.80869	-0.065218
1	3.619898	1.795915	-0.702152
1	2.28295	2.313338	-1.769261
6	2.282953	-0.792269	-1.420419
1	2.053303	-0.540826	-2.462248

1	3.366975	-0.856308	-1.292158
1	1.816347	-1.751358	-1.184778

TS_{Va-r} 2

E = -3732.504760 ZPVE = 0.140972 NIMAG = 1.

17	-1.053635	-0.862954	-1.705142
6	-0.14543	2.075603	0.471603
1	-1.177542	2.403938	0.568142
1	0.30246	1.937715	1.461884
6	0.659048	2.972724	-0.466349
1	1.688269	2.623805	-0.621673
1	0.180962	3.073013	-1.447707
1	0.745686	3.990859	-0.050698
15	-2.072349	-0.112863	0.942661
12	0.540012	0.116305	-0.348985
35	2.718776	-0.580579	0.310063
6	-3.445472	0.860724	0.183228
1	-3.245569	1.932189	0.222649
1	-3.620235	0.557104	-0.852699
1	-4.352364	0.649821	0.764862
6	-2.790907	-1.811336	0.774134
1	-3.457882	-1.921132	1.643784
1	-3.35948	-1.97798	-0.142374
1	-2.00802	-2.567849	0.861236

PC_{Va-r} 2

E = -3732.599362 ZPVE = 0.144562 NIMAG = 0.

17	1.856773	2.921765	0.286615
6	-2.939713	-1.42866	-0.108536
1	-4.014614	-1.651112	-0.129251
1	-2.485796	-2.1109	-0.838244
6	-2.371395	-1.699091	1.290236
1	-1.285349	-1.565356	1.32541
1	-2.820949	-1.051797	2.049953
1	-2.572206	-2.734765	1.585902
15	-2.793668	0.284047	-0.861491
12	1.595549	0.741201	0.017538
35	2.16539	-1.539195	-0.087231
6	-3.492666	1.36816	0.483733
1	-4.570163	1.189701	0.55835
1	-3.039882	1.206131	1.46743
1	-3.351378	2.416567	0.20339
6	-0.960195	0.635001	-0.604984
1	-0.76028	1.661588	-0.926911
1	-0.70376	0.51458	0.460734
1	-0.407172	-0.0804	-1.226906

P_{Va-r} 2

E = -500.431220 ZPVE = 0.141299 NIMAG = 0.

6	1.209136	-0.000052	-0.708447
1	1.484719	-0.873662	-1.313431
1	1.484767	0.873475	-1.31353
6	2.001727	0.000002	0.60501
1	1.785149	0.884535	1.212665

1	1.785073	-0.884428	1.212787
1	3.079446	-0.000058	0.403163
15	-0.670262	-0.000002	-0.657375
6	-1.016201	-1.426678	0.496883
1	-0.698771	-2.363222	0.026651
1	-0.522949	-1.334669	1.4708
1	-2.096609	-1.491405	0.661269
6	-1.016132	1.426727	0.496837
1	-2.09654	1.491529	0.661196
1	-0.522909	1.33471	1.470768
1	-0.69863	2.363237	0.026587

R1 + b SN2@P-b pathways 2 and 3 in the gas phase

RC1b-i 2

E = -4543.911005 ZPVE = 0.490191 NIMAG = 0.

6	1.328587	-2.064608	0.525775
6	-1.088443	-2.577312	-0.127637
6	-0.424222	-2.587054	2.343996
6	1.037827	-2.724895	1.891624
6	-1.344999	-3.17395	1.264418
6	0.658882	-2.173666	-2.012825
6	-0.651224	-3.237429	3.713518
6	2.061666	-2.579516	-2.499498
6	-0.38767	-2.681067	-3.021476
1	2.367816	-2.284193	0.263409
1	-1.718694	-3.099815	-0.852271
1	-1.416727	-1.531568	-0.150441
1	-0.653505	-1.514557	2.442097

1	1.715084	-2.338215	2.657272
1	1.271037	-3.794774	1.783055
1	-2.39626	-3.02195	1.54038
1	-1.189326	-4.263151	1.227143
1	0.597355	-1.075173	-2.01883
1	-0.016007	-2.783293	4.481995
1	-1.693835	-3.130664	4.03384
1	-0.42301	-4.31027	3.680132
1	2.151161	-3.672864	-2.537882
1	2.242255	-2.197685	-3.50984
1	2.863792	-2.196977	-1.863984
1	-0.465191	-3.775854	-2.992507
1	-0.093481	-2.39987	-4.038349
1	-1.379671	-2.260602	-2.8415
6	2.637263	0.405231	-0.457191
6	2.404392	1.41644	-1.401235
6	3.937929	-0.106327	-0.312066
6	3.441839	1.881719	-2.213063
1	1.421939	1.869131	-1.492535
6	4.975403	0.36762	-1.113401
1	4.148718	-0.862305	0.438816
6	4.726905	1.356632	-2.072066
1	3.244285	2.663503	-2.939991
1	5.977755	-0.031403	-0.988693
1	5.53629	1.7234	-2.696414
17	1.938336	0.292938	2.499979
6	0.388343	-2.677163	-0.565502
1	0.644892	-3.750354	-0.565773
15	1.222728	-0.160917	0.572248
12	-0.937711	1.49678	0.09664

35	0.024938	3.452663	1.085585
6	-2.322258	0.905552	-1.390695
6	-2.720339	0.779014	-2.727556
6	-3.311085	0.614501	-0.445496
6	-4.022529	0.385949	-3.077695
1	-2.012417	0.996656	-3.525882
6	-4.617466	0.226605	-0.727643
6	-4.963651	0.112642	-2.082396
1	-4.304699	0.300072	-4.123925
1	-5.350367	0.01739	0.045312
1	-5.972926	-0.186573	-2.350746
8	-2.803682	0.751684	0.882677
6	-3.711706	0.90986	1.976947
1	-3.103233	1.121121	2.856809
1	-4.39494	1.744518	1.787724
1	-4.28222	-0.010598	2.13862

TS_{1b-i} 2

E = -4543.867859 ZPVE = 0.490831 NIMAG = 1.

6	-1.888368	-0.728016	-1.159831
6	-1.890357	-2.546599	0.66671
6	-0.700377	-2.99476	-1.556762
6	-1.490231	-1.830989	-2.174857
6	-1.478732	-3.596969	-0.377066
6	-3.323405	-0.35742	1.002296
6	-0.357561	-4.051396	-2.61504
6	-4.605422	0.227952	0.378602
6	-3.665784	-0.93832	2.384601

1	-2.573823	-0.052609	-1.679683
1	-2.523453	-3.031501	1.416112
1	-1.009676	-2.176748	1.19591
1	0.244439	-2.596751	-1.159477
1	-0.94683	-1.394256	-3.016271
1	-2.426916	-2.228592	-2.593044
1	-0.88476	-4.386081	0.103169
1	-2.382277	-4.088021	-0.770516
1	-2.619402	0.463928	1.166693
1	0.22582	-3.621353	-3.437106
1	0.223112	-4.874508	-2.182101
1	-1.269489	-4.482544	-3.046586
1	-5.391251	-0.536798	0.336938
1	-4.986901	1.0653	0.973012
1	-4.45288	0.590806	-0.642753
1	-4.35568	-1.787777	2.304628
1	-4.159578	-0.17459	2.99609
1	-2.776638	-1.270911	2.926835
6	-0.850704	2.134733	-0.326064
6	0.151657	2.933262	0.246693
6	-2.122223	2.691423	-0.519193
6	-0.111291	4.251353	0.623444
1	1.150367	2.53959	0.416651
6	-2.391561	4.003689	-0.126756
1	-2.901029	2.118995	-1.007047
6	-1.387382	4.789472	0.444242
1	0.683379	4.851656	1.056058
1	-3.384045	4.415349	-0.28523
1	-1.595052	5.813773	0.739184
17	-0.715632	1.225698	-3.213081

6	-2.665214	-1.378586	0.025695
1	-3.509858	-1.860771	-0.497718
15	-0.387254	0.468688	-0.972087
12	1.971149	0.05802	-0.583678
35	4.180962	0.877164	-0.543654
6	0.419808	-0.099661	1.28043
6	-0.134051	0.539476	2.400765
6	1.321525	-1.133014	1.581371
6	0.154015	0.149101	3.713446
1	-0.820178	1.368603	2.253428
6	1.663927	-1.54111	2.87051
6	1.052006	-0.893234	3.947041
1	-0.314712	0.662023	4.548563
1	2.382282	-2.332157	3.052574
1	1.291453	-1.200105	4.960705
8	1.923745	-1.724828	0.431247
6	2.968568	-2.701601	0.593122
1	3.270301	-2.98967	-0.413765
1	3.819006	-2.268632	1.126679
1	2.578361	-3.573916	1.123417

PC_{1b-i} 2

E = -4543.978525 ZPVE = 0.493369 NIMAG = 0.

6	-1.835649	-0.634327	-1.152467
6	-2.536906	-2.116188	0.800532
6	-0.989223	-3.083156	-1.005665
6	-1.384322	-1.90705	-1.915918
6	-2.089147	-3.368149	0.029717

6	-3.740306	0.213857	0.438649
6	-0.653393	-4.329496	-1.83377
6	-4.797708	0.734534	-0.554986
6	-4.416408	-0.060953	1.792114
1	-2.230034	0.059624	-1.903631
1	-3.364426	-2.387876	1.462845
1	-1.728454	-1.758145	1.447998
1	-0.081388	-2.793993	-0.458983
1	-0.559396	-1.679811	-2.599685
1	-2.232195	-2.21942	-2.543894
1	-1.743748	-4.137816	0.732138
1	-2.962123	-3.794579	-0.488049
1	-3.014162	1.015829	0.607821
1	0.174456	-4.131769	-2.520463
1	-0.359227	-5.163001	-1.185373
1	-1.523033	-4.654754	-2.419318
1	-5.625982	0.019927	-0.636356
1	-5.216098	1.692298	-0.226212
1	-4.396164	0.874946	-1.564711
1	-5.156893	-0.86634	1.716107
1	-4.944781	0.836273	2.133637
1	-3.694941	-0.334845	2.566983
6	-0.518318	2.101405	-1.023536
6	0.638072	2.904618	-1.032068
6	-1.738064	2.676449	-1.411357
6	0.562912	4.249539	-1.395885
1	1.598787	2.492065	-0.736184
6	-1.80612	4.020624	-1.790068
1	-2.64732	2.090257	-1.427222
6	-0.657362	4.813097	-1.778035

1	1.466313	4.851986	-1.387171
1	-2.760663	4.443809	-2.089508
1	-0.710319	5.857728	-2.070472
17	2.526663	-2.286459	-2.259697
6	-2.989612	-1.009105	-0.172442
1	-3.726761	-1.500902	-0.829463
15	-0.291664	0.330706	-0.54584
12	2.145886	-0.618424	-0.785512
35	3.676652	0.983404	0.175798
6	-0.143373	0.390691	1.300897
6	-0.756354	1.367459	2.09642
6	0.751965	-0.501246	1.931952
6	-0.540258	1.430928	3.473643
1	-1.399528	2.103622	1.626213
6	0.972811	-0.453343	3.308175
6	0.316547	0.511448	4.076436
1	-1.029938	2.197809	4.065155
1	1.665404	-1.134198	3.785755
1	0.498448	0.549695	5.14608
8	1.405662	-1.415726	1.109719
6	2.320832	-2.365306	1.704146
1	2.66643	-2.98738	0.877587
1	3.163654	-1.84018	2.161261
1	1.793329	-2.981887	2.43611

RC1b-i 3

E = -4543.901546 ZPVE = 0.489768 NIMAG = 0.

6	3.145089	0.258324	0.285358
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6	3.018114	-0.665006	-2.090042
6	4.634272	-1.73706	-0.406974
6	4.505825	-0.461189	0.443776
6	4.344595	-1.414858	-1.88202
6	1.70836	1.530665	-1.498735
6	6.01102	-2.388009	-0.226395
6	1.982246	2.961537	-1.000653
6	1.29472	1.599047	-2.978979
1	3.18779	1.180392	0.873023
1	2.929208	-0.399585	-3.147621
1	2.176541	-1.333782	-1.863835
1	3.877615	-2.457703	-0.061406
1	4.70131	-0.686542	1.495483
1	5.283586	0.250385	0.128141
1	4.346456	-2.339167	-2.474149
1	5.166544	-0.795566	-2.273037
1	0.839653	1.145835	-0.946417
1	6.191214	-2.652735	0.821375
1	6.097826	-3.302994	-0.823406
1	6.811206	-1.706788	-0.542898
1	1.081987	3.576721	-1.079166
1	2.31067	2.991929	0.042223
1	2.769783	3.426624	-1.607507
1	2.126312	1.938593	-3.609895
1	0.469724	2.307905	-3.096425
1	0.954014	0.634322	-3.368384
6	0.495328	0.374935	1.703124
6	0.779744	1.647174	2.216117
6	-0.814456	-0.126504	1.846868
6	-0.219069	2.416915	2.818711

1	1.784452	2.05074	2.154353
6	-1.811312	0.633487	2.473392
1	-1.04345	-1.133804	1.505729
6	-1.515778	1.91856	2.944073
1	0.018961	3.409441	3.189265
1	-2.801952	0.209025	2.615037
1	-2.287703	2.516448	3.418209
17	2.530519	-1.551723	2.76921
6	2.934779	0.612563	-1.226264
1	3.821623	1.211857	-1.492703
15	1.704221	-0.807913	0.938257
12	-2.694917	0.642333	-0.206594
35	-1.929685	2.803651	-0.844599
6	-4.096593	-0.909039	0.027165
6	-3.366833	-1.799393	-0.767888
6	-5.293473	-1.413711	0.549036
6	-3.731891	-3.109251	-1.062922
6	-5.717368	-2.726617	0.284768
1	-5.922854	-0.781166	1.172753
6	-4.940061	-3.566305	-0.514805
1	-3.130487	-3.764046	-1.685001
1	-6.65207	-3.09239	0.701428
1	-5.265823	-4.581979	-0.719976
8	-2.172908	-1.184539	-1.246832
6	-1.323672	-1.890092	-2.155286
1	-1.877196	-2.160479	-3.060714
1	-0.509797	-1.211282	-2.408967
1	-0.917547	-2.788739	-1.679761

TS_{lb-i} 3

E = -4543.856328 ZPVE = 0.490331 NIMAG = 1.

6	-2.26045	0.987283	0.430042
6	-2.994695	-1.440086	0.849369
6	-4.028857	-0.136091	-1.0962
6	-3.550895	1.160425	-0.422882
6	-4.227732	-1.239453	-0.046775
6	-1.496625	-0.227277	2.640244
6	-5.302044	0.103079	-1.917728
6	-1.524195	1.028926	3.534476
6	-1.700563	-1.463578	3.535667
1	-2.084686	1.938734	0.936101
1	-3.248625	-2.167183	1.626968
1	-2.182568	-1.880635	0.263386
1	-3.242897	-0.468917	-1.791257
1	-3.406683	1.952766	-1.160949
1	-4.340418	1.517753	0.255689
1	-4.488565	-2.186685	-0.537217
1	-5.088042	-0.970148	0.585447
1	-0.503101	-0.319141	2.190913
1	-5.139155	0.863135	-2.689594
1	-5.634894	-0.817005	-2.412694
1	-6.121504	0.450842	-1.27592
1	-0.720534	1.00062	4.279994
1	-1.423991	1.960942	2.970757
1	-2.473842	1.084134	4.080963
1	-2.713907	-1.487507	3.955679
1	-0.999979	-1.44031	4.37854
1	-1.543271	-2.403605	2.998319

6	0.71579	1.797685	-0.207675
6	1.13438	1.880935	1.139338
6	1.59344	2.315837	-1.195908
6	2.352244	2.489202	1.482496
1	0.494192	1.504779	1.926432
6	2.804601	2.91833	-0.847737
1	1.281434	2.29255	-2.236029
6	3.183408	3.017507	0.494743
1	2.642805	2.545764	2.527307
1	3.446915	3.315693	-1.627154
1	4.127176	3.480179	0.76401
17	-1.376963	3.620043	-1.070352
6	-2.54369	-0.113741	1.497498
1	-3.44924	0.27417	1.997342
15	-0.847966	1.027636	-0.917312
12	1.967423	-0.127608	-0.272495
35	4.232505	-0.797118	-0.405203
6	-0.06078	-1.034839	-1.048756
6	0.393928	-2.044188	-0.169263
6	-0.539054	-1.511029	-2.287901
6	0.320665	-3.411282	-0.434957
6	-0.615851	-2.869452	-2.600996
1	-0.895339	-0.779621	-3.009712
6	-0.20879	-3.818834	-1.661893
1	0.67917	-4.149449	0.273073
1	-1.002108	-3.185242	-3.565205
1	-0.280072	-4.879237	-1.884515
8	1.052975	-1.538432	0.971447
6	1.68155	-2.444294	1.900897
1	2.462878	-3.02285	1.401466

1	2.124866	-1.815401	2.672146
1	0.926588	-3.096914	2.345254

PC_{1b-i} 3

E = -4543.871345 ZPVE = 0.491286 NIMAG = 0.

6	-2.385421	0.715817	0.072794
6	-3.642348	-1.447136	0.561999
6	-4.342865	-0.005239	-1.446706
6	-3.571428	1.165788	-0.81843
6	-4.790255	-0.995468	-0.35826
6	-1.866881	-0.545823	2.289268
6	-5.526455	0.486214	-2.289478
6	-1.694142	0.671929	3.219227
6	-2.201223	-1.785722	3.136973
1	-1.983728	1.631673	0.522868
1	-4.058864	-2.079162	1.352875
1	-2.939003	-2.078157	0.004087
1	-3.651564	-0.536215	-2.12164
1	-3.220049	1.855679	-1.594071
1	-4.249774	1.752752	-0.18309
1	-5.263803	-1.871459	-0.82127
1	-5.56599	-0.513887	0.256344
1	-0.907637	-0.737417	1.796114
1	-5.193412	1.159716	-3.087029
1	-6.058447	-0.351453	-2.755785
1	-6.246442	1.035266	-1.670001
1	-0.851018	0.527929	3.906381
1	-1.5388	1.611426	2.679161

1	-2.592584	0.806746	3.834257
1	-3.184408	-1.687891	3.613494
1	-1.465811	-1.904402	3.941992
1	-2.203258	-2.708893	2.549277
6	0.408543	1.33493	-0.834059
6	0.665438	2.024923	0.38443
6	1.249483	1.606951	-1.941526
6	1.832511	2.813211	0.513099
1	0.087521	1.802563	1.266542
6	2.375086	2.439762	-1.827856
1	1.026473	1.138253	-2.896454
6	2.673078	3.031468	-0.586001
1	2.034672	3.298491	1.46169
1	3.020175	2.602992	-2.684097
1	3.557591	3.65023	-0.476296
17	-1.163338	4.012944	0.691908
6	-2.91127	-0.237163	1.180152
1	-3.698438	0.354333	1.677875
15	-1.020471	0.186927	-1.170463
12	2.544362	0.489692	-0.122611
35	4.701959	-0.459052	-0.125541
6	-0.269479	-1.498591	-0.826345
6	0.78488	-1.884314	0.024917
6	-0.776407	-2.510962	-1.668358
6	1.307136	-3.179475	0.033162
6	-0.301272	-3.820557	-1.644997
1	-1.566926	-2.245743	-2.364552
6	0.753921	-4.154597	-0.795437
1	2.148793	-3.424689	0.670278
1	-0.736468	-4.566198	-2.302901

1	1.159261	-5.161378	-0.783131
8	1.362172	-0.908636	0.869878
6	1.81108	-1.33742	2.185637
1	2.785311	-1.825502	2.117701
1	1.889613	-0.42922	2.785851
1	1.062262	-2.001892	2.619055

R1_{II} + b S_{N2}@P-b pathways 2 and 3 in the gas phase

RC_{IIb-i} 2

E = -4235.421739 ZPVE = 0.370945 NIMAG = 0.

15	-1.552059	-0.388426	-0.068136
17	-3.09579	0.617821	-1.072493
6	-2.048579	-0.150503	1.758477
6	-0.950122	-0.804817	2.627651
1	-1.135053	-0.535816	3.674731
1	-0.956131	-1.89489	2.565753
1	0.051656	-0.447716	2.368348
6	-3.431977	-0.701228	2.136961
1	-3.677634	-0.373584	3.154727
1	-4.216579	-0.330674	1.471232
1	-3.455718	-1.793949	2.132035
6	-2.013273	1.378086	1.99832
1	-2.136001	1.565292	3.07171
1	-1.068065	1.829383	1.679445
1	-2.817784	1.894048	1.469028
12	0.83931	0.784606	-0.662534
35	0.25495	3.096429	-0.953905
6	2.373089	-0.674367	-0.79243
6	3.072516	-1.685429	-1.468022

6	2.863759	-0.364396	0.480957
6	4.196785	-2.310188	-0.906698
6	3.973037	-0.946569	1.089272
6	4.646226	-1.93876	0.36397
1	4.727087	-3.080385	-1.461047
1	4.312499	-0.659834	2.080191
1	5.519072	-2.41862	0.797548
6	-1.763325	-2.162226	-0.743722
6	-3.194571	-2.722263	-0.698985
1	-3.206505	-3.693409	-1.209005
1	-3.54661	-2.884199	0.321866
1	-3.906263	-2.069567	-1.210826
6	-1.295007	-2.068647	-2.21624
1	-0.256523	-1.729703	-2.291307
1	-1.34763	-3.067249	-2.666381
1	-1.928606	-1.402889	-2.808925
6	-0.798854	-3.093148	0.023121
1	0.216075	-2.687293	0.084147
1	-1.155107	-3.313331	1.03256
1	-0.735773	-4.046585	-0.514951
8	2.059515	0.624097	1.126577
6	2.688046	1.597741	1.973257
1	3.551213	2.041107	1.466178
1	1.938878	2.366853	2.164815
1	3.003286	1.142517	2.917339
1	2.757957	-1.988848	-2.46567

TS_{nb-i} 2

E = -4235.356037 ZPVE = 0.371328 NIMAG = 1.

15	1.268113	-0.365474	-0.13985
17	2.425508	-2.506514	-0.486986
6	1.612994	-0.142875	1.756992
6	1.968806	1.306377	2.147171
1	2.010597	1.363808	3.242884
1	2.955836	1.593084	1.776513
1	1.230379	2.028126	1.804454
6	2.739522	-1.06318	2.272856
1	2.865389	-0.860204	3.344247
1	2.50551	-2.119513	2.143869
1	3.694284	-0.874039	1.779539
6	0.29814	-0.572075	2.446185
1	0.42433	-0.514223	3.534477
1	-0.539316	0.083352	2.190651
1	0.048506	-1.617857	2.224339
12	-1.019131	-1.1701	-0.349235
35	-2.938814	-2.431411	0.120368
6	-0.576918	1.112698	-0.445897
6	-1.026992	0.827358	-1.752036
6	-1.314561	2.115191	0.235626
6	-2.096119	1.479912	-2.386368
6	-2.386879	2.785141	-0.373408
6	-2.768571	2.471598	-1.682666
1	-2.386384	1.213887	-3.397929
1	-2.9435	3.544598	0.163307
1	-3.604719	2.998122	-2.133157
6	2.516448	0.640439	-1.251307
6	3.962843	0.413693	-0.759274
1	4.637479	0.919526	-1.460843

1	4.13889	0.847765	0.227418
1	4.227007	-0.64407	-0.734932
6	2.400411	0.102115	-2.693704
1	1.430166	0.330193	-3.143102
1	3.162358	0.595391	-3.309832
1	2.571727	-0.975325	-2.737113
6	2.232244	2.156061	-1.251874
1	1.26579	2.399469	-1.694246
1	2.270995	2.591465	-0.251838
1	3.009078	2.641789	-1.855992
8	-0.934176	2.385819	1.521165
6	-1.669812	3.335129	2.288412
1	-2.717693	3.031747	2.398993
1	-1.192764	3.353729	3.269012
1	-1.619921	4.335517	1.842058
1	-0.4872	0.075077	-2.341883

PC_{IIb-i} 2

E = -4235.475300 ZPVE = 0.373233 NIMAG = 0.

15	-0.200191	0.633091	0.054988
17	3.438316	1.701605	-1.520588
6	-0.328521	0.806207	1.967126
6	-1.436472	1.736255	2.492647
1	-1.415613	1.715945	3.589681
1	-1.288108	2.775348	2.187012
1	-2.423904	1.411265	2.166224
6	1.043407	1.348732	2.438819
1	1.020403	1.490282	3.526023

1	1.853536	0.637081	2.236308
1	1.295135	2.31462	1.990103
6	-0.518532	-0.610266	2.550778
1	-0.403462	-0.557519	3.640503
1	-1.514065	-1.004205	2.335151
1	0.227539	-1.316132	2.173653
12	2.330346	0.117697	-0.371036
35	2.870161	-1.977556	0.64692
6	-1.234395	-0.778316	-0.544976
6	-0.586466	-1.706532	-1.376871
6	-2.608159	-0.993579	-0.276179
6	-1.255228	-2.784118	-1.959441
6	-3.285905	-2.075823	-0.852427
6	-2.610152	-2.961834	-1.694727
1	-0.715454	-3.477373	-2.59557
1	-4.337035	-2.237336	-0.648147
1	-3.15156	-3.795234	-2.132557
6	-0.763892	2.187305	-0.914234
6	0.08214	3.391245	-0.446182
1	-0.153506	4.252052	-1.083667
1	-0.140154	3.682092	0.584234
1	1.155685	3.203665	-0.540633
6	-0.429318	1.89387	-2.395294
1	-0.98374	1.03082	-2.776675
1	-0.714762	2.764123	-2.998752
1	0.640812	1.727515	-2.550802
6	-2.261617	2.525729	-0.807028
1	-2.888618	1.71716	-1.188727
1	-2.572464	2.745023	0.215461
1	-2.458513	3.41728	-1.415904

8	-3.216107	-0.113423	0.572037
6	-4.603161	-0.2694	0.862532
1	-4.802059	-1.229302	1.353048
1	-4.855279	0.543848	1.544168
1	-5.211825	-0.184692	-0.045332
1	0.475204	-1.597349	-1.572945

RC_{nb-i} 3

E = -4235.421339 ZPVE = 0.370731 NIMAG = 0.

15	1.510678	-0.404708	0.14795
17	2.820385	0.755462	1.306623
6	-4.138287	-1.033055	0.526607
6	-2.953998	-0.367126	0.222754
6	-2.31235	-0.365287	-1.021168
6	-2.943993	-1.124607	-2.015871
6	-4.135658	-1.825001	-1.769024
6	-4.73031	-1.774835	-0.505623
1	-4.597539	-0.993156	1.509654
1	-4.605629	-2.399967	-2.562849
1	-5.656438	-2.309672	-0.3149
12	-0.799382	0.961607	-0.34572
35	-0.083326	3.244483	-0.187087
1	-2.516064	-1.170596	-3.016342
8	-2.220168	0.393273	1.18165
6	-2.9052	0.995807	2.285867
1	-2.190971	1.669283	2.760774
1	-3.770518	1.564829	1.930133
1	-3.227224	0.233477	3.002502

6	1.34318	-1.980473	1.210749
6	0.308859	-2.902614	0.524947
1	-0.619945	-2.379494	0.278704
1	0.695787	-3.359724	-0.388108
1	0.058102	-3.715905	1.216499
6	0.750092	-1.501829	2.557933
1	-0.172213	-0.92884	2.418064
1	0.50566	-2.38329	3.162745
1	1.45692	-0.890928	3.124369
6	2.652951	-2.741974	1.467681
1	3.030734	-3.225167	0.563023
1	3.434466	-2.09106	1.870125
1	2.465592	-3.5326	2.204906
6	2.515922	-0.629524	-1.45938
6	3.985522	-1.039881	-1.268365
1	4.088584	-2.036548	-0.834967
1	4.475019	-1.054192	-2.249967
1	4.527688	-0.33105	-0.637616
6	2.460872	0.752367	-2.153926
1	2.915857	1.539411	-1.547154
1	3.011361	0.690387	-3.100296
1	1.438079	1.065324	-2.387189
6	1.783301	-1.663444	-2.342168
1	1.92779	-2.685968	-1.984521
1	0.70748	-1.470239	-2.415257
1	2.195617	-1.610071	-3.356747

TS_{nb-i} 3

E = -4235.363210 ZPVE = 0.369212 NIMAG = 1.

15	-1.458399	-0.303596	0.160083
17	-0.515548	-2.591208	1.183174
6	1.778918	3.101605	0.304075
6	1.322728	1.786897	0.278469
6	0.719016	1.17519	-0.832072
6	0.526726	1.998454	-1.949837
6	0.942505	3.338184	-1.964829
6	1.566227	3.883751	-0.840696
1	2.281273	3.525368	1.167811
1	0.794038	3.947873	-2.852136
1	1.899066	4.917571	-0.847264
12	1.082797	-0.844164	0.19672
35	3.257291	-1.69791	-0.335636
1	0.064867	1.594175	-2.849895
8	1.474098	0.897768	1.371212
6	2.516895	1.138512	2.331673
1	2.536047	0.265863	2.984669
1	3.479508	1.243543	1.823614
1	2.290736	2.03113	2.92209
6	-2.688123	0.696361	1.229135
6	-2.67323	2.159485	0.715505
1	-1.660659	2.569103	0.663636
1	-3.134626	2.262683	-0.269265
1	-3.248763	2.773534	1.420441
6	-2.062082	0.655504	2.644279
1	-1.036618	1.037075	2.643713
1	-2.658129	1.284496	3.316898
1	-2.045395	-0.359954	3.051133
6	-4.130942	0.168217	1.299809

1	-4.653904	0.239629	0.343593
1	-4.171248	-0.868804	1.645634
1	-4.688577	0.777873	2.022592
6	-2.289434	-0.944733	-1.43368
6	-3.301593	-2.0751	-1.133234
1	-4.175702	-1.726659	-0.581559
1	-3.654198	-2.477777	-2.091155
1	-2.83727	-2.891935	-0.57523
6	-1.150264	-1.532891	-2.300045
1	-0.667369	-2.383437	-1.808787
1	-1.576766	-1.903453	-3.240049
1	-0.388799	-0.788391	-2.548009
6	-2.980378	0.19866	-2.209426
1	-3.856727	0.588481	-1.686189
1	-2.299877	1.029498	-2.415643
1	-3.323935	-0.196914	-3.173665

PC_{III-i} 3

E = -4235.495754 ZPVE = 0.373820 NIMAG = 0.

15	0.935874	-0.567341	0.06965
17	-2.1106	-1.892654	-2.347353
6	0.037041	3.406051	-0.619996
6	0.018498	2.00933	-0.594008
6	1.078538	1.274722	-0.012929
6	2.159311	2.003246	0.506894
6	2.198783	3.397757	0.469551
6	1.13038	4.094981	-0.091569
1	-0.785163	3.964922	-1.047709

1	3.050549	3.92959	0.881204
1	1.136447	5.180265	-0.12018
12	-1.594292	-0.691275	-0.493863
35	-2.940954	-0.114701	1.424483
1	2.988447	1.469124	0.956822
8	-1.031611	1.289567	-1.147315
6	-2.124298	1.997086	-1.776065
1	-2.76714	1.224161	-2.198377
1	-2.672873	2.582542	-1.034173
1	-1.744707	2.630106	-2.581805
6	2.13699	-1.213293	-1.274734
6	3.587987	-0.71502	-1.144148
1	3.6475	0.376344	-1.183612
1	4.077444	-1.057713	-0.230895
1	4.167791	-1.102273	-1.991365
6	1.566909	-0.713814	-2.622259
1	1.56873	0.379228	-2.684176
1	2.205488	-1.088822	-3.431536
1	0.551519	-1.076625	-2.803963
6	2.096935	-2.755554	-1.261949
1	2.54029	-3.177348	-0.35517
1	1.076238	-3.136682	-1.365759
1	2.676551	-3.132212	-2.113365
6	1.378587	-1.1205	1.853766
6	0.651403	-2.472248	2.059145
1	0.985142	-3.242112	1.357618
1	0.857132	-2.837954	3.072427
1	-0.433079	-2.361003	1.963435
6	0.772571	-0.094706	2.836451
1	-0.285204	0.096805	2.63386

1	0.845243	-0.504703	3.85126
1	1.306355	0.858625	2.822469
6	2.876577	-1.302414	2.159319
1	3.331917	-2.094219	1.55881
1	3.453532	-0.384748	2.015208
1	2.984453	-1.590511	3.212364

R1_{III} + b S_{N2}@P-b pathway 2 in the gas phase

R1_{IIIb-i} 2

E = -1264.903326 ZPVE = 0.183787 NIMAG = 0.

15	0.063678	1.068272	0.893116
6	-1.442016	0.136885	0.352956
6	-2.137072	0.322641	-0.850194
6	-1.919391	-0.811008	1.275273
6	-3.276856	-0.436791	-1.131042
1	-1.796248	1.065993	-1.563155
6	-3.050588	-1.576726	0.987645
1	-1.408357	-0.951053	2.225401
6	-3.733205	-1.390349	-0.217914
1	-3.807592	-0.280036	-2.065901
1	-3.404264	-2.307684	1.709017
1	-4.619918	-1.977317	-0.438929
17	0.123111	2.645114	-0.539789
6	1.424052	-0.010708	0.260035
6	1.313835	-0.874059	-0.842267
6	2.642977	0.055451	0.955452
6	2.402767	-1.649535	-1.24145
1	0.376712	-0.94349	-1.385522
6	3.733905	-0.71977	0.553698

1	2.737676	0.715792	1.813848
6	3.614292	-1.572833	-0.545629
1	2.306943	-2.314608	-2.095006
1	4.67117	-0.658813	1.099086
1	4.459612	-2.178999	-0.858549

RC_{mb-i} 2

E = -4383.012221 ZPVE = 0.307512 NIMAG = 0.

15	1.544664	1.316197	0.097987
6	1.370033	0.111856	1.482338
6	1.234038	-1.280699	1.355403
6	1.347946	0.687692	2.764998
6	1.069988	-2.077873	2.490447
1	1.225539	-1.751275	0.377655
6	1.221127	-0.117196	3.899503
1	1.418008	1.76684	2.877934
6	1.081577	-1.500857	3.763257
1	0.937991	-3.148928	2.372568
1	1.210402	0.339232	4.884865
1	0.960169	-2.124421	4.644105
17	0.462136	0.228251	-1.470215
6	-4.281875	2.243733	-0.522345
6	-3.39997	1.169534	-0.457953
6	-2.685041	0.768194	0.676631
6	-2.908883	1.532887	1.826407
6	-3.785109	2.631597	1.824706
6	-4.465548	2.981743	0.65737
1	-4.81407	2.516446	-1.428051

1	-3.939726	3.208738	2.732684
1	-5.145503	3.829176	0.653338
12	-1.743118	-0.820231	-0.337151
35	-1.2786	-3.118089	-0.84047
1	-2.39395	1.281125	2.751996
8	-3.110974	0.317432	-1.5595
6	-3.770152	0.50191	-2.811158
1	-3.40683	-0.288813	-3.468263
1	-4.855067	0.411753	-2.689443
1	-3.522477	1.481048	-3.23561
6	3.256253	1.046009	-0.518576
6	4.021179	-0.115587	-0.319374
6	3.824277	2.127314	-1.216552
6	5.319585	-0.196804	-0.821916
1	3.606724	-0.954608	0.228498
6	5.123296	2.042647	-1.721617
1	3.24614	3.035726	-1.36622
6	5.871773	0.879863	-1.524217
1	5.901921	-1.099843	-0.664172
1	5.549779	2.882827	-2.261467
1	6.883907	0.812408	-1.912423

TS_{imb-i} 2

E = -4382.974169 ZPVE = 0.306602 NIMAG = 1.

15	1.205575	0.055178	-0.517356
6	1.695323	-1.568203	0.186634
6	1.094784	-2.776756	-0.218853
6	2.591354	-1.594306	1.279761

6	1.393795	-3.970539	0.438045
1	0.412426	-2.782951	-1.060562
6	2.865926	-2.787527	1.947406
1	3.056278	-0.677753	1.62747
6	2.272373	-3.980184	1.525043
1	0.934079	-4.894258	0.099793
1	3.546225	-2.78375	2.79398
1	2.494147	-4.911005	2.038753
17	-0.519736	-0.87349	-2.504564
6	-1.576703	2.622048	2.045333
6	-1.503802	1.670335	1.033624
6	-1.039642	0.350518	1.19675
6	-0.583137	0.032796	2.487219
6	-0.610097	0.962294	3.537124
6	-1.105932	2.249206	3.314143
1	-1.977461	3.617482	1.882164
1	-0.258337	0.681842	4.526419
1	-1.136363	2.971399	4.125099
12	-1.981312	-0.245565	-0.694132
35	-4.31009	-0.830826	-0.740068
1	-0.201475	-0.966731	2.68909
8	-1.94226	1.899649	-0.285935
6	-2.840212	2.98366	-0.558059
1	-3.149744	2.867833	-1.596644
1	-3.715172	2.926088	0.09654
1	-2.329738	3.943757	-0.43081
6	2.848045	0.834484	-0.693493
6	4.078786	0.170836	-0.904616
6	2.822012	2.247666	-0.763002
6	5.240192	0.898621	-1.149873

1	4.117817	-0.912844	-0.88621
6	3.990781	2.973733	-0.978595
1	1.876812	2.769735	-0.636332
6	5.199747	2.298381	-1.177385
1	6.177844	0.378899	-1.323142
1	3.960327	4.058599	-1.007634
1	6.109648	2.861475	-1.363824

PC_{nv-i} 2

E = -4383.098363 ZPVE = 0.310816 NIMAG = 0.

