Supporting Information

A Computational Study of Activation of Allenoates by Lewis Bases and Reactivity of Intermediate Adducts

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1 Assessment of performance of M06-2X

The reaction of trimethylphosphine with methyl allenoate yielding the $PMe_3 \cdot$ allenoate adduct is used to evaluate the accuracy of the chosen computational method (Figure S1). The M06-2X/6-31+G* method was used to optimize all geometries discussed in this paper. Additional single point calculations with the optimized geometries employing more sophisticated methods, M06-2X/6-311++G**, CCSD(T)/6-31+G* and CCSD(T)/6-311++G**, were done to obtain more reliable values for the electronic properties of the discussed structures. The M06-2X/6-311++G**//M06-2X/6-31+G* calculations show that the size of the basis set has only a small influence on the relative electronic energies of the discussed reaction (Figure S1). The range of energy difference is between 0.1 and 1.9 kcal mol^{-1}. The influence of the chosen correlation method is also small as the comparison of the M06-2X results with those obtained from CCSD(T) calculations shows. The M06-2X energies are up to 3 kcal mol^{-1} lower than the CCSD(T) energies, but the two methods show the same chemical trend.
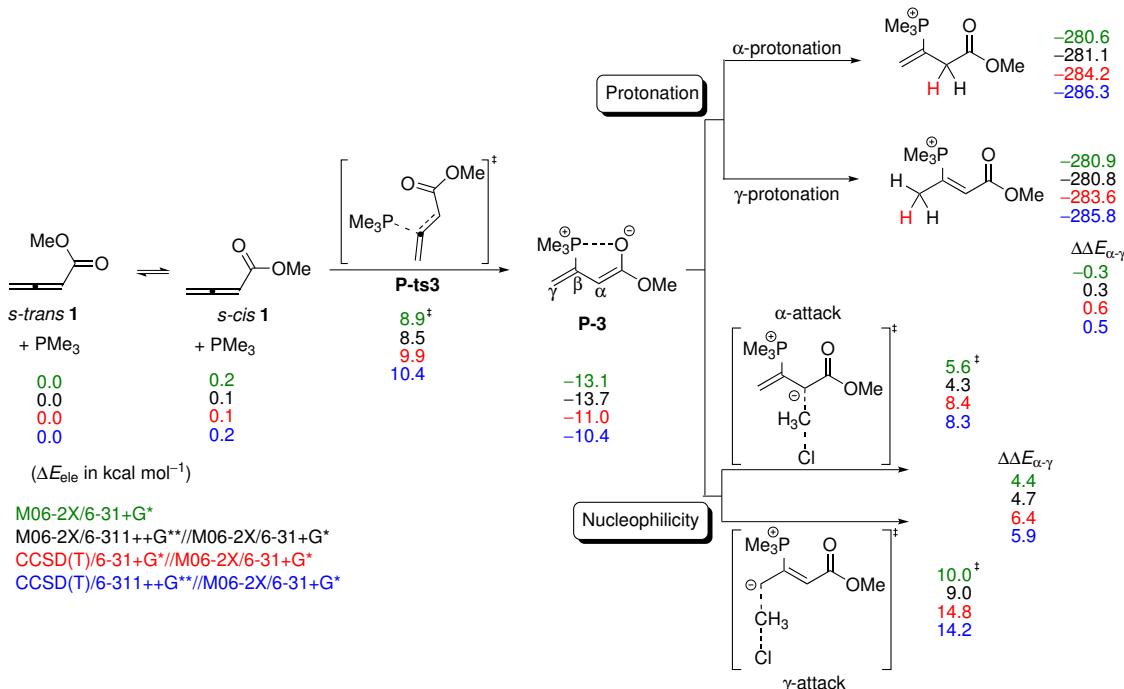
Figure S1: Evaluation of the M06-2X and CCSD(T) methods for the addition of PMe_3 to methyl allenoate. The electronic energies, ΔE_{ele} in kcal mol^{-1}, are realtive to separated reactants.

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The α- and γ-carbon atoms in $PMe_3 \cdot$ allenoate have both basic and nucleophilic properties. The protonated α- and γ-adducts differ less than 1 kcal mol^{-1} in energy, and hence the C_α and C_γ atoms have similar proton affinities (Figure S1). However, the barrier for the nucleophilic attack of C_α at the carbon atom of CH_3Cl is 4 to 5 kcal mol^{-1} lower in energy than that for the corresponding reaction of C_γ, which indicates that C_α is significantly more nucleophilic than C_γ. The M06-2X data are qualitatively reproduced by the high level CCSD(T) calculations displaying the same reactivity.

Similar tests for the addition of the allenoate to pyridine **Py**, 1,3-dimethylimidazolin-2-ylidene **IMe** and 1,4-diazabicyclo[2.2.2]octane **Dabco** (Figure S2) show that the CCSD(T) calculations essentially reproduce the M06-2X data with a maximum error of 3 kcal mol^{-1} in ΔE_{ele} while predicting the same chemical reactivity. Hence, the less expensive M06-2X/6-31+G* method was used for calculations discussed in this study.
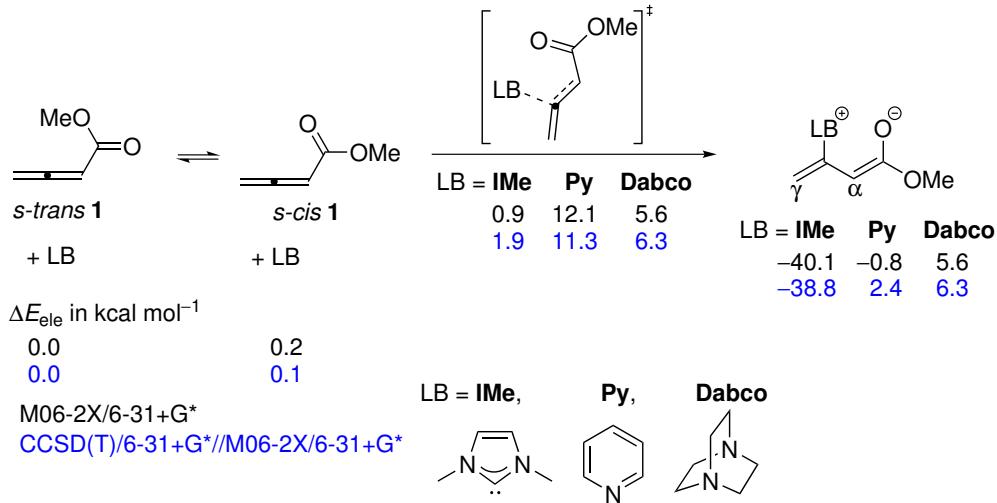
Figure S2: Addition of pyridine (**Py**), 1,3-dimethylimidazolin-2-ylidene (**IMe**) and DABCO (**Dabco**) to methyl allenoate calulated at the M06-2X and CCSD(T) levels. The electronic energies, ΔE_{ele} in kcal mol^{-1}, are relative to separated reactants.

2 Addition of Lewis bases to *s-trans* methyl allenoate

Figure S3 shows the mechanism of the addition of the Lewis base to *s-trans* methyl allenoate **1**. Table S1 summarizes the barriers of the *Z/E*-type addition and the energies of the forming adducts. The addition to *s-trans* **1** is less favorable than that to *s-cis* **1** (Scheme 2 and Table 1 in the main text).
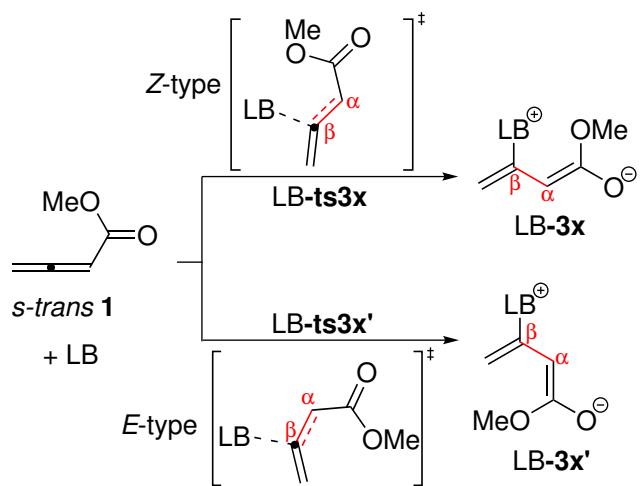
Figure S3: Addition of the Lewis base to *s-trans* methyl allenoate. LB-**ts3x** and LB-**3x** are the *Z*-type structures, and LB-**ts3x′** and LB-**3x′** are the *E*-type structures.

	Z-type addition		E-type addition	
	LB-**ts3x**	LB-**3x**	LB-**ts3x**′	LB-**3x**′
LB = NHC				
IMe	17.3 [3.3]	−18.5 [−32.6]		
IPr	18.8 [3.8]	−14.4 [−30.7]	17.0 [1.1]	−14.0 [−28.7]
phosphine				
Pbu	22.8 [8.4]	9.6 [−6.8]		
Pph	26.0 [9.8]	16.6 [−1.2]	28.9 [13.1]	17.2 [2.4]
Hmpt	28.3 [14.1]	6.5 [−7.0]	29.1 [15.5]	9.8 [−3.9]
amine				
Quin	23.5 [9.6]	23.0 [7.7]	24.5 [10.2]	21.9 [7.1]
Dabco	24.0 [10.9]	23.4 [9.5]	24.0 [11.5]	22.5 [9.0]
aza-heterocycle				
Dmap	24.1 [11.0]	14.7 [0.4]	25.3 [12.6]	16.5 [2.7]
Py	25.5 [13.2]	18.9 [5.5]	28.6 [15.4]	22.3 [8.5]
Dbu	21.1 [7.3]	4.6 [−10.2]	22.5 [8.4]	8.5 [−5.8]
Mtbd	26.4 [11.6]	7.8 [−7.4]	22.7 [9.5]	12.3 [−1.6]

Table S1: Free energies and enthalpies (ΔG [ΔH] in kcal mol^{-1}) for the addition of the Lewis bases to *s-trans* **1**. All energies are relative to the separated Lewis bases and methyl allenoate **1**.

3   Electrostatic potential surface maps for the addition of LBs to *s-cis* **1**

Figure S4 shows electrostatic potential surface maps for the transition states (TSs) and the adducts in the addition of **Pph** and **Hmpt** to *s-cis* **1**. The P⋯O distance in the *Z*-type TSs is closer than that in in the *E*-type TSs, which suggests stronger electrostatic interactions in the *Z*-type structures. The carbonyl oxygen atom rests on the top of the phenyl ring or the dimethylamino group in the *E*-type TSs, and interacts therefore less with the P atom.

Pph-ts3
24.2 [9.9]‡
P⋯O: 3.18 Å

Pph-3
9.7 [−5.8]
P⋯O: 2.65 Å

Pph-ts3'
28.3 [13.0]‡
P⋯O: 3.25 Å

Pph-3'
14.4 [0.2]
P⋯O: 4.66 Å

−0.10   0.00   0.15

Hmpt-ts3
25.6 [11.9]‡
P⋯O: 3.34 Å

Hmpt-3
3.8 [−13.2]
P⋯O: 2.86 Å

Hmpt-ts3'
28.6 [14.3]‡
P⋯O: 4.39 Å

Hmpt-3'
8.0 [−6.3]
P⋯O: 4.68 Å
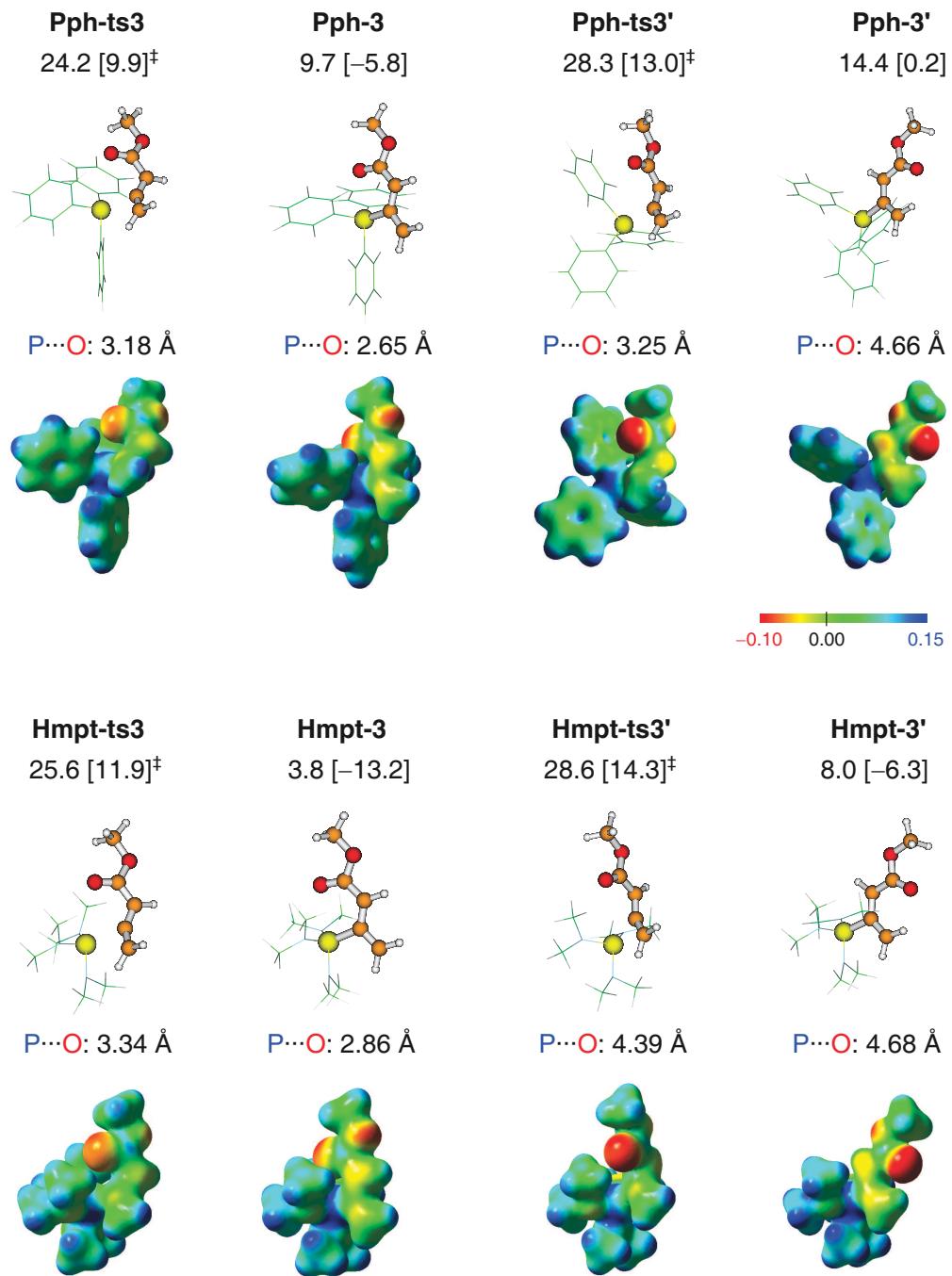
Figure S4: *Z*/*E*-type transition structures (LB-**ts3**/LB-**ts3**′) and adducts (LB-**3**/LB-**3**′) for the the addition of **Pph** and **Hmpt** to *s-cis* **1**. Electrostatic potential is mapped onto the total electron density with the isosurface of 0.02.

The structures for the addition of **Dabco** to **1**, as shown in Figure S5, reveal that the carbonyl oxygen atom interacts with two methylene groups ($-CH_2-$) of **Dabco** in the *Z*-type addition, and with one methylene group in the *E*-type addition. The barrier for the rotation of the ester is 1.5 kcal mol^{-1} higher than that for the the *E*-type addition of **Dabco** to the allenoate. The two-step addition process was also observed in the case of **Quin**. Hence, only the activation energies of the rate-determining TSs are listed for **Dabco** and **Quin** in Table 1 of the main text.

Dabco-ts3
21.4 [8.3]‡

Dabco-3
14.8 [0.6]

−0.10   0.00   0.15

Dabco-ts3i'
22.1 [9.6]‡

Dabco-3i'
21.8 [8.7]

Dabco-ts3'
23.6 [9.4]‡
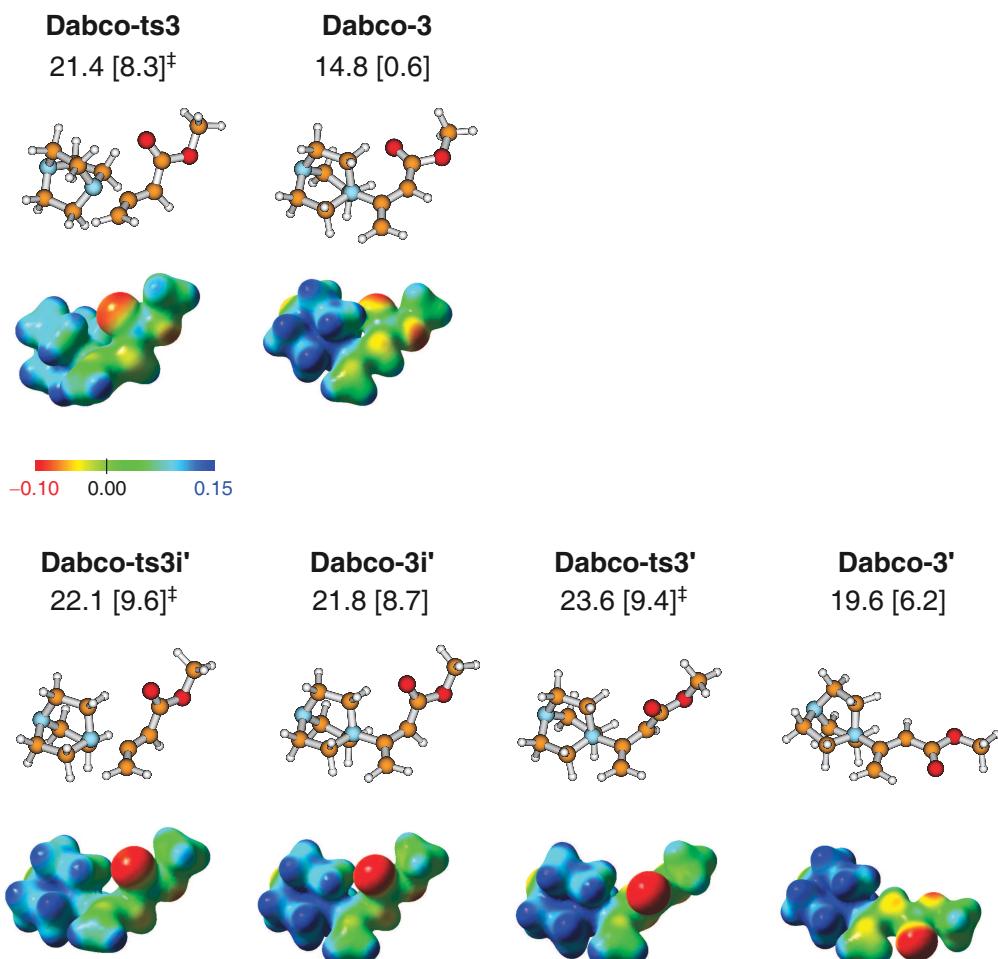
Dabco-3'
19.6 [6.2]

Figure S5: *Z*/*E*-type transition structures (LB-**ts3**/LB-**ts3**′) and adducts (LB-**3**/LB-**3**′) for the the addition of **Dabco** to *s-cis* **1**. Electrostatic potential is mapped onto the total electron density with the isosurface of 0.02.

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Figure S6 shows geometries for the addition of **Dmap/Mtbs** to *s-cis* **1** and electrostatic potential surface maps. The carbonyl oxygen atom in **1** is oriented towards the pyridine ring in the *Z*-type structures (**Dmap-ts3** and **Dmap-3**), but points away from the pyridin ring in **Dmap-ts3**′ and **Dmap-3**′. The carbonyl oxygen atom points towards the guanidine carbon atom in **Mtbd-ts3**, and towards the methyl group in **Mtbd-ts3**′. All of the *Z*-type TSs have favorable electrostatic interactions between the carbonyl oxygen atom and the LBs, stabilizing the structures.

| **Damp-ts3** | **Damp-3** | **Damp-ts3'** | **Damp-3'** |
| 22.6 [9.9]‡ | 9.3 [−3.9] | 24.7 [12.2]‡ | 14.6 [0.9] |

−0.10   0.00   0.15

| **Mtbd-ts3** | **Mtbd-ts3** | **Mtbd-ts3'** | **Mtbd-ts3'** |
| 20.5 [5.8]‡ | 0.3 [−15.4] | 22.3 [8.7]‡ | 9.6 [−3.3] |
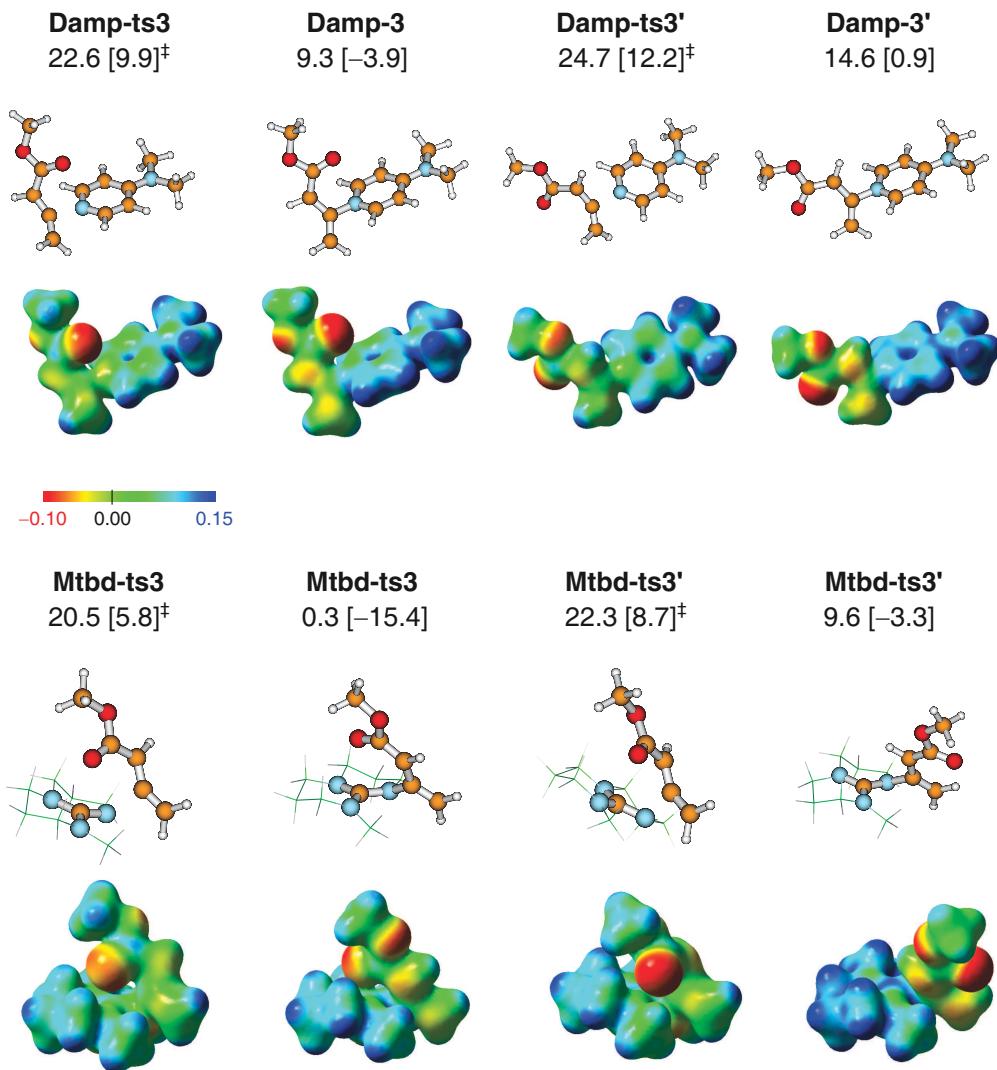
Figure S6: *Z/E*-type transition structures (LB-**ts3**/LB-**ts3**′) and adducts (LB-**3**/LB-**3**′) for the the addition of **Dmap** and **Mtbd** to *s-cis* **1**. Electrostatic potential is mapped onto the total electron density with the isosurface of 0.02.

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4 Solvent effect

Table S2 lists the free energies and enthalpies of selected stationary points in the addition of the four Lewis Bases, **IPr**, **Pph**, **Dabco** and **Dmap** to *s-cis* **1** in five different solvents. The computed dipole moments of the TSs and adducts optimized using the IEFPCM model are listed in Table S3. The dipole moment is larger in the *E*-type structures than that in the corresponding *Z*-type ones.

	vacuum $\varepsilon = 1$	toluene 2.4	CHCl$_3$ 4.7	THF 7.4	CH$_2$Cl$_2$ 8.9	MeCN 35.7
IPr-ts3	17.7 [3.3]	19.2 [4.6]	19.7 [5.3]	20.4 [5.7]	20.5 [5.8]	20.4 [5.8]
IPr-ts3′	17.1 [2.3]	18.6 [3.1]	19.2 [3.6]	19.3 [3.8]	19.3 [3.6]	19.4 [4.3]
IPr-3	−21.3 [−36.3]	−20.7 [−36.3]	−21.0 [−36.4]	−20.7 [−36.5]	−20.6 [−36.6]	−20.3 [−36.6]
IPr-3′	−17.2 [−30.9]	−19.3 [−32.9]	−21.3 [−34.8]	−21.1 [−36.6]	−22.3 [−36.0]	−22.7 [−37.3]
Pph-ts3	24.2 [9.0]	24.6 [9.4]	24.4 [9.5]	24.2 [9.5]	22.8 [8.8]	22.8 [8.7]
Pph-ts3′	28.3 [13.0]	25.9 [11.8]	26.6 [11.2]	26.3 [10.8]	26.0 [10.7]	25.2 [10.2]
Pph-3	9.7 [−5.8]	8.8 [−6.5]	8.3 [−7.0]	8.2 [−7.3]	7.9 [−7.4]	7.6 [−7.9]
Pph-3′	14.4 [0.2]	11.5 [−3.1]	9.8 [−4.9]	9.1 [−5.7]	8.6 [−5.9]	7.5 [−7.0]
Dabco-ts3	21.4 [8.3]	21.6 [7.1]	19.6 [7.3]	19.6 [7.3]	19.6 [7.2]	19.1 [7.0]
Dabco-ts3′	23.6 [9.4]	21.8 [7.6]	18.3 [7.4]	19.1 [7.2]	19.0 [7.2]	18.7 [6.8]
Dabco-3	14.8 [0.6]	13.8 [−1.5]	11.6 [−1.9]	11.2 [−2.3]	11.0 [−2.4]	10.5 [−2.9]
Dabco-3′	19.6 [6.2]	15.3 [0.5]	11.5 [−1.5]	10.3 [−2.7]	10.0 [−3.0]	8.4 [−4.5]
Dmap-ts3	22.6 [9.9]	22.6 [9.9]	22.3 [9.7]	22.0 [9.6]	21.8 [9.5]	22.1 [9.3]
Dmap-ts3′	24.7 [12.2]	23.0 [10.5]	23.0 [10.5]	22.9 [10.3]	22.9 [10.3]	22.7 [10.0]
Dmap-3	9.3 [−3.9]	7.4 [−6.6]	6.2 [−8.0]	5.5 [−8.6]	5.3 [−8.8]	4.2 [−9.6]
Dmap-3′	14.6 [0.9]	9.2 [−4.6]	7.0 [−7.8]	5.2 [−8.3]	4.9 [−8.7]	3.6 [−10.0]

The stcutures with considering solvent effects were optimized in the IEFPCM model, rather than single-point caculations on the gas-optimized geometries.

Table S2: Solvent effect on free energies and enthalpies (ΔG [ΔH] in kcal mol^{-1}) for the addition of the four Lewis bases, **IPr**, **Pph**, **Dabco** and **Dmap**, to *s-cis* **1**.

	vacuum	toluene	CHCl$_3$	THF	CH$_2$Cl$_2$	MeCN
	$\varepsilon = 1$	2.4	4.7	7.4	8.9	35.7
IPr-ts3	3.40	4.21	4.99	5.26	5.36	7.03
IPr-ts3$'$	4.89	5.74	6.37	6.61	6.68	7.40
IPr-3	6.26	7.57	8.44	8.91	9.06	9.73
IPr-3$'$	9.58	11.49	12.75	13.43	13.65	14.65
Pph-ts3	3.95	4.69	5.16	5.39	5.79	6.14
Pph-ts3$'$	5.71	6.44	6.91	7.05	7.09	7.31
Pph-3	5.73	7.03	7.82	8.20	8.33	8.87
Pph-3$'$	10.44	12.35	13.41	13.91	14.07	14.72
Dabco-ts3	3.97	4.59	4.87	5.04	5.10	5.34
Dabco-ts3$'$	5.46	5.67	5.71	5.72	5.82	8.72
Dabco-3	5.88	6.95	7.56	7.84	7.93	8.31
Dabco-3$'$	9.77	11.17	11.88	12.18	12.27	12.62
Dmap-ts3	7.11	8.24	8.70	8.90	9.29	9.59
Dmap-ts3$'$	10.53	11.13	11.40	11.51	11.55	11.71
Dmap-3	10.51	12.32	13.24	13.63	13.75	14.24
Dmap-3$'$	14.42	17.93	19.16	19.68	19.85	20.48

Table S3: Computed dipole moments (unit in Debye) for the transition states and adducts in five different solvents.

5 Protonation and nucleophilicity

Figure S7 shows the mechanism of α/γ-protonation of the *E*-type adducts LB-**3**′ and the S_N2 reaction with CH_3Cl. Table S4 summarizes proton affinities and the barrier heights for the α/γ-attack of LB-**3**′ on CH_3Cl. The C_γ atom usually has a higher proton affinity than C_α. However, the α-carbon is more nucleophilic than C_γ, as revealed by the lower barriers for the α-attack.

Tables S5 and S6 show the charges and the contributions of C_α and C_γ to the HOMO π-orbital in LB-**3**. Both the charges on and orbital coefficients of C_α are larger than those of C_γ.
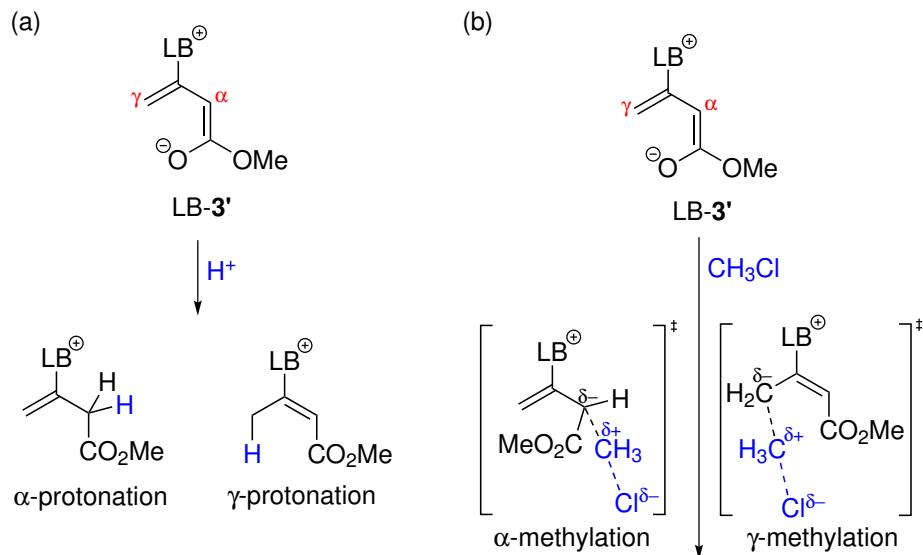
Figure S7: Protonation and methylation for the α- and γ-carbon atoms of the *E*-type adducts, LB-**3**′.

	proton affinity (ΔH)		methylation ($\Delta G^{\ddagger}$)	
LB-**3**′	C_α	C_γ	C_α	C_γ
LB = NHC				
IMe	*xx*	*xx*	*xx*	*xx*
IPr	275.4	277.9	10.0	13.2
phosphine				
Pbu	*xx*	*xx*	*xx*	*xx*
Pph	270.4	271.0	42.8	45.9
Hmpt	268.3	268.4	36.1	39.5
amine				
Quin	266.9	266.6	49.0	52.1
Dabco	264.8	264.5	49.8	53.2
aza-heterocycle				
Dmap	266.7	269.9	41.7	45.2
Py	259.6	262.3	50.2	52.9
Dbu	275.5	273.2	33.8	36.5
Mtbd	275.1	277.7	34.7	41.1

Table S4: Proton affinities calculated according to the formula, $\Delta H = (H^{298}_{\text{LB-}\mathbf{3}'} + H^{298}_{\text{proton}}) - H^{298}_{\text{LB-}\mathbf{3}'\text{-H}}$ where $\Delta H^{298}_{\text{proton}}$ is equal to 1.5 kcal mol^{-1}. The activation free energies, $\Delta G^{\ddagger}$ in kcal mol^{-1}, for the the S_N2 attack on MeCl are reported relative to the separated reactants, Lewis bases and allenoates.

LB · allenoate	Hirshfeld charge with H		Hirshfeld charge withouth H	
	C_α	C_γ	C_α	C_γ
LB = NHC				
IMe	−0.15	−0.13	−0.18	−0.17
IPr	−0.14	−0.09	−0.17	−0.14
phosphine				
Pbu	−0.14	−0.09	−0.17	−0.14
Pph	−0.14	−0.08	−0.17	−0.14
Hmpt	−0.14	−0.09	−0.17	−0.14
amine				
Quin	−0.15	−0.11	−0.18	−0.17
Dabco	−0.15	−0.11	−0.18	−0.17
aza-heterocycle				
Dmap	−0.16	−0.14	−0.19	−0.18
Py	−0.16	−0.12	−0.18	−0.17
Dbu	−0.15	−0.14	−0.18	−0.17
Mtbd	−0.16	−0.12	−0.18	−0.17

Table S5: Hirshfeld atomic charges on the C_α and C_γ in LB-**3** with and without summing the attached hydrogen atoms.

LB · allenoate	HOMO coefficient	
	C_α	C_γ
LB = NHC		
IMe	0.13	−0.10
IPr	0.13	−0.08
phosphine		
Pbu	0.14	−0.09
Pph	0.15	−0.10
Hmpt	0.14	−0.08
amine		
Quin	0.14	−0.09
Dabco	0.14	−0.09
aza-heterocycle		
Dmap	0.13	−0.09
Py	0.14	−0.09
Dbu	0.13	−0.09
Mtbd	0.13	−0.09

Table S6: HOMO-orbital contributions on the C_α and C_γ atoms in LB-**3**.

6 [3 + 2] cycloadditions with ethylene 2a

The adducts, LB-**3** and LB-**3**′, react with ethylene **2a** to form five-membered rings with exocyclic C=C bonds or ylidic bonds. Free energies and enthalpies for the [3 + 2] cycloaddition are listed in Table S7. The formation of the [3+2] intermediates obtained with the NHCs, phosphines and aza-arenes is exergonic.

	[3+2] cycloaddition starting from LB-**3**			[3+2] cycloaddition starting from LB-**3**′		
	LB-**3** + **2a**	LB-**ts4a**	LB-**4a**	LB-**3**′ + **2a**	LB-**ts4a**′	LB-**4a**′
LB = NHC						
IMe	−23.3 [−38.0]	10.6 [−17.4]	−44.1 [−72.6]			
IPr	−21.3 [−36.3]	10.8 [−19.2]	−49.9 [−80.5]	−17.2 [−30.9]	9.9 [−19.1]	−52.1 [−82.5]
phosphine						
Pbu	1.4 [−13.9]	31.7 [3.6]	−12.9 [−40.2]			
Pph	9.7 [−5.8]	40.1 [11.2]	−6.6 [−36.5]	14.4 [0.2]	42.4 [14.5]	−8.5 [−39.3]
Hmpt	3.8 [−13.2]	33.1 [4.3]	−15.7 [−45.9]	8.0 [−6.3]	35.1 [7.9]	−15.4 [−44.1]
amine						
Quin	14.8 [−1.0]	49.0 [20.4]	13.4 [−16.3]	19.0 [4.2]	51.0 [22.5]	14.1 [−14.7]
Dabco	14.8 [0.6]	49.2 [22.1]	13.5 [−14.8]	19.6 [6.2]	51.6 [24.5]	14.1 [−13.1]
aza-heterocycle						
Dmap	9.9 [−3.9]	45.4 [18.7]	−3.0 [−31.0]	14.6 [0.9]	46.2 [19.5]	−2.6 [−30.0]
Py	15.4 [1.3]	47.3 [20.8]	−10.9 [−38.0]	20.1 [6.5]	48.5 [21.9]	−10.3 [−37.6]
Dbu	−1.0 [−16.6]	36.4 [8.3]	8.6 [−21.3]	6.7 [−7.3]	41.3 [14.1]	6.0 [−20.7]
Mtbd	0.3 [−15.4]	39.2 [11.8]	6.3 [−21.8]	9.6 [−3.3]	45.5 [18.8]	11.1 [−17.0]

Table S7: Free energies and enthalpies, ΔG [ΔH] in kcal mol^{-1}, for the [3 + 2] cycloaddition of the adducts (LB-**3** and LB-**3**′) and ethylene **2a**.

7   Cycloadditions with enone 2b

The **Pph-3** adduct reacts with enone **2b** to forms either α- or γ-[3 + 2] ylides, as shown in Figure S8. The γ-[3 + 2] cycloaddition ($\Delta G^{\ddagger}$: 21.6 kcal mol^{-1}) requires a higher activation energy than the α-[3 + 2] addition ($\Delta G^{\ddagger}$: 18.9 kcal mol^{-1}). The energy profiles of the PPh$_3$-catalyzed γ-[3 + 2] and γ-[2 + 4] cyclizations are shown in Figure S9. The γ-[3 + 2] cycloaddition starting with the *E*-type adduct **Pph-3**$'$ is shown in Figure S10. The rate-determining step is the addition of PPh$_3$ to **1** in both γ-[3 + 2] cycloadditions starting from **Pph-3** and **Pph-3**$'$. The free energy of **Pph-ts3** is 24.2 kcal mol^{-1}, and thereby lower than that of **Pph-ts3**$'$, being 28.3 kcal mol^{-1}. Hence, the [3 + 2] cycloaddition starting from **Pph-3** dominates in kinetics.
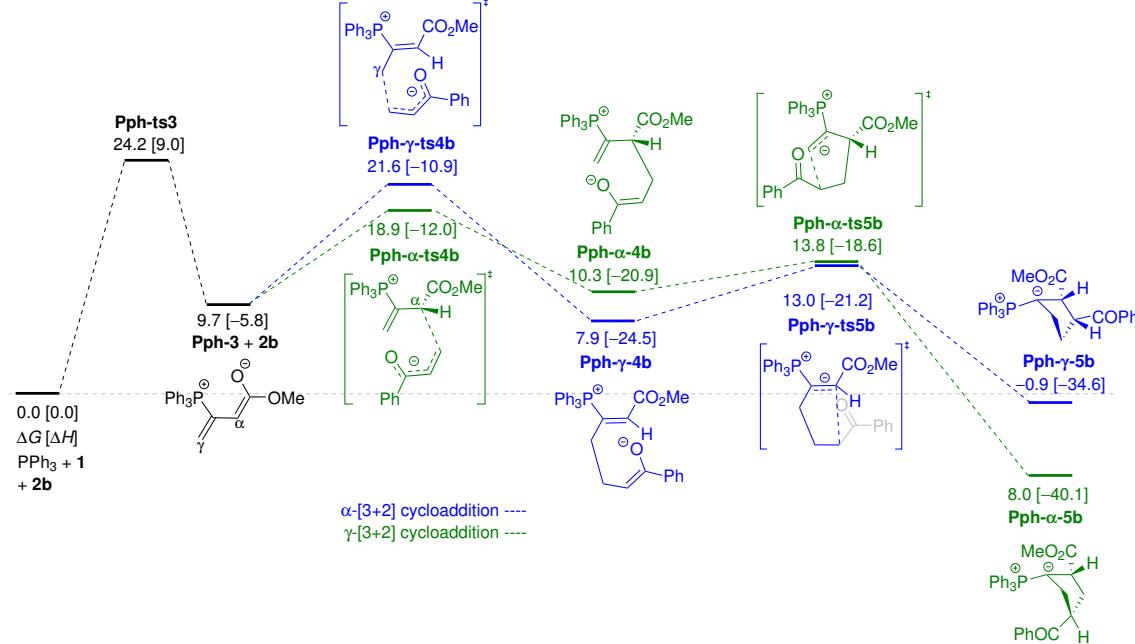
Figure S8: Energy profiles for the PPh$_3$-catalyzed α- and γ-[3 + 2] cycloadditions.
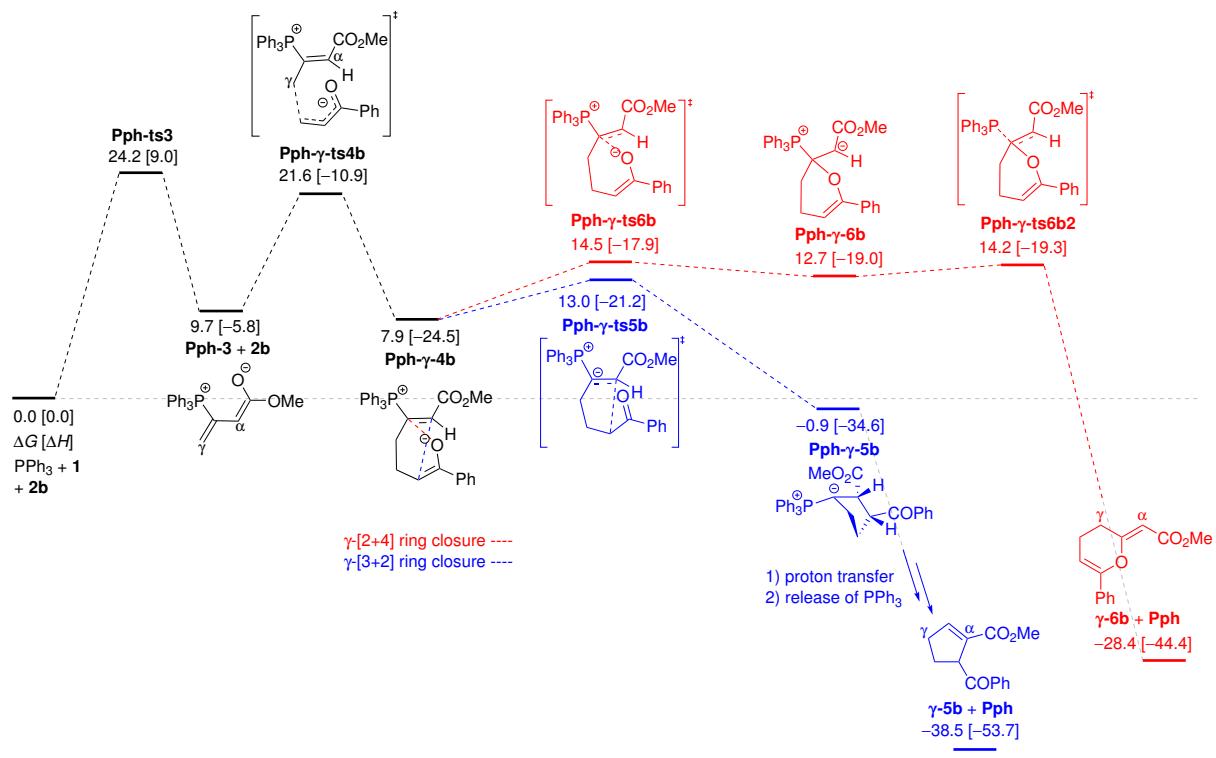
Figure S9: Energy profiles for the PPh$_3$-catalyzed γ-[3 + 2] and γ-[2 + 4] cycloadditions.

19
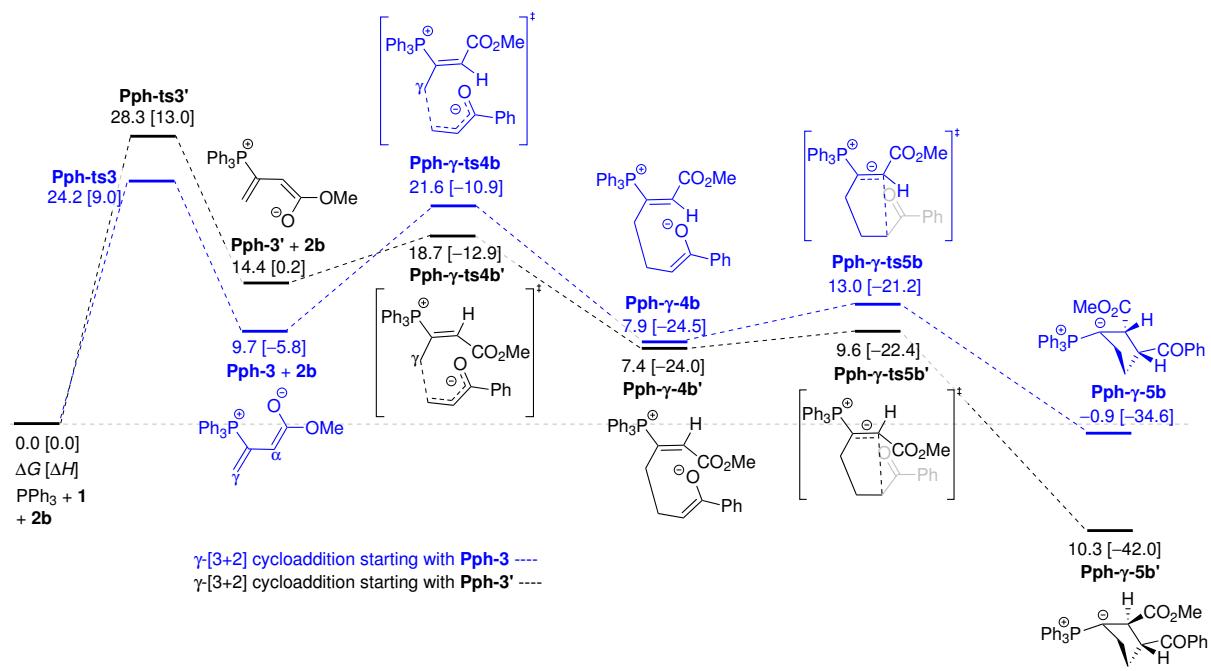
Figure S10: Energy profiles for the PPh$_3$-catalyzed γ-[3 + 2] cycloadditions starting from **Pph-3** and **Pph-3′**.

Figure S11 shows the energy profiles for the γ-[2 + 4] cycloaddition starting from **Dabco-3** and **Dabco-3′**. The formation of **Dabco-3** is more favorable than that of **Dabco-3′**. However, the rate-determining step (rds) is the Michael addition of **Dabco-3/Dabco-3′** to **2b** in the overall reaction. The activation energy of **Dabco-γ-ts4b′**, being 23.8 kcal mol^{-1}, is lower than that of **Dabco-γ-ts4b**, being 25.1 kcal mol^{-1}. The calculations show that the formation of *E*-form dihydropyran products **γ-6b′** is kinetically more favorable, which agrees with experimental observation.[1–4]
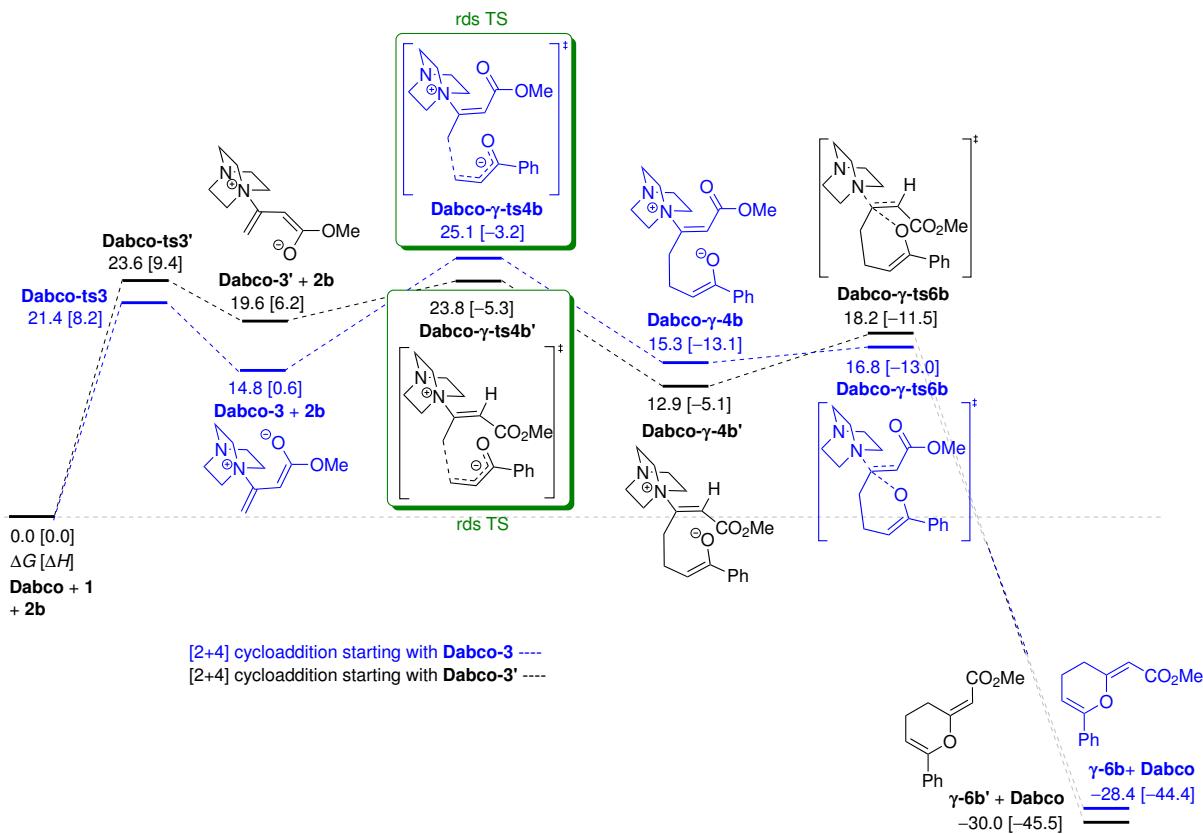
Figure S11: Energy profiles for the DABCO-catalyzed γ-[2 + 4] cycloadditions starting from **Dabco-3** and **Dabco-3′**.

8 Cycloadditions with ketone 2c

Figure S12 shows the energy profiles and mechanism for the DABCO-catalyzed γ-[2 + 2], γ-[3 + 2] and γ-[2 + 2 + 2] cycloadditions of methyl allenoate **1** and ketone **2c**. The highest barrier along the γ-[2 + 2] pathway is 26.2 kcal mol^{-1}. The γ-[2 + 2] pathway is kinetically more favorable than the γ-[3 + 2] and γ-[2 + 2 + 2] pathways with barriers of 35.2 and 28.3 kcal mol^{-1}.
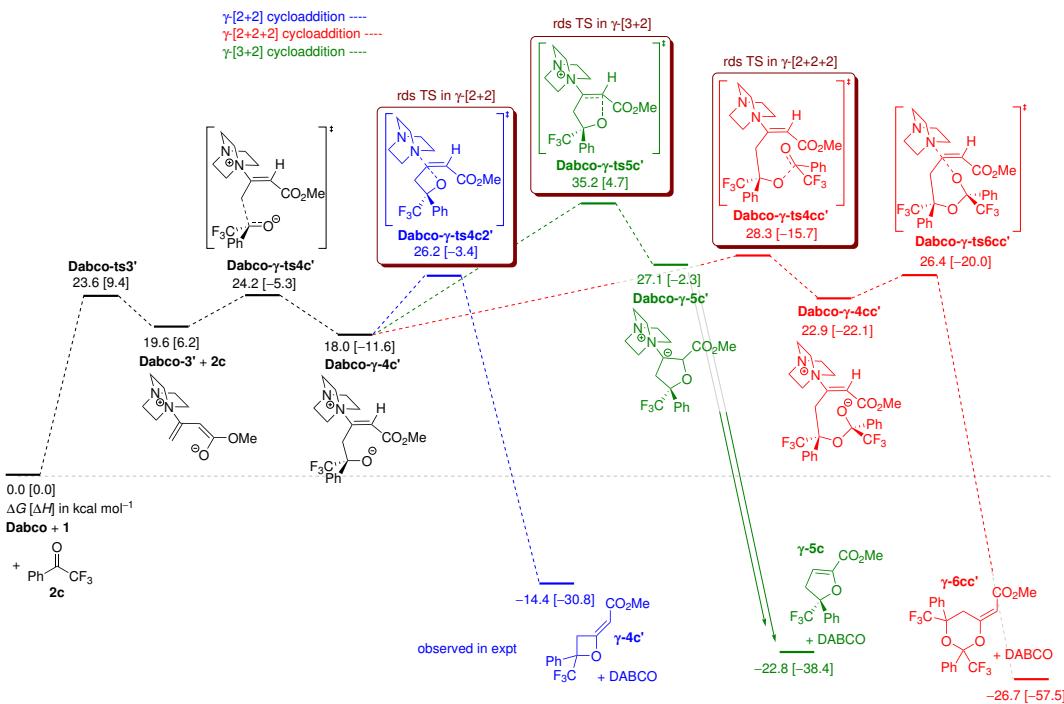
Figure S12: Energy profiles for the DABCO-catalyzed γ-[2 + 2], γ-[3 + 2] and γ-[2 + 2 + 2] cycloadditions of **1** and ketone **2c**.

Figure S13 shows the energy profiles and the mechanism for the NHC-catalyzed γ-[2 + 2], γ-[3 + 2] and γ-[2 + 2 + 2] cycloadditions of methyl allenoate **1** and ketone **2c**. The highest barrier along the γ-[2 + 2] pathway is 5.3 kcal mol^{-1} higher than that along the γ-[2 + 2 + 2] pathway. In regard of the stereochemistry of the [2 + 2 + 2] cycloaddition, the formation of the *trans*-product with the two trifluoromethyl groups on the same sides of the dioxane ring is kinetically more favorable than the formation of the [2 + 2 + 2] *cis*-product (Figure S14).
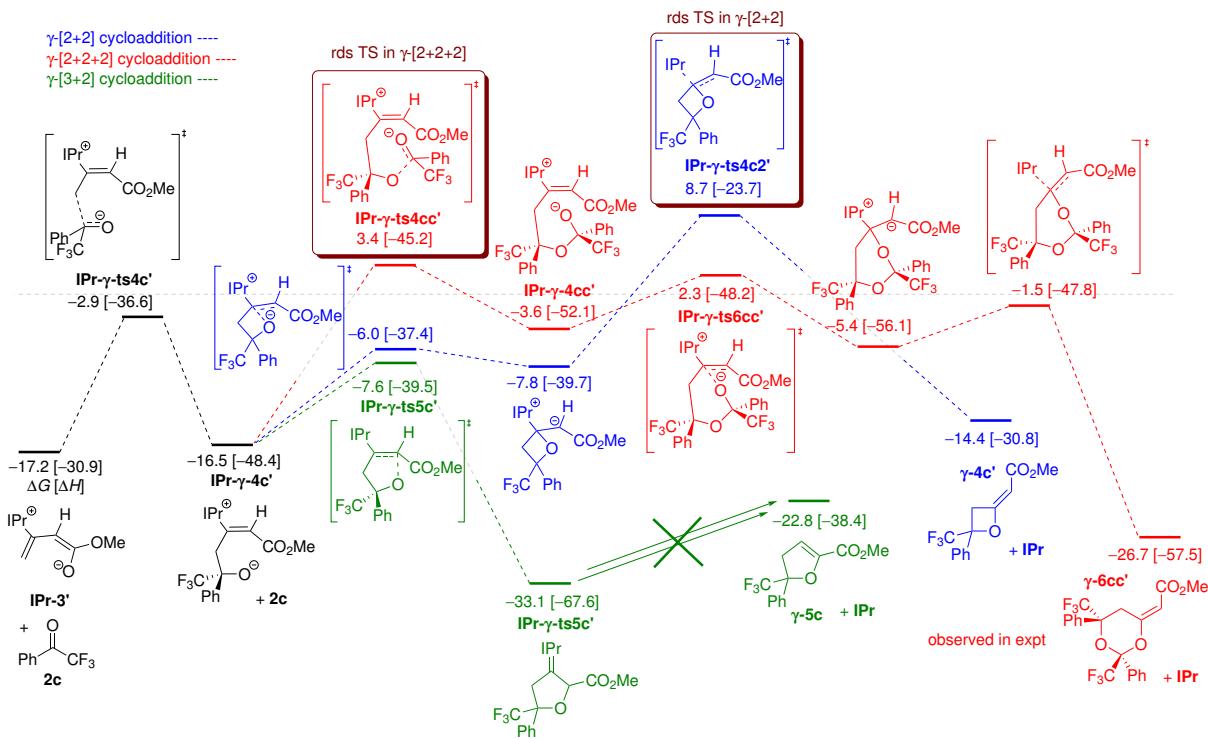
Figure S13: Energy profiles for the **IPr**-catalyzed γ-[2 + 2], γ-[3 + 2] and γ-[2 + 2 + 2] cycloadditions of **1** and ketone **2c**.
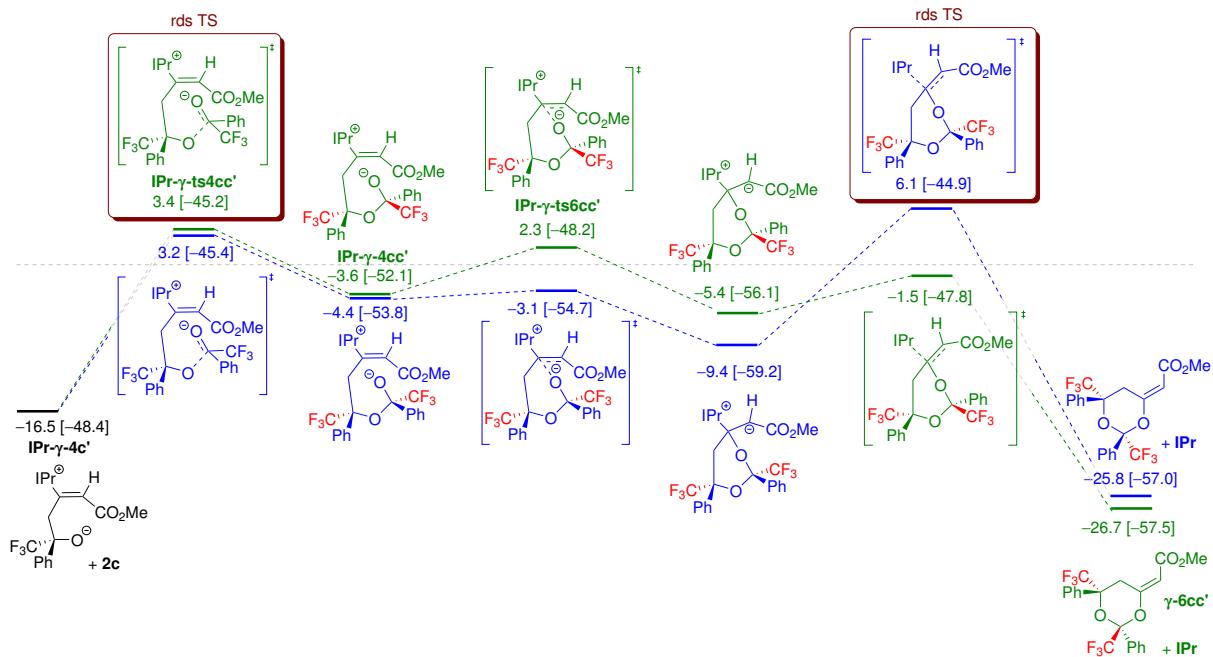
Figure S14: Energy profiles for the **IPr**-catalyzed γ-[2 + 2 + 2] cycloadditions, yielding *trans*- and *cis*-products.

