**Supplementary information for**

# Sigmatropic rearrangements in 5-allyloxytetrazoles

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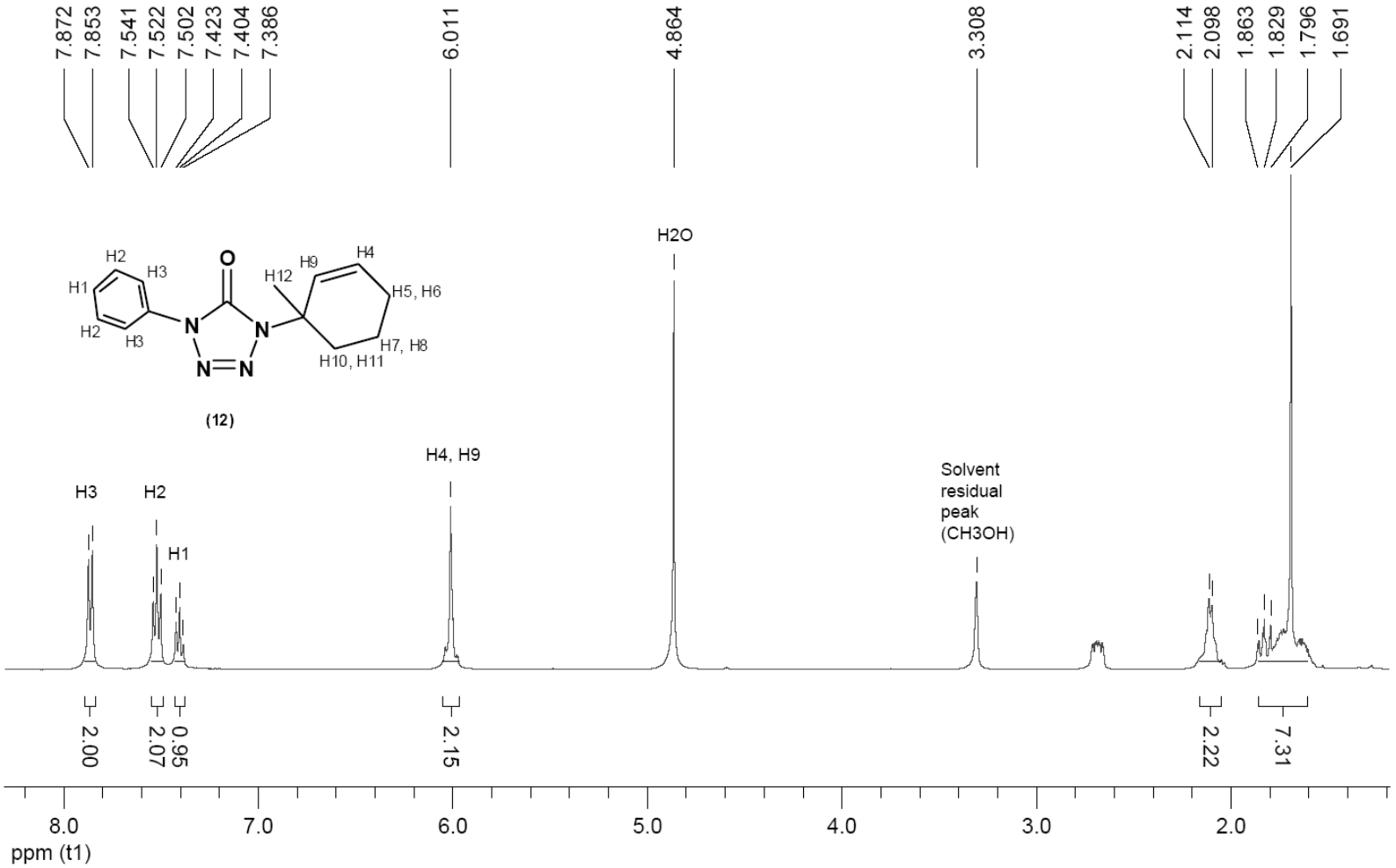


**Figure 1S.** $^{1}$H-NMR spectrum of 4-(3-methylcyclohex-2-enyl)-1-phenyl-1*H*-tetrazol-5(4*H*)-one (**12**) (400 MHz, $CD_3OD$).