15	-0.620981	0.070375	-0.205813
6	-1.344542	1.738556	-0.463753
6	-0.465468	2.783516	-0.801572
6	-2.721545	1.993355	-0.377952
6	-0.964032	4.068052	-1.02334
1	0.602057	2.594229	-0.883439
6	-3.213745	3.280639	-0.610991
1	-3.412275	1.190861	-0.139521
6	-2.336055	4.320104	-0.927772
1	-0.277367	4.869513	-1.27882
1	-4.281758	3.467389	-0.545722
1	-2.719457	5.320104	-1.108927
17	1.575497	-2.471285	-2.606972
6	1.628035	-0.805203	3.124421
6	1.084654	-0.769086	1.841678
6	0.005796	0.083149	1.528674
6	-0.486195	0.924362	2.533269
6	0.049805	0.899252	3.823234

6	1.099651	0.029256	4.114245
1	2.460701	-1.456124	3.359933
1	-0.347596	1.557026	4.589545
1	1.52814	0.002795	5.111451
12	1.661549	-0.707365	-1.199678
35	3.097557	1.198074	-0.875523
1	-1.292348	1.612713	2.298185
8	1.570824	-1.555974	0.802559
6	2.482311	-2.636809	1.101277
1	2.615246	-3.168624	0.158806
1	3.439634	-2.244969	1.455691
1	2.033517	-3.299361	1.845829
6	-2.01629	-1.125132	-0.21246
6	-2.264647	-1.818758	-1.408543
6	-2.82136	-1.379852	0.909535
6	-3.318326	-2.732137	-1.487158
1	-1.623447	-1.664219	-2.271566
6	-3.869787	-2.298945	0.828866
1	-2.626626	-0.870483	1.848308
6	-4.122654	-2.9721	-0.370357
1	-3.497953	-3.265154	-2.415875
1	-4.485693	-2.490688	1.70282
1	-4.936811	-3.688535	-0.429813

Результат 2

E = -1150.877424 ZPVE = 0.305833 NIMAG = 0.

15	0.203951	0.017404	-1.044332
6	1.911532	-0.457265	-0.485859

6	2.593016	-1.405177	-1.26943
6	2.572948	0.091101	0.624793
6	3.888031	-1.812606	-0.940351
1	2.105185	-1.823744	-2.14649
6	3.874044	-0.305263	0.947926
1	2.074098	0.834355	1.238709
6	4.533536	-1.260723	0.169905
1	4.395309	-2.549869	-1.556444
1	4.371205	0.133138	1.809025
1	5.544622	-1.567435	0.422432
6	-3.105073	-2.001137	0.377718
6	-2.251668	-1.095799	-0.262598
6	-0.853067	-1.136606	-0.046948
6	-0.352855	-2.112955	0.82225
6	-1.197941	-3.025463	1.465076
6	-2.571276	-2.965161	1.240319
1	-4.175401	-1.965036	0.212731
1	-0.78065	-3.771755	2.134151
1	-3.239872	-3.665784	1.732427
1	0.716079	-2.165082	1.000119
8	-2.683213	-0.120188	-1.115494
6	-4.069444	-0.019811	-1.4141
1	-4.160567	0.807934	-2.118287
1	-4.44504	-0.939131	-1.880444
1	-4.656207	0.20176	-0.513938
6	-0.048359	1.6435	-0.18589
6	0.334461	2.800523	-0.885196
6	-0.609477	1.78839	1.092315
6	0.181067	4.066714	-0.315749
1	0.752708	2.708646	-1.884681

6	-0.775607	3.055611	1.658943
1	-0.920831	0.908762	1.647843
6	-0.37752	4.19781	0.958984
1	0.487437	4.949054	-0.870857
1	-1.213879	3.148668	2.649059
1	-0.505861	5.181868	1.400943

R1_{IV} + b S_{N2}@P-b pathways 2 and 3 in the gas phase

RC_{IVb-i} 2

E = -4191.276335 ZPVE = 0.254857 NIMAG = 0.

17	1.330985	-1.767151	2.415651
15	0.891156	-1.090295	0.467579
12	-0.997997	0.876783	0.589574
35	0.22723	2.933225	0.80341
6	0.255925	-2.647538	-0.281141
1	0.09069	-2.472073	-1.349196
1	0.940194	-3.488558	-0.148647
1	-0.703378	-2.882617	0.185702
6	2.531728	-0.828745	-0.29273
6	2.946786	0.503282	-0.465148
6	3.367901	-1.876749	-0.715788
6	4.181479	0.777592	-1.059042
1	2.318322	1.320115	-0.11952
6	4.596659	-1.595177	-1.310774
1	3.070248	-2.911234	-0.576927
6	5.004108	-0.267163	-1.483791
1	4.49639	1.808785	-1.186701
1	5.238258	-2.409081	-1.635346
1	5.963041	-0.05107	-1.945875

6	-2.764534	-0.288215	0.564456
6	-3.760848	-1.043243	1.197567
6	-2.915325	-0.148747	-0.820701
6	-4.831594	-1.603141	0.481504
6	-3.954746	-0.672984	-1.583695
6	-4.928861	-1.414644	-0.899282
1	-5.593654	-2.178251	1.001092
1	-4.02687	-0.526574	-2.657091
1	-5.760972	-1.840804	-1.452548
1	-3.720643	-1.196988	2.274546
8	-1.832927	0.593676	-1.379299
6	-1.990644	1.265817	-2.631883
1	-1.109408	1.897078	-2.751914
1	-2.045146	0.544908	-3.454301
1	-2.893005	1.886592	-2.620183

TS_{IVb-i} 2

E = -4191.246087 ZPVE = 0.255072 NIMAG = 1.

17	-1.27569	-3.390114	0.670545
15	-0.685437	-1.093615	0.852233
12	1.531865	-0.536098	-0.001422
35	3.827211	-0.907362	-0.332402
6	-1.071982	-1.026011	2.659927
1	-1.752065	-0.206878	2.899178
1	-1.527127	-1.974858	2.939593
1	-0.141809	-0.89157	3.218294
6	-2.154874	-0.514214	-0.105854
6	-2.384357	-1.072727	-1.372212

6	-3.034019	0.46555	0.374771
6	-3.466929	-0.650421	-2.145956
1	-1.738822	-1.864562	-1.73758
6	-4.126897	0.874814	-0.392799
1	-2.868964	0.927605	1.342158
6	-4.344559	0.320611	-1.656562
1	-3.633181	-1.095095	-3.122856
1	-4.804387	1.628469	-0.001869
1	-5.193772	0.640246	-2.253525
6	0.055965	1.109788	0.932403
6	-0.103578	1.959387	2.039248
6	0.415499	1.754554	-0.26396
6	0.028272	3.349883	1.943588
6	0.560641	3.13289	-0.409081
6	0.344366	3.934462	0.716308
1	-0.116222	3.972518	2.821852
1	0.836483	3.586319	-1.354352
1	0.442825	5.012266	0.629419
1	-0.358107	1.539607	3.009077
8	0.706614	0.847165	-1.314445
6	1.135749	1.337881	-2.595624
1	1.287897	0.457184	-3.218978
1	0.354187	1.967028	-3.029129
1	2.073873	1.892744	-2.502524

PC_{IVb-i} 2

E = -4191.352321 ZPVE = 0.257268 NIMAG = 0.

17	-0.751711	-3.221361	1.337932
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15	0.62241	-0.004951	-0.932336
12	-1.297845	-1.375349	0.146996
35	-3.133633	-0.625353	-1.211268
6	0.664874	0.402056	-2.731207
1	1.398611	1.17452	-2.976081
1	0.923579	-0.51046	-3.275471
1	-0.334544	0.72054	-3.038797
6	2.371471	-0.32844	-0.46499
6	2.696327	-1.630805	-0.053074
6	3.383153	0.643706	-0.532327
6	4.014766	-1.955727	0.279649
1	1.919573	-2.385964	0.032114
6	4.697672	0.316317	-0.19829
1	3.14826	1.660686	-0.833069
6	5.015758	-0.985784	0.204162
1	4.252965	-2.96502	0.601492
1	5.472914	1.075337	-0.25081
1	6.039612	-1.238195	0.46432
6	0.147145	1.578883	-0.113125
6	0.442218	2.848016	-0.626758
6	-0.598839	1.508701	1.082296
6	0.045168	4.012799	0.033871
6	-1.002431	2.662916	1.752312
6	-0.670271	3.914166	1.226014
1	0.289749	4.984613	-0.382654
1	-1.57977	2.603171	2.666398
1	-0.989425	4.810192	1.749328
1	0.987487	2.933548	-1.561303
8	-0.912289	0.236898	1.5489
6	-1.384098	0.08036	2.907064

1	-1.405372	-0.995668	3.08018
1	-0.682642	0.558392	3.595566
1	-2.385913	0.505081	3.014616

PIVb-i 2

E = -959.133318 ZPVE = 0.252569 NIMAG = 0.

15	0.223995	-1.041484	1.231096
6	0.430105	-2.844898	0.789244
1	0.431279	-3.03822	-0.288482
1	1.391419	-3.168224	1.199513
1	-0.353396	-3.441045	1.267341
6	1.600771	-0.324559	0.205367
6	2.738107	0.148794	0.876918
6	1.573587	-0.259598	-1.196901
6	3.828284	0.662746	0.167313
1	2.767057	0.121013	1.963424
6	2.657721	0.259379	-1.908281
1	0.697355	-0.608535	-1.736835
6	3.789617	0.720095	-1.227654
1	4.701353	1.023376	0.704366
1	2.619286	0.304702	-2.993458
1	4.632677	1.123393	-1.781637
6	-1.276883	-0.586929	0.24492
6	-2.107221	-1.515867	-0.393481
6	-1.676849	0.771571	0.229032
6	-3.289618	-1.129126	-1.037046
6	-2.85172	1.170401	-0.416811
6	-3.655436	0.214267	-1.048309

1	-3.911139	-1.874564	-1.523728
1	-3.149228	2.212201	-0.431549
1	-4.567747	0.531412	-1.545311
1	-1.835442	-2.566097	-0.394344
8	-0.837859	1.632892	0.876131
6	-1.161256	3.016203	0.923114
1	-0.359005	3.487885	1.491685
1	-1.198531	3.451253	-0.083333
1	-2.118251	3.185686	1.432315

RC_{IVb-i} 3

E = -4191.268604 ZPVE = 0.254134 NIMAG = 0.

17	0.687729	-1.118336	-0.308871
15	1.649193	0.837194	-0.054253
12	-1.951428	-0.820868	-0.300194
35	-2.539295	-3.123726	-0.192854
6	1.501509	1.41971	-1.802906
1	2.090726	2.339584	-1.893755
1	1.845348	0.695326	-2.544942
1	0.451674	1.659431	-1.98857
6	3.399273	0.28438	0.04861
6	3.999281	0.383091	1.316332
6	4.164097	-0.194568	-1.029219
6	5.333992	0.015899	1.503976
1	3.418841	0.752241	2.158026
6	5.496766	-0.559624	-0.84203
1	3.723158	-0.292801	-2.015892
6	6.083543	-0.454813	0.424168
1	5.784702	0.097936	2.48846

1	6.077671	-0.929593	-1.681785
1	7.121573	-0.741054	0.565997
6	-2.244405	1.218946	-0.768195
6	-2.444524	2.254801	-1.688482
6	-2.26584	1.60449	0.577835
6	-2.631699	3.585583	-1.27671
6	-2.453232	2.900778	1.047882
6	-2.634169	3.90351	0.082749
1	-2.784191	4.369289	-2.014269
1	-2.462418	3.148822	2.104421
1	-2.783984	4.930297	0.404382
1	-2.460964	2.03555	-2.75517
8	-2.07336	0.477924	1.422737
6	-2.149796	0.613351	2.841368
1	-2.012096	-0.387044	3.252469
1	-1.358675	1.277091	3.20666
1	-3.130096	1.002957	3.136605

TS_{IVb-i} 3

E = -4191.234079 ZPVE = 0.253803 NIMAG = 1.

17	-0.136102	-2.663419	0.267603
15	1.433741	-0.536861	-0.233221
12	-1.668486	-0.819462	-0.011065
35	-4.042386	-1.095683	-0.170128
6	1.40646	-1.034514	-2.016454
1	1.879208	-0.259856	-2.628892
1	1.936835	-1.979994	-2.160593
1	0.373267	-1.155251	-2.339516

6	3.246902	-0.380156	0.006502
6	3.613628	0.038399	1.306396
6	4.274743	-0.635314	-0.929345
6	4.952304	0.198047	1.660724
1	2.833756	0.235412	2.038357
6	5.611621	-0.4795	-0.57485
1	4.032255	-0.958842	-1.935702
6	5.951652	-0.06211	0.719134
1	5.216508	0.52008	2.663345
1	6.392534	-0.680945	-1.302247
1	6.996548	0.058046	0.990274
6	-0.716862	1.032298	-0.75879
6	-0.401163	1.880968	-1.834115
6	-1.076948	1.6883	0.435815
6	-0.45016	3.277961	-1.722554
6	-1.16522	3.066823	0.591839
6	-0.827177	3.864159	-0.512702
1	-0.203541	3.904763	-2.575122
1	-1.479727	3.528876	1.521913
1	-0.87286	4.945462	-0.420466
1	-0.120152	1.451119	-2.794812
8	-1.400748	0.766206	1.448902
6	-2.157797	1.197702	2.588401
1	-2.386336	0.297322	3.158299
1	-1.564005	1.88169	3.202697
1	-3.08725	1.677552	2.267571

PCIVb-i 3

E = -4191.352321 ZPVE = 0.257268 NIMAG = 0.

17	-0.751572	-3.221179	1.338243
15	0.62245	-0.004935	-0.932259
12	-1.297778	-1.375358	0.147052
35	-3.133582	-0.625634	-1.211342
6	0.664907	0.40196	-2.731158
1	1.39862	1.174431	-2.97608
1	0.923641	-0.510584	-3.275363
1	-0.33452	0.720393	-3.038771
6	2.371508	-0.328444	-0.46491
6	2.696347	-1.630841	-0.05308
6	3.383202	0.643696	-0.532165
6	4.014779	-1.955801	0.279634
1	1.919586	-2.385998	0.032052
6	4.697714	0.316267	-0.198135
1	3.148326	1.6607	-0.832833
6	5.015783	-0.985864	0.204228
1	4.252962	-2.965119	0.601411
1	5.472963	1.075284	-0.250591
1	6.039631	-1.238304	0.464382
6	0.147178	1.578947	-0.113147
6	0.442336	2.848043	-0.626825
6	-0.598947	1.508858	1.082194
6	0.045241	4.012878	0.033683
6	-1.002593	2.663128	1.752084
6	-0.670341	3.914337	1.225748
1	0.289893	4.984659	-0.382876
1	-1.58004	2.603458	2.666106
1	-0.989537	4.810403	1.748968
1	0.987709	2.933505	-1.561315

8	-0.912468	0.237099	1.548853
6	-1.384621	0.080684	2.906908
1	-1.405938	-0.995328	3.080122
1	-0.68334	0.558768	3.595551
1	-2.386463	0.505416	3.014169

R1_v + b S_{N2}@P-b pathway 2 in the gas phase

RC_{v_b-i 2}

E = -3999.532798 ZPVE = 0.201327 NIMAG = 0.

17	-0.923657	2.79407	1.102911
15	-1.433425	1.449822	-0.431891
12	-0.142915	-0.962961	-0.236076
35	-2.161606	-2.245668	-0.040007
6	-3.269955	1.469628	-0.338167
1	-3.589413	1.013231	0.601221
1	-3.668973	2.484452	-0.418286
1	-3.652248	0.850078	-1.156374
6	-1.091908	2.463428	-1.93213
1	-1.603312	3.429271	-1.898804
1	-0.014215	2.617191	-2.026048
1	-1.437301	1.897731	-2.805124
6	1.838499	-0.613968	-0.868088
6	2.28245	-0.343066	0.431552
6	2.815687	-0.516982	-1.865307
6	3.578184	0.017697	0.787644
6	4.140819	-0.154964	-1.569994
1	2.553994	-0.723231	-2.901924
6	4.516067	0.111969	-0.252211
1	3.874309	0.219843	1.811906

1	4.878252	-0.085359	-2.365403
1	5.540164	0.390546	-0.020353
8	1.218968	-0.491775	1.368151
6	1.440311	-0.227036	2.753779
1	1.760735	0.810063	2.898456
1	0.487065	-0.390057	3.257345
1	2.193025	-0.912396	3.157745

TS_{vb-i} 2

E = -3999.505169 ZPVE = 0.201791 NIMAG = 1.

17	-3.212673	-2.261091	0.516373
15	-1.850027	-0.398319	-0.045121
12	0.540716	-0.84937	-0.061077
35	2.505106	-2.024036	-0.59964
6	-2.730172	-0.03733	-1.63273
1	-2.022184	-0.062054	-2.464955
1	-3.489519	-0.804316	-1.780791
1	-3.206126	0.946024	-1.597101
6	-2.663438	0.631579	1.268337
1	-3.727301	0.389181	1.267858
1	-2.252345	0.352436	2.241136
1	-2.510931	1.696479	1.091478
6	-0.398095	1.359666	-0.417695
6	0.576999	1.659734	0.548833
6	-0.626919	2.3719	-1.363726
6	1.271234	2.865859	0.627841
6	0.03941	3.60261	-1.322985
1	-1.357256	2.215332	-2.153446

6	0.979639	3.850273	-0.321765
1	2.020587	3.050872	1.389049
1	-0.174178	4.36296	-2.068699
1	1.500417	4.802044	-0.279168
8	0.849965	0.571969	1.422815
6	1.907481	0.67501	2.393192
1	1.682657	1.476779	3.101322
1	1.930785	-0.281771	2.914128
1	2.867408	0.851489	1.899652

PC_{vbi} 2

E = -3999.608408 ZPVE = 0.203708 NIMAG = 0.

17	-2.86573	0.428132	2.180147
15	0.451089	1.692481	0.050147
12	-1.572035	0.095618	0.359846
35	-1.843459	-0.712956	-1.89317
6	0.674516	2.55323	-1.564935
1	0.433279	1.85308	-2.368497
1	-0.034172	3.385709	-1.612954
1	1.686191	2.945382	-1.703012
6	1.066581	2.910313	1.29959
1	0.395829	3.774692	1.309235
1	1.044736	2.451337	2.291168
1	2.085043	3.242464	1.076525
6	1.728541	0.360051	0.053369
6	1.390425	-0.910737	0.564764
6	3.019615	0.538182	-0.460137
6	2.316505	-1.955105	0.569124

6	3.957248	-0.496008	-0.457784
1	3.301131	1.503478	-0.870715
6	3.599098	-1.740508	0.058799
1	2.052785	-2.931914	0.954087
1	4.952098	-0.331236	-0.858754
1	4.313233	-2.558195	0.062777
8	0.109277	-1.063515	1.080301
6	-0.221376	-2.267547	1.808373
1	0.4948	-2.417441	2.620205
1	-1.214196	-2.090745	2.223153
1	-0.235345	-3.129163	1.135489

R1 + b SN2@P-f pathway 2 in the gas phase

RC1b-r 2

E = -4543.905946 ZPVE = 0.489578 NIMAG = 0.

6	-1.518784	-2.258248	0.862075
6	-1.5959	-0.743576	0.489877
6	-2.8249	-2.991944	0.497617
6	-4.167745	-0.846553	0.831115
6	-2.847728	-0.13254	1.177577
6	-4.054167	-2.34594	1.152657
6	-0.229231	-3.014315	0.424456
6	-5.35339	-0.194458	1.552552
6	0.195479	-4.039402	1.491136
6	-0.304885	-3.698366	-0.951794
1	-1.479515	-2.230574	1.96261
1	-0.710059	-0.236508	0.891807
1	-2.753774	-4.041213	0.807183

1	-2.956593	-3.00197	-0.592105
1	-4.34186	-0.749253	-0.253089
1	-2.928711	0.936534	0.962251
1	-2.683353	-0.213588	2.262208
1	-4.966864	-2.866277	0.835164
1	-3.990374	-2.46653	2.244848
1	0.580937	-2.27374	0.37902
1	-5.451079	0.863817	1.285522
1	-6.294832	-0.694172	1.298103
1	-5.228137	-0.254463	2.641029
1	-0.581498	-4.797847	1.64789
1	1.109708	-4.556519	1.182816
1	0.395055	-3.555	2.453689
1	-0.957244	-4.578163	-0.915867
1	0.69256	-4.031092	-1.254183
1	-0.681156	-3.040491	-1.739928
15	-1.646474	-0.373111	-1.371108
6	-1.918571	1.446862	-1.411135
6	-2.910822	1.897579	-2.297058
6	-1.219347	2.385609	-0.631386
6	-3.21716	3.259299	-2.388904
1	-3.444936	1.182852	-2.918005
6	-1.518544	3.74314	-0.732618
1	-0.440584	2.062347	0.052865
6	-2.520749	4.182011	-1.607208
1	-3.989603	3.594526	-3.074737
1	-0.971569	4.458094	-0.125018
1	-2.751689	5.240898	-1.680169
17	0.501422	-0.371732	-1.851968
6	1.190562	2.58287	3.391102

6	1.169147	1.29856	2.820851
6	1.780833	1.024983	1.5916
6	2.413307	2.116951	0.983691
6	2.467898	3.410001	1.496453
6	1.834722	3.630088	2.729763
1	0.710157	2.76361	4.349072
1	2.973832	4.224195	0.987329
1	1.856546	4.623695	3.168714
12	2.335073	-0.295449	0.030392
35	3.670403	-2.113821	-0.745427
1	0.665142	0.500698	3.364526
8	3.00306	1.733989	-0.249829
6	3.838363	2.643168	-0.968044
1	4.667925	2.978507	-0.336496
1	4.225922	2.09092	-1.824427
1	3.258798	3.505338	-1.314927

TS_{1b-r} 2

E = -4543.860852 ZPVE = 0.488563 NIMAG = 1.

6	-2.313201	-1.998222	0.69839
6	-2.2082	-0.441822	0.61618
6	-3.374401	-2.544986	-0.276824
6	-4.711249	-0.376655	-0.138168
6	-3.637336	0.175071	0.817737
6	-4.753739	-1.911089	-0.052813
6	-0.951929	-2.761457	0.651506
6	-6.078017	0.252473	0.15702
6	-0.965529	-3.954816	1.623475

6	-0.5235	-3.241775	-0.747608
1	-2.713359	-2.161922	1.711515
1	-1.578264	-0.08898	1.437004
1	-3.447227	-3.632523	-0.161075
1	-3.059046	-2.371054	-1.314133
1	-4.432286	-0.107335	-1.170105
1	-3.603842	1.267232	0.756398
1	-3.929376	-0.069337	1.850073
1	-5.471982	-2.303623	-0.783372
1	-5.131165	-2.196702	0.940968
1	-0.180439	-2.069049	1.009713
1	-6.049236	1.343113	0.053651
1	-6.843105	-0.129417	-0.527712
1	-6.401761	0.021409	1.179679
1	-1.74512	-4.679145	1.355731
1	-0.005263	-4.479996	1.602607
1	-1.147439	-3.631523	2.654969
1	-1.168011	-4.051905	-1.106495
1	0.499679	-3.630651	-0.708146
1	-0.539166	-2.451913	-1.505005
15	-1.516566	0.207216	-0.989321
6	-1.250625	1.957702	-0.708073
6	-1.054231	2.705663	-1.896881
6	-1.269169	2.641609	0.531484
6	-0.92226	4.090964	-1.850094
1	-0.988164	2.184237	-2.847344
6	-1.131555	4.022403	0.571471
1	-1.361072	2.089471	1.45902
6	-0.962635	4.749036	-0.617416
1	-0.775243	4.65306	-2.766884

1	-1.139253	4.537792	1.526831
1	-0.849531	5.828631	-0.576586
17	0.925364	-0.275507	-2.79866
6	1.136151	1.094906	3.431696
6	0.76607	0.229669	2.38801
6	1.296611	0.341304	1.10127
6	2.256125	1.351659	0.931182
6	2.667508	2.227436	1.934926
6	2.075065	2.100525	3.197673
1	0.70835	0.967916	4.422867
1	3.416752	2.99236	1.757184
1	2.37135	2.772758	3.997925
12	2.019979	-0.595876	-0.773135
35	3.817366	-2.131306	-0.311561
1	0.064644	-0.569995	2.624499
8	2.803455	1.363274	-0.365261
6	4.083203	1.966034	-0.590152
1	4.819396	1.58059	0.121987
1	4.370674	1.692427	-1.605396
1	4.011658	3.055682	-0.512956

PC_{1b-r} 2

E = -4543.987073 ZPVE = 0.492667 NIMAG = 0.

6	-1.473399	2.501666	-0.548189
6	-1.37281	1.07956	-1.184492
6	-2.489193	2.487878	0.609916
6	-3.876262	0.684185	-0.564398
6	-2.775175	0.606486	-1.640487

6	-3.881022	2.060441	0.118773
6	-0.114245	3.186191	-0.23718
6	-5.246149	0.341936	-1.164422
6	0.747178	3.335649	-1.503637
6	-0.291554	4.569565	0.415368
1	-1.928515	3.115328	-1.345294
1	-0.744526	1.166198	-2.076242
1	-2.564247	3.481529	1.059205
1	-2.144808	1.815427	1.409347
1	-3.654631	-0.063526	0.205334
1	-2.733123	-0.413136	-2.0415
1	-3.067899	1.253021	-2.48201
1	-4.590472	2.05058	0.955855
1	-4.250344	2.815908	-0.591777
1	0.44492	2.566976	0.478025
1	-5.248083	-0.658257	-1.612907
1	-6.027907	0.363993	-0.397018
1	-5.525621	1.060511	-1.945445
1	0.223097	3.945819	-2.251613
1	1.69368	3.827043	-1.264216
1	1.008193	2.378421	-1.962394
1	-0.92651	5.219239	-0.20125
1	0.682284	5.058787	0.517562
1	-0.732521	4.51293	1.414187
15	-0.379068	-0.167677	-0.150119
6	-1.493759	-1.409342	0.64072
6	-1.745056	-1.291024	2.017592
6	-2.058478	-2.483748	-0.0664
6	-2.575739	-2.208671	2.665494
1	-1.27195	-0.50211	2.594394

6	-2.885894	-3.400596	0.584292
1	-1.84676	-2.614853	-1.122919
6	-3.152082	-3.260699	1.950135
1	-2.755805	-2.107022	3.73148
1	-3.318077	-4.226137	0.025889
1	-3.793476	-3.976953	2.455452
17	1.47071	-0.046692	3.524213
6	0.955772	-2.068402	-3.630578
6	0.195856	-1.295029	-2.748832
6	0.532746	-1.185852	-1.39412
6	1.678604	-1.878223	-0.943536
6	2.445505	-2.653337	-1.812081
6	2.076682	-2.746727	-3.157012
1	0.671944	-2.135155	-4.675973
1	3.331547	-3.168481	-1.463887
1	2.680048	-3.346857	-3.831067
12	1.761223	0.239138	1.297258
35	3.502531	1.32781	0.049136
1	-0.674177	-0.771136	-3.130165
8	1.988449	-1.740645	0.403424
6	3.124317	-2.454949	0.94227
1	4.048818	-2.090101	0.487062
1	3.11604	-2.240427	2.011458
1	2.99693	-3.528271	0.781165

R1_{IV} + b SN2@P-f pathways 2 to 6 in the gas phase

RC_{IVb-r} 2

E = -4191.268452 ZPVE = 0.254105 NIMAG = 0.

17	0.032197	-1.707043	0.893397
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15	1.579185	-0.367549	1.661085
12	-1.706166	-0.314631	-0.573797
35	-3.160252	-2.143279	-1.035453
6	2.283448	-1.567659	2.887563
1	1.556359	-1.73006	3.687569
1	2.562812	-2.530882	2.453505
1	3.176673	-1.101447	3.319038
6	2.814184	-0.458508	0.30419
6	3.389393	-1.646089	-0.181071
6	3.209979	0.770718	-0.248797
6	4.350788	-1.60097	-1.188944
1	3.07665	-2.608587	0.212951
6	4.182063	0.81413	-1.252813
1	2.74898	1.691768	0.096565
6	4.752468	-0.369791	-1.722118
1	4.785116	-2.523528	-1.562809
1	4.481675	1.769962	-1.671969
1	5.502421	-0.338572	-2.507126
6	-0.820136	1.578995	-0.861622
6	-0.026491	2.466947	-1.596839
6	-1.440264	2.127207	0.267573
6	0.137313	3.807791	-1.208541
6	-1.320885	3.444286	0.700548
6	-0.504818	4.290163	-0.066175
1	0.756883	4.476405	-1.801019
1	-1.824657	3.821766	1.584699
1	-0.383671	5.327473	0.233132
8	-2.229238	1.147573	0.929524
6	-3.069882	1.510752	2.023956
1	-3.782072	2.285491	1.719551

1	-3.608341	0.606514	2.309068
1	-2.469828	1.867167	2.868252
1	0.479643	2.121399	-2.496657

TS_{IVb-r} 2

E = -4191.231066 ZPVE = 0.253641 NIMAG = 1.

17	-0.191457	-2.317416	-1.084557
15	-1.628974	0.265896	-1.480803
12	1.285938	-0.926572	0.023237
35	3.129525	-1.479465	1.444335
6	-2.251992	-0.875942	-2.802811
1	-1.464991	-1.0557	-3.53746
1	-2.675674	-1.824911	-2.476326
1	-3.040416	-0.27375	-3.284192
6	-2.854388	-0.023612	-0.170619
6	-3.371698	-1.284107	0.191558
6	-3.360991	1.130392	0.464717
6	-4.37697	-1.381319	1.149831
1	-2.958664	-2.184104	-0.250761
6	-4.388682	1.029456	1.403917
1	-2.962369	2.107058	0.206622
6	-4.893375	-0.226006	1.750515
1	-4.75766	-2.358005	1.433305
1	-4.784946	1.926707	1.869579
1	-5.680618	-0.30791	2.494202
6	0.431348	1.092582	0.15785
6	-0.135921	2.013854	1.043538
6	1.493109	1.555839	-0.634888

6	0.330418	3.332728	1.123212
6	1.98084	2.860265	-0.598341
6	1.370879	3.755061	0.28999
1	-0.110354	4.026677	1.833841
1	2.809555	3.185189	-1.218672
1	1.725734	4.780399	0.33838
8	2.056829	0.530463	-1.415346
6	3.36825	0.709886	-1.971578
1	4.083781	0.969155	-1.185541
1	3.6386	-0.24772	-2.416292
1	3.349749	1.481686	-2.747013
1	-0.946558	1.704866	1.700712

PC_{IVb-r} 2

E = -4191.337765 ZPVE = 0.256621 NIMAG = 0.

17	-2.539906	0.587753	2.572196
15	1.398457	-2.332449	-0.02128
12	-1.291572	0.654451	0.673356
35	-1.122001	2.069606	-1.244035
6	1.142284	-2.670724	1.789115
1	2.130158	-2.770064	2.24893
1	0.574943	-1.911288	2.329659
1	0.634769	-3.635133	1.88996
6	-0.304844	-1.907101	-0.628277
6	-1.459426	-1.869133	0.179633
6	-0.458608	-1.706062	-2.012528
6	-2.723701	-1.613893	-0.38368
1	-1.399245	-2.067018	1.245784

6	-1.712016	-1.455453	-2.568601
1	0.414306	-1.737212	-2.658845
6	-2.849501	-1.403747	-1.75774
1	-3.594831	-1.579938	0.263519
1	-1.799391	-1.282722	-3.637003
1	-3.822705	-1.196919	-2.190853
6	2.225082	-0.666275	-0.07336
6	3.361034	-0.578772	-0.89978
6	1.808191	0.516745	0.55771
6	4.044416	0.62344	-1.088314
6	2.460311	1.731721	0.358902
6	3.586038	1.783931	-0.463493
1	4.919028	0.654845	-1.730591
1	2.07879	2.632413	0.827554
1	4.090679	2.731828	-0.6221
8	0.682593	0.487876	1.408469
6	0.965852	0.832986	2.797116
1	1.281733	1.876047	2.866872
1	0.032853	0.687666	3.340478
1	1.751048	0.172408	3.172133
1	3.706893	-1.478569	-1.400642

RC_{IVb-r} 3

E = -4191.268283 ZPVE = 0.254029 NIMAG = 0.

17	-0.046255000	0.167661000	0.686238000
15	0.991136000	1.387410000	2.179978000
12	-2.593336000	-0.079543000	1.430866000
35	-3.107787000	-2.110584000	0.299412000

6	0.555861000	3.052550000	1.499377000
1	0.791448000	3.168516000	0.438539000
1	-0.508417000	3.234461000	1.666293000
1	1.128494000	3.790356000	2.073646000
6	2.715455000	1.179798000	1.571009000
6	3.153160000	1.483203000	0.269981000
6	3.645227000	0.700227000	2.508477000
6	4.493289000	1.322796000	-0.077663000
1	2.447329000	1.831820000	-0.477994000
6	4.991194000	0.548445000	2.161550000
1	3.315435000	0.445047000	3.512330000
6	5.415006000	0.858339000	0.868619000
1	4.820615000	1.554618000	-1.087026000
1	5.700834000	0.181204000	2.896865000
1	6.458415000	0.734853000	0.593682000
6	-2.788724000	1.549369000	2.766773000
6	-3.349923000	2.378729000	1.786399000
6	-2.655077000	2.131221000	4.033025000
6	-3.769961000	3.692222000	1.975588000
6	-3.056107000	3.454516000	4.285804000
1	-2.233550000	1.552123000	4.852701000
6	-3.610360000	4.227350000	3.263512000
1	-4.205165000	4.290821000	1.181542000
1	-2.942481000	3.878255000	5.280271000
1	-3.927087000	5.247983000	3.458911000
8	-3.428042000	1.698000000	0.542633000
6	-4.140546000	2.261616000	-0.558381000
1	-5.177119000	2.473786000	-0.274849000
1	-3.653013000	3.179630000	-0.904183000
1	-4.119346000	1.510903000	-1.348758000

TS_{IVb-r} 3

E = -4191.223572 ZPVE = 0.253294 NIMAG = 1.

17	0.065904	0.875993	-2.474527
15	-0.103638	2.014561	0.487562
12	-0.169885	-0.910536	-1.022355
35	1.600199	-2.51475	-0.767685
6	0.040901	3.468596	-0.635689
1	0.857124	3.452581	-1.355483
1	-0.905372	3.600205	-1.165125
1	0.165577	4.323814	0.048138
6	1.585162	1.442261	0.704945
6	2.664468	1.662982	-0.183446
6	1.828264	0.739281	1.912463
6	3.939885	1.222366	0.143353
1	2.489262	2.130612	-1.144986
6	3.111293	0.311349	2.238306
1	1.002755	0.538913	2.588681
6	4.166071	0.550682	1.353116
1	4.758158	1.374523	-0.553492
1	3.28551	-0.225584	3.165143
1	5.16364	0.194989	1.592985
6	-1.62277	-0.598018	0.52867
6	-2.926714	-0.205713	0.147323
6	-1.445404	-0.962762	1.875197
6	-3.994268	-0.158757	1.057094
6	-2.492488	-0.941239	2.800492
1	-0.464617	-1.297515	2.209305

6	-3.76353	-0.525101	2.385545
1	-4.987879	0.150794	0.752309
1	-2.329536	-1.256832	3.827338
1	-4.583873	-0.487087	3.097107
8	-3.065388	0.093762	-1.183669
6	-4.33911	0.472063	-1.690747
1	-5.075649	-0.330036	-1.556694
1	-4.70602	1.387576	-1.209673
1	-4.190681	0.657419	-2.755157

PC_{IVb-r} 3

E = -4191.321290 ZPVE = 0.256269 NIMAG = 0.

17	0.3431	-1.154636	2.657028
15	1.325491	2.05022	-0.652974
12	-0.847883	-0.968612	0.759783
35	-2.841637	-1.726418	-0.31407
6	2.008963	2.442223	1.038629
1	1.824856	1.664301	1.784161
1	3.084712	2.594322	0.950094
1	1.549063	3.379762	1.365904
6	-0.503012	2.079439	-0.306017
6	-1.059704	1.806824	0.963149
6	-1.371995	2.423279	-1.352779
6	-2.444884	1.868098	1.165475
1	-0.41586	1.594536	1.812067
6	-2.755501	2.473386	-1.150807
1	-0.962396	2.659681	-2.331443
6	-3.294479	2.199653	0.106882

1	-2.853158	1.667482	2.152019
1	-3.410622	2.727583	-1.978885
1	-4.367918	2.237922	0.261917
6	1.559027	0.207559	-0.799485
6	2.812792	-0.396598	-0.544321
6	0.530145	-0.623787	-1.28483
6	2.983205	-1.780346	-0.684121
6	0.699397	-2.01118	-1.442515
1	-0.408704	-0.180251	-1.611707
6	1.92817	-2.58425	-1.120711
1	3.935209	-2.240194	-0.448517
1	-0.120377	-2.611758	-1.821987
1	2.07605	-3.65541	-1.214252
8	3.813369	0.446765	-0.168972
6	5.102458	-0.086153	0.129097
1	5.056125	-0.783964	0.972886
1	5.536425	-0.585028	-0.745354
1	5.719002	0.771478	0.399187

RC_{IVb-r} 4

E = -4191.274231 ZPVE = 0.254446 NIMAG = 0.