Figure S15 shows the structure of **IPr-γ-5c'**. **IPr** and the trifluoromethyl group block the access to C_α and C_β which might aid the generally unfavorable [1,2] proton transfer.

top view   bottom view
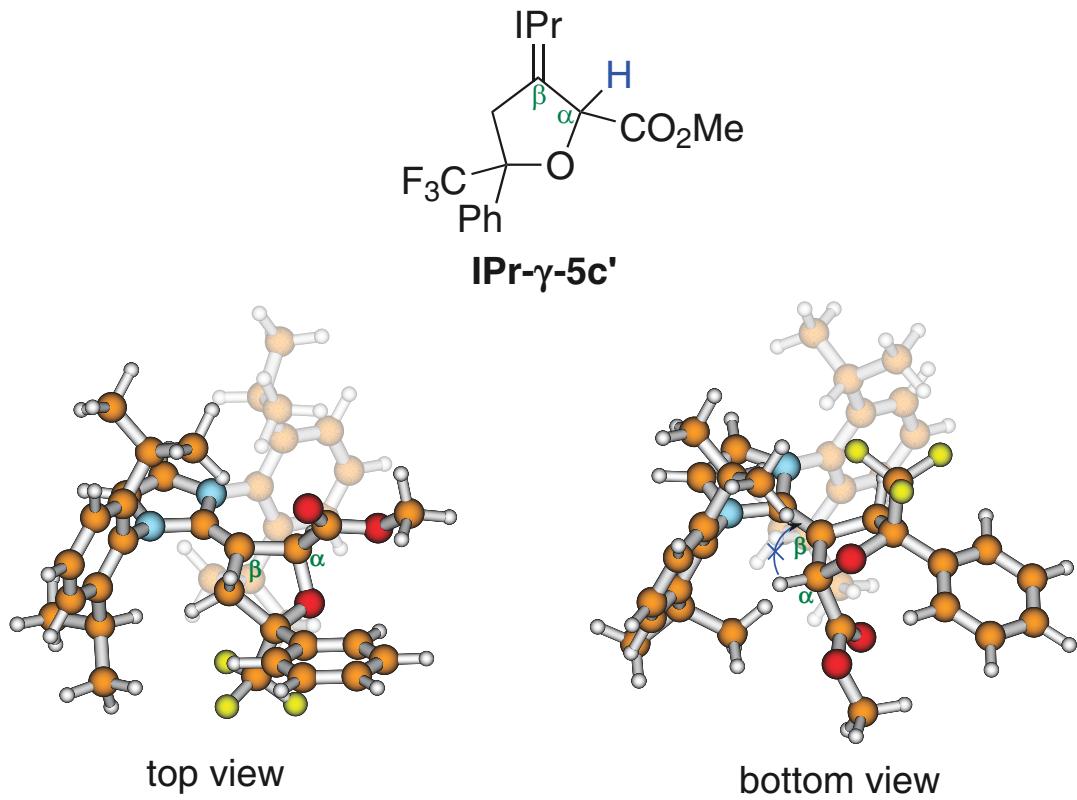
Figure S15: Geometry of **IPr-γ-5c'**.

Figure S16 shows the energy profiles and the mechanism for the PPh$_3$-catalyzed γ-[2 + 2], γ-[3 + 2] and γ-[2 + 2 + 2] cycloadditions of methyl allenoate **1** and ketone **2c**. The cycloadditions start from the Z-type adduct, **Pph-3**. The highest barrier along the γ-[2 + 2 + 2] pathway is 28.9 kcal mol^{-1}, and the γ-[2 + 2 + 2] cycloaddition is hence the kinetically least favorable. The barriers for the γ-[3 + 2] and γ-[2 + 2] cycloadditions are similar. The formation of the γ-[3 + 2] products **γ-5c** is thermodynamically more favorable than that of the γ-[2 + 2] products **γ-4c**.

Figure S16: Energy profiles for the PPh$_3$-catalyzed γ-[2 + 2], γ-[3 + 2] and γ-[2 + 2 + 2] cycloadditions of **1** and ketone **2c**.

9 Cartesian coordinates of optimized structures

Gas-phase geometry optimization was performed at the level M06-2X/6-31+G* (6d and 7f polarization functions). The listed energies are as follows:

E_e: electronic energy (au)

E_{zpe}: electronic energy with a zero-point correction (au)

H: enthalpy (au) under 1 atm and at 298 K

G: free energy (au) under 1 atm and at 298 K

9.1 LBs and methyl allenoate

IPr

E(ele) = -1159.550803
E(ele+zpe) = -1158.974016
H = -1158.943490
G = -1159.033882

```
C   -0.675993    0.029138    1.921802
C    0.675958   -0.028726    1.921822
C   -0.000007   -0.000171   -0.280214
N   -1.057827    0.037698    0.585213
N    1.057818   -0.037637    0.585213
C   -2.427136    0.116709    0.164935
C   -3.201958   -1.056155    0.179356
C   -2.937698    1.358480   -0.234414
C   -4.536362   -0.954217   -0.215908
C   -4.277581    1.408466   -0.632732
C   -5.070330    0.267443   -0.619640
H   -5.167420   -1.837681   -0.216220
H   -4.704444    2.353395   -0.958350
H   -6.110289    0.326582   -0.928637
C    2.427128   -0.116699    0.164975
C    2.937600   -1.358463   -0.234470
C    3.202034    1.056127    0.179453
C    4.277457   -1.408486   -0.632901
C    4.536427    0.954123   -0.215792
C    5.070298   -0.267538   -0.619684
H    4.704222   -2.353401   -0.958690
H    5.167554    1.837537   -0.216027
H    6.110237   -0.326713   -0.928737
C   -2.070559    2.604387   -0.295325
H   -1.149418    2.407287    0.265243
C   -2.749787    3.822812    0.338942
H   -3.072178    3.613588    1.364245
H   -2.052437    4.667222    0.362884
H   -3.627558    4.140784   -0.234432
C   -1.679036    2.890204   -1.751598
H   -1.143134    2.038261   -2.181793
H   -2.573634    3.078694   -2.357645
H   -1.035380    3.775480   -1.809798
C    2.573659    2.394772    0.532311
H    1.806625    2.218496    1.295520
H    1.870160    2.973345   -0.705568
H    2.606454    3.190799   -1.488817
H    1.138654    2.267403   -1.111762
H    1.353583    3.906854   -0.450873
C    3.569020    3.406625    1.104046
H    4.278897    3.748443    0.342585
H    3.031150    4.290172    1.462899
H    4.138886    2.988454    1.940668
C   -2.573527   -2.394754    0.532247
H   -1.806292   -2.218352    1.295225
C   -3.568764   -3.406477    1.104443
H   -4.138402   -2.988100    1.941115
H   -4.278849   -3.748442    0.343244
H   -3.030826   -4.289960    1.463352
C   -1.870337   -2.973531   -0.705705
H   -1.138897   -2.267647   -1.112124
H   -1.353709   -3.907006   -0.450992
H   -2.606800   -3.191086   -1.488769
C    2.070474   -2.604387   -0.295327
H    1.149238   -2.407201    0.265053
C    1.679159   -2.890490   -1.751598
H    1.143318   -2.038616   -2.182004
H    2.573823   -3.079096   -2.357502
H    1.035501   -3.775767   -1.809726
C    2.749672   -3.822644    0.339299
H    3.071760   -3.613202    1.364653
H    2.052415   -4.667132    0.363197
H    3.627636   -4.140580   -0.233796
H   -1.393500    0.062974    2.728521
H    1.393448   -0.062231    2.728572
```

IMe

E(ele) = -304.670098
E(ele+zpe) = -304.542127
H = -304.534075
G = -304.573677

```
C    0.000000   -0.983855   -0.000152
C    0.677634    1.208339   -0.000067
C   -0.677634    1.208339    0.000074
N   -1.058936   -0.123411   -0.000017
N    1.058936   -0.123412   -0.000016
C    2.440373   -0.565882    0.000075
H    2.959301   -0.203533   -0.892302
H    2.959100   -0.203900    0.892720
H    2.434191   -1.655595   -0.000148
C   -2.440373   -0.565882    0.000029
H   -2.959132   -0.203855    0.892636
H   -2.959269   -0.203578   -0.892385
H   -2.434191   -1.655595   -0.000141
H   -1.386291    2.023732    0.000170
H    1.386291    2.023732   -0.000076
```

Pbu

E(ele) = -814.621036
E(ele+zpe) = -814.247000
H = -814.227402
G = -814.295814

```
P   -0.412696   -0.169716    1.239551
C   -1.797661    0.615845    0.270133
C   -2.097449    1.525525    0.809092
H   -1.452251    0.929028   -0.724460
C    0.383502    2.016664    1.868693
C    0.829269    1.226005    1.248915
H    0.352248   -0.739399   -1.046754
H    1.699533    0.867698    1.815219
C    0.299958   -1.270764   -0.085910
C   -0.402659   -2.103272   -0.222162
C    1.288523    1.812284   -0.085904
H    1.744444    1.027317   -0.705294
H    0.425620    2.190116   -0.650494
C    1.674359   -1.830041    0.286159
H    2.393297   -1.006075    0.402037
C    1.616320   -2.326713    1.264962
C   -3.006198   -0.312829    0.127950
H   -2.712701   -1.225262   -0.410408
H   -3.338429   -0.636288    1.123789
C   -4.174778    0.341846   -0.609794
H   -4.473166    1.252267   -0.072985
H   -3.839041    0.664907   -1.604196
C   -5.375597   -0.591930   -0.748885
H   -6.203102   -0.107756   -1.276671
H   -5.105085   -1.495866   -1.306176
H   -5.742217   -0.905752    0.234825
C    2.215700   -2.814809   -0.751067
H    1.504915   -3.643947   -0.864664
H    2.267998   -2.315603   -1.727970
C    3.591766   -3.361866   -0.376604
H    3.963472   -4.065067   -1.128301
H    4.323140   -2.550951   -0.285010
H    3.555079   -3.886101    0.584860
C    2.300239    2.946750    0.090717
H    1.851238    3.738287    0.705220
H    3.165671    2.572140    0.653551
C    2.764891    3.529316   -1.242651
H    3.487732    4.338321   -1.098595
H    3.241332    2.759784   -1.860480
H    1.918180    3.932903   -1.809237
```

Pph

E(ele) = -1035.980878
E(ele+zpe) = -1035.704472
H = -1035.687783
G = -1035.750569

```
P    0.000791    0.001468   -1.280760
C   -0.981782   -1.317414   -0.442909
C   -1.737990   -1.121382    0.717809
C   -0.948436   -2.592326   -1.020859
C   -2.435981   -2.183646    1.292968
C   -1.781768   -0.136983    1.178207
C   -1.636315   -3.655846   -0.441203
H   -0.376540   -2.752806   -1.933026
C   -2.383413   -3.452074    0.718398
H   -3.019617   -2.017649    2.194423
H   -1.596120   -4.639807   -0.900231
C   -0.652632    1.513017   -0.446335
H   -0.070295    2.113433    0.674894
C   -1.814728    2.077781   -0.988650
C   -0.647269    3.247209    1.248600
H    0.835922    1.694029    1.104656
C   -2.399102    3.200979   -0.408053
H   -2.267531    1.629209   -1.870772
C   -1.813559    3.789652    0.713013
H   -0.184593    3.703948    2.119040
H   -3.305249    3.621469   -0.834804
H   -2.263326    4.669778    1.163591
C    1.636060   -0.188532   -0.447423
C    2.702960    0.552251   -0.973061
C    1.871348   -1.020396    0.652013
C    3.970495    0.483696   -0.399853
H    2.538075    1.189875   -1.840098
C    3.144665   -1.099736    1.218439
C    1.060238   -1.610193    1.071869
C    4.194858   -0.346959    0.697879
H    4.783991    1.070368   -0.817268
H    3.312156   -1.751733    2.071599
H    5.184605   -0.411214    1.140867
```

Hmpt

E(ele) = -744.848128
E(ele+zpe) = -744.595182
H = -744.579953
G = -744.635360

```
P    0.012698   -0.000063   -0.758601
N   -1.524789   -0.029193    0.079371
N    0.679380   -1.391705   -0.012031
N    0.621716    1.420606   -0.016817
C    1.727888    2.087422   -0.679569
C    1.698266    1.880605   -1.753193
H    1.653128    3.173171   -0.534636
H    2.705569    1.760778   -0.288661
C    0.574508    1.674652    1.412426
H   -0.290450    1.171559    1.851052
H    1.487596    1.328177    1.923076
H    0.477232    2.754331    1.592506
C   -2.347407    1.149784   -0.177360
H   -1.786321    2.059649    0.043939
H   -2.696904    1.202024   -1.223644
H   -3.228542    1.114132    0.472922
C   -2.295454   -1.245696   -0.162736
H   -1.697333   -2.127850    0.073002
H   -3.179195   -1.237986    0.484870
H   -2.639517   -1.327553   -1.208981
C    0.652336   -1.635830    1.419381
H    1.556065   -1.251109    1.920006
H   -0.227235   -1.162328    1.861099
H    0.597595   -2.716852    1.609091
C    1.798610   -2.299716   -0.680814
H    2.769685   -1.676510   -0.297231
H    1.754325   -3.117102   -0.533249
H    1.756135   -1.826296   -1.754590
```

Quin

E(ele) = -329.162039
E(ele+zpe) = -328.964695
H = -328.957241
G = -328.995433

```
C   -0.791707   -0.921651   -1.027314
C   -0.791615    1.350383   -0.284836
C   -0.792395   -0.428543    1.311157
C    0.756513   -0.851238   -1.160708
C   -1.283396   -0.673667   -1.974366
H   -1.117930   -1.929957   -0.747952
C    0.756440    1.431063   -0.156502
C   -1.283499    2.045823    0.404175
H   -1.117838    1.613575   -1.297579
H   -1.118463    0.317350    2.044890
C   -1.284632   -1.372539    1.569359
C    0.755428   -0.580090    1.317920
H    1.047629   -0.397172   -2.116163
H    1.198533   -1.854228   -1.132434
H    1.046941    2.031715    0.714575
H    1.199153    1.907786   -1.038988
H    1.197007   -0.054100    2.172609
H    1.046561   -1.634526    1.402973
N   -1.288737    0.000301   -0.000501
C    1.291417   -0.000205    0.000561
H    2.386610   -0.000463    0.000737
```

Dabco

E(ele) = -345.181640
E(ele+zpe) = -344.995946
H = -344.989542
G = -345.025195

```
C   -0.778998   -0.729487   -1.169411
C   -0.779312    1.377572   -0.046284
C   -0.778855   -0.649155    1.215868
C    0.779431   -0.728618   -1.169667
H   -1.182660   -0.249360   -2.068103
H   -1.181135   -1.748219   -1.130783
C    0.778161    1.378220   -0.046101
H   -1.182687    1.914471    0.819788
H   -1.182361    1.854473   -0.946942
H   -1.181887   -0.109033    2.080148
C   -1.181366   -1.667998    1.246580
C    0.779573   -0.648794    1.215608
H    1.182256   -0.247723   -2.068325
H    1.182721   -1.746913   -1.131529
H    1.180872    1.915108    0.820287
H    1.181031    1.855823   -0.946465
H    1.182665   -0.108867    2.079979
H    1.182550   -1.667470    1.245735
N   -1.283127   -0.000006    0.000061
N    1.283128    0.001047   -0.000125
```

Dmap

E(ele) = -382.093875
E(ele+zpe) = -381.930051
H = -381.920544
G = -381.963696

```
C   -1.950723    1.129480    0.013401
C   -1.950728   -1.129484    0.013503
C   -0.564164    1.196154   -0.021582
C   -2.524956    2.053844    0.033218
H   -0.564168   -1.196168   -0.021468
C   -2.524963   -2.053845    0.033418
C    0.183047   -0.000009   -0.052524
H   -0.084660    2.167470   -0.023790
H   -0.084673   -2.167487   -0.023542
N   -2.664067    0.000000    0.028908
N    1.554491    0.000006   -0.113531
```

```
C      2.270531    1.250205    0.043654
H      3.340237    1.061740   -0.054622
H      1.983537    1.962754   -0.737240
H      2.086164    1.714937    1.023448
C      2.270579   -1.250188    0.043461
H      2.086557   -1.714900    1.023332
H      1.983301   -1.962746   -0.737314
H      3.340251   -1.061737   -0.055215
```

Py

```
E(ele)      =  -248.180089
E(ele+zpe)  =  -248.090298
H           =  -248.085096
G           =  -248.117692
C      1.139571   -0.721256   -0.000001
C     -1.139550   -0.721290    0.000001
C      1.196383    0.671955    0.000001
H      2.054596   -1.309255    0.000002
C     -1.196403    0.671919   -0.000001
H     -2.054557   -1.309317   -0.000001
C     -0.000021    1.383282    0.000000
H      2.155676    1.179725    0.000002
H     -2.155711    1.179662   -0.000002
N      0.000022   -1.416867    0.000000
H     -0.000037    2.469601    0.000000
```

Dbu

```
E(ele)      =  -461.888397
E(ele+zpe)  =  -461.639337
H           =  -461.628629
G           =  -461.674797
C      2.133255    1.176928    0.339080
C      0.968804    1.581340   -0.609229
C     -0.322860    0.822912   -0.389755
C      1.922981   -0.126533    1.119123
C      1.890506   -1.379605    0.240124
C      0.971700   -1.191749   -0.976963
H      3.066815    1.106869   -0.234343
H      0.714499    2.633149   -0.470216
H      0.982562   -0.053611    1.680809
H      1.557319   -2.236324    0.839636
H      2.279794    1.982002    1.066279
H      1.271622    1.467383   -1.656644
H      2.718114   -0.231075    1.866324
H      2.899321   -1.620970   -0.120104
H      0.732882   -2.157824   -1.436182
H      1.486889   -0.608746   -1.745413
C     -2.580053    0.712811    0.163185
C     -2.298419   -0.664675    0.759217
C     -1.354054   -1.415421   -0.169315
H     -3.259235    1.283873    0.803260
H     -1.830624   -0.532654    1.742497
H     -3.218293   -1.241419    0.900223
H     -0.899306   -2.265005    0.357653
H     -1.904248   -1.821340   -1.030208
H     -3.080483    0.594800   -0.811277
N     -0.285864   -0.537475   -0.648483
N     -1.358249    1.481024   -0.009387
```

Mtbd

```
E(ele)      =  -477.929684
E(ele+zpe)  =  -477.692770
H           =  -477.681858
G           =  -477.727838
C     -2.328423    1.100941    0.201622
C     -0.054751    0.472966   -0.040925
C     -1.713025   -1.284421    0.175151
C     -2.685580   -0.260942   -0.383532
H     -2.643216    1.145356    1.254831
H     -2.879216    1.894722   -0.315688
H     -1.884129   -2.276270   -0.258741
H     -1.842445   -1.374664    1.268950
H     -2.590135   -0.238451   -1.475562
H     -3.716307   -0.538570   -0.138024
C      2.327153   -0.093648    0.203478
C      2.016222   -1.500788   -0.272039
C      0.641128   -1.887564    0.236427
H      3.273980    0.255896   -0.220539
H      2.026609   -1.526778   -1.366968
H      2.767026   -2.204743    0.101189
H      0.325391   -2.850017   -0.182391
H      0.666392   -2.003380    1.336015
H      2.437295   -0.080238    1.304098
N     -0.348961   -0.894459   -0.151301
N     -0.912934    1.413302    0.124356
N      1.284557    0.822895   -0.231513
C      1.603069    2.227090   -0.038768
H      0.913061    2.842167   -0.614321
H      1.526548    2.528112    1.016878
H      2.625758    2.392893   -0.388998
```

s-trans methyl allenoate **1**

```
E(ele)      =  -344.396253
E(ele+zpe)  =  -344.295473
H           =  -344.286854
G           =  -344.327977
C     -0.856377    0.995681   -0.000050
H     -1.026279    2.068358   -0.000096
C     -1.855334    0.144463    0.000003
C     -2.851116   -0.695386    0.000050
H     -3.274034   -1.059942    0.932162
H     -3.274099   -1.059937   -0.932038
C      0.569529    0.583490   -0.000034
O      0.731472   -0.747932   -0.000101
C      2.088119   -1.193026    0.000033
H      2.606357   -0.829384   -0.890377
H      2.606310   -0.828964    0.890295
H      2.038110   -2.280774    0.000280
O      1.487868    1.370347    0.000072
```

s-cis methyl allenoate **1**

```
E(ele)      =  -344.395985
E(ele+zpe)  =  -344.295156
H           =  -344.286572
G           =  -344.327549
C     -0.783242   -0.809212   -0.000911
H     -0.622834   -1.883450   -0.001713
C     -1.992032   -0.298039   -0.000102
C     -3.189211    0.213336    0.000877
H     -3.700476    0.439501   -0.930768
H     -3.699554    0.437702    0.933474
C      0.414782    0.069457   -0.000530
O      1.536298   -0.674478    0.000206
C      2.755829    0.068509    0.000775
H      2.814158    0.698598   -0.889716
H      2.812518    0.699943    0.890406
H      3.551914   -0.674553    0.002076
O      0.414642    1.276722   -0.000757
```

9.2 Addition of LBs to *s-cis* methyl allenoate

9.2.1 Z-type addition

IMe-ts3

E(ele) = −649.063755
E(ele+zpe) = −648.833042
H = −648.817027
G = −648.876221

Atom	X	Y	Z
C	1.583022	0.253555	0.129411
C	1.228639	-1.936089	0.622593
C	1.501839	-1.861698	-0.704801
H	0.997495	-2.781655	1.253132
H	1.569087	-2.630783	-1.460140
N	1.730306	-0.525232	-0.976349
N	1.289787	-0.642323	1.104621
C	1.032202	-0.276682	2.487660
H	0.892432	0.803260	2.528070
H	0.112169	-0.756734	2.824309
H	1.876163	-0.569411	3.119301
C	1.919901	0.018933	-2.305357
H	2.714725	-0.520334	-2.827085
H	0.989617	-0.051433	-2.878959
H	2.198709	1.068129	-2.200834
C	-0.900032	1.362732	-0.722516
C	0.770525	2.941936	0.473396
H	0.210556	3.858778	0.646622
H	1.808691	2.887588	0.773498
H	-1.052903	1.516520	-1.786475
C	0.147482	1.927960	-0.088726
C	-1.728554	0.383023	-0.040195
O	-2.678475	-0.128894	-0.864243
O	-1.620339	0.021789	1.119477
C	-3.527272	-1.104573	-0.272384
H	-4.045998	-0.688466	0.595024
H	-4.240679	-1.385343	-1.047170
H	-2.946715	-1.974965	0.046450

IMe-3

E(ele) = −649.131661
E(ele+zpe) = −648.897044
H = −648.881505
G = −648.938754

Atom	X	Y	Z
C	-1.080191	0.299794	-0.020948
C	-2.107967	-1.509053	0.731568
C	-2.083939	-1.576997	-0.624164
N	-1.464436	-0.430136	-1.072568
N	-1.501142	-0.322278	1.084396
C	-1.099736	0.067939	2.429344
H	-1.877009	-0.234754	3.132503
H	-0.151024	-0.420356	2.666403
H	-0.976787	1.151327	2.449924
C	-1.003137	-0.179442	-2.431415
H	-0.022165	-0.645003	-2.556499
H	-1.724947	-0.600276	-3.132522
H	-0.925169	0.898782	-2.575387
C	-1.070209	2.696715	-0.134803
H	-0.605441	3.676270	-0.181051
H	1.100770	1.411431	-0.053987
H	1.730412	2.292282	-0.086720
H	-2.154160	2.649777	-0.141087
C	-0.310282	1.565242	-0.073344
C	1.710399	0.140125	0.006529
O	1.149600	-0.973266	0.047550
O	3.080713	0.204721	0.018599
C	3.746065	-1.044689	0.070725
H	3.498510	-1.660019	-0.799507
H	4.811999	-0.811827	0.075988
H	3.475946	-1.599039	0.974501
H	-2.462811	-2.323314	-1.304611
H	-2.511466	-2.184974	1.469051

IPr-ts3

E(ele) = −1503.942588
E(ele+zpe) = −1503.263759
H = −1503.225035
G = −1503.333639

Atom	X	Y	Z
C	-1.047113	-0.334963	2.180145
C	0.188400	-0.888718	2.164765
C	-0.303212	-0.277234	0.025391
N	-1.319910	0.031436	0.868945
N	0.624056	-0.836531	0.845356
C	-2.613642	0.452759	0.405856
C	-3.546450	-0.547467	0.095466
C	-2.870209	1.821261	0.239661
C	-4.801708	-0.137127	-0.363434
C	-4.138951	2.179969	-0.221822
C	-5.097281	1.213216	-0.514684
H	-5.551697	-0.883597	-0.614661
H	-4.376190	3.229711	-0.367319
H	-6.076710	1.515728	-0.874828
C	1.862563	-1.398769	0.378202
C	1.809684	-2.544155	-0.439837
C	3.068014	-0.791240	0.756563
C	3.024017	-3.078598	-0.872929
C	4.256518	-1.377161	0.308276
C	4.237299	-2.506035	-0.499222
H	3.026518	-3.956995	-1.510045
H	5.207892	-0.929401	0.581698
H	5.170191	-2.940308	-0.847685
C	-1.811835	2.859559	0.558792
H	-0.829534	2.395984	0.430895
C	-1.944579	3.319154	2.017511
H	-1.855863	2.478195	2.714420
H	-1.158711	4.043673	2.256900
H	-2.917810	3.796767	2.185843
C	-1.844334	4.056807	-0.392051
H	-1.804774	3.726064	-1.435039
H	-2.739818	4.674067	-0.248966
H	-0.965429	4.681279	-0.209843
C	3.114863	0.459354	1.619474
H	2.127652	0.935597	1.580493
H	4.139425	1.478039	1.105033
H	5.165383	1.148475	1.306454
H	4.039155	1.643605	0.029284
H	3.996925	2.433376	1.621561
C	3.444581	0.110008	3.079051
H	4.438068	-0.350258	3.139916
H	3.452051	1.015821	3.694988
H	2.730051	-0.592712	3.516081
C	-3.218169	-2.029180	0.200305
H	-2.208161	-2.134210	0.611191
C	-4.177857	-2.754271	1.150430
H	-4.168675	-2.297481	2.145658
H	-5.207435	-2.725631	0.776257
H	-3.887659	-3.805933	1.251840
C	-3.218155	-2.685053	-1.186498
H	-2.494680	-2.203603	-1.853663
H	-2.955546	-3.746455	-1.106265
H	-4.207050	-2.618024	-1.654555
C	0.487216	-3.214887	-0.787303
H	-0.247739	-2.425092	-0.972059
C	0.546051	-4.073578	-2.051556
H	0.955128	-3.514554	-2.899540
H	1.150002	-4.976996	-1.906607
H	-0.465934	-4.398701	-2.315885
C	-0.001842	-4.057308	0.401149
H	-0.120530	-3.452192	1.306180
H	-0.970509	-4.518027	0.172393
H	0.714752	-4.858472	0.618758
C	-1.755796	-0.180652	2.980186
H	0.781640	-1.329615	2.950431
C	0.249767	0.681009	-1.939162
C	1.530017	1.106622	-1.931146
C	-0.911089	0.568086	-2.551379
H	2.328161	0.494565	-2.340895
H	-1.769396	0.070561	-2.117958
H	-1.011320	1.019213	-3.536866
C	1.859511	2.401340	-1.366995
O	1.155288	3.094867	-0.650777
O	3.099681	2.810913	-1.751339
C	3.482980	4.099184	-1.286651
H	4.487095	4.266772	-1.676726
H	2.794850	4.861788	-1.660628
H	3.485787	4.133357	-0.193523

IPr-3

E(ele) = −1504.008506
E(ele+zpe) = −1503.326562
H = −1503.288162
G = −1503.395767

Atom	X	Y	Z
C	-0.778001	-0.301236	2.041042
C	0.543060	-0.601444	2.001114
C	-0.094547	-0.075971	-0.065248
N	-1.166459	-0.007727	0.746422
N	0.947658	-0.479417	0.685726
C	-2.553306	0.093442	0.338198
C	-3.263181	-1.113246	0.196751
C	-3.131444	1.350408	0.135775
C	-4.604048	-1.027124	-0.176319
C	-4.477220	1.377701	-0.246806
C	-5.206857	0.207220	-0.403584
H	-5.184545	-1.938352	-0.294276
H	-4.954486	2.338044	-0.422997
H	-6.250555	0.252522	-0.701585
C	2.230148	-0.931013	0.188356
C	2.269148	-2.179050	-0.461543
C	3.373284	-0.161853	0.435793
C	3.510535	-2.623926	-0.916784
C	4.592627	-0.663066	-0.032559
C	4.662576	-1.871440	-0.711711
H	3.579687	-3.578606	-1.429580
H	5.499736	-0.090481	0.140064
H	5.619049	-2.236267	-1.075143
C	-2.363526	2.643573	0.307622
H	-1.344107	2.411959	0.625517
C	-3.004207	3.529716	1.382892
H	-3.074531	3.007011	2.343214
H	-2.397387	4.429691	1.528338
H	-4.013905	3.848115	1.097060
C	-2.255896	3.389587	-1.028318
H	-1.811751	2.751843	-1.799014
H	-3.239249	3.730490	-1.376096
H	-1.614343	4.269638	-0.908810
C	3.345632	1.135156	1.221395
H	2.305327	1.438129	1.363821
C	4.030410	2.270523	0.454192
H	5.101776	2.080415	0.318823
H	3.575904	2.409107	-0.531771
H	3.929742	3.204475	1.016943
C	4.004736	0.935704	2.593817
H	5.063608	0.670204	2.488160
H	3.944302	1.859180	3.179553
H	3.520007	0.136276	3.166142
C	-2.641601	-2.473642	0.474696
H	-1.555950	-2.352775	0.551515
C	-3.136554	-3.025327	1.819691
H	-2.923891	-2.334087	2.641663
H	-4.220127	-3.187842	1.792253
H	-2.652108	-3.982752	2.041735
C	-2.910725	-3.487694	-0.643630
H	-2.625666	-3.097178	-1.625041
H	-2.340482	-4.404927	-0.458302
H	-3.969539	-3.764999	-0.686984
C	1.051197	-3.079650	-0.583531
H	0.157755	-2.456668	-0.533061
C	0.980795	-3.820464	-1.920292
H	1.079389	-3.121700	-2.756631
H	1.758362	-4.587395	-2.006992
H	0.012988	-4.326528	-2.009622
C	1.001000	-4.059542	0.597734
H	0.984476	-3.528603	1.556491
H	0.101766	-4.684731	0.538937
H	1.876733	-4.718876	0.591408
H	-1.484333	-0.274222	2.855810
C	1.235592	-0.900027	2.772811
H	-0.054762	0.229794	-1.516597
C	0.667363	1.402941	-1.887612
C	-0.694955	-0.644703	-2.339681
H	0.841543	1.580913	-2.942397
H	-1.195714	-1.528365	-1.961173
C	-0.713406	-0.477448	-3.411878
C	0.940547	2.444691	-0.986613
O	0.730420	2.480348	0.243698
O	1.496286	3.546112	-1.601275
C	1.642288	4.691473	-0.783033
H	2.108101	5.449630	-1.415012
H	0.669922	5.048670	-0.426516
H	2.271180	4.485629	0.086987
C	2.247918	0.744801	-1.472431
H	2.061718	1.181678	-2.464024
O	3.253926	1.270421	-2.236826
C	4.035689	2.273065	-1.611620
H	4.495685	1.898087	-0.692525
H	4.805741	2.541294	-2.336590
H	3.430454	3.150689	-1.364880
C	-1.540529	2.000064	1.033173
C	-2.419045	1.404306	1.319177
H	-0.849151	1.973501	1.886479
C	1.846244	-1.563474	1.336592
H	1.380184	-2.532383	1.107255
H	2.460678	-1.294547	0.469783
C	-2.981352	-1.039839	-0.510763
H	-3.395441	-0.034466	-0.352302
C	-2.645784	-1.079918	-1.554087
C	2.729196	-1.695952	2.576684
H	2.107988	-1.939518	3.449538
H	3.196598	-0.724557	2.783598
C	3.809283	-2.761223	2.398928
H	4.450519	-2.523522	1.543550
H	4.444653	-2.837734	3.286703
H	3.362879	-3.745374	2.217927
C	-1.980781	3.444694	0.790882
H	-1.103561	4.043263	0.516280
H	-2.660099	3.472722	-0.071310
C	-2.666532	4.054271	2.011250
H	-2.970853	5.087989	1.822081
H	-3.562766	3.485342	2.283350
H	-1.995807	4.055294	2.877561
C	-4.083126	-2.076988	-0.290912
H	-3.673720	-3.077722	-0.483754
H	-4.391267	-2.064934	0.763314
C	-5.293456	-1.833064	-1.188825
H	-6.066846	-2.590627	-1.031469
H	-5.738589	-0.851906	-0.989288
H	-5.006064	-1.860105	-2.245586

Pbu-ts3

E(ele) = −1159.006757
E(ele+zpe) = −1158.530945
H = −1158.503003
G = −1158.591538

Atom	X	Y	Z
C	0.878515	-0.397038	-2.250604
P	-0.286891	-0.457404	-0.100504
C	0.676770	-1.031487	1.368123
H	1.396935	-0.236658	1.594707
H	0.012895	-1.158885	2.235229
H	0.383583	1.795491	0.302603
C	-0.607281	1.325448	0.244166
C	-2.289430	-1.088006	1.178359
H	-1.090701	1.750635	-0.646317
C	-1.940339	-1.260967	0.150181
H	-1.790380	-2.344503	0.046452
C	-0.052892	-2.300905	-2.361584
C	0.660946	-1.593079	-2.767863
C	1.444892	0.830819	-2.365571
C	1.073939	1.549019	-3.089136
H	1.239673	-1.889306	-3.640542
C	2.401093	1.255375	-1.370646
O	2.719670	0.617573	-0.373912
C	3.371412	3.064284	0.324153
C	3.838756	2.968357	-0.660108
H	4.689408	2.358673	-0.581551
H	4.162032	3.943419	-1.023923
O	2.901059	2.491327	-1.617727
C	-1.415719	1.645741	1.501882
H	-2.422362	1.211426	1.422361
H	-0.943978	1.179077	2.378099
C	-2.982610	-0.780518	-0.860976
H	-3.140279	0.301434	-0.742634
C	-2.598106	-0.923998	-1.880915
C	1.434049	-2.327683	1.068664
H	0.728401	-3.120095	0.775268
H	2.095175	-2.155258	0.209924
C	2.258509	-2.808527	2.262194
H	2.969847	-2.019849	2.540144
C	1.597771	-2.953993	3.127973
C	3.012867	-4.102880	1.965542
H	3.602202	-4.430866	2.827614
H	2.318232	-4.910370	1.706958
C	3.697669	-3.969114	1.120905
C	-4.325468	-1.496823	-0.714520
H	-4.172634	-2.577314	-0.837389
C	-4.702518	-1.351144	0.306621
C	-5.361353	-1.003526	-1.722583
H	-6.317136	-1.522822	-1.603205
H	-5.545071	0.069823	-1.599985
C	-5.015674	-1.166437	-2.749464
H	-1.544614	3.150778	1.742827
C	-0.541474	3.587019	1.836036
H	-2.004419	3.617681	0.861585
C	-2.367630	3.474424	2.987932
H	-2.449998	4.554323	3.144954
H	-3.382399	3.069725	2.902009
H	-1.910483	3.038856	3.883526

Pbu-3

E(ele) = −1159.043549
E(ele+zpe) = −1158.563492
H = −1158.536394
G = −1158.621626

Atom	X	Y	Z
C	1.519579	-0.266127	-2.110647
C	-0.110681	-2.130613	-1.959687
C	0.288118	-2.584989	-2.862422
H	-0.951321	-2.631042	-1.498162
C	1.836630	-0.586252	-3.096771
C	0.456004	-0.983262	-1.489302
P	-0.280084	-0.304450	0.035960
C	0.770625	-0.488913	1.524936
H	0.110498	-0.739964	2.365354
C	1.242332	0.478535	1.709597
C	-1.797186	-1.256697	0.437983
H	-2.077988	-0.965463	1.458015
C	-1.519098	-2.316366	0.492337
C	-0.858995	1.406927	-0.203233
H	-1.542694	1.384095	-1.061344
H	0.021829	1.990204	-0.483050

Pph-ts3

E(ele) = −1380.364030
E(ele+zpe) = −1379.985011
H = −1379.960371
G = −1380.040017

Atom	X	Y	Z
C	1.852378	-0.634333	2.300056
C	-0.377307	0.104754	3.333547
C	0.555865	-0.221095	2.450184
P	-0.478350	-0.036949	0.386238
C	2.720652	0.115451	1.435365
C	2.424646	1.171590	0.882727
O	3.919721	-0.483724	1.229281
C	4.755355	0.160351	0.275737
H	4.984056	1.182922	0.587135
H	5.665732	-0.437790	0.229859
H	4.264550	0.186690	-0.702447
C	-0.978602	1.626706	-0.172208
C	-2.068955	1.839961	-1.026307
H	-0.217130	2.715647	0.270551
C	-2.390996	3.131066	-1.436219
C	-2.662503	0.998171	-1.374100
C	-0.545043	4.005281	-0.146821
H	0.641781	2.539399	0.912939
C	-1.629603	4.214584	-0.995890
H	-3.233708	3.290799	-2.102916
H	0.051312	4.846665	0.193843
C	-1.883178	5.221159	-1.316653
C	-1.997418	-1.042665	0.194312
H	-2.043415	-2.210130	-0.574603
C	-3.147258	-0.647960	0.896109
C	-3.211649	-2.970371	-0.633775
H	-1.171367	-2.523018	-1.141158
C	-4.312705	-1.404223	0.829671
C	-3.140785	0.270503	1.479557
C	-4.346641	-2.573052	0.067880
C	-3.232026	-3.872223	-1.238837
H	-5.195601	-1.080868	1.373551
H	-5.255336	-3.165769	0.019473
C	0.692927	-0.672412	-0.846562
C	1.324916	-1.894993	-0.585441
C	1.057744	0.061156	-1.983332
C	2.295088	-2.383835	-1.460643
C	1.065392	-2.463255	0.304356
C	2.014933	-0.433801	-2.856957
H	0.587616	1.024605	-2.175418
C	2.638869	-1.655279	-2.596829
H	2.785173	-3.329101	-1.246814
H	2.284989	0.138918	-3.739413
H	3.395707	-2.034878	-3.277451
H	2.159754	-1.615187	2.646789
H	-1.429218	0.204249	3.087506
H	-0.078057	0.284467	4.363601

Pph-3

E(ele) = −1380.389064
E(ele+zpe) = −1380.008578
H = −1379.983933
G = −1380.063079

Atom	X	Y	Z
C	-1.766386	0.080004	-2.226859
C	0.583090	-0.178818	-3.021728
C	-0.357520	-0.016040	-2.047827
P	0.279516	-0.018682	-0.336927
C	-2.641549	0.287222	-1.151533
C	-2.299825	0.487430	0.033119
O	-3.965285	0.264176	-1.483899
C	-4.863111	0.467220	-0.404525
H	-4.704214	1.444695	0.060304

```
H     -5.862394    0.413210   -0.838897
H     -4.739327   -0.306447    0.358712
C      0.251640    1.598655    0.480669
C      1.015580    1.805510    1.632955
C     -0.465286    2.653280   -0.089129
C      1.036171    3.062214    2.234118
H      1.608331    0.995981    2.054141
C     -0.418279    3.912404    0.501732
H     -1.055009    2.481268   -0.985634
C      0.321373    4.115366    1.666567
H      1.620086    3.219460    3.136155
H     -0.969069    4.734547    0.054887
H      0.346897    5.097934    2.129183
C      2.070972   -0.388758   -0.397649
C      2.566532   -1.661513   -0.101947
C      2.962306    0.628680   -0.766168
C      3.935834   -1.915323   -0.180326
H      1.890656   -2.458253    0.194359
C      4.326552    0.369590   -0.850284
C      2.586967    1.624087   -0.991436
C      4.815307   -0.903724   -0.556331
H      4.311618   -2.906739    0.054588
H      5.007829    1.163068   -1.142589
H      5.881098   -1.104074   -0.617622
C     -0.438074   -1.379159    0.617008
C     -0.761143   -2.550128   -0.072555
C     -0.635648   -1.288745    1.995193
C     -1.271068   -3.641217    0.629680
H     -0.630503   -2.601613   -1.151476
C     -1.141125   -2.384213    2.688705
H     -0.429161   -0.359947    2.519250
C     -1.455477   -3.561026    2.008259
H     -1.530892   -4.549600    0.094443
H     -1.303623   -2.313984    3.760123
H     -1.855704   -4.411698    2.552438
H     -2.171573   -0.060848   -3.222327
H      1.637608   -0.312776   -2.825925
H      0.264374   -0.189771   -4.060698


     Hmpt-ts3

E(ele)       = -1089.226707
E(ele+zpe)   = -1088.871005
H            = -1088.847807
G            = -1088.922463
C     -1.961945    1.438717   -0.826186
C     -0.707929    1.806165   -0.439003
P      0.843171    0.008187   -0.067761
C     -2.707436    0.515360   -0.015919
O     -2.315571    0.011244    1.030795
O     -3.905498    0.179964   -0.562810
C     -4.673531   -0.751500    0.188508
H     -4.863059   -0.372262    1.196030
H     -5.609395   -0.871850   -0.357166
H     -4.151838   -1.709994    0.265832
N      2.418033    0.311831   -0.710206
N      1.258205   -0.168524    1.556719
N      0.561479   -1.462276   -0.869258
C     -0.821048   -1.880485   -1.082375
H     -1.425132   -1.029112   -1.397891
H     -0.835694   -2.623547   -1.888053
H     -1.272197   -2.324689   -0.183821
C      1.486392   -2.579853   -0.738384
H      2.513861   -2.211462   -0.702026
H      1.283694   -3.181035    0.161601
H      1.385716   -3.232381   -1.614486
C      2.526145    0.387846   -2.162140
H      1.931303   -0.399724   -2.627475
H      2.188385    1.364199   -2.548290
H      3.575668    0.251301   -2.448441
C      3.307964    1.266576   -0.063508
H      3.092358    1.337462    1.004284
H      4.347020    0.935246   -0.189859
H      3.225187    2.271893   -0.506849
C      2.364717   -0.982393    2.036928
H      2.008312   -1.939672    2.443765
H      3.076312   -1.181133    1.232929
H      2.893017   -0.448772    2.839430
C      0.327244    0.229188    2.606203
H     -0.132673   -0.647853    3.081592
H      0.869113    0.800541    3.371893
H     -0.474609    0.839245    2.191703
C      0.086571    2.831811   -0.168746
H      1.162434    2.754236   -0.064192
H     -0.368071    3.809862   -0.027617
H     -2.327139    1.701233   -1.813409


     Hmpt-3

E(ele)       = -1089.270276
E(ele+zpe)   = -1088.909922
H            = -1088.887778
G            = -1088.957251
C     -1.523378   -1.144660   -1.152700
C     -0.100239   -1.153327   -1.105422
P      0.814464   -0.050431    0.005731
C     -2.329780   -0.294064   -0.380728
O     -1.948576    0.585752    0.417340
O     -3.673330   -0.498109   -0.569386
C     -4.526580    0.358615    0.168184
H     -4.340897    1.408466   -0.078341
H     -5.542681    0.079643   -0.114678
N      2.472247   -0.295124   -0.051373
N      0.718689    1.522707   -0.496193
N      0.444352   -0.389759    1.593442
C     -0.397200   -1.538647    1.931946
H     -0.267385   -2.336809    1.198670
H     -0.079935   -1.910983    2.913034
H     -1.454300   -1.252739    1.967607
C      0.269306    0.741569    2.502201
H      1.092391    1.452581    2.397775
H     -0.688298    1.243547    2.314543
H      0.292956    0.361283    3.528332
C      3.129774   -1.330625    0.734384
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H      2.521978   -1.586243    1.601924
H      3.303381   -2.236195    0.135600
H      4.098770   -0.953855    1.083193
C      3.270578    0.152666   -1.186625
C      2.690417    0.822058   -1.823550
H      4.159415    0.685086   -0.822987
H      3.604301   -0.699300   -1.794005
C      1.578695    2.564778    0.049316
H      1.006082    3.243420    0.695100
H      2.401435    2.131749    0.621616
H      2.004979    3.148713   -0.776620
C     -0.332564    2.036714   -1.371728
H     -1.063288    2.619277   -0.802859
H      0.143647    2.669663   -2.131011
C     -0.850017    1.216805   -1.869288
C      0.724029   -1.990144   -1.802653
H      1.801328   -1.974615   -1.709112
H      0.297525   -2.716830   -2.488810
H     -2.010282   -1.866569   -1.799327


     Quin-ts3

E(ele)       = -673.548787
E(ele+zpe)   = -673.247754
H            = -673.232692
G            = -673.288715
C      0.611419    1.687187   -0.131410
C      0.161412    2.801440    0.420002
C     -0.878455    3.004601    0.648819
H      0.883062    3.573670    0.666157
C      1.739075    1.124158   -0.675722
H      2.128746    1.484327   -1.620914
H      2.423385    0.077787    0.024215
O      2.048743   -0.479561    1.054925
O      3.589362   -0.281356   -0.581494
C      4.323288   -1.305034    0.075314
H      4.571307   -1.010276    1.098266
H      3.748637   -2.235193    0.108515
C     -3.352055    0.129855   -0.472404
H     -2.118452    1.023164   -0.754956
H     -3.951440    0.017993   -1.382454
H     -3.995387    0.589552    0.287444
C     -1.891916    1.083520   -1.824443
C     -2.279983    2.040931   -0.395036
C     -1.758758   -1.703242   -0.956336
H     -1.474637   -2.740811   -0.752165
H     -2.141465   -1.668030   -1.983804
H      0.242954   -1.251547   -0.174805
C     -0.070635   -0.505102   -1.741486
C     -1.216185    0.153568    1.324006
H     -0.261029   -0.056888    1.812220
C     -1.638374    1.059064    1.771654
C     -2.204580   -1.036417    1.403302
H     -1.677736   -1.949963    1.702391
H     -2.972595   -0.841742    2.159813
O     -0.917539    0.465431   -0.094007
C     -0.528611   -0.782662   -0.787408
H      5.231269   -1.441582   -0.512856
C     -2.844988   -1.231269    0.020023
H     -3.664826   -1.954417    0.071533


     Quin-3

E(ele)       = -673.565122
E(ele+zpe)   = -673.260228
H            = -673.245645
G            = -673.299894
C      1.574018    1.252489   -0.009710
C     -0.218721    2.938100    0.016207
H      0.537538    3.713148    0.050282
H     -1.245947    3.265250    0.030226
C      2.250575    2.098644    0.010415
C      0.202083    1.648113   -0.020026
C      2.218674    0.001395   -0.007421
H      1.744318   -1.154689   -0.025910
O      3.586347    0.149304    0.015583
C      4.325833   -1.058511    0.013581
H      4.114764   -1.649609   -0.882611
H      5.375325   -0.760534    0.029386
H      4.092476   -1.666132    0.892960
C     -0.695638   -0.317505   -1.253111
H     -0.722873   -0.227596    1.265697
H     -2.272764    1.082441   -0.078841
C     -1.427393   -1.640590   -1.006515
H      0.362669   -0.469906   -1.431035
C     -1.130324    0.262105   -2.073040
H     -1.889346   -1.220768    1.401351
H     -0.699045    0.522640    2.059368
H      0.237922   -0.735900    1.204824
H     -2.459965    1.581515    0.874307
H     -2.322973    1.819414   -0.879734
C     -3.243680   -0.089741   -0.326436
H     -0.711803   -2.384422   -0.639060
H     -1.839671   -2.005269   -1.952923
H     -2.633217   -0.863747    2.123473
H     -1.499339   -2.172806    1.773799
H     -4.137899    0.052380    0.288731
H     -3.567435   -0.102031   -1.373142
N     -0.855249    0.569211   -0.026767
C     -2.538963   -1.403132    0.025968
H     -3.249564   -2.234315    0.039305


     Dabco-ts3

E(ele)       = -689.747057
E(ele+zpe)   = -689.459464
H            = -689.444886
G            = -689.499514
C      0.596272    1.678113   -0.122508
C      0.148819    2.797593    0.421879
C     -0.890971    3.007674    0.644816
H      0.873443    3.568204    0.665806
C      1.727714    1.121214   -0.669177
H      2.126674    1.504344   -1.601282
C      2.416879    0.073546    0.022141
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O      2.038016   -0.504368    1.040856
O      3.593242   -0.262285   -0.575764
C      4.335673   -1.283575    0.075444
H      4.573340   -0.995925    1.102865
H      3.772807   -2.221212    0.095336
C     -3.318523    0.057320   -0.492121
C     -2.122925    1.025490   -0.729573
C     -3.872704   -0.109111   -1.421555
H     -4.017001    0.471284    0.242696
H     -1.893164    1.152657   -1.792438
C     -2.325083    2.012286   -0.308572
C     -1.781768   -1.700253   -0.889875
H     -1.516613   -2.726048   -0.616300
C     -2.192652   -1.724120   -1.905046
O      0.269256   -1.237265   -0.229433
C     -0.140410   -0.493813   -1.779406
C     -1.213233    0.125464    1.324661
H     -0.265751   -0.148896    1.796691
C     -1.591329    1.033016    1.806231
C     -2.261917   -1.024848    1.344565
H     -1.798753   -1.966091    1.657560
H     -3.072471   -0.803903    2.046494
N     -0.915044    0.463854   -0.086359
C     -2.838095   -1.227967    0.010706
C     -0.537961   -0.776563   -0.800031
H      5.249113   -1.402078   -0.508063


     Dabco-3

E(ele)       = -689.583114
E(ele+zpe)   = -689.289813
H            = -689.275391
G            = -689.329533
C     -0.195818    1.651366   -0.015800
C      0.235425    2.937621    0.013510
C      1.266026    3.254521    0.024098
H     -0.513690    3.719752    0.041236
C     -1.568157    1.258935   -0.008456
C     -2.243559    2.106069    0.006710
C     -2.212596    0.007703   -0.006165
O     -1.735188   -1.147965   -0.020356
O     -3.579133    0.153361    0.011741
C     -4.317952   -1.055406    0.011194
H     -4.104743   -1.647967   -0.883419
C      3.215247   -0.153242   -0.262645
C      2.276748    1.066311   -0.064496
C      4.081043   -0.063680    0.400332
H      3.587701   -0.190749   -1.291151
C      2.461646    1.587065    0.877299
C      2.354929    1.776797   -0.887632
C      1.866421   -1.277147    1.321900
H      1.459354   -2.250078    1.610457
C      2.627752   -1.000221    2.058922
H     -0.254817   -0.705723    1.235550
C      0.768937    0.503715    2.069344
H      0.701787   -0.310038   -1.251708
H     -0.353283   -0.504400   -1.411035
C      1.103697    0.287748   -2.075159
H      1.490937   -1.607975   -1.005532
H      0.810412   -2.393059   -0.662520
H      1.964281   -1.943030   -1.933719
N      0.856702    0.567382   -0.020919
C      2.521080   -1.404716    0.019664
C      0.725855   -0.234822    1.265109
H     -5.367489   -0.757884    0.024525


     Dmap-ts3

E(ele)       = -726.475165
E(ele+zpe)   = -726.209216
H            = -726.191547
G            = -726.255584
C      2.029274    3.074806   -0.117004
C      2.909331    3.602105    0.237893
C      2.880140    0.681340   -0.565631
H      3.563774    0.681425   -1.407129
H      1.126814    3.644856   -0.308367
C      2.112481    1.771578   -0.323479
C     -0.130006    0.149847   -1.094178
C     -0.689847    1.660127    0.531496
H     -1.364897   -0.466967   -1.030931
H      0.659185   -0.214843   -1.752744
C     -1.951771    1.116125    0.685326
C     -0.355147    2.489835    1.152097
C     -2.333237    0.017246   -0.119792
H     -1.558811   -1.322784   -1.665121
H     -2.615689    1.529754    1.433882
N      0.194346    1.204926   -0.353072
C      2.750008   -0.516788    0.235144
O      1.976152   -0.694624    1.161519
O      3.602014   -1.496235   -0.180116
C      3.533551   -2.705362    0.562840
H      4.286406   -3.363626    0.128756
H      3.747705   -2.522654    1.619204
C      2.540028   -3.155145    0.479640
H     -4.485755   -0.092998    1.011079
H     -4.727554    0.967237    0.872455
H     -5.412551   -0.662199    0.940218
C     -4.071350   -0.228838    2.018838
C     -3.880758   -1.740914   -0.786416
H     -3.793147   -1.543013   -1.860953
H     -3.220437   -2.580164   -0.529969
H     -4.909662   -2.036379   -0.581260
N     -3.567106   -0.554487   -0.012555


     Dmap-3

E(ele)       = -726.499877
E(ele+zpe)   = -726.230948
H            = -726.213592
G            = -726.275835
C     -1.642761    3.111026    0.308286
H     -2.582115    3.649020    0.271242
C     -2.703217    0.824519    0.288890
```

```
H     -3.683154    1.200881    0.552660
H     -0.731578    3.675761    0.472355
C     -1.638046    1.753146    0.262518
C      0.061288    0.205442    1.093511
C      0.568220    1.517445   -0.762482
C      1.301581   -0.376853    1.073269
H     -0.707517   -0.054282    1.812353
C      1.820983    0.964656   -0.863238
H      0.190051    2.254610   -1.460499
C      2.235903   -0.019851    0.068778
H      1.521586   -1.132577    1.814802
C      2.457022    1.280951   -1.678578
N     -0.289176    1.162406    0.211778
C     -2.607327   -0.519434   -0.148001
O     -1.605302   -1.147329   -0.522228
C     -3.825349   -1.157337   -0.098793
H     -4.848569   -2.851530   -0.439588
C     -3.440429   -2.619047   -1.524813
H     -3.181145   -3.117074    0.159232
N      3.458085   -0.597011   -0.003847
C      3.820473   -1.648179    0.933806
H      4.830405   -1.989456    0.709678
C      3.805333   -1.277334    1.964994
H      3.139324   -2.503654    0.854042
C      4.369406   -0.232819   -1.076352
H      3.945774   -0.474197   -2.058931
H      4.604986    0.837051   -1.045102
H      5.298743   -0.788347   -0.956325


     Py-ts3

E(ele)       = -592.558262
E(ele+zpe)   = -592.366515
H            = -592.353270
G            = -592.406560
C      0.392774    2.989049   -0.006852
C     -0.192667    3.839434   -0.341205
C     -1.405133    1.235907    0.569778
C     -1.998461    1.852534    0.255437
H      1.461058    3.120091    0.128560
C     -0.235140    1.263450    1.063450
C      2.099040    0.513608   -0.728227
C      1.923733   -1.602906    0.996092
H      0.244642   -0.440577    1.777437
C      2.993582   -0.540796   -0.876535
C      2.089510    1.375179   -1.392683
C      2.904730   -1.614093    0.007020
H      1.814699   -2.425384    1.694691
H      3.728628   -0.522883   -1.674052
N      1.180940    0.515756    0.232009
C     -1.842714    0.066208   -0.156920
O     -1.244002   -0.490537   -1.065288
C     -3.031782   -0.406326    0.306777
H     -3.529312   -1.553796   -0.368822
H     -4.479856   -1.789576    0.110076
C     -3.678210   -1.342406   -1.431091
H     -2.833818   -2.392163   -0.272256
H      3.583966   -2.456644   -0.083218


     Py-3

E(ele)       = -592.577598
E(ele+zpe)   = -592.382684
H            = -592.369840
G            = -592.421149
C      0.735553    2.875665    0.130122
H      0.136022    3.777056    0.096848
C     -1.235228    1.300607    0.268573
H     -1.937187    2.077435    0.542039
C      1.809580    2.075595    0.240620
C      0.124390    1.662851    0.159916
C      0.995249   -0.418360    1.075806
C      1.934736    0.416397   -0.901151
C      1.850539   -1.503535    1.060673
C      0.229910   -0.251078    1.824699
C      2.804854   -0.657584   -0.976893
C      1.874937    1.206979   -1.639168
C      2.764058   -1.035680    0.017768
H      1.777291   -2.245640    1.846557
C      3.487166   -0.729205   -1.815721
N      1.072122    0.525450    0.122717
C     -1.748969    0.029141   -0.092887
O     -1.123682   -0.975381   -0.465025
C     -3.112561   -0.029622    0.037689
H     -3.698502   -1.274961   -0.301328
H     -4.771811   -1.145028   -0.155654
H     -3.486006   -1.538676   -1.341339
H     -3.323714   -2.075084    0.344048
H      3.428829   -2.487734   -0.026848


     Dbu-ts3

E(ele)       = -806.278656
E(ele+zpe)   = -805.926626
H            = -805.908113
G            = -805.972290
C      1.441943    0.783065   -2.071704
C      1.316426   -0.705335   -1.637457
C      1.049663   -0.933101   -0.168725
C      1.677061    1.813632   -0.961241
C      2.995995    1.648943   -0.206332
C      3.203020    0.192253    0.229036
H      2.242134    0.862567   -2.819541
H      0.496372   -1.173353   -2.181156
H      0.838131    1.757015   -0.259943
H      3.003128    2.312783    0.667427
H      0.507699    1.058503   -2.567174
H      2.223644   -1.261998   -1.903627
H      1.634570    2.815651   -1.403991
H      3.848403    1.943771   -0.832086
H      3.941506    0.120236    1.036573
H      3.598914   -0.394730   -0.602946
C     -0.220058   -1.760803    1.629976
```

C	0.191923	-0.499866	2.383498
C	1.668752	-0.249386	2.123629
H	-1.285851	-1.966625	1.775979
H	-0.404693	0.341503	2.008950
H	0.011923	-0.595488	3.458648
H	1.939558	0.778720	2.397427
H	2.289591	-0.927140	2.726574
H	0.347714	-2.627844	1.999045
N	1.980298	-0.442453	0.707967
N	0.006869	-1.607194	0.205263
C	-1.773934	-1.699911	-0.816164
C	-2.624406	-0.833735	-0.213841
H	-3.478207	-1.196093	0.348188
C	-1.552832	-2.652274	-1.700863
C	-2.311664	0.572906	-0.194281
O	-1.339647	1.105457	-0.713972
O	-3.221681	1.296904	0.511313
H	-2.278877	-2.795255	-2.496928
H	-0.680121	-3.292573	-1.661005
C	-2.971745	2.694743	0.566317
H	-2.013258	2.898164	1.053316
H	-2.952133	3.124504	-0.438822
H	-3.790497	3.119543	1.147269

Dbu-3

E(ele)	=	-806.315710	
E(ele+zpe)	=	-805.960047	
H	=	-805.941926	
G	=	-806.004394	
C	-0.503420	-1.679967	-1.575121
C	-0.782214	-0.171380	-1.817542
C	-0.977372	0.586119	-0.530966
C	-1.075695	-2.276271	-0.283067
C	-2.585847	-2.114241	-0.090110
C	-3.057473	-0.664504	-0.290384
H	-0.871361	-2.231921	-2.448649
H	0.045839	0.275285	-2.365905
H	-0.542598	-1.822028	0.559426
H	-2.848992	-2.451494	0.919822
H	0.583093	-1.810120	-1.545127
H	-1.678450	-0.033765	-2.430117
H	-0.829521	-3.343949	-0.258048
H	-3.144539	-2.748964	-0.789598
H	-3.987323	-0.472243	0.252133
H	-3.273577	-0.470732	-1.342854
C	-0.129830	2.072666	1.208559
C	-0.940748	1.207240	2.156858
C	-2.281800	0.880865	1.523185
H	0.908925	2.144162	1.538091
H	-0.381398	0.285997	2.341897
H	-1.096008	1.733534	3.102949
H	-2.813831	0.129183	2.114282
H	-2.921153	1.771468	1.452345
H	-0.540534	3.086044	1.118855
N	-2.083376	0.323023	0.182730
N	-0.090011	1.467282	-0.128836
C	1.125558	1.737480	-0.900882
C	2.193610	0.821178	-0.710653
H	3.095732	0.978687	-1.289515
C	1.058438	2.841271	-1.685516
C	2.188818	-0.244244	0.209096
O	1.307579	-0.576939	1.027766
O	3.344787	-0.991251	0.141904
H	1.918593	3.157837	-2.264947
H	0.149351	3.429092	-1.744128
C	3.415226	-2.079931	1.042972
H	3.324244	-1.743268	2.080110
H	2.622598	-2.809978	0.846143
H	4.392568	-2.537125	0.879635