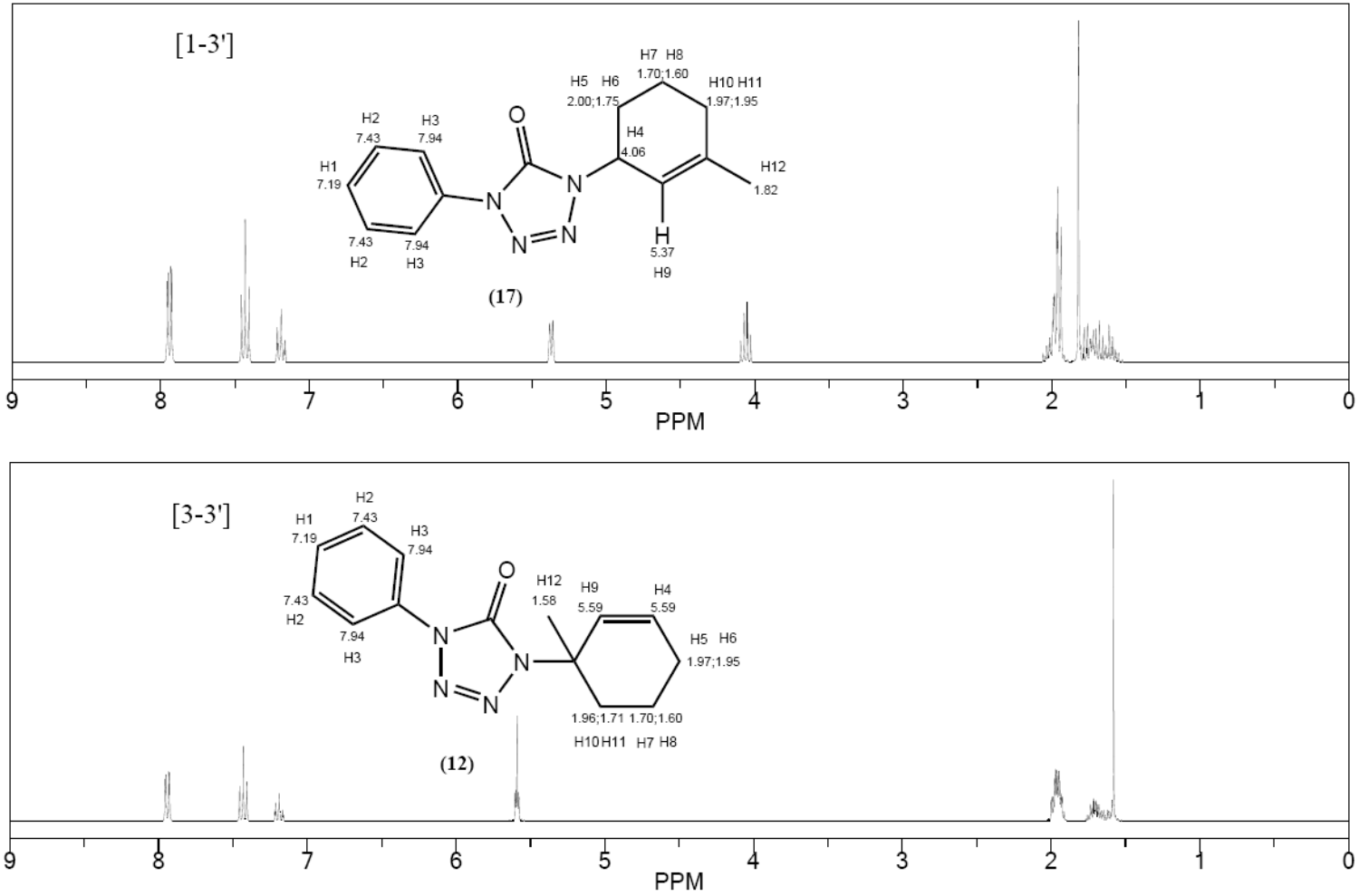


**Figure 2S.** Predicted $^{1}$H-NMR spectra of tetrazolones **17** and **12** ([1,3]- and [3,3]- migration products).
($^{1}$H-NMR shifts were acquired using the ChemDraw (Ultra 9.0) software)