17	-0.303311	-0.113909	1.970784
15	-2.500569	-0.333923	2.06081
12	1.223596	-0.883498	-0.014721
35	-0.152607	-2.264254	-1.45071
6	-2.627828	-2.068446	1.436601
1	-2.052775	-2.261409	0.527382
1	-2.289106	-2.745761	2.225564

1	-3.690321	-2.261303	1.246824
6	-3.028106	0.670141	0.619277
6	-2.809349	0.34425	-0.731967
6	-3.737777	1.842758	0.937289
6	-3.312228	1.171434	-1.736229
1	-2.248267	-0.543037	-1.007457
6	-4.239746	2.666688	-0.072942
1	-3.903565	2.105514	1.978977
6	-4.025689	2.331013	-1.411207
1	-3.141322	0.911976	-2.777103
1	-4.789542	3.566766	0.185509
1	-4.415914	2.967028	-2.200596
6	3.123348	-0.217714	0.608812
6	4.281182	-0.329894	1.387595
6	3.097098	0.869546	-0.271554
6	5.33704	0.589144	1.273284
6	4.10891	1.811138	-0.430118
6	5.251233	1.649181	0.367817
1	6.227138	0.476009	1.886724
1	4.038198	2.637876	-1.130081
1	6.068746	2.358893	0.277663
1	4.379462	-1.148627	2.098109
8	1.865081	0.911002	-0.988532
6	1.759582	1.658938	-2.200872
1	2.56257	1.38021	-2.891995
1	0.792653	1.40116	-2.634116
1	1.798277	2.733817	-1.995863

E = -4191.226924 ZPVE = 0.253139 NIMAG = 1.

17	-0.389017	1.858367	2.104285
15	0.138931	2.005868	-0.852118
12	0.068439	-0.304287	1.3156
35	-1.458095	-2.130107	1.537859
6	-0.367056	3.73096	-0.430809
1	-1.285768	3.84309	0.142651
1	0.453694	4.217199	0.101449
1	-0.476831	4.227435	-1.407706
6	-1.424012	1.135649	-1.101962
6	-2.678894	1.498336	-0.559773
6	-1.353222	0.022954	-1.976014
6	-3.823242	0.795706	-0.913727
1	-2.745474	2.297921	0.168835
6	-2.506845	-0.671821	-2.331659
1	-0.387843	-0.297496	-2.355497
6	-3.740469	-0.2837	-1.805002
1	-4.780231	1.069302	-0.480525
1	-2.441372	-1.524002	-3.000426
1	-4.637969	-0.837185	-2.064829
6	1.972287	0.06295	0.39213
6	2.914497	0.946412	0.952492
6	2.437264	-0.801448	-0.624065
6	4.262891	0.932417	0.578586
6	3.778825	-0.835187	-1.020496
6	4.686195	0.04055	-0.409829
1	4.973117	1.606825	1.048679
1	4.12921	-1.517583	-1.787343
1	5.727638	0.023049	-0.719441

1	2.586266	1.653181	1.71254
8	1.466723	-1.602018	-1.180884
6	1.855964	-2.668559	-2.039571
1	2.561017	-3.340896	-1.536204
1	0.940524	-3.214711	-2.271649
1	2.306525	-2.296368	-2.968596

PC_{IVb-r} 4

E = -4191.324663 ZPVE = 0.256196 NIMAG = 0.

17	-1.429606	3.17183	0.833243
15	0.060183	-0.351011	-2.555041
12	-0.501707	1.112802	0.835526
35	0.092864	-0.631631	2.354135
6	-0.616727	1.162848	-3.398994
1	-1.019112	1.946344	-2.750815
1	0.177304	1.594575	-4.015828
1	-1.414278	0.829236	-4.069871
6	-1.326566	-0.810636	-1.391266
6	-2.25364	0.11495	-0.867868
6	-1.419333	-2.149828	-0.981936
6	-3.225434	-0.288891	0.060577
1	-2.266603	1.146935	-1.208543
6	-2.394245	-2.551123	-0.065644
1	-0.716746	-2.876345	-1.377799
6	-3.293142	-1.623318	0.464974
1	-3.92414	0.443724	0.453785
1	-2.440857	-3.590229	0.247219
1	-4.038354	-1.935959	1.189554

6	1.215204	0.396052	-1.289518
6	1.29227	1.770464	-0.993189
6	2.112744	-0.474831	-0.616022
6	2.210016	2.274117	-0.056078
6	3.04784	0.028962	0.295707
6	3.079945	1.394021	0.585061
1	2.225567	3.335962	0.164052
1	3.721177	-0.639636	0.816796
1	3.791489	1.764276	1.316361
1	0.646201	2.47305	-1.508303
8	1.9766	-1.793418	-0.901773
6	2.724175	-2.748157	-0.145507
1	2.518004	-2.638695	0.924226
1	2.380983	-3.724405	-0.488759
1	3.798704	-2.651745	-0.340204

PIVb-r 4

E = -959.133318 ZPVE = 0.252569 NIMAG = 0.

15	-0.224023	1.041314	-1.231173
6	-0.430115	2.844797	-0.789579
1	0.353438	3.440848	-1.267708
1	-1.391392	3.168102	-1.19995
1	-0.431344	3.038274	0.288119
6	1.276861	0.586902	-0.244932
6	1.676924	-0.771565	-0.228965
6	2.107108	1.515934	0.393453
6	2.851812	-1.170274	0.416926
6	3.289515	1.129313	1.03707

1	1.835247	2.566143	0.394261
6	3.655437	-0.214052	1.048403
1	3.149395	-2.212053	0.431717
1	3.910963	1.87482	1.523738
1	4.56776	-0.531104	1.545443
8	0.838022	-1.632996	-0.876036
6	1.161553	-3.016281	-0.922934
1	1.198844	-3.451274	0.083537
1	0.359363	-3.488071	-1.491501
1	2.118578	-3.1857	-1.4321
6	-1.600825	0.32452	-0.205383
6	-2.738085	-0.149032	-0.876927
6	-1.573739	0.259813	1.1969
6	-3.828276	-0.662931	-0.167309
1	-2.76696	-0.121446	-1.963439
6	-2.65789	-0.25911	1.908295
1	-0.69758	0.608914	1.736842
6	-3.789705	-0.720028	1.227672
1	-4.701283	-1.023715	-0.70436
1	-2.619529	-0.304234	2.993482
1	-4.632777	-1.123284	1.781667

RC_{IVb-r} 5

E = -4191.268939 ZPVE = 0.254180 NIMAG = 0.

17	0.667881	-1.117989	-0.170397
15	1.654827	0.828657	-0.059543
12	-1.982561	-0.819656	-0.249668
35	-2.538621	-3.128379	-0.129754

6	1.522567	1.280363	-1.849201
1	1.907271	0.511486	-2.523868
1	0.474714	1.488768	-2.078602
1	2.100627	2.201249	-1.989989
6	3.401092	0.259116	0.053708
6	4.017932	-0.622225	-0.851203
6	4.151956	0.775169	1.122703
6	5.35943	-0.966632	-0.694822
1	3.44891	-1.053783	-1.669239
6	5.500992	0.438887	1.271601
1	3.681192	1.443643	1.83911
6	6.104114	-0.433007	0.364117
1	5.825444	-1.653188	-1.395561
1	6.072507	0.849536	2.098585
1	7.1496	-0.702728	0.481417
6	-2.2409	1.203369	-0.797053
6	-2.412707	2.206409	-1.758401
6	-2.279711	1.639155	0.532988
6	-2.587742	3.55402	-1.399771
1	-2.415035	1.947656	-2.816326
6	-2.456091	2.954489	0.951307
6	-2.606476	3.922784	-0.053394
1	-2.717364	4.311438	-2.16848
1	-2.479581	3.242172	1.997505
1	-2.746304	4.962885	0.227329
8	-2.123311	0.541471	1.422966
6	-2.183969	0.739168	2.835247
1	-1.376593	1.402095	3.164561
1	-3.153658	1.160585	3.121565
1	-2.062063	-0.244876	3.288598

TS_{IVb-r} 5

E = -4191.222398 ZPVE = 0.253165 NIMAG = 1.

17	0.602258	-1.227203	1.658653
15	1.117053	0.278777	-1.099381
12	-1.475012	-0.791946	0.754239
35	-2.902296	-2.585785	0.040469
6	0.564519	-1.280832	-1.917338
1	0.613865	-2.156044	-1.264251
1	-0.460045	-1.165514	-2.274155
1	1.222466	-1.447808	-2.780418
6	2.775027	-0.143956	-0.529457
6	3.357059	-1.431219	-0.483536
6	3.581182	0.977595	-0.224034
6	4.703402	-1.581133	-0.178207
1	2.751515	-2.310402	-0.671122
6	4.929394	0.822364	0.094225
1	3.142083	1.971794	-0.246289
6	5.490656	-0.456647	0.1146
1	5.143833	-2.573077	-0.149459
1	5.537696	1.691261	0.325229
1	6.540186	-0.583918	0.363519
6	-1.531751	1.071418	-0.313972
6	-2.013566	1.294377	-1.616408
6	-1.311728	2.218059	0.483821
6	-2.228286	2.57877	-2.120324
1	-2.231745	0.442553	-2.258625
6	-1.510731	3.521385	0.005003

6	-1.962692	3.688745	-1.306613
1	-2.614748	2.720433	-3.125707
1	-1.32609	4.392216	0.624434
1	-2.11407	4.693563	-1.691493
8	-0.915421	1.938979	1.767363
6	-0.652202	3.005556	2.672313
1	0.151804	3.653302	2.301715
1	-1.552879	3.605855	2.850539
1	-0.335865	2.533693	3.603075

PC_{IVb-r} 5

E = -4191.318365 ZPVE = 0.256182 NIMAG = 0.

17	-1.181891	0.783642	2.713704
15	1.585573	-0.241186	-1.902409
12	-2.074125	0.067319	0.794578
35	-3.526993	-1.583721	-0.103334
6	0.529311	-1.693241	-2.413014
1	-0.164168	-2.036587	-1.638758
1	-0.030406	-1.452471	-3.322227
1	1.21296	-2.512548	-2.653022
6	2.42134	-0.955421	-0.409746
6	1.848467	-1.040496	0.867557
6	3.712797	-1.473042	-0.603114
6	2.541822	-1.637083	1.92287
1	0.867017	-0.620803	1.065467
6	4.404136	-2.081266	0.448248
1	4.183769	-1.393249	-1.579963
6	3.819424	-2.164347	1.714463

1	2.08029	-1.684356	2.904797
1	5.400227	-2.480566	0.279259
1	4.357343	-2.630144	2.53515
6	0.310426	0.905679	-1.199653
6	-1.062089	0.768886	-1.460556
6	0.731819	2.089209	-0.532648
6	-2.002836	1.74676	-1.060885
1	-1.425876	-0.09771	-2.002004
6	-0.192067	3.066327	-0.136619
6	-1.552008	2.894045	-0.398779
1	-3.047822	1.632082	-1.336763
1	0.137907	3.951608	0.392094
1	-2.256407	3.65864	-0.086567
8	2.062201	2.185974	-0.323101
6	2.589517	3.303289	0.394444
1	2.396682	4.240964	-0.139293
1	2.169595	3.350152	1.404938
1	3.663735	3.129676	0.451231

RC_{IVb-r} 6

E = -4191.268282 ZPVE = 0.254018 NIMAG = 0.

17	-0.71787	-1.00837	0.257044
15	-1.784964	0.73171	-0.53562
12	1.837612	-0.82772	-0.480323
35	2.404464	-3.139042	-0.401542
6	-1.397479	1.916372	0.832487
1	-1.639136	1.532989	1.826951
1	-0.338118	2.178776	0.781992

1	-1.988538	2.820915	0.646701
6	-3.50434	0.229635	-0.112773
6	-3.953309	-0.101664	1.177561
6	-4.41835	0.206885	-1.179249
6	-5.28935	-0.43383	1.394808
1	-3.259072	-0.114702	2.012457
6	-5.760461	-0.11743	-0.958807
1	-4.079278	0.443541	-2.184547
6	-6.195712	-0.43891	0.327474
1	-5.625316	-0.693771	2.394434
1	-6.457987	-0.126922	-1.790981
1	-7.235985	-0.698233	0.501046
6	1.991528	1.237342	-0.913927
6	2.52698	1.535046	0.346484
6	1.844051	2.333735	-1.771806
6	2.910126	2.797699	0.789629
6	2.208009	3.633946	-1.380833
6	2.738132	3.862	-0.109404
1	3.326514	2.973464	1.776524
1	2.084409	4.46534	-2.06999
1	3.026242	4.8652	0.191877
1	1.440653	2.187409	-2.772191
8	2.621359	0.360063	1.138184
6	3.314659	0.36998	2.385905
1	3.311933	-0.660596	2.741751
1	4.345768	0.712945	2.247796
1	2.800825	1.014051	3.107819

E = -4191.225320 ZPVE = 0.253415 NIMAG = 1.

17	0.933429	1.449047	-1.431917
15	1.321556	-0.619862	0.649834
12	-1.233038	0.982665	-0.718837
35	-2.919112	2.576329	-0.189403
6	0.750813	0.605015	1.913986
1	0.905344	1.649126	1.631057
1	-0.304844	0.421182	2.12515
1	1.329191	0.40317	2.825478
6	3.043352	-0.116978	0.368547
6	3.639275	1.113564	0.71754
6	3.861405	-1.144505	-0.149632
6	5.010358	1.29455	0.578887
1	3.028091	1.932802	1.079301
6	5.236412	-0.957617	-0.296585
1	3.413051	-2.094017	-0.431383
6	5.811085	0.260528	0.071077
1	5.460528	2.243909	0.853086
1	5.853663	-1.75666	-0.695486
1	6.88056	0.412317	-0.042278
6	-1.140868	-1.153128	-0.56515
6	-1.903411	-1.823893	0.417523
6	-0.833134	-1.875354	-1.734149
6	-2.374916	-3.128209	0.231199
6	-1.293692	-3.179126	-1.94792
6	-2.056873	-3.799979	-0.956454
1	-2.970262	-3.631435	0.985022
1	-1.056761	-3.705355	-2.86819
1	-2.414246	-4.816078	-1.099885

1	-0.216952	-1.40535	-2.499712
8	-2.135734	-1.094574	1.560167
6	-3.039527	-1.603621	2.53693
1	-3.118635	-0.830616	3.302419
1	-4.02856	-1.78437	2.09977
1	-2.662244	-2.528891	2.989735

PC_{IVb-r} 6

E = -4191.323891 ZPVE = 0.256208 NIMAG = 0.

17	-1.682486	3.343218	0.93382
15	-0.198834	-2.467139	0.141299
12	-0.162234	1.92443	0.109084
35	1.265335	1.561332	-1.767006
6	0.417364	-2.47782	-1.621142
1	0.587126	-1.480772	-2.034354
1	1.35098	-3.03948	-1.664815
1	-0.336002	-2.99854	-2.219835
6	-1.871414	-1.692472	-0.075459
6	-2.142218	-0.669945	-1.005811
6	-2.919845	-2.162056	0.72981
6	-3.429688	-0.140869	-1.12477
1	-1.357179	-0.304707	-1.663685
6	-4.207199	-1.624695	0.61758
1	-2.728756	-2.958789	1.444157
6	-4.462688	-0.610841	-0.306727
1	-3.624587	0.645216	-1.848582
1	-5.005742	-1.999141	1.251604
1	-5.46005	-0.190966	-0.396126

6	0.709231	-1.031416	0.90266
6	2.123225	-0.956463	0.843765
6	0.045714	-0.053576	1.664491
6	2.815583	0.113642	1.426376
6	0.738387	1.007778	2.286778
6	2.125091	1.10192	2.128294
1	3.890297	0.193187	1.32121
1	0.195453	1.72301	2.897497
1	2.673999	1.922333	2.579487
1	-1.029296	-0.131943	1.80922
8	2.737919	-1.97214	0.188063
6	4.162515	-1.990286	0.096635
1	4.409033	-2.903431	-0.445106
1	4.532277	-1.122579	-0.460672
1	4.619607	-2.021109	1.0924

R1v + b S_{N2}@P-f pathway 2 in the gas phase

RC_{v_{b-r}} 2

E = -3999.525038 ZPVE = 0.200656 NIMAG = 0.

17	-0.614791	1.996174	0.013336
15	1.490852	2.355142	0.395327
12	-1.082015	-0.637146	-0.332033
35	-3.452876	-0.480447	-0.340758
6	2.120311	2.264889	-1.342566
1	2.067659	1.230588	-1.690716
1	1.57284	2.919445	-2.026995
1	3.175436	2.564512	-1.321976
6	1.37401	4.195307	0.59764
1	0.884425	4.686728	-0.248101

1	0.836223	4.434257	1.518719
1	2.397176	4.578939	0.692455
6	0.81831	-1.392574	-0.850819
6	1.166976	-1.650706	0.480264
6	1.782536	-1.74941	-1.800803
6	2.368684	-2.204017	0.911539
6	3.018197	-2.305826	-1.4281
1	1.580825	-1.597854	-2.860162
6	3.307413	-2.527634	-0.08033
1	2.592553	-2.385101	1.957867
1	3.748626	-2.572171	-2.187602
1	4.259882	-2.961553	0.210722
8	0.109255	-1.278594	1.354752
6	0.238299	-1.459018	2.76502
1	1.074678	-0.866918	3.15174
1	-0.696382	-1.111266	3.205686
1	0.387129	-2.517619	3.003587

TS_{vb-r} 2

E = -3999.485029 ZPVE = 0.200002 NIMAG = 1.

17	-1.077338	-2.419314	0.422592
15	-2.740589	-0.065073	0.080146
12	0.590316	-0.898529	-0.050808
35	2.8705	-1.170246	-0.702677
6	-3.119987	-0.532336	-1.666049
1	-2.599598	0.105602	-2.379355
1	-2.875076	-1.58021	-1.859628
1	-4.202358	-0.40311	-1.799833

6	-3.845392	-1.312614	0.911203
1	-3.94455	-2.276405	0.409619
1	-3.542156	-1.465022	1.948796
1	-4.82049	-0.796113	0.921329
6	-0.43662	1.031287	-0.448598
6	0.220121	1.518901	0.69519
6	-0.710889	1.974676	-1.448655
6	0.55799	2.856088	0.891901
6	-0.377622	3.325313	-1.298519
1	-1.19071	1.667299	-2.375444
6	0.236846	3.765015	-0.122245
1	1.065268	3.19499	1.78873
1	-0.589909	4.030539	-2.097004
1	0.484461	4.814567	0.005324
8	0.561573	0.492759	1.593697
6	1.52694	0.747413	2.626512
1	1.123764	1.457162	3.354725
1	1.704053	-0.212092	3.111916
1	2.458676	1.123663	2.193948

PC_{Vb-r} 2

E = -3999.583583 ZPVE = 0.202731 NIMAG = 0.

17	-3.276397	1.621537	0.78962
15	1.641747	1.544859	-1.528458
12	-1.785695	0.073005	0.147013
35	-1.542644	-2.090705	-0.793632
6	-0.190581	1.474367	-1.894385
1	-0.481322	0.446823	-2.14246

1	-0.81507	1.898563	-1.095987
1	-0.383388	2.078907	-2.78614
6	1.705435	3.102869	-0.503224
1	0.964525	3.132286	0.300654
1	2.707111	3.216402	-0.078671
1	1.527178	3.95417	-1.168438
6	1.927018	0.206903	-0.259234
6	1.159118	-0.135868	0.863919
6	3.082599	-0.566608	-0.482837
6	1.503659	-1.180687	1.717854
6	3.45957	-1.603239	0.372096
1	3.693807	-0.339211	-1.351565
6	2.660113	-1.920364	1.470677
1	0.857864	-1.431949	2.553378
1	4.359267	-2.174567	0.165791
1	2.926369	-2.739809	2.13077
8	-0.035874	0.574925	1.133896
6	-0.0429	1.343815	2.371568
1	0.801786	2.035779	2.362871
1	-0.989747	1.883386	2.38626
1	0.02785	0.672309	3.230068

R1 + b S_{N2}@Cl pathway, followed by S_{N2}@C pathway, in the gas phase

RC1

E = -4543.910169 ZPVE = 0.489496 NIMAG = 0.

6	-2.49791	-0.449945	-1.146687
6	-3.108781	-2.388103	0.398854
6	-1.26542	-2.716112	-1.346411

6	-1.805198	-1.473737	-2.072258
6	-2.392608	-3.374423	-0.537263
6	-4.487777	-0.184146	0.535951
6	-0.617358	-3.69616	-2.331508
6	-5.211831	0.882092	-0.30603
6	-5.520442	-0.920544	1.408483
1	-2.927781	0.33129	-1.779612
1	-3.934874	-2.91131	0.888947
1	-2.420715	-2.075125	1.195593
1	-0.491949	-2.396017	-0.634875
1	-1.007945	-0.991265	-2.645964
1	-2.559606	-1.796765	-2.806086
1	-1.98975	-4.209196	0.049006
1	-3.125763	-3.806688	-1.236302
1	-3.801608	0.333387	1.226215
1	0.208803	-3.226114	-2.877453
1	-0.217647	-4.572055	-1.808661
1	-1.346223	-4.052167	-3.071057
1	-5.914852	0.407306	-1.002469
1	-5.788617	1.55409	0.338456
1	-4.527934	1.503596	-0.889248
1	-6.183319	-1.541752	0.792261
1	-6.147657	-0.197605	1.941138
1	-5.053924	-1.564626	2.158024
6	-1.775544	2.198851	-0.136711
6	-1.91762	2.965274	1.031787
6	-1.926742	2.829933	-1.383711
6	-2.247952	4.322007	0.958521
1	-1.778369	2.49539	2.002102
6	-2.237045	4.186986	-1.457949

1	-1.793299	2.264665	-2.301773
6	-2.403432	4.934673	-0.285876
1	-2.371283	4.897948	1.871018
1	-2.346363	4.663707	-2.427809
1	-2.650726	5.990554	-0.346134
17	0.553405	0.452019	-0.988158
6	-3.651667	-1.151809	-0.351018
1	-4.339349	-1.526571	-1.128383
15	-1.356732	0.418577	0.113315
6	4.98519	-0.725641	-1.738354
6	6.164754	0.008257	-1.949481
6	6.501347	1.056451	-1.091146
6	5.667977	1.385897	-0.011139
6	4.515998	0.621958	0.146209
6	4.118703	-0.437944	-0.677688
1	4.751275	-1.538521	-2.42381
1	6.819542	-0.23894	-2.781096
1	7.413374	1.624494	-1.25202
1	5.930034	2.200909	0.656138
8	3.564933	0.834482	1.184141
6	3.836821	1.748363	2.244912
1	3.002795	1.662709	2.942255
1	4.770684	1.480114	2.751025
1	3.900209	2.773885	1.864892
12	2.362382	-0.784044	0.441929
35	0.961631	-1.900077	2.047127

TS1_t

E = -4543.841228 ZPVE = 0.488556 NIMAG = 1.

6	2.356309	-0.031885	1.262528
6	2.875956	-2.402116	0.478641
6	0.903264	-2.013441	2.061756
6	1.51681	-0.646825	2.406951
6	2.004996	-2.98057	1.604927
6	4.461729	-0.474713	-0.229196
6	0.078198	-2.575904	3.224619
6	5.201455	0.781999	0.264451
6	5.498033	-1.516876	-0.688875
1	2.824743	0.87475	1.653612
1	3.672619	-3.11799	0.256543
1	2.278497	-2.307573	-0.43816
1	0.221734	-1.881227	1.203283
1	0.735235	0.052125	2.721809
1	2.182245	-0.784258	3.273593
1	1.55791	-3.927711	1.27828
1	2.641591	-3.21686	2.471669
1	3.864617	-0.194704	-1.110409
1	-0.731578	-1.893781	3.507911
1	-0.36761	-3.542387	2.9633
1	0.708231	-2.729117	4.109649
1	5.791834	0.556078	1.162363
1	5.894065	1.144826	-0.502823
1	4.525772	1.607127	0.50147
1	6.062951	-1.915882	0.16408
1	6.218358	-1.055428	-1.37323
1	5.042635	-2.359372	-1.215922
6	1.709568	2.24557	-0.549286
6	1.512651	2.710655	-1.865679

6	2.134955	3.174597	0.420492
6	1.760906	4.040948	-2.206752
1	1.184777	2.01467	-2.633739
6	2.378961	4.505573	0.080522
1	2.265785	2.866272	1.453369
6	2.196962	4.945448	-1.234809
1	1.614888	4.369704	-3.231961
1	2.706457	5.203032	0.846737
1	2.391695	5.98113	-1.497236
17	-1.039399	0.962533	0.698307
6	3.486965	-1.032975	0.844987
1	4.08735	-1.184906	1.759723
15	1.306944	0.48552	-0.23799
6	-4.053882	2.048609	1.715208
6	-5.444501	2.234722	1.653277
6	-6.205348	1.459319	0.77792
6	-5.591877	0.497745	-0.036201
6	-4.206947	0.343124	0.059624
6	-3.429033	1.091885	0.924239
1	-3.465596	2.662426	2.395847
1	-5.926528	2.980004	2.281
1	-7.281191	1.593969	0.717058
1	-6.202868	-0.092309	-0.710868
8	-3.513335	-0.630658	-0.742888
6	-4.301254	-1.498265	-1.591352
1	-3.596504	-2.182998	-2.062549
1	-5.018504	-2.055915	-0.983538
1	-4.820468	-0.905949	-2.349375
12	-1.480501	-0.831057	-0.643648
35	-0.805545	-2.703583	-1.928969

INT_t

E = -4543.891717 ZPVE = 0.490251 NIMAG = 0.

17	2.95725	-1.678675	1.149806
15	-0.588667	0.43786	0.685196
12	1.011192	-0.965431	-0.563124
35	0.971929	-2.408313	-2.48628
6	3.767727	-0.109532	1.095112
6	3.593762	0.710576	-0.028636
6	4.587713	0.273507	2.149794
6	4.256637	1.937859	-0.079227
6	5.249661	1.502465	2.091177
1	4.702207	-0.384118	3.004373
6	5.084745	2.325252	0.977543
1	4.127166	2.593677	-0.931225
1	5.889542	1.806784	2.912448
1	5.593314	3.282467	0.925627
8	2.746681	0.257165	-1.018482
6	2.748946	0.921583	-2.307042
1	3.769941	0.966334	-2.692949
1	2.133583	0.292708	-2.950885
1	2.318001	1.922035	-2.215934
6	-2.46832	2.346105	-0.578381
6	-1.65962	1.034232	-0.817356
6	-3.760546	2.036703	0.202911
6	-3.890322	-0.302571	-0.813143
6	-2.556577	-0.009014	-1.522426
6	-4.637238	1.008705	-0.52802

6	-1.653055	3.522559	0.023556
6	-4.744938	-1.279632	-1.630461
6	-0.347605	3.785428	-0.749247
6	-2.470731	4.82699	0.076886
1	-2.782014	2.678621	-1.585986
1	-0.867915	1.286921	-1.535196
1	-4.34338	2.949907	0.359427
1	-3.496839	1.658352	1.200321
1	-3.671085	-0.774094	0.151595
1	-2.004514	-0.942228	-1.683625
1	-2.792307	0.379446	-2.528009
1	-5.542716	0.801778	0.057916
1	-4.976762	1.443879	-1.481448
1	-1.376844	3.246587	1.049894
1	-4.217141	-2.225675	-1.797418
1	-5.687075	-1.507085	-1.117767
1	-4.993173	-0.858613	-2.613528
1	-0.547474	3.965403	-1.814542
1	0.161544	4.671622	-0.35303
1	0.350011	2.946578	-0.666646
1	-2.817625	5.116947	-0.924021
1	-1.856044	5.648127	0.463393
1	-3.3481	4.748538	0.724321
6	-1.525375	-0.86723	1.639728
6	-2.136211	-0.505426	2.856637
6	-1.564072	-2.230538	1.282787
6	-2.771435	-1.450469	3.666879
1	-2.103428	0.533775	3.1721
6	-2.191318	-3.183131	2.091626
1	-1.115521	-2.560337	0.347685

6	-2.802126	-2.795212	3.286791
1	-3.237015	-1.136756	4.597626
1	-2.203601	-4.225526	1.784449
1	-3.291481	-3.532918	3.916618

TS2_i

E = -4543.850825 ZPVE = 0.489131 NIMAG = 1.

17	-2.033872	-0.264123	2.313688
15	0.331499	0.189878	0.121356
12	-1.928728	1.146335	0.300617
35	-3.071743	3.045404	-0.58034
6	-1.492672	-1.721519	0.919667
6	-2.396314	-1.775725	-0.148948
6	-1.000096	-2.883833	1.498107
6	-2.738058	-3.000742	-0.708244
6	-1.344606	-4.117583	0.930447
1	-0.350397	-2.827849	2.364758
6	-2.21162	-4.180822	-0.160864
1	-3.402988	-3.049687	-1.563499
1	-0.941601	-5.028201	1.363792
1	-2.490746	-5.13787	-0.588534
8	-2.831875	-0.54043	-0.627197
6	-3.853797	-0.499331	-1.644981
1	-4.736043	-1.048589	-1.305371
1	-4.089911	0.556008	-1.777518
1	-3.470396	-0.923225	-2.57734
6	2.352563	-0.669171	-1.932563
6	1.267092	0.368873	-1.527978

6	3.698613	-0.362463	-1.241822
6	3.114157	2.122859	-1.057185
6	1.782842	1.813253	-1.757583
6	4.165198	1.08342	-1.474833
6	1.89236	-2.14639	-1.806448
6	3.578571	3.55474	-1.351651
6	0.649395	-2.429911	-2.668837
6	3.000574	-3.148517	-2.177122
1	2.515	-0.494683	-3.011843
1	0.416744	0.237432	-2.20986
1	4.469629	-1.041777	-1.618731
1	3.617149	-0.549029	-0.164929
1	2.960467	2.033057	0.02669
1	1.01593	2.536028	-1.457123
1	1.925639	1.945145	-2.843148
1	5.103857	1.26001	-0.933586
1	4.392588	1.221814	-2.543567
1	1.612642	-2.324886	-0.758132
1	2.834486	4.29015	-1.024804
1	4.520405	3.778994	-0.837586
1	3.742752	3.702115	-2.426821
1	0.854602	-2.219775	-3.726931
1	0.356229	-3.481914	-2.587765
1	-0.214155	-1.833571	-2.363671
1	3.379019	-2.96219	-3.190806
1	2.609251	-4.171652	-2.155128
1	3.850488	-3.109718	-1.490307
6	1.405944	0.260696	1.61355
6	2.162436	-0.850397	2.033431
6	1.405021	1.403387	2.436126

6	2.908013	-0.811762	3.214055
1	2.164725	-1.755775	1.43461
6	2.14367	1.442372	3.620776
1	0.823737	2.273021	2.142629
6	2.902473	0.335933	4.011782
1	3.487228	-1.681105	3.513521
1	2.127932	2.338367	4.235114
1	3.479293	0.365341	4.93165

PC_i

E = -4543.979310 ZPVE = 0.492818 NIMAG = 0.

17	2.906637	0.793578	2.61227
15	-0.231565	0.115177	0.319008
12	2.357345	-0.189508	0.649848
35	3.504365	-1.900288	-0.61242
6	-0.044994	1.914593	-0.096866
6	1.170227	2.313649	-0.695479
6	-0.964818	2.92037	0.224966
6	1.42139	3.645037	-1.024518
6	-0.722771	4.260105	-0.085881
1	-1.88368	2.657893	0.735853
6	0.463583	4.616725	-0.724461
1	2.355773	3.935997	-1.488246
1	-1.457437	5.016184	0.172087
1	0.663124	5.65405	-0.975076
8	2.108137	1.308532	-0.917098
6	3.224542	1.566453	-1.801923
1	3.915708	2.277576	-1.340796

1	3.708887	0.599202	-1.933798
1	2.853623	1.946858	-2.756939
6	-2.280958	-0.725803	-1.809718
6	-0.8199	-0.769314	-1.267968
6	-3.206006	-1.668671	-1.006462
6	-1.222754	-3.16098	-0.377209
6	-0.329768	-2.238588	-1.218987
6	-2.659656	-3.102927	-0.915495
6	-2.851931	0.696379	-2.068483
6	-0.674457	-4.593153	-0.355027
6	-2.020416	1.456547	-3.118324
6	-4.323225	0.669674	-2.522604
1	-2.19023	-1.184567	-2.810238
1	-0.175763	-0.248438	-1.987744
1	-4.190888	-1.702677	-1.481668
1	-3.363566	-1.280956	0.004822
1	-1.229956	-2.787309	0.658753
1	0.70891	-2.287367	-0.880726
1	-0.323017	-2.613804	-2.253578
1	-3.325214	-3.70957	-0.288078
1	-2.67472	-3.560248	-1.916742
1	-2.808314	1.271337	-1.134541
1	0.34735	-4.621349	0.038004
1	-1.296871	-5.246009	0.267437
1	-0.652419	-5.017771	-1.36661
1	-2.029887	0.922146	-4.076844
1	-2.437696	2.454247	-3.290872
1	-0.979103	1.592042	-2.816313
1	-4.450985	0.035878	-3.409433
1	-4.65416	1.679055	-2.78996

1	-4.99842	0.299107	-1.746393
6	-1.361417	0.055155	1.772259
6	-2.717069	0.430244	1.78303
6	-0.773455	-0.364661	2.979204
6	-3.46207	0.378384	2.961952
1	-3.2045	0.759645	0.873136
6	-1.520424	-0.41508	4.158979
1	0.279863	-0.623917	3.010139
6	-2.865894	-0.045768	4.153403
1	-4.508174	0.670723	2.948484
1	-1.042626	-0.73663	5.079341
1	-3.447519	-0.084092	5.069784

R1_{II} + b S_{N2}@Cl pathway, followed by S_{N2}@C pathway, in the gas phase

RC_{II}

E = -4235.414484 ZPVE = 0.370233 NIMAG = 0.

17	-0.429937	-0.655801	0.791207
15	-2.24932	-0.191598	-0.329084
12	1.530927	1.003696	0.144257
35	0.350746	2.898814	-0.71815
6	-2.721042	-1.988306	-0.813262
6	-3.349022	0.485235	1.083143
6	3.150085	-0.026378	1.017889
6	3.533708	-0.599615	-0.20002
6	3.951838	-0.364326	2.114394
6	4.617487	-1.450612	-0.392675
6	5.057701	-1.221095	1.984974
1	3.723731	0.042786	3.097971

6	5.387317	-1.758627	0.739293
1	4.873704	-1.868084	-1.361307
1	5.663006	-1.465335	2.85417
1	6.244267	-2.418432	0.636972
8	2.649484	-0.202405	-1.244994
6	2.991015	-0.444169	-2.609558
1	3.004995	-1.519126	-2.819389
1	2.219264	0.038158	-3.210374
1	3.968462	-0.007338	-2.841845
6	-1.73658	-2.330627	-1.957486
1	-1.996247	-3.310358	-2.377457
1	-1.780809	-1.594196	-2.766737
1	-0.70391	-2.386037	-1.6
6	-2.634066	-3.080837	0.265561
1	-3.353913	-2.933322	1.072026
1	-2.850909	-4.052763	-0.196346
1	-1.635068	-3.141323	0.70483
6	-4.150748	-1.931047	-1.395925
1	-4.27261	-1.123016	-2.126778
1	-4.360251	-2.873777	-1.916099
1	-4.908972	-1.812089	-0.617154
6	-2.566174	1.659064	1.71736
1	-2.140429	2.332253	0.967205
1	-3.253264	2.237441	2.347155
1	-1.751816	1.303983	2.354114
6	-4.589687	1.074022	0.365556
1	-5.216326	0.308795	-0.099614
1	-5.207064	1.595967	1.106757
1	-4.308355	1.803551	-0.401059
6	-3.78294	-0.494252	2.183086

1	-4.472801	-1.256858	1.811417
1	-2.926162	-0.993641	2.645397
1	-4.306271	0.061178	2.972039

TS1_{II}

E = -4235.342216 ZPVE = 0.368956 NIMAG = 1.