Mtdb-ts3

E(ele)	=	-822.317891	
E(ele+zpe)	=	-821.978092	
H	=	-821.959478	
G	=	-822.023226	
C	-0.121336	1.695896	1.940823
C	-1.102174	0.323234	0.213796
C	-0.296464	-0.732644	2.224623
C	-0.525153	0.597120	2.917291
H	0.973911	1.781542	1.950450
H	-0.525296	2.664070	2.260845
H	-0.577813	-1.574796	2.864451
H	0.764543	-0.854894	1.947500
H	-1.584485	0.674609	3.187304
H	0.067074	0.670596	3.835358
C	-1.986336	-1.053746	-1.625349
C	-2.384540	-2.099127	-0.600948
C	-1.338589	-2.118428	0.495153
H	-2.786329	-0.914413	-2.359246
H	-3.364086	-1.850838	-0.176930
H	-2.451548	-3.084885	-1.071804
H	-1.649642	-2.769245	1.319614
H	-0.381161	-2.488845	0.096625
H	-1.074625	-1.355751	-2.158680
N	-1.147795	-0.781186	1.043653
N	-0.544351	1.467200	0.563032
N	-1.769974	0.233408	-0.975019
C	1.049837	2.016097	-0.549598
C	2.085416	1.164635	-0.298871
H	2.955671	1.526271	0.238902
C	0.688498	3.168203	-1.082272
C	1.996085	-0.238238	-0.583690
O	1.045304	-0.828278	-1.091202
O	3.110931	-0.915435	-0.193160
H	1.329909	3.608174	-1.841783
H	-0.217884	3.687317	-0.797010
C	3.105119	-2.309310	-0.464311
H	2.296071	-2.808645	0.077618
H	2.979367	-2.496012	-1.534279
H	4.071236	-2.681398	-0.123153
C	-1.861792	1.380587	-1.856883
H	-1.885751	2.291531	-1.261608
H	-1.014382	1.429902	-2.550513
H	-2.791234	1.293799	-2.429006

Mtdb-3

E(ele)	=	-822.354812	
E(ele+zpe)	=	-822.011430	
H	=	-821.993217	
G	=	-822.055411	
C	1.323858	1.967646	-1.101199
C	0.932244	0.011251	0.355080
C	1.885468	-0.299226	-1.839837
C	2.400238	1.123678	-1.754374
H	0.496157	2.133110	-1.801420
H	1.705006	2.945192	-0.796200
H	2.625712	-0.965350	-2.292260
H	0.947481	-0.357167	-2.409816
H	3.327408	1.142279	-1.170701
H	2.615605	1.522950	-2.749897
C	0.152196	-1.910744	1.604843
C	1.278256	-2.728177	0.998434
C	1.507403	-2.239669	-0.418732
H	0.009120	-2.154412	2.659841
H	2.186659	-2.603438	1.598442
H	1.021154	-3.791618	0.979866
H	2.419322	-2.674946	-0.839605
H	0.655401	-2.517186	-1.055690
H	-0.794030	-2.081215	1.074753
N	1.650556	-0.784280	-0.482652
N	0.752166	1.318476	0.091091
N	0.497417	-0.493173	1.527232
C	-0.480631	1.989688	0.525898
C	-1.717743	1.320838	0.282660
H	-2.607569	1.802541	0.671463
C	-0.310650	3.219682	1.067408
C	-1.910010	0.156368	-0.472740
O	-1.067850	-0.574262	-1.045206
O	-3.241228	-0.200878	-0.546672
H	-1.168955	3.835746	1.309488
H	0.679126	3.611823	1.276383
C	-3.519396	-1.360939	-1.305504
H	-3.162505	-1.258386	-2.334722
H	-3.052069	-2.248736	-0.864772
H	-4.605310	-1.469997	-1.292703
C	0.201607	0.326407	2.696440
H	0.758482	1.259949	2.647268
H	-0.866702	0.557125	2.767346
H	0.525115	-0.235116	3.578006

9.2.2 *E*-type addition

IPr-ts3′

E(ele) = −1503.943816
E(ele+zpe) = −1503.265357
H = −1503.226677
G = −1503.334527

```
C   -1.500903   -0.208035   -2.170859
C   -0.170617   -0.128946   -2.401935
C   -0.463027   -0.028463   -0.146102
N   -1.655329   -0.149757   -0.790920
N    0.439349   -0.033795   -1.158069
C   -2.941178   -0.138622   -0.147675
C   -3.456514    1.092103    0.294237
C   -3.626005   -1.353665   -0.002322
C   -4.719048    1.078546    0.890700
C   -4.887716   -1.312293    0.597743
C   -5.429711   -0.109465    1.036440
H   -5.151666    2.005519    1.253887
H   -5.451217   -2.231117    0.728200
H   -6.411038   -0.097083    1.502514
C    1.846387    0.240235   -1.014006
C    2.240640    1.581677   -0.924040
C    2.751943   -0.831207   -1.012294
C    3.609954    1.841769   -0.832011
C    4.109118   -0.518534   -0.920706
C    4.533942    0.804826   -0.836109
H    3.956455    2.867389   -0.743464
H    4.842621   -1.319903   -0.899371
H    5.595346    1.026717   -0.760804
C   -2.986871   -2.670597   -0.414609
H   -2.333153   -2.477717   -1.273053
C   -4.006519   -3.728928   -0.842773
H   -4.700245   -3.343775   -1.597596
H   -3.484630   -4.593369   -1.265414
H   -4.593850   -4.091340    0.008218
C   -2.105435   -3.202418    0.725598
H   -1.329132   -2.481976    1.001312
H   -2.714503   -3.396341    1.616522
H   -1.623393   -4.140465    0.427649
C    2.279593   -2.270974   -1.129103
H    1.255506   -2.313552   -0.736076
C    3.134841   -3.246809   -0.313347
H    4.113643   -3.403835   -0.782132
H    3.298276   -2.886829    0.706328
H    2.638987   -4.222689   -0.269412
C    2.251903   -2.716329   -2.599366
H    3.258989   -2.661048   -3.029624
H    1.904094   -3.752632   -2.677807
H    1.592010   -2.090883   -3.207286
C   -2.669031    2.384760    0.131110
H   -1.605837    2.141371    0.246518
C   -2.864895    2.973188   -1.273607
H   -2.556959    2.270232   -2.053751
H   -3.918614    3.228613   -1.437948
H   -2.268423    3.886114   -1.386988
C   -3.004062    3.433113    1.194319
H   -2.932922    3.020680    2.206449
H   -2.298614    4.266627    1.119457
H   -4.010367    3.845501    1.058772
C    1.231789    2.717386   -0.886331
H    0.277072    2.340659   -1.274964
C    1.006204    3.176626    0.560743
H    0.679512    2.348787    1.196972
H    1.940200    3.558329    0.988746
H    0.257161    3.978692    0.588437
C    1.644301    3.897243   -1.773842
H    1.869361    3.574084   -2.795790
H    0.832619    4.631796   -1.815373
H    2.526673    4.410746   -1.377047
C   -2.344661   -0.296283   -2.839500
H    0.398201   -0.105532   -3.318824
C    0.127579   -0.401629    1.935194
C    1.295516   -1.082385    2.017819
C   -0.864930    0.180741    2.578011
H    1.325856   -2.164146    1.923036
H   -1.666862    0.718059    2.089075
H   -0.872566    0.112284    3.663758
C    2.538541   -0.354828    2.177851
O    2.690332    0.854293    2.173941
O    3.591788   -1.204141    2.366701
C    4.841375   -0.567963    2.596012
H    5.570021   -1.373094    2.699847
H    5.102475    0.082064    1.756328
H    4.805496    0.032252    3.509571
```

IPr-3′

E(ele) = −1503.999564
E(ele+zpe) = −1503.318323
H = −1503.279542
G = −1503.389224

```
C   -1.209579   -1.168483    1.984579
C    0.099727   -1.512602    2.025853
C   -0.223735   -0.299690    0.178357
N   -1.395725   -0.422572    0.833356
N    0.697552   -0.961214    0.907120
C   -2.674596    0.142269    0.464126
C   -3.669433   -0.741921    0.020809
C   -2.871190    1.523101    0.597946
C   -4.928731   -0.203300   -0.247605
C   -4.147770    2.009238    0.304272
C   -5.169209    1.158871   -0.102136
H   -5.726832   -0.856400   -0.590050
H   -4.338699    3.075676    0.388715
H   -6.153964    1.561547   -0.321293
C    2.088861   -1.172405    0.574151
C    2.403405   -2.097204   -0.428763
C    3.053702   -0.467605    1.308749
C    3.760086   -2.331857   -0.669384
C    4.392460   -0.748967    1.035143
C    4.744454   -1.674905    0.058577
H    4.047076   -3.036487   -1.445464
H    5.170719   -0.222406    1.580530
```

```
H    5.792450   -1.874042   -0.145815
C   -1.771693    2.491984    0.994741
C   -0.851219    1.929654    1.182999
C   -2.128029    3.239815    2.285706
H   -2.319307    2.545828    3.111650
H   -1.304109    3.901173    2.573523
H   -3.021756    3.859819    2.152661
C   -1.476359    3.466148   -0.154068
H   -1.259934    2.929156   -1.082814
H   -2.328862    4.135382   -0.323448
H   -0.602878    4.078364    0.093584
C    2.692234    0.584291    2.344788
H    1.619388    0.797476    2.260180
H    3.439964    1.902628    2.100863
H    4.513405    1.787888    2.287455
C    3.308381    2.263342    1.075992
C    3.067250    2.669978    2.787679
C    2.964818    0.070408    3.765157
H    4.030942   -0.148643    3.894908
H    2.681096    0.825464    4.506216
H    2.408966   -0.848053    3.982273
C   -3.413473   -2.224836   -0.200947
H   -2.334870   -2.406763   -0.121007
C   -4.122897   -3.073733    0.862716
H   -3.811955   -2.802308    1.876844
H   -5.208305   -2.934474    0.801470
H   -3.908390   -4.136999    0.711315
C   -3.842272   -2.667816   -1.606010
H   -3.383855   -2.045832   -2.380323
H   -3.543356   -3.707440   -1.776769
H   -4.929498   -2.612722   -1.726905
C    1.357400   -2.816230   -1.262188
H    0.361394   -2.492541   -0.939966
C    1.498045   -2.438552   -2.742262
H    1.459758   -1.352986   -2.873647
H    2.443892   -2.811519   -3.152222
H    0.680182   -2.882390   -3.320382
C    1.435946   -4.334754   -1.059562
H    1.317007   -4.603434   -0.004091
H    0.647465   -4.833321   -1.633585
H    2.398526   -4.731187   -1.401399
C   -2.027703   -1.369298    2.658130
H    0.668663   -2.099004    2.730160
C    0.015849    0.454871   -1.061776
C    1.095080    1.372176   -0.952810
C   -0.843560    0.182088   -2.091977
H    1.629103    1.466947   -0.017230
H   -1.614978   -0.573463   -1.979155
H   -0.739847    0.689939   -3.041817
C    1.419732    2.270906   -1.994822
O    0.894628    2.353698   -3.106034
O    2.441376    3.133864   -1.641472
C    2.804722    4.062195   -2.647444
H    3.610700    4.663782   -2.222932
H    3.151323    3.548995   -3.549728
H    1.958072    4.700531   -2.918202
```

Pph-ts3′

E(ele) = −1380.357039
E(ele+zpe) = −1379.978608
H = −1379.953912
G = −1380.033474

```
C    1.848263    1.013760    1.595965
C    0.162483   -0.007055    3.227521
C    0.692363    0.420522    2.088310
P   -0.563555   -0.038195    0.455669
C    2.951201    0.179915    1.195449
O    3.046317   -1.033248    1.318587
O    3.955647    0.913202    0.622135
C    5.088367    0.156414    0.223467
H    4.804028   -0.611486   -0.502746
H    5.780648    0.870671   -0.224403
H    5.552447   -0.332825    1.084745
C   -2.170758   -0.925403    0.336367
C   -2.478881   -1.838742   -0.678565
C   -3.129994   -0.642095    1.317070
C   -3.726421   -2.459265   -0.706293
H   -1.748451   -2.062499   -1.451213
C   -4.377168   -1.260142    1.283992
C   -2.904301    0.075131    2.104675
C   -4.675466   -2.173650    0.273441
H   -3.956610   -3.165187   -1.499260
H   -5.114247   -1.031411    2.048251
H   -5.646029   -2.660588    0.249104
C    0.570460   -0.879294   -0.678783
C    1.413354   -0.149662   -1.521545
C    0.749718   -2.262468   -0.547270
C    2.415065   -0.803179   -2.239101
H    1.305035    0.928384   -1.603852
C    1.740344   -2.910915   -1.272869
H    0.132197   -2.828976    0.146423
C    2.576918   -2.180066   -2.117734
H    3.075503   -0.227133   -2.880984
H    1.880166   -3.981400   -1.157493
H    3.364174   -2.685800   -2.669753
C   -0.939784    1.585686   -0.291438
C   -0.847805    2.748597    0.477693
C   -1.394811    1.665293   -1.612763
C   -1.201270    3.980246   -0.072350
H   -0.500791    2.692526    1.506856
C   -1.746550    2.895472   -2.159988
H   -1.471235    0.762067   -2.214991
C   -1.648354    4.054722   -1.389366
H   -1.126713    4.880665    0.530180
H   -2.097699    2.949803   -3.186298
H   -1.922595    5.014988   -1.816767
H    1.882641    2.071730    1.358045
H    0.716742    0.140707    4.151783
H   -0.794941   -0.518241    3.279651
```

Pph-3′

E(ele) = −1380.379514
E(ele+zpe) = −1379.999212
H = −1379.974305
G = −1380.055670

```
C   -2.277975   -0.060462   -0.440937
C   -0.820471    0.308435   -2.503950
C   -1.072175    0.060630   -1.181625
P    0.379480   -0.004900   -0.122029
C   -3.540675    0.125923   -1.065204
O   -3.758995    0.389122   -2.246612
O   -4.586743   -0.017545   -0.178850
C   -5.873029    0.146608   -0.749719
H   -6.050538   -0.593294   -1.536033
H   -6.582576    0.006536    0.067485
H   -5.986694    1.144695   -1.183400
C    1.929064   -0.173291   -1.050190
C    2.550505   -1.416854   -1.192852
C    2.478558    0.959294   -1.664418
H    3.714386   -1.527155   -1.951665
C    3.639255    0.841808   -2.422342
C    1.995556    1.927356   -1.554701
H    4.257056   -0.400900   -2.566065
H    4.060646    1.720548   -2.900857
H    5.163786   -0.488967   -3.157502
C    0.254584   -1.436967    0.981128
C    0.771510   -1.421441    2.278678
C   -0.351368   -2.594032    0.475434
C    0.698227   -2.569104    3.065628
H    1.213329   -0.515890    2.684768
C   -0.415621   -3.738344    1.266373
C   -0.788618   -2.585083   -0.520575
C    0.110838   -3.726552    2.557737
H    1.092701   -2.554953    4.077068
H   -0.890245   -4.633975    0.877472
H    0.053018   -4.618941    3.174185
C    0.552689    1.512987    0.855482
C   -0.514688    2.412333    0.942610
C    1.768190    1.796638    1.493038
C   -0.364168    3.584625    1.681530
H   -1.450571    2.186504    0.435944
C    1.906035    2.966304    2.234417
C    2.612014    1.116651    1.394393
C    0.838014    3.858994    2.330215
H   -1.191298    4.284916    1.745986
H    2.848495    3.183997    2.727898
H    0.947615    4.774047    2.905225
H   -2.267055   -0.321813    0.611463
H   -1.652932    0.450258   -3.182479
H    0.188192    0.353656   -2.896763
```

Hmpt-ts3′

E(ele) = −1089.223171
E(ele+zpe) = −1088.867107
H = −1088.844035
G = −1088.917752

```
C    1.843820   -0.990806    0.515357
C    0.798162   -0.654661    1.332133
P   -1.058815    0.006954    0.117593
C    2.975055   -0.104544    0.366366
O    3.151027    0.976448    0.909280
O    3.901765   -0.625904   -0.487990
C    5.071515    0.162534   -0.657370
H    5.572737    0.321746    0.301065
H    5.712998   -0.402054   -1.334556
H    4.823831    1.136443   -1.089155
C   -2.738465    0.182551    0.512598
N   -0.802349    1.516063   -0.567326
C   -1.071856   -1.177576   -1.090387
H   -0.795714   -2.569083   -0.766954
H   -1.711950   -3.178375   -0.808849
H   -0.075492   -2.985477   -1.482306
C   -0.379249   -2.657941    0.239529
H   -1.794397   -1.009369   -2.339109
H   -1.798631    0.037734   -2.641762
H   -1.292820   -1.586146   -3.125352
C   -2.837015   -1.358749   -2.266320
H   -3.441837   -1.057886    0.813926
H   -3.281121   -1.789007    0.018622
H   -3.130390   -1.505161    1.773053
C   -4.515749   -0.849263    0.869919
H   -3.064569    1.235858    1.469447
C   -2.501684    2.142602    1.236811
H   -4.134871    1.462017    1.400451
C   -2.844282    0.944365    2.509498
C   -1.749240    2.229083   -1.413209
H   -1.420035    2.241372   -2.462662
C   -2.736819    1.767965   -1.349013
H   -1.825241    3.270860   -1.074234
C    0.554558    2.053070   -0.611792
H    0.494664    3.147191   -0.606440
H    1.134295    1.744348    0.259613
H    1.089717    1.737596   -1.519576
C    0.431445   -0.522088    2.598767
H   -0.516679   -0.089745    2.902061
H    1.121928   -0.848989    3.373758
H    1.827640   -1.891902   -0.087950
```

Hmpt-3′

E(ele) = −1089.258549
E(ele+zpe) = −1088.899959
H = −1088.876772
G = −1088.950572

```
C    1.704266    0.026920   -0.187971
C    0.617953    0.018737    0.726117
P   -1.005070    0.010648   -0.021563
O    3.047257    0.049136    0.268052
O    3.441885    0.071483    1.433660
O    3.953747    0.041676   -0.772697
```

```
C    5.312567    0.061324   -0.374169
H    5.557458   -0.815002    0.233650
H    5.894518    0.054368   -1.297480
H    5.539194    0.959215    0.208764
C   -2.297323   -0.281192    0.997122
N   -1.389114    1.497296   -0.646270
C   -1.002745   -1.181958   -1.180074
C   -0.220061   -2.412329   -1.048887
H   -0.881214   -3.268937   -0.854639
H    0.323852   -2.592290   -1.982478
H    0.508632   -2.321007   -0.243031
C   -2.095188   -1.278887   -2.136726
H   -2.494844   -0.290577   -2.370580
H   -1.711968   -1.714716   -3.065240
H   -2.912594   -1.915318   -1.765139
C   -2.599361   -1.647931    1.407859
H   -2.319997   -2.354353    0.624039
H   -2.067373   -1.917857    2.329973
H   -3.677802   -1.735530    1.580940
C   -2.784793    0.725630    1.936874
H   -2.380498    1.708684    1.689396
H   -3.880623    0.766105    1.891695
H   -2.487046    0.480409    2.964084
C   -2.743333    1.887466   -1.019642
H   -2.823414    2.022169   -2.106828
H   -3.466900    1.136469   -0.697462
H   -2.993061    2.841919   -0.538668
C   -0.368224    2.462610   -1.056217
H   -0.663138    3.454562   -0.695886
H    0.600837    2.200493   -0.630005
C   -0.280941    2.494355   -2.149820
C    0.576813    0.020256    2.096939
H   -0.363105   -0.013572    2.635559
H    1.498996    0.053836    2.663445
H    1.528931   -0.015036   -1.257370
```

Quin-ts3i′

E(ele) = −673.546736
E(ele+zpe) = −673.245461
H = −673.230467
G = −673.286763

```
C    1.619027    0.829428    0.794626
C    0.294051    2.717204   -0.283297
C    1.099406    3.444566   -0.317316
H   -0.664531    3.021868   -0.684133
C    1.820076    0.899660    1.857904
C    0.568655    1.529177    0.227193
C    2.506575    0.069921   -0.033202
O    2.412812   -1.133591   -1.240279
C    3.548949   -0.453205    0.684543
C    4.491575   -1.190767   -0.078216
H    4.965875   -0.555081   -0.831340
H    5.233605   -1.550915    0.635476
C    4.011319   -2.032142   -0.585621
C   -0.639370   -0.598835   -0.875954
C   -1.242190   -0.098369    1.416370
C   -2.218917    1.168005   -0.383957
C   -1.870297   -1.495160   -1.141663
H    0.186550   -1.152252   -0.424240
C   -0.245677   -0.127961   -1.779707
C   -2.228319   -1.282959    1.308773
H   -1.636694    0.707567    2.045191
H   -0.269373   -0.399970    1.815984
C   -2.353219    2.070694    0.219229
H   -0.049292    1.468244   -1.422678
C   -3.438326    0.219033   -0.261169
H   -1.575238   -2.549500   -1.127396
H   -2.292335   -1.290904   -2.132948
H   -2.963248   -2.232812    2.119227
H   -1.698267   -2.237259    1.408310
C   -4.067119    0.512650    0.587539
H   -4.056359    0.283729   -1.162811
N   -0.990502    0.486835    0.080280
C   -2.919663   -1.210723   -0.059428
H   -3.742859   -1.929397   -0.117204
```

Quin-3i′

E(ele) = −673.551293
E(ele+zpe) = −673.247766
H = −673.232738
G = −673.289301

```
C    1.545380    0.897015    0.638586
C    0.161675    2.692841   -0.386868
C    1.039043    3.326901   -0.438388
H   -0.778817    3.144487   -0.677721
C    1.971710    1.465741    1.457645
C    0.346610    1.440650    0.050137
C    2.410168    0.014391   -0.043491
O    2.238131   -0.555950   -1.130496
C    3.586865   -0.190911    0.648034
C    4.523407   -1.030690   -0.000009
H    4.795167   -0.634587   -0.984099
H    5.399120   -1.057737    0.649989
C    4.123118   -2.040574   -0.135241
C   -0.582204   -0.711785   -0.831775
C   -1.178972    0.021399    1.433728
C   -2.157629    1.130058   -0.490816
C   -1.841287   -1.572299   -1.029398
H    0.215630   -1.243034   -0.315469
C   -0.152255   -0.233849   -1.759684
C   -2.141318   -1.178956    1.405024
H   -1.598495    0.884422    1.960685
H   -0.202955   -0.209445    1.864698
C   -2.285667    2.075799    0.035224
H   -1.988412    1.337269   -1.550797
C   -3.368480    0.202862   -0.252953
H   -1.563091   -2.628978   -0.968084
H   -2.274546   -1.408173   -2.022930
H   -2.858785   -1.087907    2.226867
H   -1.589642   -2.113633    1.555233
```

```
H    -3.972873    0.577070    0.581126
H    -4.006195    0.202133   -1.142500
N    -0.901885    0.494439    0.028520
C    -2.861978   -1.208802    0.051625
H    -3.691052   -1.922200    0.066694
```

Quin-ts3′

```
E(ele)        = -673.549379
E(ele+zpe)    = -673.246387
H             = -673.232050
G             = -673.286255
C     1.479087    0.374728    0.897634
C     0.457835    2.449483   -0.039779
H     1.387143    2.986187    0.109398
H    -0.320470    2.959293   -0.596411
C     1.533187    0.041832    1.927197
C     0.410645    1.190913    0.403758
O     2.628676    0.316758   -1.190383
O     3.560521   -0.617938    0.649412
C     4.627988   -1.009606   -0.194077
H     5.105037   -0.140878   -0.657166
H     5.338863   -1.531995    0.449159
H     4.280179   -1.676028   -0.990072
C    -0.665470   -0.625134   -0.886606
C    -1.365642   -0.258759    1.435642
C    -2.083918    1.275918   -0.306707
C    -1.981661   -1.298520   -1.313054
H     0.045041   -1.312789   -0.425507
H    -0.139421   -0.117444   -1.698433
C    -2.435861   -1.324340    1.131874
H    -1.731575    0.531508    2.098196
H    -0.460951   -0.689926    1.864114
C    -2.125669    2.153642    0.341716
H    -1.829279    1.601453   -1.318009
C    -3.395410    0.466025   -0.284516
H    -1.817417   -2.374396   -1.429832
H    -2.320304   -0.915698   -2.282726
H    -3.202877   -1.303606    1.912621
H    -1.990268   -2.325416    1.137267
H    -3.999413    0.736477    0.589017
H    -3.984592    0.706494   -1.174837
N    -0.945454    0.426345    0.165959
C    -3.046474   -1.025861   -0.242250
H    -3.936998   -1.637179   -0.414628
```

Quin-3′

```
E(ele)        = -673.556342
E(ele+zpe)    = -673.252420
H             = -673.237437
G             = -673.293184
C     1.418446   -0.215216   -0.061807
C     0.630776    2.172008    0.000502
H     1.652084    2.527499    0.017632
H    -0.165003    2.898573    0.047696
C     1.141204   -1.259687   -0.088775
C     0.457129    0.826768   -0.047995
C     2.808900    0.055856   -0.012671
O     3.374923    1.147124    0.031992
O     3.552950   -1.108804   -0.017593
C     4.955005   -0.913871    0.031199
H     5.246412   -0.378819    0.940071
H     5.395425   -1.912622    0.022796
H     5.302090   -0.339772   -0.833259
C    -1.244381   -0.564939   -1.253521
C    -1.177797   -0.531694    1.220768
C    -2.030870    1.374043   -0.035231
C    -2.516006   -1.402653   -1.037071
H    -0.357964   -1.169461   -1.429299
C    -1.336677    0.138579   -2.085734
C    -2.660577   -0.902155    1.396035
H    -0.776594    0.070684    2.038494
H    -0.543474   -1.410085    1.113436
H    -1.948425    1.883751    0.926983
H    -1.762532    2.075211   -0.824478
C    -3.427259    0.764852   -0.260283
H    -2.255923   -2.424086   -0.736588
H    -3.066274   -1.471592   -1.980675
H    -3.135032   -0.265464    2.151327
H    -2.733240   -1.935374    1.749543
H    -4.148075    1.269566    0.390451
H    -3.754066    0.926540   -1.293613
N    -0.981047    0.294195   -0.035046
C    -3.369459   -0.733476    0.047682
H    -4.373026   -1.166508    0.078488
```

Dabco-ts3i′

```
E(ele)        = -689.565632
E(ele+zpe)    = -689.275959
H             = -689.261072
G             = -689.317946
C     1.609032    0.846180    0.780041
C     0.265138    2.724057   -0.289752
H     1.068093    3.453581   -0.327997
H    -0.700192    3.031269   -0.672639
C     1.826796    0.957681    1.836480
C     0.548568    1.531951    0.207580
C     2.492134    0.071228   -0.035745
O     2.386472   -0.163855   -1.236941
O     3.544412   -0.428615    0.683666
C     4.483832   -1.180406   -0.069174
H     4.953578   -0.559568   -0.837422
H     5.230221   -1.525067    0.647665
H     4.002257   -2.032594   -0.556910
C    -0.634275   -0.619324   -0.865232
C    -1.242694   -0.077660    1.411934
C    -2.217036    1.144515   -0.412075
H    -1.871612   -1.540656   -1.035030
H     0.221976   -1.139453   -0.431621
C    -0.294630   -0.169611   -1.801454
H    -2.277057   -1.226276    1.286490
H    -1.607011    0.743737    2.038696
```

```
H    -0.279232   -0.414348    1.806616
H    -2.394185    2.031448    0.203605
H    -2.041510    1.461759   -1.444631
C    -3.397130    0.130816   -0.312527
H    -1.590286   -2.591658   -0.918671
H    -2.316132   -1.425067   -2.028938
H    -3.059599   -1.126240    2.045135
H    -1.800484   -2.201677    1.426408
H    -4.080480    0.411146    0.495887
H    -3.970746    0.115067   -1.244316
N    -0.982471    0.486343    0.067790
N    -2.898800   -1.215942   -0.040469
```

Dabco-3i′

```
E(ele)        = -689.569493
E(ele+zpe)    = -689.277397
H             = -689.262547
G             = -689.318326
C     1.534265    0.868805    0.667460
C     0.177919    2.676046   -0.387076
H     1.054354    3.312716   -0.417953
H    -0.756998    3.123457   -0.702204
C     1.947310    1.423948    1.502472
C     0.354724    1.425804    0.054961
C     2.412911    0.014088   -0.034632
O     2.243936   -0.526996   -1.136622
O     3.588577   -0.200351    0.652230
C     4.529894   -1.022004   -0.014146
H     4.795081   -0.606547   -0.990875
H     5.407484   -1.053741    0.633869
C     4.136271   -2.032233   -0.164458
C    -0.548483   -0.786217   -0.718726
C    -1.271243    0.126117    1.432528
C    -2.117113    1.079629   -0.624874
C    -1.809651   -1.670970   -0.831159
H     0.249860   -1.253598   -0.144082
H    -0.118135   -0.492375   -1.676760
C    -2.311532   -1.019682    1.399430
H    -1.661920    1.041781    1.886940
H    -0.334087   -0.141254    1.926242
C    -2.314088    2.036914   -0.141813
H    -1.869462    1.254881   -1.675149
C    -3.314374    0.107931   -0.436048
H    -1.566334   -2.704273   -0.568102
H    -2.200334   -1.673417   -1.853610
H    -3.125688   -0.811001    2.100076
H    -1.852332   -1.967672    1.696001
H    -4.030578    0.520816    0.281197
H    -3.838143   -0.033303   -1.385940
N    -0.902736    0.486726    0.018211
N    -2.869587   -1.190099    0.056500
```

Dabco-ts3′

```
E(ele)        = -689.567005
E(ele+zpe)    = -689.275602
H             = -689.261427
G             = -689.315495
C     1.474474    0.340761    0.891035
C     0.459085    2.440048   -0.007055
H     1.386271    2.977308    0.152963
H    -0.321601    2.957585   -0.553073
C     1.519987   -0.016118    1.912996
C     0.415941    1.173067    0.411230
C     2.552905    0.067604    0.016472
O     2.651342    0.348287   -1.182465
O     3.560049   -0.641544    0.639418
C     4.650977   -0.986414   -0.195104
H     5.133648   -0.092788   -0.601790
H     5.348511   -1.536113    0.439719
C     4.327583   -1.613632   -1.031809
C    -0.692721   -0.618678   -0.903912
C    -1.370616   -0.283661    1.421097
C    -2.089385    1.273162   -0.290849
C    -2.034364   -1.302542   -1.257861
H     0.049149   -1.297868   -0.480474
H    -0.219528   -0.097587   -1.739996
C    -2.492602   -1.291854    1.076690
H    -1.695400    0.497610    2.114992
H    -0.478138   -0.767925    1.819129
C    -2.158674    2.123655    0.391636
H    -1.833600    1.639117   -1.287741
C    -3.379361    0.413339   -0.309197
H    -1.900993   -2.386307   -1.321716
H    -2.411137   -0.958272   -2.226179
H    -3.290481   -1.240863    1.823525
H    -2.106223   -2.315657    1.070372
H    -4.021314    0.655790    0.543555
H    -3.948832    0.612430   -1.221690
N    -0.950811    0.418010    0.163060
N    -3.054383   -1.009910   -0.245248
```

Dabco-3′

```
E(ele)        = -689.573735
E(ele+zpe)    = -689.281265
H             = -689.266454
G             = -689.321975
C     1.416875   -0.218972   -0.034772
C     0.624599    2.169262    0.005207
H     1.644190    2.529559    0.021807
H    -0.175266    2.892418    0.031220
C     1.140943   -1.264063   -0.043818
C     0.456792    0.822979   -0.028729
C     2.807945    0.055607   -0.007762
O     3.370087    1.149174    0.014226
O     3.554113   -1.106506   -0.007496
C     4.956693   -0.908001    0.017319
H     5.259910   -0.358316    0.913379
H     5.398957   -1.905865    0.017879
H     5.289199   -0.346699   -0.861067
C    -1.238043   -0.567592   -1.240973
C    -1.199455   -0.534593    1.226011
C    -2.033070    1.366167   -0.031052
```

```
C    -2.565119   -1.335119   -1.036483
H    -0.379449   -1.221752   -1.375629
C    -2.688430   -0.948594    1.309090
H    -0.865843    0.086982    2.060090
H    -0.531287   -1.391301    1.157732
H    -1.939621    1.902409    0.915399
H    -1.791671    2.047061   -0.847121
C    -3.424491    0.711899   -0.209476
H    -2.373498   -2.378163   -0.765854
H    -3.146294   -1.334697   -1.963229
H    -3.216795   -0.372852    2.075323
H    -2.767987   -2.006231    1.576543
H    -4.139430    1.160578    0.486153
H    -3.803517    0.873497   -1.223335
N    -0.982671    0.290393   -0.023447
N    -3.362228   -0.727282    0.030069
```

Dmap-ts3′

```
E(ele)        = -726.471481
E(ele+zpe)    = -726.205636
H             = -726.187938
G             = -726.252289
C    -1.670269    2.598978    0.343049
H    -2.540618    3.228737    0.189361
H    -2.403837    0.374385   -0.719498
C    -2.168177   -0.076188   -1.678029
H    -0.880828    2.960269    0.992923
C    -1.669952    1.394036   -0.203901
C     0.405783   -0.478883    0.073354
C     1.227097    1.641252   -0.237419
C     1.674476   -1.022570    0.138781
H    -0.495441   -1.087978    0.153172
C     2.537108    1.203831   -0.191522
C     0.984666    2.690273   -0.400705
C     2.800641   -0.174047    0.008845
H     1.781740   -2.089255    0.289828
H     3.335957    1.923222   -0.319586
N     0.185446    0.821753   -0.100285
H    -3.525061   -0.158946    0.028951
O    -3.942499    0.197706    1.115854
O    -4.119884   -1.181939   -0.657655
H    -5.253534   -1.750134   -0.017340
H    -5.615251   -2.528351   -0.690202
H    -4.978753   -2.178729    0.950664
H    -6.026870   -0.994047    0.142864
H     4.071737   -0.656861    0.066195
C     4.297356   -2.079472    0.247072
H     5.370090   -2.270722    0.254899
H     3.879017   -2.432546    1.197572
H     3.851038   -2.660285   -0.569583
C     5.196737    0.249544   -0.073132
H     5.194306    0.744401   -1.052630
H     5.185318    1.019259    0.708275
H     6.123305   -0.316288    0.020772
```

Dmap-3′

```
E(ele)        = -726.492194
E(ele+zpe)    = -726.223352
H             = -726.205929
G             = -726.268414
C     1.558658    2.065344   -0.865535
C     2.575933    2.417327   -0.966045
H     2.139504   -0.171369    0.230617
C     1.704410   -0.960122    0.832686
C     0.747174    2.628452   -1.315192
C     1.325167    0.860613   -0.280808
C    -0.585051   -0.588690   -0.760369
C    -1.912731   -0.933158   -0.693135
H     0.161143   -1.173761   -1.287097
C    -2.285871    1.045970    0.637547
C    -0.472060    2.185965    0.981234
C    -2.824934   -0.111189    0.020314
H    -2.234604   -1.831137   -1.203350
C    -2.900147    1.718729    1.220872
N    -0.110648    0.524825   -0.168095
C     3.550392   -0.130509    0.069707
O     4.213829    0.729852   -0.504250
O     4.169991   -1.217002    0.650212
C     5.580936   -1.229922    0.527071
H     5.917927   -2.124042    1.054668
H     5.883729   -1.273889   -0.523693
C     6.022964   -0.335347    0.976073
N    -4.138694   -0.420040    0.109815
C    -4.645705   -1.630856   -0.517562
H    -5.713232   -1.712575   -0.317634
H    -4.499888   -1.605643   -1.603725
C    -4.151410   -2.521631   -0.112943
H    -5.041573    0.453488    0.843170
H    -4.766214    0.510374    1.902957
H    -5.039729    1.464882    0.420744
H    -6.053314    0.056530    0.772391
```

Py-ts3′

```
E(ele)        = -592.553284
E(ele+zpe)    = -592.361192
H             = -592.348054
G             = -592.401119
C     0.002642    2.388968    0.234123
H    -0.745767    3.145264    0.022928
C    -1.122383    0.280360   -0.704961
C    -0.960156   -0.294739   -1.610807
H     0.826676    2.650003    0.889554
C    -0.198640    1.165633   -0.237893
C     1.423028   -1.004652    0.252873
C     2.617905    0.900658   -0.301138
C     2.588536   -1.752912    0.376750
C     0.421433   -1.409768    0.396571
C     3.828402    0.223886   -0.209487
H     2.544604    1.951191   -0.575741
C     3.809544   -1.125516    0.139998
```

```
H     2.535483   -2.800813    0.651480
H     4.758947    0.742051   -0.414514
N     1.461374    0.284778   -0.066023
C    -2.368743    0.093044    0.009056
O    -2.737740    0.635441    1.035367
C    -3.154999   -0.825758   -0.629636
C    -4.414374   -1.064847   -0.017160
H    -4.920644   -1.790273   -0.654819
H    -4.286140   -1.467610    0.991462
H    -4.995612   -0.141022    0.046616
H     4.738031   -1.682932    0.220612
```

Py-3′

```
E(ele)        = -592.569047
E(ele+zpe)    = -592.374549
H             = -592.361535
G             = -592.413665
C     0.068147    2.033089   -0.593033
C     1.030205    2.517886   -0.684792
C     0.965715   -0.228864    0.208495
H     0.656242   -1.127761    0.728050
H    -0.824779    2.533272   -0.953026
C     0.017186    0.767683   -0.151715
C    -1.702884   -0.860629   -0.780147
C    -2.244090    0.821145    0.764563
C    -2.986226   -1.375203   -0.715282
C    -0.903608   -1.263067   -1.393061
C    -3.544609    0.348548    0.867830
H    -1.851296    1.668993    1.313976
C    -3.920432   -0.762704    0.119849
H    -3.244441   -2.237328   -1.318634
N    -1.365001    0.219271   -0.052892
C     2.355395    0.014030    0.019385
O     2.875505    1.016005   -0.462967
C     3.127053   -1.039711    0.449085
C     4.524497   -0.850809    0.301767
H     4.989405   -1.759550    0.687140
H     4.791517   -0.703475   -0.748888
H     4.863266    0.020016    0.870791
H    -4.930770   -1.153599    0.189899
```

Dbu-ts3′

```
E(ele)        = -806.273736
E(ele+zpe)    = -805.921855
H             = -805.903451
G             = -805.967326
C    -0.419985   -1.810825    0.897088
C     0.162045   -0.509654    1.515860
C     1.191076    0.222970    0.681352
C     0.161432   -2.192300   -0.467442
C     1.597407   -2.722803   -0.363202
C     2.437357   -1.884059    0.606480
H    -0.274213   -2.646538    1.594456
H    -0.647618    0.192559    1.723630
H     0.122106   -1.314139   -1.126732
H     2.068351   -2.739115   -1.354445
H    -1.500170   -1.675595    0.803220
H     0.640237   -0.723926    2.480523
H    -0.473209   -2.950227   -0.939200
H     1.591796   -3.757791    0.002410
H     3.498368   -2.147173    0.544688
H     2.128983   -2.075176    1.638218
C     1.980758    2.192801   -0.380221
C     2.669526    1.272752   -1.383381
C     3.277333    0.100735   -0.627929
H     1.483281    3.029706   -0.879843
H     1.923550    0.908263   -2.099858
H     3.448927    1.800704   -1.940952
H     3.559122   -0.697978   -1.323662
H     4.186651    0.412437   -0.096191
N     2.721889    2.619548    0.311644
C     2.322642   -0.454481    0.334992
H     0.975371    1.463967    0.372927
C    -0.869620    2.079831    0.084358
C    -1.551983    1.219028   -0.724896
C    -1.260491    1.068958   -1.759890
C    -0.905352    1.595244    0.789483
C    -2.591767    0.384973   -0.182592
H    -3.003021    1.364962    0.969046
O    -3.109000   -0.447149   -1.139517
O    -1.765662    3.847968    0.671267
H    -0.127591    3.471001    1.491942
C    -4.170618   -1.281261   -0.700259
H    -3.836145   -1.956072    0.094294
H    -5.003553   -0.683814   -0.319697
H    -4.480197   -1.853106   -1.575668
```

Dbu-3′

```
E(ele)        = -806.300763
E(ele+zpe)    = -805.945717
H             = -805.927195
G             = -805.992178
C    -0.769876    2.186158    0.785773
C    -0.833221    0.814658    1.510641
C    -1.259416   -0.311651    0.604200
C    -1.572814    2.281808   -0.516050
C    -3.081713    2.060048   -0.364777
C    -3.417004    0.810210    0.463468
H    -1.098739    2.965884    1.483391
H     0.141583    0.564639    1.928424
H    -1.168141    1.555009   -1.233321
H    -3.534812    1.979900   -1.360529
H     0.280368    2.381007    0.549512
H    -1.541518    0.844701    2.344941
H    -1.401755    3.265517   -0.965700
H    -3.549256    2.923365    0.124270
H    -4.439209    0.471285    0.272614
H    -3.359590    1.027035    1.531647
C    -0.795673   -2.361467   -0.610780
C    -1.809247   -1.854065   -1.623875
C    -2.988266   -1.243147   -0.884685
```

```
H          0.122511   -2.709809   -1.085859
H         -1.330197   -1.100637   -2.259908
H         -2.155532   -2.669472   -2.264529
H         -3.624284   -0.678426   -1.574253
H         -3.605915   -2.021948   -0.419336
H         -1.207044   -3.181820   -0.009082
N         -2.528991   -0.314267    0.154956
N         -0.412653   -1.261472    0.277624
C          1.015358   -1.158139    0.620901
C          1.675973   -0.233842   -0.225260
H          1.119137    0.272605   -1.006383
C          1.417727   -1.969348    1.631499
C          3.065206    0.022347   -0.101851
O          3.851061   -0.476178    0.701858
O          3.505936    0.961512   -1.015158
H          2.461748   -2.003176    1.912187
H          0.694266   -2.586693    2.154514
C          4.888116    1.259313   -0.934596
H          5.149661    1.652747    0.052555
H          5.494245    0.367407   -1.121330
H          5.077115    2.011081   -1.703144
```

Mtdb-ts3′

```
E(ele)         = -822.313257
E(ele+zpe)     = -821.973741
H              = -821.954785
G              = -822.020377
C         -2.520862   -1.520654   -0.431796
C         -1.094086    0.185767    0.502294
C         -2.501425    0.738441   -1.396841
C         -3.406474   -0.368059   -0.884009
H         -2.103060   -2.019080   -1.318601
H         -3.107234   -2.275393    0.105148
H         -3.078528    1.619236   -1.696894
H         -1.928593    0.397233   -2.273703
H         -4.004606    0.014485   -0.048754
H         -4.092067   -0.699197   -1.670686
C          0.606738    1.779293    1.282226
C         -0.290547    2.897354    0.783077
C         -0.958819    2.449089   -0.503077
H          1.012564    2.018799    2.268891
H         -1.051289    3.123399    1.538570
H          0.293975    3.804064    0.600566
H         -1.729147    3.164334   -0.811910
H         -0.216488    2.383431   -1.313982
H          1.459639    1.618211    0.606503
N         -1.603737    1.153226   -0.325873
N         -1.424027   -1.093136    0.429929
N         -0.160634    0.546272    1.414830
C          0.162119   -2.065519   -0.106409
C          0.918143   -1.310411   -0.969045
H          0.513778   -1.009810   -1.932666
C          0.050205   -3.226065    0.513135
C          2.135825   -0.688250   -0.540215
O          2.747161   -0.845091    0.510927
O          2.604749    0.194935   -1.484427
H          0.728712   -4.027291    0.234173
H         -0.680157   -3.400416    1.295201
C          3.878184    0.754245   -1.198797
H          3.853714    1.343668   -0.277065
H          4.630677   -0.030999   -1.084929
H          4.120924    1.391515   -2.050055
C          0.297717   -0.393342    2.433373
H         -0.479749   -1.135272    2.608692
H          1.223128   -0.890537    2.121964
H          0.477002    0.174996    3.351833
```

Mtdb-3′

```
E(ele)         = -822.335268
E(ele+zpe)     = -821.993063
H              = -821.973996
G              = -822.040534
C          1.139745    2.444856   -0.045529
C          1.258114   -0.004611    0.254744
C          2.493295    1.043489   -1.536729
C          2.513045    2.301969   -0.683311
H          0.418712    2.832057   -0.773522
H          1.160834    3.138630    0.799472
H          3.447827    0.875869   -2.041528
H          1.704250    1.100730   -2.298743
H          3.299132    2.205683    0.074507
H          2.730358    3.188998   -1.285525
C          1.327637   -2.394331    0.432125
C          2.826271   -2.363183    0.172184
C          3.115871   -1.267730   -0.843886
H          1.066909   -3.151935    1.172806
H          3.341056   -2.159970    1.116889
H          3.187675   -3.321119   -0.212548
H          4.162671   -0.945915   -0.784984
H          2.941540   -1.641803   -1.861215
H          0.761972   -2.610905   -0.485110
N          2.257700   -0.097910   -0.655135
N          0.608548    1.157020    0.426984
N          0.931311   -1.096898    0.966607
C         -0.857502    1.144125    0.607066
C         -1.501194    0.290015   -0.328305
H         -0.925775   -0.158457   -1.132333
C         -1.336906    1.955983    1.581971
C         -2.891082    0.032533   -0.275716
O         -3.713584    0.469216    0.529998
O         -3.297659   -0.837653   -1.275543
H         -2.404480    2.061433    1.717628
H         -0.656214    2.482218    2.244744
C         -4.686051   -1.111171   -1.289526
H         -5.009611   -1.566798   -0.348428
H         -5.266740   -0.196228   -1.444690
H         -4.846860   -1.803519   -2.118417
C          0.067264   -1.063764    2.143441
H          0.155815   -0.098235    2.637895
H         -0.981399   -1.216413    1.866405
H          0.408324   -1.851389    2.820672
```

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9.3 Proton affinity and methylation

9.3.1 Protonated Z-type adducts

```
        IMe-3-Hα

  E(ele)      = -649.563039
  E(ele+zpe)  = -649.314507
  H           = -649.298635
  G           = -649.357536
C   -1.125217  -0.110941   0.255972
C   -2.570643   0.015283  -1.422809
C   -2.385341   1.268233  -0.931479
N   -1.489865   1.169747   0.109887
N   -1.782596  -0.828544  -0.670942
C   -1.701148  -2.279809  -0.845016
H   -2.682460  -2.649293  -1.142839
H   -0.965904  -2.523043  -1.615010
H   -1.421645  -2.736453   0.105170
C   -0.959951   2.324347   0.841626
H   -0.331752   2.907013   0.167457
H   -1.798815   2.916431   1.209879
H   -0.355230   1.969951   1.673091
C   -0.499115  -0.691570   2.531399
H    0.186703  -1.084877   3.276672
C    1.151056  -1.172403   0.705008
H    1.766048  -1.567188   1.519130
H   -1.460404  -0.327015   2.884024
H   -0.166989  -0.666323   1.239074
C    1.920890  -0.077330  -0.015086
O    1.469817   1.023923  -0.244183
O    3.128994  -0.487685  -0.363779
C    3.952581   0.470404  -1.054349
H    4.131541   1.333564  -0.411131
H    4.881237  -0.052398  -1.270903
H    3.458949   0.789221  -1.973853
H   -2.807547   2.216234  -1.229364
H   -3.196386  -0.349451  -2.223269
H    1.015645  -2.000358  -0.004016


        IMe-3-Hγ

  E(ele)      = -649.565913
  E(ele+zpe)  = -649.317367
  H           = -649.301251
  G           = -649.360286
C    1.051355   0.233854  -0.000141
C    2.249870  -1.494988  -0.678157
C    2.249959  -1.493979   0.680302
N    1.513362  -0.400640   1.082330
N    1.513246  -0.402243  -1.081725
C    1.146051  -0.097022  -2.464240
H    1.977396  -0.371012  -3.113567
H    0.252646  -0.664884  -2.732368
H    0.950277   0.971083  -2.559346
C    1.146492  -0.093271   2.464464
H    0.253343  -0.660947   2.733822
H    1.978119  -0.365934   3.113988
H    0.950424   0.974931   2.557866
C    0.944455   2.763933  -0.001894
H    0.249971   3.605885  -0.002440
C   -1.129832   1.342442  -0.001048
H   -1.758466   2.228283  -0.001660
H    1.594003   2.843858   0.877756
C    0.204050   1.453929  -0.001012
O   -1.821938   0.018794  -0.000246
O   -1.247970  -1.052020  -0.000242
C   -3.136428   0.170280   0.000417
C   -3.915129  -1.039906   0.001144
H   -3.686788  -1.624755   0.893734
H   -4.952618  -0.714701   0.001602
H   -3.687725  -1.625205  -0.891397
H    2.711327  -2.162899   1.390815
H    2.711119  -2.164985  -1.387734
H    1.593897   2.842673  -0.881739


        IPr-3-Hα

  E(ele)      = -1504.456651
  E(ele+zpe)  = -1503.759448
  H           = -1503.721143
  G           = -1503.827982
C   -0.852739  -0.327919   2.087681
C    0.457915  -0.677686   2.068935
C   -0.127440  -0.119603  -0.002150
N   -1.206928  -0.003836   0.793349
N    0.888358  -0.558707   0.762736
C   -2.584129   0.165016   0.370838
C   -3.325825  -1.012587   0.166695
C   -3.103064   1.452967   0.206803
C   -4.652372  -0.858168  -0.237387
C   -4.435704   1.546221  -0.208154
C   -5.200831   0.407798  -0.429353
H   -5.267138  -1.738771  -0.403322
H   -4.878861   2.527361  -0.354313
H   -6.234315   0.504254  -0.748223
C    2.170277  -1.019212   0.270934
C    2.184044  -2.205377  -0.490620
C    3.318867  -0.283113   0.589591
C    3.423844  -2.621435  -0.977127
C    4.534571  -0.761672   0.087970
C    4.586464  -1.907532  -0.694316
H    3.487561  -3.523297  -1.576712
H    5.450737  -0.223090   0.312417
H    5.539180  -2.256431  -1.080982
C   -2.283739   2.705123   0.450502
H   -1.303423   2.411589   0.836323
C   -2.947281   3.611577   1.495140
H   -3.132141   3.074763   2.431040
H   -2.299098   4.466024   1.713352
H   -3.904952   4.004190   1.137049
C   -2.055159   3.464604  -0.862578


        IPr-3-Hγ

  E(ele)      = -1504.454780
  E(ele+zpe)  = -1503.758339
  H           = -1503.719636
  G           = -1503.826823
C   -0.731088  -0.331283   2.072947
C    0.605837  -0.565537   2.028509
C   -0.067643  -0.095122  -0.029303
N   -1.137683  -0.066446   0.781148
N    0.999640  -0.437752   0.710647
C   -2.519554  -0.048685   0.333655
C   -3.122287  -1.301662   0.108091
C   -3.177646   1.173337   0.157063
C   -4.432429  -1.293326  -0.370418
C   -4.488993   1.119300  -0.326960
C   -5.105285  -0.095280  -0.599680
H   -4.939285  -2.235749  -0.557271
H   -5.035437   2.045667  -0.481244
H   -6.123783  -0.112856  -0.975586
C    2.309262  -0.796480   0.195781
C    2.428886  -2.047927  -0.443824
C    3.387226   0.071161   0.406557
C    3.684792  -2.376649  -0.953090
C    4.624645  -0.318658  -0.118680
C    4.770093  -1.516359  -0.803612
H    3.825114  -3.325383  -1.460587
H    5.486388   0.327994   0.020460
H    5.738487  -1.795866  -1.207597
C   -2.550658   2.504979   0.520849
H   -1.518501   2.329631   0.835479
C   -3.296135   3.137940   1.704536
H   -3.303391   2.472220   2.573785
H   -2.811994   4.075459   1.995693
H   -4.336394   3.362165   1.444756
C   -2.520643   3.462780  -0.675942
H   -2.044685   3.006852  -1.551140
H   -3.531000   3.765841  -0.971177
H   -1.969391   4.372126  -0.413874
C    3.285844   1.344412   1.226045
H    2.232219   1.550910   1.427627
C    3.852857   2.553094   0.473768
H    4.938619   2.478594   0.350982
H    3.410718   2.650917  -0.523821
H    3.646911   3.467745   1.039028
C    4.008400   1.162520   2.569451
H    5.077230   0.976042   2.418144
H    3.905761   2.065556   3.179633
H    3.603631   0.317869   3.137859
C   -2.438664  -2.620041   0.444620
H   -1.371329  -2.434244   0.611014
C   -3.012091  -3.177832   1.757020
H   -2.922103  -2.456781   2.575946
H   -4.074610  -3.417062   1.640199
H   -2.485185  -4.093513   2.044491
C   -2.551024  -3.667553  -0.668742
H   -2.154764  -3.304337  -1.622395
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H   -1.988634  -4.564467  -0.387639
H   -3.588854  -3.975104  -0.831363
C    1.294637  -3.063873  -0.479367
H    0.342247  -2.528921  -0.555474
C    1.368477  -4.023033  -1.671302
H    1.531523  -3.498470  -2.618682
H    2.174382  -4.754177  -1.550041
H    0.433059  -4.586329  -1.747826
C    1.260138  -3.861844   0.834323
H    1.120665  -3.212540   1.704733
H    0.437468  -4.585781   0.816337
H    2.197046  -4.412797   0.969346
C   -1.435568  -0.342870   2.890720
H    1.315811  -0.823495   2.799888
C   -0.084566   0.220100  -1.484749
H    0.273766   1.437239  -1.914404
C   -0.553215  -0.842895  -2.440989
H    0.257496   1.652842  -2.979097
H   -1.507911  -1.262724  -2.107210
H   -0.691670  -0.415826  -3.436022
C    0.642060   2.576456  -1.031291
O    0.630241   2.554240   0.182348
O    0.951681   3.645806  -1.757442
C    1.246320   4.845821  -1.027544
H    1.437399   5.604417  -1.783318
H    0.391569   5.120721  -0.406198
H    2.123452   4.693710  -0.396334
H    0.171491  -1.659572  -2.513944


        Pbu-3-Hα

  E(ele)      = -1159.477329
  E(ele+zpe)  = -1158.983859
  H           = -1158.956335
  G           = -1159.042677
C    0.501814  -1.753353  -2.074942
C    0.995286  -1.955806  -3.022962
C   -0.010640  -2.592799  -1.613013
C    0.538378  -0.533034  -1.532983
P   -0.302090  -0.259441   0.060628
C    0.710235  -0.715780   1.507937
C   -0.001322  -0.906941   2.321997
H    1.313632   0.156747   1.772934
H   -1.795233  -1.304834   0.100273
H   -2.228295  -1.175309   1.100647
C   -1.474066  -2.352711   0.043844
C   -0.822206   1.479706   0.176633
C   -1.361707   1.732134  -0.745283
H    0.094466   2.080226   0.205372
C    2.361491   1.182615  -1.360524
O    2.389304   1.072149  -0.151087
O    3.265653   1.820627  -2.079333
C    4.353330   2.423138  -1.352167
H    4.911957   1.651429  -0.820370
H    4.972124   2.902177  -2.107278
H    3.964102   3.155126  -0.642917
C   -1.692681   1.767121   1.408201
H   -2.619367   1.179419   1.362657
H   -1.163979   1.462674   2.321524
H    1.605788  -1.937246   1.274058
H    1.009810  -2.793007   0.924434
C    2.330295  -1.706087   0.484063
H   -2.831183  -0.983863  -0.982287
H   -3.176801   0.052867  -0.868655
C   -2.372778  -1.058582  -1.976705
H    2.348457  -2.331114   2.552515
H    1.620258  -2.545812   3.345074
C    2.943649  -1.475350   2.895028
C    3.253128  -3.541832   2.338215
H    4.003944  -3.341126   1.566600
H    3.782114  -3.804189   3.258090
H    2.673534  -4.417120   2.025666
C   -2.048443   3.252786   1.504053
H   -1.123903   3.842183   1.544794
H   -2.575195   3.555813   0.590015
H   -2.911905   3.556103   2.725978
C   -3.159886   4.619389   2.775897
H   -3.851880   2.994917   2.693907
H   -2.391087   3.290195   3.651859
C   -4.035932  -1.924958  -0.905607
H   -3.690111  -2.960078  -1.015321
H   -4.490831  -1.850148   0.090342
C   -5.076646  -1.609819  -1.977048
H   -5.925871  -2.294816  -1.912447
H   -5.460986  -0.590339  -1.866026
H   -4.648091  -1.701890  -2.980628
C    1.243439   0.617424  -2.213307
H    0.548315   1.442261  -2.424535
H    1.644009   0.296392  -3.178646


        Pbu-3-Hγ

  E(ele)      = -1159.476503
  E(ele+zpe)  = -1158.983045
  H           = -1158.956284
  G           = -1159.040484
C    1.804804   0.107955  -1.972335
C    0.207176  -1.727970  -2.380850
H    0.766470  -1.801725  -3.315616
H    0.347392  -2.666462  -1.830532
H    2.275751  -0.164150  -2.914340
C    0.713889  -0.559555  -1.568354
P   -0.190245  -0.193751  -0.004294
C    0.797395  -0.679755   1.448151
H    0.111123  -0.646531   2.304501
H    1.567762   0.081000   1.598273
C   -1.672896  -1.264960  -0.007466
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H   -1.996227  -1.349313   1.037686
H   -1.365431  -2.271000  -0.313539
C   -0.809086   1.517009   0.090389
H   -1.488002   1.650799  -0.760914
H    0.034698   1.296780  -0.036020
C    2.487262   1.188629  -1.212175
O    2.172651   1.537304  -0.090099
O    3.490020   1.700157  -1.903723
C    4.249189   2.736611  -1.256265
H    4.670350   2.356883  -0.323901
H    5.033766   3.000837  -1.961319
H    3.604062   3.592370  -1.049852
C   -1.531750   1.792723   1.418087
H   -2.306385   1.036560   1.608197
H   -0.814368   1.732165   2.246430
C    1.414163  -2.077466   1.300379
H    0.630799  -2.826151   1.117413
H    2.085137  -2.093716   0.430984
C   -2.831511  -0.759212  -0.879927
H   -3.289246   0.119657  -0.407656
H   -2.469620  -0.423844  -1.861859
C    2.201328  -2.473961   2.551992
H    1.532461  -2.451582   3.421479
H    2.981177  -1.724505   2.735576
C    2.830202  -3.858535   2.416314
H    3.522496  -3.895414   1.568426
H    3.390681  -4.124587   3.316081
H    2.064457  -4.625929   2.260833
C   -2.181494   3.178573   1.411755
H   -1.412285   3.935049   1.212917
H   -2.899794   3.234524   0.583541
C   -2.884911   3.485527   2.731566
H   -3.345951   4.476348   2.708335
H   -3.673908   2.754157   2.937079
H   -2.178568   3.464557   3.568092
C   -3.896178  -1.839902  -1.077418
H   -3.441016  -2.704585  -1.578557
H   -4.237629  -2.192649  -0.095871
C   -5.084233  -1.333862  -1.891229
H   -5.829836  -2.120922  -2.029103
H   -5.575295  -0.493098  -1.390101
H   -4.766982  -0.996072  -2.883710
H   -0.855832  -1.643959  -2.623651


        Pph-3-Hα

  E(ele)      = -1380.824432
  E(ele+zpe)  = -1380.429143
  H           = -1380.404338
  G           = -1380.484308
C    0.530162   0.182808  -2.976699
C   -0.292769  -0.076723  -1.956841
P    0.414061  -0.079202  -0.267459
C   -2.699494   0.328382  -1.255932
C   -2.337594   1.067685  -0.367027
O   -3.963402   0.050523  -1.538160
C   -4.949934   0.684509  -0.705754
H   -4.876063   1.768906  -0.804116
H   -5.909109   0.325069  -1.071202
H   -4.794298   0.396941   0.335764
C    0.601431   1.583275   0.409740
C    1.331484   1.714325   1.599843
C    0.103754   2.711753  -0.244132
C    1.537993   2.977125   2.144528
H    1.746071   0.837748   2.094189
C    0.329192   3.973791   0.301378
C   -0.462745   2.609332  -1.163532
H    1.037317   4.105786   1.493980
H    2.095703   3.079664   3.070029
H   -0.054906   4.853414  -0.205235
C    1.204259   5.091297   1.917911
C    2.103632  -0.740528  -0.341296
C    2.389359  -2.077466  -0.039154
C    3.138423   0.127020  -0.722865
C    3.698565  -2.543024  -0.138786
H    1.608922  -2.751068   0.296543
C    4.441157  -0.349301  -0.826185
C    2.933868   1.177483  -0.916992
H    4.720984  -1.685250  -0.537960
H    3.918027  -3.577676   0.104983
H    5.238837   0.325767  -1.119779
C    5.739417  -2.053865  -0.612182
C   -0.610670  -1.136722   0.777083
C   -0.928851  -2.428461   0.335775
C   -1.108550  -0.665140   1.995106
C   -1.732975  -3.249499   1.121431
C   -0.554680  -2.798327  -0.617575
C   -1.905979  -1.496199   2.778231
H   -0.899124   0.349890   2.319427
C   -2.217006  -2.783568   2.344217
H   -1.980597  -4.249418   0.779320
H   -2.292657  -1.130976   3.724254
C   -2.842883  -3.425024   2.956907
H    1.594276   0.359092  -2.847757
H    0.153231   0.215861  -3.996660
C   -1.751735  -0.408076  -2.177613
H   -1.936623  -1.481153  -2.045845
H   -2.024815  -0.181160  -3.213630


        Pph-3-Hγ
```

```
E(ele)      = -1380.826567
E(ele+zpe)  = -1380.431677
H           = -1380.406662
G           = -1380.487022
C  -1.533016   0.122931  -2.270743
C   0.800215  -0.274503  -3.031790
C  -0.236872  -0.030289  -1.965868
P   0.374714  -0.021497  -0.229730
C  -2.601989   0.430128  -1.279805
O  -2.390948   0.955731  -0.207481
O  -3.796467   0.072247  -1.727467
C  -4.897207   0.315545  -0.835170
H  -4.965834   1.382154  -0.614094
H  -5.781172  -0.030977  -1.365620
H  -4.749694  -0.244253   0.090851
C   0.626313   1.655794   0.379178
C   1.456934   1.832896   1.495082
C   0.041565   2.756738  -0.252050
C   1.681755   3.114507   1.986342
H   1.934855   0.979466   1.971415
C   0.286608   4.036877   0.238013
H  -0.605401   2.619730  -1.112562
C   1.098771   4.214778   1.356315
H   2.319257   3.254290   2.853661
H  -0.162823   4.894176  -0.252642
H   1.282270   5.214605   1.737785
C   2.012613  -0.800963  -0.261154
C   2.170934  -2.148673   0.078013
C   3.121614  -0.044831  -0.669061
C   3.430950  -2.739440  -0.004657
H   1.325424  -2.737299   0.420276
C   4.374595  -0.642342  -0.749120
C   3.012042   1.010142  -0.909957
H   4.528573  -1.990336  -0.420945
H   3.552306  -3.783866   0.264596
H   5.232194  -0.054581  -1.060741
H   5.508926  -2.452826  -0.482566
C  -0.698349  -1.026115   0.820358
C  -1.215762  -2.225248   0.315327
C  -1.000556  -0.610412   2.118392
C  -2.028666  -3.015437   1.124037
H  -0.997337  -2.541009  -0.702530
C  -1.812296  -1.409919   2.919903
H  -0.633497   0.339980   2.495012
C  -2.323824  -2.608683   2.425363
H  -2.431222  -3.945923   0.736275
H  -2.054777  -1.088127   3.927683
H  -2.958907  -3.225976   3.053204
H  -1.855174   0.027036  -3.305784
H   1.574281   0.500866  -3.009034
H   1.305103  -1.235457  -2.890360
H   0.330164  -0.261531  -4.017500
```