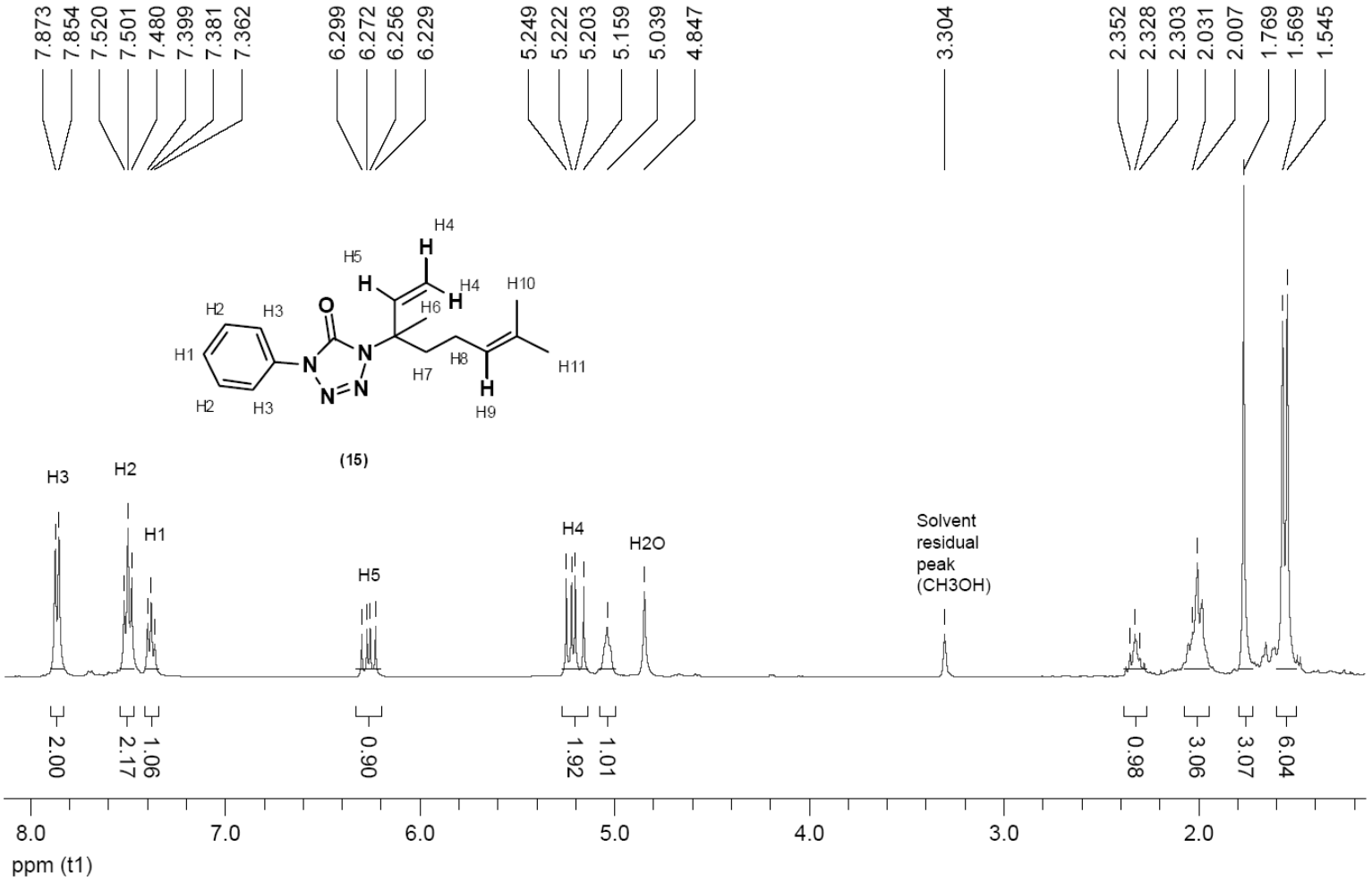


**Figure 3S.** $^{1}$H-NMR spectrum of 1-(3,7-dimethylocta-1,6-dien-3-yl)-4-phenyl-1*H*-tetrazol-5(4*H*)-one (**15**) (400 MHz, $CD_3OD$).