17	0.079846	-1.199764	0.694177
15	-2.016645	-0.159126	-0.17384
12	0.589461	0.94107	-0.002549
35	0.567261	3.30959	0.113372
6	-2.568357	-1.309632	-1.596095
6	-3.196284	-0.142053	1.331704
6	2.522584	-1.297871	0.842348
6	3.150908	-0.614957	-0.188751
6	3.273802	-2.233623	1.549084
6	4.490718	-0.80844	-0.530831
6	4.625472	-2.460594	1.241865
1	2.814237	-2.802001	2.356341
6	5.226165	-1.749472	0.202544
1	4.97714	-0.260477	-1.330955
1	5.201598	-3.189069	1.807137
1	6.269951	-1.916116	-0.04677
8	2.341066	0.345009	-0.891147
6	2.932761	1.088763	-1.973426
1	3.246247	0.404458	-2.766725
1	2.161315	1.767042	-2.340015
1	3.78207	1.675361	-1.613334
6	-1.323818	-1.481214	-2.496057

1	-1.609652	-2.02531	-3.404947
1	-0.913184	-0.514351	-2.811606
1	-0.533481	-2.049484	-1.998694
6	-3.071295	-2.695691	-1.159467
1	-4.011045	-2.633757	-0.603989
1	-3.259271	-3.313015	-2.047946
1	-2.335718	-3.216394	-0.539037
6	-3.658382	-0.581529	-2.418221
1	-3.321038	0.407027	-2.746653
1	-3.89168	-1.172528	-3.314258
1	-4.587003	-0.452873	-1.857186
6	-2.625062	0.956754	2.25688
1	-2.56778	1.928684	1.757349
1	-3.276235	1.063381	3.133682
1	-1.626673	0.69749	2.625144
6	-4.618493	0.265378	0.891779
1	-5.102125	-0.512272	0.293839
1	-5.239116	0.424408	1.783634
1	-4.619293	1.196774	0.316395
6	-3.247247	-1.470597	2.110165
1	-3.676037	-2.283764	1.520837
1	-2.252389	-1.77852	2.443365
1	-3.87559	-1.341696	3.001605

INT1II

E = -4235.397233 ZPVE = 0.371210 NIMAG = 0.

17	1.628455	-1.846806	1.06047
15	-2.220278	-0.36689	-0.724513

12	-0.04925	0.175049	0.33277
35	1.052394	2.110237	1.271124
6	-3.039094	-1.900274	0.113119
6	-3.240673	1.247092	-0.426606
6	3.012406	-1.168043	0.197164
6	2.779337	-0.324314	-0.897339
6	4.299147	-1.477107	0.618175
6	3.874755	0.216883	-1.57199
6	5.390051	-0.937929	-0.068441
1	4.441431	-2.128339	1.473441
6	5.172416	-0.094453	-1.15691
1	3.725671	0.887646	-2.408423
1	6.39816	-1.173599	0.25524
1	6.013599	0.336734	-1.689936
8	1.46521	-0.08728	-1.241248
6	1.190131	0.788351	-2.360375
1	1.679925	0.409221	-3.260334
1	0.108617	0.74936	-2.493591
1	1.519373	1.804992	-2.130162
6	-1.937802	-2.976952	0.198011
1	-2.376225	-3.942275	0.485262
1	-1.427849	-3.11657	-0.762139
1	-1.185352	-2.725004	0.953708
6	-3.611708	-1.67492	1.523747
1	-4.454283	-0.978023	1.518776
1	-3.980669	-2.626158	1.934513
1	-2.854139	-1.283566	2.210912
6	-4.155553	-2.443503	-0.807863
1	-3.765386	-2.6746	-1.803969
1	-4.580737	-3.36443	-0.383655

1	-4.972613	-1.727748	-0.928963
6	-2.541359	2.30036	-1.316516
1	-2.568422	2.013609	-2.373201
1	-3.042551	3.271967	-1.212879
1	-1.494203	2.451128	-1.023912
6	-4.692268	1.08684	-0.920876
1	-5.266813	0.403284	-0.288193
1	-5.204367	2.059042	-0.895339
1	-4.728782	0.711955	-1.948953
6	-3.255479	1.775609	1.02328
1	-3.727862	1.07351	1.713976
1	-2.245211	1.982759	1.391318
1	-3.821192	2.717665	1.074145

INT2_{II}

E = -4235.397607 ZPVE = 0.370827 NIMAG = 0.

17	-1.866413	0.949934	1.871825
15	1.446204	-1.256989	0.486054
12	0.138388	0.78478	-0.006935
35	0.426083	3.087984	-0.651295
6	2.955802	-0.487649	1.426762
6	1.953981	-1.826123	-1.295778
6	-2.879828	-0.227526	1.040681
6	-2.745395	-0.376223	-0.345937
6	-3.815973	-0.968496	1.754449
6	-3.569485	-1.279191	-1.019266
6	-4.638417	-1.8705	1.075249
1	-3.898297	-0.833835	2.827304

6	-4.516524	-2.018414	-0.306762
1	-3.468703	-1.413486	-2.089739
1	-5.370687	-2.448925	1.628435
1	-5.151575	-2.718944	-0.839226
8	-1.765458	0.368485	-0.974597
6	-1.923903	0.682542	-2.382073
1	-2.945883	1.02179	-2.564204
1	-1.21996	1.492083	-2.57614
1	-1.685614	-0.191752	-2.993051
6	3.156898	-2.789349	-1.257087
1	3.330436	-3.218121	-2.254684
1	4.078873	-2.28246	-0.957778
1	2.982537	-3.615585	-0.560381
6	0.727987	-2.617133	-1.803178
1	-0.174504	-1.993438	-1.837058
1	0.910935	-2.988177	-2.821391
1	0.510368	-3.474544	-1.158877
6	2.24841	-0.690533	-2.298551
1	2.440814	-1.101922	-3.30126
1	1.406042	0.007794	-2.387961
1	3.122038	-0.101198	-2.011706
6	3.776058	-1.61694	2.088492
1	4.23628	-2.275659	1.346748
1	4.583964	-1.191807	2.7016
1	3.145207	-2.234956	2.735308
6	2.333449	0.368171	2.552286
1	3.114131	0.711435	3.244616
1	1.843887	1.268648	2.156734
1	1.598999	-0.199571	3.13547
6	3.895854	0.405449	0.596861

1	4.420466	-0.160816	-0.17818
1	3.359347	1.228485	0.113534
1	4.663493	0.847728	1.248494

TS2_{II}

E = -4235.355712 ZPVE = 0.370440 NIMAG = 1.

17	0.554706	0.856265	2.34963
15	-0.996062	-0.877466	-0.133638
12	1.378708	-0.450261	0.410163
35	3.519073	-1.420463	-0.00022
6	-2.134397	-1.891496	1.035998
6	-1.600624	-0.910843	-1.950014
6	-0.514976	1.775255	0.813707
6	0.360132	2.288807	-0.152558
6	-1.606756	2.522073	1.242135
6	0.084856	3.501485	-0.773668
6	-1.891596	3.736638	0.606734
1	-2.239233	2.156503	2.042907
6	-1.054245	4.227527	-0.396329
1	0.736223	3.880579	-1.553417
1	-2.765865	4.301415	0.916436
1	-1.265874	5.177038	-0.876223
8	1.446718	1.475008	-0.468029
6	2.485452	1.984664	-1.329042
1	2.864872	2.928878	-0.929552
1	3.268213	1.226716	-1.320194
1	2.098799	2.121047	-2.343039
6	-3.098	-0.572496	-2.087494

1	-3.364431	-0.514183	-3.151509
1	-3.740932	-1.332063	-1.635463
1	-3.33472	0.392578	-1.628579
6	-0.794079	0.17962	-2.688448
1	0.284997	-0.000977	-2.629245
1	-1.065674	0.171467	-3.751931
1	-1.003558	1.178206	-2.296333
6	-1.295225	-2.265158	-2.629273
1	-1.563493	-2.209254	-3.694024
1	-0.231123	-2.511662	-2.56242
1	-1.858298	-3.090737	-2.190714
6	-3.367569	-1.06358	1.45677
1	-3.99268	-0.789478	0.60321
1	-3.988702	-1.64675	2.150623
1	-3.071667	-0.142688	1.967171
6	-1.313814	-2.234945	2.297653
1	-1.936621	-2.828145	2.980102
1	-0.429863	-2.834131	2.052586
1	-0.992016	-1.342684	2.838772
6	-2.595708	-3.221517	0.405486
1	-3.245014	-3.075429	-0.460831
1	-1.746727	-3.841358	0.101608
1	-3.172168	-3.786328	1.150963

PC_{II}

E = -4235.495390 ZPVE = 0.373775 NIMAG = 0.

17	1.54612	0.605579	3.008422
15	-0.735744	-0.74527	-0.008211

12	1.577649	0.137835	0.787581
35	3.42647	-0.393569	-0.670261
6	-1.694656	-1.716822	1.339476
6	-0.828583	-1.522991	-1.757494
6	-1.52553	0.915975	-0.209543
6	-0.686584	2.052351	-0.278618
6	-2.909724	1.131426	-0.287884
6	-1.216556	3.337848	-0.411589
6	-3.452466	2.410337	-0.423383
1	-3.580844	0.281421	-0.241005
6	-2.600133	3.511638	-0.482796
1	-0.567558	4.203511	-0.450395
1	-4.52833	2.541461	-0.479662
1	-3.003873	4.514507	-0.582624
8	0.683961	1.838367	-0.210078
6	1.587389	2.920256	-0.533506
1	1.556832	3.687334	0.244683
1	2.576266	2.463951	-0.584491
1	1.326464	3.337944	-1.509263
6	-2.24646	-1.61997	-2.349984
1	-2.171096	-2.012839	-3.37173
1	-2.899031	-2.291807	-1.790197
1	-2.727723	-0.639944	-2.415436
6	0.020931	-0.612133	-2.673488
1	1.054678	-0.521659	-2.329217
1	0.040876	-1.050908	-3.678637
1	-0.4114	0.389625	-2.762356
6	-0.173772	-2.91882	-1.701602
1	-0.101681	-3.317826	-2.72056
1	0.841073	-2.873478	-1.294306

1	-0.758916	-3.632196	-1.113779
6	-2.972564	-2.443983	0.88274
1	-2.764396	-3.234111	0.156517
1	-3.433373	-2.920221	1.75704
1	-3.716792	-1.76795	0.45303
6	-2.037989	-0.731226	2.478364
1	-2.41349	-1.308573	3.332133
1	-1.161501	-0.172304	2.818893
1	-2.815187	-0.018847	2.190795
6	-0.691259	-2.759626	1.891653
1	-0.353856	-3.466222	1.12811
1	0.185894	-2.278964	2.334753
1	-1.183091	-3.339303	2.682411

R1_{III} + b S_N2@Cl pathway, followed by S_N2@C pathway, in the gas phase

RC_{III}

E = -4383.014977 ZPVE = 0.307981 NIMAG = 0.

17	-0.049706	0.541147	0.599169
15	-1.798121	0.076037	-0.672851
12	2.064898	-0.798579	-0.222743
35	1.038091	-2.358684	-1.739335
6	3.544252	-0.076682	1.093281
6	4.014443	0.85863	0.164163
6	4.212865	-0.086803	2.32234
6	5.062983	1.749801	0.368303
6	5.278476	0.789148	2.589781
1	3.908226	-0.786246	3.099021
6	5.699058	1.69934	1.618404
1	5.39118	2.457258	-0.386564

1	5.780444	0.759214	3.553382
1	6.524059	2.375936	1.822986
8	3.26558	0.783403	-1.045157
6	3.644097	1.556489	-2.182625
1	4.67201	1.321665	-2.479985
1	2.957207	1.281103	-2.983501
1	3.553675	2.626921	-1.968138
6	-2.75359	1.628853	-0.410166
6	-2.827879	2.366256	0.78397
6	-3.454857	2.085174	-1.53918
6	-3.60014	3.526375	0.846942
1	-2.273949	2.041783	1.659311
6	-4.246677	3.234868	-1.466547
1	-3.382759	1.5413	-2.477958
6	-4.315651	3.959352	-0.275283
1	-3.643982	4.093286	1.772398
1	-4.791297	3.570859	-2.343907
1	-4.91766	4.861662	-0.220712
6	-2.638531	-1.139579	0.423323
6	-3.766013	-0.856799	1.213546
6	-2.147409	-2.459533	0.374834
6	-4.377769	-1.869123	1.955639
1	-4.173618	0.147217	1.246866
6	-2.753955	-3.461547	1.132295
1	-1.288924	-2.698144	-0.247336
6	-3.870078	-3.170411	1.92228
1	-5.250697	-1.639184	2.559826
1	-2.359876	-4.472846	1.096539
1	-4.345591	-3.955027	2.50376

TS1m

E = -4382.947218 ZPVE = 0.307195 NIMAG = 1.

17	0.294792	-1.02053	-0.165799
15	-1.77412	0.35213	0.683714
12	1.383244	0.831436	0.609202
35	1.487445	2.989473	1.55754
6	2.377901	-1.891727	-0.696408
6	3.500213	-1.15096	-0.374862
6	2.532424	-3.137568	-1.285889
6	4.792533	-1.616433	-0.628938
6	3.816028	-3.638483	-1.556213
1	1.658003	-3.73319	-1.542794
6	4.936758	-2.875845	-1.226357
1	5.679312	-1.042851	-0.382315
1	3.936928	-4.614077	-2.019786
1	5.935109	-3.251127	-1.429828
8	3.274237	0.130804	0.23129
6	4.430395	0.940925	0.555231
1	4.993578	1.161032	-0.355259
1	4.040953	1.861108	0.989966
1	5.058888	0.416249	1.279239
6	-2.928815	-1.047708	0.949106
6	-2.502687	-2.153806	1.71106
6	-4.279541	-0.999134	0.550317
6	-3.386647	-3.180369	2.044692
1	-1.467755	-2.218445	2.035372
6	-5.161809	-2.028092	0.885476
1	-4.646232	-0.149811	-0.017214

6	-4.721472	-3.124474	1.632285
1	-3.030429	-4.026401	2.625966
1	-6.198494	-1.968213	0.565119
1	-5.409478	-3.923985	1.891065
6	-2.263392	1.100426	-0.917524
6	-2.741359	0.384255	-2.033548
6	-2.049042	2.487203	-1.057734
6	-3.012227	1.035895	-3.236381
1	-2.894856	-0.68806	-1.960179
6	-2.318044	3.137439	-2.264787
1	-1.683075	3.060647	-0.20972
6	-2.80098	2.41459	-3.35827
1	-3.380591	0.465657	-4.08498
1	-2.153044	4.208105	-2.347145
1	-3.013276	2.918401	-4.296808

INT_{III}

E = -4383.005103 ZPVE = 0.308720 NIMAG = 0.

17	0.195978	2.680915	-1.247186
15	-0.334016	-1.802723	-1.443179
12	1.150842	0.135198	-0.998093
35	3.47391	0.503885	-1.45868
6	-0.467897	2.744241	0.387746
6	0.037664	1.873396	1.361965
6	-1.477382	3.653119	0.682198
6	-0.475284	1.938138	2.658816
6	-1.98531	3.712955	1.981826
1	-1.852756	4.307958	-0.096374

6	-1.479597	2.860287	2.963574
1	-0.103469	1.265341	3.422225
1	-2.769552	4.423689	2.219474
1	-1.872176	2.898792	3.974521
8	1.014931	0.981421	0.974705
6	1.91478	0.446397	1.987414
1	1.411763	-0.34011	2.552908
1	2.759728	0.040191	1.432429
1	2.249961	1.262455	2.630986
6	-2.1111	-1.31963	-1.263779
6	-2.584301	-0.078189	-1.728484
6	-3.07033	-2.257374	-0.82889
6	-3.950702	0.216037	-1.759069
1	-1.879192	0.665739	-2.089322
6	-4.432995	-1.955963	-0.832505
1	-2.746236	-3.239391	-0.495572
6	-4.88315	-0.716523	-1.299979
1	-4.284134	1.180419	-2.133855
1	-5.146977	-2.698289	-0.485293
1	-5.944599	-0.486777	-1.314562
6	0.162894	-2.441572	0.232615
6	-0.586777	-2.33398	1.42302
6	1.426409	-3.070612	0.317915
6	-0.097809	-2.833022	2.633926
1	-1.564224	-1.861779	1.402412
6	1.923316	-3.546497	1.532262
1	2.021125	-3.198567	-0.583891
6	1.163053	-3.435615	2.701752
1	-0.708725	-2.749707	3.529969
1	2.899986	-4.022557	1.559844

1	1.538793	-3.825379	3.643289
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TS2_{III}

E = -4382.967060 ZPVE = 0.307141 NIMAG = 1.

17	0.598026	-2.300952	1.360033
15	-0.561779	-0.103677	-0.995824
12	1.698425	-0.893756	-0.289495
35	3.700135	-1.007686	-1.557917
6	-0.142628	-0.419764	1.809863
6	0.861484	0.507835	2.114858
6	-1.328888	-0.446728	2.533365
6	0.650572	1.477129	3.086314
6	-1.542836	0.533647	3.511034
1	-2.077888	-1.202963	2.325769
6	-0.5611	1.483928	3.794413
1	1.404701	2.229928	3.289184
1	-2.479079	0.53331	4.061305
1	-0.723769	2.229946	4.564844
8	1.998501	0.424953	1.309854
6	3.173548	1.190646	1.649263
1	3.941796	0.873948	0.94435
1	2.971198	2.258936	1.533069
1	3.474927	0.964717	2.675288
6	-0.921788	1.659605	-1.213649
6	-2.126496	2.162702	-1.747919
6	0.107133	2.582425	-0.92683
6	-2.297764	3.530257	-1.962154
1	-2.925705	1.480589	-2.016755

6	-0.065406	3.948015	-1.149354
1	1.053977	2.227664	-0.528908
6	-1.272382	4.432576	-1.661362
1	-3.235001	3.891066	-2.377055
1	0.745255	4.6349	-0.922098
1	-1.409179	5.496277	-1.831118
6	-2.099529	-1.055842	-0.872568
6	-2.095657	-2.383642	-1.348174
6	-3.279455	-0.567466	-0.27338
6	-3.234717	-3.182143	-1.254974
1	-1.201512	-2.781676	-1.819852
6	-4.420905	-1.36828	-0.189885
1	-3.30543	0.439266	0.130052
6	-4.406249	-2.676433	-0.681569
1	-3.210357	-4.197753	-1.639716
1	-5.322649	-0.967904	0.26582
1	-5.296484	-3.295254	-0.618933

PCIII

E = -4383.097268 ZPVE = 0.310504 NIMAG = 0.

17	1.250288	-2.872418	-1.836466
15	-0.595408	0.143535	-0.192186
12	1.70689	-0.828086	-0.97412
35	3.416667	0.82673	-1.325212
6	-0.674169	-0.912723	1.319669
6	0.544451	-1.359603	1.869483
6	-1.865349	-1.326645	1.927767
6	0.573439	-2.161073	3.009875

6	-1.8514	-2.131587	3.069625
1	-2.813199	-1.017908	1.497541
6	-0.631755	-2.539259	3.609207
1	1.513011	-2.50656	3.423569
1	-2.785478	-2.439327	3.528563
1	-0.607355	-3.167518	4.494348
8	1.701002	-0.977367	1.198506
6	2.975982	-1.078158	1.875109
1	3.679316	-0.539915	1.23935
1	2.908073	-0.597469	2.854072
1	3.271151	-2.126625	1.972175
6	-0.620559	1.871751	0.433855
6	0.00603	2.853371	-0.351744
6	-1.214681	2.242712	1.650919
6	0.014972	4.187074	0.062144
1	0.506961	2.575098	-1.274262
6	-1.198047	3.576526	2.064678
1	-1.682891	1.49289	2.280931
6	-0.586514	4.550423	1.269616
1	0.506901	4.935654	-0.55145
1	-1.658703	3.852784	3.008827
1	-0.571032	5.586434	1.59531
6	-2.196412	-0.139102	-1.044735
6	-2.297295	-1.272901	-1.870812
6	-3.292279	0.728597	-0.923601
6	-3.491314	-1.543695	-2.540957
1	-1.44773	-1.941301	-1.988145
6	-4.479704	0.458731	-1.609894
1	-3.219992	1.617521	-0.305004
6	-4.583166	-0.67961	-2.41322

1	-3.561408	-2.424456	-3.172184
1	-5.321597	1.138354	-1.51435
1	-5.507212	-0.888145	-2.94466

R1_{IV} + b S_{N2}@Cl pathway, followed by S_{N2}@C pathway, in the gas phase

RC_{IV}

E = -4191.271037 ZPVE = 0.254249 NIMAG = 0.

17	-0.29682	-1.150674	-0.810898
15	-2.119913	-0.201403	-1.611741
12	1.248983	0.649531	0.374098
35	-0.174628	2.585247	0.367443
6	-2.537862	-1.553345	-2.811054
1	-1.809312	-1.520572	-3.625238
1	-2.540466	-2.557702	-2.380774
1	-3.526989	-1.332145	-3.228235
6	2.79032	-0.611804	1.059712
6	3.611046	-0.332118	-0.038605
6	3.331519	-1.494748	2.000595
6	4.883481	-0.851186	-0.255234
6	4.609638	-2.055076	1.837461
1	2.756383	-1.76273	2.885244
6	5.377734	-1.734989	0.716601
1	5.482851	-0.601176	-1.124844
1	5.005116	-2.738367	2.5845
1	6.366876	-2.165936	0.589511
8	2.967425	0.577624	-0.926377
6	3.654279	1.076765	-2.072573
1	3.898753	0.260062	-2.760649

1	2.974926	1.777939	-2.558309
1	4.57043	1.597723	-1.773586
6	-3.2844	-0.512588	-0.22585
6	-4.090213	-1.656801	-0.089485
6	-3.392224	0.516594	0.729159
6	-4.988478	-1.766167	0.972387
1	-4.025578	-2.468385	-0.806381
6	-4.283549	0.397157	1.796984
1	-2.762674	1.398193	0.646307
6	-5.084226	-0.740937	1.918841
1	-5.609264	-2.65271	1.06424
1	-4.351926	1.194535	2.530876
1	-5.782096	-0.829762	2.74641

TS1iv

E = -4191.201610 ZPVE = 0.253751 NIMAG = 1.

17	-0.29244	-1.236869	0.836702
15	2.086592	-0.384866	1.563704
12	-0.502987	0.988338	0.392097
35	0.197258	3.242975	0.283458
6	2.416394	-1.86781	2.643241
1	1.82921	-1.752899	3.558666
1	2.139606	-2.817278	2.174634
1	3.475532	-1.901455	2.921172
6	-2.469416	-1.538372	0.12968
6	-3.139622	-0.427952	-0.350305
6	-3.103984	-2.771485	0.121916
6	-4.447418	-0.507103	-0.835997

6	-4.418453	-2.888896	-0.357298
1	-2.586146	-3.655358	0.490901
6	-5.080774	-1.757162	-0.833462
1	-4.984387	0.356414	-1.212798
1	-4.916636	-3.854907	-0.360634
1	-6.096889	-1.833298	-1.208538
8	-2.429013	0.820049	-0.321636
6	-3.106819	1.992343	-0.83575
1	-4.009651	2.184956	-0.250769
1	-2.404961	2.818609	-0.727256
1	-3.3557	1.842152	-1.889466
6	3.008637	-0.741339	0.027834
6	3.661044	-1.954934	-0.267652
6	3.071866	0.293247	-0.932999
6	4.347737	-2.125564	-1.471408
1	3.637502	-2.77457	0.443269
6	3.753807	0.118179	-2.13657
1	2.613261	1.256491	-0.717109
6	4.394583	-1.094201	-2.413971
1	4.846287	-3.06967	-1.67443
1	3.793348	0.932237	-2.855196
1	4.930665	-1.229942	-3.348621

INT_{IV}

E = -4191.258527 ZPVE = 0.255371 NIMAG = 0.

17	2.332086	1.573032	-0.876445
15	-1.304889	-0.393577	-2.301181
12	-0.360537	1.150339	-0.608083

35	-1.035603	3.133057	0.559195
6	0.103734	-1.532354	-2.81606
1	0.691175	-1.002685	-3.572905
1	0.781627	-1.835934	-2.010447
1	-0.294142	-2.437356	-3.288578
6	2.779314	0.065168	-0.076724
6	1.874655	-0.519707	0.820973
6	4.022298	-0.506596	-0.325452
6	2.239591	-1.696336	1.479103
6	4.379576	-1.684061	0.335968
1	4.699208	-0.030054	-1.026012
6	3.490297	-2.269838	1.237328
1	1.54873	-2.170494	2.165467
1	5.349585	-2.131851	0.148024
1	3.760316	-3.185347	1.753631
8	0.654749	0.097695	0.987474
6	-0.134455	-0.212415	2.169934
1	0.508272	-0.163498	3.051541
1	-0.891598	0.5694	2.218081
1	-0.60103	-1.193624	2.060128
6	-2.065747	-1.310654	-0.880763
6	-1.691272	-2.604553	-0.458548
6	-3.125412	-0.686611	-0.178557
6	-2.333255	-3.233416	0.614053
1	-0.898762	-3.1359	-0.976484
6	-3.757103	-1.310516	0.896237
1	-3.46675	0.299034	-0.490146
6	-3.360834	-2.589312	1.308472
1	-2.026681	-4.235534	0.905237
1	-4.565331	-0.798174	1.411554

1	-3.860495	-3.081306	2.137793
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TS2_{iv}

E = -4191.221274 ZPVE = 0.253766 NIMAG = 1.

17	1.204392	2.539073	0.997126
15	-0.356765	-0.517352	1.704646
12	1.650082	0.216049	0.40555
35	3.597705	-1.064204	-0.062364
6	-1.363091	0.398789	2.953402
1	-0.689518	1.035534	3.533252
1	-2.13323	1.031837	2.494788
1	-1.843095	-0.303233	3.641959
6	-0.563812	1.902272	0.124153
6	-0.416498	1.432757	-1.189377
6	-1.6581	2.684835	0.475313
6	-1.404008	1.669971	-2.134563
6	-2.65852	2.921086	-0.479321
1	-1.730683	3.112675	1.469408
6	-2.532506	2.425157	-1.775237
1	-1.320449	1.260381	-3.135136
1	-3.523348	3.515809	-0.200647
1	-3.298709	2.622875	-2.517135
8	0.72386	0.666154	-1.408902
6	1.00272	0.150944	-2.727505
1	1.954413	-0.371915	-2.637865
1	0.213278	-0.542812	-3.028761
1	1.085756	0.979318	-3.435687
6	-1.507136	-1.549917	0.763177

6	-2.90922	-1.500658	0.90206
6	-0.966107	-2.471728	-0.16293
6	-3.733473	-2.336336	0.145098
1	-3.363447	-0.806238	1.601312
6	-1.792149	-3.300808	-0.918147
1	0.113529	-2.556097	-0.27098
6	-3.183225	-3.239344	-0.768181
1	-4.811379	-2.280797	0.271782
1	-1.350276	-4.007289	-1.615682
1	-3.826831	-3.890804	-1.351736

PC_{IV}

E = -4191.352509 ZPVE = 0.257517 NIMAG = 0.

17	2.665841	1.389052	2.166649
15	-0.721631	0.072706	1.05997
12	1.840052	-0.019293	0.602841
35	2.615756	-1.990589	-0.552093
6	-1.383116	0.477153	2.73282
1	-0.780092	1.284976	3.155483
1	-2.436836	0.767323	2.725813
1	-1.269248	-0.408536	3.363915
6	-1.019098	1.601878	0.064482
6	-0.074957	1.945918	-0.925062
6	-2.110731	2.459465	0.252957
6	-0.231283	3.090362	-1.708232
6	-2.28001	3.607957	-0.522515
1	-2.844536	2.230878	1.019318
6	-1.338396	3.916996	-1.503342

1	0.503533	3.35447	-2.458441
1	-3.135753	4.254672	-0.357714
1	-1.452953	4.808915	-2.111641
8	1.021006	1.102321	-1.072631
6	1.811616	1.186122	-2.28253
1	2.439501	0.295065	-2.276236
1	1.151014	1.171102	-3.152727
1	2.424666	2.091481	-2.271937
6	-1.855609	-1.206484	0.379335
6	-3.254676	-1.084652	0.420319
6	-1.282649	-2.360371	-0.178998
6	-4.06705	-2.099737	-0.084829
1	-3.719026	-0.199793	0.846207
6	-2.100596	-3.373103	-0.689797
1	-0.20193	-2.465559	-0.227712
6	-3.489618	-3.246829	-0.640769
1	-5.14759	-1.99625	-0.046785
1	-1.645815	-4.260506	-1.119481
1	-4.122846	-4.03718	-1.033472

R1_v + b S_N2@Cl pathway, followed by S_N2@C pathway, in the gas phase

RC_v

E = -3999.526806 ZPVE = 0.200592 NIMAG = 0.

17	1.082577	-1.553256	-0.089319
15	3.192329	-1.192029	0.318256
12	-0.383842	0.629754	0.494912
35	1.379582	2.250651	0.599359
6	3.804251	-2.873807	-0.176271

1	3.456077	-3.622252	0.540198
1	3.499878	-3.163866	-1.186152
1	4.899838	-2.843521	-0.128355
6	3.621476	-0.240054	-1.209927
1	4.710671	-0.107054	-1.210041
1	3.320461	-0.746458	-2.131727
1	3.155401	0.745941	-1.146945
6	-2.240944	-0.288049	0.862426
6	-2.699061	-0.051087	-0.438246
6	-3.155316	-0.922214	1.710939
6	-3.953218	-0.392321	-0.934029
6	-4.436128	-1.294223	1.269429
1	-2.879076	-1.136561	2.741786
6	-4.829497	-1.032366	-0.044195
1	-4.261231	-0.185126	-1.953878
1	-5.125797	-1.786416	1.950204
1	-5.820129	-1.318151	-0.386352
8	-1.696242	0.604574	-1.211236
6	-1.983391	1.054197	-2.534524
1	-2.826497	1.753616	-2.526999
1	-1.086601	1.563496	-2.888774
1	-2.210111	0.205268	-3.18861

TS1v

E = -3999.451281 ZPVE = 0.200002 NIMAG = 1.

17	-0.09029	-1.601231	0.000367
15	-2.665774	-1.684963	-0.00034
12	-0.636891	0.620971	0.000128

35	-1.980832	2.567427	0.000233
6	-2.837836	-2.860413	-1.437364
1	-2.644466	-2.325546	-2.371814
1	-2.145501	-3.706558	-1.3676
1	-3.86209	-3.249077	-1.479701
6	-2.838428	-2.860488	1.436548
1	-3.862759	-3.248983	1.478561
1	-2.146209	-3.706741	1.366929
1	-2.645245	-2.325716	2.371092
6	2.153645	-1.062558	0.0006
6	2.463593	0.285593	-0.000081
6	3.186223	-1.990639	0.000755
6	3.783972	0.744314	-0.000562
6	4.525188	-1.568735	0.000294
1	2.961758	-3.056373	0.00125
6	4.815482	-0.204304	-0.000371
1	4.038697	1.798189	-0.001092
1	5.331064	-2.29833	0.00044
1	5.845979	0.138038	-0.000747
8	1.357721	1.206887	-0.000203
6	1.673875	2.620586	-0.000578
1	2.243251	2.872412	-0.899049
1	0.719024	3.144481	-0.000388
1	2.243794	2.872751	0.897451

INT1v

E = -3999.488030 ZPVE = 0.201644 NIMAG = 0.

17	-0.412704	-1.419811	-0.000147
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15	3.443967	-1.588037	0.000104
12	1.835874	0.30176	0.000146
35	1.63937	2.678444	0.000322
6	2.908619	-2.678619	1.443311
1	3.086193	-2.149667	2.385489
1	1.860292	-2.993466	1.413949
1	3.533481	-3.579158	1.453348
6	2.908818	-2.678384	-1.443355
1	3.53368	-3.578922	-1.453453
1	1.860487	-2.993236	-1.414188
1	3.086521	-2.149278	-2.385422
6	-2.152249	-1.070917	-0.000233
6	-2.586711	0.26572	-0.000146
6	-3.041978	-2.137528	-0.000385
6	-3.9698	0.501917	-0.000218
6	-4.416934	-1.884717	-0.000455
1	-2.660992	-3.153134	-0.000448
6	-4.870869	-0.566054	-0.000371
1	-4.343596	1.518365	-0.000155
1	-5.117413	-2.713016	-0.000574
1	-5.936196	-0.356928	-0.000424
8	-1.632682	1.225419	0
6	-2.036671	2.599678	0.000091
1	-2.620168	2.832518	0.89793
1	-1.106109	3.16404	0.0002
1	-2.62005	2.83267	-0.897785

INT2v

E = -3999.505344 ZPVE = 0.202190 NIMAG = 0.

17	0.697454	-0.47464	1.932788
15	-0.916556	2.512346	-0.719857
12	-1.17064	0.148609	-0.00656
35	-2.695028	-1.695848	0.231263
6	-0.010854	3.357076	0.706094
1	0.997864	2.94065	0.79986
1	0.097563	4.425438	0.485801
1	-0.514447	3.260933	1.674808
6	-2.632587	3.261976	-0.495192
1	-3.037637	3.149356	0.516533
1	-2.598302	4.331526	-0.732874
1	-3.329277	2.791525	-1.196705
6	2.048334	-0.365629	0.804557
6	1.813811	-0.623298	-0.553775
6	3.322904	-0.060471	1.269607
6	2.881986	-0.567434	-1.45069
6	4.388375	-0.008729	0.367009
1	3.473672	0.131263	2.326313
6	4.164011	-0.263487	-0.985894
1	2.718143	-0.745995	-2.506248
1	5.384066	0.22924	0.725727
1	4.98602	-0.220916	-1.693062
8	0.515162	-0.895026	-0.927072
6	0.261174	-1.459049	-2.23587
1	0.901257	-2.330963	-2.389275
1	-0.784498	-1.767031	-2.213878
1	0.426646	-0.705496	-3.010525

TS2v

E = -3999.460837 ZPVE = 0.199620 NIMAG = 1.

17	1.104715	0.05617	2.314661
15	0.591542	1.742244	-0.3017
12	-1.371947	0.242448	-0.307716
35	-3.695744	-0.168742	-0.226652
6	0.5183	3.422623	0.491437
1	0.013449	3.343072	1.457492
1	1.531075	3.802844	0.661786
1	-0.025172	4.140029	-0.133249
6	1.535862	2.024565	-1.868283
1	1.035195	2.744105	-2.52292
1	2.540335	2.39497	-1.633478
1	1.642568	1.07691	-2.402903
6	1.777115	-0.1002	0.524694
6	1.209149	-1.177704	-0.217992
6	3.194078	0.031239	0.414879
6	1.94038	-1.940632	-1.1188
6	3.923531	-0.747208	-0.473452
1	3.692826	0.772704	1.030167
6	3.314595	-1.735791	-1.264553
1	1.423337	-2.700981	-1.698759
1	4.997018	-0.589907	-0.538691
1	3.89292	-2.337733	-1.956017
8	-0.193751	-1.402828	-0.094689
6	-0.578454	-2.593769	0.650616
1	-0.182254	-2.526138	1.665898
1	-1.66945	-2.611623	0.658149
1	-0.188056	-3.476311	0.140442

PCv

E = -3999.607747 ZPVE = 0.203651 NIMAG = 0.

17	-1.021154	0.355426	2.916218
15	0.582842	1.568104	-0.336424
12	-1.313343	0.109646	0.686474
35	-3.127135	-0.287735	-0.840462
6	1.285721	2.996038	0.595071
1	1.364331	2.721022	1.649921
1	2.262044	3.314272	0.218971
1	0.587866	3.834726	0.512298
6	0.627256	2.114774	-2.10254
1	-0.08838	2.930267	-2.243955
1	1.625891	2.451506	-2.396837
1	0.323308	1.281986	-2.741612
6	1.891683	0.267063	-0.259503
6	1.503455	-1.08018	-0.107883
6	3.262141	0.550347	-0.332043
6	2.453719	-2.100759	-0.032094
6	4.222744	-0.459991	-0.262205
1	3.588441	1.579903	-0.445985
6	3.811697	-1.783698	-0.108627
1	2.152256	-3.131962	0.102302
1	5.278062	-0.214135	-0.321413
1	4.545396	-2.58132	-0.044478
8	0.141138	-1.341238	-0.031012
6	-0.322532	-2.703949	-0.178235
1	-0.079861	-3.284917	0.715582

1	-1.40221	-2.628278	-0.309522
1	0.125266	-3.14986	-1.069683

S.11.4 Alternative solvent-phase reactions in manuscript

R1₁ + a S_N2@P-b pathways 2, 3 and 4 in THF

RC_{Ia-i} 2

E = -4303.614906 ZPVE = 0.461914 NIMAG = 0.