Hmpt-3-Hα
```
E(ele)      = -1089.699478
E(ele+zpe)  = -1089.325742
H           = -1089.302847
G           = -1089.375570
C   1.537120  -0.852429   1.416585
C   0.070185  -0.482908   1.484591
P  -0.872828  -0.030417  -0.008110
C   2.393974  -0.023969   0.480841
O   2.002325   0.915279  -0.175614
O   3.644341  -0.468620   0.477792
C   4.573104   0.253338  -0.349064
H   4.616614   1.297302  -0.034365
H   5.532470  -0.237540  -0.202667
H   4.262498   0.196724  -1.394236
N  -2.449277  -0.546899   0.038787
N  -0.997127   1.596392  -0.119360
C   0.269740  -2.166497  -1.253422
H  -0.086321  -2.658330  -0.342876
H  -0.148200  -2.704777  -2.112017
H   1.364175  -2.244100  -1.295794
C   0.299863  -0.028257  -2.473039
H   0.184450   1.045431  -2.321561
H   1.364560  -0.223539  -2.640584
C  -0.270145  -0.340502  -3.354895
H  -2.864938  -1.856534  -0.464111
H  -2.290934  -2.129628  -1.349668
H  -2.765001  -2.639322   0.299306
C  -3.916786  -1.791004  -0.756057
H  -3.446882   0.095835   0.898178
H  -3.063542   1.037289   1.297368
H  -4.343770   0.309740   0.306589
H  -3.731877  -0.558756   1.731305
H  -1.909769   2.200256  -1.098181
H  -1.343642   2.835321  -1.788309
H  -2.432941   1.431595  -1.670067
H  -2.650250   2.818935  -0.578562
C  -0.180329   2.573150   0.605285
H   0.562920   3.024403  -0.057704
H   0.849770   3.346566   0.996130
H   0.337850   2.102698   1.439287
C  -0.604600  -0.567637   2.635973
H  -1.671403  -0.379047   2.706302
H  -0.102084  -0.835867   3.563222
H   1.977486  -0.780285   2.417686
H   1.655865  -1.902796   1.123325
```

Hmpt-3-Hγ
```
E(ele)      = -1089.703542
E(ele+zpe)  = -1089.330328
H           = -1089.307058
G           = -1089.380163
C  -1.454617  -1.307586  -0.933966
C  -0.115520  -1.257134  -0.877222
P   0.825578   0.033185   0.032344
C  -2.378860  -0.271381  -0.394521
O  -2.047375   0.856298  -0.091183
O  -3.615584  -0.741526  -0.305491
C  -4.609124   0.174460   0.184288
```

```
H  -4.652487   1.053857  -0.460495
H  -5.546620  -0.376015   0.159114
H  -4.363039   0.476945   1.204355
N   2.382281  -0.482893   0.256970
H   0.957713   1.376425  -0.894731
N   0.181820   0.233720   1.532378
C  -0.342596  -0.905641   2.282613
H   0.069330  -1.848060   1.910228
H  -0.063144  -0.805439   3.336888
H  -1.437815  -0.948328   2.209050
C  -0.228012   1.543552   2.040243
H  -0.025901   2.321512   1.302504
H  -1.305674   1.539944   2.230553
H   0.312594   1.771405   2.964873
C   2.895121  -1.027756   1.513806
H   2.269413  -0.719791   2.351023
H   2.950423  -2.123313   1.478709
H   3.903343  -0.634876   1.678574
C   3.322412  -0.592459  -0.860180
H   2.893906  -0.169273  -1.771320
H   4.234076  -0.034774  -0.617605
H   3.591777  -1.638904  -1.045413
C   1.967824   2.395137  -0.577104
H   1.476897   3.330083  -0.284839
H   2.612259   2.062746   0.238852
H   2.584046   2.583019  -1.462795
C  -0.007163   1.804013  -1.912335
H  -0.693398   2.555250  -1.510869
H   0.556845   2.226397  -2.749410
H  -0.587783   0.956629  -2.275058
C   0.719811  -2.356574  -1.485160
H   1.386941  -2.808678  -0.743056
H   0.077254  -3.137465  -1.897280
H  -1.939004  -2.159592  -1.406714
H   1.347441  -1.971773  -2.296730
```

Quin-3-Hα
```
E(ele)      = -673.995872
E(ele+zpe)  = -673.677016
H           = -673.662159
G           = -673.717439
C   1.595736   0.966910  -0.804333
C   0.271799   2.511084   0.607689
C   1.120937   3.185564   0.607161
H  -0.594532   2.828765   1.177914
C   2.211707   1.859158  -0.940046
C   0.347075   1.364593  -0.060080
C   2.414637  -0.074021  -0.053210
O   1.952888  -0.815827   0.786890
O   3.674555  -0.070809  -0.450660
C   4.543270  -1.031122   0.182114
H   4.168363  -2.040677   0.006862
H   5.515512  -0.888437  -0.283311
H   4.588846  -0.833183   1.254093
C  -0.681649  -0.750358  -0.982335
C  -1.098641  -0.093022   1.355533
C  -2.080257   1.208457  -0.512953
C  -1.801628  -1.772284  -0.719951
H   0.296243  -1.184892  -0.790028
H  -0.718263  -0.349984  -1.999393
C  -2.497340  -0.729934   1.418685
H  -0.991993   0.749491   2.038294
H  -0.284548  -0.794455   1.547088
H  -2.307113   1.924013   0.278548
H  -1.791365   1.763891  -1.407342
C  -3.246364   0.236901  -0.750787
H  -1.421843  -2.599706  -0.112101
H  -2.126928  -2.191655  -1.676201
H  -3.210620  -0.049098   1.895323
H  -2.446117  -1.630903   2.036379
H  -4.169916   0.699462  -0.391507
H  -3.374928   0.042223  -1.820537
N  -0.841409   0.445062  -0.053466
H   1.396130   0.587205  -1.812625
C  -2.957326  -1.069539  -0.004063
H  -3.845128  -1.705107   0.017996
```

Quin-3-Hγ
```
E(ele)      = -673.993170
E(ele+zpe)  = -673.674304
H           = -673.659282
G           = -673.715069
C   1.570308   1.191844  -0.003228
C  -0.145294   2.959033   0.005125
C   0.741627   3.579870   0.131062
H  -0.630390   3.262210  -0.928252
C   2.250176   2.037358   0.016637
C   0.267682   1.512241  -0.017544
C   2.301980  -0.112779  -0.009197
O   1.818097  -1.226627  -0.033525
O   3.604461   0.126531   0.015362
C   4.462367  -1.029465   0.016271
C   4.300256  -1.608292  -0.894625
C   5.474528  -0.634198   0.054398
C   4.247802  -1.646564   0.890269
H  -0.742596  -0.405250  -1.257420
C  -0.757362  -0.326918   1.270037
C  -2.227437   1.108710  -0.056403
C  -1.572368  -1.670561  -1.010485
H   0.300998  -0.631120  -1.443185
H  -1.133639   0.204038  -2.077393
C  -2.002587  -1.220060   1.399760
H  -0.669825   0.403409   2.078141
H   0.159360  -0.907158   1.203471
H  -2.383088   1.578978   0.916571
H  -2.238758   1.876005  -0.829174
C  -3.269524   0.009165  -0.334432
H  -0.923252  -2.476724  -0.651864
H  -2.009046  -1.993989  -1.959840
H  -2.711784  -0.801033   2.121010
H  -1.690672  -2.197836   1.777041
H  -4.159679   0.214023   0.266843
H  -3.576006   0.028877  -1.385128
```

```
N  -0.831366   0.494881  -0.021897
H  -0.828275   3.181214   0.830379
C  -2.660705  -1.350158   0.022171
H  -3.428022  -2.127278   0.034293
```

Dabco-3-Hα
```
E(ele)      = -690.189201
E(ele+zpe)  = -689.884401
H           = -689.869932
G           = -689.924030
C   1.591590   0.976196  -0.799927
C   0.258997   2.521052   0.606381
H   1.107467   3.196411   0.609751
H  -0.609627   2.838058   1.173272
C   2.209864   1.867789  -0.929559
C   0.339838   1.375253  -0.061508
C   2.406395  -0.070346  -0.051634
O   1.940391  -0.817219   0.782036
O   3.666725  -0.067260  -0.445083
C   4.531621  -1.035555   0.181954
H   4.152653  -2.042291  -0.000512
H   5.504574  -0.893407  -0.282018
H   4.577090  -0.844820   1.255205
C  -0.683720  -0.738004  -0.990557
C  -1.095020  -0.094466   1.348407
C  -2.093627   1.197228  -0.506716
C  -1.854496  -1.723195  -0.745679
C   0.276980  -1.200787  -0.774377
C  -0.688200  -0.333976  -2.006530
C  -2.467304  -0.814381   1.358660
H  -1.062121   0.756468   2.029082
H  -0.247215  -0.747408   1.563465
H  -2.302816   1.946180   0.257796
H  -1.839336   1.709503  -1.437293
C  -3.257164   0.184166  -0.655658
H  -1.511133  -2.590646  -0.175540
H  -2.238314  -2.084014  -1.703423
H  -3.223037  -0.208156   1.866362
H  -2.382362  -1.760872   1.898591
H  -4.164752   0.599691  -0.210248
H  -3.466443  -0.016538  -1.710042
N  -0.846225   0.449709  -0.056324
N  -2.926487  -1.076009  -0.002427
H   1.396122   0.601056  -1.810683
```

Dabco-3-Hγ
```
E(ele)      = -690.007070
E(ele+zpe)  = -689.699917
H           = -689.685048
G           = -689.740604
C   1.567413   1.193817  -0.010305
C  -0.154957   2.956610  -0.011305
H   0.731845   3.583459   0.080829
H  -0.659971   3.235608  -0.941976
C   2.245307   2.041060   0.005564
C   0.264550   1.511965  -0.013232
C   2.301735  -0.109329  -0.033112
O   1.819860  -1.220605  -0.129170
O   3.600227   0.128558   0.059296
C   4.461568  -1.025539   0.046698
H   4.338755  -1.564990  -0.893836
H   5.469509  -0.629713   0.143209
H   4.213648  -1.678774   0.884842
C  -0.783547  -0.363546  -1.273942
C  -0.725102  -0.376413   1.247267
C  -2.227920   1.099529   0.026496
C  -1.687448  -1.596314  -1.049474
C   0.248475  -0.640221  -1.462698
C  -1.143895   0.290313  -2.073381
C  -1.951307  -1.323086   1.303473
H  -0.677942   0.319200   2.088840
H   0.210527  -0.922886   1.166857
H  -2.342802   1.572993   1.003538
H  -2.290841   1.859089  -0.751794
C  -3.260782  -0.038146  -0.194781
H  -1.082223  -2.464932  -0.775747
H  -2.222020  -1.833483  -1.973322
H  -2.657987  -1.008315   2.076626
H  -1.617803  -2.334710   1.547351
H  -4.097656   0.093530   0.495959
H  -3.660638  -0.004015  -1.211997
H  -0.833341   0.490554  -0.007438
N  -2.647865  -1.340499   0.021918
H  -0.821768   3.195479   0.822074
```

Dmap-3-Hα
```
E(ele)      = -727.126344
E(ele+zpe)  = -726.844225
H           = -726.827345
G           = -726.887605
C  -1.720615   2.782407  -0.742977
C  -2.710003   3.222388  -0.810628
C  -2.577135   0.879314   0.676568
C  -3.522764   1.429548   0.677733
C  -0.904467   3.287904  -1.250309
C  -1.528199   1.660375  -0.059957
C   0.521556   1.065996   1.118753
C   0.337300   0.533945  -1.160040
H   1.775177   0.529833   1.186344
C   1.588861  -0.014694  -1.168577
H  -0.304107   0.543855  -2.032270
C   2.372862  -0.045796   0.022737
C   2.295472   0.562834   2.134201
H   1.951662  -0.433043  -2.097733
N  -0.195135   1.078574  -0.034985
C  -2.800509  -0.481477   0.033201
O  -2.203843  -0.872678  -0.944092
C  -3.727802  -1.170274   0.682627
H  -4.044879  -2.467084   0.146383
H  -4.802429  -2.875469   0.811336
H  -4.431683  -2.362415  -0.868637
```

```
H  -3.152046  -3.094378   0.138726
H   3.595600  -0.583618   0.052388
C   4.366583  -0.594262   1.294788
H   5.323043  -1.079788   1.112167
H   4.559098   0.425972   1.642661
H   3.840012  -1.153166   2.075050
C   4.172753  -1.164232  -1.159379
H   3.556518  -1.992055  -1.524817
H   4.272265  -0.407868  -1.944545
H   5.163233  -1.550336  -0.927289
H  -2.311418   0.721605   1.729735
```

Dmap-3-Hγ
```
E(ele)      = -726.942711
E(ele+zpe)  = -726.659251
H           = -726.641533
G           = -726.704847
C  -1.723641   3.138805   0.221005
H  -2.761966   3.473467   0.215245
C  -2.685765   0.811997   0.071799
C  -3.690042   1.222412   0.107288
C  -1.241800   3.486571   1.141910
C  -1.646418   1.647929   0.125440
C   0.230206   0.534135   1.211044
C   0.426995   1.146768  -1.044244
H   1.478470  -0.016697   1.211918
C   1.677598   0.605825  -1.123400
H  -0.058247   1.609540  -1.896987
C   2.264535  -0.079181   0.020553
H   1.837039  -0.463652   2.129268
C   2.196024   0.653410  -2.071559
N  -0.292802   1.119597   0.105261
C  -2.580952  -0.671981  -0.063581
O  -1.547415  -1.302723  -0.114913
C  -3.794479  -1.207829  -0.128087
H  -3.844542  -2.636035  -0.274832
H  -4.902537  -2.886320  -0.300949
H  -3.349969  -2.930150  -1.202423
H  -3.349965  -3.113352   0.573026
N   3.481084  -0.566059  -0.023386
C   4.043872  -1.203336   1.166327
H   5.029565  -1.594717   0.922950
H   4.151649  -0.479746   1.980838
H   3.413711  -2.035558   1.496133
C   4.253827  -0.546406  -1.264689
H   3.727536  -1.084388  -2.059679
H   4.447889   0.482342  -1.585191
H   5.209710  -1.036881  -1.092697
H  -1.199484   3.609968  -0.618571
```

Py-3-Hα
```
E(ele)      = -593.003815
E(ele+zpe)  = -592.794513
H           = -592.781416
G           = -592.834060
C   0.307516   2.642343  -0.709818
C  -0.452094   3.412778  -0.790237
C  -1.217734   1.155551   0.659698
C  -1.910867   2.001255   0.630799
C   1.266579   2.823472  -1.186077
C   0.056478   1.523530  -0.042424
C   1.737390   0.272391   1.185354
C   1.424861  -2.182765  -1.106854
H   2.734268  -0.678334   1.269980
C   1.423697   0.883486   2.024742
C   2.424818  -1.139434  -1.075012
H   0.836335   0.050157  -1.985139
C   3.085243  -1.394225   0.123672
C   3.229727  -0.844937   2.219451
H   2.665429  -1.680536  -1.982712
N   1.109520   0.550518   0.010893
C  -1.875532  -0.052792   0.007548
O  -1.380284  -0.668766  -0.910158
C  -3.034690  -0.331581   0.576044
H  -3.760207  -1.450499   0.029785
H  -4.671533  -1.515597   0.619327
H  -3.985876  -3.263681  -1.021169
H  -3.164679  -2.359758   0.126031
H   3.867840  -1.345319   0.169019
H  -1.054007   0.928239   1.721076
```

Py-3-Hγ
```
E(ele)      = -593.005247
E(ele+zpe)  = -592.796585
H           = -592.783166
G           = -592.836780
C  -0.684044   2.944010   0.000755
H   0.091163   3.711696   0.000837
C   1.230966   1.284128   0.000195
C   1.953055   2.094969   0.000345
H  -1.317676   3.082379  -0.883049
C  -0.068279   1.581977   0.000385
C  -1.468399  -0.010289  -1.177593
C  -1.466489  -0.012306   1.177930
C  -2.360503  -1.064652  -1.205252
C  -1.054886   0.450689  -2.068188
C  -2.358585  -1.066692   1.205232
H  -1.051555   0.447158   2.068643
C  -2.808230  -1.603390  -0.000106
H  -2.687249  -1.458781  -2.160502
H  -2.683821  -1.462412   2.160345
H  -1.045495   0.490734   0.000266
C   1.780455  -0.010148  -0.000258
H   1.108490  -1.117404  -0.000570
O   3.103352  -0.075838  -0.000245
C   3.767703  -1.352632  -0.000633
H   4.830317  -1.122395  -0.000732
H   3.487975  -1.914071   0.892259
H   3.487710  -1.913671  -0.893691
H  -3.501397  -2.438739  -0.000267
H  -1.317478   3.081946   0.884767
```

Dbu-3-Hα

```
    E(ele)        = -806.750699
    E(ele+zpe)    = -806.380752
    H             = -806.362541
    G             = -806.425485
C     -0.542633   -1.743489   -1.606177
C     -0.806725   -0.233514   -1.879291
C     -0.973030    0.573482   -0.616099
C     -0.951361   -2.228952   -0.210153
C     -2.445776   -2.095356    0.100803
C     -3.005460   -0.711680   -0.259675
H     -1.063799   -2.326010   -2.373177
H     -0.015737    0.204724   -2.487129
H     -0.371672   -1.680436    0.546752
H     -2.610636   -2.298390    1.164802
H      0.525185   -1.946121   -1.735319
H     -1.721715   -0.101867   -2.462987
H     -0.658193   -3.278339   -0.105846
H     -3.021103   -2.844132   -0.455294
H     -3.939983   -0.509054    0.267889
H     -3.231745   -0.642117   -1.324705
C     -0.222167    2.284555    0.965998
C     -0.991462    1.493482    2.007065
C     -2.299007    1.008707    1.412727
H      0.778622    2.526205    1.321471
H     -0.378953    0.646731    2.330500
H     -1.192520    2.123669    2.877044
H     -2.766502    0.264410    2.063024
H     -3.012051    1.828955    1.269332
H     -0.742475    3.211723    0.697062
N     -2.067298    0.362953    0.108941
N     -0.055699    1.468637   -0.257826
C      1.196202    1.632159   -0.967608
C      2.154465    0.463964   -0.973940
H      3.170018    0.837848   -1.148240
C      1.470821    2.813663   -1.512778
C      2.176258   -0.312893    0.327625
O      1.801315    0.119778    1.394026
O      2.673074   -1.533433    0.146785
H      2.435055    3.000375   -1.974027
H      0.747742    3.623695   -1.510660
C      2.832626   -2.331585    1.331555
H      3.503187   -1.829070    2.030743
H      1.862242   -2.492715    1.805963
H      3.259706   -3.272248    0.991067
H      1.954691   -0.234976   -1.792869
```

Dbu-3-H$_\gamma$

```
    E(ele)        = -806.757197
    E(ele+zpe)    = -806.387330
    H             = -806.368707
    G             = -806.433337
C     -0.486900   -1.740168   -1.534566
C     -0.778643   -0.237257   -1.795933
C     -0.996382    0.530255   -0.518834
C     -1.113408   -2.321245   -0.261309
C     -2.629432   -2.141608   -0.131633
C     -3.093733   -0.687502   -0.327202
H     -0.818821   -2.299491   -2.415537
H      0.040365    0.206536   -2.361626
H     -0.618055   -1.875727    0.609668
H     -2.937701   -2.496168    0.857796
H      0.598973   -1.873017   -1.471176
H     -1.673707   -0.121464   -2.412240
H     -0.883489   -3.390819   -0.222222
H     -3.158810   -2.761400   -0.864173
H     -4.020882   -0.491865    0.216001
H     -3.305377   -0.474337   -1.376106
C     -0.251508    2.135519    1.180382
C     -1.049012    1.280652    2.149929
C     -2.354882    0.863713    1.499823
H      0.752338    2.328470    1.564385
H     -0.460092    0.398230    2.413546
H     -1.256195    1.849358    3.059811
H     -2.849283    0.090048    2.093571
H     -3.047682    1.707402    1.396352
H     -0.745377    3.095619    0.988228
N     -2.108564    0.293006    0.165475
N     -0.094216    1.412679   -0.097629
C      1.141923    1.646816   -0.808910
C      2.206949    0.862648   -0.613209
H      3.125776    1.072205   -1.151773
C      1.122206    2.849679   -1.700469
C      2.236327   -0.302947    0.312522
O      1.368605   -0.591571    1.112655
O      3.358454   -0.994968    0.151091
H      2.089871    3.004226   -2.180512
H      0.352066    2.739907   -2.473251
C      3.520104   -2.144361    0.996722
H      3.505228   -1.839943    2.044628
H      2.715655   -2.859208    0.810226
H      4.485164   -2.567505    0.727089
H      0.871365    3.746304   -1.121449
```

Mtbd-3-H$_\alpha$

```
    E(ele)        = -822.794559
    E(ele+zpe)    = -822.436903
    H             = -822.418084
    G             = -822.484123
C      0.083044   -0.526782    2.313177
C     -1.007481    0.159947    0.191985
C     -1.077343   -2.156251    0.878012
C     -0.932811   -1.654838    2.305411
H      1.095600   -0.930042    2.203922
H      0.037698    0.034981    3.249031
H     -1.813500   -2.959074    0.804787
H     -0.123296   -2.509599    0.473355
H     -1.906241   -1.313153    2.673745
H     -0.583460   -2.451022    2.968154
C     -1.956166    0.743747   -1.933928
C     -3.176162   -0.093787   -1.579868
C     -2.682143   -1.336566   -0.856556
H     -2.214598    1.651771   -2.480399
H     -3.842283    0.494800   -0.939217
H     -3.738323   -0.388329   -2.469660
H     -3.482456   -1.799253   -0.269882
H     -2.317862   -2.079650   -1.575449
H     -1.249352    0.168331   -2.544095
N     -1.565920   -1.042769    0.057424
N     -0.128715    0.417878    1.192604
N     -1.296250    1.143472   -0.687589
C      0.948320    1.352510    0.986657
H      2.560875    1.968659   -0.273170
C      1.318699    2.158046    1.981533
C      2.163354   -0.102069   -0.683089
O      1.440883   -1.078072   -0.664504
O      3.438528   -0.126700   -1.041141
H      2.193248    2.791582    1.884318
H      0.767915    2.205729    2.915939
C      3.962808   -1.403310   -1.444857
H      3.882780   -2.114992   -0.621371
H      3.408955   -1.774723   -2.308902
H      5.003971   -1.218896   -1.699456
C     -1.421226    2.542785   -0.270129
H     -1.335454    2.624125    0.812251
H     -0.651317    3.166313   -0.737107
H     -2.406781    2.908888   -0.573219
H      1.068747    1.635691   -1.157136
```

Mtbd-3-H$_\gamma$

```
    E(ele)        = -822.800882
    E(ele+zpe)    = -822.443191
    H             = -822.424269
    G             = -822.488968
C      1.213674    2.266805   -0.773559
C      0.886123    0.026965    0.290890
C      1.856495    0.164935   -1.892170
C      2.317645    1.576116   -1.564588
H      0.470145    2.675090   -1.465601
H      1.611705    3.088370   -0.170468
H      2.604742   -0.382563   -2.467890
H      0.908033    0.157902   -2.444831
H      3.245829    1.522606   -0.986984
H      2.520252    2.151575   -2.471652
C      0.637438   -2.117256    1.345987
C      2.042999   -2.465115    0.879857
C      2.232476   -1.890096   -0.513471
H      0.438230   -2.490218    2.351526
H      2.772043   -2.042627    1.579332
H      2.192076   -3.547504    0.849372
H      3.292578   -1.839123   -0.780678
H      1.721609   -2.511340   -1.259416
H     -0.117587   -2.531229    0.666842
N      1.673665   -0.537517   -0.622600
N      0.488632    1.323060    0.115757
N      0.502121   -0.656726    1.378810
C     -0.803946    1.769106    0.521727
C     -1.931861    1.069801    0.307793
C     -0.827660    3.128223    1.162883
C     -2.062483   -0.175205   -0.484221
O     -1.174349   -0.736761   -1.100174
O     -3.325002   -0.597580   -0.471890
H     -1.804341    3.324786    1.607760
H     -0.056347    3.216003    1.935576
C     -3.613374   -1.759109   -1.262577
H     -3.374657   -1.565349   -2.309903
H     -3.030350   -2.610604   -0.905230
H     -4.678438   -1.939052   -1.133865
C      0.081137   -0.035924    2.630762
H      0.360623    1.017224    2.644431
H     -1.000310   -0.124702    2.774907
H      0.598983   -0.537575    3.452304
H     -0.639248    3.912884    0.421324
```

9.3.2 Transition structures for the attack of the Z-type adducts on MeCl

```
IMe-3-tsα

E(ele)      = -1149.152677
E(ele+zpe)  = -1148.878037
H           = -1148.859039
G           = -1148.925103

C   -1.271355  -0.692714   0.321925
C   -1.883028  -1.979269  -1.374922
C   -2.799538  -0.984883  -1.254899
N   -2.412704  -0.211373  -0.186021
N   -0.947386  -1.791149  -0.379587
C    0.198450  -2.681617  -0.154602
H   -0.140169  -3.707515  -0.305225
H    1.020091  -2.445551  -0.836142
H    0.543140  -2.558056   0.871068
C   -3.050777   1.033956   0.222766
H   -2.817211   1.804486  -0.513509
H   -4.126824   0.870224   0.302074
H   -2.649339   1.324924   1.193918
C   -0.699694  -0.758246   2.655542
H   -0.183983  -0.419627   3.549401
C    0.404536   0.958258   1.218672
H    0.864296   1.401264   2.097001
H   -1.357511  -1.617022   2.748450
C   -0.524723  -0.123927   1.474531
C    0.250665   1.823489   0.079116
O   -0.390928   1.580388  -0.943809
O    1.002629   2.946336   0.184887
C    1.033102   3.776118  -0.972281
H    0.035150   4.162327  -1.196942
H    1.709793   4.594415  -0.727688
H    1.401805   3.218626  -1.836749
H   -3.685320  -0.760669  -1.828516
H   -1.813286  -2.803645  -2.067379
C    2.049863  -0.144481   0.390125
H    1.461074  -0.317005  -0.496740
H    2.722972   0.701191   0.403893
H    1.992180  -0.790198   1.251843
Cl   3.612068  -1.542004  -0.483175


IMe-3-tsγ

E(ele)      = -1149.146564
E(ele+zpe)  = -1148.871467
H           = -1148.852588
G           = -1148.918562

C    0.144649   0.997358   0.139125
C   -0.155884   2.059997  -1.776381
C    0.485360   2.907696  -0.931980
N    0.648393   2.232563   0.259734
N   -0.367759   0.883835  -1.092391
C   -0.915130  -0.337000  -1.692685
H   -2.008127  -0.306267  -1.718075
H   -0.500534  -0.427399  -2.697154
H   -0.588386  -1.187917  -1.095825
C    1.411392   2.711222   1.407063
H    1.177337   3.763446   1.574100
H    1.126744   2.126563   2.281963
H    2.478367   2.585359   1.209738
C   -0.959888   0.161191   2.136358
H   -0.971629  -0.472206   3.019678
H    0.985250  -1.073267   1.158510
C   -1.373972   1.157846   2.267248
C    0.099046  -0.015026   1.226883
C    2.005640  -1.164374   0.140175
O    2.209360  -0.359860  -0.767563
O    2.772021  -2.269290   0.286725
C    3.811689  -2.426273  -0.673267
H    4.493738  -1.572775  -0.645468
H    4.332370  -3.341922  -0.394825
H    3.394743  -2.514604  -1.679786
H    0.834257   3.919562  -1.066427
H   -0.484316   2.186797  -2.796250
C   -2.614782  -0.591518   0.989160
H   -2.581082   0.299379   0.386777
H   -2.038023  -1.468327   0.742731
H   -3.248103  -0.599042   1.863859
Cl  -4.270862  -1.321680  -0.366947
H    0.961713  -1.841564   1.923352


IPr-3-tsα

E(ele)      = -2004.032174
E(ele+zpe)  = -2003.310131
H           = -2003.267972
G           = -2003.384096

C   -1.539892  -0.337712   2.140757
C   -0.229654  -0.610446   2.354765
C   -0.476987  -0.158610   0.190079
N   -1.682363  -0.084354   0.789725
N    0.411745  -0.509081   1.137708
C   -2.973764   0.038587   0.146903
C   -3.670803  -1.152918  -0.120560
C   -3.482455   1.309652  -0.137663
C   -4.931353  -1.035012  -0.706161
C   -4.747353   1.369138  -0.732253
C   -5.464888   0.213926  -1.013057
H   -5.502534  -1.931230  -0.931190
H   -5.172862   2.339604  -0.974049
H   -6.446185   0.284398  -1.473444
C    1.801159  -0.853215   0.925446
C    2.080426  -2.033665   0.210591
C    2.796977  -0.024293   1.458798
C    3.420172  -2.318867  -0.044988
C    4.124426  -0.380014   1.195528
C    4.434336  -1.492505   0.426896
H    3.680678  -3.186291  -0.642411
H    4.925435   0.252437   1.567441
H    5.466416  -1.708709   0.172576
C   -2.722440   2.583602   0.171926
H   -1.768403   2.322890   0.637480
C   -3.500402   3.464033   1.157754
```

```
H   -3.731689   2.921777   2.080985
H   -2.905731   4.345444   1.419129
H   -4.445672   3.812408   0.725683
C   -2.402539   3.351732  -1.116449
H   -1.872036   2.718017  -1.834504
H   -3.316469   3.722840  -1.595784
H   -1.766860   4.214137  -0.888778
C    2.506108   1.208822   2.295331
H    1.444273   1.449634   2.208303
H    3.281807   2.428080   1.782324
H    4.349784   2.353772   2.016242
H    3.178389   2.531452   0.698095
C    2.896512   3.338127   2.254338
C    2.843848   0.947133   3.770122
H    3.910606   0.725895   3.890749
H    2.609218   1.828920   4.376447
H    2.286140   0.095071   4.175424
C   -3.117153  -2.525466   0.231094
H   -2.041107  -2.428955   0.421043
C   -3.769414  -3.058221   1.515648
H   -3.630081  -2.373549   2.357885
C   -4.847181  -3.191080   1.367432
H   -3.339196  -4.028062   1.788000
H   -3.294852  -3.543239  -0.902995
H   -2.934346  -3.158449  -1.861591
H   -2.741413  -4.458774  -0.669222
H   -4.346881  -3.821036  -1.028358
C    1.003385  -3.028081  -0.190885
H    0.044727  -2.507880  -0.239568
C    1.242851  -3.647714  -1.570069
H    1.449720  -2.878600  -2.320725
H    2.085305  -4.347233  -1.558439
H    0.355255  -4.209297  -1.882984
C    0.873892  -4.113164   0.888554
H    0.641677  -3.676461   1.867032
H    0.075541  -4.818410   0.628520
H    1.809852  -4.674962   0.984039
C   -2.387546  -0.303428   2.806668
H    0.313801  -0.874365   3.248487
C   -0.239341   0.073860  -1.259100
C    0.559896   1.210830  -1.684652
C   -0.788084  -0.817301  -2.113475
H    0.428171   1.463875  -2.732996
H   -1.336819  -1.687447  -1.771771
H   -0.682664  -0.684914  -3.186603
C    0.703323   2.351504  -0.820347
O    0.461740   2.407779   0.387038
O    1.196355   3.430016  -1.481845
C    1.373604   4.609733  -0.707627
H    1.733746   5.365897  -1.404947
H    0.427504   4.925001  -0.257943
H    2.104425   4.449672   0.088363
C    2.539287   0.512197  -2.103079
H    2.858263   0.498331  -1.073586
H    2.070479  -0.360423  -2.532636
H    2.731483   1.389362  -2.701224
Cl   4.562536  -0.343650  -2.752124


IPr-3-tsγ

E(ele)      = -2004.025174
E(ele+zpe)  = -2003.302783
H           = -2003.260816
G           = -2003.376278

C    0.027750   0.568171  -2.385040
C    1.347948   0.674924  -2.097084
C    0.277483   0.169469  -0.211193
N   -0.624618   0.280038  -1.202420
N    1.487281   0.440716  -0.742797
C   -2.066075   0.359621  -1.052409
C   -2.611073   1.641916  -0.861720
C   -2.836069  -0.809204  -1.086169
C   -3.988024   1.719787  -0.652574
C   -4.210030  -0.670450  -0.867925
C   -4.778439   0.574278  -0.638021
H   -4.447914   2.688300  -0.477364
H   -4.834810  -1.557296  -0.824693
H   -5.838450   0.648641  -0.418058
C    2.725158   0.633712  -0.015283
C    2.867919   1.821053   0.726001
C    3.743505  -0.321265  -0.134823
C    4.064814   1.999923   1.420375
C    4.924619  -0.085156   0.576006
C    5.081145   1.051968   1.356444
H    4.208815   2.900402   2.010015
H    5.733385  -0.807764   0.511330
H    6.004310   1.210036   1.906586
C   -2.236377  -2.184403  -1.301180
H   -1.156738  -2.080932  -1.437241
C   -2.815301  -2.835558  -2.563893
H   -2.657549  -2.206023  -3.446688
C   -2.332139  -3.802282  -2.740914
H   -3.892248  -3.011911  -2.463397
H   -2.459191  -3.073117  -0.070797
H   -2.019222  -2.630346   0.829072
H   -3.525146  -3.222292   0.132724
H   -1.998268  -4.053489  -0.235768
C    3.641719  -1.537685  -1.035376
H    2.605393  -1.648030  -1.363093
C    4.013988  -2.825478  -0.294286
H    5.080007  -2.852183  -0.040699
H    3.440052  -2.931131   0.632015
H    3.803949  -3.689253  -0.933539
C    4.537298  -1.353646  -2.269267
H    5.592492  -1.282983  -1.980106
H    4.427996  -2.206438  -2.947822
H    4.286867  -0.442496  -2.823952
C   -1.776554   2.911503  -0.919026
H   -0.719178   2.641043  -0.820242
C   -1.944157   3.598515  -2.282610
H   -1.679607   2.929223  -3.107630
H   -2.984994   3.910007  -2.426186
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H   -1.307748   4.488508  -2.343878
C   -2.108357   3.897163   0.207937
H   -2.112208   3.412516   1.189084
H   -1.370775   4.707711   0.223132
H   -3.091793   4.355621   0.060052
C    1.832073   2.931909   0.703473
H    0.870658   2.500058   0.422331
C    1.633068   3.599598   2.066370
C    1.454792   2.854087   2.847102
C    2.498294   4.206774   2.353608
H    0.765474   4.267365   2.026733
C    2.196751   3.967267  -0.370365
H    2.279161   3.504795  -1.360436
H    1.429334   4.748574  -0.422034
H    3.156230   4.444307  -0.139565
C   -0.519424   0.677617  -3.308355
H    2.202404   0.905325  -2.714239
C    0.050829  -0.150172   1.226826
C    0.451217  -1.396754   1.673149
C   -0.596545   0.819251   2.023087
H    0.389283  -1.612445   2.734711
H   -0.745616   1.810992   1.607682
C    0.761040  -2.503162   0.803406
O    0.805361  -2.495388  -0.425973
O    0.971965  -3.643878   1.503747
C    1.105101  -4.831653   0.732165
H    1.251910  -5.634114   1.454623
H    0.199726  -5.009844   0.145381
H    1.959145  -4.765990   0.054437
C   -0.386216   0.801718   3.089417
C   -2.537694   0.024648   2.290739
H   -2.124742  -0.707006   2.969575
H   -2.913360   0.967849   2.658472
H   -2.624574  -0.227342   1.252116
Cl  -4.619468  -0.908993   2.616389


Pbu-3-tsα

E(ele)      = -1659.062886
E(ele+zpe)  = -1658.542770
H           = -1658.512163
G           = -1658.605725

C    1.258719   1.301691  -1.542476
C    0.456475  -0.736191  -2.679846
H    0.807696  -0.343762  -3.630864
H   -0.065600  -1.684585  -2.715840
H    1.584522   1.665322  -2.513320
C    0.683361  -0.032898  -1.548845
P    0.077607  -0.784686   0.007043
H    1.417690  -1.594622   0.954316
H    0.982046  -2.483073   1.429750
H    1.728158  -0.892551   1.732785
C   -1.095839  -2.124007  -0.421114
H   -1.303400  -2.643956   0.523219
H   -0.578483  -2.850861  -1.058948
H   -0.865467   0.343546   1.088378
H   -1.619147   0.863260   0.482615
H   -0.150419   1.089228   1.446952
C    2.039146   1.730565  -0.420608
O    2.014354   1.215989   0.703709
O    2.763708   2.841826  -0.665755
C    3.469557   3.381542   0.447905
H    4.174409   2.649327   0.849435
H    4.000525   4.251452   0.062638
H    2.773820   3.678992   1.236530
C   -1.526162  -0.372695   2.272428
H   -2.276502  -1.092208   1.919399
H   -0.778577  -0.943648   2.841787
C    2.616321  -1.977801   0.081991
H    2.293362  -2.606620  -0.759845
H    3.040418  -1.064403  -0.352366
C   -2.405298  -1.647044  -1.059025
H   -2.946655  -1.000549  -0.355725
H   -2.194613  -1.029752  -1.940434
C    3.686094  -2.712557   0.889120
H    3.254927  -3.624097   1.324538
H    3.996232  -2.079587   1.730468
C    4.901195  -3.072365   0.036957
H    5.362982  -2.172023  -0.382274
H    5.659678  -3.596510   0.625842
H    4.616653  -3.721394  -0.798675
C   -2.207622   0.636819   3.199315
H   -1.456816   1.343709   3.573325
C   -2.925629   1.227813   2.617271
C   -2.911507  -0.043295   4.370809
H   -3.392775   0.691564   5.022509
H   -3.685551  -0.733841   4.017279
H   -2.202205  -0.616984   4.978275
C   -3.301954  -2.820230  -1.457117
H   -2.762359  -3.461658  -2.167054
H   -3.506983  -3.438047  -0.572377
C   -4.615768  -2.352155  -2.078641
H   -5.245779  -3.200942  -2.360057
H   -5.181574  -1.729241  -1.377778
H   -4.431354  -1.755296  -2.978169
C   -0.484663   2.528708  -1.257771
H   -0.316072   2.563839  -0.196201
H   -0.107652   3.337199  -1.867097
H   -1.055160   1.740014  -1.720604
Cl  -2.480351   3.549975  -0.842995


Pbu-3-tsγ

E(ele)      = -1659.055061
E(ele+zpe)  = -1658.535589
H           = -1658.504696
G           = -1658.599460

C   -1.706197   1.573159  -1.433279
C   -0.732276  -0.229502  -2.803808
C   -1.303161   0.133898  -3.656246
H    0.168014  -0.773258  -3.069319
H   -2.303919   1.901795  -2.277786


Pph-3-tsα

E(ele)      = -1880.409089
E(ele+zpe)  = -1879.987434
H           = -1879.959513
G           = -1880.045786

P    0.661094  -0.128197  -0.170616
C    1.675085   1.310833   0.257250
C    2.558178   1.213868   1.336648
C    1.660995   2.454928  -0.542400
C    3.405893   2.277761   1.633993
H    2.593454   0.307267   1.937550
C    2.525147   3.507105  -0.251421
H    0.977142   2.523327  -1.384243
C    3.390189   3.422994   0.838600
H    4.084154   2.207099   2.478802
H    2.517038   4.396298  -0.874195
H    4.057375   4.249181   1.066111
C    1.923977  -1.425928  -0.407608
H    1.803071  -2.695356   0.162733
C    3.057995  -1.114730  -1.172414
C    2.800659  -3.649282  -0.042817
H    0.942807  -2.945515   0.774914
C    4.045582  -2.070959  -1.379362
C    3.167430  -0.123282  -1.606155
H    3.916792  -3.341433  -0.814910
C    2.699424  -4.632876   0.405462
H    4.917800  -1.822810  -1.976288
H    4.690213  -4.087076  -0.973348
C   -0.427766  -0.685001   1.156271
C   -1.280849  -1.761986   0.891135
C   -0.462088  -0.040885   2.395447
C   -2.170966  -2.198791   1.869226
H   -1.300381  -2.232478  -0.090691
C   -1.332326  -0.502768   3.378093
H    0.149501   0.838235   2.574915
C   -2.184722  -1.576094   3.115405
H   -2.875494  -2.988129   1.628171
H   -1.367961  -0.001334   4.340588
C   -2.883483  -1.910823   3.876368
C    0.127654  -0.732100  -2.755858
H   -0.408538  -0.680148  -3.700884
C   -1.408778   0.953903  -1.809488
H    0.937744  -1.446537  -2.689703
C   -0.248938   0.080480  -1.740790
C   -3.019463  -0.346991  -1.318292
C   -2.868534  -0.211788  -0.259662
H   -3.763417   0.255710  -1.819666
C   -1.640739   1.953162  -0.806045
O   -1.104520   1.984347   0.302782
O   -2.597949   2.841033  -1.152388
C   -2.968194   3.771412  -0.138274
H   -3.357103   3.247679   0.738460
H   -2.109288   4.378142   0.159458
H   -3.742223   4.395919  -0.583320
H   -1.742063   1.196544  -2.814691
H   -2.497646  -1.119719  -1.861755
Cl  -4.564290  -1.958695  -0.771814


Pph-3-tsγ
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E(ele)        = -1880.401771
E(ele+zpe)    = -1879.980955
H             = -1879.952874
G             = -1880.040639
C    0.530772   -1.717013   -1.876952
C   -0.958056    0.147026   -2.526133
C   -0.031954   -0.470468   -1.663504
P    0.291644    0.405696   -0.086248
C    1.246899   -2.454743   -0.869883
O    1.371769   -2.114692    0.305146
O    1.784201   -3.599408   -1.338428
C    2.483623   -4.385334   -0.377707
H    1.825456   -4.651690    0.452908
H    2.808663   -5.277957   -0.911097
H    3.344786   -3.835914    0.011919
C   -0.660346   -0.234828    1.309315
C   -0.748190    0.530756    2.479497
C   -1.404222   -1.408963    1.175783
C   -1.562535    0.100954    3.522220
H   -0.208309    1.471488    2.566392
C   -2.250227   -1.809266    2.206545
H   -1.349537   -1.996352    0.264043
C   -2.318826   -1.063507    3.381006
H   -1.625509    0.688667    4.433021
H   -2.867571   -2.691435    2.071764
H   -2.978772   -1.379094    4.183635
C   -0.307371    2.120138   -0.273361
C    0.550525    3.132821   -0.714686
C   -1.653341    2.417354   -0.017570
C    0.065958    4.424658   -0.909273
H    1.599366    2.923524   -0.900871
C   -2.133180    3.708016   -0.219786
H   -2.330064    1.648852    0.346881
C   -1.275415    4.712260   -0.667462
H    0.740531    5.205005   -1.248221
H   -3.178353    3.926177   -0.023369
H   -1.652831    5.718951   -0.820974
C    2.075525    0.536713    0.199563
C    2.915283    0.694780   -0.906357
C    2.604068    0.510010    1.490883
C    4.286790    0.846343   -0.713104
H    2.505265    0.681982   -1.913890
C    3.975060    0.665845    1.675159
H    1.958316    0.331432    2.345730
C    4.815636    0.838703    0.576186
H    4.940799    0.962829   -1.572076
H    4.387964    0.636454    2.678933
H    5.885173    0.955143    0.724705
H    0.418487   -2.177464   -2.853643
H   -1.145991    1.212949   -2.460397
H   -1.028138   -0.273012   -3.527550
C   -2.750000   -0.686604   -1.789139
H   -3.336595   -0.227440   -2.571820
H   -2.316744   -1.665976   -1.928962
H   -2.678258   -0.190076   -0.838134
Cl  -4.607024   -1.723740   -0.935082


Hmpt-3-tsα

E(ele)        = -1589.282999
E(ele+zpe)    = -1588.882791
H             = -1588.856756
G             = -1588.936661
C   -1.208078    0.444781   -1.229032
C   -0.012359   -0.389210   -1.200303
P    1.329411   -0.234057    0.018093
C   -1.359425    1.556292   -0.330616
O   -0.717906    1.743030    0.704794
O   -2.368126    2.378894   -0.691553
C   -2.685770    3.416208    0.231897
H   -1.825500    4.072979    0.385977
H   -3.510180    3.966408   -0.220265
N    2.516749   -1.381466   -0.236764
N    2.164663    1.171327   -0.228670
C    0.814335   -0.527111    1.564745
C   -0.479762   -1.162195    1.822007
C   -0.801695   -1.764372    0.969442
H   -0.377284   -1.827034    2.686598
H   -1.241881   -0.405070    2.036320
C    1.227855    0.383159    2.632656
H    2.287536    0.631571    2.550271
H    0.626589    1.299663    2.613048
C    1.083775   -0.130779    3.587743
H    1.857627   -2.680318    1.277960
H    2.052619   -3.449878   -0.320331
H    3.482886   -3.010011    0.646121
C    3.434095   -1.296006   -1.367924
H    3.333199   -0.332627   -1.871022
H    4.466258   -1.405256   -1.011292
H    3.237730   -2.091823   -2.098363
C    3.472818    1.397765    0.379235
H    3.415398    2.189701    1.136541
H    3.848346    0.483467    0.842633
H    4.183302    1.708373   -0.396993
C    1.633179    2.345340   -0.918461
H    1.290250    3.102480   -0.206209
C    2.434286    2.759040   -1.541511
H    0.803617    2.068491   -1.568879
C    0.167906   -1.417371   -2.062928
H    1.030448   -2.070423   -2.037786
H   -0.578106   -1.617021   -2.829089
H   -1.632931    0.585864   -2.218932
C   -2.787332   -0.753456   -0.554853
H   -2.723540   -0.422264    0.467127
H   -3.514247   -0.282817   -1.199238
H   -2.248374   -1.627707   -0.888639
Cl  -4.407452   -2.233400    0.193534


Hmpt-3-tsγ

E(ele)        = -1589.282627
E(ele+zpe)    = -1588.881883
H             = -1588.856236
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G             = -1588.935106
C   -1.065614   -1.364793   -1.315165
C   -0.134169   -0.340378   -1.299041
P   -0.087436    0.958882   -0.016538
C   -2.066978   -1.561791   -0.300634
O   -2.229004   -0.860177    0.695985
C   -2.853078   -2.632145   -0.547418
C   -3.843267   -2.903437    0.438381
H   -4.548151   -2.071183    0.515494
H   -4.353551   -3.805026    0.101182
H   -3.378513   -3.067572    1.413855
N    1.092611    2.107209   -0.307637
N   -1.455814    1.891984   -0.102677
N    0.419692    0.312529    1.415231
C    0.440224   -1.115363    1.748132
H    0.275620   -1.723795    0.861269
H    1.430292   -1.363954    2.147722
C   -0.339777   -1.341621    2.482025
C    0.610318    1.169421    2.582656
H    0.807946    2.201528    2.285026
H   -0.271237    1.142612    3.235923
C    1.476905    0.806968    3.146841
C    2.493544    1.942310    0.074390
C    2.604600    1.196285    0.860872
C    3.104202    1.634472   -0.785012
C    2.874044    2.901810    0.444192
C    0.913924    3.153324   -1.310077
H   -0.126183    3.205444   -1.632274
H    1.204907    4.121851   -0.884427
C    1.544841    2.960038   -2.187899
C   -1.604791    3.034095    0.795134
H   -2.194638    2.766778    1.681580
H   -0.630508    3.413018    1.110331
C   -2.122568    3.838440    0.260147
C   -2.704447    1.521600   -0.763144
H   -3.446069    1.175448   -0.036366
H   -3.083134    2.409030   -1.284322
C   -2.533966    0.735971   -1.497897
C    0.990093   -0.281747   -2.148192
H    1.520860    0.655157   -2.280668
H   -1.030429   -2.083235   -2.128537
H    0.973743   -0.926158   -3.024555
C    2.394410   -1.354238   -0.999587
H    1.756936   -2.226144   -1.027794
H    3.157842   -1.208537   -1.749449
H    2.335950   -0.672348   -0.172154
Cl   3.883725   -2.511530    0.303112


Quin-3-tsα

E(ele)        = -1173.580067
E(ele+zpe)    = -1173.234661
H             = -1173.216474
G             = -1173.279930
C    1.088055    0.502182    1.116679
C   -0.288195   -0.775994    2.680057
H    0.556697   -0.752017    3.358782
H   -1.138785   -1.359092    2.997163
C    1.735896    0.590794    1.983174
C   -0.177157   -0.114480    1.513339
C    1.335312    1.559550    0.162351
O    0.670680    1.880747   -0.825042
O    2.532179    2.142466    0.403859
C    2.972539    3.077816   -0.577427
H    2.259957    3.900321   -0.672088
H    3.934191    3.443394   -0.218623
H    3.088139    2.589625   -1.548133
C   -1.903050    1.252330    0.371932
C   -0.850265   -0.720865   -0.782488
C   -2.488748   -1.006978    1.002428
C   -2.742035    1.290684   -0.910188
H   -1.079144    1.956553    0.337157
C   -2.497365    1.426149    1.273662
C   -2.040509   -0.951699   -1.726625
H   -0.316995   -1.642577   -0.538763
H   -0.154598    0.012014   -1.184778
C   -2.136332   -2.040913    0.982152
H   -2.720728   -0.728648    2.029176
C   -3.705310   -0.773650    0.082770
H   -2.134377    1.678741   -1.735063
C   -3.583856    1.974679   -0.763271
H   -2.305457   -2.013825   -1.771010
C   -1.750095   -0.644261   -2.735273
H   -4.192796   -1.733979   -0.109687
H   -4.438293   -0.129422    0.580731
H   -1.330004   -0.147819    0.548891
C    2.213840   -1.011784    0.205450
H    1.893449   -0.781160   -0.797076
H    3.152962   -0.606322    0.551193
H    1.697852   -1.750237    0.800662
Cl   3.337715   -2.800247   -0.754259
H   -3.229836   -0.130649   -1.222916
H   -4.034588   -0.115366   -1.962643


Quin-3-tsγ

E(ele)        = -1173.575145
E(ele+zpe)    = -1173.230010
H             = -1173.211839
G             = -1173.275532
C    0.865194   -1.415807    0.959391
C   -1.198297   -0.603788    1.982381
C   -1.173223   -1.510792    2.578566
H   -1.719166    0.214303    2.461778
H    0.675715   -2.312921    1.537966
C   -0.035153   -0.394424    1.219781
O    1.980565   -1.555488    0.052285
O    2.451187   -0.736635   -0.738329
C    2.524467   -2.788774    0.167707
C    3.626481   -3.058523   -0.692756
H    4.451158   -2.370793   -0.489070
H    3.920710   -4.084533   -0.474927
H    3.329555   -2.958840   -1.739753
C    1.467177    1.545845    0.755005
C   -0.152648    0.707254   -0.981767
```

```
C   -0.898425    1.973136    0.978571
H    1.730190    2.614150   -0.312143
H    2.210779    0.758535    0.728695
H    1.412706    1.962157    1.765118
C   -0.252963    2.057348   -1.709455
H   -1.068263    0.118427   -1.052543
H    0.688965    0.115011   -1.333075
H   -1.885928    1.632871    0.663534
H   -0.860049    1.991370    2.067343
C   -0.538290    3.346527    0.377809
C    2.313562    2.178069   -1.130670
C    2.323226    3.420564    0.130805
C   -1.296982    2.309305   -1.925884
H    0.270108    1.977352   -2.667021
H   -1.460652    3.855228    0.082254
H   -0.045668    3.974027    1.128796
N    0.095866    0.931026    0.511067
C   -2.638569   -1.233260    0.598620
H   -1.922108   -1.894224    0.133130
H   -2.810206   -0.242089    0.214993
H   -3.274685   -1.594660    1.392171
Cl  -4.181774   -1.919990   -0.946723
C    0.382209    3.136795   -0.828596
H    0.509491    4.068972   -1.385166


Dabco-3-tsα

E(ele)        = -1189.597123
E(ele+zpe)    = -1189.263283
H             = -1189.245263
G             = -1189.308628
C    1.093680    0.508483    1.113315
C   -0.308504   -0.718883    2.698089
H    0.525891   -0.680364    3.388888
H   -1.167010   -1.289361    3.017028
C    1.742273    0.597252    1.979292
C   -0.177746   -0.088870    1.516533
C    1.345395    1.562159    0.155384
O    0.676987    1.886113   -0.829021
O    2.547513    2.134628    0.388251
C    2.991069    3.065827   -0.596406
H    2.286407    3.896120   -0.684636
H    3.958976    3.420486   -0.244789
H    3.093111    2.576573   -1.567962
C   -1.909653    1.254323    0.358655
C   -0.845952   -0.709191   -0.784711
C   -2.477964   -1.002062    0.991844
C   -2.801439    1.229312   -0.898592
H   -1.092194    1.961750    0.261703
C   -2.468588    1.451674    1.277726
C   -2.059525   -0.875052   -1.727462
H   -0.348372   -1.654012   -0.551915
H   -0.126292    0.004112   -1.178794
C   -2.114677   -2.032252    1.008003
H   -2.751575   -0.698789    2.001723
C   -3.659877   -0.792469    0.007033
H   -2.253002    1.632891   -1.754946
C   -3.687911    1.850324   -0.737770
H   -2.341136   -1.927269   -1.831495
C   -1.802930   -0.498678   -2.721002
H   -4.106993   -1.759397   -0.240015
H   -4.437033   -0.174461    0.467217
H   -1.324754   -0.137211    0.544154
C   -3.215411   -0.139146   -1.217530
C    2.199020   -1.023642    0.215084
H    1.890315   -0.791928   -0.790654
H    3.143102   -0.633273    0.564679
H    1.669937   -1.754023    0.808585
Cl   3.296579   -2.834613   -0.736687


Dabco-3-tsγ

E(ele)        = -1189.592137
E(ele+zpe)    = -1189.258896
H             = -1189.240739
G             = -1189.304708
C    0.897905   -1.392616    0.968720
C   -1.182066   -0.620320    1.993902
H   -1.135397   -1.520894    2.598433
H   -1.715681    0.192619    2.468732
C    0.734172   -2.289734    1.555185
C   -0.025659   -0.392754    1.226543
O    2.009420   -1.511919    0.053383
O    2.452112   -0.686543   -0.746949
C    2.583429   -2.729653    0.172594
C    3.685123   -2.979867   -0.694909
H    4.487245   -2.259771   -0.515629
H    4.016594   -3.990326   -0.459033
H    3.372694   -2.913392   -1.739983
C    1.425589    1.580509    0.747790
C   -0.177793    0.704339   -0.980134
C   -0.941454    1.954715    0.968487
H    1.605537    2.694536   -0.301650
H    2.198142    0.824492    0.670073
H    1.381681    1.962369    1.771810
C   -0.228351    2.077136   -1.690053
H   -1.115217    0.150261   -1.055010
H    0.645303    0.088563   -1.334508
H   -1.927330    1.583870    0.685077
H   -0.879632    2.017439    2.055198
C   -0.607431    3.311477    0.292677
C    2.212205    2.328507   -1.135283
C    2.121859    3.548400    0.147378
C   -1.253922    2.345916   -1.960417
H    0.359833    2.034534   -2.610480
H   -1.529213    3.777659   -0.066043
H   -0.145391    3.996415    1.010283
N    0.072077    0.931480    0.509087
C    0.309075    3.128483   -0.826794
C   -2.601153   -1.284460    0.610975
H   -1.856538   -1.880025    0.103716
H   -2.844534   -0.290834    0.275300
H   -3.201917   -1.722747    1.393514
Cl  -4.119726   -1.995185   -0.953760


Dmap-3-tsα
```

```
E(ele)        = -1226.520774
E(ele+zpe)    = -1226.211436
H             = -1226.190569
G             = -1226.262300
C   -1.324978   -0.158929    3.155087
H   -2.294565   -0.203209    3.638607
C   -2.273704   -0.575970    0.867377
C   -0.458200    0.087294    3.758515
C   -1.216358   -0.398735    1.837087
C    0.854369   -1.413425    1.029791
C    0.654105    0.914536    0.967133
C    2.099382   -1.361957    0.460396
H    0.373319   -2.346522    1.294514
C    1.879730    1.042955    0.369922
H    0.034502    1.776076    1.189992
C    2.652951   -0.112285    0.076944
H    2.613612   -2.295164    0.276358
H    2.215869    2.039775    0.118784
N    0.143837   -0.296598    1.290033
C   -2.096255   -1.350676   -0.335088
H   -1.035333   -1.670597   -0.868498
O   -3.286541   -1.630329   -0.925254
O   -3.206172   -2.275178   -2.191487
H   -4.236541   -2.391115   -2.527062
H   -2.639871   -1.664863   -2.899443
N    3.850507   -0.022443   -0.535767
C    4.599968   -1.230538   -0.848524
H    5.529444   -0.951568   -1.342744
H    4.849336   -1.785158    0.062927
H    4.032343   -1.884268   -1.520793
C    4.356503    1.277510   -0.957976
H    3.669312    1.756781   -1.663996
H    5.317374    1.138395   -1.451154
H    5.283759   -0.603324    1.294608
C   -2.244993    1.368795   -0.072262
H   -1.359889    1.075630   -0.612928
H   -3.207154    1.238214   -0.547481
H   -2.205545    1.785373    0.921557
Cl  -1.913837    3.460206   -0.875000


Dmap-3-tsγ

E(ele)        = -1226.514747
E(ele+zpe)    = -1226.205326
H             = -1226.184499
G             = -1226.256236
C   -1.830074    1.099827    2.072846
C   -2.821083    1.127376    2.516368
C   -2.365909   -0.937420    0.710386
H   -3.415096   -0.891041    0.977565
C   -1.035754    1.555904    2.657231
C   -1.520006   -0.015351    1.282719
C    0.839259   -0.444262    1.731834
C    0.216344    0.280868   -0.400873
C    2.161209   -0.492240    1.374148
H    0.488996   -0.721460    2.719814
C    1.517909    0.282707   -0.823906
H   -0.606353    0.564831   -1.047757
C    2.553470   -0.118510    0.059631
H    2.880332   -0.821084    2.112136
H    1.719375    0.583316   -1.842969
N   -0.116100   -0.056575    0.865145
C   -1.961448   -2.011338   -0.170930
H   -0.835572   -2.261023   -0.588995
O   -3.024196   -2.780183   -0.513728
O   -2.737374   -3.866054   -1.386737
H   -3.690905   -4.365935   -1.554756
H   -2.325061   -3.502063   -2.331360
H   -2.020453   -4.551851   -0.927862
N    3.844555   -0.141704   -0.327350
C    4.877495   -0.570014    0.604204
H    5.845347   -0.517852    0.107851
H    4.907982    0.081199    1.485159
H    4.711467   -1.603631    0.928988
C    4.204108    0.247372   -1.684936
H    3.726879   -0.408787   -2.421373
H    3.912853    1.283912   -1.887121
H    5.283863    0.165863   -1.800745
C   -1.897378    2.590903    0.542505
H   -2.366464    3.298978    1.209085
H   -0.822894    2.573218    0.477581
H   -1.945767   -0.068980    1.045767
Cl  -1.848742    4.096589   -1.159823


Py-3-tsα

E(ele)        = -1092.594470
E(ele+zpe)    = -1092.359360
H             = -1092.342973
G             = -1092.403822
C    0.728731   -0.104346    2.901296
H    0.029593   -0.078711    3.729313
H   -1.070897   -0.461962    1.716510
H    1.776917    0.083999    3.105824
C    0.287276   -0.359674    1.658797
C    1.806481   -1.534308    0.915618
C    1.754420    0.815091    0.101323
C    2.762304   -1.569209   -0.832950
C    1.386464   -2.418548    0.627757
C    2.691391    0.835420   -0.915618
C    1.310014    1.715965    0.510769
C    3.202286   -0.371345   -1.388296
H    3.131044   -2.527102   -1.179256
H    2.998735    1.790532   -1.324939
N    1.334472   -0.358860    0.616684
C   -1.417820   -1.262123    0.025581
O   -0.660274   -1.651842   -0.861368
O   -2.751914   -1.475706   -0.047750
C   -3.202776   -2.152680   -1.217649
H   -4.283438   -2.236713   -1.107617
H   -2.952178   -1.579331   -2.113299
H   -2.746871   -3.143399   -1.288944
H   -1.820285   -0.424778    1.961367
```

```
C   -1.277228    1.470347    0.279555
H   -0.698653    1.132571   -0.564496
H   -2.355580    1.431852    0.206959
H   -0.829769    1.873178    1.173784
Cl  -1.088911    3.556394   -0.607055
H    3.936682   -0.377077   -2.187887
```