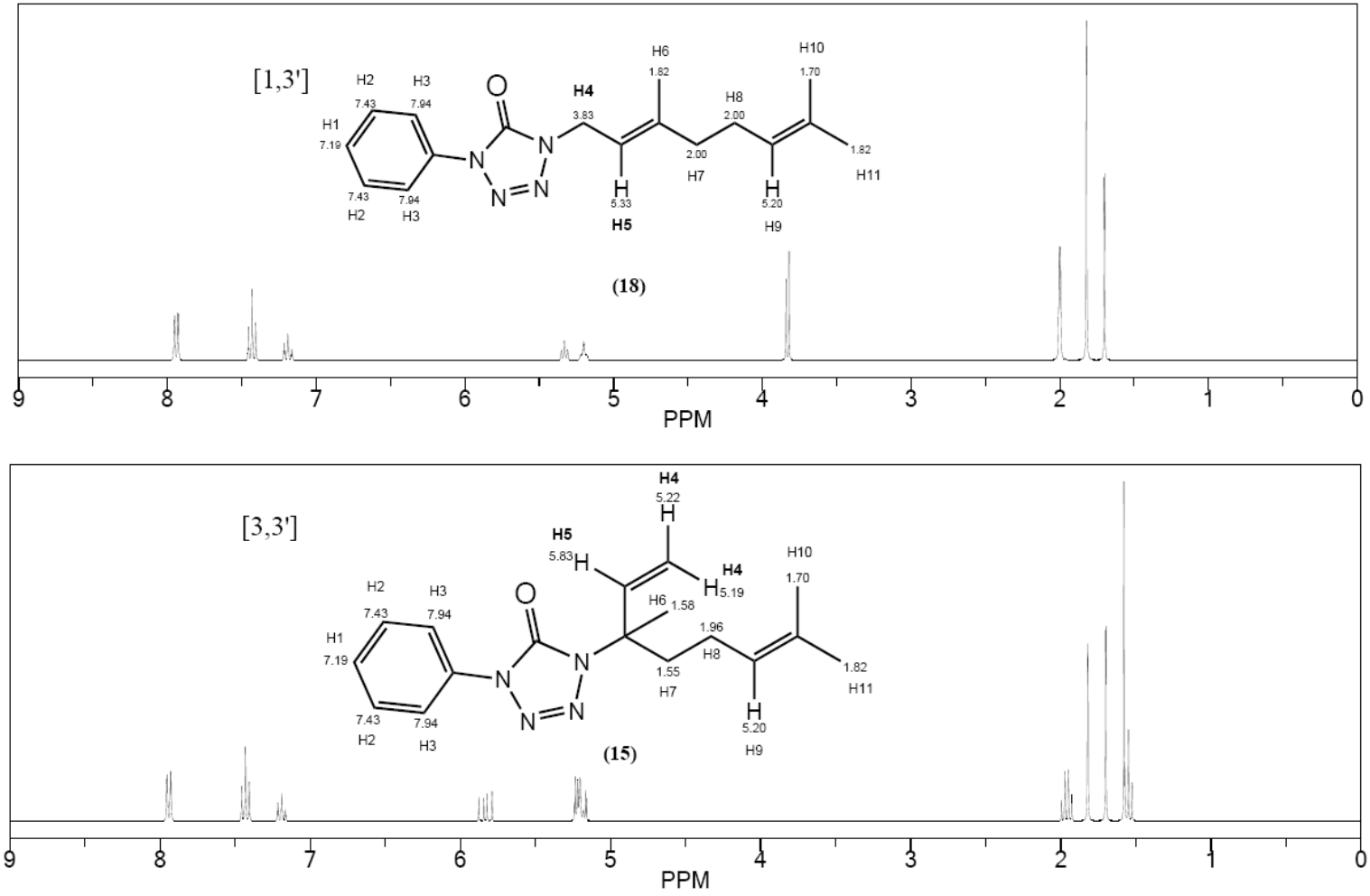


**Figure 4S.** Predicted $^{1}$H-NMR spectra of tetrazolones **18** and **15** ([1,3]- and [3,3]- migration products).
($^{1}$H-NMR shifts were acquired using the ChemDraw (Ultra 9.0) software)

**Table 1S.** Conformationally relevant geometric parameters and relative energies of conformers of 5-(Cyclohex-2-enyloxy)-1-phenyl-1*H*-tetrazole **9** [in brief: Ether **9** (R)] and corresponding isomeric 1-(cyclohex-2-enyl)-4-phenyltetrazol-5-one **16** [in brief: Tetrazolone **16** (R)] calculated at the DFT(B3LYP)/6-31G(d,p) level of theory.