17	-3.389002	1.236146	-2.122316
15	-1.814777	0.461789	-0.964668
5	-0.699065	-0.601097	-2.160912
1	0.220407	-0.997996	-1.48183
1	-0.357432	0.194077	-3.007273
1	-1.403162	-1.487189	-2.58114
6	6.306065	-1.445992	-2.021472
1	5.662706	-1.987885	-2.732388
1	6.72839	-0.608617	-2.598357
6	7.446255	-2.373222	-1.554537
1	7.06701	-3.243162	-1.002951
1	8.045992	-2.767174	-2.390515
1	8.144535	-1.855854	-0.883957
12	5.023082	-0.627716	-0.539773
35	3.286041	0.320406	0.922621
6	-4.104149	-0.805826	0.278391
6	-1.844129	-1.348212	1.313717
6	-4.129916	-2.125765	-0.506827
1	-4.715998	-0.049383	-0.21968
1	-4.565496	-0.973969	1.262448
6	-1.861131	-2.686242	0.542772

6	-0.430764	-0.894067	1.777967
1	-2.424612	-1.512143	2.237306
6	-3.28422	-3.174852	0.229981
6	-5.568907	-2.605935	-0.732207
1	-3.674407	-1.951886	-1.492512
1	-1.358847	-3.451514	1.140694
1	-1.288145	-2.589443	-0.385894
6	-0.497165	0.284769	2.76564
6	0.361196	-2.038788	2.437888
1	0.148193	-0.572575	0.902734
1	-3.234589	-4.09785	-0.361554
1	-3.791888	-3.434457	1.171759
1	-6.154266	-1.864633	-1.28809
1	-5.586172	-3.542747	-1.300499
1	-6.075962	-2.785729	0.224366
1	-1.028605	-0.009322	3.680187
1	0.514409	0.592249	3.049768
1	-0.998338	1.16423	2.353791
1	-0.20297	-2.48017	3.270155
1	1.304248	-1.652577	2.836868
1	0.60854	-2.838918	1.735007
6	-1.010214	2.002266	-0.395308
6	0.360375	2.179336	-0.632654
6	-1.736704	3.010465	0.263287
6	0.997316	3.351352	-0.213161
1	0.931887	1.408963	-1.136256
6	-1.097526	4.177653	0.677114
1	-2.801723	2.895642	0.442397
6	0.270615	4.351478	0.434054
1	2.061331	3.473372	-0.387914

1	-1.666407	4.954271	1.179133
1	0.766969	5.261295	0.758523
6	-2.683956	-0.261167	0.557696
1	-2.792228	0.610101	1.211132

TS_{1a-i} 2

E = -4303.545178 ZPVE = 0.466034 NIMAG = 1.

17	-1.527969	3.204067	0.63565
15	-0.898661	1.108148	-0.526388
5	-1.533473	1.900179	-2.273975
1	-1.495295	1.056044	-3.129714
1	-0.758126	2.810771	-2.442399
1	-2.645768	2.275656	-2.006577
6	-0.079101	-0.830811	-1.964671
1	-1.158285	-0.89125	-2.045299
1	0.225488	-0.272802	-2.860627
6	0.469822	-2.290981	-2.037156
1	0.149063	-2.902856	-1.192772
1	0.10005	-2.772189	-2.951425
1	1.566397	-2.382736	-2.091792
12	1.806739	-0.395138	-0.928301
35	3.991164	-1.315583	-0.448123
6	-3.485315	0.551263	0.409911
6	-1.938789	-1.346229	1.080732
6	-4.125796	-0.314543	-0.685492
1	-3.564572	1.609554	0.157175
1	-4.054841	0.415543	1.340949
6	-2.607581	-2.241603	0.01675

6	-0.556407	-1.822035	1.61366
1	-2.613871	-1.406612	1.951098
6	-4.04369	-1.795911	-0.295215
6	-5.570239	0.129083	-0.949916
1	-3.558367	-0.170764	-1.616535
1	-2.634869	-3.270202	0.388374
1	-2.025649	-2.26727	-0.907557
6	-0.330611	-1.338399	3.060644
6	-0.356915	-3.347922	1.594033
1	0.218132	-1.379998	0.967543
1	-4.457835	-2.421737	-1.095732
1	-4.674765	-1.96258	0.590996
1	-5.611388	1.177646	-1.264872
1	-6.031084	-0.478176	-1.737153
1	-6.182999	0.025672	-0.045306
1	-0.944413	-1.934226	3.746391
1	0.715774	-1.457658	3.35984
1	-0.609849	-0.293066	3.219312
1	-1.117769	-3.846324	2.206222
1	0.621952	-3.59906	2.016183
1	-0.404238	-3.777841	0.591249
6	0.790008	1.553061	0.108293
6	1.68185	2.16804	-0.802926
6	1.178878	1.437445	1.457274
6	2.927357	2.638847	-0.369095
1	1.380167	2.324052	-1.834893
6	2.42534	1.905759	1.87717
1	0.507494	1.005599	2.185222
6	3.300168	2.510795	0.970298
1	3.596092	3.108573	-1.083037

1	2.709606	1.796657	2.918879
1	4.266889	2.873136	1.303906
6	-2.014384	0.180398	0.747397
1	-1.749564	0.725716	1.655773

PC_{Ia-i} 2

E = -4303.688597 ZPVE = 0.465396 NIMAG = 0.

17	-7.72641	-1.62521	-1.435764
15	2.562305	1.017384	-0.87343
5	3.107716	1.366525	-2.724418
1	4.21307	0.88851	-2.874989
1	3.109224	2.579606	-2.797668
1	2.270986	0.861744	-3.44459
6	3.842165	1.824625	0.210234
1	4.76661	1.282639	-0.017524
1	3.963547	2.804989	-0.265589
6	3.689844	2.001251	1.727969
1	3.741096	1.055467	2.267542
1	4.510465	2.630102	2.089868
1	2.753984	2.489504	2.006951
12	-5.999124	-0.777659	-0.198824
35	-3.965836	-0.066883	0.922767
6	3.063118	-1.702019	-1.55107
6	2.331309	-1.438429	0.870546
6	4.52778	-1.913785	-1.138804
1	3.010298	-1.283747	-2.559433
1	2.570812	-2.68514	-1.592082
6	3.802029	-1.642185	1.296574

6	1.399828	-0.753036	1.913251
1	1.926051	-2.456975	0.744314
6	4.586719	-2.490256	0.283378
6	5.264521	-2.802921	-2.148202
1	5.028574	-0.933846	-1.131689
1	3.835773	-2.137975	2.27114
1	4.309132	-0.679799	1.423512
6	-0.078329	-1.075044	1.626215
6	1.71616	-1.144334	3.367628
1	1.522438	0.333906	1.835475
1	5.630832	-2.582925	0.608963
1	4.17229	-3.509818	0.26835
1	5.246565	-2.363238	-3.151751
1	6.312735	-2.942965	-1.860147
1	4.798741	-3.794878	-2.207749
1	-0.277622	-2.140338	1.799109
1	-0.734283	-0.499626	2.287676
1	-0.37472	-0.84104	0.601297
1	1.682348	-2.233156	3.501016
1	0.970265	-0.707476	4.040622
1	2.700378	-0.796297	3.694781
6	0.960942	1.887791	-0.596808
6	0.891141	3.131568	0.051797
6	-0.210769	1.374661	-1.181263
6	-0.322018	3.819721	0.150635
1	1.778618	3.586416	0.474903
6	-1.422176	2.059547	-1.078824
1	-0.189127	0.43914	-1.731479
6	-1.484652	3.281772	-0.404286
1	-0.352723	4.776112	0.664374

1	-2.314581	1.638446	-1.529849
1	-2.428041	3.81223	-0.318744
6	2.244797	-0.831856	-0.563641
1	1.201359	-0.903997	-0.88799

P_{1a-i} 2

E = -1071.474465 ZPVE = 0.462528 NIMAG = 0.

6	-0.873611	-0.135403	-0.834069
6	-2.491184	1.252557	0.581977
6	-2.086447	-0.993359	-1.277738
6	-3.664005	0.372673	0.121441
6	-0.20477	2.314363	-0.185375
6	-4.397454	-1.894573	-0.766781
6	0.528992	2.681464	-1.489244
6	-0.680444	3.610451	0.494755
1	-0.226296	-0.049424	-1.713229
1	-2.863534	2.264702	0.764733
1	-2.122442	0.882762	1.544586
1	1.303955	0.827361	2.661704
1	-1.761364	-2.00308	-1.540936
1	-2.477812	-0.538536	-2.199866
1	-4.430693	0.338695	0.906116
1	-4.13729	0.835127	-0.758103
1	0.525465	1.844645	0.484718
1	-4.080541	-2.918807	-0.993007
1	-5.204094	-1.946942	-0.026571
1	-4.813955	-1.461154	-1.685008
1	-0.144127	3.221877	-2.16676

1	1.385581	3.331649	-1.280818
1	0.908773	1.806115	-2.022076
1	-1.456521	4.108606	-0.099961
1	0.157926	4.308615	0.593875
1	-1.084311	3.438306	1.496705
6	1.996292	-0.649339	-0.046268
6	2.419102	-0.51058	-1.379936
6	2.966828	-0.586886	0.968339
6	3.760783	-0.27345	-1.686529
1	1.710937	-0.602481	-2.197086
6	4.309943	-0.350822	0.661636
1	2.692645	-0.734036	2.006261
6	4.711173	-0.184875	-0.665812
1	4.061263	-0.166111	-2.724586
1	5.040289	-0.301708	1.463902
1	5.754461	-0.000312	-0.903676
6	-1.355246	1.301499	-0.463808
1	-1.836907	1.657208	-1.390446
6	-0.014204	-0.859193	2.148755
1	0.581861	-1.663153	2.596296
15	0.255361	-1.129973	0.32733
5	0.109001	-3.061684	0.022009
1	0.995466	-3.522778	0.71379
1	-0.995832	-3.4069	0.386308
1	0.299983	-3.251241	-1.161652
6	0.290862	0.46868	2.856263
1	-0.40072	1.262372	2.572989
1	0.195001	0.320253	3.937229
1	-1.056234	-1.151589	2.317598
6	-3.225494	-1.051946	-0.248282

1	-2.84305	-1.539601	0.661032
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RC_{1a-i} 3

E = -4303.613699 ZPVE = 0.463604 NIMAG = 0.

6	-1.242806	-1.683187	-0.109594
6	0.2673	-1.778584	1.961084
6	1.16096	-2.62067	-0.29375
6	-0.293805	-2.705409	-0.777665
6	1.205728	-2.756945	1.235391
6	-2.200764	-0.973837	2.239476
6	2.033697	-3.676199	-0.983059
6	-3.655587	-1.351263	1.904645
6	-2.001477	-1.071506	3.763322
1	-2.258708	-1.908564	-0.449165
1	0.280946	-2.016903	3.0281
1	0.648769	-0.756382	1.867969
1	1.566038	-1.635699	-0.561395
1	-0.343092	-2.623866	-1.866597
1	-0.695224	-3.69775	-0.526166
1	2.232738	-2.612965	1.592765
1	0.923122	-3.786645	1.503035
1	-2.047499	0.079468	1.967074
1	2.022122	-3.55197	-2.071959
1	3.073647	-3.600145	-0.647952
1	1.678026	-4.68948	-0.756236
1	-3.858763	-2.387586	2.202773
1	-4.353338	-0.705804	2.448418
1	-3.889875	-1.255881	0.841534

1	-2.044504	-2.114945	4.100802
1	-2.797915	-0.524003	4.278506
1	-1.048007	-0.648325	4.089854
6	-2.648887	0.858745	-0.830343
6	-2.886668	2.087517	-0.194666
6	-3.676523	0.250632	-1.572513
6	-4.144855	2.689264	-0.285427
1	-2.099916	2.57285	0.371854
6	-4.926435	0.860877	-1.667231
1	-3.505396	-0.688605	-2.089654
6	-5.163608	2.079204	-1.020384
1	-4.322276	3.636748	0.213741
1	-5.71339	0.386923	-2.245548
1	-6.138543	2.551363	-1.093895
17	-0.448955	-0.098916	-2.707909
6	-1.187492	-1.851374	1.448551
1	-1.516078	-2.893436	1.595803
6	2.970211	3.94233	0.903395
1	2.421771	4.56415	0.177399
15	-0.995483	0.095527	-0.700661
12	2.985066	1.951073	0.153309
35	4.255924	-0.044389	-0.624754
5	0.290614	1.294096	0.132499
1	0.3379	2.257437	-0.592293
1	-0.108234	1.535162	1.243096
1	1.323797	0.654231	0.149204
6	2.376631	4.166389	2.309763
1	2.928326	3.608562	3.078276
1	2.385426	5.223245	2.622836
1	1.333116	3.830415	2.368672

1	4.004557	4.321426	0.881745
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TS_{1a-i} 3

E = -4303.563373 ZPVE = 0.466512 NIMAG = 1.

6	-2.200431	0.182319	-0.448233
6	-2.486391	-1.620889	1.333122
6	-2.736983	-2.297523	-1.109267
6	-2.858567	-0.803992	-1.461755
6	-3.1765	-2.564322	0.336921
6	-2.562594	0.927715	2.077994
6	-3.52301	-3.1493	-2.115086
6	-3.395491	2.186901	1.764602
6	-2.939342	0.421403	3.481722
1	-2.518505	1.190419	-0.725259
1	-2.849673	-1.840085	2.339971
1	-1.410684	-1.815193	1.333138
1	-1.681173	-2.584128	-1.190904
1	-2.4867	-0.627725	-2.472125
1	-3.923748	-0.5329	-1.481036
1	-2.968172	-3.608979	0.601064
1	-4.266207	-2.432892	0.415352
1	-1.510644	1.225362	2.127081
1	-3.16629	-2.987946	-3.138543
1	-3.423074	-4.216774	-1.888237
1	-4.591485	-2.900727	-2.088862
1	-4.466593	1.956871	1.819603
1	-3.187335	2.97918	2.491517
1	-3.201714	2.596557	0.768118

1	-3.963536	0.028665	3.501718
1	-2.888135	1.246894	4.199683
1	-2.266828	-0.364657	3.836142
6	0.558751	1.869182	-0.486192
6	1.820743	2.092025	-1.063524
6	0.00817	2.848821	0.348039
6	2.524973	3.262961	-0.785275
1	2.258803	1.36312	-1.736142
6	0.715417	4.024729	0.618246
1	-0.972475	2.720426	0.784593
6	1.977232	4.233415	0.060104
1	3.50041	3.416981	-1.236562
1	0.272075	4.77411	1.267064
1	2.526903	5.14473	0.274435
17	-0.960165	1.403064	-2.954307
6	-2.765341	-0.148805	0.96899
1	-3.85087	-0.111364	0.777379
6	0.812646	-0.319377	1.39658
1	-0.075081	0.214947	1.711364
15	-0.328698	0.31145	-0.903985
12	1.995668	-1.486028	-0.059541
35	4.382418	-1.67088	0.408072
5	0.573347	-1.16437	-1.887191
1	1.727699	-0.792232	-2.004671
1	0.474922	-2.158285	-1.181694
1	0.08889	-1.362965	-2.957928
6	1.044648	-1.479081	2.407569
1	1.997236	-2.010137	2.262919
1	1.095004	-1.08625	3.432177
1	0.248795	-2.228649	2.387747

1	1.624488	0.417678	1.474469
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PC_{1a-i} 3

E = -4303.704701 ZPVE = 0.467699 NIMAG = 0.

6	-1.750046	-0.672797	-0.874492
6	-3.411063	-2.252545	0.253332
6	-1.246102	-3.211638	-0.738105
6	-1.097176	-1.909931	-1.538421
6	-2.726847	-3.458716	-0.411706
6	-4.073777	0.259203	-0.06445
6	-0.619791	-4.394905	-1.486836
6	-4.137306	1.3775	-1.121531
6	-5.509285	-0.122077	0.34262
1	-1.699782	0.137626	-1.610824
1	-4.473099	-2.482469	0.373411
1	-3.015374	-2.110152	1.266215
1	-0.69981	-3.095117	0.208375
1	-0.04241	-1.718676	-1.75652
1	-1.594181	-2.039486	-2.510656
1	-2.825464	-4.341145	0.233018
1	-3.257354	-3.695413	-1.346309
1	-3.585407	0.66893	0.829405
1	0.44764	-4.227876	-1.669637
1	-0.720943	-5.322226	-0.911801
1	-1.108677	-4.547506	-2.457211
1	-4.646094	1.019922	-2.025566
1	-4.702712	2.233536	-0.738526
1	-3.151079	1.746802	-1.413109

1	-6.032815	-0.623717	-0.481143
1	-6.07762	0.779549	0.594749
1	-5.538849	-0.782232	1.213709
6	-0.865968	1.895215	0.339255
6	-1.526809	2.667399	1.307588
6	-0.328081	2.535999	-0.790202
6	-1.655116	4.049325	1.143156
1	-1.954158	2.20847	2.192101
6	-0.460549	3.915957	-0.953523
1	0.207977	1.966767	-1.542956
6	-1.124373	4.676358	0.01321
1	-2.170272	4.632118	1.900771
1	-0.03351	4.394789	-1.829084
1	-1.222731	5.750474	-0.111049
17	3.636637	2.57568	-1.191927
6	-3.25497	-0.960458	-0.576592
1	-3.671365	-1.193757	-1.571015
6	-1.113653	-0.328854	2.239514
1	-2.197139	-0.24851	2.358793
15	-0.655468	0.074294	0.486176
12	3.440444	0.48534	-0.235007
35	4.993675	-1.295504	0.402186
5	1.210897	-0.40226	0.208556
1	1.820713	0.230943	1.061396
1	1.369181	-1.581257	0.359232
1	1.513603	-0.058775	-0.924224
6	-0.595452	-1.661088	2.798715
1	0.491901	-1.730646	2.722229
1	-0.865447	-1.726146	3.857242
1	-1.028119	-2.527543	2.29379

1	-0.667642	0.48795	2.816923
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RC_{1a-i} 4

E = -4303.614906 ZPVE = 0.461914 NIMAG = 0.

17	-3.389002	1.236146	-2.122316
15	-1.814777	0.461789	-0.964668
5	-0.699065	-0.601097	-2.160912
1	0.220407	-0.997996	-1.48183
1	-0.357432	0.194077	-3.007273
1	-1.403162	-1.487189	-2.58114
6	6.306065	-1.445992	-2.021472
1	5.662706	-1.987885	-2.732388
1	6.72839	-0.608617	-2.598357
6	7.446255	-2.373222	-1.554537
1	7.06701	-3.243162	-1.002951
1	8.045992	-2.767174	-2.390515
1	8.144535	-1.855854	-0.883957
12	5.023082	-0.627716	-0.539773
35	3.286041	0.320406	0.922621
6	-4.104149	-0.805826	0.278391
6	-1.844129	-1.348212	1.313717
6	-4.129916	-2.125765	-0.506827
1	-4.715998	-0.049383	-0.21968
1	-4.565496	-0.973969	1.262448
6	-1.861131	-2.686242	0.542772
6	-0.430764	-0.894067	1.777967
1	-2.424612	-1.512143	2.237306
6	-3.28422	-3.174852	0.229981

6	-5.568907	-2.605935	-0.732207
1	-3.674407	-1.951886	-1.492512
1	-1.358847	-3.451514	1.140694
1	-1.288145	-2.589443	-0.385894
6	-0.497165	0.284769	2.76564
6	0.361196	-2.038788	2.437888
1	0.148193	-0.572575	0.902734
1	-3.234589	-4.09785	-0.361554
1	-3.791888	-3.434457	1.171759
1	-6.154266	-1.864633	-1.28809
1	-5.586172	-3.542747	-1.300499
1	-6.075962	-2.785729	0.224366
1	-1.028605	-0.009322	3.680187
1	0.514409	0.592249	3.049768
1	-0.998338	1.16423	2.353791
1	-0.20297	-2.48017	3.270155
1	1.304248	-1.652577	2.836868
1	0.60854	-2.838918	1.735007
6	-1.010214	2.002266	-0.395308
6	0.360375	2.179336	-0.632654
6	-1.736704	3.010465	0.263287
6	0.997316	3.351352	-0.213161
1	0.931887	1.408963	-1.136256
6	-1.097526	4.177653	0.677114
1	-2.801723	2.895642	0.442397
6	0.270615	4.351478	0.434054
1	2.061331	3.473372	-0.387914
1	-1.666407	4.954271	1.179133
1	0.766969	5.261295	0.758523
6	-2.683956	-0.261167	0.557696

1	-2.792228	0.610101	1.211132
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TS_{1a-i} 4

E = -4303.537655 ZPVE = 0.465416 NIMAG = 1.

17	1.476145	3.107226	-0.954254
15	0.890165	1.124024	0.493321
5	1.926721	1.864525	2.049776
1	2.185548	0.90637	2.73659
1	1.154585	2.639737	2.565111
1	2.886385	2.390577	1.554351
6	-0.35763	-0.207476	2.335758
1	-0.019968	0.686939	2.853386
1	-1.448603	-0.18158	2.591787
6	0.23687	-1.451941	2.995231
1	0.056949	-2.375285	2.435096
1	1.316304	-1.342888	3.121688
1	-0.187281	-1.594739	3.998606
12	-1.78735	-0.398087	0.618138
35	-3.798748	-1.531965	-0.077988
6	3.185426	0.376925	-1.034557
6	1.712868	-1.623238	-0.683216
6	4.193999	-0.11276	0.017805
1	3.253998	1.457708	-1.141851
1	3.463912	-0.048743	-2.009962
6	2.646896	-2.078628	0.456615
6	0.350509	-2.357021	-0.789683
1	2.230593	-1.914882	-1.611842
6	4.092076	-1.630495	0.204807

6	5.61495	0.321549	-0.365856
1	3.946565	0.361686	0.975033
1	2.626658	-3.167461	0.543081
1	2.303178	-1.680652	1.414342
6	-0.276998	-2.17855	-2.186218
6	0.435452	-3.864296	-0.486361
1	-0.324231	-1.948814	-0.017035
1	4.732682	-1.950378	1.036377
1	4.472715	-2.134397	-0.696885
1	5.689418	1.411453	-0.450046
1	6.341567	-0.008344	0.385388
1	5.911202	-0.111185	-1.330159
1	0.344273	-2.686221	-2.932727
1	-1.277448	-2.6191	-2.222515
1	-0.36657	-1.134201	-2.496862
1	1.176292	-4.346806	-1.134982
1	-0.534121	-4.334207	-0.678824
1	0.704086	-4.073123	0.551674
6	-0.815133	1.723723	0.03626
6	-1.496292	2.529062	0.978118
6	-1.407365	1.519481	-1.227731
6	-2.718302	3.116363	0.650829
1	-1.052965	2.720659	1.94881
6	-2.639487	2.10637	-1.541938
1	-0.890177	0.9528	-1.993077
6	-3.292102	2.911577	-0.609312
1	-3.2171	3.744571	1.382025
1	-3.07275	1.936305	-2.52197
1	-4.24101	3.375166	-0.857995
6	1.700977	-0.059712	-0.815024

1	1.158871	0.213433	-1.724215
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PC_{1a-i} 4

E = -4303.689660 ZPVE = 0.466261 NIMAG = 0.

17	-3.257433	-1.845772	-2.617276
15	1.17622	0.596148	0.852893
5	1.906593	1.621009	2.353051
1	2.690611	0.901812	2.930366
1	0.922466	1.863057	3.02534
1	2.42345	2.625386	1.918949
6	0.032305	-0.72333	1.512717
1	-0.913395	-0.194899	1.672593
1	-0.149409	-1.472341	0.737175
6	0.460812	-1.376768	2.834869
1	1.427974	-1.881151	2.765842
1	0.530997	-0.63191	3.630454
1	-0.284582	-2.122864	3.129762
12	-3.905019	-0.827234	-0.684802
35	-5.046996	-0.075474	1.314613
6	3.239982	1.057348	-1.009597
6	3.164109	-1.372629	-0.298902
6	4.469279	1.324628	-0.119911
1	2.67193	1.985943	-1.143217
1	3.58594	0.767357	-2.012673
6	4.308768	-1.09868	0.697015
6	2.381024	-2.695862	-0.068511
1	3.649122	-1.509256	-1.281299
6	5.226283	0.021436	0.180088

6	5.384616	2.375721	-0.761535
1	4.113915	1.727076	0.834753
1	4.90859	-2.001171	0.841587
1	3.902558	-0.828908	1.68053
6	1.384996	-2.978964	-1.209278
6	3.326414	-3.905906	0.063954
1	1.819641	-2.627046	0.868769
1	6.022943	0.220388	0.908359
1	5.723348	-0.327598	-0.738353
1	4.851777	3.318547	-0.931664
1	6.246913	2.590008	-0.119697
1	5.767055	2.02713	-1.729662
1	1.911268	-3.065358	-2.168387
1	0.859874	-3.923881	-1.033736
1	0.62267	-2.203516	-1.324247
1	3.998359	-3.977132	-0.801061
1	2.745507	-4.833471	0.109095
1	3.941281	-3.863016	0.966619
6	0.017731	1.636541	-0.142664
6	-0.152234	2.992369	0.175141
6	-0.732113	1.091716	-1.201005
6	-1.048277	3.786324	-0.54919
1	0.416544	3.428753	0.988674
6	-1.626727	1.884316	-1.924719
1	-0.624504	0.046944	-1.478846
6	-1.788462	3.235327	-1.597432
1	-1.166386	4.834236	-0.289718
1	-2.186147	1.446606	-2.746418
1	-2.480627	3.853445	-2.161463
6	2.310332	-0.084673	-0.512018

1	1.602487	-0.287381	-1.321352
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R1_{II} + a S_N2@P-b pathways 2 and 3 in THF

RC_{IIa-i} 2

E = -3995.124328 ZPVE = 0.343432 NIMAG = 0.

17	3.603498	1.807158	0.318362
15	1.876848	0.641514	0.078076
6	2.096659	-0.121675	-1.650951
6	2.014694	-0.592257	1.52237
5	0.313027	1.79842	0.190702
1	0.283854	2.440175	-0.833324
1	0.446773	2.474244	1.181929
1	-0.609352	1.013098	0.278205
6	-4.675523	2.244236	-0.455785
1	-3.973177	2.926479	-0.95897
1	-5.499187	2.098572	-1.172113
6	-5.219446	2.918438	0.820688
1	-5.97039	2.2942	1.32219
1	-4.425357	3.107058	1.554475
1	-5.700537	3.88898	0.619849
12	-3.696095	0.380177	-0.218917
35	-2.810539	-1.914099	-0.076897
6	0.730964	-0.721582	-2.063159
1	-0.052324	0.039519	-2.086733
1	0.834861	-1.131687	-3.074333
1	0.401308	-1.531813	-1.410564
6	3.196916	-1.194752	-1.721
1	3.321269	-1.493329	-2.768351

1	4.161489	-0.817783	-1.368697
1	2.940147	-2.093486	-1.155396
6	2.445003	1.021504	-2.632147
1	2.417536	0.613354	-3.648729
1	1.727342	1.844055	-2.579786
1	3.446856	1.420096	-2.457255
6	1.633928	0.193007	2.798744
1	1.719404	-0.485717	3.65495
1	2.302783	1.040582	2.975096
1	0.608046	0.56487	2.759758
6	0.989441	-1.727416	1.307128
1	-0.027228	-1.358563	1.150143
1	1.25864	-2.379707	0.472736
1	0.978932	-2.346237	2.211948
6	3.425217	-1.185093	1.705509
1	4.173739	-0.411527	1.891692
1	3.402642	-1.843648	2.581394
1	3.749493	-1.783374	0.853102

TS_{IIa-i} 2

E = -3995.031611 ZPVE = 0.347799 NIMAG = 1.

17	3.508987	0.565623	-1.028935
15	1.430699	-0.14437	0.402245
6	0.91696	1.775021	0.432575
6	0.910805	-1.308599	-1.127727
5	2.763413	-0.849108	1.789464
1	2.656893	-0.028776	2.67476
1	3.849334	-0.887886	1.288162

1	2.341318	-1.930683	2.110812
6	-0.200345	-0.863936	2.100068
1	0.595766	-0.439529	2.705084
1	-1.070367	-0.346749	2.569154
6	-0.31829	-2.371767	2.391984
1	-1.251789	-2.820383	2.034322
1	0.506001	-2.933343	1.949299
1	-0.28161	-2.550778	3.473484
12	-1.767956	-0.389849	0.647921
35	-3.753125	0.346581	-0.490017
6	-0.361448	2.078573	1.237803
1	-0.357792	1.68526	2.253872
1	-0.442674	3.168023	1.325208
1	-1.290503	1.810277	0.712326
6	0.705133	2.34602	-0.981998
1	0.533643	3.425011	-0.887202
1	1.570029	2.190928	-1.624735
1	-0.182396	1.921658	-1.461018
6	2.0661	2.515816	1.15593
1	1.828932	3.586397	1.149548
1	2.157862	2.197216	2.197253
1	3.024075	2.369662	0.660819
6	1.925477	-2.47123	-1.063534
1	1.715176	-3.157016	-1.892982
1	2.948428	-2.108156	-1.16818
1	1.850336	-3.034625	-0.130212
6	-0.50619	-1.899354	-1.010442
1	-0.694841	-2.420617	-0.068556
1	-1.284132	-1.16014	-1.268977
1	-0.639442	-2.658559	-1.788653

6	0.969207	-0.6403	-2.51765
1	1.951618	-0.230144	-2.735825
1	0.742052	-1.414572	-3.260589
1	0.224129	0.149422	-2.632771

PC_{IIa-i} 2

E = -3995.208311 ZPVE = 0.346569 NIMAG = 0.

17	-7.045019	0.026958	0.246462
15	2.729326	0.082392	-0.334373
6	2.489619	-1.705409	0.296396
6	2.264538	1.390553	0.977663
5	4.561414	0.362108	-0.977382
1	4.662227	-0.264574	-2.011836
1	5.312224	-0.049533	-0.116734
1	4.688832	1.555688	-1.159395
6	1.48821	0.230222	-1.718326
1	1.397599	-0.776016	-2.138932
1	0.505837	0.472466	-1.300517
6	1.857886	1.19747	-2.853752
1	1.914677	2.235381	-2.519275
1	2.822043	0.935769	-3.296501
1	1.095785	1.141782	-3.638684
12	-4.770309	-0.099686	-0.032929
35	-2.342295	-0.067799	-0.197283
6	1.006616	-2.108381	0.433088
1	0.465829	-2.037442	-0.514106
1	0.960247	-3.155631	0.756972
1	0.469783	-1.511663	1.171373

6	3.207135	-1.905078	1.647393
1	3.189398	-2.972096	1.900375
1	4.253814	-1.590458	1.604276
1	2.714712	-1.369967	2.463258
6	3.158581	-2.634652	-0.744303
1	3.017524	-3.67403	-0.424109
1	2.717167	-2.536113	-1.74107
1	4.230577	-2.443818	-0.82782
6	2.043706	2.731216	0.238841
1	1.89787	3.519039	0.987604
1	2.904	3.010208	-0.375458
1	1.150387	2.711894	-0.391428
6	0.984334	1.060428	1.768498
1	0.120725	0.890692	1.119862
1	1.107789	0.189988	2.417562
1	0.745102	1.914517	2.414424
6	3.447031	1.571842	1.955033
1	4.362144	1.857156	1.430505
1	3.196062	2.371278	2.662897
1	3.654102	0.670706	2.536268

RCIIa-i 3

E = -3995.124634 ZPVE = 0.342989 NIMAG = 0.

17	-4.311822	0.291137	-1.091024
15	-2.864946	0.336542	0.427682
6	-2.219613	-1.453174	0.456322
6	-1.632773	1.633192	-0.226626
5	-3.71237	0.868496	2.10342

1	-2.777427	1.125312	2.834388
1	-4.354805	-0.081772	2.483691
1	-4.388321	1.837457	1.852321
6	6.194678	1.192261	0.789473
1	6.131643	1.199878	1.888659
6	7.601995	0.731355	0.358877
1	7.720957	0.744376	-0.732208
1	8.403249	1.365434	0.770678
1	7.814134	-0.294508	0.686479
6	-1.324114	-1.605463	1.709655
1	-1.845339	-1.312643	2.624528
1	-1.051143	-2.663053	1.801088
1	-0.395424	-1.03688	1.631592
6	-1.436056	-1.846266	-0.807158
1	-1.213387	-2.918448	-0.755784
1	-2.012439	-1.670718	-1.720267
1	-0.4815	-1.322506	-0.878535
6	-3.443352	-2.386224	0.607752
1	-3.071436	-3.406709	0.75289
1	-4.05946	-2.125056	1.471512
1	-4.072727	-2.382786	-0.285229
6	-2.329788	3.004439	-0.068341
1	-1.645241	3.778206	-0.434098
1	-3.250781	3.068133	-0.655223
1	-2.56791	3.224734	0.974285
6	-0.372674	1.599246	0.66712
1	-0.614548	1.658291	1.732053
1	0.236334	0.71129	0.484498
1	0.241694	2.472611	0.41804
6	-1.230449	1.441371	-1.701584

1	-2.097387	1.4225	-2.366445
1	-0.606456	2.293928	-1.994269
1	-0.643168	0.536884	-1.862294
12	4.536627	0.074626	0.06674
35	2.460215	-1.073246	-0.603051
1	6.04372	2.239762	0.485706

TS_{IIa-i} 3

E = -3995.051438 ZPVE = 0.345592 NIMAG = 1.

17	4.160732	0.503945	0.632893
15	1.729035	-0.000036	0.449994
6	1.356617	1.779731	-0.306201
6	2.13254	-1.430481	-0.868222
5	1.810145	-0.208333	2.502411
1	0.677948	-0.228167	2.917553
1	2.430458	0.757942	2.860253
1	2.409121	-1.243179	2.677779
6	-0.669323	-0.639677	0.669078
1	-0.704362	0.277582	1.246513
6	-0.681039	-1.981802	1.40736
1	-1.165412	-2.771702	0.821608
1	0.318105	-2.341027	1.670512
1	-1.225656	-1.905409	2.354278
6	-0.074109	1.926258	-0.865355
1	-0.835183	1.881111	-0.084722
1	-0.1538	2.919647	-1.321635
1	-0.30245	1.196404	-1.647349
6	2.311261	2.195234	-1.445876

1	2.151144	3.264018	-1.634011
1	3.36022	2.046989	-1.196569
1	2.086397	1.667778	-2.37532
6	1.518847	2.758533	0.876645
1	1.287085	3.770233	0.521513
1	0.837744	2.526104	1.700429
1	2.538683	2.753727	1.26512
6	2.830133	-2.550539	-0.066351
1	3.080327	-3.363441	-0.759224
1	3.753585	-2.198603	0.396136
1	2.187964	-2.963144	0.714974
6	0.888772	-2.019759	-1.56571
1	0.215886	-2.541278	-0.887052
1	0.329384	-1.26641	-2.129376
1	1.242542	-2.758337	-2.294744
6	3.066118	-0.963683	-2.007618
1	3.961787	-0.462591	-1.648023
1	3.373739	-1.858439	-2.562679
1	2.548457	-0.310591	-2.713133
12	-2.860334	-0.310464	0.299716
35	-5.177735	0.157033	-0.17326
1	-0.656598	-0.587574	-0.412952

PCIIa-i 3

E = -3995.205206 ZPVE = 0.346483 NIMAG = 0.

17	6.096745	1.174669	-0.840184
15	-2.618501	0.066412	0.213238
6	-2.309643	-1.170135	-1.216303

6	-1.887417	1.794935	-0.148948
5	-4.530922	0.164234	0.633164
1	-4.92626	-0.983606	0.676138
1	-5.066857	0.801068	-0.251005
1	-4.626676	0.714273	1.709773
6	-1.657574	-0.65097	1.637241
1	-2.077994	-1.652325	1.76638
6	-1.741292	0.082884	2.984711
1	-1.202216	1.033613	2.977767
1	-2.776967	0.279321	3.27417
1	-1.286769	-0.542312	3.76055
6	-0.880719	-1.118686	-1.792102
1	-0.112171	-1.288815	-1.033432
1	-0.780337	-1.91439	-2.541171
1	-0.665682	-0.174106	-2.297491
6	-3.337387	-0.91525	-2.341727
1	-3.188994	-1.667868	-3.125634
1	-4.363178	-1.004443	-1.975748
1	-3.224916	0.067021	-2.80429
6	-2.556062	-2.598097	-0.670141
1	-2.558662	-3.293696	-1.517622
1	-1.767097	-2.922804	0.013228
1	-3.520866	-2.686853	-0.163092
6	-2.5328	2.790309	0.845675
1	-2.113223	3.786294	0.657893
1	-3.615525	2.845358	0.712732
1	-2.333212	2.537924	1.888879
6	-0.355724	1.83126	0.023301
1	-0.044013	1.556564	1.034384
1	0.161176	1.170798	-0.675274

1	-0.004579	2.854009	-0.162278
6	-2.25901	2.264379	-1.571702
1	-3.338208	2.223565	-1.745501
1	-1.944201	3.3088	-1.685822
1	-1.756815	1.68723	-2.351241
12	4.364171	-0.057923	0.000893
35	2.30769	-1.168823	0.683532
1	-0.611761	-0.781258	1.342108

R1III + a S_N2@P-b pathway 2 in THF

RCIIIa-i 2

E = -4142.718661 ZPVE = 0.279860 NIMAG = 0.