Py-3-ts$_\gamma$

```
E(ele)       =  -1092.588543
E(ele+zpe)   =  -1092.353558
H            =  -1092.337119
G            =  -1092.398660
```

```
C   -1.052976   -0.485010    2.151868
H   -1.020675   -1.330652    2.832504
C    1.063979   -1.191230    0.989177
H    1.100212   -2.134304    1.521511
H   -1.563615    0.399671    2.522649
C    0.065350   -0.310121    1.323810
C    0.377041    2.093397    1.140241
C   -0.376657    0.897531   -0.736997
C    0.345443    3.281053    0.433926
H    0.694669    2.009673    2.173337
C   -0.449198    2.060135   -1.483228
H   -0.631084   -0.081854   -1.127984
C   -0.077061    3.264298   -0.894450
H    0.649007    4.199043    0.923048
H   -0.785920    2.004525   -2.511421
N    0.013628    0.942405    0.549511
C    2.107354   -0.939734    0.014184
O    2.258460    0.063816   -0.674479
O    2.958805   -1.985537   -0.064290
C    4.020028   -1.842809   -1.004221
H    4.594470   -2.766046   -0.938910
H    3.621892   -1.709201   -2.013029
H    4.643735   -0.982329   -0.750235
C   -2.486881   -1.055041    0.700952
H   -3.175626   -1.419865    1.448615
H   -2.577102   -0.033844    0.372770
H   -1.779229   -1.736646    0.254314
Cl  -3.923930   -1.556599   -0.999347
H   -0.114161    4.186140   -1.466255
```

Dbu-3-ts$_\alpha$

```
E(ele)       =  -1306.336420
E(ele+zpe)   =  -1305.940587
H            =  -1305.918999
G            =  -1305.990051
```

```
C   -0.670118    2.459395   -0.214420
C   -0.862869    1.536619    1.027133
C   -1.422716    0.162336    0.737396
C   -1.103324    1.847296   -1.549728
C   -2.630080    1.767761   -1.678449
C   -3.267212    1.304075   -0.366868
H   -1.221885    3.393177   -0.048350
H    0.081367    1.416800    1.552922
H   -0.658166    0.848670   -1.661838
H   -2.912816    1.091451   -2.494679
H    0.386317    2.741502   -0.263473
H   -1.546499    1.996081    1.752316
H   -0.699186    2.451408   -2.367861
H   -3.044908    2.754260   -1.920240
H   -4.329000    1.072142   -0.487479
H   -3.199681    2.085751    0.393386
C   -1.300197   -2.277220    0.816879
C   -2.173768   -2.256290   -0.422160
C   -3.231977   -1.182799   -0.260640
H   -0.433475   -2.924788    0.676120
H   -1.543123   -2.040111   -1.288499
H   -2.649738   -3.231137   -0.559238
H   -3.753103   -1.010559   -1.206815
H   -3.980842   -1.462810    0.491907
H   -1.850945   -2.623242    1.701303
N   -2.617116    0.088740    0.136795
N   -0.778528   -0.931949    1.106322
C    0.519773   -0.929451    1.770287
C    1.687939   -1.158969    0.943848
H    2.564225   -1.504617    1.483040
C    0.511684   -0.727240    3.100694
C    1.608133   -1.577509   -0.428980
O    0.660645   -1.432268   -1.203724
O    2.790723   -2.081746   -0.867098
H    1.437300   -0.743310    3.666568
H   -0.414707   -0.546433    3.635243
C    2.864805   -2.352929   -2.262481
H    2.123094   -3.102444   -2.551092
H    2.694149   -1.441634   -2.841566
H    3.872807   -2.729905   -2.434020
C    2.375892    0.818209    0.468752
H    1.560570    0.937928   -0.228190
H    2.264653    1.064976    1.513532
H    3.321992    0.447971    0.101996
Cl   2.979669    2.969044    0.068364
```

Dbu-3-ts$_\gamma$

```
E(ele)       =  -1306.331207
E(ele+zpe)   =  -1305.935180
H            =  -1305.913519
G            =  -1305.985739
```

```
C   -0.201261    0.790603   -2.151110
C    0.724584    0.288081   -1.005883
C    0.281946    0.676509    0.380894
C   -1.160367    1.942279   -1.831699
C   -0.476020    3.240600   -1.402784
C    0.592631    2.985410   -0.334859
H    0.440315    1.061019   -2.997789
H    0.785724   -0.795080   -1.057953
H   -1.850397    1.608992   -1.049824
H   -1.229071    3.942947   -1.025475
H   -0.809461   -0.059307   -2.475661
H    1.755013    0.641656   -1.143475
H   -1.772859    2.137155   -2.719122
H    0.012976    3.728492   -2.254414
```

```
H    0.826545    3.894376    0.227399
H    1.526424    2.651862   -0.791085
C   -0.464054    0.158373    2.639796
C   -1.330249    1.397582    2.490729
C   -0.498359    2.492444    1.850299
H   -1.040935   -0.690449    3.012109
H   -2.185970    1.152510    1.853598
H   -1.693507    1.727631    3.467498
H   -1.130852    3.329560    1.535828
H    0.258014    2.881512    2.544238
H    0.375124    0.334589    3.324998
N    0.171489    1.980974    0.650928
N    0.054450   -0.230436    1.321147
C    0.173536   -1.667481    1.100335
C   -0.790365   -2.291530    0.329212
H   -0.707466   -3.361005    0.174514
C    1.313245   -2.234740    1.681896
C   -1.943247   -1.639577   -0.231543
O   -2.287563   -0.462211   -0.110174
O   -2.696462   -2.504270   -0.959629
H    1.768809   -1.719226    2.522489
H    1.377171   -3.319144    1.700441
C   -3.864803   -1.950475   -1.550480
H   -4.534807   -1.550283   -0.784999
H   -3.603299   -1.146520   -2.244996
H   -4.342365   -2.772027   -2.083818
C    2.875984   -1.610458    0.311845
H    3.623436   -2.150641    0.874109
H    2.362054   -2.107795   -0.493567
H    2.645207   -0.599672    0.595849
Cl   4.355035   -0.753458   -1.153934
```

Mtbd-3-ts$_\alpha$

```
E(ele)       =  -1322.373400
E(ele+zpe)   =  -1321.989353
H            =  -1321.967552
G            =  -1322.039312
```

```
C    0.878822   -2.110031    0.907460
C   -1.155973   -0.814913    0.297196
C    0.024152   -1.997694   -1.416314
C    0.623528   -2.913862   -0.365473
H    1.891329   -1.703707    0.885158
H    0.791097   -2.742628    1.796813
H   -0.221964   -2.549415   -2.326502
H    0.701202   -1.174895   -1.683101
H   -0.072892   -3.738933   -0.182415
H    1.572956   -3.328684   -0.715207
C   -3.155856    0.452041   -0.223353
C   -3.522948   -0.635280   -1.219332
C   -2.251333   -1.139435   -1.875687
H   -4.033181    0.780364    0.337834
H   -4.033609   -1.453056   -0.698914
H   -4.198392   -0.243295   -1.985117
H   -2.444315   -2.045555   -2.458266
H   -1.838048   -0.373889   -2.546803
H   -2.712392    1.317889   -0.728858
N   -1.228071   -1.459867   -0.882939
N   -0.048769   -0.959503    1.059607
C   -2.194652   -0.084207    0.741926
C    0.474003    0.148432    1.844150
C    0.813006    1.390681    1.159499
H    1.185842    2.163757    1.825415
C    0.821590   -0.115114    3.116922
C    0.230963    1.894513   -0.050201
O   -0.314344    1.258487   -0.959243
O    0.459548    3.228375   -0.195949
H    1.322421    0.636714    3.716801
H    0.630351   -1.082084    3.570074
C    0.107378    3.777041   -1.459713
H    0.644089    3.270466   -2.265951
H   -0.968140    3.685341   -1.637690
H    0.393168    4.827787   -1.413236
C   -2.363731    0.297456    2.139504
H   -1.877984   -0.428846    2.787910
H   -1.945744    1.289047    2.346087
H   -3.435734    0.301818    2.352532
C    2.527824    0.625768    0.110782
H    2.894148    1.568660   -0.273063
H    2.909196    0.260289    1.051134
H    1.823115    0.070973   -0.480896
Cl   4.109044   -0.637388   -0.956176
```

Mtbd-3-ts$_\gamma$

```
E(ele)       =  -1322.366342
E(ele+zpe)   =  -1321.982951
H            =  -1321.960888
G            =  -1322.033493
```

```
C    1.038922   -1.687594   -0.434502
C   -1.188258   -0.878815    0.316832
C   -0.931537   -1.766446   -1.900521
C    0.258616   -2.562067   -1.400220
C    1.665872   -0.982556   -0.990602
H    1.691193   -2.291355    0.202136
H   -1.536379   -2.347816   -2.600519
H   -0.624127   -0.828552   -2.383453
H   -0.099821   -3.473655   -0.910727
H    0.916604   -2.853899   -2.223065
C   -3.296674    0.107646    0.984504
C   -4.012045   -0.958730    0.173715
C   -3.188039   -1.240904   -1.068338
C   -3.806422    0.295737    1.931402
H   -4.120428   -1.866341    0.777333
H   -5.010027   -0.621361   -0.120266
H   -3.552121   -2.133380   -1.586203
H   -3.242918   -0.389902   -1.761696
H   -3.234116    1.052081    0.429336
N   -1.777637   -1.460959   -0.749041
N    0.156145   -0.884792    0.437021
C   -1.946461   -0.357584    1.300021
C    0.841626    0.225795    1.082663
C    0.521033    1.523432    0.715153
H    1.046820    2.319183    1.231505
C    1.905752   -0.117505    1.932254
```

```
C   -0.367489    1.944598   -0.332079
O   -1.073606    1.253211   -1.073036
O   -0.377327    3.296859   -0.449337
H    2.263021    0.675858    2.581651
H    1.906581   -1.113202    2.370291
H   -1.192652    3.821366   -1.488455
H   -0.874866    3.437040   -2.460908
H   -2.242483    3.558409   -1.329381
H   -1.062524    4.902290   -1.445876
C   -1.476553   -0.160452    2.666354
H   -0.605130   -0.784260    2.858061
H   -1.208580    0.884831    2.851340
H   -2.282273   -0.462570    3.341554
C    3.654827   -0.138330    0.747219
H    3.266515    0.653400    0.124588
H    4.265346    0.104405    1.602451
H    3.530771   -1.171504    0.477055
Cl   5.536909   -0.159533   -0.568853
```

9.4 [3 + 2] cycloaddition with ethylene 2a

```
        ethylene 2a

  E(ele)      = -78.541283
  E(ele+zpe)  = -78.489664
  H           = -78.485688
  G           = -78.511190
C    0.000000   0.665185   0.000000
H    0.924990   1.235281   0.000000
H   -0.924951   1.235324   0.000000
C    0.000000  -0.665185   0.000000
H   -0.924990  -1.235281   0.000000
H    0.924951  -1.235324   0.000000


        IMe-ts4a

  E(ele)      = -727.641340
  E(ele+zpe)  = -727.352116
  H           = -727.334415
  G           = -727.396014
C    1.195836  -0.142630   0.316879
C    2.876938  -0.887388  -0.958443
C    2.453227  -1.920270  -0.189976
H    3.654974  -0.828547  -1.703317
H    2.788404  -2.944054  -0.133336
N    1.433202  -1.443015   0.602206
C    2.071233   1.460957  -1.368688
H    2.517800   2.265920  -0.781493
H    2.633419   1.322945  -2.293316
C    1.035735   1.710288  -1.603585
C    0.665417  -2.237282   1.545719
H   -0.180005  -2.699924   1.031144
H    1.319777  -3.000730   1.970476
H    0.297447  -1.575043   2.330714
C    0.599731   1.989427   1.408294
H    0.034149   2.399219   2.241800
C   -1.163898   0.452550   0.828469
H   -1.856472   0.835201   1.568922
H    1.660118   2.247117   1.455194
C    0.222213   0.701735   0.971272
C   -0.484567   3.213229   0.094722
H   -0.728861   4.001345   0.803593
H    0.340378   3.477015  -0.562579
C   -1.528579   2.417855  -0.386197
H   -1.449571   1.912882  -1.346612
C   -2.541221   2.544277  -0.016736
H   -1.677233  -0.548677  -0.074757
O   -1.037757  -1.198162  -0.900039
C   -3.025801  -0.693997   0.031418
C   -3.620560  -1.576069  -0.910333
H   -3.440892  -1.229899  -1.931996
H   -3.216442  -2.586884  -0.806503
H   -4.687926  -1.568875  -0.688613


        IMe-4a

  E(ele)      = -727.734500
  E(ele+zpe)  = -727.439365
  H           = -727.422386
  G           = -727.483058
C   -1.127244  -0.299036   0.215874
C   -3.302349   0.022210  -0.396667
C   -2.952522   1.056124   0.382009
H   -4.234075  -0.198186  -0.894542
H   -3.526153   1.906154   0.718946
N   -1.618961   0.890297   0.761544
N   -2.204618  -0.839423  -0.499791
C   -2.041063  -1.721610  -1.635844
H   -1.878653  -2.758010  -1.329084
H   -2.950992  -1.678603  -2.237899
H   -1.193085  -1.393272  -2.250221
C   -1.062770   1.549613   1.921293
H   -0.162985   2.116287   1.665951
H   -1.812304   2.240565   2.312701
H   -0.827224   0.812940   2.699939
C    0.483218  -2.299044   0.056713
H    0.004442  -2.968486   0.789014
C    1.361362  -0.117744   0.862526
H    1.184433   0.527236   1.726901
H    0.195481  -2.663631  -0.932987
C    0.118763  -0.845741   0.345275
C    2.013527  -2.350795   0.201334
H    2.372223  -3.334795   0.518824
C    2.484070  -2.109095  -0.757216
C    2.339998  -1.246730   1.207662
H    3.383616  -0.922411   1.163329
H    2.124334  -1.588918   2.227250
C    1.884261   0.760531  -0.256664
O    2.787601   0.500411  -1.017760
C    1.167668   1.902139  -0.342876
C    1.494745   2.749195  -1.442416
H    2.537149   3.071165  -1.380480
H    1.340483   2.219205  -2.385630
H    0.822579   3.603500  -1.369098


        IPr-ts4a

  E(ele)      = -1582.524430
  E(ele+zpe)  = -1581.786850
  H           = -1581.746602
  G           = -1581.855863
C    0.458156   1.104616  -2.074080
C   -0.866280   0.850113  -2.121108
C   -0.134339   0.241160  -0.081633
N    0.904472   0.731133  -0.817173
C   -1.225620   0.314146  -0.891844
C    2.205831   1.112508  -0.324871
C    2.289071   2.214139   0.544497
C    3.337624   0.442083  -0.809880
C    3.559604   2.599672   0.974374
C    4.586794   0.880718  -0.359191
C    4.700687   1.938878   0.532753
```

```
H    3.655805   3.440821   1.656288
H    5.482889   0.377249  -0.711805
H    5.680286   2.256920   0.878058
C   -2.585164  -0.079902  -0.615757
C   -3.532890   0.938228  -0.437382
C   -2.911861  -1.446979  -0.615564
C   -4.870475   0.555736  -0.299061
C   -4.262020  -1.772645  -0.472335
C   -5.233094  -0.784621  -0.328100
H   -5.633852   1.316968  -0.161323
H   -4.560230  -2.815909  -0.459535
H   -6.277046  -1.065653  -0.221404
H    3.260336  -0.695118  -1.812778
H    2.227834  -1.052930  -1.846508
C    3.679133  -0.216169  -3.210470
H    3.048198   0.601097  -3.575299
H    3.614416  -1.040840  -3.928909
H    4.714071   0.145921  -3.201045
C    4.136251  -1.877739  -1.381625
H    4.000672  -2.094379  -0.319135
H    5.199314  -1.676369  -1.560588
H    3.863754  -2.770358  -1.954181
C   -1.834640  -2.511676  -0.733735
H   -0.988389  -2.197621  -0.112753
C   -2.281856  -3.883404  -0.227114
H   -3.023487  -4.341859  -0.893002
H   -2.702131  -3.832352   0.783321
H   -1.412423  -4.548510  -0.196739
C   -1.311629  -2.640311  -2.171583
H   -0.891411  -1.702510  -2.545672
H   -2.117102  -2.954351  -2.847361
H   -0.513708  -3.388752  -2.200976
C    1.082173   3.022933   0.990810
H    0.173728   2.541310   0.619698
C    1.128111   4.435166   0.391718
H    1.169164   4.400189  -0.702497
H    2.007720   4.986099   0.743704
C    0.236413   5.000664   0.685314
H    0.974519   3.073772   2.518778
H    1.006165   2.066050   2.943007
H    0.030028   3.544278   2.814743
H    1.791972   3.659819   2.954701
C   -3.153833   2.410817  -0.381628
H   -2.060901   2.483451  -0.327500
C   -3.720265   3.098992   0.867346
H   -3.336442   4.122634   0.934727
H   -3.442626   2.568103   1.782800
C   -4.813387   3.158088   0.829021
H   -3.619046   3.149508  -1.643966
H   -3.198459   2.709047  -2.553237
H   -3.318892   4.202229  -1.604181
H   -4.711153   3.110622  -1.729607
H    1.131855   1.524143  -2.803884
H   -1.592356   0.961652  -2.910793
C   -0.074073  -0.102864   1.312175
C    0.904857  -0.984799   1.833830
C   -1.144469   0.245968   2.162649
H    1.244229  -0.878740   2.857289
H   -1.929214   0.911357   1.801909
H   -0.883893   0.423017   3.204316
C    1.521138  -2.008866   1.041688
O    1.273050  -2.290542  -0.132712
C    2.397968  -2.768064   1.764465
C    2.684455  -4.050771   1.224658
H    3.401653  -4.505911   1.908599
H    3.106687  -3.982040   0.220092
H    1.772567  -4.656353   1.181412
C   -1.901662  -1.616797   2.705613
H   -2.643880  -1.711357   1.917061
H   -2.311148  -1.275213   3.653796
C   -0.808359  -2.477743   2.724998
H   -0.264311  -2.672033   3.644573
H   -0.629800  -3.183397   1.918504


        IPr-4a

  E(ele)      = -1582.627792
  E(ele+zpe)  = -1581.883779
  H           = -1581.844380
  G           = -1581.952533
C   -0.051010   1.343168  -2.191744
C   -1.351989   1.057735  -2.050378
C   -0.277424   0.219171  -0.198639
N    0.636527   0.792641  -1.101873
N   -1.513922   0.346588  -0.854185
C    1.953838   1.227407  -0.765416
C    2.121828   2.458274  -0.115245
C    3.034999   0.392016  -1.096879
C    3.426544   2.855457   0.197007
C    4.318903   0.830991  -0.771531
C    4.513447   2.053086  -0.129930
H    3.591795   3.801226   0.707712
H    5.178160   0.209574  -1.005031
H    5.519723   2.375509   0.122989
C   -2.758100  -0.260015  -0.502682
C   -3.815554   0.579244  -0.104587
C   -2.893257  -1.656347  -0.601876
C   -5.038749  -0.020226   0.203449
C   -4.132072  -2.208590  -0.264318
C   -5.193793  -1.401663   0.130127
H   -5.879248   0.591692   0.514435
H   -4.270563  -3.284164  -0.310877
H   -6.150191  -1.851794   0.382140
C    2.784985  -0.946367  -1.772422
H    1.849677  -1.348961  -1.362170
C    2.593517  -0.768483  -3.285455
H    1.730400  -0.136232  -3.511273
H    2.433194  -1.741166  -3.763897
H    3.485147  -0.310336  -3.730261
C    3.894559  -1.965076  -1.503749
H    4.155317  -2.001207  -0.441373
H    4.804043  -1.728187  -2.069112
```

```
H    3.563661  -2.961556  -1.814236
C   -1.730316  -2.523309  -1.062853
H   -0.815720  -2.147900  -0.589132
C   -1.859521  -3.988679  -0.644144
H   -2.667008  -4.501039  -1.181515
H   -2.040810  -4.086527   0.431921
C   -0.924695  -4.510502  -0.870041
C   -1.548118  -2.423936  -2.584917
H   -1.352743  -1.395696  -2.905448
C   -2.445478  -2.782640  -3.104069
H   -0.699871  -3.042000  -2.901027
C    0.941125   3.328159   0.282494
H    0.026380   2.866494  -0.104728
C    1.043992   4.730498  -0.328203
H    1.132739   4.681382  -1.418619
C    1.915223   5.272297   0.057673
H    0.151473   5.315788  -0.081473
C    0.812559   3.397945   1.808754
H    0.674798   2.396125   2.229151
H   -0.051482   4.008894   2.093071
H    1.707021   3.842818   2.260697
C   -3.602091   2.081728   0.039377
H   -3.037186   2.430877  -0.833414
C   -2.753719   2.397770   1.281451
H   -2.594125   3.480013   1.361119
H   -1.772966   1.911046   1.246095
H   -3.270411   2.062513   2.189415
C   -4.905932   2.881009   0.082022
H   -5.555311   2.648091  -0.768530
H   -4.681378   3.952127   0.055768
H   -5.466250   2.689932   1.004399
C    0.480812   1.872305  -2.967826
H   -2.193597   1.238868  -2.701729
C   -0.046553  -0.318887   1.031308
C    1.298452  -0.555243   1.681524
C   -1.126345  -0.875488   1.956223
H    2.083990   0.167862   1.446654
H   -1.613697  -1.772387   1.554644
H   -1.927429  -0.149028   2.139999
C    1.841838  -1.949288   1.379894
O    1.257362  -2.835182   0.797593
C    3.069251  -2.124778   1.911437
C    3.586556  -3.453595   1.843389
H    4.591564  -3.400569   2.261079
H    3.614251  -3.806715   0.810091
H    2.960972  -4.129216   2.432874
C   -0.388353  -1.235717   3.266842
H   -0.215476  -2.317799   3.306214
H   -0.962379  -0.966407   4.158214
C    0.954635  -0.505502   3.189931
H    0.838831   0.545160   3.478124
H    1.734180  -0.945979   3.818525


        Pbu-ts4a

  E(ele)      = -1237.558268
  E(ele+zpe)  = -1237.023816
  H           = -1236.994222
  G           = -1237.084494
C    0.072511  -0.539858  -2.647278
H   -0.493753  -0.734319  -3.555638
H   -1.871764  -1.011505  -1.370674
H   -2.425058  -1.214222  -2.281736
C    1.028753  -0.059634  -2.846813
H   -0.688960  -0.235851  -1.500890
C    0.343934  -2.623366  -2.343685
H    0.451966  -2.876839  -3.395606
C    1.290090  -2.576452  -1.806662
H   -0.799873  -3.038360  -1.658040
C   -0.761496  -3.244772  -0.591359
H   -1.621254  -3.514117  -2.185515
P    0.194456   0.358995  -0.088999
H   -0.674136   1.694268   0.809535
H   -1.512082   1.235252   1.341318
H    0.029915   2.094970   1.551265
C    0.722873  -0.927027   1.103325
H    1.419913  -1.578180   0.559541
H   -0.166553  -1.515783   1.342266
H    1.751191   1.154849  -0.656773
C    1.510294   1.699575  -1.576996
H    2.014598   1.911598   0.093905
H   -2.623753  -1.171574  -0.155951
C   -2.279494  -0.821353   0.975668
O   -3.793841  -1.827338  -0.348556
C   -4.551283  -2.087231   0.825970
C   -3.985910  -2.715988   1.519245
H   -4.815894  -1.154273   1.330851
H   -5.448794  -2.605863   0.488769
C   -1.159264   2.804433  -0.126896
H   -0.313124   3.231918  -0.684007
C   -1.837374   3.733316  -0.873197
C    2.939007   0.212021  -0.881035
H    2.633422  -0.654854  -1.480081
C    3.285485  -0.183944   0.083434
C    1.361635  -0.370826   2.379566
H    2.147969   0.361003   2.139557
H    0.599849   0.166220   2.959967
C   -1.871097   3.921234   0.637731
H   -2.716746   3.492580   1.190922
H   -1.188481   4.342461   1.388106
C   -2.366826   5.028624  -0.293518
H   -3.067859   4.630759  -1.031187
H   -2.879586   5.818198   0.268160
H   -1.532973   5.488217  -0.832067
C    1.963083  -1.480538   3.242450
H    1.186850  -2.226397   3.455321
H    2.743047  -1.998636   2.668597
C    2.547059  -0.949638   4.549706
H    2.978813  -1.755791   5.150417
H    3.337185  -0.214774   4.357793
H    1.774251  -0.459042   5.151836
C    4.100648   0.921937  -1.577255
```

```
H    4.391521   1.803818  -0.990664
H    3.757807   1.295706  -2.551154
C    5.306363   0.005594  -1.770694
H    6.125461   0.524806  -2.276962
H    5.682654  -0.356255  -0.807343
H    5.038839  -0.868883  -2.373760


        Pbu-4a

  E(ele)      = -1237.632331
  E(ele+zpe)  = -1237.093234
  H           = -1237.064059
  G           = -1237.155539
P   -0.311319  -0.146380  -0.526526
H   -0.483052  -0.344498   1.294562
H    0.395982   0.128424   1.748454
C   -1.356440   0.221972   1.638900
C   -0.634559   1.668797  -0.870298
H   -1.347863   1.725013  -1.705596
H    0.322842   2.051579  -1.236902
C   -1.792109  -0.940837  -1.275539
C   -1.745895  -0.750714  -2.356283
H   -1.679109  -2.022778  -1.138407
C   -0.593029  -1.809646   1.718588
H   -1.516238  -2.246484   1.309698
H    0.235844  -2.379458   1.279399
C   -3.131415  -0.459354  -0.714792
H   -3.228913   0.627858  -0.843173
C   -3.174514  -0.648586   0.367568
H   -1.111887   2.539641   0.292993
H   -2.071058   2.170971   0.685230
C   -0.595598  -1.975092   3.238700
H    0.334532  -1.557484   3.646589
C   -1.415271  -1.384166   3.669583
H   -0.734979  -3.435522   3.663004
C    0.086073  -4.038798   3.259743
H   -0.726104  -3.540661   4.752367
C   -1.673806  -3.862059   3.291957
H   -1.274038   4.005364  -0.111323
H   -0.315751   4.375640  -0.497793
H   -1.991814   4.075643  -0.940130
H   -1.738415   4.883311   1.049236
C   -1.849725   5.928604   0.744040
H   -2.705479   4.541484   1.435635
H   -1.019368   4.848907   1.875422
C   -4.321422  -1.147527  -1.385681
H   -4.229077  -2.233730  -1.254128
H   -4.280753  -0.961658  -2.467090
C   -5.661009  -0.670699  -0.828695
H   -6.500498  -1.172962  -1.318972
H   -5.731605  -0.871127   0.246380
C   -5.783658   0.408427  -0.974926
C    1.208100  -1.459533  -2.518513
H    0.398840  -2.141200  -2.813623
C    2.435351  -0.850744  -0.440096
H    2.539673  -1.557016   0.409262
H    1.266600  -0.680486  -3.301146
C    1.069921  -0.924273  -1.099212
C    2.556577  -2.193579  -2.454593
H    2.418206  -3.169648  -1.972907
C    3.409367  -1.291933  -1.560690
C    3.722204  -0.407435  -2.131075
H    4.311520  -1.770675  -1.169827
C    2.836274   0.479998   0.162030
O    2.085326   1.395317   0.432967
C    4.152047   0.537008   0.435014
C    4.603143   1.733325   1.068218
H    5.677378   1.609724   1.200535
H    4.389401   2.601033   0.439766
H    4.108656   1.862582   2.034260
H    3.007769  -2.357751  -3.439249


        Pph-ts4a

  E(ele)      = -1458.904817
  E(ele+zpe)  = -1458.469346
  H           = -1458.442454
  G           = -1458.526055
C   -1.847602  -0.184207  -1.848765
H   -2.264147  -0.229042  -2.849090
C    0.119650  -1.342872  -2.566052
H   -0.444711  -0.376220  -1.711638
C   -2.377329  -2.420415  -1.695587
C   -1.209559  -3.004115  -2.180598
H   -0.538357  -3.532653  -1.508813
H   -1.200878  -3.395332  -3.194984
C   -0.239075  -1.339865  -3.592279
H   -3.251333  -2.316823  -2.331138
P    0.384353   0.003382  -0.196184
C   -2.642604   0.487735  -0.858371
H   -2.235520   0.898589   0.288462
O   -3.945759   0.607885  -1.208564
C   -4.786210   1.203737  -0.227918
H   -4.790593   0.608344   0.688947
H   -4.447344   2.215709   0.009783
C   -5.782266   1.229236  -0.670158
C    1.154671  -1.657719  -2.466600
C    2.120493  -0.549590  -0.348111
C    2.901778   0.030168  -1.358068
C    2.702070  -1.467951   0.527874
C    4.238415  -0.323795  -1.500329
H    2.456771   0.755981  -2.034870
C    4.045921  -1.818623   0.383702
H    2.117567  -1.910940   1.328279
C    4.812614  -1.252135  -0.629357
H    4.833488   0.126828  -2.289105
H    4.488145  -2.535139   1.069517
C    5.857701  -1.526744  -0.740028
C    0.589862   1.788153   0.100010
C   -0.068119   2.725191  -0.696999
C    1.480538   2.213521   1.090811
```

```
C     0.153169    4.084895   -0.490351        C    -2.054588   -0.688491    2.396687
H    -0.746227    2.386495   -1.475002        H    -2.476291    0.086202    3.051415
C     1.689458    3.574038    1.302277        H    -2.857894   -1.089065    1.775314
H     2.018918    1.483474    1.692821        H    -1.654843   -1.491909    3.030651
C     1.024534    4.510066    0.511057        N    -0.691611   -1.813731   -0.609773
H    -0.359716    4.812975   -1.111769        N    -2.565545    0.041782   -0.460085
H     2.377155    3.901239    2.076470        C    -0.632169   -2.890287    0.375104
H     1.191694    5.571379    0.671343        H    -0.782064   -3.841035   -0.146899
C    -0.250402   -0.798755    1.309974        H     0.340252   -2.900597    0.884146
C    -0.444566   -2.181634    1.262119        C    -1.430856   -2.793708    1.111876
C    -0.570749   -0.088321    2.468381        C    -3.087760   -0.371784   -1.754541
C    -0.935365   -2.857459    2.377014        H    -2.943139    0.407548   -2.517204
H    -0.222489   -2.727754    0.348439        C    -2.594513   -1.289451   -2.079803
C    -1.051937   -0.768678    3.583940        H    -4.161175   -0.571938   -1.657676
C    -0.478570    0.993370    2.488164        C     0.089366    0.475592    2.339102
C    -1.232137   -2.151199    3.541208        H    -0.330732    1.186119    3.062990
H    -1.091775   -3.931114    2.329982        H     0.658215   -0.297148    2.868207
H    -1.304895   -0.214040    4.482635        H     0.767098    1.008225    1.674905
H    -1.616472   -2.675690    4.411441
H    -2.580300   -2.383911   -0.627778
```

Pph-4a

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E(ele)        = -1458.986549
E(ele+zpe)    = -1458.544521
H             = -1458.518523
G             = -1458.600330
C     1.636790    1.012828   -1.877756
H     2.040806    0.691935   -2.847865
C    -0.607942    1.225235   -2.630358
C     0.261007    0.353944   -1.723923
C     1.354169    2.537891   -1.917970
C    -0.105045    2.673943   -2.415088
H    -0.715526    3.168600   -1.650931
H    -0.177436    3.273822   -3.328824
H    -0.443515    0.932984   -3.679954
H     2.070376    3.061286   -2.561728
P    -0.414325   -0.054095   -0.214177
C     2.672569    0.661339   -0.837600
O     2.729667    1.126065    0.281040
O     3.561997   -0.243170   -1.279845
C     4.558837   -0.630669   -0.334163
H     5.176010    0.229480   -0.063147
H     4.090283   -1.037153    0.566019
H     5.157020   -1.392003   -0.834258
H    -1.685190    1.135708   -2.445874
C    -1.936800   -1.036690   -0.491794
C    -2.202994   -1.564066   -1.756921
C    -2.769661   -1.367990    0.583111
C    -3.313095   -2.384473   -1.952895
H    -1.526134   -1.336549   -2.575973
C    -3.869911   -2.198110    0.388095
H    -2.559260   -0.976497    1.576409
C    -4.147423   -2.701623   -0.883081
H    -3.518807   -2.784103   -2.941816
H    -4.509433   -2.452454    1.228347
H    -5.007517   -3.347567   -1.035859
C     0.671207   -1.186871    0.718228
C     1.409415   -2.123229   -0.014483
C     0.698908   -1.223572    2.114956
C     2.187637   -3.069910    0.647970
H     1.367953   -2.097851   -1.100486
C     1.480120   -2.171471    2.772941
H     0.116021   -0.512927    2.694003
C     2.227285   -3.093409    2.041540
H     2.762280   -3.790574    0.072504
H     1.502961   -2.189427    3.858663
H     2.833265   -3.833190    2.557205
C    -0.953607    1.266517    0.966809
C    -2.254240    1.783642    0.902922
C     0.006824    1.941815    1.735029
C    -2.597034    2.931871    1.615993
H    -3.008150    1.293610    0.291235
C    -0.341457    3.082727    2.453597
H     1.035832    1.591079    1.745243
C    -1.643944    3.579651    2.398773
H    -3.610342    3.319251    1.556795
H     0.411783    3.590908    3.049134
H    -1.911313    4.472545    2.956611
H     1.459916    2.941429   -0.905915
```

Hmpt-4a

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E(ele)        = -1167.869518
E(ele+zpe)    = -1167.449385
H             = -1167.425570
G             = -1167.499475
C    -0.204000    2.569263   -0.037508
H    -0.538386    3.216216   -0.865521
C     1.494479    0.905225   -0.783243
H     1.691184    0.592727   -1.818228
H    -0.943776    2.683155    0.767469
C     0.027728    1.121545   -0.457651
C     1.194644    3.014088    0.418355
H     1.327049    4.101671    0.428437
C     1.390391    2.636958    1.430482
H     2.122084    2.319039   -0.579500
H     3.168090    2.274398   -0.258652
C     2.092886    2.848740   -1.538575
P    -1.020650   -0.125139   -0.090868
C     2.238148   -0.101164    0.081325
H     1.926554   -0.501130    1.180667
C     3.371350   -0.513311   -0.530090
C     4.182667   -1.413169    0.220877
H     4.519985   -0.940858    1.147102
H     3.621080   -2.317349    0.470056
H     5.031411   -1.652854   -0.418729
C     0.157305   -1.703447   -2.004212
H    -0.262613   -2.579433   -2.518980
H    -0.056754   -0.811225   -2.596248
H     1.249842   -1.829367   -1.952462
C    -3.325264    1.212766   -0.330543
H    -2.964168    2.097806   -0.879945
H    -4.393336    1.087692   -0.541894
H    -3.204807    1.392631    0.741506
C    -2.559147   -1.170067    1.962243
H    -3.293111   -0.570980    2.521189
H    -3.059863   -1.620097    1.104710
H    -2.197221   -1.966475    2.629534
N    -0.414224   -1.581239   -0.672827
N    -2.619350   -0.006138   -0.716657
C    -1.451246   -0.337633    1.521634
C    -0.091192   -2.697115    0.200517
C    -0.619880   -3.605103   -0.120575
H     0.989905   -2.894330    0.178838
C    -0.361514   -2.469133    1.231916
C    -2.770596   -0.273442   -2.139876
H    -2.254501    0.472438   -2.768432
C    -2.391648   -1.269901   -2.378295
H    -3.837514   -0.252166   -2.386777
C    -0.645656    0.192224    2.607971
H    -1.290815    0.750884    3.300602
H    -0.144547   -0.612958    3.163443
H     0.125708    0.850113    2.208845
```

Hmpt-ts4a

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E(ele)        = -1167.784643
E(ele+zpe)    = -1167.370517
H             = -1167.345617
G             = -1167.421814
C    -0.407120    2.105608   -1.293232
H     0.110478    2.621217   -2.099756
C     1.546991    0.775177   -0.907990
H     2.084343    1.272696   -1.707863
C    -1.482417    2.269184   -1.308065
C     0.130634    0.861750   -0.904178
C     0.495739    3.366460    0.098828
H     0.306446    4.259386   -0.492367
C    -0.192742    3.239783    0.933523
H     1.802939    2.904152    0.230996
H     2.155564    2.420588    1.135887
H     2.586729    3.276274   -0.422779
P    -0.951259   -0.247484   -0.083340
C     2.284968   -0.228992   -0.192626
O     1.830194   -1.034166    0.621543
O     3.613092   -0.207436   -0.477996
C     4.407282   -1.140017    0.241468
H     4.302661   -0.989497    1.319352
H     4.115545   -2.166420    0.000157
H     5.435342   -0.955594   -0.070927
C     0.097795   -2.094913   -1.805609
H    -0.327015   -2.975719   -2.302900
H     0.065676   -1.250049   -2.494373
H     1.145573   -2.299346   -1.548943
C    -3.303732    1.151819    0.130440
H    -3.474424    1.951611   -0.602998
H    -4.281794    0.797777    0.482482
H    -2.755562    1.572914    0.976181
```

Quin-ts4a

```
E(ele)        = -752.073616
E(ele+zpe)    = -751.714154
H             = -751.697235
G             = -751.756489
C     0.095089    2.399767   -0.962147
H     0.867056    2.867852   -1.567219
C     1.501191    0.537394   -0.712726
H     2.239981    1.115998   -1.254227
C    -0.854224    2.920558   -1.061486
C     0.179236    0.989031   -0.951594
C     0.971510    2.931746    0.777319
H     0.098509    3.018286    1.425614
C     1.925148    1.937524    1.070556
H     1.744705    1.205749    1.854425
C     2.973161    2.097833    0.835543
H     1.336312    3.904081    0.451323
C     2.044177   -0.719682   -0.245711
O     1.462853   -1.681982    0.258321
O     3.396620   -0.735168   -0.372008
C     4.049123   -1.878820    0.162116
H     3.707425   -2.789776   -0.336524
H     5.112260   -1.720976   -0.019443
H     3.855416   -1.969494    1.234479
C    -1.111048   -1.110156   -1.093992
H    -0.872749    0.022528    1.113758
C    -2.293157    0.945532   -0.628446
C    -2.055553   -2.026644   -0.305876
H    -0.115132   -1.530342   -1.181755
H    -1.487806   -0.867675   -2.091519
C    -2.186871   -0.544716    1.682272
H    -0.621431    1.000905    1.524375
C    -0.034154   -0.655933    1.259649
C    -2.300482    1.805912    0.043904
C    -2.268980    1.307406   -1.657610
H    -3.479168    0.002276   -0.357484
C    -1.473804   -2.691985    0.342247
C    -2.618723   -2.652986   -1.005594
H    -2.770408    0.237402    2.182524
H    -1.952404   -1.306692    2.432305
```

```
H    -4.280166    0.565172    0.131982
H    -3.884028   -0.389076   -1.297689
N    -0.989822    0.225967   -0.388716
O     2.593139    0.830884   -0.971071
C    -2.996461   -1.150274    0.531035
H    -3.842919   -1.729830    0.910732
```

Quin-4a

```
E(ele)        = -752.136614
E(ele+zpe)    = -751.771951
H             = -751.755798
G             = -751.813182
C     1.116757   -1.866439   -0.861450
H     0.583785   -2.760112   -1.213777
C     1.638169   -0.346628    0.935310
H     1.457270    0.007070    1.956528
C     1.208751   -1.186651   -1.732174
C     0.511578   -1.250290    0.391836
C     2.541213   -2.226051   -0.381376
C     2.606100   -3.286658   -0.121512
C     2.806377   -1.348314    0.868929
H     3.775716   -0.842108    0.821508
C     2.778784   -1.954624    1.777486
H     1.973072    0.855312    0.078255
O     2.599560    0.848265   -0.960173
O     1.398323    2.005870    0.541025
C     1.612696    3.160516   -0.265535
H     1.132494    3.986328    0.259296
H     2.681736    3.350169   -0.387067
H     1.168563    3.026950   -1.257378
C    -1.196542    0.271328    1.328353
C    -0.928470    0.305113   -1.111150
C    -1.865835   -1.636507    0.000501
C    -2.693091    0.631481    1.301041
H    -0.561208    1.157490    1.304660
C    -0.917906   -0.336076    2.192499
C    -2.216506    1.145670   -1.080041
H    -0.917140   -0.386879   -1.956799
H    -0.029988    0.917228   -1.178046
C    -1.475324   -2.369480   -0.705710
H    -1.910322   -2.110403    0.982371
C    -3.213699   -1.039669   -0.450608
H    -2.825456    1.663770    1.641260
H    -3.262717   -0.010856    1.982825
C    -2.629102    1.228934   -2.089247
H    -2.004233    2.163196   -0.727113
C    -3.372926   -1.196378   -1.524104
N    -0.822173   -0.557833    0.130370
H     3.276128   -2.027495   -1.166166
C    -3.210567    0.460823   -0.131635
H    -4.212259    0.887371   -0.239799
```

Dabco-ts4a

```
E(ele)        = -768.091483
E(ele+zpe)    = -767.743600
H             = -767.726826
G             = -767.785961
C     0.082776    2.398876   -0.969634
H     0.854057    2.870414   -1.572716
C     1.498670    0.542855   -0.710705
H     2.236160    1.122599   -1.252787
C    -0.869531    2.913433   -1.072386
C     0.175847    0.989773   -0.953905
C     0.953683    2.936386    0.776334
H     0.077542    3.018322    1.420893
C     1.909521    1.945505    1.070990
H     1.729667    1.213240    1.854536
C     2.957686    2.109879    0.839488
H     1.314849    3.910009    0.450484
C     2.043194   -0.714451   -0.246093
O     1.461273   -1.678456    0.255124
O     3.394886   -0.728094   -0.369210
C     4.048236   -1.873405    0.161481
H     3.707699   -2.782584   -0.341042
H     5.111251   -1.713760   -0.018713
H     3.853569   -1.967978    1.233252
C    -1.115851   -1.108315   -1.092608
H    -0.874219    0.014414    1.113679
C    -2.296981    0.935396   -0.613617
C    -2.106966   -1.986321   -0.306753
H    -0.128012   -1.554295   -1.148894
H    -1.463373   -0.864335   -2.100094
C    -2.187555   -0.618141    1.634846
H    -0.675241    0.998607    1.540225
C    -0.012609   -0.632762    1.267562
C    -2.299191    1.810295    0.039380
C    -2.306919    1.269866   -1.652796
H    -3.455780   -0.035273   -0.279532
C    -1.566641   -2.680380    0.344539
C    -2.718307   -2.576847   -0.996301
H    -2.801359    0.116557    2.166798
H    -1.958168   -1.427491    2.333780
C    -4.240004    0.497767    0.266240
H    -3.904451   -0.438031   -1.193298
N    -0.989491    0.224517   -0.386255
C    -2.981288   -1.156504    0.528775
```

Dabco-4a

```
E(ele)        = -768.154644
E(ele+zpe)    = -767.801642
H             = -767.785626
G             = -767.842926
C     1.099853   -1.878294   -0.856178
H     0.560618   -2.771218   -1.200617
C     1.632986   -0.351217    0.932753
H     1.454926    0.006681    1.953077
C     1.194338   -1.204965   -1.731448
C     0.501692   -1.250528    0.394479
C     2.523164   -2.242957   -0.376253
C     2.583008   -3.302570   -0.111474
C     2.795030   -1.360721    0.869425
H     3.767343   -0.860745    0.818642
```

```
H     2.764753   -1.962455    1.780908
H     1.974668    0.845920    0.071747
O     2.593139    0.830884   -0.971071
C     1.418332    2.003238    0.539989
C     1.650131    3.158545   -0.261520
H     1.182283    3.988978    0.267038
H     2.721976    3.332441   -0.381543
C     1.205094    3.036393   -1.254372
C    -1.204050    0.282639    1.322019
C    -0.936588    0.318039   -1.105657
C    -1.878606   -1.617708   -0.001433
C    -2.698656    0.665832    1.231211
H    -0.551360    1.156805    1.316273
C    -0.965304   -0.331556    2.193885
C    -2.269401    1.099506   -1.063881
H    -0.882824   -0.360390   -1.960268
H    -0.067015    0.973244   -1.143371
C    -1.517415   -2.334451   -0.740235
H    -1.906329   -2.117376    0.968298
C    -3.224493   -0.970154   -0.403351
H    -2.838813    1.713276    1.515605
H    -3.306833    0.055991    1.907212
C    -2.724268    1.133986   -2.059036
H    -2.107282    2.132541   -0.737297
C    -3.432863   -1.109536   -1.469403
H    -4.046180   -1.429337    0.155039
N    -3.205832    0.469962   -0.129666
H    -0.827259   -0.549997    0.130349
C     3.257631   -2.051879   -1.163200
```

Dmap-ts4a

```
E(ele)        = -805.006719
E(ele+zpe)    = -804.682813
H             = -804.663206
G             = -804.730473
C    -1.484220   -2.592552   -0.581981
H    -2.392642   -3.040190   -0.978726
H    -2.411181   -0.387666   -0.497672
C    -3.387472   -0.795387   -0.727802
H    -0.613397   -3.244099   -0.667326
C    -1.325183   -1.210669   -0.831645
C    -2.013273   -2.582226    1.346915
H    -1.030527   -2.688592    1.809649
C    -2.735580   -1.404961    1.622662
H    -2.305968   -0.609913    2.226882
C    -3.820703   -1.402618    1.585086
C    -2.562374   -3.521855    1.317190
C    -2.372852    1.058339   -0.394617
H    -1.383155    1.781447   -0.355044
O    -3.622404    1.585652   -0.301981
O    -3.676530    2.995126   -0.136062
H    -3.199706    3.503562   -0.978496
H    -4.736232    3.246606   -0.088636
H    -3.172146    3.296186    0.786643
C     1.014320   -0.968550   -1.427196
C     0.311810   -0.095983    0.610516
C     2.314844   -0.595919   -1.189182
H     0.702471   -1.464821   -2.338808
C     1.585620    0.316238    0.916377
C    -0.525151    0.051686    1.279833
C     2.646963    0.085190    0.008923
C     3.056897   -0.812708   -1.946220
H     1.743115    0.820184    1.860541
N     0.021219   -0.728158   -0.547290
C     4.197699    1.230491    1.490617
H     5.254622    1.494044    1.507426
H     3.610236    2.154944    1.540974
H     3.980137    0.625057    2.378407
C     4.970162    0.243330   -0.694379
H     5.093290   -0.831234   -0.874240
H     4.766226    0.740608   -1.650651
H     5.909032    0.630949   -0.300637
N     3.912947    0.495313    0.269499
```

Dmap-4a

```
E(ele)        = -805.090434
E(ele+zpe)    = -804.761203
H             = -804.742563
G             = -804.807590
C    -1.946710   -2.264348    0.474098
H    -1.351709   -3.170424    0.286139
C    -2.353214   -0.170214   -0.824648
H    -2.228172   -0.128579   -1.919401
C    -2.066517   -2.186024    1.570810
H    -1.346598   -1.037822   -0.135623
C    -3.315126   -2.330375   -0.223391
C    -4.069006   -2.868892   -0.358385
H    -3.690602   -0.861063   -0.450573
C    -4.061358   -0.431173    0.487337
C    -4.456124   -0.717786   -1.217560
H    -3.205850   -2.839592   -1.187981
C    -2.366680    1.285755   -0.374873
O    -2.481238    2.235157   -1.115430
O    -2.244772    1.403872    0.956119
C    -2.241363    2.742170    1.453702
H    -3.185762    3.238589    1.216944
H    -2.109856    2.655298    2.531203
H    -1.417696    3.305370    1.008375
C     0.834010   -1.470974    0.732496
C     0.505915    0.381004   -0.691559
C     2.170649   -1.175500    0.813263
H     0.387898   -2.281310    1.289675
C     1.854535    0.670895   -0.625590
C    -0.164406    0.968724   -1.300210
C     2.748749   -0.097476    0.124218
C     2.781611   -1.795863    1.463117
H     2.187053    1.537200   -1.188169
N    -0.051491   -0.719008   -0.004819
C     4.562160    1.468924   -0.224084
H     5.607438    1.624429    0.057945
H     4.488624    1.570239   -1.323104
H     3.958718    2.252887    0.241899
C     4.992282   -0.889616   -0.272731
```

```
   H      4.687696    -1.858082     0.128791
   H      4.949755    -0.942032    -1.375409
   H      6.026797    -0.702307     0.031546
   N      4.137695     0.168856     0.254238

        Py-ts4a

   E(ele)          -  -671.088991
   E(ele+zpe)      -  -670.839753
   H               -  -670.824416
   G               -  -670.881540
   C      0.325912     2.341425     1.037682
   H     -0.406639     2.873220     1.637279
   C     -1.185124     0.478349     0.846481
   H     -1.951413     0.959205     1.440953
   H      1.333599     2.747151     1.140122
   C      0.134372     0.950079     0.990653
   C     -0.602457     2.921899    -0.723549
   H      0.252030     2.944366    -1.399722
   C     -1.602835     1.972129    -0.959947
   H     -1.460567     1.196407    -1.707316
   H     -2.630876     2.160051    -0.666229
   H     -0.894173     3.908991    -0.372593
   C     -1.591289    -0.720417     0.149286
   O     -0.892718    -1.477000    -0.518864
   O     -2.930732    -0.926786     0.261667
   C     -3.440696    -2.019579    -0.490460
   H     -2.995349    -2.961305    -0.158039
   H     -4.515906    -2.023830    -0.311208
   H     -3.231071    -1.887147    -1.555287
   C      1.360616    -1.121134     0.885107
   C      2.069481     0.667471    -0.450596
   C      2.388266    -1.912673     0.417973
   H      0.637215    -1.449145     1.619722
   C      3.131520    -0.078392    -0.929578
   H      1.851923     1.673455    -0.781751
   C      3.301061    -1.389925    -0.497374
   H      2.470446    -2.929482     0.783680
   H      3.800929     0.370519    -1.654697
   N      1.210187     0.158075     0.465042
   H      4.123186    -1.994080    -0.866697

        Py-4a

   E(ele)          -  -671.088991
   E(ele+zpe)      -  -670.839753
   H               -  -670.824416
   G               -  -670.881540
   C      0.325912     2.341425     1.037682
   H     -0.406639     2.873220     1.637279
   C     -1.185124     0.478349     0.846481
   H     -1.951413     0.959205     1.440953
   H      1.333599     2.747151     1.140122
   C      0.134372     0.950079     0.990653
   C     -0.602457     2.921899    -0.723549
   H      0.252030     2.944366    -1.399722
   C     -1.602835     1.972129    -0.959947
   H     -1.460567     1.196407    -1.707316
   H     -2.630876     2.160051    -0.666229
   H     -0.894173     3.908991    -0.372593
   C     -1.591289    -0.720417     0.149286
   O     -0.892718    -1.477000    -0.518864
   O     -2.930732    -0.926786     0.261667
   C     -3.440696    -2.019579    -0.490460
   H     -2.995349    -2.961305    -0.158039
   H     -4.515906    -2.023830    -0.311208
   H     -3.231071    -1.887147    -1.555287
   C      1.360616    -1.121134     0.885107
   C      2.069481     0.667471    -0.450596
   C      2.388266    -1.912673     0.417973
   H      0.637215    -1.449145     1.619722
   C      3.131520    -0.078392    -0.929578
   H      1.851923     1.673455    -0.781751
   C      3.301061    -1.389925    -0.497374
   H      2.470446    -2.929482     0.783680
   H      3.800929     0.370519    -1.654697
   N      1.210187     0.158075     0.465042
   H      4.123186    -1.994080    -0.866697

        Dbu-ts4a

   E(ele)          -  -884.818307
   E(ele+zpe)      -  -884.408548
   H               -  -884.387995
   G               -  -884.456011
   C      1.729169     1.444021    -1.568120
   C      1.442671    -0.053553    -1.834096
   C      1.167398    -0.791756    -0.553434
   C      2.434278     1.745339    -0.240573
   C      3.724606     0.960165     0.019416
   C      3.556801    -0.567535    -0.115838
   H      2.312632     1.831595    -2.411993
   H      0.569612    -0.161344    -2.477258
   H      1.722949     1.557318     0.571496
   H      4.075384     1.200526     1.030154
   H      0.770254     1.974016    -1.565750
   H      2.290487    -0.527027    -2.335786
   H      2.662635     2.816425    -0.199663
   H      4.517707     1.275145    -0.670467
   H      4.261045    -1.093518     0.534199
   H      3.783428    -0.894945    -1.132263
   C     -0.370161    -1.741107     1.068564
   C      0.654040    -1.323830     2.108640
   C      2.051525    -1.609741     1.590867
   H     -1.361857    -1.376435     1.338871
   H      0.537610    -0.252334     2.294620
   H      0.483785    -1.867851     3.042237
   H      2.803606    -1.152002     2.240932
   H      2.251609    -2.689147     1.551176
   H     -0.420211    -2.831773     0.955170
   N      2.218337    -1.038912     0.251900
   N     -0.059380    -1.145506    -0.241180
   C     -1.192511    -0.820678    -1.101355
   C     -1.925632     0.342691    -0.798335
   H     -2.684325     0.648724    -1.508356

   C     -1.963989    -1.921841    -1.546168
   C     -1.509284     1.366965     0.131393
   O     -0.582728     1.319243     0.940935
   O     -2.309194     2.464748     0.069975
   H     -2.628805    -1.703415    -2.380376
   H     -1.464974    -2.887536    -1.659503
   C     -2.035986     3.475425     1.029244
   H     -2.111315     3.076567     2.044579
   H     -1.032861     3.888081     0.886696
   H     -2.788690     4.247224     0.867513
   C     -3.391628    -2.064605    -0.206772
   H     -4.158664    -2.481354    -0.858297
   H     -2.976540    -2.821216     0.460275
   C     -3.639675    -0.782042     0.336356
   H     -3.329161    -0.531498     1.348358
   H     -4.452409    -0.172749    -0.047609

        Dbu-4a

   E(ele)          -  -884.869907
   E(ele+zpe)      -  -884.454559
   H               -  -884.435071
   G               -  -884.500215
   C     -1.822919     1.362258     1.355978
   C     -1.269746     0.003949     1.829242
   C     -0.817601    -0.875969     0.700589
   C     -2.590602     1.302488     0.029884
   C     -3.691361     0.238939    -0.041162
   C     -3.196047    -1.202431     0.227438
   H     -2.467975     1.765212     2.146951
   H     -0.398077     0.143143     2.471808
   H     -1.875669     1.126563    -0.782848
   H     -4.150679     0.288459    -1.035431
   H     -0.981647     2.058198     1.250332
   H     -2.050184    -0.535967     2.377840
   H     -3.044430     2.281983    -0.167304
   H     -4.487434     0.463625     0.680140
   H     -3.761123    -1.913547    -0.382883
   H     -3.379848    -1.486913     1.265644
   C      0.721488    -2.255443    -0.443935
   C     -0.037530    -1.989851    -1.737466
   C     -1.522947    -1.993732    -1.411361
   H      1.794579    -2.317073    -0.606562
   H      0.269808    -1.016509    -2.127102
   H      0.176751    -2.757753    -2.487298
   H     -2.086341    -1.407840    -2.149833
   H     -1.920118    -3.017456    -1.423031
   H      0.386259    -3.200234     0.008329
   N     -1.784152    -1.429646    -0.081940
   N      0.457411    -1.152123     0.506293
   C      1.499691    -0.368661     1.182313
   C      2.101242     0.731668     0.273355
   H      2.653470     1.412347     0.932153
   C      2.738549    -1.227671     1.439985
   C      1.116942     1.561295    -0.491042
   O      0.398892     1.163751    -1.389748
   O      1.095973     2.850178    -0.096038
   H      3.223487    -0.895466     2.365932
   C      2.477163    -2.281044     1.606186
   H      0.207594     3.702698    -0.813957
   H      0.467841     3.716204    -1.875430
   H     -0.826031     3.361296    -0.707996
   H      0.329302     4.692291    -0.374939
   C      3.751690    -1.041514     0.254499
   H      4.721764    -0.696436     0.629017
   H      3.944963    -1.974971    -0.288704
   C      3.122088     0.028244    -0.658980
   H      2.584349    -0.420673    -1.503836
   H      3.866748     0.715890    -1.077585