| Compound / Conformer | | Dihedral angle / degrees | | | | Relative energy / kJ mol$^{-1}$ | | |
|---|---|---|---|---|---|---|---|---|
| Nº | Ether **9** (R) | A | B | C | D | $\Delta E_{el}$ | $\Delta E_{ZPE}$ | $\Delta E_G$ |
| 1 | $Ph^+TG^-G^-$ | 22.3 | 179.1 | −83.6 | −59.6 | 0.00 | 0.00 | 0.00 |
| 2 | $Ph^+TTG^-$ | 28.3 | 177.6 | −158.0 | −58.9 | 0.14 | 0.04 | 0.53 |
| 3 | $Ph^-TTG^-$ | −27.0 | −176.9 | −163.3 | −59.6 | 0.21 | 0.37 | 0.83 |
| 4 | $Ph^-TG^-G^-$ | −20.5 | −175.8 | −82.6 | −59.4 | 0.34 | 0.47 | 0.99 |
| 5 | $Ph^-TG^-G^+$ | −24.9 | −176.3 | −81.2 | 60.7 | 0.82 | 0.63 | 1.05 |
| 6 | $Ph^+TG^-G^+$ | 21.9 | 177.8 | −80.7 | 60.7 | 1.39 | 1.23 | 0.73 |
| 7 | $Ph^+TTG^+$ | 27.6 | 176.8 | −155.6 | 60.9 | 2.01 | 1.81 | 1.65 |
| 8 | $Ph^-TTG^+$ | −26.4 | −178.8 | −158.6 | 60.9 | 2.42 | 2.27 | 2.28 |
| 9 | $Ph^+TG^+G^+$ | 28.7 | 170.2 | 68.0 | 60.8 | 11.63 | 11.55 | 12.57 |
| 10 | $Ph^-TG^+G^+$ | −28.2 | 179.6 | 65.6 | 61.0 | 12.22 | 11.86 | 12.27 |
| 11 | $Ph^+TG^+G^-$ | 30.5 | 160.5 | 77.4 | −52.9 | 17.00 | 16.65 | 17.25 |
| 12 | $Ph^-TG^+G^-$ | −28.3 | 172.7 | 71.9 | −52.3 | 18.11 | 17.58 | 16.85 |
| Nº | Tetrazolone **16** (R) | A | | C | D | $\Delta E_{el}$ | $\Delta E_{ZPE}$ | $\Delta E_G$ |
| 1 | $CG^+$ | −0.7 | | 5.0 | 60.8 | −69.31 | −68.22 | −68.35 |
| 2 | $CG^-$ | 0.1 | | 9.9 | −59.2 | −68.08 | −66.70 | −66.66 |
| 3 | $TG^+$ | 1.7 | | 178.7 | 60.9 | −65.43 | −64.54 | −64.84 |
| 4 | $TG^-$ | 3.6 | | −171.5 | −57.5 | −62.46 | −61.06 | −61.25 |
| | | Distance / pm | | | | | | |
| Nº | TS type | OC(1) | OC(3) | NC(1) | NC(3) | $\Delta E_{el}$ | $\Delta E_{ZPE}$ | $\Delta E_G$ |
| 1 | 1,3'-shift | 273.7 | 338.0 | 270.5 | 394.1 | 161.89 | 150.32 | 149.67 |
| 2 | 1,3'-shift | 266.1 | 400.0 | 267.8 | 332.8 | 160.49 | 149.06 | 148.31 |
| 3 | 3,3'-shift | 230.5 | 331.6 | 339.5 | 244.8 | 115.41 | 107.50 | 110.76 |
| 4 | 3,3'-shift | 224.0 | 328.3 | 333.6 | 239.1 | 107.37 | 100.06 | 102.77 |