17	4.91466	0.422311	1.252171
15	2.843168	0.190884	1.001082
5	1.975575	0.015156	2.722258
1	0.808937	-0.123521	2.417782
1	2.205652	1.031585	3.334021
1	2.455734	-0.982226	3.208193
6	-2.372135	-0.78545	-0.077261
1	-1.84672	-0.09203	0.59673
6	-1.979658	-2.236215	0.270666
1	-2.45713	-2.960588	-0.402202
1	-0.895059	-2.413287	0.207187
1	-2.282257	-2.507563	1.290144
6	2.375639	1.640067	0.005526
6	1.335646	2.46053	0.47036
6	3.037179	1.961548	-1.192746
6	0.952466	3.584775	-0.26672
1	0.828531	2.223382	1.399222

6	2.652699	3.08681	-1.920401
1	3.852332	1.341873	-1.553294
6	1.608775	3.897952	-1.459158
1	0.146558	4.215206	0.09585
1	3.167597	3.332099	-2.844098
1	1.312573	4.774156	-2.028019
6	2.724491	-1.279508	-0.073843
6	3.327448	-2.477602	0.34837
6	1.96066	-1.264882	-1.25122
6	3.182973	-3.638433	-0.4106
1	3.914445	-2.504739	1.261068
6	1.816118	-2.433691	-2.0042
1	1.476647	-0.353626	-1.584226
6	2.427734	-3.618218	-1.588588
1	3.65758	-4.557655	-0.081528
1	1.224399	-2.413488	-2.914209
1	2.315691	-4.523658	-2.177305
12	-4.43974	-0.328076	0.012177
35	-6.827736	0.213848	0.162888
1	-2.012678	-0.53812	-1.088064

TS_{IIIa-i} 2

E = -4142.683234 ZPVE = 0.281472 NIMAG = 1.

17	-3.560768	1.566145	-1.075331
15	-1.543158	0.317133	-0.905265
5	-1.351697	0.13463	-2.885958
1	-0.410274	-0.582336	-3.123053
1	-1.192462	1.283832	-3.229235

1	-2.410087	-0.317326	-3.250156
6	0.585267	-0.931792	-0.516881
1	0.823351	-0.240015	-1.319367
6	0.280894	-2.391294	-0.841034
1	-0.295607	-2.845637	-0.030093
1	-0.323783	-2.461554	-1.752779
1	1.152757	-3.038995	-1.005611
6	-0.746465	1.678338	0.031403
6	0.347278	2.333135	-0.558606
6	-1.214666	2.120246	1.279038
6	0.973505	3.397031	0.097905
1	0.694581	2.039848	-1.544502
6	-0.578237	3.174576	1.93711
1	-2.091432	1.66697	1.727054
6	0.519298	3.813877	1.351735
1	1.808998	3.902562	-0.377175
1	-0.952451	3.505571	2.901278
1	1.006444	4.639028	1.86236
6	-2.358479	-0.937092	0.154501
6	-3.30579	-1.768837	-0.463229
6	-2.055063	-1.135229	1.509702
6	-3.942382	-2.776589	0.264516
1	-3.552099	-1.625577	-1.510134
6	-2.704153	-2.13493	2.238204
1	-1.311294	-0.522522	2.007414
6	-3.649239	-2.958302	1.618743
1	-4.671116	-3.413306	-0.22801
1	-2.465799	-2.271211	3.288889
1	-4.149879	-3.736934	2.186322
12	2.791466	-0.775847	-0.17365

35	5.196296	-0.773378	0.075795
1	0.5005	-0.557427	0.498502

PCIIIa-i 2

E = -4142.735465 ZPVE = 0.283944 NIMAG = 0.

17	8.352504	-0.954724	0.555957
15	0.806474	0.104306	0.833889
5	1.116855	0.070747	2.757458
1	1.440216	-1.066545	3.019495
1	0.043855	0.370655	3.244229
1	1.982553	0.880129	3.003249
6	-0.654235	-0.955558	0.384055
1	-1.472349	-0.527252	0.978561
6	-0.452541	-2.439997	0.722245
1	0.366994	-2.873172	0.143083
1	-0.222543	-2.573698	1.782126
1	-1.35505	-3.017561	0.497399
6	0.359234	1.774338	0.204072
6	-0.161553	2.719486	1.104097
6	0.514161	2.130031	-1.146078
6	-0.53345	3.990896	0.657286
1	-0.261807	2.467735	2.154656
6	0.14327	3.401959	-1.58917
1	0.943033	1.42746	-1.853113
6	-0.38349	4.333884	-0.689305
1	-0.926739	4.715037	1.364584
1	0.277533	3.66728	-2.633591
1	-0.662876	5.325117	-1.033784

6	2.203519	-0.495194	-0.183722
6	3.504494	-0.398356	0.338379
6	2.018855	-1.047355	-1.46319
6	4.602875	-0.834807	-0.407996
1	3.660076	0.012905	1.330664
6	3.116298	-1.486415	-2.207113
1	1.023998	-1.147675	-1.886077
6	4.407318	-1.378508	-1.681089
1	5.608027	-0.762259	0.001428
1	2.960779	-1.914055	-3.193314
1	5.260662	-1.722403	-2.257801
12	-4.383691	-0.928149	0.053894
35	-6.770243	-0.939681	-0.132411
1	-0.886003	-0.809505	-0.675872

R1iv + a SN2@P-b pathways 2, 3 and 4 in THF

RC_{iv}-i 2

E = -3950.979882 ZPVE = 0.227613 NIMAG = 0.

15	-1.412982	-1.311588	0.545089
5	0.517768	-1.209194	0.47114
6	1.305693	2.714522	0.560039
12	2.20334	0.825281	0.145214
1	0.940191	-2.296912	0.756136
1	0.818807	-0.85447	-0.648725
1	0.762862	-0.381066	1.331074
6	-2.050258	-1.638083	2.218966
6	-2.318803	0.088677	-0.168085
17	-2.061936	-2.973264	-0.529585
6	0.9124	2.960891	2.032166

1	0.409331	2.817597	-0.072728
1	1.985718	3.515273	0.228638
35	4.257608	-0.418227	-0.479105
1	-3.124085	-1.832125	2.211932
1	-1.827193	-0.77681	2.855085
1	-1.525613	-2.51238	2.61085
6	-1.888685	0.599335	-1.406112
6	-3.42252	0.667713	0.479454
1	1.787035	2.942394	2.695917
1	0.415404	3.931257	2.195564
1	0.221644	2.192216	2.405124
6	-2.557974	1.675969	-1.986509
1	-1.039005	0.158468	-1.917439
6	-4.081924	1.751397	-0.10442
1	-3.771467	0.289029	1.433622
6	-3.652773	2.254174	-1.335667
1	-2.222381	2.065466	-2.942393
1	-4.930315	2.199229	0.403224
1	-4.169429	3.095128	-1.78784

TS_{IVa-i} 2

E = -3950.952618 ZPVE = 0.230002 NIMAG = 1.

15	-1.168632	-1.13195	-0.076257
5	0.191008	-1.673339	-1.408333
6	0.542788	-0.096407	1.58971
12	1.763796	-0.38238	-0.237757
1	-0.266624	-2.346116	-2.280055
1	0.622521	-0.629813	-1.880836

1	1.028604	-2.282881	-0.765528
6	-1.598389	-2.242216	1.319856
6	-1.856235	0.558747	0.004347
17	-3.000731	-1.902429	-1.270927
6	1.474728	-0.868341	2.554391
1	-0.419429	0.045109	2.07446
1	0.891795	0.946692	1.459725
35	4.019153	0.512329	-0.379688
1	-2.596761	-1.999902	1.687113
1	-0.874202	-2.185809	2.128915
1	-1.623576	-3.25487	0.912946
6	-1.482742	1.492399	-0.972994
6	-2.764865	0.929306	1.00622
1	2.525364	-0.876334	2.235195
1	1.468139	-0.422199	3.557948
1	1.173333	-1.916476	2.664951
6	-2.006511	2.787047	-0.940136
1	-0.790898	1.221898	-1.76367
6	-3.285462	2.224743	1.032448
1	-3.078193	0.220407	1.765624
6	-2.906543	3.15737	0.06254
1	-1.710536	3.502294	-1.701425
1	-3.987208	2.502261	1.81308
1	-3.311985	4.164111	0.086728

PC_{IVa-i} 2

E = -3951.079788 ZPVE = 0.232100 NIMAG = 0.

15	-1.413541	-0.855586	0.315509
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5	0.30906	0.008359	0.524706
6	-1.900706	-1.757815	1.850608
12	2.468049	-0.040836	-0.679327
1	0.499745	0.652933	-0.495178
1	0.298963	0.725404	1.488509
1	1.111645	-0.901044	0.671394
6	-1.439731	-2.072002	-1.054207
6	-2.754258	0.340401	-0.015828
17	2.482173	-1.164633	-2.701148
6	-0.912323	-2.848032	2.288883
1	-2.897989	-2.180034	1.687343
1	-1.998318	-0.990524	2.626115
35	3.991676	1.10734	0.867536
1	-1.215035	-1.557117	-1.991073
1	-2.417243	-2.554208	-1.132072
1	-0.674167	-2.832119	-0.881312
6	-2.47646	1.715343	-0.069043
6	-4.073194	-0.104371	-0.214019
1	0.085608	-2.439124	2.469917
1	-1.261968	-3.301824	3.22102
1	-0.826657	-3.644878	1.544118
6	-3.503254	2.630472	-0.31865
1	-1.464243	2.075976	0.081315
6	-5.095195	0.812729	-0.463431
1	-4.312265	-1.163246	-0.177001
6	-4.811139	2.181538	-0.516577
1	-3.277653	3.691605	-0.359366
1	-6.110093	0.458804	-0.616588
1	-5.607141	2.893708	-0.712034

RC_{IVa-i} 3

E = -3950.979439 ZPVE = 0.226530 NIMAG = 0.

17	-5.041137	0.592584	0.391392
15	-2.959733	0.754598	0.583533
6	-2.553269	2.007907	-0.67831
1	-2.940935	1.739162	-1.66244
1	-2.976797	2.965239	-0.366337
1	-1.46244	2.089784	-0.721725
5	-2.441521	1.23906	2.380288
1	-1.233075	1.317972	2.277328
1	-2.805942	0.362445	3.127006
1	-2.967509	2.309968	2.576457
6	1.395611	1.735544	-0.803037
1	0.863507	1.999702	0.12365
6	1.512559	2.979212	-1.706457
1	2.004684	2.746541	-2.65944
1	0.535472	3.422625	-1.958416
1	2.102611	3.773952	-1.232586
6	-2.334147	-0.840001	-0.031648
6	-1.721223	-1.713706	0.881204
6	-2.443799	-1.210416	-1.38316
6	-1.215345	-2.940377	0.442978
1	-1.637524	-1.436025	1.926446
6	-1.939969	-2.437564	-1.813983
1	-2.924318	-0.552825	-2.100473
6	-1.323627	-3.302365	-0.902104
1	-0.740169	-3.610231	1.152939
1	-2.028215	-2.718655	-2.858837

1	-0.931524	-4.256591	-1.240939
12	3.196651	0.765866	-0.211926
35	5.25875	-0.387948	0.460445
1	0.76831	0.97711	-1.296105

TS_{IVa-i} 3

E = -3950.942673 ZPVE = 0.227877 NIMAG = 1.

17	4.413769	-0.005052	0.037705
15	2.183101	-0.834324	0.089286
6	2.479344	-1.579195	-1.574585
1	2.747751	-0.803244	-2.292757
1	3.334727	-2.248831	-1.468075
1	1.617421	-2.139992	-1.93207
5	2.451557	-1.805481	1.812024
1	1.417385	-2.344394	2.121924
1	2.795171	-0.933643	2.57647
1	3.347217	-2.576095	1.552371
6	-0.168165	-1.516353	-0.063558
1	-0.146212	-1.056097	0.920659
6	-0.189141	-3.037303	-0.19533
1	-0.417708	-3.336865	-1.22333
1	0.772408	-3.493179	0.073685
1	-0.938141	-3.514422	0.447791
6	1.521107	0.874161	0.003521
6	1.165267	1.50318	1.207417
6	1.336753	1.557706	-1.208034
6	0.634642	2.796263	1.197601
1	1.316229	0.991473	2.153061

6	0.804821	2.849939	-1.213103
1	1.610733	1.097818	-2.152056
6	0.450866	3.472354	-0.011802
1	0.3696	3.273524	2.136402
1	0.670469	3.369711	-2.157146
1	0.040059	4.477356	-0.018676
12	-2.272294	-0.810584	-0.027781
35	-4.554366	-0.00131	0.018566
1	-0.118118	-0.886648	-0.947855

PC_{IVa-i} 3

E = -3951.079780 ZPVE = 0.231915 NIMAG = 0.

17	-2.877983	1.881226	-2.066273
15	1.429491	0.813691	0.337921
6	1.393018	2.117327	-0.948613
1	1.192515	1.65479	-1.917862
1	0.592469	2.826871	-0.727213
1	2.345971	2.650046	-0.992826
5	-0.272224	-0.096429	0.534969
1	-0.185169	-0.977917	1.344956
1	-0.565739	-0.539183	-0.566117
1	-1.052156	0.756404	0.930179
6	1.949635	1.626699	1.911602
1	2.038608	0.82115	2.648401
6	0.990807	2.716982	2.411355
1	0.918719	3.551033	1.707061
1	-0.015228	2.323548	2.581421
1	1.358375	3.116671	3.361131

6	2.778332	-0.335489	-0.107701
6	2.519361	-1.709056	-0.237671
6	4.085539	0.141601	-0.310153
6	3.554592	-2.592376	-0.557233
1	1.5155	-2.092946	-0.091122
6	5.115344	-0.743844	-0.631764
1	4.310531	1.20061	-0.220822
6	4.851417	-2.112302	-0.754003
1	3.343917	-3.653086	-0.653099
1	6.121249	-0.365634	-0.786141
1	5.654414	-2.799957	-1.001608
12	-2.496254	0.245322	-0.479317
35	-3.861632	-1.480329	0.60304
1	2.954393	2.033909	1.757139

RC_{IVa-i} 4

E = -3950.979552 ZPVE = 0.226799 NIMAG = 0.

17	5.066495	-0.505729	-0.251793
15	3.357173	0.667332	0.062668
5	3.550106	1.816627	1.602984
1	2.498463	2.426693	1.587075
1	4.504846	2.513808	1.348186
1	3.689389	1.12187	2.580911
6	-3.005124	3.13718	-0.634809
1	-1.99489	3.207532	-1.066651
1	-3.685605	3.457151	-1.439163
6	-3.12461	4.110889	0.555765
1	-4.133672	4.105842	0.987664

1	-2.432974	3.851885	1.367618
1	-2.90695	5.154496	0.277692
12	-3.40725	1.086216	-0.245761
35	-3.943813	-1.307106	-0.033461
6	3.220303	1.566207	-1.520137
1	2.306019	2.16614	-1.488403
1	4.080525	2.232837	-1.613164
1	3.187989	0.891246	-2.376687
6	1.996776	-0.538158	0.119809
6	1.540361	-1.206422	-1.029814
6	1.399295	-0.807458	1.36281
6	0.497553	-2.127894	-0.933893
1	1.996618	-1.021871	-1.997058
6	0.35477	-1.730624	1.4514
1	1.747419	-0.296779	2.254412
6	-0.097344	-2.389719	0.305349
1	0.148243	-2.639822	-1.825171
1	-0.103702	-1.933108	2.414334
1	-0.911682	-3.103542	0.375296

TS_{IVa-i} 4

E = -3950.934416 ZPVE = 0.229228 NIMAG = 1.

17	-3.690194	1.031781	-0.467552
15	-1.980405	-0.590979	-0.121471
5	-2.994173	-1.453995	1.367885
1	-2.30993	-2.292217	1.888885
1	-3.938737	-1.902804	0.757507
1	-3.283808	-0.529777	2.086148

6	-0.334254	-2.474605	-0.045516
1	-1.300811	-2.938747	-0.234813
1	0.248036	-2.785159	-0.937772
6	0.262478	-3.106309	1.230867
1	1.312729	-2.841977	1.414175
1	-0.305069	-2.811485	2.117018
1	0.236959	-4.202359	1.174394
12	1.063632	-0.781169	-0.158031
35	3.41932	-0.221948	-0.380438
6	-2.077428	-0.99061	-1.922955
1	-1.24102	-1.600356	-2.260421
1	-3.009733	-1.544268	-2.060919
1	-2.143678	-0.074126	-2.508136
6	-0.777327	0.771719	0.189376
6	-0.343644	1.652474	-0.824561
6	-0.377772	1.012942	1.523444
6	0.483725	2.73362	-0.511404
1	-0.663248	1.50842	-1.851056
6	0.453379	2.095442	1.824107
1	-0.732279	0.364797	2.319316
6	0.879051	2.958576	0.810141
1	0.812352	3.400345	-1.302008
1	0.755819	2.268159	2.851782
1	1.523591	3.798663	1.047639

PC_{IVa-i} 4

E = -3951.072743 ZPVE = 0.229983 NIMAG = 0.

17	6.267447	0.957203	-0.001708
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15	-2.695373	-1.047217	-0.422454
5	-4.524194	-1.616106	-0.752109
1	-5.198066	-1.293362	0.203591
1	-4.43754	-2.822924	-0.873471
1	-4.877852	-1.07259	-1.779235
6	-1.915868	-1.853531	1.048959
1	-1.970999	-2.93085	0.851914
1	-0.853793	-1.585328	1.053708
6	-2.576994	-1.517344	2.39086
1	-2.521698	-0.445935	2.607653
1	-3.630143	-1.812562	2.404749
1	-2.066171	-2.048526	3.200385
12	4.26561	-0.156452	-0.005836
35	1.959732	-0.952933	-0.035155
6	-1.566001	-1.49853	-1.801164
1	-0.52201	-1.342114	-1.51832
1	-1.717168	-2.555531	-2.038035
1	-1.805736	-0.900742	-2.683627
6	-2.499575	0.761607	-0.181759
6	-1.236458	1.347112	0.014429
6	-3.638791	1.581791	-0.197215
6	-1.120568	2.727825	0.189688
1	-0.337887	0.737524	0.031594
6	-3.518888	2.963841	-0.02041
1	-4.618206	1.139971	-0.347739
6	-2.260445	3.538844	0.173099
1	-0.139859	3.170053	0.339673
1	-4.407933	3.587395	-0.034647
1	-2.166392	4.612239	0.309736

R1v + a S_N2@P-b pathways 2 in THF

RC_{Va-i} 2

E = -3759.236255 ZPVE = 0.172771 NIMAG = 0.

17	-5.127725	-0.935682	-0.657241
15	-3.392335	-0.209838	0.247563
6	-2.068092	-0.944467	-0.77199
1	-2.080042	-2.03029	-0.655034
1	-2.186164	-0.681379	-1.825264
1	-1.113083	-0.559096	-0.401602
6	-3.426743	1.564936	-0.176838
1	-3.490449	1.711476	-1.257228
1	-4.279536	2.038552	0.314407
1	-2.504879	2.017722	0.201589
5	-3.293206	-0.610286	2.129779
1	-2.225214	-0.095325	2.407461
1	-3.279506	-1.814767	2.234052
1	-4.233379	-0.064442	2.658687
6	1.464217	2.319304	0.351795
1	0.464734	1.971242	0.047669
1	1.378404	2.532578	1.428467
6	1.805701	3.619826	-0.40426
1	2.776636	4.027891	-0.095597
1	1.861475	3.460857	-1.488911
1	1.063758	4.417566	-0.24025
12	2.809397	0.690926	0.132304
35	4.343039	-1.213591	-0.059931

TS_{Va-i} 2

E = -3759.181589 ZPVE = 0.177216 NIMAG = 1.

17	-3.454887	-1.736933	-0.302935
15	-1.931224	0.085281	0.114122
6	-1.354349	-0.863253	1.597291
1	-2.240463	-1.261529	2.092006
1	-0.722011	-1.705796	1.303971
1	-0.816527	-0.209853	2.286814
6	-1.161064	-0.309661	-1.52815
1	-0.4611	-1.149325	-1.454684
1	-1.955862	-0.604043	-2.213526
1	-0.660462	0.575422	-1.926729
5	-3.41456	1.405281	0.297638
1	-2.962156	2.489377	0.566798
1	-4.062597	0.918689	1.196776
1	-3.977818	1.363261	-0.771885
6	-0.284238	1.802024	0.556647
1	-1.010805	2.01831	1.340206
1	0.635734	1.974636	1.171213
6	-0.349742	2.896876	-0.525095
1	0.38828	2.769825	-1.326172
1	-1.334668	2.903729	-0.999462
1	-0.189983	3.895497	-0.099947
12	1.389248	0.377017	0.127878
35	3.610573	-0.526745	-0.038691

PC_{Va-i} 2

E = -3759.323898 ZPVE = 0.175222 NIMAG = 0.

17	-0.537176	-0.702559	0.686467
15	3.936439	-0.238547	-0.209592
6	3.147668	-1.52513	-1.253491
1	3.658252	-2.479397	-1.098414
1	2.088786	-1.634495	-1.003159
1	3.245853	-1.246858	-2.306386
6	3.60056	-0.769834	1.515219
1	2.526649	-0.887325	1.684959
1	4.102948	-1.723764	1.697782
1	4.00169	-0.031721	2.214293
5	5.823744	-0.000802	-0.598355
1	6.24546	0.839525	0.170726
1	5.885079	0.356064	-1.759829
1	6.334959	-1.089862	-0.419325
6	2.895298	1.262052	-0.4859
1	2.970627	1.48733	-1.556238
1	1.854553	0.98453	-0.283313
6	3.306507	2.486111	0.344279
1	3.205076	2.29983	1.418185
1	4.342637	2.774747	0.146485
1	2.664798	3.337676	0.095968
12	-2.739952	-0.28136	0.259389
35	-5.056613	0.205616	-0.239124

R1_{IV} + a S_N2@P-f pathway 2 in THF

RC_{IVa-r} 2

E = -3950.981262 ZPVE = 0.227867 NIMAG = 0.

17	1.314569	2.411279	0.444912
6	-3.157201	2.135343	1.357742

1	-4.044068	1.971833	1.990962
1	-2.345811	2.387261	2.059502
6	-3.413563	3.339867	0.427714
1	-2.539184	3.564188	-0.198034
1	-4.250161	3.154586	-0.259062
1	-3.654086	4.268208	0.971471
15	1.364513	0.672077	-0.696384
12	-2.683618	0.277811	0.417375
35	-3.624243	-1.938046	-0.242744
6	1.812772	1.281891	-2.354076
1	1.013807	1.929337	-2.721905
1	2.755221	1.831827	-2.337046
1	1.907123	0.413883	-3.013451
5	-0.326976	-0.261161	-0.636422
1	-0.54571	-0.525162	0.527474
1	-1.134064	0.486734	-1.151827
1	-0.158886	-1.251767	-1.300669
6	2.771054	-0.278479	-0.056753
6	4.084831	0.214978	-0.144713
6	2.533173	-1.535733	0.522472
6	5.147404	-0.547719	0.337729
1	4.283769	1.191032	-0.576116
6	3.604191	-2.29587	0.998652
1	1.523604	-1.924563	0.596163
6	4.90821	-1.803938	0.907099
1	6.160111	-0.163196	0.269624
1	3.415982	-3.269218	1.440438
1	5.738569	-2.396232	1.279188

TS_{IVa-r} 2

E = -3950.925514 ZPVE = 0.229989 NIMAG = 1.

17	0.728702	-0.023415	1.953227
6	-1.190184	1.697702	0.477204
1	-1.774881	1.271882	1.31613
1	-0.515858	2.372994	0.999812
6	-2.09628	2.475529	-0.496744
1	-1.572406	2.777389	-1.409329
1	-2.97781	1.906836	-0.821446
1	-2.483947	3.3899	-0.027487
15	0.873141	0.600229	-0.263403
12	-1.873633	-0.350875	-0.180528
35	-4.236346	-0.876231	0.01582
6	1.307921	2.299782	-0.831073
1	0.439481	2.789301	-1.263973
1	1.672989	2.902679	0.004373
1	2.10015	2.211492	-1.578347
5	-0.037689	-0.513595	-1.612607
1	-0.441077	-1.51356	-1.021396
1	-0.954618	0.176046	-2.022901
1	0.696155	-0.861348	-2.493044
6	2.618571	-0.097154	-0.187501
6	3.717438	0.688113	0.197017
6	2.84175	-1.441186	-0.525849
6	5.006538	0.149394	0.225376
1	3.58296	1.724972	0.487863
6	4.130869	-1.980979	-0.498167
1	2.013046	-2.076601	-0.818971
6	5.218387	-1.187556	-0.123619

1	5.84289	0.775567	0.522711
1	4.281806	-3.021908	-0.769563
1	6.220167	-1.60632	-0.102434

PC_{IVa-r} 2

E = -3951.079256 ZPVE = 0.232717 NIMAG = 0.

17	2.225913000	1.944854000	-2.113522000
6	-1.540359000	2.280563000	-0.049722000
1	-1.252211000	2.130572000	-1.095655000
1	-2.593243000	2.580955000	-0.043983000
6	-0.668862000	3.363056000	0.603159000
1	-0.980005000	3.570881000	1.631029000
1	0.387872000	3.084007000	0.609492000
1	-0.761013000	4.292849000	0.034190000
15	-1.427100000	0.621661000	0.751704000
12	2.443559000	0.263669000	-0.527585000
35	4.047167000	-1.305912000	0.455462000
6	-1.870538000	0.850280000	2.515488000
1	-1.099189000	1.445791000	3.009970000
1	-2.836028000	1.351802000	2.616902000
1	-1.919196000	-0.130168000	2.995021000
5	0.309332000	-0.227552000	0.599296000
1	0.497056000	-0.428811000	-0.591922000
1	1.119306000	0.547444000	1.085439000
1	0.301064000	-1.265527000	1.205620000
6	-2.747401000	-0.401505000	0.008545000
6	-4.079687000	0.047754000	-0.005317000
6	-2.439069000	-1.653373000	-0.546853000

6	-5.083156000	-0.741786000	-0.568931000
1	-4.345768000	1.010794000	0.420427000
6	-3.447111000	-2.440955000	-1.110257000
1	-1.417507000	-2.018021000	-0.540153000
6	-4.767965000	-1.986895000	-1.123283000
1	-6.108362000	-0.384515000	-0.575483000
1	-3.196588000	-3.406933000	-1.537720000
1	-5.549851000	-2.599216000	-1.562303000

R1_{II} + b S_N2@P-b pathway 2 in THF

RC_{IIb-i} 2

E = -4262.101947 ZPVE = 0.402007 NIMAG = 0.

17	-5.700521	-0.580957	0.474105
15	-3.617119	-0.710729	0.680007
12	2.958758	1.048291	-0.167943
35	1.048781	2.174114	-1.195686
6	-3.086098	-1.401984	-1.013614
6	-3.104294	1.090111	1.015286
6	4.609172	0.272978	0.916734
6	4.87949	-0.751174	-0.001047
6	5.474145	0.340925	2.015541
6	5.91461	-1.677119	0.108567
6	6.537131	-0.566116	2.178971
1	5.33203	1.110687	2.772938
6	6.751862	-1.568279	1.230689
1	6.085368	-2.455912	-0.627298
1	7.19198	-0.490493	3.043368
1	7.570544	-2.271974	1.352972
8	3.957596	-0.724734	-1.071265

6	4.066359	-1.672702	-2.138881
1	3.953163	-2.692854	-1.758437
1	3.257389	-1.447059	-2.833254
1	5.030478	-1.56868	-2.646975
5	-3.188593	-1.907168	2.160106
1	-1.997974	-2.10915	2.031889
1	-3.454252	-1.309414	3.176268
1	-3.851673	-2.903711	1.999832
6	-1.547038	-1.312094	-1.120934
1	-1.238076	-1.873475	-2.010394
1	-1.193959	-0.285814	-1.246516
1	-1.0448	-1.758374	-0.257931
6	-3.50539	-2.890375	-1.021997
1	-4.586132	-3.012995	-0.905658
1	-3.222124	-3.318856	-1.990165
1	-3.006063	-3.461016	-0.236355
6	-3.738075	-0.694529	-2.216598
1	-3.40993	-1.206428	-3.128603
1	-4.828819	-0.747816	-2.180864
1	-3.443972	0.351855	-2.303706
6	-3.295179	2.028567	-0.189154
1	-4.31675	1.997555	-0.579105
1	-3.096645	3.055321	0.139033
1	-2.597293	1.808943	-0.99998
6	-1.618058	1.069215	1.442083
1	-0.958749	0.779941	0.622323
1	-1.335623	2.087684	1.731487
1	-1.445507	0.409893	2.296405
6	-3.954357	1.60632	2.199027
1	-3.565653	2.589633	2.486892

1	-5.005624	1.7273	1.927289
1	-3.891611	0.950185	3.070526

TS_{nb-i} 2

E = -4262.008111 ZPVE = 0.404292 NIMAG = 1.

17	-4.385333	-0.494016	-0.152525
15	-1.764956	0.130908	-0.07919
12	2.080363	-0.204249	0.060132
35	3.645362	-2.025294	-0.094435
6	-1.58823	-0.125008	1.842872
6	-1.500653	-1.532571	-1.120042
6	0.388088	1.105663	-0.659311
6	1.11025	2.05606	0.104199
6	0.197996	1.491163	-2.010122
6	1.458875	3.332621	-0.335783
6	0.579593	2.734498	-2.51112
1	-0.30856	0.814831	-2.689208
6	1.161537	3.674819	-1.657423
1	1.987826	4.031205	0.301895
1	0.395789	2.980423	-3.552131
1	1.422051	4.663223	-2.023219
8	1.64749	1.509727	1.289827
6	2.350366	2.35005	2.232144
1	1.688628	3.147639	2.576461
1	2.614309	1.698832	3.064139
1	3.252173	2.767862	1.777567
5	-2.512938	1.967903	-0.663236
1	-1.634173	2.755275	-0.428583

1	-2.733172	1.817255	-1.842324
1	-3.494713	2.125525	0.009579
6	-0.299917	-0.875753	2.228046
1	-0.318263	-1.070173	3.306721
1	-0.20119	-1.844571	1.733653
1	0.576385	-0.257251	2.048779
6	-1.570382	1.293205	2.454356
1	-2.517568	1.808801	2.282515
1	-1.423765	1.200585	3.537307
1	-0.767923	1.915875	2.057059
6	-2.767869	-0.891106	2.484736
1	-2.561817	-0.948102	3.560867
1	-3.716729	-0.380238	2.337345
1	-2.868822	-1.90855	2.106213
6	-2.095727	-2.762517	-0.396489
1	-3.156578	-2.645471	-0.187535
1	-1.965071	-3.62668	-1.058966
1	-1.567422	-2.989634	0.532893
6	-0.021044	-1.871592	-1.375779
1	0.509366	-2.111027	-0.4493
1	0.020892	-2.785493	-1.978801
1	0.509847	-1.100646	-1.930402
6	-2.199474	-1.351007	-2.485549
1	-2.058007	-2.271954	-3.063997
1	-3.268092	-1.176588	-2.366761
1	-1.778094	-0.52848	-3.068227

PC_{11b-i} 2

E = -4262.155207 ZPVE = 0.407411 NIMAG = 0.

17	3.056723	3.213871	-0.048036
15	-2.31896	-0.206853	0.044082
12	2.469015	1.009417	0.229177
35	3.282678	-1.108897	1.102138
6	-2.495389	1.637424	-0.4514
6	-1.881245	-0.471231	1.894815
6	-0.949658	-1.076916	-0.914673
6	0.351361	-0.688408	-1.308277
6	-1.298514	-2.410185	-1.233746
6	1.229866	-1.575135	-1.93477
6	-0.433525	-3.298356	-1.869706
1	-2.290358	-2.755866	-0.97509
6	0.848859	-2.882731	-2.218617
1	2.227703	-1.234383	-2.187036
1	-0.76848	-4.307939	-2.085306
1	1.547406	-3.558943	-2.700494
8	0.848252	0.629456	-1.121302
6	1.118783	1.334579	-2.386573
1	0.353986	1.071207	-3.114749
1	1.092448	2.398101	-2.156425
1	2.103992	1.052492	-2.76317
5	-4.056795	-1.073842	-0.341276
1	-4.318111	-0.819414	-1.497479
1	-3.977171	-2.261043	-0.136711
1	-4.829182	-0.554285	0.432632
6	-1.424028	2.573833	0.134102
1	-1.589472	3.58347	-0.260081
1	-1.48721	2.638244	1.223369
1	-0.416078	2.270822	-0.139974

6	-2.474337	1.690719	-1.994674
1	-3.272677	1.082603	-2.427122
1	-2.62954	2.728702	-2.311238
1	-1.527778	1.354527	-2.415512
6	-3.883889	2.149898	0.004641
1	-3.973672	3.193048	-0.321125
1	-4.698465	1.581253	-0.444681
1	-4.008942	2.132472	1.088516
6	-2.850521	0.338372	2.781726
1	-3.897229	0.138321	2.539782
1	-2.685375	0.043524	3.82473
1	-2.67282	1.414812	2.718192
6	-0.431518	-0.107409	2.24782
1	-0.191922	0.938086	2.03618
1	-0.284102	-0.260773	3.323613
1	0.281214	-0.758469	1.735254
6	-2.080901	-1.974995	2.19273
1	-1.822157	-2.153455	3.242996
1	-3.114121	-2.290353	2.036406
1	-1.427771	-2.604582	1.581376

P11b-i 2

E = -1029.943131 ZPVE = 0.401144 NIMAG = 0.

15	0.832183	-0.499746	0.427315
6	1.484905	1.218233	1.003886
6	1.412968	-0.991711	-1.330365
6	-1.026623	-0.501789	0.403308
6	-1.86443	0.447732	-0.234773

6	-1.653	-1.564407	1.077393
6	-3.259441	0.304518	-0.202656
6	-3.041842	-1.710102	1.115236
1	-1.033849	-2.295325	1.581797
6	-3.842935	-0.772041	0.468127
1	-3.895139	1.030662	-0.693433
1	-3.483916	-2.547394	1.645697
1	-4.924983	-0.865101	0.482706
8	-1.2565	1.496094	-0.855387
6	-2.050902	2.465027	-1.543912
1	-2.73233	2.979036	-0.857654
1	-1.343286	3.183417	-1.958462
1	-2.620363	2.002558	-2.357243
5	1.447145	-1.854356	1.725768
1	1.097297	-1.458631	2.819338
1	0.940898	-2.916551	1.443826
1	2.652481	-1.898743	1.621056
6	1.673982	2.272401	-0.104391
1	1.998008	3.207995	0.368468
1	2.453128	1.98673	-0.815854
1	0.752961	2.468689	-0.649339
6	0.488116	1.750684	2.05696
1	0.305264	1.02122	2.851856
1	0.916353	2.647982	2.520013
1	-0.469086	2.02783	1.609984
6	2.852551	1.004669	1.695434
1	3.21795	1.981901	2.033607
1	2.77478	0.348766	2.563432
1	3.602286	0.585999	1.019036
6	2.955548	-0.943233	-1.38523

1	3.412003	-1.540724	-0.592106
1	3.282435	-1.35525	-2.347593
1	3.343681	0.076524	-1.319754
6	0.827839	-0.131707	-2.466538
1	1.099743	0.921137	-2.385568
1	1.222282	-0.509034	-3.418353
1	-0.261312	-0.200344	-2.506946
6	0.95723	-2.452941	-1.549745
1	1.260938	-2.763312	-2.556761
1	1.411888	-3.136556	-0.830113
1	-0.130377	-2.55627	-1.483508

R1_{III} + b S_N2@P-b pathway 2 in THF

RC_{IIIb-i} 2

E = -4409.703025 ZPVE = 0.339289 NIMAG = 0.

17	5.131973	0.574851	1.791052
15	3.131582	0.073645	1.414463
12	-2.870833	-0.539433	-0.918498
35	-0.826347	0.138479	-2.094464
6	-4.559438	-1.219693	0.177425
6	-4.952527	0.071168	0.557372
6	-5.387693	-2.256002	0.62455
6	-6.073408	0.380366	1.32409
6	-6.532996	-2.005647	1.402718
1	-5.152267	-3.288797	0.370963
6	-6.870396	-0.69541	1.748312
1	-6.337343	1.397845	1.593183
1	-7.157741	-2.830286	1.736433
1	-7.753935	-0.49771	2.348836

8	-4.052353	1.037465	0.05297
6	-4.286055	2.433268	0.268129
1	-4.275658	2.662996	1.338234
1	-3.47061	2.956682	-0.230321
1	-5.243635	2.733339	-0.169469
5	2.189747	-0.26634	3.072002
1	2.771444	-1.201026	3.57122
1	2.227156	0.751774	3.722086
1	1.078154	-0.555862	2.677054
6	2.519602	1.463938	0.412958
6	1.488399	2.262648	0.931043
6	3.071169	1.760596	-0.845507
6	1.010437	3.347681	0.191132
1	1.064571	2.041363	1.904577
6	2.591807	2.845858	-1.576636
1	3.869677	1.14831	-1.252878
6	1.560799	3.639072	-1.058942
1	0.211369	3.962246	0.593629
1	3.017552	3.070637	-2.549507
1	1.186664	4.481442	-1.633164
6	3.255245	-1.362827	0.293226
6	2.256602	-1.541485	-0.677635
6	4.237829	-2.34952	0.472637
6	2.254882	-2.69002	-1.4724
1	1.48317	-0.796997	-0.833344
6	4.2329	-3.49128	-0.330941
1	5.011174	-2.226176	1.223582
6	3.243616	-3.662511	-1.30502
1	1.482933	-2.813878	-2.225855
1	5.002373	-4.245055	-0.195019

1	3.245296	-4.550754	-1.929701
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TS_{IIIb-i} 2

E = -4409.658627 ZPVE = 0.341320 NIMAG = 1.