        Mtdb-ts4a

   E(ele)          -  -900.853817
   E(ele+zpe)      -  -900.456482
   H               -  -900.435608
   G               -  -900.504505
   C      0.578737    -2.031527    -0.929692
   C     -1.087281    -0.687934     0.278578
   C     -1.402906    -1.170453    -2.074725
   C     -0.561406    -2.410749    -1.852881
   H      1.311359    -1.417824    -1.466588
   H      1.096589    -2.915918    -0.547847
   H     -2.258234    -1.378219    -2.724634
   H     -0.809154    -0.356074    -2.514790
   H     -1.183157    -3.198713    -1.412938
   H     -0.155742    -2.784337    -2.797758
   C     -2.473313     1.001570     1.331787
   C     -3.626284     0.593397     0.433154
   C     -3.050171     0.199231    -0.913079
   H     -2.816120     1.220695     2.345522
   H     -4.159513    -0.250376     0.884759
   H     -4.333670     1.417757     0.299663
   H     -3.811884    -0.274607    -1.540837
   H     -2.677632     1.092178    -1.437807
   H     -1.966270     1.893947     0.938780
   N     -1.940699    -0.745667    -0.786201
   N      0.127142    -1.245269     0.228742
   C     -1.525971    -0.104357     1.419844
   C      1.202812    -0.676675     1.030127
   C      1.642718     0.623746     0.716103
   H      2.356280     1.073206     1.397106
   C      2.243122    -1.550747     1.440460
   C      0.988259     1.565710    -0.162732
   O      0.013302     1.380013    -0.895961
   O      1.599348     2.780214    -0.142001
   H      2.856963    -1.164379     2.253509
   H      1.999409    -2.606252     1.593138
   C      1.094965     3.740339    -1.057571
   H      1.189033     3.382535    -2.086760
   H      0.042194     3.958738    -0.855467
   H      1.701104     4.634675    -0.910752
   C     -1.010349    -0.443788     2.739019
   H     -0.562957    -1.436030     2.720934
   H     -0.250948     0.266957     3.079294
   H     -1.863332    -0.446006     3.426875

   C      3.498192    -0.086086    -0.513461
   H      3.067837     0.050821    -1.502766
   H      4.178766     0.701174    -0.202930
   C      3.581523    -1.378246     0.072650
   H      4.469265    -1.578276     0.672825
   H      3.343605    -2.227157    -0.569956

        Mtdb-4a

   E(ele)          -  -900.911202
   E(ele+zpe)      -  -900.509202
   H               -  -900.489108
   G               -  -900.556942
   C     -0.381387    -2.537936    -0.644136
   C     -1.047639    -0.389588     0.294881
   C     -2.582468    -1.563136    -1.163709
   C     -1.867568    -2.826979    -0.735794
   H      0.064330    -2.450176    -1.640645
   H      0.132891    -3.338202    -0.111356
   H     -3.658934    -1.725987    -1.277688
   H     -2.181582    -1.207885    -2.132210
   H     -2.260102    -3.149960     0.234874
   H     -2.026597    -3.635901    -1.455607
   C     -1.477223     1.912643     0.926691
   C     -2.966779     1.662898     0.722220
   C     -3.108644     0.672063    -0.422106
   H     -1.278671     2.573222     1.775658
   H     -3.414627     1.244161     1.631449
   H     -3.489562     2.594487     0.478482
   H     -4.157194     0.402510    -0.584913
   H     -2.724833     1.127001    -1.356011
   H     -1.070325     2.399108     0.028511
   N     -2.388817    -0.566632    -0.126875
   N     -0.079028    -1.273593     0.058662
   C     -0.750826     0.672367     1.149026
   C      1.248135    -1.109396     0.425129
   C      1.890079     0.256087     0.407376
   H      1.798684     0.818740     1.349801
   C      2.276973    -2.184325     0.158800
   C      1.367715     1.174598    -0.677132
   O      0.900486     0.826834    -1.739616
   O      1.510356     2.480703    -0.349875
   C      2.114534    -3.116946     0.716066
   C      2.385942    -2.466919    -0.908367
   C      1.166307     3.406073    -1.376360
   H      1.821360     3.274527    -2.242281
   H      0.130842     3.264922    -1.698312
   H      1.301315     4.396465    -0.942217
   C     -0.551692     0.262471     2.535079
   H     -1.484796    -0.061096     3.020230
   H      0.172243    -0.564524     2.546745
   H     -0.120490     1.099594     3.093167
   C      3.381194    -0.060098     0.116416
   H      3.549062    -0.039379    -0.968332
   H      4.057651     0.665497     0.577996
   C      3.567274    -1.494249     0.614730
   H      3.627197    -1.509940     1.709438
   H      4.470261    -1.965395     0.213223
```

9.5 [3 + 2] and [2 + 4] cycloadditions with enone 2b

9.5.1 Cycloadditions starting from Pph-3

enone 2b

E(ele) = −422.798857
E(ele+zpe) = −422.653699
H = −422.644270
G = −422.687866

```
C   -2.255262   -0.737497    0.224058
C   -3.559015   -0.565738    0.001266
H   -3.928520    0.389060   -0.363347
H   -4.277093   -1.360763    0.176219
H   -1.874689   -1.684209    0.594490
C   -1.298727    0.388417   -0.012213
O   -1.707355    1.519700   -0.205465
C    0.174049    0.108735    0.004353
C    1.044055    1.200480    0.107688
C    0.701377   -1.182062   -0.108105
C    2.419728    1.003777    0.112577
H    0.617345    2.196032    0.183232
C    2.081267   -1.377433   -0.116207
H    0.045092   -2.040440   -0.213507
C    2.940418   -0.286894    0.000001
H    3.089278    1.854317    0.200591
H    2.484423   -2.380916   -0.214631
H    4.015669   -0.441393    0.000159
```

Pph-γ-ts4b

E(ele) = −1803.198105
E(ele+zpe) = −1802.669024
H = −1802.636317
G = −1802.731904

```
C   -0.886300    0.247886   -2.008772
H   -1.354695   -0.042356   -2.941991
C    0.809869   -1.415474   -2.440544
C    0.300646   -0.383652   -1.647285
C   -1.905029   -2.408119   -1.845988
C   -0.744683   -3.047055   -2.212196
H   -0.118557   -3.485114   -1.443209
H   -0.636846   -3.458379   -3.211867
H    0.548906   -1.379522   -3.494159
H   -2.662547   -2.160582   -2.581556
C   -2.005613   -1.894551   -0.501811
O   -1.070455   -2.045862    0.308540
P    1.229031    0.027578   -0.123057
C   -1.457784    1.349616   -1.298075
O   -0.933018    1.917939   -0.341041
C   -2.657148    1.734444   -1.781749
C   -3.280044    2.812062   -1.091852
H   -3.411983    2.562647   -0.036279
H   -2.678926    3.722149   -1.177743
H   -4.249187    2.945748   -1.572384
H    1.725342   -1.940823   -2.203631
C    2.474673   -1.302724    0.060841
C    3.843761   -1.037675   -0.026493
C    2.037279   -2.620467    0.265202
C    4.767797   -2.073953    0.113936
H    4.201812   -0.031323   -0.217440
C    2.964977   -3.647825    0.403555
H    0.970171   -2.831753    0.288276
C    4.331985   -3.376990    0.333511
H    5.829490   -1.856894    0.042611
H    2.615725   -4.664511    0.559174
H    5.053721   -4.181584    0.441025
C    2.167858    1.547286   -0.480368
C    2.091828    2.136984   -1.743296
C    3.002441    2.103234    0.497602
C    2.846138    3.274799   -2.025801
H    1.435923    1.714824   -2.498982
C    3.757685    3.236110    0.208920
H    3.063141    1.651762    1.485571
C    3.679412    3.823245   -1.054300
H    2.775179    3.733603   -3.007454
H    4.404553    3.660553    0.970968
H    4.265583    4.709778   -1.278437
C    0.549758    0.261205    1.569475
C    0.384648   -0.830243    2.429172
C    0.289646    1.552507    2.046828
C   -0.056764   -0.634829    3.735441
H    0.565991   -1.839663    2.088987
C   -0.144635    1.741279    3.355854
H    0.404245    2.408124    1.393812
H   -0.326227    0.649099    4.201773
H   -0.196131   -1.495215    4.382853
H   -0.348582    2.748239    3.707699
H   -0.674512    0.798245    5.220060
C   -3.224947   -1.133557   -0.066034
C   -3.126261   -0.318907    1.067888
C   -4.444591   -1.204607   -0.746576
C   -4.223561    0.415351    1.508047
H   -2.175247   -0.266802    1.590386
C   -5.544323   -0.472420   -0.304554
H   -4.547045   -1.845143   -1.617802
C   -5.436701    0.341749    0.822376
H   -4.129967    1.050107    2.385742
H   -6.488317   -0.541630   -0.838098
H   -6.295072    0.913486    1.165188
```

Pph-γ-4b

E(ele) = −1803.223405
E(ele+zpe) = −1802.690445
H = −1802.658001
G = −1802.753748

```
C    0.763348   -0.499314   -2.349311
H    1.205579   -0.206404   -3.298961
C   -0.561106    1.543801   -2.522901
C   -0.191485    0.266283   -1.805078
C    1.535584    2.494788   -1.439705
C    0.139808    2.793863   -1.897526
H   -0.462839    3.143224   -1.053672
H    0.131695    3.587872   -2.650642
H   -0.238638    1.431613   -3.564573
H    2.383205    2.837594   -2.023422
C    1.730805    1.675629   -0.383151
O    0.720555    1.166448    0.335893
P   -0.859820    0.120115   -0.073852
C    1.351163   -1.683078   -1.700565
O    0.861555   -2.272561   -0.758954
O    2.507893   -2.038135   -2.272764
C    3.191714   -3.124446   -1.646600
H    3.433317   -2.863494   -0.613197
H    2.570464   -4.022953   -1.660281
H    4.101259   -3.271306   -2.227018
C   -1.644060    1.707360   -2.530688
C   -1.898350    1.597478    0.343599
C   -3.108274    1.829700   -0.322263
C   -1.486707    2.516187    1.316430
C   -3.877871    2.955572   -0.032366
H   -3.462908    1.132735   -1.075443
C   -2.274096    3.620162    1.632584
C   -0.528480    2.391142    1.801728
C   -3.469531    3.848680    0.954639
H   -4.804048    3.123708   -0.574253
H   -1.937546    4.313072    2.398205
H   -4.075515    4.718640    1.191077
C   -2.324975   -1.008443   -0.515260
C   -2.408417   -1.733399   -1.704296
C   -3.367205   -1.155158    0.415876
C   -3.494809   -2.576853   -1.963305
H   -1.618553   -1.660075   -2.444899
C   -4.450812   -1.987151    0.164865
H   -3.325729   -0.612000    1.358737
C   -4.518157   -2.705265   -1.032642
H   -3.530352   -3.134377   -2.895205
H   -5.241692   -2.082153    0.903751
H   -5.361804   -3.360254   -1.231539
C   -0.402249   -0.837478    1.464525
C    0.182887   -0.212883    2.574508
C   -0.713991   -2.199641    1.560716
C    0.413109   -0.920618    3.752783
H    0.496824    0.819082    2.515113
C   -0.460939   -2.910705    2.730383
H   -1.134235   -2.724206    0.711520
C    0.092525   -2.272366    3.837405
H    0.862013   -0.408512    4.599034
H   -0.698728   -3.969758    2.768929
H    0.283160   -2.825228    4.753088
C    3.080815    1.215327    0.049324
C    3.205813   -0.015824    0.705906
C    4.237246    1.967768   -0.193161
C    4.459419   -0.493024    1.084698
H    2.311119   -0.594684    0.919746
C    5.488247    1.490744    0.186442
H    4.152528    2.943551   -0.663707
C    5.606082    0.254868    0.824248
H    4.537726   -1.450184    1.594619
H    6.373784    2.090565   -0.005528
H    6.582194   -0.113510    1.127033
```

Pph-γ-ts5b

E(ele) = −1803.216507
E(ele+zpe) = −1802.684376
H = −1802.652659
G = −1802.745647

```
C   -0.760829    0.124162   -2.145734
H   -1.019434   -0.022974   -3.191017
C    0.731440   -1.647763   -2.455264
C    0.448745   -0.380855   -1.697250
C   -1.788161   -1.878216   -1.956015
C   -0.549620   -2.604946   -2.369010
H   -0.328159   -3.380646   -1.628452
H   -0.681538   -3.090406   -3.340795
H    0.858658   -1.381381   -3.512393
H   -2.611026   -1.750113   -2.650650
C   -1.961338   -1.674823   -0.568603
O   -1.008492   -1.905925    0.220022
P    1.253819    0.016869   -0.165785
C   -1.502226    1.210487   -1.488688
O   -1.085454    1.842062   -0.536965
C   -2.695598    1.428864   -2.050290
C   -3.534557    2.356449   -1.358745
H   -3.718026    2.000103   -0.341186
H   -3.063701    3.342251   -1.325991
H   -4.464139    2.388634   -1.925387
H    1.636572   -2.174464   -2.153848
C    2.485412   -1.312548    0.096253
C    3.856898   -1.047321    0.107670
C    2.033442   -2.629942    0.272121
C    4.769027   -2.084169    0.310802
H    4.227045   -0.039187   -0.049599
C    2.949236   -3.657085    0.476412
H    0.964846   -2.836428    0.228081
C    4.318436   -3.386756    0.499910
H    5.833202   -1.867250    0.315258
H    2.590031   -4.673350    0.610710
H    5.030846   -4.191540    0.657401
C    2.234787    1.545151   -0.422905
C    2.954855    2.117246    0.634609
C    2.315512    2.113356   -1.694830
C    3.744314    3.242231    0.417510
H    2.896808    1.682944    1.630016
C    3.101217    3.245993   -1.908646
H    1.759371    1.664982   -2.513286
C    3.816076    3.809972   -0.855597
H    4.299154    3.678902    1.242866
H    3.153198    3.685733   -2.900382
H    4.428371    4.691497   -1.023824
C    0.514426    0.295709    1.505361
C    0.393084   -0.765256    2.409760
C    0.135707    1.580563    1.911303
C   -0.112640   -0.547277    3.688567
H    0.664949   -1.771729    2.121762
C   -0.377150    1.793308    3.189253
H    0.225263    2.416835    1.229293
C   -0.506671    0.730627    4.080431
H   -0.207199   -1.384690    4.373375
C   -0.676763    2.795268    3.482323
H   -0.909645    0.896629    5.075728
C   -3.203190   -1.021890   -0.024103
C   -3.122638   -0.386287    1.220069
C   -4.427201   -1.021609   -0.703433
C   -4.238992    0.236535    1.774257
C   -2.169977   -0.392266    1.741608
C   -5.546494   -0.405896   -0.147390
C   -4.515132   -1.516973   -1.666218
C   -5.456712    0.225784    1.094086
H   -4.155337    0.728582    2.739892
H   -6.492743   -0.424549   -0.681542
H   -6.331348    0.702938    1.527943
```

Pph-γ-5b

E(ele) = −1803.240422
E(ele+zpe) = −1802.705897
H = −1802.674005
G = −1802.767805

```
C   -0.859529    0.034070   -2.123810
H   -0.865468    0.296782   -3.197867
C    0.781146   -1.564199   -2.571274
C    0.532499   -0.337798   -1.709788
C   -1.641334   -1.345701   -2.079863
C   -0.581050   -2.325812   -2.620788
H   -0.552682   -3.221751   -1.994697
H   -0.828713   -2.634348   -3.642010
H    1.027938   -1.235469   -3.593787
H   -2.539642   -1.287907   -2.701376
C   -2.012519   -1.641141   -0.639948
O   -1.288906   -2.311337    0.075892
P    1.323179    0.018391   -0.249343
C   -1.524374    1.198011   -1.448415
O   -1.016743    1.888688   -0.593813
C   -2.754464    1.422489   -1.932279
C   -3.509508    2.420899   -1.243799
H   -3.577196    2.166967   -0.181658
H   -3.038319    3.400004   -1.358513
H   -4.497951    2.408992   -1.701802
H    1.606006   -2.201643   -2.253506
C    2.648056   -1.232397   -0.043274
C    3.998284   -0.882365    0.022999
C    2.289666   -2.586865    0.043003
C    4.974813   -1.866011    0.191833
H    4.300089    0.156785   -0.064443
C    3.264681   -3.563905    0.215639
H    1.242588   -2.873716   -0.046005
C    4.611012   -3.204692    0.295139
H    6.021378   -1.578925    0.238353
H    2.972455   -4.608106    0.281073
H    5.371762   -3.968420    0.429028
C    2.203010    1.640706   -0.247055
C    2.868503    2.122602    0.886620
C    2.256210    2.368084   -1.434586
C    3.580759    3.317066    0.827467
H    2.832746    1.561151    1.818173
C    2.960137    3.571335   -1.492295
H    1.738879    1.973626   -2.306668
C    3.624396    4.044991   -0.363395
H    4.098471    3.682290    1.710082
H    2.990139    4.137203   -2.419182
H    4.176419    4.979781   -0.407719
C    0.515656    0.078833    1.438539
C    0.394732   -1.076055    2.220274
C    0.031801    1.287223    1.958859
C   -0.189628   -1.027833    3.484917
H    0.748404   -2.031239    1.852961
C   -0.562931    1.334615    3.218208
H    0.117076    2.198757    1.379036
C   -0.674195    0.177961    3.987945
H   -0.267453   -1.938706    4.071579
H   -0.935113    2.282417    3.597237
H   -1.131028    0.216911    4.973286
C   -3.236056   -0.997895   -0.049013
C   -3.168725   -0.583471    1.285353
C   -4.422533   -0.818658   -0.767479
C   -4.270349    0.014575    1.891306
H   -2.243055   -0.733199    1.833853
C   -5.534874   -0.251645   -0.149915
H   -4.488036   -1.129696   -1.806065
C   -5.457980    0.172998    1.177232
H   -4.200834    0.350271    2.922288
H   -6.460961   -0.135511   -0.705982
H   -6.323348    0.626959    1.652253
```

γ-5b

E(ele) = −767.287102
E(ele+zpe) = −767.032992
H = −767.016776
G = −767.077277

```
C    1.851155   -0.373601   -0.229791
C    2.523567   -2.592837   -0.604757
C    2.919588   -1.172053   -0.309006
C    0.551104   -1.119495   -0.452141
C    1.006152   -2.596772   -0.321167
H    0.836099   -2.908602    0.713673
H    0.446845   -3.263866   -0.981743
H    0.171411   -0.913634   -1.459173
C    2.747698   -2.826421   -1.655105
C   -0.509788   -0.773733    0.597963
O   -0.281354   -1.013441    1.767546
C    3.068536   -3.321579    0.004304
H    1.846019    1.089739   -0.038634
O    0.840552    1.763649   -0.119633
O    3.059299    1.598361    0.221273
C    3.097557    3.013791    0.411977
H    4.140514    3.253441    0.613560
H    2.749102    3.526755   -0.487394
H    2.465333    3.297792    1.256115
C   -1.834418   -0.217616    0.178910
C   -2.017775    0.481373   -1.017830
C   -2.920688   -0.408048    1.040506
C   -3.276350    0.976198   -1.351197
H   -1.172993    0.682811   -1.668399
C   -4.179925    0.072691    0.699169
H   -2.756407   -0.938010    1.974083
C   -4.359112    0.764720   -0.499363
H   -3.410067    1.531896   -2.274677
H   -5.021302   -0.088705    1.366783
H   -5.341500    1.144306   -0.766273
H    3.946238   -0.830868   -0.217086
```

Pph-γ-ts6b

E(ele) = −1803.210914
E(ele+zpe) = −1802.679719
H = −1802.647477
G = −1802.743314

```
C    0.486703   -1.106604   -1.896513
H    1.066950   -1.090440   -2.812600
C   -0.075557    1.269823   -2.338330
C    0.070978    0.103839   -1.357805
C    2.194115    2.148778   -1.787079
C    0.768456    2.532549   -2.051486
H    0.349489    3.060064   -1.185738
H    0.681602    3.200736   -2.914512
H    0.219994    0.878471   -3.316555
H    3.005356    2.491747   -2.419648
C    2.382730    1.260313   -0.786272
O    1.322597    0.801552   -0.125731
P   -1.095869    0.142827    0.079060
C    0.256565   -2.373327   -1.271910
C   -0.530524   -2.580178   -0.346880
O    0.942435   -3.389454   -1.846459
O    0.675080   -4.682179   -1.316477
H    0.940093   -4.727256   -0.256931
H   -0.383304   -4.934345   -1.426547
H    1.293246   -5.369417   -1.894012
C   -1.137339    1.539857   -2.424472
C    3.695256    0.681137   -0.396678
H   -2.054679   -1.382758   -2.250744
C   -5.125496   -0.539390   -0.033763
H   -3.725171    0.423131    1.281511
C   -5.297261   -1.238378   -1.229477
H   -4.325790   -2.076720   -2.959050
C   -5.981443   -0.303202    0.591251
H   -6.291307   -1.549080   -1.538021
C   -1.401873    1.907223    0.461237
C   -0.629654    2.582010    1.411427
C   -2.380108    2.611780   -0.251068
C   -0.833089    3.939337    1.643953
H    0.146929    2.057767    1.955066
C   -2.571685    3.972969   -0.025659
H   -2.997145    2.105342   -0.987838
C   -1.798509    4.639229    0.922150
H   -0.225497    4.451740    2.383678
H   -3.328546    4.508730   -0.590745
H   -1.948856    5.700238    1.099426
C   -0.642598   -0.689372    1.644575
C   -1.553910   -1.608294    2.180322
C    0.551369   -0.428294    2.327699
C   -1.294409   -2.225413    3.399116
H   -2.447698   -1.881641    1.631327
C    0.805026   -1.058297    3.545402
H    1.293805    0.225564    1.866566
C   -0.116533   -1.947948    4.089911
H   -2.008048   -2.940961    3.796447
H    1.739762   -0.853873    4.059396
H    0.088065   -2.436244    5.038478
```

Pph-γ-6b

	E(ele)	=	-1803.214216	
	E(ele+zpe)	=	-1802.681769	
	H	=	-1802.649249	
	G	=	-1802.746134	
C	0.581850	-1.052352	-1.900745
H	0.815787	-1.127319	-2.954113
C	-0.142182	1.247742	-2.453113
C	0.223462	0.236787	-1.334974
C	2.299915	1.902883	-2.214392
C	0.925698	2.357409	-2.629714
H	0.637276	3.233501	-2.033418
H	0.924269	2.686663	-3.672904
H	-0.212470	0.674308	-3.380209
H	3.170903	2.139189	-2.815745
C	2.405714	1.177202	-1.094559
O	1.242611	0.856179	-0.434105
P	-1.093607	0.140162	0.083594
C	0.565728	-2.194969	-1.107404
O	0.178546	-2.222877	0.083218
O	0.948043	-3.350187	-1.726357
C	0.832398	-4.526492	-0.943691
H	1.439442	-4.457196	-0.036384
H	-0.208451	-4.707458	-0.656607
H	1.193114	-5.338590	-1.576741
H	-1.121002	1.711828	-2.296813
C	-2.459028	-0.986205	-0.294686
C	-3.356195	-1.370335	0.709400
C	-2.674942	-1.394965	-1.614752
H	-3.210671	-1.032241	1.732000
C	-3.767473	-2.207475	-1.916421
H	-1.979817	-1.104896	-2.396570
C	-4.649008	-2.603419	-0.913791
H	-5.134288	-2.477087	1.184247
H	-3.924336	-2.532570	-2.940613
H	-5.497839	-3.236750	-1.154997
C	-1.880719	1.805712	0.112067
C	-1.079101	2.957986	0.124256
C	-3.271569	1.951463	0.107070
C	-1.659423	4.221985	0.149353
H	0.002907	2.863105	0.093088
C	-3.849919	3.220953	0.133412
H	-3.915602	1.078419	0.073552
C	-3.047625	4.357614	0.157795
H	-1.023955	5.102912	0.155951
H	-4.931846	3.315408	0.129138
H	-3.499231	5.345284	0.176141
C	-0.518062	-0.091385	1.805346
C	-0.665579	-1.320958	2.458711
C	0.069935	0.979414	2.485842
C	-0.257478	-1.459396	3.782160
H	-1.063921	-2.174414	1.923525
C	0.499970	0.826874	3.801438
H	0.215090	1.934401	1.996323
C	0.329245	-0.389966	4.456140
H	-0.379691	-2.417984	4.277652
H	0.970449	1.662997	4.309796
H	0.661327	-0.507671	5.483748
C	3.621990	0.626825	-0.468021
C	3.514549	-0.492117	0.367636
C	4.880410	1.198306	-0.693401
C	4.656889	-1.040473	0.946397
H	2.534715	-0.928048	0.548588
C	6.018063	0.645350	-0.114781
H	4.963634	2.088914	-1.311256
C	5.909536	-0.477650	0.706778
H	4.566727	-1.913247	1.587209
H	6.989642	1.097376	-0.294106
H	6.797810	-0.906699	1.161956

C	3.704371	-3.951807	-0.396861
H	1.829851	-5.013655	-0.266668
H	5.398130	-2.625880	-0.493247
H	4.298428	-4.852128	-0.524661
C	0.668986	-0.148851	1.891677
C	0.284852	1.029546	2.548848
C	0.719282	-1.344577	2.621443
C	-0.034852	1.001094	3.904107
H	0.224606	1.959741	1.999385
C	0.378427	-1.366847	3.971395
H	1.035623	-2.270383	2.157278
C	0.000252	-0.193969	4.618465
H	0.417815	-2.306126	4.515075
H	-0.263384	-0.210715	5.672162
C	-3.648108	-0.790302	-0.424381
C	-3.602048	0.353659	0.382291
C	-4.871442	-1.442426	-0.624138
C	-4.772085	0.847002	0.956003
H	-2.648340	0.849907	0.546034
C	-6.036195	-0.944261	-0.050005
H	-4.906348	-2.352270	-1.217812
C	-5.990406	0.204823	0.741196
H	-4.729988	1.739385	1.574488
H	-6.980091	-1.457955	-0.210094
H	-6.900156	0.591566	1.191983

γ-6b

	E(ele)	=	-767.272485	
	E(ele+zpe)	=	-767.017806	
	H	=	-767.001935	
	G	=	-767.061098	
C	-2.508527	0.775034	-0.216190
H	-3.366927	1.431877	-0.285287
C	-1.000750	2.770476	-0.509388
C	-1.277174	1.308385	-0.309473
C	1.207754	2.269362	0.481738
C	0.066363	3.246077	0.480805
H	-0.362167	3.342627	1.487657
H	0.417051	4.242488	0.191726
H	2.183677	2.583401	0.833884
H	-0.616812	2.901946	-1.530097
O	1.042397	1.004420	0.077264
O	-0.194471	0.500732	-0.278027
C	-1.930248	3.337087	-0.421176
C	-2.778402	-0.657927	-0.022667
C	-1.971162	-1.555619	0.078464
O	-4.113255	-0.872582	0.039015
C	-4.499669	-2.230532	0.233554
H	-4.084856	-2.615396	1.168341
H	-4.146183	-2.850149	-0.594369
H	-5.588409	-2.223851	0.270396
C	2.069761	-0.055435	0.013982
C	1.679759	-1.400891	0.014239
C	3.431798	0.264927	-0.038725
C	2.646280	-2.404042	-0.017305
H	0.622384	-1.650049	0.043702
C	4.390932	-0.741231	-0.066588
H	3.744212	1.304695	-0.079134
C	4.001090	-2.080891	-0.053962
H	2.335053	-3.444717	-0.012777
H	5.444258	-0.479650	-0.110902
H	4.750412	-2.866950	-0.081286

Pph-γ-ts6b2

	E(ele)	=	-1803.213672	
	E(ele+zpe)	=	-1802.681250	
	H	=	-1802.649576	
	G	=	-1802.743774	
C	-0.636846	1.022776	-1.884860
H	-0.646607	1.168546	-2.956143
C	0.103369	-1.259762	-2.454062
C	-0.284167	-0.261495	-1.336194
C	-2.278097	-2.047387	-2.141668
C	-0.886938	-2.443337	-2.555767
H	-0.539822	-3.265052	-1.914796
H	-0.875997	-2.829577	-3.579126
H	0.079994	-0.702661	-3.393599
H	-3.142921	-2.355648	-2.718576
C	-2.407560	-1.283346	-1.050704
O	-1.253514	-0.874696	-0.415812
P	1.124803	-0.138465	0.113379
C	-0.816703	2.125097	-1.044889
O	-0.660091	2.101195	0.191689
O	-1.134970	3.291583	-1.675882
C	-1.260208	4.423480	-0.831311
H	-2.035041	4.265015	-0.075592
H	-0.314050	4.641139	-0.325533
H	-1.536017	5.251723	-1.485393
H	1.121271	-1.645832	-2.346260
C	2.247112	1.243075	-0.214645
C	2.904077	1.926813	0.814355
C	2.510432	1.575396	-1.549362
C	3.798528	2.949271	0.509100
H	2.722674	1.661167	1.851441
C	3.404961	2.601910	-1.847058
H	2.014560	1.042318	-2.354250
C	4.044231	3.292785	-0.820181
H	4.303645	3.477342	1.312385
H	3.598204	2.860599	-2.883809
H	4.738397	4.094834	-1.054409
C	2.173114	-1.629842	-0.073454
C	1.558484	-2.890480	-0.094039
C	3.560035	-1.544882	-0.219635
C	2.318968	-4.043801	-0.251666
H	0.477565	-2.961870	0.010311
C	4.320812	-2.704116	-0.379898
H	4.052702	-0.576575	-0.213245

9.5.2 Cycloadditions starting from Dabco-3′

Dabco-γ-ts4b′

E(ele)	= −1112.392940		
E(ele+zpe)	= −1111.952104		
H	= −1111.929102		
G	= −1112.003067		

C	0.046802	1.161613	−0.649397
H	0.223375	0.383506	−1.375620
C	−1.288257	2.070958	1.213184
C	−1.100578	1.230412	0.124210
C	1.128154	0.564206	2.061386
C	0.021109	1.053192	2.719187
H	−0.767307	0.359044	2.995461
H	0.100680	1.954093	3.319416
H	−0.649901	2.942980	1.241780
H	2.020319	1.173324	1.983930
C	1.054522	−0.700734	1.387213
O	0.021331	−1.407161	1.409048
H	−2.248389	2.170767	1.707104
C	1.084652	2.168832	−0.597543
O	1.141051	3.181498	0.085321
O	2.080665	1.862291	−1.480499
C	3.174179	2.766934	−1.494437
H	3.626378	2.847259	−0.500782
H	2.851055	3.763425	−1.808508
H	3.889897	2.354646	−2.206164
C	−3.289837	0.962908	−0.940575
C	−1.748865	−0.925652	−1.048122
C	−2.815173	−0.375734	1.064804
C	−4.321742	−0.067574	−1.460378
C	−2.793740	1.519296	−1.738579
H	−3.720949	1.678586	−0.237148
C	−2.903022	−1.947643	−1.155133
H	−0.860420	−1.345848	−0.571043
H	−1.497614	−0.503580	−2.022800
H	−2.042724	−1.033829	1.468312
H	−2.998965	0.424456	1.776620
C	−4.128098	−1.091920	0.673560
H	−4.189451	−0.244988	−2.532283
H	−5.336491	0.312470	−1.309331
H	−2.716341	−2.805974	−0.502934
H	−2.976179	−2.317394	−2.182205
H	−4.200275	−2.043648	1.207751
H	−5.003294	−0.492016	0.943921
N	−4.178208	−1.346032	−0.765777
N	−2.204534	0.231290	−0.184287
C	2.251414	−1.225767	0.637579
C	2.235759	−2.565429	0.233093
C	3.363240	−0.438719	0.315400
C	3.305525	−3.109342	−0.472372
H	1.370686	−3.167979	0.493365
C	4.431426	−0.978721	−0.395481
H	3.393910	0.608144	0.599485
C	4.407414	−2.315796	−0.790925
H	3.282686	−4.153674	−0.772099
H	5.283281	−0.352305	−0.646006
H	5.242839	−2.736745	−1.343689

Dabco-γ-ts5b′

E(ele)	= −1112.390812		
E(ele+zpe)	= −1111.947970		
H	= −1111.925568		
G	= −1111.999555		

C	−0.128385	1.097713	−0.262350
C	−1.304921	1.637823	1.740491
C	−1.399292	1.254633	0.301053
C	0.905490	0.414306	1.543314
C	−0.269740	0.648064	2.432169
H	−0.754324	−0.307399	2.663968
H	0.034980	1.100960	3.382044
H	1.705534	1.143366	1.628506
H	−0.862253	2.635513	1.782034
H	1.286287	−0.923857	1.178263
O	0.546093	−1.911012	1.348999
H	−2.247782	1.685847	2.291556
C	−2.796367	0.449652	−1.547495
C	−1.949325	−1.237622	0.008771
C	−3.667825	0.331977	0.711209
C	−3.695760	−0.707250	−2.039924
C	−1.872136	0.537293	−2.118259
H	−3.293287	1.422761	−1.563115
C	−3.149682	−2.176652	−0.256185
H	−1.496055	−1.367868	0.989593
H	−1.153898	−1.368782	−0.726947
H	−3.424353	−0.039570	1.708972
H	−3.903010	1.396282	0.777300
C	−4.794388	−0.494642	0.047381
H	−3.131042	−1.405129	−2.665813
H	−4.518052	−0.311035	−2.643808
H	−3.529874	−2.599100	0.679185
H	−2.841330	−3.011023	−0.892270
H	−5.360406	−1.032479	0.813481
H	−5.494343	0.156737	−0.485946
N	−2.412845	0.207770	−0.107910
N	−4.245120	−1.453768	−0.908049
C	0.805358	2.246540	−0.372396
O	0.765766	3.298207	0.228271
O	1.771614	1.966291	−1.276077
H	0.047491	0.377366	−1.060333
C	2.788619	2.954190	−1.409936
H	3.504408	2.544585	−2.121953
H	2.366084	3.891868	−1.779549
H	3.269523	3.141200	−0.445331
C	2.614702	−1.152587	0.489219
C	3.569944	−0.151364	0.276553
C	2.894896	−2.448835	0.042385
C	4.767882	−0.437796	−0.373900
H	3.391257	0.862440	0.618914
C	4.089896	−2.737847	−0.610125
H	2.152628	−3.219942	0.223581
C	5.031392	−1.731056	−0.822787
H	5.499539	0.351185	−0.526957
H	4.289746	−3.750230	−0.950869
H	5.966240	−1.953075	−1.330073

Dabco-γ-ts6b′

E(ele)	= −1112.404669		
E(ele+zpe)	= −1111.961305		
H	= −1111.939041		
G	= −1112.012035		

C	−0.180843	1.394914	−0.483602
H	−0.181390	1.092316	−1.522610
C	−0.870379	1.052454	1.913962
C	−0.850730	0.656541	0.457563
C	1.299612	−0.199694	2.245956
C	−0.022799	0.145415	2.852369
H	−0.586608	−0.778448	3.047261
H	0.090579	0.671169	3.805153
H	2.227741	0.157641	2.676944
H	−0.457622	2.059525	1.963907
C	1.251851	−0.874039	1.070043
O	0.079150	−1.139741	0.528802
H	−1.899261	1.107870	2.291149
C	0.761652	2.472224	−0.206802
O	0.969102	3.084991	0.826004
C	1.426541	2.788961	−1.351487
C	2.401489	3.816307	−1.219041
H	3.169047	3.522711	−0.498182
H	1.938826	4.748333	−0.883919
H	2.836885	3.938850	−2.210556
C	−3.234321	0.950562	−0.173332
C	−1.926014	−0.693594	−1.398884
C	−2.588390	−1.155471	0.902721
C	−4.419267	0.286041	−0.916028
C	−2.818737	1.808032	−0.704413
H	−3.502823	1.263059	0.838291
C	−3.162440	−1.565426	−1.713264
H	−0.989693	−1.248963	−1.346121
H	−1.837631	0.127216	−2.111796
H	−1.851539	−1.951527	0.818221
H	−2.549874	−0.765771	1.918584
C	−4.017833	−1.573763	0.494172
H	−4.450538	0.604723	−1.962655
H	−5.363633	0.583135	−0.450559
H	−2.954504	−2.623190	−1.526508
H	−3.429384	−1.459662	−2.769054
H	−4.120064	−2.659402	0.581095
H	−4.771466	−1.117962	1.144900
N	−2.119543	−0.062231	−0.037326
N	−4.303598	−1.171375	−0.883767
C	2.468502	−1.260135	0.301633
C	2.417629	−1.314752	−1.095061
C	3.674258	−1.573025	0.940861
C	3.547642	−1.648424	−1.837692
H	1.480260	−1.077693	−1.590162
C	4.805355	−1.908536	0.200913
H	3.716147	−1.569236	2.026940
C	4.747490	−1.946156	−1.192466
H	3.493561	−1.675065	−2.922957
H	5.732005	−2.152487	0.713643
H	5.628597	−2.212280	−1.769603

Dabco-γ-4b′

E(ele)	= −1112.413083		
E(ele+zpe)	= −1111.969309		
H	= −1111.946317		
G	= −1112.020542		

C	−0.180033	1.240444	−0.841138
H	−0.063312	0.571854	−1.682589
C	−1.125284	1.830189	1.374858
C	−1.158538	1.119745	0.066022
C	1.130515	0.626977	1.840592
C	−0.157950	1.112360	2.410684
H	−0.705959	0.273049	2.856517
H	0.014290	1.849502	3.201746
H	−0.721021	2.824919	1.190933
H	2.028617	1.208532	2.013521
C	1.153077	−0.570160	1.156633
O	0.092707	−1.278136	0.960984
H	−2.117514	1.959804	1.818499
C	0.935475	2.214933	−0.722607
O	0.925352	3.294895	−0.171414
O	1.988936	1.757577	−1.419823
C	3.162037	2.564055	−1.354639
H	3.428501	2.756528	−0.312232
H	2.996291	3.518238	−1.862119
H	3.941298	1.987520	−1.851374
C	−3.493817	0.940171	−0.650697
C	−1.976137	−0.889444	−1.216136
C	−2.682371	−0.569224	1.109082
C	−4.722326	−0.006934	−0.672641
C	−3.232147	1.326514	−1.639255
H	−3.623892	1.785638	0.028398
C	−3.269617	−1.679010	−1.537203
H	−1.158831	−1.477017	−0.782881
H	−1.631408	−0.368744	−2.107687
H	−1.745858	−0.986340	1.493287
H	−3.079743	0.189339	1.783619
C	−3.751167	−1.629763	0.771761
H	−5.278276	0.130379	−1.604764
H	−5.399751	0.220804	0.155980
H	−3.057196	−2.751429	−1.538419
H	−3.650341	−1.413473	−2.528781
H	−3.315119	−2.632669	0.790991
H	−4.554103	−1.599891	1.514494
N	−4.317536	−1.405482	−0.558162
N	−2.292403	0.159804	−0.172679
C	2.437831	−1.101163	0.570084
C	2.438462	−2.396142	0.041438
C	3.629106	−0.365577	0.513436
C	3.589649	−2.942954	−0.524027
H	1.513363	−2.962010	0.092702
C	4.780181	−0.905548	−0.052648
H	3.661351	0.644721	0.910464
C	4.767119	−2.199538	−0.576175
H	3.567895	−3.954331	−0.922541
H	5.692724	−0.315011	−0.084368
H	5.666412	−2.621869	−1.016316

Dabco-γ-5b′

E(ele)	= −1112.414330		
E(ele+zpe)	= −1111.969816		
H	= −1111.947158		
G	= −1112.021727		

C	0.106259	0.770909	0.402883
C	−1.292227	0.751011	2.340766
C	−1.351680	0.994272	0.834586
C	0.873767	0.003508	1.556190
C	−0.173753	−0.274103	2.639848
H	−0.525347	−1.307611	2.564465
H	0.251875	−0.152699	3.641912
H	1.643087	0.673077	1.950162
H	−0.997291	1.706787	2.793978
C	1.512207	−1.230854	0.964160
O	0.969659	−2.324234	1.020653
H	−2.247445	0.491743	2.809860
C	−2.418037	0.569401	−1.328848
C	−1.900830	−1.431996	−0.027738
C	−3.653532	0.073902	0.682012
C	−3.234239	−0.419707	−2.187431
H	−1.415320	0.743266	−1.719862
H	−2.892417	1.546114	−1.215505
C	−3.068796	−2.228644	−0.663380
H	−1.653354	−1.775885	0.975724
H	−0.993058	−1.487754	−0.631248
H	−3.607335	−0.512495	1.601641
H	−3.842878	1.118543	0.939313
C	−4.678729	−0.519646	−0.311748
H	−2.583730	−1.028536	−2.823672
H	−3.918246	0.127760	−2.843848
H	−3.620682	−2.788862	0.098524
H	−2.685136	−2.950096	−1.390664
H	−5.401005	−1.144832	0.222123
H	−5.238613	0.272705	−0.819095
N	−2.282039	0.033685	0.071816
N	−4.007664	−1.325428	−1.333338
C	0.674603	2.152189	0.181178
O	1.230299	2.835761	1.012254
O	0.468778	2.569642	−1.084371
H	0.202559	0.248362	−0.556868
C	0.825163	3.926028	−1.340720
H	0.609999	4.095597	−2.395352
H	0.229916	4.594722	−0.713857
H	1.885508	4.090054	−1.133794
C	2.804148	−1.082612	0.206510
C	3.451044	0.148244	0.045063
C	3.365376	−2.231934	−0.363249
C	4.639306	0.224282	−0.679955
H	3.041835	1.055282	0.481189
C	4.552610	−2.155212	−1.081820
H	2.852165	−3.178862	−0.225647
C	5.191750	−0.924293	−1.242702
H	5.133509	1.183777	−0.801020
H	4.982949	−3.053149	−1.515899
H	6.120035	−0.862638	−1.803831

γ-6b′

E(ele)	= −767.273998		
E(ele+zpe)	= −767.019573		
H	= −767.003580		
G	= −767.063676		

C	2.068322	−0.630496	−0.150515
H	1.775609	−1.602111	−0.532504
C	1.261367	1.655204	0.676642
C	1.106008	0.261923	0.147163
C	−1.045430	2.031192	−0.120812
C	0.337845	2.613176	−0.081961
H	0.721556	2.786496	−1.096783
H	0.328878	3.585126	0.420658
H	−1.911925	2.682060	−0.144385
H	0.962799	1.640910	1.734388
C	−1.231339	0.707737	−0.066326
O	−0.173526	−0.181578	−0.027035
C	2.308598	1.947932	0.626772
O	3.507158	−0.382943	0.002055
O	4.051632	0.608638	0.445624
C	4.209006	−1.450377	−0.433848
C	5.626040	−1.326464	−0.335606
H	5.923495	−1.171801	0.704407
H	5.976181	−0.482536	−0.934912
H	6.029362	−2.263347	−0.716996
C	−2.529726	0.000404	−0.049709
C	−2.622706	−1.291190	0.481609
C	−3.684638	0.610572	−0.555059
C	−3.851017	−1.946197	0.529842
H	−1.729065	−1.776410	0.859746
C	−4.909841	−0.045099	−0.504164
H	−3.621023	1.594543	−1.010476
C	−4.998711	−1.325954	0.041522
H	−3.910030	−2.945829	0.950622
H	−5.795881	0.439534	−0.903885
H	−5.955174	−1.839233	0.077318

9.6 [2 + 2], [3 + 2] and [2 + 2 + 2] cycloadditions with ketone 2c

9.6.1 Cycloadditions starting from IPr-3′

ketone 2c

```
E(ele)     = -682.381443
E(ele+zpe) = -682.264790
H          = -682.254170
G          = -682.301143

C  -0.738879   0.806797   0.000115
O  -1.042901   1.974236  -0.000023
C   2.331627  -1.433077  -0.000007
C   0.992916  -1.050181   0.000040
C   0.661525   0.310400   0.000064
C   1.674822   1.277794   0.000032
C   3.007773   0.889658  -0.000014
C   3.336383  -0.467568  -0.000034
H   2.588773  -2.487684  -0.000025
H   0.221261  -1.812604   0.000058
H   1.394863   2.326755   0.000049
H   3.791761   1.640778  -0.000036
H   4.378926  -0.772432  -0.000072
C  -1.888024  -0.235124  -0.000002
F  -3.074273   0.354504  -0.000150
F  -1.812805  -1.026206  -1.084916
F  -1.813059  -1.026161   1.084961
```

IPr-γ-ts4c′

```
E(ele)     = -2186.390908
E(ele+zpe) = -2185.590109
H          = -2185.542803
G          = -2185.667553

C  -2.125894  -1.730448   1.772684
C  -0.898687  -1.979120   2.283627
C  -0.621680  -0.714025   0.462618
H  -3.110290  -2.047373   2.077894
H  -0.583422  -2.548227   3.143064
N  -1.941828  -0.948349   0.650758
N   0.025215  -1.351167   1.470225
C  -3.045640  -0.669373  -0.248912
C   1.449894  -1.528009   1.699860
C   0.947588  -0.588824  -1.392208
C  -0.717778   1.240728  -1.004935
H  -0.554671   1.697633  -1.972193
H  -1.625543   1.511484  -0.475424
H   1.435567  -1.456532  -0.984299
C  -0.108821   0.011844  -0.727204
C   1.421670  -0.164217  -2.692089
O   0.977641   0.723452  -3.399195
O   2.469210  -0.942489  -3.100582
C   2.994626  -0.611429  -4.379561
H   3.319993   0.431769  -4.400974
H   3.840635  -1.281863  -4.535598
H   2.240642  -0.762839  -5.157495
O   0.727820   2.410755   0.311542
O   0.917932   1.725709   1.327237
C  -3.173641  -1.450681  -1.406010
C  -3.978871   0.305570   0.131416
C  -4.311093  -1.243645  -2.189833
C  -5.103632   0.459250  -0.681474
C  -5.273650  -0.309477  -1.827614
H  -4.439737  -1.825583  -3.098737
H  -5.850388   1.203440  -0.420134
H  -6.153888  -0.168632  -2.448355
C   2.087840  -2.583548   1.022369
C   2.087882  -0.744507   2.673202
C   3.458249  -2.741407   1.229054
C   3.461882  -0.949656   2.840666
C   4.145910  -1.912676   2.110019
H   3.990670  -3.528515   0.703703
H   3.999858  -0.344470   3.564020
H   5.215429  -2.041073   2.250884
C  -3.788687   1.194466   1.349525
C  -2.745927   1.109212   1.680288
C  -4.701604   0.755582   2.503049
H  -4.515181  -0.279615   2.806665
H  -4.545924   1.398624   3.375641
H  -5.754341   0.831717   2.206808
C  -4.043884   2.668846   1.010134
H  -3.469967   2.983757   0.133651
H  -5.105644   2.852229   0.811767
H  -3.746359   3.300006   1.852091
C   1.343971   0.182515   3.618514
H   0.405259   0.482592   3.147591
C   2.126999   1.462214   3.937784
H   2.950226   1.263760   4.635153
H   2.522582   1.919319   3.028618
H   1.459785   2.186376   4.415966
C   1.040688  -0.564708   4.928935
H   1.971137  -0.868120   5.423182
H   0.489342   0.089052   5.613729
H   0.442901  -1.468286   4.770332
C  -2.142971  -2.475481  -1.843009
C  -1.314080  -2.464526  -1.130925
C  -2.727057  -3.893237  -1.837973
C  -3.108928  -4.163690  -0.847242
C  -3.550993  -3.985921  -2.554385
H  -1.955474  -4.618695  -2.119654
H  -1.560494  -2.109888  -3.214496
H  -1.213954  -1.071842  -3.233916
H  -0.707898  -2.759155  -3.444758
C  -2.309421  -2.240495  -4.004507
C   1.322395  -3.600337   0.185208
H   0.371429  -3.154338  -0.125749
C   2.060789  -4.035975  -1.085656
H   2.381443  -3.184376  -1.693667
H   2.942530  -4.640326  -0.845950
H   1.397792  -4.658987  -1.695718
C   0.994214  -4.827140   1.051063
H   0.418265  -4.553815   1.941226
H   0.410143  -5.553545   0.475113
H   1.916748  -5.315197   1.385427
C  -0.253791   3.590479   0.506253
F  -1.169496   3.294194   1.439383
F  -0.929243   3.993034  -0.587894
F   0.426911   4.667546   0.950036
C   1.783060   2.552939  -0.731976
C   1.755053   3.513486  -1.753940
C   2.856089   1.655841  -0.661166
C   2.779243   3.566897  -2.687484
H   0.931640   4.215587  -1.828981
C   3.876163   1.703732  -1.612673
H   2.881758   0.939801   0.155912
C   3.838037   2.655649  -2.625728
H   2.749902   4.314163  -3.475233
H   4.694833   0.990711  -1.560120
H   4.632847   2.697138  -3.366499
```

IPr-γ-4c′

```
E(ele)     = -2186.413274
E(ele+zpe) = -2185.609795
H          = -2185.561661
G          = -2185.689283

C   2.065201   1.482251   2.066189
C   0.804928   1.748451   2.475506
C   0.656038   0.624017   0.553496
H   3.026982   1.736952   2.481671
H   0.427020   2.250976   3.351430
N   1.957923   0.787654   0.874787
N  -0.060925   1.226884   1.531131
C   3.084521   0.575170  -0.006100
C  -1.495714   1.260779   1.727354
C  -0.493795   0.895165  -1.559438
C   0.626605  -1.314244  -1.101386
H   0.600300  -1.490901  -2.176333
H   1.625080  -1.553701  -0.724249
C  -0.842206   1.857379  -1.209857
C   0.251591   0.104460  -0.777626
C  -0.940923   0.548381  -2.936875
O  -0.311449  -0.066871  -3.765759
O  -2.147087   1.087855  -3.170924
C  -2.688577   0.830542  -4.468422
H  -2.761918  -0.246041  -4.633909
H  -3.677305   1.287460  -4.468196
H  -2.052275   1.278074  -5.234612
C  -0.418870  -2.130724  -0.256798
O  -0.443291  -1.625804   0.985705
C   3.341797   1.560965  -0.969483
C   3.879223  -0.567619   0.171817
C   4.460907   1.377838  -1.785183
C   4.987742  -0.696297  -0.668098
C   5.277460   0.264382  -1.633196
H   4.691864   2.117022  -2.547441
H   5.625746  -1.569401  -0.577144
H   6.142475   0.136814  -2.277823
C  -2.225340   2.292030   1.114574
C  -2.069400   0.334686   2.616337
C  -3.612330   2.283855   1.281634
C  -3.458222   0.391339   2.766265
C  -4.225702   1.326558   2.081139
H  -4.214270   3.049092   0.800206
H  -3.945107  -0.320011   3.426644
H  -5.305892   1.330926   2.198316
C   3.555689  -1.616464   1.225805
C   2.466347  -1.632228   1.374415
C   4.224693  -1.264743   2.564303
H   3.877507  -0.308829   2.966158
H   4.002271  -2.038180   3.306782
H   5.313125  -1.207717   2.443462
C   3.987767  -3.023141   0.800393
H   3.622155  -3.276861  -0.198788
H   5.079199  -3.126587   0.812831
H   3.577400  -3.755999   1.500021
C  -1.255226  -0.618465   3.476071
H  -0.271386  -0.740600   3.016801
C  -1.868803  -2.018684   3.565120
H  -2.818751  -2.015093   4.113800
H  -2.005589  -2.433545   2.564887
H  -1.181426  -2.676459   4.108001
C  -1.110518  -0.021909   4.886913
H  -2.090878   0.071722   5.369403
H  -0.488573  -0.674781   5.508932
H  -0.654165   0.974443   4.879409
C   2.488889   2.809194  -1.124064
C   1.580161   2.690745  -0.523683
C   3.232310   4.038369  -0.583807
H   3.506264   3.907769   0.468617
H   4.152356   4.216917  -1.151891
C   2.602933   4.931431  -0.667330
H   2.052751   3.025620  -2.578285
H   1.616356   2.116881  -3.004289
H   1.308326   3.828226  -2.630603
H   2.900117   3.322448  -3.206009
C  -1.556523   3.479589   0.437171
C  -0.532773   3.201977   0.160083
C  -2.286482   3.954410  -0.825240
H  -2.523344   3.128366  -1.503708
H  -3.225286   4.457841  -0.570379
C  -1.667361   4.680534  -1.363362
H  -1.435004   4.632891   1.445961
H  -0.859145   4.333373   2.328057
H  -0.935847   5.492783   0.985392
H  -2.427269   4.950768   1.784662
C   0.044729  -3.600949  -0.201475
F   1.188963  -3.729457   0.500065
F   0.304100  -4.141785  -1.421125
F  -0.863451  -4.393148   0.387314
C  -1.778603  -2.074378  -1.000891
C  -1.962735  -2.518150  -2.315960
F  -2.855844  -1.485518  -0.340060
C  -3.201738  -2.387233  -2.942315
H  -1.137941  -2.963258  -2.865402
C  -4.092172  -1.337697  -0.968138
C  -2.692110  -1.140538   0.674267
C  -4.271469  -1.791653  -2.273041
H  -3.328665  -2.751742  -3.959155
C  -4.913765  -0.865901  -0.434123
H  -5.234700  -1.684698  -2.765660
```

[2 + 2 + 2] cycloaddition
IPr-γ-ts4cc′

```
E(ele)     = -2868.791667
E(ele+zpe) = -2867.868729
H          = -2867.810788
G          = -2867.958671

C   3.332791  -0.920818  -1.927248
C   2.415713  -1.876327  -2.200553
C   1.590603  -0.606497  -0.571994
H   4.313543  -0.733692  -2.333510
H   2.407164  -2.679456  -2.920833
C   2.813008  -0.136819  -0.912465
N   1.341405  -1.680771  -1.348407
C   3.626605   0.799600  -0.152443
C   0.300685  -2.698972  -1.219717
C   0.627222  -0.966963   1.545378
C   0.402405   1.383322   0.606833
H   0.173724   1.603661   1.649496
H   1.261445   2.006154   0.317673
C   0.923923  -1.998996   1.391339
H   0.799764  -0.074390   0.560586
C   0.109079  -0.710332   2.917466
O   0.080055   0.355552   3.484078
O  -0.203228  -1.876205   3.501226
C  -0.896411  -1.748989   4.743251
H  -1.828614  -1.201538   4.578984
H  -1.099938  -2.766890   5.073145
H  -0.280673  -1.218834   5.473698
O  -0.860437   1.795323  -0.239823
O  -1.838487   0.851698  -0.305247
C  -2.850947  -0.249521   1.094883
C  -2.087776  -1.060963   1.606939
O   4.156217   0.353701   1.072621
O   3.915670   2.063490  -0.692855
C   4.961676   1.242998   1.786716
H   4.737670   2.905279   0.062320
H   5.248376   2.508384   1.291729
H   5.376341   0.931525   2.741157
H   4.972631   3.893608  -0.319994
H   5.875855   3.185798   1.863520
C   0.652431  -3.844844  -0.482502
C  -0.927195  -2.557784  -1.891872
C  -0.294696  -4.865895  -0.385619
C  -1.828600  -3.619284  -1.760258
C  -1.525847  -4.752489  -1.014760
H  -0.059504  -5.759545   0.185650
H  -2.797655  -3.549428  -2.240053
H  -2.256709  -5.551603  -0.927015
C   3.417141   2.524251  -2.051658
C   2.521096   1.949174  -2.302749
C   4.483137   2.266917  -3.129775
H   4.745807   1.208866  -3.219512
H   4.119704   2.607784  -4.104814
H   5.400490   2.819042  -2.894798
C   3.046291   4.013202  -2.062377
H   2.425680   4.286601  -1.205105
H   3.942154   4.644379  -2.060529
H   2.482665   4.244422  -2.970475
C  -1.288203  -1.331815  -2.717472
C  -1.209284  -0.473546  -2.040561
C  -2.731598  -1.348328  -3.220155
H  -2.883258  -2.116339  -3.990790
H  -3.447691  -1.512325  -2.414830
C  -2.958201  -0.374481  -3.665249
H  -0.367565  -1.150616  -3.934671
H  -0.404827  -2.041845  -4.574746
H  -0.714733  -0.295577  -4.524132
C   0.673168  -0.951493  -3.675577
C   3.963901  -1.053508   1.608050
H   3.139744  -1.518498   1.069218
C   5.213259  -1.902454   1.335024
H   5.438912  -1.946554   0.263359
H   6.087662  -1.486375   1.848232
C   5.061874  -2.926536   1.695827
H   3.591433  -1.070062   3.095018
H   2.791856  -0.355245   3.313949
H   3.248738  -2.070308   3.382918
H   4.451707  -0.823730   3.727129
C   2.015981  -4.051254   0.164340
C   2.567002  -3.106067   0.139980
C   1.916347  -4.495161   1.631161
H   1.267506  -3.845252   2.227113
H   1.522888  -5.514290   1.708134
C   2.914376  -4.497557   2.084468
H   2.841006  -5.071755  -0.633886
H   2.973388  -4.762068  -1.675511
H   3.832301  -5.195869  -0.183965
H   2.343409  -6.047932  -0.637782
C  -3.219741   0.950155   1.995906
C  -0.380694   2.050171  -1.702238
F   0.430576   1.055255  -2.171735
F   0.355509   3.174325  -1.835401
F  -1.389771   2.139493  -2.573327
F  -3.917920   0.455921   3.047803
F  -2.144442   1.557198   2.496272
F  -4.002406   1.879632   1.435120
C  -1.348866   3.193182   0.221965
C  -2.581099   3.637320  -0.263318
C  -0.611878   4.048758   1.044107
C  -3.075644   4.892763   0.076596
H  -3.155205   2.972560  -0.900464
C  -1.106132   5.304821   1.394210
H   0.355191   3.747933   1.435502
C  -2.340523   5.732176   0.912621
H  -4.041092   5.213900  -0.305041
```

IPr-4cc′

```
E(ele)     = -2868.803460
E(ele+zpe) = -2867.879879
H          = -2867.821751
G          = -2867.969885