Definition of the geometric parameters (see also Figure 1 for the graphical representation). Compound "Ether" (R-enantiomer): A is defined as CCNC dihedral angle; B is defined as N−COC dihedral angle; C is defined as COC(1)C(6); D is defined as C(1)C(6)C(5)C(4) dihedral angle. Compound "Tetrazolone" resulting from 1,3'-shift (R-enantiomer): A is defined as CCNC dihedral angle; dihedral angle "B" (analogous of ether) is not applicable; C is defined as C−NC(1)H dihedral angle; D is defined as C(1)C(6)C(5)C(4). By the nature of compound, the structures resulting from the 3,3'-shift represent S-enantiomeric variety and otherwise are symmetrically identical to R-structures resulting from the 1,3'-shift. "TS" stands for transition state. Numbering of the carbon atoms corresponds to that of the starting compound. Nitrogen atom is N(5) of the ether. All relative energies are calculated with respect to $Ph^+TG^-G^-$ conformer (Nº1) of Ether **9**. $\Delta E_{el}$, $\Delta E_{ZPE}$, $\Delta E_G$ state for the relative electronic, zero-point-corrected and Gibbs free energy (at 298.15 K), respectively. The absolute values calculated for the most stable conformer $Ph^+TG^-G^-$ of Ether **9** at the DFT(B3LYP)/6-31G(d,p) level are: $E_{el}$=−797.995940; $E_{ZPE}$=−797.736523, $E_G$=−797.780470 hartree.

**Table 2S.** Conformationally relevant geometric parameters and relative energies of conformers of 5-(Cyclohex-2-enyloxy)-1-phenyl-1*H*-tetrazole **9** [in brief: Ether **9** (R)] and corresponding isomeric 1-(cyclohex-2-enyl)-4-phenyltetrazol-5-one **16** [in brief: Tetrazolone **16** (R)] calculated at the MP2/6-31G(d,p) level of theory.

| Compound / Conformer | | Dihedral angle / degrees | | | | Relative Energy |
|---|---|---|---|---|---|---|
| Nº | Ether **9** (R) | A | B | C | D | $\Delta E_{el}$ |
| 1 | $Ph^{+}TTG^{-}$ | 36.6 | −180.0 | −164.9 | −62.2 | 0.00 |
| 2 | $Ph^{-}TTG^{-}$ | −35.2 | −173.7 | −168.4 | −62.6 | 0.06 |
| 3 | $Ph^{+}TG^{-}G^{-}$ | 33.7 | 174.4 | −78.9 | −62.8 | 0.96 |
| 4 | $Ph^{-}TG^{-}G^{-}$ | −34.1 | −177.1 | −79.9 | −62.6 | 1.32 |
| 5 | $Ph^{-}TG^{-}G^{+}$ | −34.6 | −177.0 | −78.2 | 63.6 | 3.90 |
| 6 | $Ph^{+}TG^{-}G^{+}$ | 34.8 | 175.9 | −76.7 | 63.6 | 4.31 |
| 7 | $Ph^{+}TTG^{+}$ | 35.6 | 177.4 | −161.4 | 63.9 | 4.32 |
| 8 | $Ph^{-}TTG^{+}$ | −35.1 | −177.7 | −163.1 | 63.8 | 4.64 |
| 9 | $Ph^{+}TG^{+}G^{+}$ | 36.8 | 167.0 | 71.1 | 63.4 | 11.16 |
| 10 | $Ph^{-}TG^{+}G^{+}$ | −37.1 | 177.6 | 67.4 | 63.5 | 11.88 |
| 11 | $Ph^{+}A^{+}G^{+}G^{-}$ | 38.6 | 91.6 | 104.6 | −60.4 | 13.03 |
| 12 | $Ph^{-}A^{+}G^{+}G^{-}$ | −39.4 | 157.3 | 86.4 | −56.4 | 19.18 |
| Nº | Tetrazolone **16** (R) | A | B | C | D | $\Delta E_{el}$ |
| 1 | $Ph^{-}CG^{+}$ | −22.2 | −25.7 | 91.4 | 62.7 | −67.54 |
| 2 | $Ph^{+}CG^{+}$ | 22.3 | −26.7 | 90.3 | 62.8 | −67.52 |
| 3 | $Ph^{-}CG^{-}$ | −22.9 | −9.6 | 108.1 | −63.6 | −65.74 |
| 4 | $Ph^{+}CG^{-}$ | 23.1 | −10.5 | 107.2 | −63.6 | −65.74 |
| 5 | $Ph^{+}TG^{+}$ | 23.8 | 179.8 | 61.7 | 63.7 | −63.52 |
| 6 | $Ph^{-}TG^{+}$ | −23.5 | −179.9 | 62.0 | 63.7 | −63.38 |
| 7 | $Ph^{+}TG^{-}$ | 25.6 | −164.5 | 78.5 | −60.8 | −62.16 |
| 8 | $Ph^{-}TG^{-}$ | −25.3 | −164.2 | 78.8 | −60.8 | −61.97 |
| | | Distance / pm | | | | |
| Nº | TS type | OC(1) | OC(3) | NC(1) | NC(3) | $\Delta E_{el}$ |
| 1 | 1,3'-shift | 271.4 | 312.5 | 264.7 | 376.6 | 213.87 |
| 2 | 1,3'-shift | 261.3 | 377.6 | 267.5 | 311.4 | 209.60 |
| 3 | 3,3'-shift | 204.6 | 310.8 | 319.8 | 213.9 | 128.27 |
| 4 | 3,3'-shift | 215.7 | 317.0 | 328.2 | 220.8 | 121.62 |