17	2.530253	-2.063157	-2.026433
15	1.266404	-0.270231	-1.099087
12	-1.595712	0.171178	0.278759
35	-2.732603	-0.56325	2.290984
6	0.025566	1.663496	-0.108264
6	-1.003255	2.355322	-0.7834
6	0.929143	2.49396	0.580039
6	-1.125124	3.739724	-0.851733
6	0.845579	3.890869	0.546042
1	1.74047	2.050741	1.146223
6	-0.164366	4.512262	-0.18967
1	-1.937706	4.218675	-1.38547
1	1.574622	4.488609	1.085059
1	-0.228127	5.595274	-0.23296
8	-1.989803	1.484105	-1.297709
6	-3.143524	2.010141	-1.982934
1	-2.824247	2.569457	-2.864829
1	-3.729214	1.142533	-2.283962
1	-3.729094	2.646799	-1.314184
5	1.519943	0.836232	-2.770332
1	2.72308	0.86096	-2.869643
1	0.994814	0.1352	-3.603181
1	1.011765	1.910614	-2.614608
6	-0.129279	-1.473637	-0.916122

6	-1.185651	-1.405154	-1.851906
6	-0.102351	-2.545838	-0.000408
6	-2.207116	-2.363527	-1.839308
1	-1.187926	-0.627162	-2.607105
6	-1.129978	-3.488182	0.009222
1	0.724977	-2.657624	0.689134
6	-2.187246	-3.396958	-0.90089
1	-3.005936	-2.299974	-2.571258
1	-1.099828	-4.299759	0.729009
1	-2.98098	-4.13679	-0.888256
6	2.363379	-0.242677	0.379309
6	1.962096	-0.526685	1.694171
6	3.697625	0.129589	0.140434
6	2.887847	-0.471452	2.740352
1	0.939235	-0.778634	1.944107
6	4.612818	0.201202	1.191155
1	4.024671	0.358173	-0.868143
6	4.213812	-0.110028	2.494348
1	2.561191	-0.70681	3.748685
1	5.638439	0.493047	0.987272
1	4.927961	-0.065152	3.31094

PC_{mb-i} 2

E = -4409.770832 ZPVE = 0.340491 NIMAG = 0.

17	-7.045562	0.707212	0.813116
15	2.4729	-0.02772	-0.353954
12	-4.843347	0.3134	0.361602
35	-2.44674	0.088185	-0.019333

6	1.186706	-0.763377	-1.438978
6	0.855725	-2.136297	-1.343451
6	0.63488	-0.014681	-2.487829
6	-0.038051	-2.711194	-2.257464
6	-0.240656	-0.588874	-3.4118
1	0.893306	1.033297	-2.5892
6	-0.575303	-1.936861	-3.288449
1	-0.302657	-3.758485	-2.182105
1	-0.6505	0.012682	-4.216465
1	-1.259214	-2.398406	-3.994876
8	1.458865	-2.833991	-0.344479
6	1.152667	-4.219769	-0.175695
1	1.445724	-4.798821	-1.058205
1	1.736452	-4.54552	0.684913
1	0.085812	-4.363582	0.027567
5	4.277511	-0.515743	-0.928068
1	4.354171	-0.103508	-2.066373
1	5.060265	0.033451	-0.182232
1	4.328585	-1.722865	-0.859318
6	2.10648	-0.465535	1.395206
6	3.189727	-0.650271	2.267398
6	0.798866	-0.577686	1.890414
6	2.967513	-0.939991	3.61731
1	4.205386	-0.57492	1.893796
6	0.580741	-0.868939	3.238322
1	-0.054693	-0.457243	1.232294
6	1.663322	-1.049058	4.106001
1	3.814345	-1.082772	4.28223
1	-0.436495	-0.95773	3.608968
1	1.490201	-1.276234	5.153963

6	2.190336	1.791423	-0.423468
6	0.925107	2.362827	-0.198906
6	3.290771	2.632284	-0.646966
6	0.771392	3.750024	-0.193866
1	0.05435	1.735192	-0.036769
6	3.133122	4.022194	-0.638838
1	4.270856	2.202709	-0.822882
6	1.874763	4.583081	-0.411559
1	-0.211097	4.180011	-0.022345
1	3.993894	4.661331	-0.811776
1	1.751302	5.66216	-0.405537

R1_{IV} + b S_N2@P-b pathway 2 in THF

RC_{IVb-i} 2

E = -4217.960469 ZPVE = 0.286798 NIMAG = 0.

17	-2.709310000	-2.865548000	1.188960000
15	-1.971158000	-1.111437000	0.347009000
12	1.928106000	-0.084751000	0.087854000
35	3.319315000	-0.891758000	-1.785070000
6	-2.011755000	0.060917000	1.739552000
1	-1.287315000	-0.262446000	2.489579000
1	-1.718225000	1.044951000	1.362861000
1	-3.004783000	0.116805000	2.188416000
6	-3.213859000	-0.586048000	-0.864066000
6	-2.965945000	-0.817951000	-2.227928000
6	-4.403823000	0.049525000	-0.468038000
6	-3.898697000	-0.411249000	-3.183983000
1	-2.052387000	-1.310463000	-2.542826000
6	-5.330139000	0.453033000	-1.429335000

1	-4.614929000	0.231683000	0.580356000
6	-5.078388000	0.223651000	-2.786459000
1	-3.700726000	-0.588584000	-4.236272000
1	-6.246499000	0.945257000	-1.119231000
1	-5.801378000	0.540531000	-3.531875000
6	1.761868000	1.174333000	1.809261000
6	1.451653000	2.322768000	1.066028000
6	1.820852000	1.361283000	3.196766000
6	1.231539000	3.593650000	1.594221000
6	1.601345000	2.618454000	3.789826000
1	2.054549000	0.519534000	3.848243000
6	1.312804000	3.726827000	2.989979000
1	1.006951000	4.455213000	0.973428000
1	1.661691000	2.732319000	4.869480000
1	1.149953000	4.701409000	3.442028000
8	1.374534000	2.022467000	-0.312614000
6	1.361644000	3.071744000	-1.285840000
1	2.245178000	3.708585000	-1.171004000
1	1.382913000	2.582580000	-2.259528000
1	0.452059000	3.673798000	-1.195131000
5	-0.219891000	-1.445409000	-0.408481000
1	0.490019000	-1.742937000	0.531867000
1	0.061636000	-0.384294000	-0.933339000
1	-0.305375000	-2.327281000	-1.217290000

TS_{IVb-i} 2

E = -4217.935038 ZPVE = 0.287917 NIMAG = 1.

17 -3.059473 -2.884671 -0.070246

15	-1.280491	-1.481997	0.371408
12	1.749148	-0.859901	-0.272825
35	4.180409	-0.653293	-0.210324
6	-1.341307	-1.856714	2.16623
1	-1.694015	-2.882478	2.269588
1	-0.339416	-1.769935	2.58378
1	-2.026433	-1.190669	2.692199
6	-2.237047	-0.046433	-0.232764
6	-2.259779	0.191919	-1.614471
6	-2.979545	0.771568	0.629061
6	-3.008583	1.254002	-2.126012
1	-1.701487	-0.445046	-2.292657
6	-3.730738	1.827493	0.109859
1	-2.973581	0.603217	1.700443
6	-3.744788	2.074194	-1.266625
1	-3.019965	1.433591	-3.196847
1	-4.301994	2.45871	0.78374
1	-4.327743	2.898465	-1.666162
6	0.347985	0.400878	0.973122
6	0.645991	1.400689	0.022318
6	0.203803	0.875214	2.290362
6	0.738548	2.7633	0.29668
6	0.295072	2.233593	2.618763
1	0.002875	0.182629	3.101868
6	0.540729	3.176319	1.618656
1	0.97238	3.489344	-0.473374
1	0.172689	2.552418	3.649814
1	0.602715	4.23281	1.861845
8	0.945347	0.85832	-1.2386
6	1.397136	1.708922	-2.308091

1	2.328196	2.2116	-2.03222
1	1.564299	1.050693	-3.159956
1	0.624358	2.440873	-2.554019
5	0.059003	-2.474949	-0.704393
1	0.950877	-2.714862	0.099602
1	0.411471	-1.746338	-1.611349
1	-0.393552	-3.49305	-1.129762

PCIVb-i 2

E = -4217.998239 ZPVE = 0.289688 NIMAG = 0.

17	4.543153000	-2.969544000	-1.677342000
15	1.176945000	-0.014756000	-0.786257000
12	-1.962456000	-1.374367000	0.328237000
35	-4.379367000	-1.553465000	0.396222000
6	2.325995000	-0.031545000	-2.201643000
1	3.002672000	-0.884316000	-2.057106000
1	1.765086000	-0.175396000	-3.128923000
1	2.908508000	0.890966000	-2.250125000
6	2.158732000	0.339147000	0.713118000
6	2.669368000	-0.734347000	1.460265000
6	2.453686000	1.657535000	1.096170000
6	3.470198000	-0.487802000	2.577780000
1	2.462125000	-1.758080000	1.166629000
6	3.249150000	1.896821000	2.218848000
1	2.067136000	2.496859000	0.526216000
6	3.757299000	0.825515000	2.960128000
1	3.869090000	-1.322578000	3.145380000
1	3.472011000	2.918320000	2.511406000

1	4.378183000	1.013983000	3.830686000
6	0.031857000	1.395991000	-1.033795000
6	-1.097158000	1.536771000	-0.211774000
6	0.211175000	2.332176000	-2.064056000
6	-2.022334000	2.559296000	-0.392382000
6	-0.701125000	3.373257000	-2.251255000
1	1.066398000	2.254490000	-2.725463000
6	-1.816276000	3.484688000	-1.418947000
1	-2.895074000	2.627024000	0.247609000
1	-0.541339000	4.089707000	-3.050121000
1	-2.532894000	4.285839000	-1.567334000
8	-1.290849000	0.575033000	0.798452000
6	-1.361451000	1.093570000	2.164833000
1	-2.311554000	1.604660000	2.323855000
1	-1.280267000	0.230608000	2.824482000
1	-0.520101000	1.768096000	2.326655000
5	0.198713000	-1.708572000	-0.687035000
1	-0.812610000	-1.542065000	-1.360601000
1	-0.026137000	-1.951005000	0.492848000
1	0.848252000	-2.595592000	-1.157174000

R1v + b S_N2@P-b pathway 2 in THF

RC_vb-i 2

E = -4026.214978 ZPVE = 0.231626 NIMAG = 0.

17	-4.65609	-2.523221	0.144773
15	-3.888909	-0.580693	0.092237
12	2.5948	-0.182223	-0.486769
35	4.127183	-2.056827	-0.212943

6	-2.846407	-0.520614	1.589543
1	-3.479468	-0.60288	2.475761
1	-2.105173	-1.322661	1.585567
1	-2.339226	0.449138	1.604337
6	-2.734471	-0.641479	-1.319577
1	-2.209338	0.317909	-1.368684
1	-2.008799	-1.448724	-1.198165
1	-3.299935	-0.784841	-2.242995
6	1.249112	1.380617	-0.978909
6	1.237136	1.929057	0.311128
6	0.457596	2.044855	-1.923849
6	0.512935	3.054244	0.699775
6	-0.295584	3.18526	-1.589339
1	0.415374	1.681424	-2.949771
6	-0.26602	3.683298	-0.285022
1	0.53544	3.445546	1.711542
1	-0.902267	3.680355	-2.343235
1	-0.845749	4.563542	-0.021794
8	2.063354	1.185034	1.182896
6	2.254178	1.613357	2.536149
1	1.303599	1.60456	3.078877
1	2.94267	0.900539	2.989127
1	2.689107	2.617593	2.561977
5	-5.265429	0.763802	-0.010898
1	-4.589113	1.775646	-0.026358
1	-5.863904	0.576538	-1.044745
1	-5.935596	0.656243	0.990041

E = -4026.170773 ZPVE = 0.234304 NIMAG = 1.

17	-3.636435	-2.480815	0.40548
15	-2.024638	-0.702943	0.061669
12	1.415263	-0.223408	-0.345584
35	3.52129	-1.402194	-0.398657
6	-0.973773	-1.466638	1.376981
1	-1.646272	-1.84521	2.147094
1	-0.396904	-2.311201	0.988641
1	-0.316077	-0.721851	1.824085
6	-1.779409	-1.467296	-1.614554
1	-1.090718	-0.89368	-2.23125
1	-1.411992	-2.486859	-1.486569
1	-2.755279	-1.515106	-2.099896
6	-0.447543	0.98669	-0.531314
6	0.168395	1.80892	0.441215
6	-1.061674	1.697579	-1.587831
6	0.117695	3.199912	0.461494
6	-1.118897	3.091659	-1.625565
1	-1.554816	1.149805	-2.386707
6	-0.555757	3.837404	-0.585869
1	0.596857	3.782837	1.239429
1	-1.617064	3.595535	-2.447946
1	-0.617287	4.921391	-0.594444
8	0.97468	1.062786	1.319758
6	1.749948	1.718355	2.345633
1	1.083185	2.228651	3.043626
1	2.29026	0.923412	2.857131
1	2.454509	2.424646	1.898514
5	-3.349547	0.709452	0.582546

1	-2.74341	1.730163	0.784404
1	-4.090455	0.760851	-0.375587
1	-3.867486	0.243266	1.569366

PC_{v_b-i} 2

E = -4026.231722 ZPVE = 0.235343 NIMAG = 0.

17	3.685585	4.096283	-0.54661
15	2.31894	-0.155666	0.340362
12	-2.258878	0.254893	0.237613
35	-4.270903	1.41957	-0.357599
6	1.307318	1.363556	0.503918
1	2.012991	2.202422	0.527441
1	0.645193	1.513797	-0.352511
1	0.738238	1.349832	1.434152
6	3.404824	0.205146	-1.091183
1	2.836773	0.246501	-2.023752
1	3.855333	1.185916	-0.907535
1	4.197297	-0.54161	-1.169349
6	1.250442	-1.55863	-0.222383
6	-0.070471	-1.805266	0.181496
6	1.83538	-2.530918	-1.057174
6	-0.781565	-2.937165	-0.213426
6	1.141089	-3.671036	-1.463586
1	2.856365	-2.399121	-1.396778
6	-0.172701	-3.879679	-1.041689
1	-1.800724	-3.076006	0.135413
1	1.630648	-4.394434	-2.107235
1	-0.7216	-4.762842	-1.351139

8	-0.759232	-0.874938	1.007721
6	-0.635768	-1.136901	2.450693
1	0.421936	-1.20401	2.703345
1	-1.09264	-0.291507	2.96531
1	-1.156472	-2.065774	2.687657
5	3.325165	-0.610385	1.945288
1	2.521329	-0.797531	2.834465
1	3.950659	-1.609713	1.658437
1	4.03051	0.355378	2.145424

R1 + b SN2@P-f pathways 2, 3 and 4 in THF

RC_{1b-r} 2

E = -4570.596661 ZPVE = 0.522097 NIMAG = 0.

6	1.893058	-0.843591	-0.085527
6	3.953568	-2.35958	0.059004
6	1.997631	-3.045213	-1.450486
6	1.124433	-2.050201	-0.672795
6	3.153806	-3.519056	-0.557046
6	3.826577	-0.254635	1.601374
6	1.159566	-4.219502	-1.971403
6	2.929299	0.427144	2.650512
6	5.086292	-0.791172	2.305402
1	1.183394	-0.294832	0.539596
1	4.693319	-2.779661	0.74601
1	4.514613	-1.837615	-0.7238
1	2.42775	-2.526918	-2.319091
1	0.288129	-1.710163	-1.289314
1	0.677112	-2.565081	0.188754

1	3.828545	-4.167069	-1.130959
1	2.73833	-4.140031	0.251573
1	4.164148	0.509018	0.88724
1	0.354819	-3.872864	-2.630026
1	1.778016	-4.924209	-2.538769
1	0.699895	-4.770488	-1.140933
1	2.66349	-0.286755	3.44026
1	3.459073	1.263019	3.120344
1	1.998753	0.818456	2.234688
1	4.841079	-1.63671	2.960892
1	5.527888	-0.006678	2.929541
1	5.853629	-1.119605	1.599328
6	2.232765	2.077704	-0.581995
6	3.239474	3.036697	-0.777518
6	1.091288	2.415506	0.165759
6	3.110425	4.313102	-0.222858
1	4.119928	2.788613	-1.35955
6	0.965174	3.6929	0.711213
1	0.30395	1.688044	0.339116
6	1.973498	4.643793	0.518109
1	3.896406	5.046365	-0.375485
1	0.081628	3.94441	1.290012
1	1.87187	5.636982	0.945233
17	0.805059	0.459055	-2.717735
6	3.057015	-1.363178	0.825389
1	2.528199	-1.951151	1.593693
15	2.421611	0.435433	-1.366998
5	4.055232	0.268678	-2.415945
1	4.013932	1.203928	-3.182393
1	4.953896	0.355038	-1.607716

1	4.004616	-0.806573	-2.961029
6	-6.719829	-0.663395	0.9289
6	-7.69996	-0.33246	-0.024729
6	-7.328474	0.283905	-1.221335
6	-5.980241	0.577331	-1.483058
6	-5.053719	0.227505	-0.502966
6	-5.36294	-0.393022	0.715475
1	-7.040316	-1.142031	1.853287
1	-8.746653	-0.554239	0.167272
1	-8.081223	0.541649	-1.961088
1	-5.695896	1.056279	-2.414107
12	-3.357142	-0.449749	1.407098
35	-1.048368	-0.557178	2.242895
8	-3.66418	0.448754	-0.618457
6	-3.13668	1.133154	-1.760759
1	-3.331971	0.562679	-2.674298
1	-3.574457	2.133204	-1.843841
1	-2.062369	1.21193	-1.599073

TS_{lb-r} 2

E = -4570.487821 ZPVE = 0.522492 NIMAG = 1.

6	1.721193	-0.146742	-0.651161
6	4.25914	-0.502524	-0.334264
6	3.43291	1.797859	-1.034111
6	2.075007	1.168794	-1.392043
6	4.56242	0.767373	-1.140614
6	2.674724	-2.615441	-0.3209
6	3.695992	3.030205	-1.90922

6	2.017048	-3.424143	-1.456132
6	3.926788	-3.367764	0.162674
1	0.878603	-0.577983	-1.198782
1	5.075122	-1.21507	-0.483623
1	4.23034	-0.273155	0.735566
1	3.382396	2.131502	0.007312
1	1.276009	1.898012	-1.257421
1	2.088259	0.908421	-2.461855
1	5.504417	1.213553	-0.796138
1	4.712683	0.495081	-2.19753
1	1.989281	-2.599324	0.53084
1	2.910246	3.78361	-1.781057
1	4.653188	3.498149	-1.651452
1	3.732634	2.759331	-2.972846
1	2.737478	-3.590222	-2.266755
1	1.679993	-4.404149	-1.100704
1	1.151962	-2.91496	-1.893238
1	4.680188	-3.457867	-0.629039
1	3.647229	-4.383025	0.465971
1	4.392427	-2.88105	1.024067
6	-0.164629	-1.400224	1.313332
6	-0.522268	-1.762228	2.622705
6	-0.709312	-2.162178	0.25481
6	-1.399822	-2.826127	2.866236
1	-0.102803	-1.220939	3.462156
6	-1.584271	-3.22918	0.499295
1	-0.381525	-2.010466	-0.769333
6	-1.942473	-3.55852	1.810313
1	-1.654842	-3.077628	3.891468
1	-1.965603	-3.804755	-0.337908

1	-2.620989	-4.383528	2.001624
17	1.259163	2.549807	1.461724
6	2.93672	-1.146967	-0.794289
1	3.02762	-1.212557	-1.891303
15	1.017032	0.058043	1.116534
5	2.23296	-0.193928	2.661621
1	1.614015	0.065605	3.668489
1	2.469	-1.384152	2.570554
1	3.17239	0.535624	2.49343
6	-1.935275	1.247446	2.093714
6	-2.607515	2.353918	2.617515
6	-2.747517	3.496461	1.825861
6	-2.237806	3.537124	0.524215
6	-1.555855	2.420908	0.023693
6	-1.391895	1.234055	0.791865
1	-1.832504	0.365237	2.720511
1	-3.012575	2.327786	3.624373
1	-3.260418	4.370474	2.217489
1	-2.370798	4.431995	-0.072215
12	-2.249391	-0.290789	-0.468012
35	-3.655344	-1.30375	-2.153436
8	-1.061705	2.359531	-1.248928
6	-1.236293	3.480073	-2.123888
1	-2.299161	3.690847	-2.284397
1	-0.73489	4.367906	-1.725804
1	-0.774093	3.191376	-3.067677

PC_{1b-r} 2

E = -4570.590460 ZPVE = 0.525702 NIMAG = 0.

6	-2.220473	0.652278	0.618122
6	-4.498513	0.862828	-0.550063
6	-2.860873	2.829396	-0.64581
6	-2.10579	2.194234	0.531592
6	-4.33127	2.388953	-0.611229
6	-3.970782	-1.295954	0.831317
6	-2.720271	4.35674	-0.623208
6	-3.594551	-1.734166	2.25853
6	-5.422917	-1.721827	0.548745
1	-1.766081	0.350315	1.56484
1	-5.56314	0.637734	-0.441692
1	-4.178874	0.415171	-1.496229
1	-2.418005	2.463789	-1.583691
1	-1.060227	2.510151	0.527575
1	-2.531302	2.582841	1.468086
1	-4.859799	2.782469	-1.488599
1	-4.810759	2.840981	0.270612
1	-3.340003	-1.849238	0.123202
1	-1.669294	4.662655	-0.676252
1	-3.246909	4.812353	-1.46912
1	-3.144267	4.774189	0.298797
1	-4.263551	-1.263007	2.989334
1	-3.692501	-2.819546	2.367934
1	-2.568841	-1.47184	2.530131
1	-6.131177	-1.155029	1.166105
1	-5.551624	-2.782872	0.788673
1	-5.70122	-1.585399	-0.499626
6	-0.503336	-1.799591	0.074239
6	-0.481225	-2.966348	-0.72516

6	-0.060889	-1.899602	1.412261
6	-0.006579	-4.179905	-0.211706
1	-0.87336	-2.933886	-1.73611
6	0.398905	-3.114484	1.918472
1	-0.064892	-1.029244	2.053507
6	0.431017	-4.255669	1.109977
1	0.00285	-5.059746	-0.846858
1	0.737869	-3.167963	2.948072
1	0.795208	-5.196296	1.510795
17	4.600488	3.936714	1.992353
6	-3.728935	0.23009	0.629523
1	-4.115886	0.71782	1.5399
15	-1.160987	-0.22888	-0.681181
5	-1.918786	-0.650314	-2.44678
1	-1.004387	-1.153925	-3.071247
1	-2.821399	-1.427858	-2.256978
1	-2.273599	0.393983	-2.935455
6	0.673543	1.184034	-2.293749
6	1.739343	2.032037	-2.580388
6	2.533402	2.511529	-1.532028
6	2.270571	2.166934	-0.207392
6	1.193242	1.317341	0.090568
6	0.396319	0.759597	-0.96143
1	0.031186	0.836096	-3.093999
1	1.935694	2.328333	-3.604896
1	3.364297	3.178652	-1.739097
1	2.896762	2.581574	0.580062
12	1.760907	-1.304333	-1.362781
35	3.854681	-2.147493	-0.545326
8	0.840755	0.983987	1.347177

6	1.622419	1.476399	2.458086
1	2.654147	1.125521	2.387655
1	1.605408	2.56768	2.486429
1	1.143196	1.067473	3.34649

RC_{1b-r} 3

E = -4570.592975 ZPVE = 0.522819 NIMAG = 0.

6	2.31583	-0.654995	1.311608
6	1.95214	-2.877909	0.080134
6	0.403541	-2.255013	2.027064
6	1.457321	-1.226485	2.466317
6	1.085498	-3.386152	1.243507
6	3.993789	-1.390713	-0.58381
6	-0.379967	-2.786143	3.233721
6	5.20554	-0.650945	0.012395
6	4.501834	-2.57564	-1.425958
1	3.099813	-0.038213	1.76343
1	2.47292	-3.733579	-0.357685
1	1.314952	-2.468399	-0.710705
1	-0.312217	-1.759909	1.356421
1	0.994028	-0.419728	3.039668
1	2.163642	-1.719479	3.149561
1	0.330505	-4.083295	0.860075
1	1.717634	-3.959528	1.938622
1	3.480477	-0.708759	-1.275373
1	-0.890952	-1.975077	3.764945
1	-1.13634	-3.514288	2.920474
1	0.289551	-3.284675	3.945914

1	5.772531	-1.320186	0.671757
1	5.88012	-0.317395	-0.78309
1	4.92702	0.23308	0.591163
1	4.948045	-3.350293	-0.78936
1	5.275673	-2.232435	-2.120807
1	3.709399	-3.038571	-2.019631
6	2.583859	1.872171	-0.289177
6	2.705136	2.18083	-1.653244
6	3.353585	2.574425	0.654456
6	3.600473	3.170326	-2.067958
1	2.106538	1.656475	-2.389787
6	4.239516	3.565551	0.234541
1	3.255467	2.364774	1.715534
6	4.367472	3.861496	-1.127502
1	3.691867	3.400849	-3.124705
1	4.827942	4.106701	0.968871
1	5.059349	4.632884	-1.451696
17	0.191145	1.62868	1.572746
6	2.995283	-1.830735	0.526046
1	3.608734	-2.319038	1.301221
15	1.396399	0.58731	0.225333
5	0.277232	-0.01478	-1.2473
1	-0.311914	0.966424	-1.641929
1	1.000526	-0.494971	-2.079641
1	-0.439824	-0.86873	-0.773542
6	-3.85935	1.141397	0.530652
6	-4.657745	1.830031	1.441714
6	-4.976988	3.161251	1.129145
6	-4.500136	3.744669	-0.047568
6	-3.701691	2.995092	-0.930722

6	-3.365963	1.658913	-0.67444
1	-5.022581	1.378573	2.358966
1	-5.598327	3.734303	1.811999
1	-4.751235	4.777074	-0.278708
12	-2.401438	-0.163039	-1.238944
35	-2.739329	-2.418967	-2.208145
8	-3.42227	-0.190806	0.725054
6	-4.115674	-1.048959	1.63814
1	-5.183481	-1.078553	1.39656
1	-3.681079	-2.040557	1.513238
1	-3.975	-0.712993	2.669991
1	-3.353283	3.476189	-1.844355

TS_{lb-r} 3

E = -4570.519620 ZPVE = 0.524236 NIMAG = 1.

6	1.654093	-1.133758	1.084065
6	1.539133	-3.319801	-0.315974
6	-0.29168	-2.844543	1.420391
6	0.635606	-1.794294	2.050642
6	0.53179	-3.909659	0.682528
6	3.619039	-1.740148	-0.570566
6	-1.196282	-3.477726	2.486037
6	4.781546	-1.221372	0.296104
6	4.161744	-2.802065	-1.543763
1	2.357901	-0.577483	1.706689
1	2.164393	-4.136027	-0.689486
1	1.017049	-2.913635	-1.185336
1	-0.942838	-2.339995	0.694106

1	0.048202	-1.028078	2.558985
1	1.235341	-2.290971	2.827987
1	-0.13645	-4.608602	0.163299
1	1.078405	-4.50141	1.433054
1	3.254814	-0.90955	-1.185213
1	-1.790975	-2.719607	3.007223
1	-1.887847	-4.20023	2.037938
1	-0.59907	-4.008016	3.238628
1	5.239163	-2.050374	0.85103
1	5.559027	-0.765972	-0.326706
1	4.465035	-0.469801	1.024021
1	4.504997	-3.697702	-1.010695
1	5.019866	-2.396352	-2.09107
1	3.416171	-3.110858	-2.281906
6	2.178704	1.479225	-0.475841
6	2.195293	1.902128	-1.818759
6	3.179498	1.958191	0.390487
6	3.18892	2.767014	-2.283336
1	1.443501	1.55157	-2.514021
6	4.178716	2.808436	-0.079551
1	3.170112	1.680456	1.436665
6	4.18559	3.219635	-1.41703
1	3.180259	3.081489	-3.322495
1	4.947476	3.157683	0.603084
1	4.959252	3.891171	-1.777329
17	0.674716	1.471383	2.243968
6	2.45181	-2.253819	0.327039
1	2.94155	-2.773609	1.169363
15	0.879128	0.284291	0.041312
5	0.191151	-0.482992	-1.668179

1	-0.360219	0.40279	-2.295875
1	1.091379	-0.969712	-2.29919
1	-0.583224	-1.361058	-1.323337
6	-2.330429	1.486204	1.204996
6	-2.91958	2.662909	1.685169
6	-2.640984	3.87395	1.041692
6	-1.799775	3.921916	-0.073556
6	-1.227105	2.734762	-0.540339
6	-1.474783	1.493584	0.075127
1	-3.581617	2.655952	2.543202
1	-3.088317	4.787302	1.42396
1	-1.595674	4.866219	-0.569367
12	-2.11944	-0.105578	-1.245456
35	-4.046814	-1.162016	-2.295599
8	-2.562055	0.252937	1.746386
6	-3.43922	0.145034	2.872059
1	-4.444775	0.501779	2.62367
1	-3.479937	-0.916186	3.115881
1	-3.047125	0.703651	3.72853
1	-0.570328	2.781437	-1.406912

PC_{1b-r} 3

E = -4570.625354 ZPVE = 0.527332 NIMAG = 0.

6	-1.460912	1.095405	0.67562
6	-0.426135	3.321606	-0.08668
6	0.479283	2.194805	2.021744
6	-0.783556	1.319056	2.049721
6	0.187701	3.521177	1.30607

6	-2.49971	2.37016	-1.377836
6	1.016044	2.425976	3.440295
6	-3.990311	2.093443	-1.109942
6	-2.374506	3.623241	-2.262853
1	-2.430179	0.633018	0.895735
1	-0.665623	4.303823	-0.50327
1	0.311778	2.874865	-0.762224
1	1.253215	1.670787	1.443729
1	-0.576829	0.361016	2.537071
1	-1.537261	1.813187	2.677575
1	1.109518	4.111499	1.226306
1	-0.507867	4.109158	1.923297
1	-2.097702	1.534618	-1.964966
1	1.23722	1.480611	3.948836
1	1.934215	3.024	3.422507
1	0.278831	2.962521	4.049825
1	-4.458873	2.97444	-0.653741
1	-4.520422	1.878577	-2.044202
1	-4.152004	1.251167	-0.433099
1	-2.708147	4.5233	-1.731705
1	-3.007536	3.511764	-3.150004
1	-1.349876	3.790429	-2.607469
6	-1.901487	-1.122038	-1.332379
6	-1.574241	-1.617855	-2.607556
6	-3.192909	-1.343761	-0.823831
6	-2.521763	-2.31201	-3.361952
1	-0.588112	-1.459708	-3.026445
6	-4.134896	-2.042157	-1.584468
1	-3.490616	-0.991183	0.161781
6	-3.805857	-2.524935	-2.853021

1	-2.254202	-2.681114	-4.347493
1	-5.128093	-2.202712	-1.176489
1	-4.543576	-3.061951	-3.441775
17	-4.509926	-0.405269	2.471
6	-1.710688	2.468604	-0.036118
1	-2.381425	2.988795	0.666703
15	-0.608182	-0.233375	-0.368286
5	0.754509	0.315227	-1.661327
1	1.256406	-0.757644	-2.006016
1	0.255346	0.838888	-2.612797
1	1.540587	1.074783	-1.133115
6	1.412709	-1.619569	1.192725
6	1.865623	-2.678987	1.980047
6	0.976898	-3.668018	2.400146
6	-0.363137	-3.59845	2.023358
6	-0.798331	-2.551459	1.213055
6	0.069802	-1.535528	0.770765
1	2.908373	-2.734122	2.268884
1	1.338134	-4.485413	3.015668
1	-1.070509	-4.353259	2.349533
12	2.98078	-0.347195	-1.169255
35	5.327027	0.172122	-1.363932
8	2.332011	-0.620094	0.813836
6	3.282948	-0.199744	1.848708
1	4.12481	-0.891249	1.891094
1	3.630339	0.790781	1.559005
1	2.76234	-0.155465	2.804621
1	-1.840132	-2.525082	0.920828

RC_{1b-r} 4

E = -4570.594752 ZPVE = 0.521049 NIMAG = 0.

6	-1.59952	0.980577	0.047315
6	-3.166822	3.003306	0.182318
6	-0.86289	3.277258	-0.909093
6	-0.44361	1.973348	-0.214475
6	-1.988617	3.947605	-0.107398
6	-3.875826	0.771488	1.349877
6	0.340506	4.209712	-1.095631
6	-3.382046	-0.252553	2.388387
6	-5.058243	1.552944	1.950438
1	-1.184696	0.167422	0.65069
1	-3.876864	3.528338	0.827284
1	-3.698893	2.775053	-0.747495
1	-1.254677	3.028951	-1.905491
1	0.360919	1.488465	-0.774167
1	-0.029445	2.215374	0.774724
1	-2.350459	4.834813	-0.642452
1	-1.572383	4.306938	0.84644
1	-4.267899	0.221321	0.483746
1	1.124979	3.732917	-1.694648
1	0.047291	5.135873	-1.602546
1	0.777324	4.482397	-0.12631
1	-3.079995	0.261248	3.309808
1	-4.183225	-0.954255	2.644646
1	-2.528319	-0.839494	2.042808
1	-4.725869	2.205751	2.767745
1	-5.794405	0.854942	2.363785
1	-5.571968	2.170879	1.209082

6	-2.645832	-1.613751	-0.983947
6	-3.84857	-2.174112	-1.44318
6	-1.785613	-2.38261	-0.180662
6	-4.191083	-3.48338	-1.094231
1	-4.515394	-1.59115	-2.068541
6	-2.129379	-3.691338	0.157121
1	-0.8505	-1.972405	0.188495
6	-3.33174	-4.243981	-0.297883
1	-5.125439	-3.906493	-1.450241
1	-1.460965	-4.27684	0.781174
1	-3.596032	-5.262929	-0.031196
17	-0.458118	-0.255352	-2.594017
6	-2.718769	1.698655	0.876182
1	-2.190714	2.005906	1.794162
15	-2.221966	0.09075	-1.49624
5	-3.524828	0.873929	-2.714263
1	-3.608937	0.071394	-3.615887
1	-4.542528	0.967392	-2.063401
1	-3.075951	1.940983	-3.054428
6	4.978444	-0.580033	-0.331171
6	6.068846	-0.772415	-1.176593
6	7.069675	0.21255	-1.160453
6	6.953548	1.326549	-0.326512
6	5.828486	1.467443	0.506422
6	4.804464	0.513172	0.528788
1	6.162725	-1.637136	-1.825189
1	7.937126	0.098569	-1.804518
1	7.734474	2.082693	-0.322677
12	2.954298	-0.174275	1.304143
35	0.86696	-0.77992	2.450534

8	3.890764	-1.477075	-0.233057
6	3.883618	-2.688135	-0.997939
1	4.732445	-3.321318	-0.720589
1	2.949262	-3.195972	-0.759645
1	3.918172	-2.464599	-2.068714
1	5.767016	2.346352	1.146717

TS_{lb-r} 4

E = -4570.485822 ZPVE = 0.521730 NIMAG = 1.

6	1.819167	-0.293283	-0.662888
6	4.230654	-1.022871	-0.039766
6	3.83961	1.349494	-0.874167
6	2.467821	0.905475	-1.410629
6	4.810404	0.164928	-0.818407
6	2.338084	-2.845508	-0.110471
6	4.394514	2.504484	-1.717567
6	1.565554	-3.5627	-1.236853
6	3.423703	-3.800669	0.417234
1	0.97915	-0.633507	-1.278519
1	4.934593	-1.857232	-0.104604
1	4.134662	-0.769415	1.019308
1	3.697344	1.718654	0.147746
1	1.792874	1.762172	-1.417934
1	2.58747	0.585517	-2.45667
1	5.758037	0.481539	-0.363784
1	5.047825	-0.157005	-1.844834
1	1.660975	-2.670586	0.730757
1	3.716855	3.365581	-1.707336

1	5.365948	2.837477	-1.334278
1	4.535271	2.197542	-2.762383
1	2.268127	-3.925648	-1.997093
1	1.012636	-4.42755	-0.854343
1	0.853019	-2.911526	-1.755295
1	4.173981	-4.026556	-0.350059
1	2.961354	-4.749135	0.713204
1	3.939905	-3.397118	1.29253
6	-0.347915	-0.95309	1.461713
6	-0.888643	-0.817854	2.752646
6	-0.831057	-2.00595	0.653322
6	-1.876749	-1.692008	3.213422
1	-0.537487	-0.02601	3.401661
6	-1.817382	-2.889867	1.124695
1	-0.39012	-2.203809	-0.317814
6	-2.347709	-2.731574	2.405998
1	-2.275915	-1.559679	4.214562
1	-2.152227	-3.698328	0.483243
1	-3.11058	-3.411632	2.770387
17	1.318711	2.752393	1.116627
6	2.875093	-1.470428	-0.619732
1	3.066227	-1.618745	-1.696216
15	1.009342	0.257293	0.98148
5	2.169045	0.104985	2.580773
1	1.561272	0.518118	3.539778
1	2.281987	-1.110965	2.609436
1	3.18735	0.706938	2.368214
6	-1.718424	2.386044	0.434326
6	-2.17724	3.581017	-0.140396
6	-1.897967	3.849235	-1.483033

6	-1.193204	2.932239	-2.266397
6	-0.755787	1.741242	-1.680907
6	-0.992157	1.422156	-0.322134
1	-2.730466	4.308176	0.441876
1	-2.242027	4.78414	-1.916431
1	-0.993213	3.137687	-3.313562
12	-2.261053	-0.348252	-0.414959
35	-3.600763	-1.597231	-1.998055
8	-1.959245	2.054775	1.734377
6	-2.607708	3.001291	2.588911
1	-3.62518	3.216179	2.243082
1	-2.64819	2.531323	3.571481
1	-2.030991	3.92986	2.65059
1	-0.226562	1.031612	-2.312506

PC_{1b-r} 4

E = -4570.642617 ZPVE = 0.523837 NIMAG = 0.