C   2.796754  -2.903622  -0.696133
C   1.769690  -3.581850  -0.133979
C   1.297035  -1.409094   0.030448
H   3.718775  -3.229671  -1.151735
H   1.575910  -4.638176  -0.031349
N   2.480640  -1.563780  -0.604177
C   0.838188  -2.652881   0.293204
C   3.347748  -0.510429  -1.078347
C  -0.533435  -3.083357   0.522579
C   0.797664  -0.043871   1.900609
C   0.832062   1.079101  -0.401080
H   1.770087   1.637090  -0.307634
H   0.800807   0.655126  -1.404474
C   0.820043  -0.961365   2.479362
H   0.868686  -0.088114   0.563897
C   0.734266   1.203742   2.706255
O   1.444672   2.164479   2.514314
O  -0.118914   1.099434   3.727132
C  -0.201888   2.252106   4.570646
H  -0.462548   3.131117   3.977360
H  -0.980955   2.025641   5.296842
H   0.756814   2.422920   5.067395
C  -0.357636   2.100466  -0.295623
O  -1.490723   1.642199   0.364199
O  -2.199911   0.393490  -0.066402
C   4.302403   0.002645  -0.195198
C   3.176191  -0.067049  -2.401472
C   5.136929   1.012670  -0.684921
C   4.034328   0.943751  -2.835522
C   5.005243   1.474977  -1.988134
H   5.890697   1.445158  -0.032966
H   3.932904   1.337175  -3.841902
H   5.657458   2.265407  -2.348639
C  -0.967268  -3.377346   1.814890
C  -1.302075  -3.296038  -0.635793
C  -2.291418  -3.808591   1.949167
C  -2.608244  -3.736679  -0.443804
C  -3.106365  -3.965384   0.836831
H  -2.684318  -4.025955   2.938655
H  -3.248020  -3.901687  -1.307144
H  -4.137348  -4.282185   0.964966
C   2.101306  -0.644829  -3.313039
C   1.245122  -0.933560  -2.689773
C   2.600333  -1.906404  -4.033533
C   2.890450  -2.697858  -3.335831
C   1.809357  -2.303843  -4.679263
H   3.467606  -1.669045  -4.660473
H   1.580285   0.367083  -4.337513
H   1.308640   1.316971  -3.869928
C   2.321698   0.560841  -5.121276
H   0.685570  -0.036787  -4.820999
C  -0.718216  -3.196759  -2.039764
C   0.267178  -2.722543  -1.979308
C  -1.533789  -2.349988  -3.018616
H  -2.540697  -2.759586  -3.164919
H  -1.612859  -1.324704  -2.649377
C  -1.037190  -2.355287  -3.997475
H  -0.514283  -4.614705  -2.599893
H  -1.481407  -5.109241  -2.746360
H  -0.005578  -4.571451  -3.569693
C   0.079037  -5.244233  -1.927320
C   4.460365  -0.506066   1.226928
H   3.597606  -1.138181   1.468393
C   5.724400  -1.368572   1.343934
H   5.696273  -2.222106   0.657504
H   6.616473  -0.777598   1.107241
C   5.831672  -1.751760   2.364104
H   4.478712   0.644088   2.239678
H   3.611815   1.301146   2.117402
H   4.464815   0.241205   3.258389
H   5.388503   1.246779   2.139642
C  -0.041414  -3.368703   3.020112
C   0.915509  -2.923940   2.719330
C  -0.595189  -2.567220   4.203368
H  -0.825419  -1.534041   3.932411
H  -1.515187  -3.022618   4.585871
C   0.133513  -2.561493   5.021933
H   0.259683  -4.813847   3.447305
H   0.687327  -5.395028   2.622667
H   0.967679  -4.826401   4.283265
H  -0.657180  -5.319233   3.770293
C  -2.805584  -0.012334   1.315733
C  -0.673549   2.511316  -1.764526
F  -1.112196   1.506246  -2.531076
F   0.455906   2.968839  -2.367530
F  -1.572909   3.495919  -1.830950
F  -3.694342  -1.019363   1.158627
```

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```
F        -1.872711   -0.475879    2.170960
F        -3.452671    0.978743    1.951185
C         0.026615    3.420319    0.408716
C        -0.875348    3.999304    1.303722
C         1.230009    4.080229    0.147538
C        -0.569328    5.199011    1.943100
H        -1.811758    3.492612    1.510925
C         1.536300    5.277596    0.787654
H         1.949133    3.666844   -0.553626
C         0.639813    5.841854    1.692971
H        -1.283688    5.631218    2.639256
```

IPr-γ-ts6cc' (transition state involving ring closure)
```
E(ele)        = -2868.797551
E(ele+zpe)    = -2867.872665
H             = -2867.815506
G             = -2867.960535
```
```
C         0.083414   -3.924802   -0.688525
C        -1.156743   -3.742790   -0.185886
C        -0.079789   -1.792479   -0.022719
H         0.576948   -4.786699   -1.108416
H        -2.003435   -4.405361   -0.102297
N         0.730239   -2.706105   -0.603113
N        -1.257235   -2.417691    0.204546
C         2.082130   -2.519359   -1.078071
C        -2.585003   -1.848385    0.366410
C         0.497429   -0.661830    1.927321
C         1.427485    0.291134   -0.239162
H         2.424427    0.071645    0.149189
H         1.387846   -0.063106   -1.267282
H        -0.141884   -1.371696    2.432756
C         0.415203   -0.509047    0.566184
C         1.296106    0.183565    2.795649
O         2.156744    0.974527    2.464190
O         0.997544   -0.048971    4.097081
C         1.714274    0.766064    5.015221
H         1.501413    1.822309    4.832756
H         1.371324    0.471835    6.006859
H         2.791214    0.605720    4.916813
C         1.255814    1.846413   -0.284452
O         0.156969    2.355402    0.410624
C        -1.157093    1.775643    0.220639
O        -1.139173    0.498677   -0.167107
C         3.136253   -2.779047   -0.200224
C         2.251885   -2.095963   -2.409206
C         4.432113   -2.637210   -0.707589
C         3.563922   -1.969145   -2.860054
C         4.642227   -2.245035   -2.021278
H         5.280071   -2.829721   -0.056744
H         3.749893   -1.630236   -3.873372
H         5.654110   -2.135562   -2.397113
C        -3.184681   -1.805440    1.623653
C        -3.251793   -1.525290   -0.827204
C        -4.488509   -1.301875    1.684065
C        -4.555372   -1.049804   -0.710847
C        -5.159956   -0.911379    0.536079
H        -4.980611   -1.224025    2.649129
H        -5.102179   -0.773647   -1.609186
H        -6.169082   -0.517992    0.606845
C         1.065167   -1.740265   -3.297976
H         0.296993   -1.278368   -2.661779
C         0.453520   -2.984461   -3.958311
H         0.089277   -3.713599   -3.229367
H        -0.393608   -2.690274   -4.587757
H         1.195877   -3.477585   -4.595752
C         1.412946   -0.710807   -4.375703
H         1.922033    0.158699   -3.956377
H         2.043157   -1.147931   -5.158339
H         0.490550   -0.363860   -4.850710
C        -2.639357   -1.742369   -2.204671
H        -1.627223   -2.140662   -2.081763
C        -2.501351   -0.449611   -3.010988
H        -3.476720    0.013414   -3.200440
H        -1.878317    0.267264   -2.471731
H        -2.045024   -0.671934   -3.983878
C        -3.441339   -2.798441   -2.976966
H        -4.461915   -2.452298   -3.172254
H        -2.967120   -3.001875   -3.942958
H        -3.507989   -3.740218   -2.421414
C         2.917480   -3.188842    1.244906
H         1.851744   -3.089656    1.475096
H         3.321220   -4.652853    1.455953
H         2.746159   -5.325213    0.810463
H         4.383471   -4.798869    1.231361
C         3.151818   -4.947481    2.496303
H         3.671628   -2.261737    2.205417
H         3.444536   -1.209074    2.011380
H         3.384694   -2.485575    3.238175
C         4.755334   -2.401266    2.123240
C        -2.531500   -2.350333    2.880083
H        -1.529483   -2.707270    2.618946
C        -2.397755   -1.281024    3.968880
H        -1.855852   -0.404976    3.608371
H        -3.385906   -0.953208    4.309985
H        -1.861112   -1.687917    4.832177
C        -3.315182   -3.564095    3.398237
H        -3.402614   -4.342265    2.632498
H        -2.815060   -3.994183    4.271876
H        -4.328215   -3.276682    3.698792
C        -1.773229    1.973738    1.638795
C         1.162231    2.230168   -1.782258
F         0.131291    1.653982   -2.416078
F         2.274361    1.823331   -2.437306
F         1.065562    3.547332   -1.958189
F        -2.958354    1.349934    1.712043
F        -1.015247    1.494298    2.637785
F        -1.973738    3.271111    1.918208
C         2.486262    2.598855    0.243384
C         2.316670    3.741598    1.023270
C         3.778978    2.191337   -0.088994
C         3.422559    4.452310    1.479080
H         1.315313    4.051671    1.295951
C         4.883492    2.903754    0.366852
H         3.936157    1.314443   -0.710290
C         4.710312    4.037317    1.154681
H         3.273671    5.334541    2.094725
```

six-membered intermediate
```
E(ele)        = -2868.810552
E(ele+zpe)    = -2867.885395
H             = -2867.828009
G             = -2867.972821
```
```
C         0.040959   -3.621189   -0.653169
C        -1.281032   -3.383471   -0.558609
C        -0.215460   -1.458923   -0.110203
H         0.597314   -4.514490   -0.887443
H        -2.138408   -4.023087   -0.698594
N         0.697818   -2.419024   -0.426512
N        -1.438123   -2.040464   -0.259831
C         2.093713   -2.326722   -0.825278
C        -2.775454   -1.475805   -0.224843
C        -0.380391   -0.574368    2.042527
C         1.416051    0.472789    0.590240
H         1.745913    0.696434    1.604725
H         2.141373   -0.230182    0.184535
H        -1.423753   -0.833457    2.139422
C         0.009867   -0.152599    0.689878
C         0.359943   -0.523715    3.239837
O         1.548117   -0.240155    3.436647
O        -0.431854   -0.885815    4.313837
C         0.220234   -0.866172    5.571385
H         0.624990    0.125797    5.790889
H        -0.542644   -1.134063    6.304936
H         1.041158   -1.590514    5.602140
C         1.525544    1.765406   -0.243237
O         0.391360    2.613160   -0.191957
C        -0.827786    2.112550    0.300838
O        -0.979256    0.752450    0.094687
C         3.092877   -2.437599    0.154890
C         2.366657   -2.246330   -2.202261
C         4.418097   -2.427554   -0.284198
C         3.711863   -2.255687   -2.584051
C         4.725894   -2.338799   -1.639078
H         5.219599   -2.491947    0.444774
H         3.964754   -2.182072   -3.637942
H         5.764266   -2.333701   -1.958367
C        -3.606608   -1.779351    0.862063
C        -3.223600   -0.791430   -1.370594
C        -4.929060   -1.321605    0.798181
C        -4.555078   -0.380562   -1.388513
C        -5.400435   -0.634091   -0.310975
H        -5.599710   -1.527710    1.627925
H        -4.932575    0.162364   -2.249816
H        -6.433286   -0.297499   -0.341437
C         1.281644   -2.185413   -3.268356
H         0.353893   -1.844540   -2.794331
C         1.031198   -3.573255   -3.881386
H         0.702315   -4.307571   -3.142247
H         0.259139   -3.506058   -4.656352
H         1.949218   -3.949803   -4.347336
C         1.615896   -1.207235   -4.404280
H         2.001865   -0.256475   -4.035092
H         2.357760   -1.635075   -5.088149
H         0.713265   -1.006720   -4.991810
C        -2.317651   -0.556351   -2.568039
H        -1.305132   -0.402722   -2.187537
C        -2.679137    0.692414   -3.376346
H        -3.609559    0.554731   -3.940381
H        -2.786007    1.574300   -2.738903
H        -1.883915    0.893178   -4.102264
C        -2.319310   -1.786434   -3.490540
H        -3.329040   -1.968051   -3.877700
H        -1.653577   -1.617662   -4.345728
H        -1.983374   -2.693988   -2.977649
C         2.748881   -2.581886    1.626204
H         1.809764   -2.050908    1.815740
C         2.527933   -4.062169    1.971955
H         1.715696   -4.503171    1.384183
H         3.440078   -4.641734    1.784622
H         2.267260   -4.161150    3.030961
C         3.804504   -1.971936    2.549514
H         4.024827   -0.935185    2.274267
H         3.417786   -1.949442    3.570750
H         4.734796   -2.553055    2.540678
C        -3.171912   -2.625303    2.050199
H        -2.088772   -2.777280    1.998926
C        -3.481988   -1.940500    3.388416
H        -3.077674   -0.925490    3.433542
H        -4.562718   -1.893347    3.565031
H        -3.029629   -2.508912    4.206664
C        -3.849649   -4.002920    1.997268
H        -3.625305   -4.538104    1.068217
H        -3.512648   -4.620507    2.836557
H        -4.939011   -3.903154    2.066498
C        -0.882592    2.567511    1.797244
C         1.676101    1.428720   -1.736795
F         0.670300    0.633944   -2.160892
F         2.820012    0.768932   -1.990356
F         1.663562    2.522091   -2.505563
F         0.237850    2.296156    2.470712
F        -1.030034    3.905689    1.830339
F        -1.918463    2.033690    2.451226
C         2.746588    2.572206    0.200061
C         2.636819    3.941618    0.439751
C         3.983172    1.941694    0.375429
C         3.751090    4.673121    0.848673
H         1.675995    4.429554    0.320029
C         5.093330    2.675061    0.782593
H         4.088375    0.874320    0.176900
C         4.981066    4.044260    1.019652
H         3.651149    5.737746    1.038961
```

transition state involving release of **IPr**
```
E(ele)        = -2868.794458
E(ele+zpe)    = -2867.872309
H             = -2867.814913
G             = -2867.961783
```
```
C        -0.020777   -3.743592   -0.643653
C        -1.337763   -3.492028   -0.495659
C        -0.247743   -1.505869   -0.295436
H         0.517899   -4.657118   -0.843243
H        -2.199268   -4.138607   -0.548598
N         0.633001   -2.520292   -0.529822
N        -1.463252   -2.124321   -0.289668
C         2.008221   -2.396776   -0.965031
C        -2.766215   -1.499266   -0.234273
C        -0.554889   -0.369339    2.164070
C         1.387979    0.552540    0.812959
H         1.762609    0.790611    1.810072
H         2.026878   -0.246125    0.430002
H        -1.631931   -0.406469    2.254753
C        -0.052235    0.093850    0.955991
C         0.217840   -0.753738    3.306874
O         1.435617   -0.727209    3.450280
O        -0.591906   -1.168179    4.325597
C         0.077132   -1.498892    5.534570
H         0.618629   -0.633861    5.927011
H        -0.704947   -1.804698    6.230501
H         0.787141   -2.315874    5.375827
C         1.577339    1.800735   -0.078596
O         0.489606    2.711766   -0.054183
C        -0.781388    2.274484    0.358899
O        -0.966443    0.900737    0.235576
C         3.045173   -2.499724   -0.023855
C         2.243544   -2.261449   -2.344588
C         4.356296   -2.429959   -0.502443
C         3.573041   -2.218571   -2.771711
C         4.619623   -2.293292   -1.861758
H         5.183133   -2.490430    0.198198
H         3.789209   -2.107638   -3.830431
H         5.646958   -2.245368   -2.211973
C        -3.594811   -1.739011    0.873620
C        -3.193284   -0.762149   -1.356977
C        -4.887911   -1.202396    0.837713
C        -4.494759   -0.262513   -1.343767
C        -5.337448   -0.477144   -0.256816
H        -5.553440   -1.365988    1.680650
H        -4.849714    0.315896   -2.191280
H        -6.347716   -0.076469   -0.264720
C         1.117607   -2.194966   -3.363189
H         0.204241   -1.900607   -2.837220
C         0.881476   -3.573651   -3.998976
H         0.625871   -4.330101   -3.251040
H         0.061682   -3.522154   -4.724579
H         1.783248   -3.907573   -4.525938
C         1.372756   -1.158432   -4.464156
H         1.682810   -0.195713   -4.052573
H         2.145025   -1.498514   -5.163508
H         0.456610   -1.004431   -5.045059
C        -2.304763   -0.577380   -2.577009
H        -1.277659   -0.463788   -2.220752
C        -2.624077    0.673905   -3.397781
H        -3.586648    0.590363   -3.916827
H        -2.639344    1.574027   -2.777022
H        -1.851449    0.805810   -4.162951
C        -2.388701   -1.823834   -3.813112
H        -1.755145   -1.699482   -4.359427
H        -2.065255   -2.731767   -2.952072
H        -3.420431   -1.974670   -3.813112
C         2.761745   -2.723271    1.450935
H         1.794243   -2.266908    1.686451
C         2.663344   -4.227343    1.747326
H         1.873846   -4.709244    1.162122
H         3.612023   -4.726146    1.515083
H         2.442522   -4.386198    2.808420
C         3.801645   -2.076674    2.367546
H         3.927869   -1.011694    2.145096
H         3.464026   -2.147598    3.403872
H         4.775433   -2.573911    2.286841
C        -3.176954   -2.584452    2.069224
H        -2.086379   -2.694837    2.051665
C        -3.561804   -1.937189    3.407813
H        -3.246119   -0.892754    3.473799
H        -4.645089   -1.979014    3.568726
H        -3.080610   -2.477902    4.227978
C        -3.817735   -3.979761    1.995727
H        -3.554533   -4.518322    1.081032
H        -3.500595   -4.586848    2.850563
H        -4.910419   -3.896203    2.026241
H        -0.920081    2.797742    1.826697
C         1.716369    1.435720   -1.569096
F         0.612171    0.836973   -2.043297
F         2.746041    0.602299   -1.789333
F         1.918526    2.529516   -2.317244
F         0.144758    2.507857    2.584047
F        -1.021459    4.136958    1.806167
F        -2.010983    2.316080    2.432290
C         2.836838    2.549272    0.355568
C         2.787092    3.911505    0.648673
C         4.049296    1.862284    0.480814
C         3.938266    4.580513    1.062677
H         1.846302    4.443780    0.564524
C         5.196322    2.534434    0.892349
H         4.105145    0.799477    0.257917
C         5.144483    3.896841    1.184398
H         3.886556    5.640393    1.294329
```

γ-6cc'
```
E(ele)        = -1709.259473
E(ele+zpe)    = -1708.914312
H             = -1708.886767
G             = -1708.972805
```
```
C        -1.382880    2.157214   -0.873780
C        -1.281714    2.486335   -1.901847
C        -0.495020    0.607498    0.959908
C        -0.555182    1.209049   -0.408764
C        -0.325364   -0.906111    0.782072
C        -1.384109    0.861807    1.532263
C         1.352430   -0.139864   -0.766633
C         0.324490    0.662511   -1.300150
H         0.375954    1.002953    1.496817
C        -2.467406    2.748088   -0.077170
O        -2.800634    2.444641    1.052559
C        -3.096697    3.705404   -0.780219
C        -4.192525    4.333064   -0.113373
```

```
H        -4.961752    3.594916    0.125580
H        -3.853056    4.808203    0.809740
H        -4.574318    5.074523   -0.813213
O         0.865275   -1.180959    0.041208
C         1.937414   -0.852957   -2.006145
C         2.422669    0.687011   -0.069821
C         3.249339    0.084482    0.878887
C         2.601681    2.029154   -0.408744
C         4.246411    0.832198    1.499992
H         3.102561   -0.960653    1.132497
C         3.597533    2.773834    0.219408
H         1.963045    2.487684   -1.158348
C         4.419166    2.176691    1.173908
H         4.886610    0.364229    2.241664
H         3.731706    3.819838   -0.039081
C         5.195099    2.758132    1.663204
C        -1.525445   -1.576075    0.117260
C        -2.824141   -1.100115    0.317260
C        -1.322229   -2.708472   -0.674405
C        -3.905293   -1.749785   -0.275028
H        -3.011427   -0.221387    0.928546
C        -2.405197   -3.354786   -1.264105
H        -0.314207   -3.076838   -0.831927
C        -3.699257   -2.877041   -1.066489
H        -4.909375   -1.367699   -0.116748
H        -2.234437   -4.232487   -1.880453
H        -4.543132   -3.379976   -1.529683
H        -0.070036   -1.549309    2.154474
F         1.001655   -1.547300   -2.654082
F         2.461079    0.036208   -2.855557
F         2.903228   -1.699405   -1.635403
F         0.178516   -2.857485    2.047368
F        -1.134624   -1.389137    2.952542
F         0.982711   -0.989287    2.771916
```

[2 + 2] cycloaddition
transition state involving a C–O ring closure
```
E(ele)        = -2186.395589
E(ele+zpe)    = -2185.591948
H             = -2185.544191
G             = -2185.672528
```
```
C        -2.377311    2.014035   -1.223172
C        -1.223032    2.576775   -1.647644
C        -0.685891    0.854311   -0.338721
C        -3.410786    2.262528   -1.402673
H        -1.026547    3.416770   -2.294475
C        -2.029328    0.947597   -0.412243
N        -0.185210    1.851805   -1.089885
C        -3.009329    0.165402    0.309141
C         1.206057    2.183441   -1.318771
C         0.647373    0.490164    1.617721
C        -0.368157   -1.573517    0.482330
C        -0.443926   -2.019259    1.472559
H        -1.299462   -1.711003   -0.071925
C         0.917352    1.535506    1.575427
C         0.068130   -0.101133    0.510084
C         1.116436   -0.221506    2.787099
O         0.853673   -1.353710    3.154051
C         1.914290    0.590145    3.542295
C         2.430149   -0.027003    4.712878
H         3.012393   -0.915002    4.453003
C         3.063174    0.720742    5.191516
C         1.620508   -0.327484    5.383817
H         0.855793   -1.964911   -0.366445
O         1.194538   -0.700595   -0.829459
C        -3.256343    0.477480    1.651816
C        -3.702224   -0.832658   -0.393913
C        -4.260965   -0.248790    2.296631
C        -4.700413   -1.518945    0.296619
C        -4.980015   -1.229273    1.627560
H        -4.479808   -0.035661    3.338870
H        -5.257858   -2.299613   -0.211884
H        -5.758983   -1.778228    2.147585
C         1.800965    3.136989   -0.482245
C         1.853171    1.594642   -2.412955
C         3.132128    3.467259   -0.744203
C         3.180601    1.964027   -2.628925
C         3.817166    2.879754   -1.799602
H         3.633583    4.198175   -0.117275
H         3.723303    1.522969   -3.459135
H         4.853679    3.145286   -1.984767
C        -3.391844   -1.174629   -1.842195
H        -2.408613   -0.759222   -2.090890
C        -4.433484   -0.549180   -2.779776
H        -4.469495    0.540523   -2.684285
H        -4.202349   -0.792069   -3.821549
H        -5.432506   -0.937521   -2.552386
C        -3.313438   -2.687823   -2.073759
H        -2.632453   -3.172295   -1.369505
H        -4.299042   -3.156512   -1.982510
H        -2.941336   -2.884930   -3.082922
C         1.142868    0.661145   -3.375724
H         0.285242    0.228793   -2.855565
C         2.026948   -0.511448   -3.802541
H         2.829599   -0.190957   -4.476698
H         2.457441   -0.991372   -2.921871
C         1.423015   -1.252011   -4.335563
H         0.652511    1.449280   -4.598108
H         1.496759    1.901096   -5.131265
H         0.128863    0.784748   -5.293225
C        -0.034054    2.256047   -4.317684
H        -1.661164    1.887987    1.802384
C        -3.430705    2.784662    2.610301
H        -3.787091    3.184482    1.654964
C        -4.307168    2.515327    3.210026
H        -2.892057    3.579502    3.136170
C        -1.957842    1.054999    3.733693
H        -1.412648    0.117290    3.595265
C        -1.265009    1.790720    4.154991
C        -2.756894    0.890811    4.465363
H         1.034661    3.873215    0.606767
C         0.114973    3.317370    0.825885
H         1.823528    3.998187    1.915687
C         2.186743    3.030942    2.275097
H         2.683382    4.665533    1.796184
```

```
H    1.182050   4.430970   2.690089
C    0.622325   5.262875   0.100278
H    0.007917   5.197023  -0.803507
H    0.050216   5.796125   0.866401
H    1.508739   5.858977  -0.141788
C    0.454131  -2.848964  -1.543536
F   -0.381081  -2.191585  -2.379360
F   -0.211623  -3.957248  -1.148031
F    1.495576  -3.253760  -2.276242
C    1.958756  -2.624073   0.456046
C    1.771771  -3.858428   1.082185
C    3.153214  -1.934131   0.644057
C    2.769877  -4.393580   1.887812
H    0.836436  -4.395622   0.954101
C    4.151447  -2.469727   1.455630
H    3.266608  -0.968825   0.162012
C    3.962594  -3.699111   2.079850
H    2.612783  -5.350844   2.376332
H    5.078548  -1.922579   1.603144
H    4.738332  -4.114918   2.716480
```

four-membered intermediate

```
E(ele)      = -2186.398999
E(ele+zpe)  = -2185.594999
H           = -2185.547841
G           = -2185.675390
C   -2.300076   0.320762  -2.215087
C   -1.507300   1.386838  -2.458430
C   -0.661050   0.302231  -0.699096
H   -3.196506  -0.036860  -2.695729
H   -1.559752   2.168348  -3.199602
N   -1.777201  -0.334753  -1.107878
N   -0.502769   1.371363  -1.506814
C   -2.440597  -1.469100  -0.496433
C    0.325378   2.525068  -1.228204
C    0.010293   0.859303   1.606301
C    0.483562  -1.531462   0.743757
H    0.342169  -1.803414   1.786497
H   -0.051398  -2.220895   0.088932
H    0.388430   1.870704   1.530471
C    0.253064  -0.027058   0.466168
C   -0.514863   0.408043   2.824080
O   -0.993058  -0.701387   3.105702
O   -0.504183   1.408366   3.783371
C   -1.014088   1.024248   5.044218
H   -0.506847   0.132806   5.422699
H   -0.835611   1.870401   5.710806
H   -2.087737   0.811641   4.998423
C    1.930878  -1.253922   0.290682
O    1.627873   0.085731  -0.085673
C   -3.222749  -1.248564   0.651284
C   -2.313527  -2.717351  -1.121682
C   -3.863236  -2.365427   1.190705
C   -2.992248  -3.792455  -0.546630
C   -3.751195  -3.619676   0.602776
H   -4.456413  -2.249865   2.090577
H   -2.912717  -4.776042  -1.000186
H   -4.260866  -4.469283   1.046993
C   -0.253535   3.534564  -0.440508
C    1.610595   2.601517  -1.772513
C    0.526876   4.662754  -0.189712
C    2.344836   3.756143  -1.492674
C    1.812924   4.770866  -0.707100
H    0.121788   5.466030   0.418273
H    3.347203   3.860203  -1.895932
H    2.404562   5.656736  -0.496689
C   -1.490010  -2.922795  -2.381828
H   -0.862123  -2.039564  -2.533691
C   -2.407852  -3.074942  -3.602320
H   -3.053710  -2.201743  -3.739515
H   -1.815144  -3.207649  -4.513082
C   -3.055575  -3.951043  -3.487190
C   -0.555085  -4.132155  -2.271273
H    0.049952  -4.097340  -1.362294
H   -1.118704  -5.071040  -2.270640
H    0.125829  -4.153383  -3.127508
C    2.165175   1.522414  -2.683363
H    1.602280   0.603541  -2.500502
C    3.634967   1.213850  -2.392232
H    4.284318   2.058690  -2.646298
H    3.775821   0.963691  -1.337093
C    3.958061   0.357953  -2.991420
H    1.969885   1.932022  -4.149272
H    2.513235   2.858068  -4.368709
C    2.344056   1.150695  -4.818549
H    0.912672   2.102432  -4.380725
C   -3.433413   0.138245   1.239079
C   -2.464836   0.653391   1.237093
C   -4.429669   0.942217   0.387265
C   -4.091239   1.090814  -0.642458
C   -5.401588   0.436198   0.356751
C   -4.579003   1.933031   0.831818
C   -3.921689   0.114780   2.688711
C   -3.285180  -0.527251   3.300288
C   -3.868055   1.130896   3.094725
H   -4.967001  -0.211209   2.757011
H   -1.685356   3.458609   0.072054
C   -2.027529   2.421157  -0.003046
C   -1.830098   3.864473   1.541763
C   -1.213660   3.245760   2.198759
H   -1.575976   4.918859   1.695820
C   -2.875678   3.737738   1.845302
C   -2.596754   4.324200  -0.810732
C   -2.551335   4.026058  -1.863338
H   -3.636677   4.242312  -0.477458
H   -2.301359   5.377670  -0.749919
C    2.299467  -2.023995  -0.971589
F    1.400487  -1.791616  -1.952840
F    2.299919  -3.352273  -0.761304
F    3.498423  -1.686726  -1.449664
C    3.015268  -1.338504   1.344562
C    3.462963  -2.571776   1.826815
C    3.543332  -0.160295   1.870287
C    4.441977  -2.620439   2.813002
```

```
H    3.045846  -3.495433   1.439178
C    4.524829  -0.215036   2.856756
H    3.161121   0.789282   1.512707
C    4.979144  -1.442572   3.327651
H    4.783527  -3.582288   3.183199
H    4.928388   0.707606   3.262586
H    5.742157  -1.484563   4.099161
```

IPr-γ-ts4c2′ (transition state involving release of **IPr**)

```
E(ele)      = -2186.373016
E(ele+zpe)  = -2185.569652
H           = -2185.522275
G           = -2185.649206
C   -2.474763  -0.229784  -2.166352
C   -1.738330   0.803149  -2.631841
C   -0.845121   0.183338  -0.640394
H   -3.344926  -0.727237  -2.565629
H   -1.820771   1.395816  -3.529746
N   -1.918556  -0.587613  -0.942502
N   -0.752816   1.041131  -1.683006
C   -2.493866  -1.580942  -0.072283
C    0.119764   2.189269  -1.717518
C    0.501228   1.498351   1.592459
C    0.687392  -1.083942   1.391014
H    0.845011  -1.144898   2.466004
H   -0.111314  -1.757560   1.076578
H    0.928356   2.418698   1.214537
C    0.604838   0.334154   0.857459
C   -0.112871   1.457854   2.880727
O   -0.633447   0.489683   3.427537
O   -0.053579   2.668274   3.514801
C   -0.620439   2.681567   4.814534
H   -0.109392   1.972446   5.471144
H   -0.494629   3.699116   5.185877
H   -1.681526   2.417537   4.783753
C    1.962631  -1.136733   0.517713
O    1.685339   0.157388  -0.040869
C   -3.089182  -1.150551   1.132035
C   -2.466676  -2.925175  -0.469583
C   -3.632875  -2.134974   1.956170
C   -3.043901  -3.865369   0.389632
C   -3.611139  -3.478158   1.592832
H   -4.083163  -1.849592   2.899649
H   -3.040102  -4.914317   0.107355
H   -4.043542  -4.222600   2.254536
C   -0.323529   3.359036  -1.078420
C    1.348541   2.098292  -2.381896
C    0.510072   4.476208  -1.135926
C    2.143989   3.246081  -2.413790
C    1.730620   4.421124  -1.799449
H    0.204880   5.397464  -0.649492
H    3.102642   3.217371  -2.922055
H    2.367027   5.300466  -1.831343
C   -1.880841  -3.391415  -1.792542
H   -1.317521  -2.565469  -2.235343
C   -3.004014  -3.785279  -2.762163
H   -3.703782  -2.962188  -2.938136
H   -2.587249  -4.093356  -3.726579
C   -3.580436  -4.625176  -2.358434
C   -0.913706  -4.567313  -1.613151
H   -0.149617  -4.349900  -0.864785
H   -1.444317  -5.475786  -1.308699
H   -0.412215  -4.783168  -2.562028
C    1.786370   0.823997  -3.081071
H    1.254382  -0.011230  -2.616167
C    3.283905   0.551792  -2.926171
H    3.888534   1.298763  -3.451499
H    3.570914   0.544231  -1.871137
C    3.526710  -0.425491  -3.352717
C    1.404725   0.882002  -4.566680
H    1.909981   1.720466  -5.059402
H    1.700662  -0.041200  -5.075428
C    0.326509   1.014322  -4.701733
C   -3.190292   0.325466   1.500320
C   -2.196310   0.771250   1.376212
C   -4.181490   1.049403   0.573750
C   -3.884391   1.019989  -0.478667
C   -5.177063   0.599558   0.662288
C   -4.260915   2.102673   0.867489
C   -3.606837   0.563484   2.951793
C   -2.945648   0.045560   3.648612
C   -3.538958   1.635353   3.165898
H   -4.646232   0.258162   3.123418
C   -1.672193   3.424233  -0.381277
C   -1.936606   2.406452  -0.075964
C   -1.665639   4.283888   0.884787
H   -0.878938   3.979850   1.580180
H   -1.543921   5.347645   0.651533
C   -2.628405   4.176165   1.397122
H   -2.746021   3.928423  -1.356533
C   -2.819887   3.293478  -2.244784
H   -3.727061   3.946952  -0.869687
H   -2.508962   4.946409  -1.684473
H    1.923186  -2.168630  -0.598788
F    0.805690  -2.053024  -1.337691
F    1.935822  -3.415829  -0.099246
F    2.960752  -2.047707  -1.430366
C    3.280595  -1.176573   1.258414
C    3.612918  -2.283908   2.042871
C    4.157386  -0.096956   1.177807
C    4.821789  -2.313924   2.728530
H    2.923425  -3.118931   2.123330
C    5.367512  -0.131615   1.866728
H    3.873634   0.771865   0.593530
C    5.703601  -1.238867   2.639256
H    5.073240  -3.176123   3.338378
H    6.045458   0.714018   1.803801
H    6.645506  -1.262221   3.178674
```

γ-4c′

```
E(ele)      = -1026.830835
E(ele+zpe)  = -1026.607191
H           = -1026.590212
G           = -1026.652125
C   -0.693038   0.434418  -0.040105
C    0.548066   0.105688   0.824843
H    0.917391   0.893417   1.483896
C    0.491305  -0.840712   1.365174
C    1.226075   0.023315  -0.511679
C    2.455730  -0.216227  -0.971421
F    2.682775  -0.205634  -2.030476
O    0.103100   0.296804  -1.244573
O    3.507753  -0.493443   0.011454
O    3.351704  -0.537452   1.216427
C    4.697843  -0.699568  -0.580097
C    5.779664  -0.977767   0.308279
H    6.655284  -1.103121  -0.327110
C    5.922396  -0.148537   1.005044
C    5.579356  -1.890276   0.874797
C   -1.866520  -0.506764   0.000237
C   -2.440816  -0.849036   1.225961
C   -2.390367  -1.021602  -1.185555
C   -3.538888  -1.704046   1.264481
H   -2.030996  -0.446795   2.149591
C   -3.487035  -1.880033  -1.142518
H   -1.932391  -0.753887  -2.132918
C   -4.062669  -2.220803   0.079784
H   -3.982610  -1.969351   2.219394
H   -3.891183  -2.282415  -2.066564
H   -4.917481  -2.889876   0.110485
C   -1.129966   1.895336   0.059593
F   -0.081353   2.724873  -0.036075
F   -1.992227   2.217663  -0.909152
F   -1.722303   2.126874   1.242394
```

[3 + 2] cycloaddition
IPr-γ-ts5c′

```
E(ele)      = -2186.399334
E(ele+zpe)  = -2185.594852
H           = -2185.547321
G           = -2185.675079
C   -2.042994   2.196951   1.476224
C   -2.726843   1.057217   1.703271
C   -1.035491   0.557160   0.315495
H   -2.203139   3.207555   1.812908
C   -3.601052   0.846541   2.298976
N   -1.001993   1.884116   0.617494
N   -2.110225   0.048556   0.978778
C   -0.263703   2.917417  -0.074954
C   -2.759043  -1.242825   0.853410
C   -0.352222  -1.344306  -1.049158
H    1.343219   0.292840  -0.528306
H    1.767729   0.373423  -1.526650
C    1.536672   1.220798   0.011786
C   -1.282777  -1.866834  -0.856863
C   -0.095212  -0.093670  -0.562781
O    0.507983  -2.011076  -2.061306
O    1.307531  -1.469685  -2.791975
H    0.208417  -3.318841  -2.140259
C    1.081109  -4.059342  -2.986271
H    2.112783  -3.955387  -2.639307
H    0.753161  -5.096134  -2.918424
H    1.017264  -3.701513  -4.016840
C    2.099521  -0.977727   0.196623
O    1.364893  -2.092331   0.188354
C   -0.612888   3.199715  -1.404283
C    0.716551   3.635209   0.628408
C    0.061676   4.249987  -2.031372
C    1.340880   4.688049  -0.041650
C    1.020129   4.993981  -1.358379
H   -0.178192   4.489827  -3.063504
H    2.105165   5.263605   0.471159
H    1.526593   5.810284  -1.863889
C   -3.900751  -1.301001   0.040117
C   -2.253270  -2.346691   1.556587
C   -4.576395  -2.522328  -0.023315
C   -2.969658  -3.539129   1.458144
C   -4.123538  -3.625533   0.686880
H   -5.459486  -2.610783  -0.648991
H   -2.603412  -4.417433   1.978679
H   -4.661434  -4.566569   0.623014
C    1.125818   3.286460   2.050359
H    0.831520   2.249365   2.243798
C    0.430101   4.198475   3.071033
H   -0.659234   4.109655   3.041423
H    0.758992   3.949383   4.084768
H    0.685577   5.246373   2.877797
C    2.644922   3.378788   2.243750
H    3.185134   2.872702   1.440992
H    2.976269   4.422003   2.285043
H    2.925317   2.903309   3.187495
C   -0.953977  -2.244929   2.326664
H   -0.289838  -1.618257   1.732535
C   -0.218243  -3.576697   2.455202
H   -0.723312  -4.269398   3.139907
H   -0.099587  -4.046760   1.475139
C    0.786265  -3.382201   2.839666
C   -1.162805  -1.590912   3.697308
H   -1.810354  -2.209094   4.329862
H   -0.197275  -1.474474   4.198296
C   -1.616431  -0.596918   3.613573
C   -1.684462   2.449188  -2.178512
H   -2.109245   1.671712  -1.536981
C   -2.832793   3.391117  -2.561398
H   -3.266706   3.866817  -1.675795
C   -2.490237   4.182409  -3.236470
H   -3.622974   2.834432  -3.076361
H   -1.093964   1.754249  -3.411630
H   -0.323748   1.028259  -3.131193
C   -1.883454   1.225100  -3.955554
F   -0.649032   2.482835  -4.097756
H   -4.347845  -0.143510  -0.840162
H   -3.879272   0.779517  -0.481657
H   -3.863503  -0.380586  -2.277465
H   -2.773111  -0.480790  -2.319539
C   -4.302232  -1.298463  -2.683843
H   -4.156203   0.454580  -2.923988
```

```
C   -5.861991   0.081744  -0.802536
H   -6.223161   0.202172   0.223434
H   -6.117547   0.984513  -1.366014
C   -6.406419  -0.751619  -1.257838
C    2.296829  -0.524341   1.656248
H    1.128781  -0.085392   2.206843
F    3.158179   0.506381   1.796454
F    2.735696  -1.510402   2.440770
C    3.485817  -1.162135  -0.444994
C    3.922334  -2.465646  -0.675543
C    4.319945  -0.098434  -0.795143
C    5.163087  -2.705209  -1.259136
H    3.257002  -3.274538  -0.391320
C    5.561248  -0.335112  -1.379413
H    3.999572   0.925736  -0.619692
C    5.986771  -1.639981  -1.614544
H    5.489889  -3.726480  -1.435734
H    6.196290   0.502523  -1.653821
H    6.954466  -1.823489  -2.072521
```

IPr-γ-5c′

```
E(ele)      = -2186.443985
E(ele+zpe)  = -2185.638336
H           = -2185.592225
G           = -2185.715770
C   -2.158588   2.765832   0.503821
C   -3.037785   1.771586   0.677864
C   -1.034901   0.804880   0.132979
C   -2.273806   3.836924   0.552838
H   -4.080750   1.776232   0.954164
N   -0.916291   2.195594   0.192232
N   -2.368483   0.560344   0.456780
C    0.120573   2.961461  -0.428485
C   -2.967526  -0.703841   0.747557
C   -0.134614  -1.571403  -0.194835
H    1.433523   0.197880  -0.194571
H    1.854584   0.276958  -1.203108
C    1.712189   1.097569   0.356628
C   -1.047789  -2.028072   0.185878
C   -0.049978  -0.081285  -0.189899
O    0.176970  -2.197309  -1.565429
O    0.496693  -1.603024  -2.565536
H    0.097658  -3.534120  -1.497470
C    0.537651  -4.217192  -2.670331
H    1.590725  -3.989839  -2.858327
H    0.402542  -5.278234  -2.464733
H   -0.054860  -3.912344  -3.535797
C    2.010053  -1.074102   0.507152
O    0.934582  -1.987562   0.674130
C    0.103238   3.121478  -1.820609
C    1.104670   3.544630   0.387374
C    1.114299   3.897101  -2.395582
C    2.084500   4.321131  -0.229283
C    2.090051   4.495537  -1.610278
H    1.131318   4.034931  -3.473591
H    2.860517   4.784928   0.372219
H    2.864910   5.097639  -2.075631
C   -3.849435  -1.253059  -0.198402
C   -2.669989  -1.339689   1.964338
C   -4.453371  -2.473103   0.109239
C   -3.293831  -2.561637   2.223156
C   -4.178554  -3.120611   1.308465
H   -5.143560  -2.926153  -0.594683
H   -3.084137  -3.083917   3.151266
H   -4.654989  -4.071159   1.529285
C    1.097168   3.322300   1.890529
H    0.564771   2.382929   2.079125
C    0.333033   4.449267   2.597654
H   -0.703028   4.510055   2.251627
H    0.320594   4.283804   3.679891
H    0.813104   5.415373   2.404422
C    2.503235   3.179999   2.478231
H    3.090621   2.428214   1.944034
H    3.050171   4.128777   2.451993
H    2.435316   2.869007   3.525260
C   -1.714709  -0.715268   2.968901
H   -1.036699  -0.051426   2.424081
C   -0.833467  -1.746830   3.677386
H   -1.418081  -2.411803   4.322364
H   -0.275138  -2.349672   2.954264
C   -0.106634  -1.229572   4.310235
C   -2.501577   0.130079   3.979139
H   -3.207789  -0.495587   4.537024
H   -1.819494   0.598456   4.696365
H   -3.068469   0.921835   3.478364
C   -0.965797   2.493405  -2.698441
H   -1.660302   1.938960  -2.057604
C   -1.776601   3.573430  -3.424295
H   -2.222544   4.278305  -2.715241
H   -1.147387   4.143359  -4.116893
C   -2.582539   3.113240  -4.005453
H   -0.349918   1.497555  -3.686325
H    0.149468   0.677282  -3.162063
C   -1.129923   1.065881  -4.322928
F    0.376166   1.993229  -4.341032
C   -4.070409  -0.570126  -1.539105
H   -4.097528   0.512958  -1.638510
C   -2.885477  -0.862165  -2.472070
H   -1.940621  -0.479426  -2.072234
H   -2.779780  -1.943962  -2.622708
C   -3.046010  -0.398280  -3.451832
C   -5.385124  -0.966485  -2.212550
H   -6.239570  -0.849112  -1.538491
H   -5.553049  -0.338450  -3.092442
C   -5.361004  -2.006081  -2.556963
C    2.439885  -0.723957   1.931010
H    1.486261  -0.027191   2.577017
F    3.545461   0.041750   1.932294
F    2.698922  -1.814330   2.653652
C    3.160498  -1.726826  -0.244527
C    3.175328  -3.108068  -0.438032
C    4.209982  -0.952265  -0.743901
C    4.222877  -3.704057  -1.138086
H    2.354995  -3.703044  -0.050134
```

```
C       5.257457   -1.550432   -1.435407
H       4.206968    0.124011   -0.594108
C       5.265151   -2.928983   -1.636913
H       4.224396   -4.779870   -1.288352
H       6.066686   -0.938104   -1.821383
H       6.080930   -3.395873   -2.180471
```

γ-5c

```
  E(ele)      = -1026.844345
  E(ele+zpe)  = -1026.619735
  H           = -1026.602270
  G           = -1026.665528
C      -1.708644    0.090044    0.711650
C       0.135150    1.125078    1.631418
C      -1.318384    0.773096    1.784612
C       0.455438    0.540852    0.222222
H       0.312397    2.205373    1.675756
C      -3.064005   -0.458122    0.452907
O      -3.981791   -0.331905    1.229023
O      -3.140419   -1.092966   -0.717222
C      -4.426951   -1.634077   -1.029058
H      -4.718404   -2.369716   -0.275929
H      -5.172075   -0.836104   -1.061488
H      -4.316635   -2.101082   -2.005958
H       0.755133    0.654478    2.401377
O      -0.735954   -0.115331   -0.231615
C       0.672306    1.684732   -0.779123
C       1.629519   -0.419641    0.185196
C       2.828748   -0.078971    0.816996
C       1.528637   -1.633679   -0.494854
C       3.915022   -0.948184    0.774937
H       2.920035    0.869823    1.340350
C       2.616511   -2.504591   -0.530007
H       0.596785   -1.892276   -0.986529
C       3.810032   -2.165231    0.102592
H       4.842515   -0.674942    1.269308
H       2.528536   -3.451088   -1.055340
H       4.656226   -2.845361    0.073425
F      -0.388164    2.507749   -0.800954
F       1.743011    2.425110   -0.437971
F       0.864136    1.235678   -2.021119
H      -1.950315    1.017839    2.626996
```

50

9.6.2 Cycloadditions starting from Dabco-3′

Dabco-γ-ts4c′

	E(ele)	− -1371.975027	
	E(ele+zpe)	− -1371.563509	
	H	− -1371.538984	
	G	− -1371.615788	

```
C    0.008763   -1.865295   -0.417883
C   -0.097017    0.449197   -1.342095
H    0.860110    0.291519   -1.823960
H   -0.733829    1.189267   -1.805088
H   -0.464542   -2.644548    0.164727
C   -0.639013   -0.696993   -0.746517
C    1.372533   -2.165642   -0.824753
O    2.101961   -1.513208   -1.546917
O    1.771340   -3.352453   -0.289782
C    3.096608   -3.745205   -0.630395
H    3.812693   -2.983898   -0.310654
H    3.270336   -4.684362   -0.104866
H    3.189535   -3.888702   -1.710359
C   -2.915696   -1.702558   -0.909811
C   -2.132848   -0.841654    1.256869
C   -2.750183    0.695623   -0.545457
C   -4.287264   -1.776841   -0.191788
C   -2.360777   -2.638019   -0.854591
H   -2.996417   -1.414926   -1.961916
C   -3.575938   -0.591772    1.747729
H   -1.405663   -0.151207    1.686471
H   -1.819748   -1.870229    1.433658
H   -2.208739    1.445946    0.036280
H   -2.621810    0.889709   -1.609682
C   -4.251759    0.593247   -0.180576
H   -4.334979   -2.657137    0.456657
H   -5.089225   -1.864986   -0.930562
H   -3.648410    0.375149    2.253983
H   -3.865127   -1.367816    2.462878
H   -4.555913    1.483829    0.375820
H   -4.868798    0.537482   -1.083055
N   -2.083342   -0.630225   -0.249135
N   -4.519647   -0.591524    0.630398
C    0.507839    1.623304    0.424784
O   -0.402677    1.593632    1.279729
C    0.555750    2.942791   -0.383845
F   -0.687584    3.392378   -0.624421
F    1.178156    2.882916   -1.575876
F    1.189107    3.887185    0.335463
C    1.800789    0.901034    0.652591
C    2.997110    1.201075   -0.014123
C    1.792565   -0.126993    1.601248
C    4.150471    0.477441    0.258273
H    3.037128    1.994991   -0.751219
C    2.946341   -0.866637    1.856764
H    0.877459   -0.325617    2.149302
C    4.128032   -0.565302    1.186251
H    5.071469    0.723054   -0.262133
H    2.919340   -1.673420    2.584374
H    5.032226   -1.132826    1.390762
```

Dabco-γ-4c′

	E(ele)	− -1371.987681	
	E(ele+zpe)	− -1371.573358	
	H	− -1371.549075	
	G	− -1371.625589	

```
C   -0.134685   -1.880318   -0.582222
C   -0.044151    0.541673   -1.238656
H    0.782721    0.233798   -1.878740
H   -0.708578    1.165640   -1.837643
H   -0.616783   -2.695553   -0.052865
C   -0.722447   -0.688932   -0.740593
C    1.233989   -2.218727   -1.064581
O    1.759404   -1.816777   -2.075551
O    1.789228   -3.116041   -0.240392
C    3.098633   -3.557802   -0.609923
H    3.772699   -2.702496   -0.679109
H    3.412438   -4.233557    0.183962
H    3.060902   -4.075327   -1.571829
C   -3.034243   -1.660810   -0.758349
C   -2.119209   -0.698338    1.310748
C   -2.786382    0.750633   -0.590552
C   -4.370880   -1.631845    0.031020
C   -2.529687   -2.619762   -0.657942
H   -3.161189   -1.447689   -1.823295
C   -3.521154   -0.340607    1.842238
H   -1.338160   -0.003778    1.639710
H   -1.848754   -1.736388    1.518375
H   -2.171986    1.512649   -0.092180
H   -2.704779    0.837731   -1.675644
C   -4.264984    0.726572   -0.137677
H   -4.412380   -2.462974    0.741885
H   -5.209767   -1.743949   -0.662272
H   -3.519510    0.668662    2.263641
H   -3.808435   -1.038014    2.635274
H   -4.504040    1.664683    0.370080
H   -4.940544    0.629151   -0.993938
N   -2.137903   -0.575083   -0.211643
N   -4.522117   -0.386304    0.773685
C    0.457911    1.410507    0.016530
O   -0.504417    1.615633    0.915529
C    0.869926    2.771242   -0.600224
F   -0.208367    3.422713   -1.085007
F    1.730942    2.660870   -1.646617
F    1.450544    3.575401    0.295642
C    1.720488    0.728996    0.601137
C    2.851471    0.394607   -0.153307
C    1.716214    0.435020    1.965409
C    3.950211   -0.217233    0.448097
H    2.886636    0.608978   -1.217765
C    2.806943   -0.192764    2.566390
H    0.842998    0.733475    2.537622
C    3.929951   -0.520771    1.809385
H    4.827054   -0.452354   -0.150712
H    2.785226   -0.413781    3.630461
H    4.786664   -0.999416    2.276583
```

[2 + 2 + 2] cycloaddition

Dabco-γ-ts4cc′

	E(ele)	− -2054.376512	
	E(ele+zpe)	− -2053.844477	
	H	− -2053.809730	
	G	− -2053.909507	

```
C   -1.310932   -1.575768    1.407021
C   -0.658301   -1.608931   -0.985194
H   -0.379782   -2.661289   -0.909742
H   -1.103901   -1.467808   -1.970890
C   -1.910653   -1.267862    2.250708
C   -1.612825   -1.326165    0.132846
O   -0.047156   -2.273729    1.789114
O    0.481603   -3.161539    1.161715
C    0.375712   -1.844518    2.978614
H    1.638158   -2.367708    3.395629
H    2.388332   -2.177294    2.624619
H    1.882453   -1.838774    4.315508
C    1.562315   -3.443934    3.570925
C   -3.847549   -1.759961   -0.786984
C   -3.637067   -0.096088    0.991384
C   -2.787111    0.398973   -1.249561
C   -5.110982   -1.063819   -1.360198
H   -4.071026   -2.449872    0.031257
C   -3.277562   -2.297126   -1.548205
C   -5.076367    0.303808    0.582179
H   -3.005540    0.738909    1.310462
H   -3.672188   -0.855561    1.769852
H   -1.999441    1.060308   -0.893813
C   -2.474113   -0.087437   -2.172544
H   -4.143628    1.110319   -1.425980
H   -6.003613   -1.628471   -1.076141
H   -5.071322   -1.031035   -2.453109
H   -5.304546    1.300510    0.969073
H   -5.806157   -0.393664    1.005210
C   -4.137309    2.079006   -0.917753
N   -4.331778    1.289929   -2.488273
N   -2.938806   -0.699823   -0.207429
N   -5.230987    0.306492   -0.867899
C    0.714837   -0.748118   -0.830226
O    0.786913   -0.057236    0.320049
C    0.092299    1.829708    0.896578
O   -1.105580    1.952701    0.646136
F    0.789001    0.186153   -2.067409
C    0.596835   -0.478515   -3.237191
F   -0.159252    1.147868   -2.044411
F    1.966751    0.805804   -2.164007
C    0.399182    1.452999    2.372963
F   -0.607298    0.750582    2.906525
F    1.537974    0.805332    2.630466
F    0.459850    2.619300    3.059176
C    1.922980   -1.709288   -0.978175
C    1.985882   -2.722348   -1.936824
C    3.000771   -1.533794   -0.111638
C    3.100104   -3.557107   -2.014240
H    1.165376   -2.869920   -2.635489
C    4.115872   -2.364332   -0.186988
H    2.927478   -0.746581    0.632214
C    4.168635   -3.382834   -1.137160
H    3.131751   -4.345671   -2.761403
H    4.945322   -2.218371    0.500541
C    5.035344   -4.035552   -1.194218
H    1.138126    2.637814    0.187933
C    2.508797    2.406877    0.332163
H    0.695421    3.689676   -0.615580
C    3.423536    3.219915   -0.328514
H    2.852571    1.569877    0.927805
C    1.611959    4.499576   -1.280450
H   -0.373113    3.857375   -0.712280
C    2.978363    4.265735   -1.136887
H    4.487352    3.027274   -0.224073
H    1.261256    5.313501   -1.908670
H    3.696080    4.894867   -1.656212
```

Dabco-γ-4cc′

	E(ele)	− -2054.388777	
	E(ele+zpe)	− -2053.854484	
	H	− -2053.819050	
	G	− -2053.918942	

```
C   -1.241287   -2.030894    0.868936
C   -0.418478   -1.023802   -1.276587
H   -0.211214   -2.005088   -1.714166
H   -0.839826   -0.406692   -2.063840
C   -1.959426   -2.118888    1.676572
C   -1.428564   -1.228966   -0.177531
O   -0.069318   -2.939899    1.017140
O    0.334660   -3.670080    0.141744
C    0.400321   -2.930996    2.264078
C    1.461954   -3.856878    2.522936
H    2.277894   -3.697378    1.815294
H    1.781172   -3.653066    3.543637
H    1.091021   -4.880831    2.428157
C   -3.746171   -1.835776   -0.671940
C   -3.359449    0.018784    0.903124
C   -2.975504    0.308544   -1.510657
C   -5.132873   -1.282120   -1.085404
H   -3.793290   -2.449900    0.229290
C   -3.263857   -2.419738   -1.459839
C   -4.886612    0.188650    0.756908
H   -2.791882    0.948625    0.963888
H   -3.102116   -0.595789    1.762098
H   -2.171356    1.040003   -1.416450
C   -2.869386   -0.284921   -2.422805
H   -4.379462    0.941174   -1.427127
H   -5.919742   -1.896811   -0.638167
H   -5.260234   -1.317600   -2.171778
H   -5.180607    1.163567    1.156063
H   -5.433876   -0.577494    1.316546
C   -4.328524    1.925913   -0.953674
N   -4.779933    1.074685   -2.436524
N   -2.828543   -0.669231   -0.352548
```

```
N   -5.290186    0.101407   -0.646856
C    0.967979   -0.381054   -0.854424
O    0.991141    0.282933    0.364929
C    0.137009    1.465627    0.657047
C   -1.045280    1.422689    0.110730
F    1.389965   -0.141192   -3.192119
C    0.486731    1.553940   -2.233411
F    2.566156    1.097133   -1.858857
F    0.031269    1.314283    2.208354
C    1.211554    1.165003    2.837531
F   -0.567482    2.395109    2.739025
F   -0.726324    0.251631    2.556972
C    2.099015   -1.429188   -0.761043
C    2.289199   -2.406052   -1.743408
C    2.992538   -1.373965    0.310879
C    3.338674   -3.313891   -1.649555
H    1.619264   -2.475027   -2.594945
C    4.049189   -2.280650    0.401108
H    2.851491   -0.622679    1.078938
C    4.225663   -3.256077   -0.575538
H    3.462659   -4.069571   -2.419645
H    4.734429   -2.218726    1.242477
C    5.047092   -3.963488   -0.504677
H    0.960328    2.734100    0.369329
C    0.287945    3.863218   -0.093914
H    2.336556    2.797530    0.589343
C    0.981696    5.045428   -0.341587
H   -0.781609    3.785124   -0.264670
C    3.033921    3.978254    0.340942
H    2.865999    1.913764    0.933581
C    2.357879    5.105507   -0.123583
H    0.450415    5.920599   -0.706610
H    4.107356    4.016027    0.505344
H    2.901886    6.025746   -0.318843
```

Dabco-γ-ts6cc′

	E(ele)	− -2054.384055	
	E(ele+zpe)	− -2053.850470	
	H	− -2053.816623	
	G	− -2053.913454	

```
C   -1.018971   -2.090527    1.059040
C   -0.080294   -1.158239   -1.066194
H    0.327154   -2.166199   -1.138716
C   -0.549218   -0.933788   -2.024482
C   -1.810142   -2.235052    1.781280
C   -1.123845   -1.191869    0.035160
O    0.233587   -2.731220    1.426452
O    1.296995   -2.687307    0.836841
C    0.081471   -3.441957    2.571167
H    1.269438   -4.064940    3.050789
H    2.039958   -3.313851    3.241541
H    0.985567   -4.568057    3.974838
C    1.648737   -4.784571    2.320913
C   -3.120117   -2.246336   -0.971799
C   -3.479387   -0.481172    0.704850
C   -2.728189    0.085782   -1.539125
C   -4.485925   -1.977128   -1.648751
H   -3.192918   -2.928542   -0.124006
C   -2.373643   -2.645796   -1.662872
C   -4.948715   -0.663927    0.267816
H   -3.203744    0.554842    0.890693
H   -3.240207   -1.055253    1.595634
H   -2.134588    0.950780   -1.252572
C   -2.318759   -0.359643   -2.446623
H   -4.232980    0.382246   -1.726722
H   -5.179901   -2.788321   -1.409876
H   -4.386113   -1.936250   -2.737917
H   -5.546783    0.169446    0.648238
H   -5.375224   -1.588540    0.670096
C   -4.518610    1.306646   -1.215692
N   -4.448678    0.511737   -2.791320
N   -2.579047   -0.942067   -0.430830
N   -5.050417   -0.708006   -1.191173
C    1.140748   -0.185906   -0.886885
O    1.238787    0.426991    0.365877
C    0.129612    1.158643    0.926808
C   -1.067963    0.689884    0.562927
C    1.064843    0.887140   -2.008711
F    1.067038    0.304121   -3.229003
C   -0.062049    1.623132   -1.967608
F    2.097181    1.728384   -1.966146
F    0.364559    0.953041    2.452731
C    0.245639   -0.326791    2.828810
F    1.581810    1.366306    2.848675
F   -0.545188    1.653477    3.152082
C    2.473904   -0.920491   -1.102115
C    2.633908   -1.823967   -2.154194
C    3.553299   -0.667129   -0.256229
C    3.849517   -2.474039   -2.351682
H    1.811087   -2.029693   -2.833433
C    4.768586   -1.317214   -0.454334
H    3.430580    0.020325    0.572394
C    4.923215   -2.223124   -1.500550
H    3.954631   -3.177928   -3.172343
H    5.597040   -1.116566    0.219483
C    5.871736   -2.730614   -1.651273
H    0.288566    2.661614    0.646905
C   -0.849470    3.457766    0.527103
H    1.550411    3.246726    0.547121
C   -0.730958    4.825543    0.292464
H   -1.825046    2.989144    0.617939
C    1.670982    4.613983    0.307125
H    2.437424    2.626753    0.638734
C    0.531727    5.406303    0.179143
H   -1.623012    5.439250    0.200257
H    2.657468    5.059990    0.217380
H    0.627444    6.472351   -0.007348
```

	E(ele)	− -1371.973279	
	E(ele+zpe)	− -1371.559973	
	H	− -1371.536011	
	G	− -1371.612564	

```
C   -0.146254   -1.816118   -0.151063
C    0.037524    0.459119   -1.231946
H    0.751121   -0.013578   -1.905471
H   -0.642374    1.084106   -1.813242
H   -0.596801   -2.503736    0.553448
C   -0.665351   -0.567203   -0.350276
C    1.165651   -2.260375   -0.622353
O    1.838446   -1.827870   -1.538242
O    1.576754   -3.326734    0.110517
C    2.872143   -3.816664   -0.223109
H    3.618367   -3.029023   -0.086272
H    3.057267   -4.645844    0.459722
H    2.899631   -4.158984   -1.260788
C   -2.933065   -1.354760   -1.053439
C   -2.492468   -0.916487    1.318977
C   -2.749802    0.935633   -0.236819
C   -4.399143   -1.477705   -0.566594
H   -2.414731   -2.312133   -1.083922
C   -2.847102   -0.886572   -2.038783
C   -3.980628   -0.626306    1.618459
H   -1.788749   -0.386607    1.962463
H   -2.292774   -1.986720    1.358013
H   -2.311817    1.516411    0.572017
H   -2.402436    1.348297   -1.181215
C   -4.293260    0.854530   -0.195648
H   -4.559531   -2.440895   -0.072128
H   -5.081583   -1.425529   -1.419852
H   -4.089119    0.268612    2.238274
H   -4.417663   -1.466302    2.166582
H   -4.685228    1.679682    0.405912
H   -4.724425    0.942515   -1.198143
N   -2.183560   -0.462784   -0.093709
N   -4.732046   -0.414940    0.380536
C    0.630988    1.208023   -0.012389
O   -0.261578    0.791903    0.961954
C    0.547525    2.728205   -0.176045
F   -0.729425    3.134924   -0.375036
F    1.000099    3.384611    0.896614
F    1.243124    3.174943   -1.245310
C    2.077240    0.788390    0.267069
C    2.358677    0.119020    1.456360
C    3.099660    0.981948   -0.666830
C    3.647067   -0.352444    1.712533
H    1.549407   -0.035981    2.162072
C    4.385452    0.517558   -0.409676
H    2.889484    1.473716   -1.612584
C    4.664002   -0.152924    0.781825
H    3.853541   -0.878483    2.641013
H    5.168663    0.665770   -1.147755
H    5.667192   -0.522024    0.978389
```

Dabco-γ-ts4c

	E(ele)	− -1371.976662	
	E(ele+zpe)	− -1371.565043	
	H	− -1371.540321	
	G	− -1371.619024	

```
C    0.465670    1.413600   -0.962042
C   -0.517570   -0.767288   -1.399617
H   -1.251077   -0.245531   -2.003998
H   -0.371338   -1.800097   -1.680750
H   -0.459741    1.783633   -1.391542
C    0.553852    0.034628   -0.963434
C    1.337569    2.478441   -0.514185
O    2.471743    2.416393   -0.042412
O    0.735097    3.675267   -0.700893
C    1.492243    4.812764   -0.303265
H    2.434375    4.860911   -0.855222
H    0.867892    5.674646   -0.536077
H    1.710034    4.775077    0.767248
C    3.011253   -0.302953   -1.094136
C    1.855436   -0.283367    1.123739
C    1.636820   -2.174991   -0.400618
C    4.212459   -0.766862   -0.240671
H    3.022283    0.770868   -1.256070
C    2.943069   -0.824003   -2.053513
C    2.982588   -1.121029    1.766409
H    0.875809   -0.491812    1.555179
H    2.076604    0.779889    1.144091
H    0.785562   -2.446798    0.230041
H    1.437601   -2.455811   -1.434418
C    2.983517   -2.773297    0.078891
H    4.643442    0.085647    0.293036
H    4.987107   -1.189319   -0.888119
H    2.568520   -1.899880    2.413992
H    3.617669   -0.475244    2.379592
H    2.791438   -3.597160    0.771807
H    3.551348   -3.174720   -0.766829
N    1.741394   -0.664385   -0.350659
N    3.806046   -1.769053    0.745634
C   -1.663688   -1.106960    0.405737
O   -0.914109   -1.515575    1.317991
C   -2.512923   -2.232275   -0.236543
F   -1.794256   -3.360019   -0.340687
F   -3.000959   -1.975505   -1.468427
F   -3.571908   -2.500127    0.546644
C   -2.264496    0.269408    0.470086
C   -3.273449    0.734729   -0.385501
C   -1.739925    1.141942    1.429243
C   -3.739864    2.040806   -0.277183
H   -3.700671    0.083272   -1.139898
C   -2.204812    2.451836    1.532754
H   -0.980011    0.768500    2.108329
C   -3.204664    2.906448    0.678362
H   -4.526971    2.384670   -0.942211
H   -1.783470    3.116371    2.281836
H   -3.569499    3.926663    0.755190
```

[2 + 2] cycloaddition
Dabco-γ-ts4c2′

Dabco-γ-4c

```
E(ele)        = -1371.987929
E(ele+zpe)    = -1371.573796
H             = -1371.549360
G             = -1371.627090
C    0.449723   1.409007  -0.969257
C   -0.541791  -0.805859  -1.263069
H   -1.127861  -0.290845  -2.026499
H   -0.221828  -1.757513  -1.685337
H   -0.501574   1.717093  -1.391986
C    0.602529   0.074124  -0.872012
C    1.271223   2.574094  -0.561414
O    2.371960   2.587696  -0.041945
O    0.607357   3.696538  -0.857625
C    1.254117   4.916832  -0.491013
H    2.218759   5.000674  -0.996522
H    0.578980   5.708939  -0.809384
H    1.407763   4.949909   0.589816
C    3.084254  -0.137798  -0.995200
C    1.898779  -0.191381   1.210139
C    1.793513  -2.086808  -0.359960
C    4.288474  -0.550931  -0.117268
H    3.057278   0.934330  -1.157852
H    3.065452  -0.658153  -1.956854
C    3.037341  -1.005796   1.856449
H    0.907747  -0.439746   1.602582
H    2.094790   0.877903   1.235584
H    0.928699  -2.390472   0.244203
H    1.635224  -2.346541  -1.407628
C    3.159050  -2.622381   0.134503
H    4.659593   0.314611   0.440387
H    5.099594  -0.916781  -0.754443
H    2.632420  -1.820586   2.463783
H    3.629566  -0.358153   2.509801
H    2.993815  -3.467626   0.808119
H    3.768238  -2.977864  -0.703263
N    1.820239  -0.564807  -0.275662
N    3.914374  -1.590138   0.839974
C   -1.427284  -1.119373   0.046354
O   -0.683359  -1.548444   1.059695
C   -2.388311  -2.247065  -0.404806
F   -1.708285  -3.385578  -0.657915
F   -3.060926  -1.963222  -1.554638
F   -3.308137  -2.531180   0.521148
C   -2.253810   0.152254   0.361113
C   -3.080411   0.801772  -0.563962
C   -2.123275   0.696582   1.638485
C   -3.750762   1.974090  -0.219362
H   -3.217530   0.391810  -1.561372
C   -2.790379   1.871502   1.986030
H   -1.495278   0.162094   2.345183
C   -3.604260   2.516733   1.057391
H   -4.392759   2.461343  -0.948549
H   -2.679233   2.280471   2.987083
H   -4.127993   3.430157   1.325760
```

Dabco-γ-ts4c2

```
E(ele)        = -1371.975989
E(ele+zpe)    = -1371.562334
H             = -1371.538383
G             = -1371.614893
C    0.380004   1.538816  -0.667193
C   -0.540294  -0.635130  -1.321843
H   -1.009951  -0.027818  -2.098566
H   -0.159975  -1.544308  -1.789594
H   -0.573282   1.849271  -1.080186
C    0.512184   0.172942  -0.552143
C    1.187385   2.668985  -0.245192
O    2.355399   2.695419   0.133873
O    0.486453   3.815540  -0.387679
C    1.188046   5.012579  -0.068220
H    2.060410   5.131969  -0.716059
H    0.475216   5.819822  -0.232499
H    1.517908   4.998306   0.973430
C    2.923481   0.038594  -1.165245
C    2.235024  -0.057616   1.231039
C    1.885441  -1.953062  -0.244469
C    4.306414  -0.313410  -0.574082
H    2.806722   1.108836  -1.304323
H    2.720565  -0.478655  -2.108159
C    3.532135  -0.801663   1.621021
H    1.373729  -0.331570   1.836914
H    2.375712   1.019078   1.232473
H    1.218145  -2.287916   0.547572
H    1.482797  -2.275027  -1.202747
C    3.552224  -2.425810  -0.083245
H    4.748870   0.573489  -0.110386
H    4.977245  -0.650893  -1.370211
H    3.323777  -1.624833   2.311570
H    4.215445  -0.109722   2.121876
H    3.385446  -3.281702   0.596998
H    3.766739  -2.749883  -1.043469
N    1.860333  -0.439227  -0.197772
N    4.198015  -1.358889   0.442864
C   -1.390079  -0.924472  -0.066755
O   -0.418280  -0.727623   0.895912
C   -1.879223  -2.375971  -0.031280
F   -0.850271  -3.250796  -0.122370
F   -2.538370  -2.666436   1.094555
F   -2.699545  -2.663728  -1.066840
C   -2.589931   0.015761   0.078349
C   -2.713498   0.749136   1.257403
C   -3.541980   0.179552  -0.932862
C   -3.777185   1.633079   1.429073
H   -1.953375   0.619885   2.020636
C   -4.603738   1.065636  -0.763028
H   -3.458315  -0.384955  -1.858830
C   -4.724414   1.794652   0.419838
H   -3.862325   2.201694   2.351229
H   -5.336705   1.188380  -1.555539
H   -5.550126   2.488535   0.550275
```

γ-4c

```
E(ele)        = -1026.823978
E(ele+zpe)    = -1026.600016
H             = -1026.582191
G             = -1026.646867
C   -0.740076   0.565753   0.218847
C   -0.027329   0.800179   1.572633
H    0.008976   1.836609   1.914651
H   -0.353491   0.136152   2.374735
C    1.180047   0.337711   0.798660
C    2.466673   0.104671   1.069577
H    2.831141   0.287364   2.073275
O    0.514032   0.178009  -0.384973
C    3.402107  -0.409295   0.059484
O    3.135020  -0.685723  -1.088127
O    4.638111  -0.552432   0.584153
C    5.620418  -1.065171  -0.314497
H    6.550528  -1.092419   0.251445
H    5.342391  -2.068030  -0.648201
H    5.716073  -0.413533  -1.186168
C   -1.777264  -0.524355   0.141196
C   -2.882058  -0.513954   0.996117
C   -1.629251  -1.543502  -0.799570
C   -3.838383  -1.521961   0.905836
H   -2.996899   0.280116   1.730375
C   -2.588189  -2.550837  -0.884682
H   -0.759234  -1.547825  -1.448896
C   -3.692283  -2.541223  -0.034998
H   -4.696316  -1.512368   1.571349
H   -2.468971  -3.344702  -1.615715
C   -1.209898   1.857244  -0.448829
F   -0.247644   2.789967  -0.433720
F   -1.566516   1.657403  -1.718853
F   -2.268146   2.361105   0.210191
```

[3 + 2] cycloaddition
Dabco-γ-ts5c'

```
E(ele)        = -1371.959962
E(ele+zpe)    = -1371.546828
H             = -1371.523124
G             = -1371.598214
C   -0.339785   1.588007  -0.152404
C    0.016136  -0.327873   1.147917
C   -0.946394   0.738611   0.751929
C    0.892970  -0.661620  -0.205855
H    0.727764   0.083503   1.864370
H   -0.413423  -1.226000   1.595469
C   -3.281246   1.512757   0.813398
C   -2.629335   0.162770  -1.094226
C   -2.833688  -0.843752   1.139372
C   -4.707680   1.243981   0.271983
H   -2.846412   2.434348   0.424284
H   -3.228196   1.550559   1.904307
C   -4.035884  -0.445737  -1.267739
H   -1.813134  -0.439626  -1.486790
C   -2.573722   1.149634  -1.557251
H   -2.314014  -1.693462   0.697519
H   -2.502589  -0.720086   2.172527
C   -4.368700  -0.974746   1.016856
H   -4.913065   1.852584  -0.614338
H   -5.451527   1.504842   1.030886
H   -3.982460  -1.531480  -1.396516
H   -4.514241  -0.028676  -2.159061
H   -4.638307  -2.021443   0.849486
H   -4.867844  -0.645147   1.933781
N   -2.376518   0.381523   0.390684
N   -4.867364  -0.164497  -0.092639
C    0.953864   2.269820   0.170492
O    1.587913   2.159706   1.192981
O    1.326060   3.070069  -0.842064
H   -0.904257   2.134120  -0.903952
C    2.597943   3.695690  -0.672435
H    2.775603   4.253727  -1.590924
H    2.580471   4.365610   0.190964
H    3.370075   2.936792  -0.520933
O    0.564190   0.212370  -1.187024
C    0.520534  -2.085097  -0.644957
F    0.782617  -3.014199   0.301449
F   -0.813015  -2.210357  -0.903675
F    1.153327  -2.470632  -1.756580
C    2.396699  -0.655167   0.114738
C    3.263017  -0.018999  -0.775356
C    2.923732  -1.254297   1.261262
C    4.631583   0.030435  -0.517269
H    2.837799   0.441165  -1.663030
C    4.292194  -1.208034   1.520170
H    2.264779  -1.759874   1.963283
C    5.150985  -0.562555   0.632255
H    5.295909   0.529883  -1.218257
H    4.687057  -1.672419   2.419659
H    6.217579  -0.523357   0.835529
```

Dabco-γ-5c'

```
E(ele)        = -1371.972915
E(ele+zpe)    = -1371.558318
H             = -1371.534183
G             = -1371.611038
C   -0.298231   0.979306  -0.767191
C    0.172590  -0.705633   0.882991
C   -0.827381   0.397545   0.531608
C    1.278252  -0.657020  -0.213137
H    0.633965  -0.555328   1.862939
H   -0.266342  -1.714447   0.902330
C   -3.170864   1.042617   0.141339
C   -2.514344  -1.157675  -0.696493
C   -2.679360  -0.734761   1.691127
C   -4.608190   0.530745  -0.110030
H   -2.778525   1.615784  -0.698143
H   -3.075668   1.669237   1.030998
C   -3.957323  -1.705975  -0.553325
H   -1.761462  -1.936933  -0.588063
H   -2.352789  -0.658998  -1.655252
H   -2.135975  -1.675203   1.798729
H   -2.332874  -0.043749   2.462219
C   -4.210452  -0.957833   1.688809
H   -4.863117   0.575038  -1.173707
H   -5.328570   1.155136   0.427527
H   -3.949325  -2.718494  -0.137110
H   -4.446557  -1.754486  -1.530814
H   -4.449863  -1.944565   2.096329
H   -4.714852  -0.211685   2.310985
C   -2.253304  -0.127806   0.381406
N   -4.752381  -0.856483   0.333532
C    0.161683   2.403678  -0.489093
O    1.263078   2.748850  -0.147007
O   -0.872866   3.261387  -0.637596
H   -1.022809   1.027976  -1.591730
C   -0.601802   4.605531  -0.243213
H   -1.522485   5.160225  -0.422445
H   -0.329924   4.638580   0.814791
H    0.217709   5.018908  -0.835751
H    0.810255   0.209869  -1.226514
C    1.410146  -2.020207  -0.908935
F    1.773681  -2.987368  -0.045000
F    0.239581  -2.418179  -1.455147
F    2.308851  -2.003812  -1.897623
C    2.659748  -0.254004   0.295095
C    3.189520  -0.834000   1.450775
C    3.430759   0.657523  -0.425614
C    4.466923  -0.493460   1.890564
H    2.609386  -1.562687   2.011572
C    4.706109   0.999959   0.015626
H    3.013480   1.111595  -1.316619
C    5.227887   0.427987   1.174372
H    4.865300  -0.948442   2.792996
H    5.292051   1.721018  -0.547096
H    6.222255   0.699002   1.517983
```

9.6.3 Cycloadditions starting from Pph-3

Pph-γ-ts4c

```
E(ele)      =  -2062.778568
E(ele+zpe)  =  -2062.279423
H           =  -2062.244899
G           =  -2062.345358

C   0.706157   2.250647  -0.825614
H   0.096082   3.039946  -1.251462
C  -0.813590   0.595114  -1.788214
C   0.322730   0.939009  -1.043727
C  -2.411616   1.389976  -0.374864
H  -1.090211   1.289289  -2.575208
P   1.166177  -0.410798  -0.150723
C   1.876355   2.636025  -0.078424
O   2.732726   1.865360   0.352092
O   1.970483   3.968707   0.101284
C   3.103758   4.405876   0.843412
H   3.095825   3.970341   1.846076
H   4.029546   4.117271   0.338468
H   3.018222   5.490739   0.896716
H  -1.091622  -0.437622  -1.953750
C   0.189064  -1.941461  -0.290757
C   0.165319  -2.631767  -1.511181
C  -0.491847  -2.459817   0.813929
C  -0.536616  -3.826772  -1.621919
H   0.702567  -2.237430  -2.370940
C  -1.177871  -3.668363   0.700422
H  -0.491113  -1.929340   1.761764
C  -1.201322  -4.350670  -0.511819
H  -0.554783  -4.354997  -2.570514
H  -1.703679  -4.065313   1.563352
H  -1.739148  -5.290838  -0.596046
C   2.742330  -0.842751  -0.941344
C   3.339340   0.036234  -1.847715
C   3.324476  -2.089921  -0.685317
C   4.522610  -0.327687  -2.483966
H   2.878084   0.997197  -2.052478
C   4.517977  -2.439905  -1.311427
H   2.839404  -2.797702  -0.016551
C   5.116514  -1.558733  -2.210856
H   4.981418   0.355442  -3.192105
H   4.970746  -3.405468  -1.107178
H   6.042205  -1.836524  -2.706582
C   1.296613  -0.098088   1.626510
C   0.341066   0.733871   2.215962
C   2.275940  -0.724823   2.398597
C   0.367077   0.922328   3.597256
H  -0.393586   1.257142   1.603529
C   2.291291  -0.527301   3.776757
H   3.036318  -1.345918   1.933011
C   1.334420   0.291647   4.376955
H  -0.368610   1.575867   4.057607
H   3.056575  -1.006653   4.379952
H   1.351184   0.445244   5.452168
O  -1.858982   2.232890   0.342489
C  -3.245969   1.987671  -1.530870
F  -2.643054   3.053882  -2.067488
F  -3.525699   1.138985  -2.542370
F  -4.433493   2.399076  -1.045704
C  -2.942428   0.099079   0.208400
C  -3.023035   0.032295   1.603246
H  -3.437715  -0.971143  -0.548801
C  -3.585464  -1.076630   2.233160
H  -2.668416   0.879278   2.182930
C  -4.013925  -2.069962   0.080792
H  -3.379617  -0.949803  -1.631961
C  -4.093008  -2.127319   1.472642
H  -3.648805  -1.105851   3.317694
H  -4.397189  -2.890034  -0.520588
H  -4.549826  -2.985401   1.958734
H  -5.840779   2.446262  -2.633834
C  -1.388594  -0.071363   1.569794
C  -0.453645  -0.949410   2.130561
C  -2.448027   0.439138   2.323119
C  -0.587464  -1.294967   3.475781
H   0.353047  -1.381948   1.523591
C  -2.565898   0.081469   3.663141
H  -3.191490   1.089141   1.869837
C  -1.632620  -0.780854   4.240506
H   0.131864  -1.978531   3.917663
H  -3.392014   0.467915   4.252633
C  -1.728710  -1.058312   5.286490
O   1.661866  -2.179032   0.195069
C   3.214713  -1.888006  -1.537645
F   2.715167  -2.962492  -2.177303
F   3.649680  -1.045520  -2.515663
F   4.303065  -2.292983  -0.871740
C   2.835815  -0.071011   0.140769
C   3.000060  -0.190120   1.522006
C   3.355268   1.061507  -0.498219
C   3.654524   0.800272   2.255243
H   2.625165  -1.093279   1.994827
C   4.027453   2.042313   0.227472
H   3.259051   1.177191  -1.575021
C   4.177719   1.918195   1.608673
H   3.776889   0.685522   3.329638
H   4.432960   2.909479  -0.288492
H   4.704482   2.684228   2.172357
```

Pph-γ-4c

```
E(ele)      =  -2062.786601
E(ele+zpe)  =  -2062.285064
H           =  -2062.250720
G           =  -2062.350659

C  -0.732479  -2.163675  -1.013658
H  -0.107840  -2.938567  -1.448363
C   1.030823  -0.638022  -1.663681
C  -0.318133  -0.881057  -1.098113
C   2.154486  -1.255062  -0.596306
H   1.120288  -1.212921  -2.589175
P  -1.138911   0.432050  -0.149968
C  -1.966677  -2.607196  -0.336561
O  -2.874400  -1.869287   0.002029
O  -1.985207  -3.926512  -0.146990
C  -3.126148  -4.431707   0.548321
H  -3.192780  -3.975932   1.539127
H  -4.038270  -4.212537  -0.011651
H  -2.967456  -5.505789   0.626650
H   1.241852   0.406876  -1.889064
C  -0.081622   1.908157  -0.111546
C   0.048033   2.674502  -1.277208
C   0.528778   2.324218   1.073563
C   0.783789   3.853764  -1.253123
H  -0.438011   2.357500  -2.197703
C   1.250522   3.516829   1.093621
H   0.452462   1.724014   1.975639
C   1.375312   4.280254  -0.063073
H   0.885563   4.443761  -2.159049
H   1.728954   3.834814   2.014537
H   1.944436   5.205237  -0.043093
C  -2.656325   1.034080  -0.944671
C  -3.286454   0.308136  -1.957092
C  -3.161727   2.280350  -0.554692
C  -4.428884   0.822768  -2.565476
H  -2.885189  -0.651443  -2.267109
C  -4.313949   2.780420  -1.153762
H  -2.647461   2.868873   0.202033
C  -4.946999   2.051272  -2.159760
H  -4.915132   0.260602  -3.356784
H  -4.707400   3.743532  -0.843409
```

[3 + 2] cycloaddition
Pph-γ-ts5c

```
E(ele)      =  -2062.781525
E(ele+zpe)  =  -2062.278514
H           =  -2062.245233
G           =  -2062.342341

C  -0.196506  -2.014375  -1.145331
H   0.382865  -2.604048  -1.849015
C   1.085248  -0.173264  -1.787153
C  -0.229597  -0.644661  -1.278852
C   2.189810  -0.889900  -0.794370
H   1.249854  -0.569708  -2.794218
P  -1.214625   0.380758  -0.214641
C  -1.207423  -2.779584  -0.367977
O  -2.333572  -2.378492  -0.142310
O  -0.746836  -3.954225   0.049512
C  -1.650379  -4.709584   0.858814
H  -1.937646  -4.127246   1.738327
C  -2.545524  -4.968193   0.288331
H  -1.102514  -5.604888   1.147272
C   1.214466   0.907597  -1.824542
C  -0.419004   2.007177  -0.051599
C  -0.420717   2.880051  -1.147310
C   0.202715   2.382705   1.141431
H   0.197489   4.121928  -1.045961
C  -0.909342   2.589372  -2.075137
C   0.807661   3.634923   1.240529
H   0.225416   1.704680   1.990128
C   0.806566   4.501372   0.151522
H   0.197727   4.794825  -1.898170
H   1.295769   3.919292   2.167564
H   1.284310   5.473725   0.231819
C  -2.842555   0.739121  -0.945959
C  -3.381586  -0.129492  -1.897228
C  -3.545697   1.891437  -0.572124
C  -4.624937   0.146135  -2.460702
H  -2.828388  -1.016225  -2.188389
C  -4.790918   2.158980  -1.134949
H  -3.116221   2.589072   0.143738
C  -5.330911   1.285322  -2.078665
H  -5.040908  -0.531780  -3.199709
H  -5.333461   3.053346  -0.843605
H  -6.299969   1.497144  -2.521380
C  -1.434251  -0.237185   1.483001
C  -0.430281  -1.042149   2.031345
C  -2.560454   0.106640   2.233569
C  -0.558532  -1.488606   3.345682
H   0.426787  -1.342284   1.424438
C  -2.676587  -0.344720   3.546451
H  -3.355476   0.704624   1.797473
C  -1.675702  -1.140001   4.103666
H   0.217596  -2.119270   3.770641
H  -3.554306  -0.082355   4.129479
C  -1.771590  -1.494731   5.125983
O   1.661754  -1.955790  -0.173127
C   3.316394  -1.376356  -1.728181
F   2.773330   0.164238   0.164100
C   3.231610   1.414408  -0.269472
C   2.897022  -0.157503   1.517268
C   3.786117   2.321563   0.629858
H   3.168919   1.686071  -1.320020
C   3.432853   0.756845   2.424486
H   2.582645  -1.145773   1.838146
C   3.881041   2.000664   1.983542
H   4.138531   3.285340   0.271248
H   3.518248   0.487938   3.474311
H   4.310443   2.710089   2.686206
F   2.879489  -2.355941  -2.544093
F   3.791380  -0.395927  -2.538878
F   4.369075  -1.861098  -1.057082
```

Pph-γ-5c

```
E(ele)      =  -2062.814488
E(ele+zpe)  =  -2062.309707
H           =  -2062.275968
G           =  -2062.374726

C  -0.528158   0.510187  -2.117887
H  -0.319876   0.286920  -3.176556
C  -1.080881  -1.525146  -1.037636
C   0.031288  -0.516038  -1.164568
C  -2.317941  -0.600270  -1.091031
H  -1.117032  -2.211549  -1.896142
P   1.287750  -0.310349  -0.052421
C   0.033597   1.891920  -1.844520
O   1.188952   2.161920  -2.097786
O  -0.813398   2.732120  -1.257913
C  -0.257155   4.001665  -0.902940
H   0.628774   3.864842  -0.277845
H   0.015325   4.555052  -1.804923
H  -1.041798   4.520469  -0.353200
H  -1.044935  -2.128096  -0.130390
C   1.196027  -1.710946   1.113102
C   1.616235  -2.967070   0.657323
C   0.644489  -1.588950   2.390469
C   1.476615  -4.089225   1.468600
H   2.049265  -3.065366  -0.335438
C   0.509180  -2.715807   3.201860
H   0.312859  -0.622724   2.758512
C   0.921147  -3.964618   2.742535
H   1.802140  -5.059813   1.106385
H   0.079886  -2.612582   4.194301
C   0.813474  -4.840281   3.376295
C   2.984005  -0.447204  -0.740466
C   3.171882  -0.334931  -2.117457
C   4.079531  -0.705617   0.092169
C   4.450271  -0.464216  -2.660249
H   2.315797  -0.140810  -2.757556
C   5.354009  -0.842467  -0.451571
H   3.935070  -0.809173   1.166666
C   5.539377  -0.718309  -1.829637
H   4.593040  -0.368362  -3.732630
H   6.199952  -1.051168   0.197157
H   6.533436  -0.825983  -2.254344
C   1.344385   1.237006   0.951444
C   0.167178   1.632055   1.599757
C   2.485438   2.039182   1.057014
C   0.146657   2.781445   2.387085
H  -0.742297   1.049608   1.473416
C   2.459717   3.195411   1.836819
H   3.389798   1.776676   0.517240
C   1.296117   3.560907   2.512757
H  -0.774216   3.067277   2.888489
H   3.349907   3.813763   1.908160
H   1.281297   4.460197   3.122151
O  -1.956091   0.448819  -1.973815
C  -3.510640  -1.299948  -1.746578
C  -2.731771  -0.044479   0.268861
C  -2.721029  -0.835119   1.421419
C  -3.123879   1.293275   0.366661
H  -2.446376  -1.884892   1.367289
C  -3.463842   1.840406   1.602003
H  -3.125702   1.903371  -0.529813
C  -3.415645   1.057025   2.755325
H  -3.023961  -0.909074   3.548499
H  -3.760541   2.884122   1.664096
H  -3.670421   1.485742   3.720782
F  -3.227127  -1.727844  -2.985373
F  -3.868686  -2.381904  -1.024068
F  -4.586131  -0.505464  -1.837058
```

[2 + 2] cycloaddition
transition state involving a C−O ring closure

```
E(ele)      =  -2062.782782
E(ele+zpe)  =  -2062.281165
H           =  -2062.247428
G           =  -2062.345342

C   1.165714   2.139819  -1.039972
H   0.805400   2.968817  -1.637438
C  -0.954877   0.928876  -1.650383
C   0.280608   1.097511  -0.741567
C  -1.905022   1.271121  -0.489728
H  -0.934659   1.651569  -2.469417
P   0.970336  -0.447644   0.027985
C   2.452668   2.251652  -0.442842
O   3.014846   1.373915   0.220943
O   3.081798   3.419343  -0.722359
C   4.392866   3.549270  -0.187724
H   4.374491   3.473540   0.902622
H   5.053239   2.772927  -0.584355
H   4.738697   4.536186  -0.495331
C  -1.093809  -0.071806  -2.063790
C  -0.322437  -1.737866  -0.080476
C  -0.488358  -2.418640  -1.295954
C  -1.144978  -2.062415   1.000125
H  -1.470290  -3.394320  -1.428946
C   0.158476  -2.194724  -2.141252
C  -2.123887  -3.045811   0.866130
H  -1.031590  -1.550704   1.949857
C  -2.291598  -3.707570  -0.346038
H  -1.591372  -3.909305  -2.377380
H  -2.764254  -3.280471   1.710862
C  -3.062859  -4.465495  -0.449784
C   2.304840  -1.222856  -0.943912
C   2.908924  -0.582739  -2.027647
C   2.668148  -2.536436  -0.619570
C   3.877388  -1.253201  -2.773594
H   2.619794   0.431077  -2.287676
C   3.649056  -3.193242  -1.355531
H   2.180095  -3.050123   0.206089
C   4.254173  -2.550871  -2.435953
H   4.342839  -0.752303  -3.617124
H   3.932431  -4.207489  -1.090870
H   5.015669  -3.064971  -3.015366
C   1.451708  -0.308178   1.778913
C   0.573250   0.208653   2.738389
C   2.725296  -0.742354   2.163261
C   0.962569   0.251771   4.076558
H  -0.387667   0.606251   2.431099
C   3.099601  -0.701629   3.501911
H   3.440462  -1.073572   1.417918
C   2.216944  -0.211483   4.463265
H   0.278789   0.661080   4.814328
H   4.092004  -1.035525   3.789496
H   2.514149  -0.175488   5.507494
O  -0.913105   1.323183   0.503107
C  -3.042958   0.317201  -0.167620
C  -3.685872  -0.428321  -1.153960
C  -3.481185   0.219801   1.156931
C  -4.743979  -1.275260  -0.821642
C  -3.364011  -0.349293  -2.190029
C  -4.541918  -0.616682   1.488744
C  -2.977800   0.806534   1.921046
C  -5.174712  -1.370496   0.498845
H  -5.232234  -1.857095  -1.598724
H  -4.878002  -0.680612   2.520223
H  -6.003077  -2.024662   0.756809
C  -2.503224   2.673381  -0.687417
F  -1.563155   3.587370  -0.966752
F  -3.374405   2.680237  -1.719909
F  -3.162364   3.102031   0.397973
```

four-membered intermediate

```
E(ele)      =  -2062.783827
E(ele+zpe)  =  -2062.281881
H           =  -2062.247649
G           =  -2062.348170

C   1.082514   2.292109  -0.804686
H   0.715867   3.177216  -1.308618
C  -0.947528   0.980641  -1.628892
C   0.176283   1.195600  -0.577772
C  -1.952368   1.279314  -0.504281
H  -0.898013   1.725116  -2.425565
P   1.037933  -0.372718   0.036472
C   2.357418   2.279030  -0.244278
C   2.871122   1.284797   0.323583
O   3.089258   3.412867  -0.408475
C   4.415580   3.363132   0.097004
H   4.416404   3.163521   1.171961
C   4.997244   2.584644  -0.405574
H   4.843865   4.345487  -0.105746
C  -1.034802  -0.017619  -2.058126
C  -0.229618  -1.702521  -0.131624
C  -0.400088  -2.332689  -1.374870
C  -1.030300  -2.108305   0.939849
H  -1.353443  -3.332035  -1.541373
C   0.226020  -2.054374  -2.219497
C  -1.983262  -3.112385   0.773350
H  -0.917809  -1.646823   1.915031
C  -2.148737  -3.723753  -0.465035
H  -1.470573  -3.806526  -2.511405
H  -2.599673  -3.407372   1.617129
C  -2.896470  -4.501287  -0.593567
C   2.338074  -1.046764  -1.048793
C   2.868892  -0.301413  -2.103810
C   2.740282  -2.373391  -0.858544
C   3.798602  -0.885806  -2.960850
H   2.551966   0.727450  -2.252625
C   3.690497  -2.942687  -1.703026
H   2.306159  -2.968540  -0.057762
C   4.216209  -2.200131  -2.758890
H   4.203743  -0.305143  -3.784351
H   4.008072  -3.968476  -1.541235
H   4.948007  -2.646528  -3.424072
C   1.469963  -0.392207   1.806185
C   0.592556   0.122050   2.765660
C   2.700234  -0.927185   2.199221
C   0.939417   0.068501   4.115501
H  -0.339803   0.583770   2.458063
C   3.030208  -0.988057   3.549042
H   3.416801  -1.259682   1.454669
C   2.148919  -0.495514   4.510958
H   0.258253   0.477941   4.855710
H   3.988551  -1.402470   3.847717
H   2.413217  -0.536487   5.563707
O  -0.927041   1.386081   0.477825
C  -3.022471   0.267610  -0.154714
C  -3.640877  -0.507424  -1.133433
C  -3.437695   0.156403   1.175800
C  -4.660765  -1.393582  -0.786789
C  -3.329474  -0.420112  -2.171888
C  -4.458261  -0.723236   1.521097
C  -2.955531   0.767816   1.934380
C  -5.072419  -1.501517   0.538727
H  -5.132712  -1.998403  -1.556197
H  -4.778408  -0.799817   2.556514
H  -5.870739  -2.187964   0.807129
C  -2.617054   2.650677  -0.690870
F  -1.729224   3.608997  -0.984317
F  -3.500229   2.604477  -1.708031
F  -3.278378   3.043047   0.406402
```

Pph-γ-ts4c2 (TS involving release of Pph)

```
E(ele)      =  -2062.777601
E(ele+zpe)  =  -2062.275725
H           =  -2062.241997
G           =  -2062.341685

C   1.194318   2.189723  -1.125516
H   1.121449   2.712406  -2.068935
C  -0.996109   1.085755  -1.722953
C   0.210739   1.226180  -0.776026
C  -1.852117   1.391937  -0.482592
H  -0.996713   1.860644  -2.490377
P   0.939719  -0.546428  -0.135032
C   2.130205   2.560025  -0.153306
O   2.288106   1.979285   0.936439
O   2.937066   3.604124  -0.500964
C   3.895778   3.967205   0.476037
H   3.420051   4.179765   1.436847
H   4.632502   3.171324   0.628167
H   4.390350   4.860487   0.091866
H  -1.203072   0.115218  -2.166634
```

```
C    -0.258631   -1.830551   -0.633747
C    -0.432790   -2.122978   -1.995503
C    -1.077020   -2.465339    0.305463
C    -1.395251   -3.038014   -2.405047
H     0.194467   -1.636707   -2.739972
C    -2.044973   -3.376959   -0.109346
H    -0.968455   -2.242881    1.361990
C    -2.203465   -3.667501   -1.460054
H    -1.513808   -3.258407   -3.461340
H    -2.683689   -3.849073    0.630297
H    -2.959796   -4.377879   -1.779927
C     2.527495   -1.049569   -0.885247
C     3.644124   -0.218106   -0.723568
C     2.677225   -2.277700   -1.543553
C     4.874147   -0.598071   -1.251734
H     3.557114    0.691423   -0.140801
C     3.913215   -2.650137   -2.062944
H     1.840620   -2.960162   -1.640792
C     5.010952   -1.805704   -1.929702
H     5.731276    0.055284   -1.121979
H     4.015708   -3.606973   -2.565389
H     5.973923   -2.096813   -2.338504
C     1.135174   -0.789524    1.661488
C     0.771333    0.176423    2.602267
C     1.656041   -2.019690    2.081939
C     0.911587   -0.107574    3.958807
H     0.417484    1.142717    2.268909
C     1.795098   -2.290897    3.438186
C     1.953721   -2.767637    1.350310
C     1.417362   -1.334439    4.377955
H     0.634141    0.645049    4.690244
C     2.200454   -3.245256    3.759377
H     1.526747   -1.543697    5.437943
O    -0.711846    1.469581    0.368120
C    -2.857998    0.360315   -0.030831
C    -3.703632   -0.264473   -0.945501
C    -2.966333    0.066098    1.328656
C    -4.648239   -1.187067   -0.504592
H    -3.625585   -0.027497   -2.003785
C    -3.912205   -0.855091    1.767762
H    -2.294308    0.553325    2.029292
C    -4.754896   -1.482131    0.852225
H    -5.300839   -1.675277   -1.222270
H    -3.993661   -1.081306    2.826761
H    -5.493994   -2.199644    1.196525
C    -2.512185    2.765671   -0.552282
F    -1.649744    3.710706   -0.928513
F    -3.514626    2.749537   -1.448817
F    -3.021426    3.118272    0.631603
```

γ-4c

```
E(ele)      = -1026.823978
E(ele+zpe)  = -1026.600016
H           = -1026.582191
G           = -1026.646867
```

```
C    -0.740076    0.565753    0.218847
C    -0.027329    0.800179    1.572633
H     0.008976    1.836609    1.914651
H    -0.353491    0.136152    2.374735
C     1.180047    0.337711    0.798660
C     2.466673    0.104671    1.069577
H     2.831141    0.287364    2.073275
O     0.514032    0.178009   -0.384973
C     3.402107   -0.409295    0.059484
O     3.135020   -0.685723   -1.088127
O     4.638111   -0.552432    0.584153
C     5.620418   -1.065171   -0.314497
H     6.550528   -1.092419    0.251445
H     5.342391   -2.068030   -0.648201
H     5.716073   -0.413533   -1.186168
C    -1.777264   -0.524355    0.141196
C    -2.882058   -0.513954    0.996117
C    -1.629251   -1.543502   -0.799570
C    -3.838383   -1.521961    0.905836
H    -2.996899    0.280116    1.730375
C    -2.588189   -2.550837   -0.884682
H    -0.759234   -1.547825   -1.448896
C    -3.692283   -2.541223   -0.034998
H    -4.696316   -1.512368    1.571349
H    -2.468971   -3.344702   -1.615715
H    -4.437827   -3.328051   -0.102474
C    -1.209898    1.857244   -0.448829
F    -0.247644    2.789967   -0.433720
F    -1.566516    1.657403   -1.718853
F    -2.268146    2.361105    0.210191
```

[2 + 2 + 2] cycloaddition
Pph-γ-ts4cc

```
E(ele)      = -2745.179807
E(ele+zpe)  = -2744.558777
H           = -2744.514486
G           = -2744.634731
```

```
C     0.583098    1.167952   -1.553771
H    -0.227945    1.538345   -2.174815
C    -0.628080   -0.968145   -1.516224
C     0.498136   -0.072004   -1.058741
H    -0.564095   -1.011974   -2.609935
P     1.759270   -0.872039    0.035872
C     1.741812    2.061647   -1.386629
O     2.812956    1.709272   -0.931111
O     1.502687    3.278253   -1.867010
C     2.575694    4.212232   -1.752059
H     2.880771    4.303400   -0.706724
H     3.426925    3.882885   -2.353526
H     2.179281    5.157295   -2.119855
C    -0.480073   -1.987693   -1.167591
C     0.874441   -2.272274    0.801912
C     1.393614   -3.569930    0.758980
C    -0.357876   -2.031485    1.424168
C     0.690034   -4.615864    1.355053
H     2.329332   -3.779917    0.250814
C    -1.055975   -3.082966    2.008259
H    -0.788258   -1.033032    1.427602
```

```
C    -0.531734   -4.373741    1.979559
H     1.094607   -5.622880    1.314232
H    -2.028264   -2.888076    2.452527
H    -1.086271   -5.194467    2.425530
C     3.014215   -1.570988   -1.081574
C     2.830326   -1.542456   -2.466300
C     4.150300   -2.191345   -0.544605
C     3.772438   -2.133795   -3.306335
H     1.961341   -1.052693   -2.895450
C     5.086423   -2.781751   -1.387926
H     4.307437   -2.207179    0.531291
C     4.897565   -2.754111   -2.769796
H     3.624763   -2.103707   -4.381457
H     5.965201   -3.258470   -0.964371
H     5.630643   -3.211753   -3.427549
C     2.668421   -0.081291    1.411535
C     3.952056    0.441698    1.211477
C     2.138356   -0.142563    2.705196
C     4.686533    0.913196    2.295100
H     4.375829    0.489293    0.215930
C     2.875584    0.342949    3.781557
H     1.150220   -0.550899    2.878583
C     4.147984    0.871919    3.579932
H     5.680153    1.318667    2.129798
C     2.448960    0.301312    4.778930
H     4.722100    1.244914    4.423457
C    -2.096437   -0.468891   -1.097379
O    -2.140931    0.626256   -0.322395
C    -1.091119    1.673346    1.204145
O    -0.096683    1.048556    1.545062
C    -2.793612   -0.087807   -2.434336
F    -2.153722    0.931468   -3.056236
F    -2.827623   -1.101259   -3.334098
F    -4.055257    0.307526   -2.244403
F    -2.338493    1.494090    2.096922
F    -3.499170    1.875201    1.567597
F    -2.457873    0.238342    2.543063
F    -2.137929    2.274233    3.187550
C    -2.901625   -1.668956   -0.536311
C    -2.755960   -2.982357   -0.994495
C    -3.848259   -1.406674    0.454148
C    -3.501106   -4.019051   -0.435921
H    -2.060679   -3.213058   -1.798375
C    -4.596827   -2.440268    1.015200
H    -3.978259   -0.379593    0.774011
C    -4.416838   -3.753049    0.581466
H    -3.365811   -5.034872   -0.797882
H    -5.324280   -2.218211    1.791744
H    -4.996305   -4.560778    1.020840
C    -0.981028    2.989694    0.492641
C     0.059444    3.818809    0.927459
C    -1.874071    3.439378   -0.484669
C     0.202265    5.098838    0.396729
H     0.741121    3.452874    1.691557
C    -1.702036    4.706731   -1.035998
H    -2.662067    2.773198   -0.819108
C    -0.674072    5.540158   -0.592559
H     0.995998    5.749322    0.755413
H    -2.381667    5.049476   -1.810956
H    -0.561717    6.535293   -1.015263
```

Pph-γ-4cc

```
E(ele)      = -2745.205193
E(ele+zpe)  = -2744.580722
H           = -2744.537028
G           = -2744.655138
```

```
C    -1.088198   -0.992937   -1.974677
H    -0.582025   -1.612338   -2.711413
C     1.017450    0.251558   -1.790960
C    -0.414993   -0.005749   -1.374386
H     1.069158    0.063032   -2.866781
P    -0.965942    1.081785    0.030791
C    -2.492031   -1.344457   -1.686257
O    -3.235020   -0.695714   -0.980869
C    -2.862044   -2.455609   -2.328435
O    -4.211670   -2.869952   -2.110880
H    -4.394071   -3.003194   -1.042434
C    -4.902245   -2.122980   -2.510460
H    -4.315409   -3.815731   -2.640896
H     1.249220    1.304927   -1.658280
C     0.343620    2.355321    0.383854
C     0.478862    3.453453   -0.479160
C     1.214689    2.265209    1.478870
C     1.437973    4.437052   -0.245252
H    -0.158572    3.554193   -1.351405
C     2.147809    3.268474    1.730156
H     1.197130    1.393149    2.116366
C     2.264122    4.357890    0.872104
H     1.526194    5.268784   -0.938337
H     2.808925    3.172421    2.586515
H     3.005457    5.129272    1.061847
C    -2.110753    2.242826   -0.923248
C    -2.417040    2.101519   -2.277327
C    -2.618351    3.366970   -0.251143
C    -3.204778    3.045737   -2.943123
H    -2.043719    1.252015   -2.839166
C    -3.400842    4.310115   -0.906383
H    -2.389220    3.514391    0.802771
C    -3.698094    4.151967   -2.262008
H    -3.427614    2.908099   -3.997514
H    -3.776399    5.171447   -0.360992
H    -4.307683    4.887970   -2.778478
C    -2.092701    0.857693    1.491490
C    -1.564476    0.725230    2.783547
C    -3.482232    0.901714    1.335218
C    -2.407309    0.634694    3.887890
H    -0.496433    0.659877    2.934593
C    -4.322293    0.785613    2.441062
H    -3.918308    1.009570    0.351328
C    -3.790222    0.653700    3.720919
H    -1.974163    0.532374    4.878402
H    -5.398100    0.801562    2.292888
C    -4.447516    0.567582    4.581647
H     2.126806   -0.604119   -1.080777
```

```
O     1.672315   -1.630809   -0.229549
O     0.670349   -1.458696    0.794925
O     0.240363   -0.195825    0.962176
C     2.776869   -1.450176   -2.204395
F     1.864526   -2.220688   -2.828233
F     3.325689   -0.658272   -3.142918
F     3.733035   -2.261852   -1.750285
F     1.392701   -1.818146    2.133072
F     2.131947   -2.931560    2.031656
F     2.200508   -0.831624    2.552698
F     0.496233   -2.013704    3.115188
C     3.254790    0.224165   -0.450163
C     3.590087    1.509239   -0.883351
C     4.061399   -0.389560    0.512298
C     4.674144    2.184977   -0.326901
H     3.023068    2.009276   -1.662642
C     5.136708    0.288340    1.077536
H     3.844177   -1.407606    0.814946
C     5.443868    1.583462    0.664394
H     4.908237    3.189113   -0.669545
H     5.739141   -0.202614    1.836355
H     6.284025    2.113841    1.103994
C    -0.385966   -2.555847    0.558028
C    -1.617064   -2.486628    1.211626
C    -0.101038   -3.664158   -0.244952
C    -2.559213   -3.501211    1.049919
H    -1.844379   -1.638895    1.848233
C    -1.044053   -4.676932   -0.406435
H     0.857104   -3.726732   -0.749282
C    -2.275923   -4.600038    0.241146
H    -3.515258   -3.425962    1.561732
H    -0.811884   -5.528606   -1.039537
H    -3.010031   -5.391938    0.116498
```

Pph-γ-ts6cc (TS involving a C—O ring closure)

```
E(ele)      = -2745.196140
E(ele+zpe)  = -2744.572285
H           = -2744.528773
G           = -2744.648809
```

```
C     0.820407    1.055097   -1.655284
H     0.154855    1.511028   -2.376180
C    -0.898212   -0.687033   -1.424752
C     0.344189    0.009490   -0.880450
H    -0.781130   -0.781464   -2.508146
P     1.547886   -1.079427    0.069853
C     2.067950    1.693230   -1.392021
O     2.925151    1.275933   -0.613237
C     2.257089    2.816866   -2.113255
O     3.487728    3.483006   -1.876050
H     3.590129    3.733356   -0.817344
C     4.333403    2.856742   -2.174217
H     3.455594    4.390381   -2.478948
C    -0.973663   -1.694425   -1.027841
C     0.624007   -2.602915    0.533790
C     1.136416   -3.860086    0.192497
C    -0.602685   -2.533179    1.216552
C     0.452818   -5.021561    0.545520
H     2.065743   -3.948311   -0.358207
C    -1.281064   -3.697543    1.558262
H    -1.049887   -1.568439    1.435017
C    -0.754150   -4.944454    1.230828
H     0.866972   -5.986948    0.271842
C    -2.238667   -3.618733    2.063645
H    -1.289481   -5.850521    1.497807
C     2.891499   -1.661686   -0.999916
C     2.804105   -1.511268   -2.386195
C     3.981821   -2.341107   -0.442195
C     3.806030   -2.028296   -3.203137
H     1.971374   -0.967964   -2.821060
C     4.977727   -2.855510   -1.265053
H     4.050101   -2.473220    0.634413
C     4.891204   -2.698054   -2.646727
H     3.736408   -1.901458   -4.278794
H     5.821424   -3.377515   -0.824933
H     5.669923   -3.098216   -3.288634
C     2.258529   -0.461035    1.636240
C     1.481316   -0.474298    2.800412
C     3.582774   -0.015205    1.693712
C     2.024230   -0.040785    4.004236
H     0.445069   -0.785520    2.767685
C     4.122074    0.401585    2.906935
H     4.177194    0.037722    0.790744
C     3.345557    0.394095    4.061586
H     1.406726   -0.038943    4.896432
H     5.149602    0.749423    2.940657
C     3.766236    0.733438    5.003347
O    -2.249126    0.050075   -1.118685
O    -2.145330    1.270278   -0.417163
O    -1.187241    1.425426    0.640605
C    -0.349622    0.376476    0.743457
O    -2.825374    0.525219   -2.466307
F    -1.988953    1.357844   -3.100035
F    -3.036465   -0.521047   -3.281837
F    -3.983978    1.164933   -2.310179
F    -1.978049    1.472877    1.969358
F    -3.013397    2.318535    1.897717
F    -2.459950    0.265709    2.307495
F    -1.189629    1.866805    2.976477
C    -3.307182   -0.873053   -0.501412
C    -3.373832   -2.232449   -0.814323
C    -4.304963   -0.317653    0.301799
C    -4.383509   -3.033042   -0.287313
H    -2.646138   -2.682649   -1.482941
C    -5.311735   -1.117165    0.831615
H    -4.276358    0.743769    0.519764
C    -5.350437   -2.479511    0.546123
H    -4.411974   -4.090159   -0.534188
H    -6.070042   -0.671629    1.468127
C    -6.136578   -3.103466    0.960661
C    -0.494215    2.775602    0.442599
C     0.728594    2.995378    1.077468
C    -1.067618    3.781725   -0.331163
C     1.383746    4.211726    0.918833
H     1.179045    2.197876    1.662427
```

```
C    -0.405308    4.996067   -0.492043
H    -2.013438    3.596879   -0.829322
C     0.820609    5.213654    0.130458
H     2.341274    4.372359    1.406497
H    -0.847224    5.771683   -1.110388
H     1.336549    6.160727    0.000718
```

six-membered intermediate

```
E(ele)      = -2745.200370
E(ele+zpe)  = -2744.576471
H           = -2744.532568
G           = -2744.654758
```

```
C     0.772127    1.120115   -1.624634
H     0.210215    1.399020   -2.503763
C    -0.898381   -0.669446   -1.388975
C     0.259701    0.107642   -0.749992
H    -0.738048   -0.704537   -2.468893
P     1.625120   -1.049190    0.073394
O     1.966350    1.770674   -1.301835
O     2.715663    1.433647   -0.366147
C     2.301264    2.804688   -2.117163
C     3.512818    3.457252   -1.782934
H     3.456797    3.888307   -0.778832
C     4.359018    2.764962   -1.818257
H     3.640937    4.247226   -2.523729
H    -0.925472   -1.695828   -1.034748
C     0.795977   -2.646860    0.446408
C     1.387693   -3.864572    0.095297
C    -0.452410   -2.657200    1.089243
C     0.755120   -5.067851    0.399935
H     2.341192   -3.882535   -0.422241
C    -1.081177   -3.861284    1.385705
H    -0.954476   -1.722984    1.326637
C    -0.476244   -5.069485    1.046802
H     1.228063   -6.004803    0.122580
C    -2.054600   -3.846462    1.866249
H    -0.969086   -6.009047    1.277263
C     2.963798   -1.473867   -1.063101
C     2.761222   -1.337978   -2.439952
C     4.157543   -2.029148   -0.585303
C     3.760158   -1.731590   -3.326981
H     1.843860   -0.894980   -2.812666
C     5.147336   -2.422270   -1.478916
H     4.310820   -2.158969    0.482443
C     4.951081   -2.269611   -2.850252
H     3.603405   -1.613505   -4.394435
H     6.072359   -2.847671   -1.102805
H     5.726463   -2.575655   -3.545905
C     2.290013   -0.508404    1.686022
C     1.502575   -0.636815    2.834388
C     3.568442    0.051664    1.785216
C     1.993376   -0.222967    4.068217
H     0.496455   -1.035192    2.775400
C     4.061574    0.437719    3.026719
H     4.153785    0.222442    0.890220
C     3.277157    0.304508    4.168922
H     1.365787   -0.311320    4.949168
H     5.055905    0.867687    3.094858
C     3.660284    0.624032    5.133295
C    -2.286648   -0.016969   -1.086561
O    -2.235352    1.198610   -0.354543
O    -1.226283    1.448510    0.600332
C    -0.240257    0.480747    0.607381
C    -2.879433    0.461648   -2.424490
F    -2.076661    1.337977   -3.036880
F    -3.049621   -0.577857   -3.256561
F    -4.062321    1.051939   -2.251286
F    -1.861471    1.312503    2.001728
F    -2.941235    2.090388    2.109180
F    -2.241783    0.047581    2.248209
F    -0.997633    1.652685    2.960897
C    -3.301160   -0.986772   -0.473061
C    -3.323933   -2.337161   -0.828168
C    -4.295458   -0.494373    0.374406
C    -4.292350   -3.190161   -0.305390
H    -2.593428   -2.737860   -1.524659
C    -5.259431   -1.347340    0.900767
H    -4.299761    0.558062    0.631269
C    -5.275634   -2.699623    0.568480
H    -4.289339   -4.239088   -0.586334
H    -6.015406   -0.951482    1.571702
C    -6.010154   -3.365497    0.979836
C    -0.694011    2.861452    0.417082
C     0.513146    3.200698    1.029594
C    -1.406682    3.809731   -0.311129
C     1.014705    4.489367    0.890818
H     1.076716    2.442427    1.565338
C    -0.899261    5.099895   -0.442629
C    -2.336055    3.526875   -0.793856
H     0.309928    5.441056    0.155699
C     1.962119    4.748171    1.354551
H    -1.447930    5.836966   -1.020985
H     0.706272    6.446190    0.046417
```

transition state involving release of Pph

```
E(ele)      = -2745.199770
E(ele+zpe)  = -2744.576566
H           = -2744.532762
G           = -2744.656961
```

```
C     0.717256    1.163615   -1.656113
C     0.282194    1.293782   -2.636819
C    -0.922915   -0.656576   -1.387729
C     0.211083    0.167977   -0.789097
H    -0.791233   -0.711685   -2.471197
P     1.679115   -1.067331    0.069580
C     1.872637    1.886397   -1.291660
O     2.574951    1.624868   -0.306584
O     2.202463    2.892106   -2.140139
C     3.362922    3.619286   -1.774688
H     3.235330    4.079257   -0.790684
C     4.242921    2.970337   -1.745643
H     3.486145    4.388594   -2.537430
H    -0.902042   -1.675032   -1.009219
```

C	0.905775	-2.700977	0.378958		F	0.352698	-0.067575	2.852218
C	1.517894	-3.891959	-0.025067		F	-1.776830	-0.428044	2.754329
C	-0.347776	-2.756971	1.009028		F	-0.391548	-2.091996	2.676526
C	0.897789	-5.115851	0.215787		F	3.048269	-2.240632	-0.604491
H	2.478428	-3.867441	-0.530464		F	2.830836	-1.110575	-2.442008
C	-0.963271	-3.981711	1.244488		F	1.336944	-2.569701	-1.878394
H	-0.861195	-1.839723	1.289156					
C	-0.339302	-5.163557	0.851660					
H	1.384538	-6.033517	-0.099929					
H	-1.939692	-4.003801	1.718667					
H	-0.820939	-6.119758	1.031991					
C	3.048050	-1.396438	-1.064140					
C	2.819070	-1.252575	-2.436506					
C	4.289664	-1.861385	-0.611743					
C	3.831996	-1.552101	-3.344477					
H	1.862661	-0.883951	-2.791855					
C	5.293882	-2.162395	-1.524674					
H	4.466011	-1.992114	0.452264					
C	5.067447	-2.002785	-2.891080					
H	3.652601	-1.429172	-4.407826					
H	6.253758	-2.523014	-1.168614					
H	5.855074	-2.234324	-3.601668					
C	2.338478	-0.553254	1.692465					
C	1.601894	-0.809589	2.853689					
C	3.546870	0.147080	1.787237					
C	2.075756	-0.389845	4.092192					
H	0.652506	-1.330893	2.804113					
C	4.024957	0.543247	3.031544					
H	4.090915	0.410707	0.888729					
C	3.292371	0.279281	4.185579					
H	1.489527	-0.589475	4.983495					
H	4.966462	1.080029	3.093761					
H	3.663060	0.603992	5.153034					
C	-2.320498	-0.045542	-1.056945					
O	-2.285624	1.143209	-0.281471					
C	-1.247970	1.420983	0.630216					
O	-0.202759	0.508405	0.571440					
C	-2.932617	0.470624	-2.370995					
F	-2.147292	1.381311	-2.953997					
F	-3.095431	-0.539568	-3.240208					
F	-4.122753	1.035816	-2.164879					
C	-1.819312	1.206047	2.048213					
F	-2.918897	1.942005	2.226838					
F	-2.152314	-0.080494	2.246265					
F	-0.933654	1.532726	2.990192					
C	-3.304926	-1.055634	-0.464195					
C	-3.303319	-2.391468	-0.870590					
C	-4.289264	-0.618124	0.423552					
C	-4.243074	-3.285306	-0.363255					
H	-2.574889	-2.747285	-1.593453					
C	-5.223968	-1.512469	0.934221					
H	-4.307840	0.423254	0.724664					
C	-5.201005	-2.849976	0.547208					
H	-4.223171	-4.322454	-0.684305					
H	-5.974120	-1.159927	1.635202					
H	-5.931219	-3.547374	0.946282					
C	-0.798926	2.862272	0.459807					
C	0.392161	3.262809	1.066520					
C	-1.567262	3.774870	-0.258401					
C	0.819440	4.579331	0.935246					
H	1.002697	2.532028	1.587740					
C	-1.133904	5.091758	-0.382739					
H	-2.483209	3.444529	-0.736368					
C	0.057834	5.495641	0.212458					
H	1.753779	4.887682	1.395301					
H	-1.726372	5.800815	-0.952789					
H	0.395907	6.522644	0.110444					

γ-6cc

E(ele)	= -1709.253911
E(ele+zpe)	= -1708.908419
H	= -1708.880953
G	= -1708.966771

C	-1.076987	2.125602	-1.293767
H	-0.817952	2.450487	-2.294638
C	0.348761	0.073071	-1.605690
C	-0.525701	1.002161	-0.815585
C	1.397099	-0.523719	-0.657115
H	0.805133	0.587582	-2.451795
C	-0.541794	-0.734290	0.751788
O	-0.690601	0.638991	0.484898
H	-0.261037	-0.746668	-2.005237
C	-2.050527	2.940583	-0.544136
O	-2.651495	2.610798	0.453478
O	-2.231956	4.131300	-1.150197
C	-3.189838	4.987132	-0.527568
H	-4.171580	4.507595	-0.510483
H	-2.886022	5.214654	0.496723
H	-3.212700	5.891542	-1.133645
O	0.736770	-1.215860	0.401121
C	-0.591336	-0.825984	2.291892
C	-1.663556	-1.541309	0.118963
C	-1.454559	-2.869347	-0.251655
C	-2.911716	-0.939238	-0.063619
C	-2.497097	-3.596547	-0.821881
H	-0.479285	-3.321967	-0.103438
C	-3.947869	-1.673578	-0.635873
H	-3.063646	0.095051	0.240242
C	-3.741869	-2.998770	-1.016617
H	-2.334826	-4.629215	-1.115865
H	-4.917765	-1.208118	-0.783273
H	-4.551953	-3.566580	-1.465321
C	2.383876	0.499015	-0.099594
C	2.781399	1.611135	-0.845371
C	2.933289	0.294113	1.168280
C	3.705297	2.514661	-0.324527
H	2.380988	1.787974	-1.838964
C	3.857561	1.196839	1.686576
H	2.626724	-0.568636	1.749481
C	4.243706	2.310764	0.943272
H	3.999669	3.378987	-0.912030
H	4.273744	1.030142	2.675555
H	4.960759	3.017332	1.350613
C	2.165972	-1.629841	-1.397095

Acknowledgement

References

(1) Pei, C.-K.; Wu, L.; Lian, Z.; Shi, M. *Org. Biomol. Chem.* **2012**, *10*, 171–80.

(2) Wang, X.; Fang, T.; Tong, X. *Angew. Chem. Int. Ed.* **2011**, *50*, 5361–4.

(3) Ashtekar, K. D.; Staples, R. J.; Borhan, B. *Org. Lett.* **2011**, *13*, 5732–5.

(4) Chen, X.-y.; Wen, M.-w.; Ye, S.; Wang, Z.-x. *Org. Lett.* **2011**, *13*, 1138–41.