6	2.164595	-0.24692	-0.847064
6	4.633424	-0.053611	-0.161929
6	3.471091	1.961584	-1.23598
6	2.389554	0.996213	-1.746413
6	4.78898	1.198157	-1.040126
6	3.425758	-2.369096	0.063285
6	3.638479	3.153878	-2.186454
6	2.751678	-3.425009	-0.832787
6	4.786061	-2.917103	0.530645
1	1.482439	-0.910889	-1.388964
1	5.58758	-0.58869	-0.15662

1	4.4297	0.239676	0.871424
1	3.155246	2.350838	-0.258276
1	1.453732	1.535374	-1.91483
1	2.700445	0.615454	-2.730594
1	5.545086	1.863168	-0.603154
1	5.169693	0.900787	-2.0298
1	2.812543	-2.238041	0.962851
1	2.701715	3.712723	-2.295787
1	4.401947	3.847515	-1.816003
1	3.947721	2.819479	-3.185052
1	3.393265	-3.657106	-1.692512
1	2.584548	-4.35555	-0.279523
1	1.783009	-3.099572	-1.220542
1	5.486334	-3.017802	-0.30843
1	4.653023	-3.91215	0.969693
1	5.253184	-2.282383	1.288579
6	0.236784	-1.342569	1.205603
6	0.109518	-1.652902	2.571444
6	-0.402806	-2.172863	0.27009
6	-0.636264	-2.759087	2.987108
1	0.59717	-1.029903	3.311363
6	-1.15085	-3.276949	0.686156
1	-0.328578	-1.984745	-0.794362
6	-1.269289	-3.57476	2.045914
1	-0.718142	-2.981153	4.047033
1	-1.642117	-3.897119	-0.056722
1	-1.848641	-4.435149	2.367688
17	-5.077721	1.058493	1.439329
6	3.527658	-1.00095	-0.676325
1	3.808139	-1.247835	-1.714686

15	1.209121	0.170539	0.74871
5	2.266494	0.722365	2.317967
1	1.477617	0.95641	3.202978
1	2.938007	-0.261591	2.547871
1	2.929152	1.681685	2.010979
6	-0.352508	2.615268	0.696379
6	-1.365006	3.444618	0.17216
6	-2.138416	3.022927	-0.902382
6	-1.931355	1.755944	-1.466981
6	-0.918765	0.938021	-0.94398
6	-0.118116	1.330531	0.138904
1	-1.541363	4.422486	0.601162
1	-2.900405	3.68402	-1.303717
1	-2.458779	1.453651	-2.367224
12	-3.830446	0.180426	-0.273694
35	-3.499878	-1.528629	-2.003374
8	0.429511	2.993886	1.724493
6	0.225761	4.263225	2.354503
1	-0.780887	4.333815	2.779359
1	0.96469	4.307141	3.153825
1	0.395764	5.084784	1.650909
1	-0.751646	-0.019118	-1.422115

R1_{III} + b S_N2@P-f pathways 2 and 3 in THF

RC_{IIIb-r 2}

E = -4409.698343 ZPVE = 0.339543 NIMAG = 0.

17	-1.23333	0.523287	1.748426
15	-1.969792	0.103002	-0.17056
12	3.197878	1.288975	-0.423256

35	2.820985	3.694486	-0.196581
5	-0.758204	0.788665	-1.517393
1	-0.754658	1.98693	-1.366951
1	0.307854	0.259084	-1.302574
1	-1.262027	0.423251	-2.558153
6	3.78626	-0.697255	-0.882259
6	4.213364	-1.639697	-1.825146
6	3.633591	-1.178278	0.425743
6	4.46945	-2.977673	-1.472549
6	3.872289	-2.489403	0.832976
6	4.298533	-3.396209	-0.15136
1	4.7998	-3.688188	-2.226197
1	3.740129	-2.818024	1.858632
1	4.495353	-4.428105	0.126329
6	-2.170294	-1.709298	-0.157004
6	-3.40614	-2.331414	0.082927
6	-1.034125	-2.496386	-0.418785
6	-3.500164	-3.724897	0.068802
1	-4.293914	-1.738584	0.272068
6	-1.134801	-3.887857	-0.425838
1	-0.076708	-2.026276	-0.618201
6	-2.367031	-4.503499	-0.182499
1	-4.459545	-4.199108	0.251439
1	-0.253537	-4.488656	-0.627654
1	-2.44408	-5.586546	-0.192663
6	-3.629755	0.854481	-0.161476
6	-4.454846	0.868459	0.975515
6	-4.085549	1.429593	-1.359751
6	-5.724483	1.443586	0.908791
1	-4.106596	0.446953	1.912762

6	-5.361054	1.996553	-1.420509
1	-3.449949	1.438588	-2.238495
6	-6.180189	2.004945	-0.288884
1	-6.354936	1.455703	1.792482
1	-5.706465	2.439822	-2.349286
1	-7.168	2.45317	-0.336419
8	3.199833	-0.15217	1.292446
6	3.004351	-0.418772	2.684822
1	2.688456	0.521243	3.136568
1	2.226108	-1.175731	2.825226
1	3.938808	-0.755031	3.145969
1	4.354298	-1.343951	-2.864015

TS_{mb-r} 2

E = -4409.636881 ZPVE = 0.339140 NIMAG = 1.

17	-0.1678	-1.664814	1.355191
15	0.851507	-0.583664	-0.432035
12	-2.095516	-1.051169	-0.087134
35	-4.371358	-1.893574	-0.259879
5	0.01472	-1.443359	-2.01559
1	0.499062	-2.540291	-2.079137
1	-1.19288	-1.527776	-1.811065
1	0.209271	-0.742534	-2.975348
6	-1.145448	0.92701	-0.194332
6	-1.654841	1.409941	-1.418581
6	-1.210117	1.815261	0.911468
6	-2.217745	2.683641	-1.557063
6	-1.763947	3.099493	0.790033

6	-2.263082	3.52484	-0.444902
1	-2.614081	3.009171	-2.514343
1	-1.809463	3.772241	1.63828
1	-2.68655	4.521879	-0.52875
6	1.677753	1.062232	-0.477344
6	2.449697	1.507472	0.606654
6	1.597898	1.843706	-1.641877
6	3.12513	2.727405	0.530038
1	2.53193	0.91054	1.508139
6	2.305344	3.043949	-1.723809
1	0.999061	1.515733	-2.483885
6	3.06001	3.495431	-0.635834
1	3.710509	3.069106	1.378434
1	2.257321	3.630252	-2.636535
1	3.596457	4.437363	-0.698719
6	2.423904	-1.554947	-0.075841
6	2.929634	-1.906839	1.182094
6	3.186408	-1.853	-1.218586
6	4.165258	-2.55223	1.296181
1	2.368406	-1.690215	2.083926
6	4.419685	-2.499716	-1.103245
1	2.820837	-1.593971	-2.207615
6	4.913436	-2.852403	0.15548
1	4.537604	-2.821229	2.280372
1	4.987035	-2.731576	-1.999814
1	5.869895	-3.358567	0.245803
8	-0.692847	1.351976	2.087041
6	-0.750691	2.178442	3.250782
1	-0.299556	1.5914	4.051167
1	-0.180809	3.103819	3.111012

1	-1.786441	2.419652	3.5153
1	-1.614415	0.773802	-2.299847

PC_{stab-r} 2

E = -4409.775783 ZPVE = 0.342739 NIMAG = 0.

17	-4.253534	3.200067	0.16086
15	0.688776	0.337914	0.214942
12	-3.489555	1.027459	0.227896
35	-4.315339	-1.283884	0.11263
5	-1.028347	1.170964	0.615765
1	-0.75633	2.235159	1.105277
1	-1.553726	1.336604	-0.476352
1	-1.6946	0.482518	1.369285
6	0.569117	-1.328732	-0.520155
6	-0.691294	-1.933391	-0.623269
6	1.711532	-2.050858	-0.946638
6	-0.833455	-3.225944	-1.130214
6	1.568163	-3.344221	-1.465483
6	0.298929	-3.92283	-1.55094
1	-1.81938	-3.673327	-1.196526
1	2.434007	-3.903771	-1.796472
1	0.204157	-4.928205	-1.950659
6	1.706953	0.227638	1.735855
6	3.103736	0.365664	1.717673
6	1.054341	-0.027252	2.953391
6	3.834246	0.25223	2.902319
1	3.620351	0.560152	0.78535
6	1.790684	-0.148882	4.134206

1	-0.025355	-0.13201	2.986104
6	3.180895	-0.007809	4.110895
1	4.913998	0.364983	2.878746
1	1.275954	-0.347005	5.06932
1	3.752407	-0.097111	5.029912
6	1.53538	1.445187	-0.972836
6	1.539203	1.14991	-2.343779
6	2.072535	2.663073	-0.526711
6	2.0917	2.053488	-3.254654
1	1.112459	0.21958	-2.704251
6	2.625753	3.562648	-1.440849
1	2.062733	2.915105	0.529071
6	2.638559	3.258807	-2.805404
1	2.09298	1.81357	-4.313645
1	3.042747	4.499927	-1.085246
1	3.06841	3.959523	-3.514811
8	2.905394	-1.417004	-0.820671
6	4.102109	-2.085725	-1.234143
1	4.912052	-1.385615	-1.031575
1	4.257293	-3.004205	-0.658961
1	4.073009	-2.314336	-2.304557
1	-1.579112	-1.401739	-0.304602

RC_{mb-r} 3

E = -4409.697117 ZPVE = 0.339878 NIMAG = 0.

17	-0.960799	0.129735	1.87812
15	-1.725234	-0.043899	-0.062515
12	2.319443	1.352938	-0.617014

35	2.125556	3.797772	-0.669782
5	-0.590737	0.905765	-1.312722
1	0.504422	0.373377	-1.243155
1	-1.109271	0.712122	-2.388392
1	-0.62174	2.053647	-0.959684
6	3.381661	-0.480271	-0.56556
6	3.8801	-1.285368	-1.601661
6	3.593442	-0.959072	0.740648
6	4.547714	-2.49956	-1.362127
6	4.255991	-2.159911	1.022845
6	4.734659	-2.929001	-0.048377
1	4.919291	-3.096687	-2.191258
1	4.409539	-2.506172	2.039275
1	5.250895	-3.863175	0.157001
6	-1.882416	-1.833659	-0.315892
6	-2.548935	-2.654249	0.611334
6	-1.310497	-2.397693	-1.467566
6	-2.65263	-4.024241	0.376734
1	-2.980736	-2.229128	1.512036
6	-1.424665	-3.77126	-1.698008
1	-0.783662	-1.772718	-2.180351
6	-2.093252	-4.58293	-0.778948
1	-3.166774	-4.655491	1.094673
1	-0.985432	-4.203006	-2.591654
1	-2.175915	-5.650616	-0.958112
6	-3.394873	0.670208	0.073121
6	-4.531742	-0.038566	-0.345289
6	-3.524589	1.99738	0.520266
6	-5.787132	0.574704	-0.307215
1	-4.446494	-1.058344	-0.703267

6	-4.781352	2.599321	0.560643
1	-2.652335	2.558244	0.841243
6	-5.914127	1.88917	0.146921
1	-6.662647	0.020974	-0.631677
1	-4.875373	3.622003	0.912028
1	-6.891318	2.361321	0.177703
8	3.082735	-0.128472	1.730412
6	3.266641	-0.485155	3.098221
1	2.791019	0.303158	3.683297
1	2.788631	-1.445087	3.327704
1	4.331491	-0.537937	3.355413
1	3.748567	-0.970885	-2.636813

TS_{mb-r} 3

E = -4409.637017 ZPVE = 0.339073 NIMAG = 1.

17	0.107208	-1.824188	1.344931
15	1.080071	-0.489814	-0.475646
12	-1.791194	-1.309268	-0.104688
35	-4.082074	-2.012813	-0.540543
5	0.309251	-1.362685	-2.082492
1	-0.894274	-1.492561	-1.920596
1	0.519564	-0.599841	-2.990801
1	0.851094	-2.424949	-2.197437
6	-1.246144	0.811478	-0.153874
6	-1.570781	1.400115	-1.390788
6	-1.632681	1.520685	1.010569
6	-2.268593	2.608106	-1.489846
6	-2.333421	2.734864	0.933278

6	-2.643303	3.271771	-0.319432
1	-2.518282	3.021041	-2.462869
1	-2.638183	3.264886	1.828268
1	-3.180515	4.214671	-0.372791
6	1.609805	1.272271	-0.51883
6	1.624161	2.092469	0.6174
6	2.087908	1.761573	-1.743987
6	2.108642	3.398282	0.525447
1	1.248162	1.7214	1.565161
6	2.563174	3.074562	-1.827723
1	2.087992	1.135747	-2.630337
6	2.576167	3.893473	-0.696756
1	2.115337	4.029782	1.4087
1	2.920788	3.4507	-2.781541
1	2.946482	4.911737	-0.765992
6	2.693745	-1.289029	-0.037561
6	3.786394	-0.549614	0.448943
6	2.857182	-2.673183	-0.251146
6	5.013549	-1.1725	0.694765
1	3.694987	0.512942	0.634456
6	4.083712	-3.288122	-0.012543
1	2.026901	-3.272265	-0.604504
6	5.167666	-2.539794	0.462406
1	5.845498	-0.582731	1.067358
1	4.192738	-4.352928	-0.19443
1	6.121818	-3.022267	0.65198
8	-1.296053	0.942188	2.205666
6	-1.717934	1.555449	3.424435
1	-1.36051	0.902016	4.220776
1	-1.276688	2.55158	3.544338

1	-2.810088	1.629858	3.475711
1	-1.282825	0.898044	-2.310744

PC_{imp-r} 3

E = -4409.773758 ZPVE = 0.342946 NIMAG = 0.

17	3.713712	-2.789553	0.377905
15	-0.694772	0.249942	0.165566
12	3.489061	-0.487218	0.24106
35	5.164903	1.267668	-0.085371
5	1.202169	0.478225	0.533598
1	1.589783	-0.604227	0.946309
1	1.774451	0.846649	-0.472829
1	1.273244	1.304691	1.405377
6	-1.044025	-0.806468	-1.281643
6	0.021839	-1.28272	-2.058876
6	-2.363545	-1.198417	-1.618812
6	-0.195824	-2.132723	-3.144236
6	-2.583222	-2.054343	-2.706272
6	-1.50031	-2.514252	-3.459653
1	0.643401	-2.491251	-3.730383
1	-3.587374	-2.361839	-2.970469
1	-1.686397	-3.176793	-4.299666
6	-1.438366	1.901009	-0.106054
6	-2.017815	2.255403	-1.332424
6	-1.349959	2.859638	0.91841
6	-2.516123	3.546717	-1.526355
1	-2.081637	1.532401	-2.138125
6	-1.854137	4.146185	0.721923

1	-0.885029	2.609714	1.866907
6	-2.43872	4.491979	-0.500658
1	-2.962749	3.810678	-2.480141
1	-1.784302	4.877443	1.521363
1	-2.82759	5.494245	-0.653148
6	-1.496278	-0.516271	1.630606
6	-2.674627	-0.009425	2.196635
6	-0.896791	-1.656687	2.190376
6	-3.239608	-0.630039	3.313417
1	-3.156883	0.862212	1.768836
6	-1.471343	-2.280482	3.299991
1	0.016197	-2.064066	1.768243
6	-2.641262	-1.76606	3.866064
1	-4.149798	-0.226813	3.747086
1	-0.999322	-3.16201	3.722832
1	-3.083248	-2.247253	4.733386
8	-3.354779	-0.692096	-0.843171
6	-4.712455	-1.06611	-1.103396
1	-5.305232	-0.555723	-0.345036
1	-5.025648	-0.735979	-2.099359
1	-4.845553	-2.148478	-1.007747
1	1.034644	-0.988041	-1.812901

R1_{IV} + b S_N2@P-f pathways 2, 3 and 4 in THF

RC_{IVb-r} 2

E = -4217.960228 ZPVE = 0.286359 NIMAG = 0.

17	1.757926	-1.637892	-1.839196
15	2.267331	0.265745	-1.173434
12	-1.832753	0.753363	-0.506773

35	-2.524205	3.097181	-0.082499
6	3.207448	0.946838	-2.577855
1	3.566299	1.939135	-2.289286
1	4.055558	0.311796	-2.838713
1	2.539707	1.040095	-3.437175
5	0.702081	1.312657	-0.738454
1	0.019062	1.292476	-1.741474
1	0.1816	0.804776	0.233372
1	1.118548	2.41525	-0.492229
6	-2.624686	-1.224941	-0.680556
6	-2.696945	-1.433162	0.704618
6	-3.061628	-2.297171	-1.469313
6	-3.174943	-2.586741	1.323875
6	-3.552547	-3.487711	-0.902112
1	-3.034473	-2.217783	-2.55573
6	-3.611766	-3.626229	0.48662
1	-3.215925	-2.69815	2.402746
1	-3.890873	-4.299693	-1.541265
1	-3.99367	-4.541836	0.92996
8	-2.194912	-0.316035	1.407909
6	-2.425614	-0.181705	2.813228
1	-1.898801	-0.963994	3.36897
1	-2.034056	0.796009	3.093516
1	-3.498161	-0.227194	3.030247
6	3.425895	-0.000756	0.196131
6	4.690452	-0.575687	-0.022193
6	3.047824	0.38606	1.49246
6	5.565808	-0.757466	1.047382
1	4.993042	-0.891204	-1.015746
6	3.932598	0.20431	2.558061

1	2.07445	0.8294	1.672451
6	5.188236	-0.366408	2.337247
1	6.540259	-1.203404	0.875197
1	3.638058	0.508595	3.557432
1	5.872983	-0.508375	3.167766

TS_{IVb-r} 2

E = -4217.904667 ZPVE = 0.287431 NIMAG = 1.

17	-0.385389	2.932113	1.357918
15	-1.123515	1.594252	-0.326802
12	1.718746	0.553421	-0.56198
35	4.087054	0.010722	-0.363123
6	-2.44222	2.895844	-0.619084
1	-2.962868	2.615836	-1.540784
1	-3.16311	2.92587	0.201471
1	-1.98121	3.877913	-0.732988
5	0.170286	1.848147	-1.794981
1	1.150441	2.369017	-1.279429
1	0.42866	0.771229	-2.286371
1	-0.283969	2.604635	-2.606247
6	0.027089	-0.071948	0.961418
6	0.319438	-1.352651	0.44028
6	-0.26227	-0.041755	2.336342
6	0.304944	-2.5266	1.191289
6	-0.291658	-1.198242	3.124284
1	-0.495477	0.906617	2.806222
6	-0.025767	-2.440728	2.547371
1	0.559552	-3.484228	0.752373

1	-0.530198	-1.126533	4.181352
1	-0.054026	-3.345178	3.147559
8	0.742535	-1.318184	-0.893667
6	1.141851	-2.527321	-1.565407
1	0.314941	-3.241159	-1.568441
1	1.376813	-2.232691	-2.587515
1	2.023664	-2.959681	-1.085105
6	-2.315691	0.179616	-0.524244
6	-3.256771	-0.120785	0.471828
6	-2.346834	-0.524939	-1.73674
6	-4.20752	-1.121518	0.263443
1	-3.246545	0.413347	1.417645
6	-3.302897	-1.526779	-1.940489
1	-1.636562	-0.299114	-2.524511
6	-4.232008	-1.829826	-0.943088
1	-4.927676	-1.348029	1.044187
1	-3.318164	-2.06487	-2.884046
1	-4.971598	-2.608474	-1.103847

PC_{IVb-r} 2

E = -4218.041518 ZPVE = 0.289312 NIMAG = 0.

17	-3.083728	2.369505	0.84233
15	1.461471	0.242077	1.323144
12	-2.189539	0.285528	0.399501
35	-3.169727	-1.883768	-0.239404
6	2.818697	0.704162	2.462632
1	2.943312	-0.125061	3.163357
1	3.759542	0.86569	1.932361

1	2.544612	1.59946	3.02619
5	-0.168791	-0.052133	2.353736
1	-0.533081	1.042867	2.701698
1	-0.978793	-0.648706	1.660777
1	0.12482	-0.774001	3.274005
6	1.327143	1.61493	0.111886
6	0.326699	1.589556	-0.872675
6	2.158054	2.745995	0.168185
6	0.149821	2.636312	-1.772235
6	2.00083	3.798378	-0.736087
1	2.936808	2.81352	0.918894
6	0.998072	3.743248	-1.705984
1	-0.647531	2.591093	-2.505987
1	2.65769	4.659955	-0.676202
1	0.863106	4.564172	-2.402724
8	-0.533019	0.480837	-0.917957
6	-0.435839	-0.325266	-2.138049
1	0.597555	-0.652558	-2.258971
1	-1.098703	-1.174219	-1.982942
1	-0.763574	0.263193	-2.996343
6	2.059376	-1.224069	0.406085
6	3.053851	-1.11031	-0.579566
6	1.534276	-2.487398	0.719021
6	3.516876	-2.248537	-1.242047
1	3.465541	-0.138463	-0.836021
6	1.999645	-3.623622	0.051019
1	0.766128	-2.588082	1.478201
6	2.987631	-3.505518	-0.929766
1	4.285306	-2.153241	-2.003231
1	1.585136	-4.596838	0.295097

1	3.34566	-4.389164	-1.449352
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RC_{IVb-r} 3

E = -4217.960430 ZPVE = 0.286746 NIMAG = 0.

17	3.092499	1.839349	-2.181465
15	1.985806	0.579449	-0.952386
12	-2.023874	0.680174	-0.350013
35	-3.14766	2.742272	0.392048
5	0.435077	1.52928	-0.289318
1	-0.250376	1.747066	-1.265574
1	-0.060527	0.746459	0.499988
1	0.796074	2.536506	0.254339
6	-2.133646	-1.364236	-0.986486
6	-2.256527	-1.87239	0.315583
6	-2.142199	-2.327236	-2.004015
6	-2.386419	-3.21937	0.649428
6	-2.269266	-3.701982	-1.730039
1	-2.053616	-2.017036	-3.04495
6	-2.392375	-4.141484	-0.409985
1	-2.482375	-3.562302	1.674656
1	-2.277268	-4.423864	-2.543109
1	-2.495054	-5.201129	-0.192512
8	-2.220477	-0.828872	1.264436
6	-2.488005	-1.08959	2.645104
1	-1.728688	-1.755915	3.067126
1	-2.452696	-0.123461	3.148139
1	-3.482073	-1.53308	2.764828
6	1.630961	-0.840246	-2.037213

1	1.058199	-0.492003	-2.89936
1	2.548763	-1.325833	-2.373345
1	1.021819	-1.549121	-1.468479
6	3.141403	0.027106	0.3324
6	4.287684	-0.720231	0.009203
6	2.874247	0.355182	1.671854
6	5.153853	-1.136693	1.018905
1	4.515452	-0.968476	-1.02279
6	3.746625	-0.067664	2.67781
1	1.991552	0.929337	1.931928
6	4.883526	-0.811507	2.353323
1	6.038342	-1.712436	0.765324
1	3.536013	0.186609	3.711751
1	5.560707	-1.13698	3.137078

TS_{IVb-r} 3

E = -4217.903907 ZPVE = 0.288186 NIMAG = 1.

17	-1.316247	-0.5999	-1.878584
15	-1.321693	-0.027748	0.349896
12	1.560426	-0.952491	0.208634
35	3.619076	-2.088802	-0.463624
5	-0.491847	-1.58067	1.234276
1	-0.031222	-2.282855	0.347088
1	0.359874	-1.134074	1.972949
1	-1.301548	-2.204111	1.859016
6	0.705438	1.143788	-0.379359
6	1.727902	1.60241	0.48053
6	0.429605	1.983459	-1.471369

6	2.433954	2.791002	0.30185
6	1.10566	3.191628	-1.681426
1	-0.345664	1.699338	-2.174353
6	2.097307	3.59977	-0.788402
1	3.232005	3.085214	0.973704
1	0.85251	3.811011	-2.536695
1	2.625266	4.536343	-0.940264
8	2.050005	0.677586	1.485449
6	3.134599	0.935047	2.398114
1	2.942461	1.855974	2.953443
1	3.150748	0.088314	3.082979
1	4.082517	1.001922	1.857772
6	-1.371778	1.46168	1.467698
1	-0.407306	1.549707	1.965632
1	-1.573943	2.383824	0.920045
1	-2.167551	1.294931	2.199696
6	-3.177608	-0.2592	0.257871
6	-4.033193	0.840283	0.084225
6	-3.737761	-1.542732	0.358016
6	-5.418204	0.663028	0.024092
1	-3.631924	1.843939	-0.015875
6	-5.123194	-1.717232	0.310547
1	-3.097546	-2.410419	0.474036
6	-5.968182	-0.616146	0.142421
1	-6.063546	1.525751	-0.113864
1	-5.539841	-2.716203	0.401131
1	-7.044533	-0.754152	0.100451

E = -4218.040069 ZPVE = 0.289381 NIMAG = 0.

17	-2.088284	0.430753	2.918612
15	1.239494	-0.576782	-0.712104
12	-2.156765	-0.433117	0.762871
35	-4.14249	-1.378864	-0.406606
5	-0.06303	-1.737303	0.165253
1	-0.231583	-1.305919	1.289607
1	-1.065847	-1.713675	-0.515816
1	0.397885	-2.847788	0.192111
6	0.999028	1.222911	-0.394764
6	-0.28027	1.803536	-0.402955
6	2.093409	2.057486	-0.109546
6	-0.472536	3.156283	-0.129721
6	1.915668	3.417593	0.145104
1	3.093414	1.639377	-0.083771
6	0.631555	3.966389	0.13803
1	-1.475479	3.568324	-0.115521
1	2.777424	4.041486	0.358317
1	0.483194	5.019741	0.352849
8	-1.388555	0.984017	-0.664226
6	-2.180422	1.366896	-1.833388
1	-1.530398	1.384019	-2.710413
1	-2.951606	0.604941	-1.929051
1	-2.635978	2.345068	-1.673687
6	1.210845	-0.792776	-2.531444
1	0.194112	-0.602729	-2.88215
1	1.896435	-0.106426	-3.031996
1	1.473414	-1.826733	-2.770376
6	2.933124	-0.954114	-0.142406

6	4.034188	-0.952867	-1.013313
6	3.127665	-1.257465	1.216225
6	5.311865	-1.248433	-0.529828
1	3.909332	-0.727743	-2.067037
6	4.406727	-1.544448	1.695454
1	2.284198	-1.276271	1.899371
6	5.50005	-1.541057	0.823427
1	6.156421	-1.249035	-1.211999
1	4.54633	-1.776115	2.74675
1	6.493689	-1.769178	1.197028

RC_{IVb-r} 4

E = -4217.957703 ZPVE = 0.285736 NIMAG = 0.

17	-1.575153	0.046117	1.795042
15	-2.195767	0.202492	-0.201184
12	2.986664	0.5951	-0.531094
35	3.910183	2.835529	-0.161605
5	-1.255174	1.616175	-1.12277
1	-0.093163	1.282848	-1.08011
1	-1.721667	1.550521	-2.242497
1	-1.495483	2.654593	-0.553659
6	2.397292	-1.379904	-1.041513
6	1.969943	-2.297758	-2.008495
6	2.542077	-1.893446	0.255307
6	1.704314	-3.642285	-1.688841
6	2.292542	-3.212194	0.630355
6	1.865552	-4.092856	-0.37693
1	1.373899	-4.332831	-2.460815

1	2.418862	-3.565677	1.648454
1	1.663079	-5.130201	-0.125052
6	-1.859687	-1.474144	-0.837074
1	-0.780133	-1.643054	-0.838869
1	-2.352669	-2.243471	-0.240302
1	-2.228957	-1.516951	-1.866324
6	-4.003335	0.377611	-0.092262
6	-4.822459	-0.654093	0.398564
6	-4.584262	1.57943	-0.528677
6	-6.205655	-0.483365	0.447572
1	-4.389965	-1.584976	0.751652
6	-5.971179	1.742761	-0.480446
1	-3.958042	2.380249	-0.906982
6	-6.781128	0.713828	0.006064
1	-6.833428	-1.282778	0.828784
1	-6.414761	2.672596	-0.82253
1	-7.858634	0.842672	0.043907
8	2.981645	-0.892252	1.145838
6	3.203654	-1.197467	2.526442
1	3.979662	-1.962793	2.630293
1	3.534961	-0.270743	2.99429
1	2.276836	-1.53955	2.9981
1	1.834032	-1.976107	-3.040252

TS_{IVb-r} 4

E = -4217.898860 ZPVE = 0.286121 NIMAG = 1.

17	-0.866076	-0.816931	-1.480932
15	-1.310204	0.028563	0.783182

12	1.247955	-1.169779	-0.3202
35	3.371668	-2.381563	-0.327994
5	-0.620293	-1.40962	1.950623
1	0.391056	-1.870627	1.440339
1	-0.358038	-0.837659	2.978564
1	-1.461919	-2.257824	2.051562
6	1.203794	0.874625	0.480454
6	1.90092	0.891795	1.70782
6	1.459999	1.950193	-0.406945
6	2.826193	1.887809	2.038424
6	2.388235	2.957501	-0.094985
6	3.065377	2.918144	1.127213
1	3.354731	1.854651	2.986588
1	2.588885	3.768514	-0.785244
1	3.777723	3.704082	1.362749
6	-1.377791	1.765924	1.398475
1	-0.533493	1.915669	2.068789
1	-1.305604	2.482474	0.577829
1	-2.328698	1.904736	1.920523
6	-3.091623	-0.194681	0.33764
6	-3.862375	0.881237	-0.139585
6	-3.702848	-1.452026	0.488402
6	-5.215504	0.708626	-0.434942
1	-3.417313	1.858359	-0.292861
6	-5.059124	-1.618106	0.202593
1	-3.125639	-2.300351	0.835471
6	-5.819303	-0.540124	-0.259542
1	-5.795685	1.550096	-0.801257
1	-5.518632	-2.59241	0.338832
1	-6.873248	-0.672512	-0.484686

8	0.751274	1.949122	-1.578192
6	0.992886	2.973057	-2.544018
1	2.034893	2.962664	-2.883429
1	0.335479	2.746064	-3.383774
1	0.746447	3.964214	-2.146116
1	1.719836	0.102574	2.432815

PC_{IVb-r} 4

E = -4218.042832 ZPVE = 0.289617 NIMAG = 0.

17	-2.281279	-3.497761	0.716709
15	1.199913	0.247902	-1.237185
12	-1.863569	-1.38163	-0.144539
35	-3.535874	0.375785	-0.666076
5	0.060841	-1.251792	-1.760487
1	0.05827	-2.063973	-0.85975
1	-1.032205	-0.768989	-1.985293
1	0.514521	-1.729721	-2.765937
6	0.41597	1.46483	-0.109103
6	0.54885	2.848305	-0.314756
6	-0.336953	1.037589	0.996935
6	-0.022982	3.765425	0.56811
6	-0.923193	1.942048	1.878057
6	-0.755158	3.311152	1.666806
1	0.098726	4.829063	0.391822
1	-1.517031	1.582825	2.710678
1	-1.210694	4.01801	2.352692
6	1.693883	1.186522	-2.731719
1	0.805502	1.605486	-3.211287

1	2.407039	1.980482	-2.502228
1	2.163008	0.475982	-3.416458
6	2.754666	-0.286631	-0.4323
6	3.491057	0.583503	0.388036
6	3.237542	-1.581664	-0.679234
6	4.69617	0.160952	0.952936
1	3.127525	1.585809	0.593111
6	4.445531	-1.998273	-0.113741
1	2.674169	-2.265157	-1.306096
6	5.174666	-1.129209	0.702556
1	5.258026	0.837994	1.589162
1	4.811249	-3.001765	-0.308373
1	6.110681	-1.456281	1.145169
8	-0.531693	-0.338429	1.165205
6	-0.146072	-0.899847	2.457126
1	-0.818779	-0.543864	3.238976
1	-0.239052	-1.979382	2.350646
1	0.886199	-0.618376	2.670622
1	1.109794	3.22051	-1.164056

R1v + b S_N2@P-f pathway 2 in THF

RC_{v_b-r} 2

E = -4026.216045 ZPVE = 0.231651 NIMAG = 0.

17	2.24689	-1.214253	1.579392
15	2.9769	-1.414531	-0.367944
12	-2.092252	0.107343	-0.453253
35	-3.634236	-1.769849	-0.251998
6	3.381407	0.304139	-0.827296
1	2.464123	0.895582	-0.877011

1	4.074353	0.750925	-0.111018
1	3.843279	0.282536	-1.819477
6	4.573383	-2.260909	-0.111519
1	5.068571	-2.340564	-1.084362
1	5.209642	-1.703848	0.579504
1	4.392479	-3.265682	0.276495
5	1.746166	-2.32519	-1.538785
1	0.774744	-1.614631	-1.651168
1	2.408081	-2.383161	-2.558398
1	1.529962	-3.409059	-1.04801
6	-0.877946	1.786534	-0.90185
6	-0.310011	2.646157	-1.849453
6	-0.557504	2.062185	0.43418
6	0.5274	3.712779	-1.474156
6	0.264591	3.101715	0.864819
6	0.811007	3.935252	-0.124979
1	0.955843	4.36431	-2.231688
1	0.486761	3.279063	1.91201
1	1.456572	4.757807	0.170261
8	-1.181505	1.138216	1.300326
6	-0.995687	1.24042	2.716232
1	-1.571624	0.429214	3.160718
1	0.06237	1.12606	2.972249
1	-1.366912	2.202934	3.082951
1	-0.512212	2.495972	-2.909139

TS_{vb-r} 2

E = -4026.159871 ZPVE = 0.232783 NIMAG = 1.

17	0.530333	-1.813807	1.504536
15	1.591903	-1.552221	-0.586328
12	-1.118738	-0.56882	0.137147
35	-3.534894	-0.209855	0.140879
6	3.051558	-0.487135	-0.973225
1	2.782471	0.266103	-1.712192
1	3.382833	0.012625	-0.059143
1	3.859245	-1.13051	-1.334853
6	2.565868	-3.071662	-0.125416
1	3.105016	-3.3719	-1.032045
1	3.291394	-2.867978	0.666469
1	1.902096	-3.879786	0.180239
5	0.223863	-2.156708	-1.87351
1	-0.848071	-1.624444	-1.598839
1	0.587131	-1.799181	-2.966806
1	0.164286	-3.350181	-1.726355
6	0.546556	0.727017	-0.481225
6	0.215028	1.191662	-1.772925
6	0.98442	1.706619	0.44745
6	0.279486	2.54173	-2.133424
6	1.052184	3.067468	0.105644
6	0.698316	3.474963	-1.183576
1	0.003456	2.857636	-3.135027
1	1.376945	3.810343	0.82459
1	0.758598	4.528963	-1.44034
8	1.339991	1.245933	1.684725
6	1.721396	2.17927	2.697166
1	1.918559	1.581928	3.58762
1	2.628951	2.725319	2.41594
1	0.913879	2.890022	2.906008

1 -0.102973 0.476338 -2.527077

PC_{vb-r} 2

E = -4026.295374 ZPVE = 0.235475 NIMAG = 0.

17 4.897 1.409503 -1.031054
15 -0.722566 1.263137 0.070356
12 3.081389 0.244722 -0.210744
35 2.429352 -1.801 1.002911
6 -1.513905 2.912894 -0.020412
1 -1.733741 3.14139 -1.06608
1 -2.433099 2.936728 0.565048
1 -0.808346 3.656676 0.359927
6 -0.459564 0.907602 1.847933
1 0.149075 1.710134 2.274905
1 -1.415072 0.853079 2.37124
1 0.080311 -0.037608 1.945687
5 0.95766 1.337289 -0.913686
1 1.29187 0.205263 -1.216542
1 0.822382 2.005931 -1.9036
1 1.730667 1.878619 -0.132457
6 -1.894689 0.0285 -0.589364
6 -1.503051 -0.805026 -1.646725
6 -3.202224 -0.109868 -0.062784
6 -2.372967 -1.759494 -2.178371
6 -4.077234 -1.06468 -0.595508
6 -3.655522 -1.885524 -1.645159
1 -2.046917 -2.396982 -2.993359
1 -5.077397 -1.179622 -0.196781

1	-4.343248	-2.624785	-2.044848
8	-3.530491	0.723089	0.964134
6	-4.847028	0.658898	1.525171
1	-4.871862	1.425245	2.299441
1	-5.606577	0.876875	0.767295
1	-5.035374	-0.322219	1.972977
1	-0.504454	-0.709973	-2.05655