For the definition of the geometric parameters see caption of Table 1S and also Figure 1 for the graphical representation. All relative electronic energies ($\Delta E_{el}$, in kJ $mol^{-1}$) are calculated with respect to $Ph^{+}TTG^{-}$ conformer (Nº1) of Ether **9**. The absolute value calculated for $Ph^{+}TTG^{-}$ conformer at the MP2/6-31G(d,p) level is $E_{el}$=−795.620869 hartree.

**Table 3S.** Conformationally relevant geometric parameters and relative energies of conformers of (E)-5-(3,7-dimethylocta-2,6-dienyloxy)-1-phenyl-1*H*-tetrazole (**14**) [in brief: Ether **14**] and corresponding isomeric 1-(3,7-dimethylocta-1,6-dien-3-yl)-4-phenyl-1*H*-tetrazol-5(4*H*)-one (**15**) [in brief: Tetrazolone **15** (R)] and isomeric (E)-1-(3,7-dimethylocta-2,6-dienyl)-4-phenyl-1H-tetrazol-5(4*H*)-one (**18**) [in brief: Tetrazolone **18**] calculated at the DFT(B3LYP)/6-31G(d,p) level of theory for selected structures.

| Compound / Form | | Dihedral angle / degrees | | | | | | | | Relative energy / kJ mol$^{-1}$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| No. | Ether **14** | A | B | C | O12=3 | 12=34 | 2=345 | 3456 | 456=7 | $\Delta E_{el}$ | $\Delta E_{ZPE}$ | $\Delta E_G$ |
| 1 | $Ph^+TG^-A^+CA^-TA^-$ | 27.4 | 171.7 | −82.9 | 131.8 | −0.7 | −104.5 | −173.6 | −111.7 | 0.00 | 0.00 | 0.00 |
| 2 | $Ph^-TG^+A^-CA^-TA^+$ | −26.8 | −171.5 | 84.2 | −120.5 | 0.3 | −89.2 | −178.5 | 119.8 | 1.45 | 1.17 | −0.98 |
| 3 | $Ph^+TG^-A^+TA^-TA^+$ | 26.1 | 171.3 | −85.1 | 119.6 | 177.2 | −115.0 | 176.2 | 115.5 | 1.50 | 1.20 | −0.95 |
| 4 | $Ph^-TG^-A^+TA^-TA^+$ | −25.8 | 175.9 | −87.2 | 118.9 | 177.1 | −114.5 | 176.4 | 116.8 | 1.64 | 1.53 | −1.53 |
| 5 | $Ph^+TG^-A^+TA^+TA^+$ | 25.4 | 171.1 | −85.1 | 118.1 | 178.7 | 103.0 | 175.0 | 115.2 | 1.91 | 1.56 | −1.50 |
| 6 | $Ph^-TG^-A^+TA^+TA^+$ | −25.0 | 175.9 | −86.5 | 118.9 | 178.2 | 105.6 | 175.8 | 118.9 | 2.11 | 1.58 | −1.89 |
| 7 | $Ph^+TG^+A^-CA^-TA^+$ | 26.0 | −176.2 | 86.8 | −120.0 | 0.3 | −90.8 | −178.8 | 119.0 | 1.49 | 1.69 | 0.87 |
| 8 | $Ph^-TG^-A^+CA^-TA^+$ | −25.3 | 176.4 | −85.6 | 117.9 | −0.5 | −119.4 | 173.2 | 112.0 | 2.53 | 2.45 | 0.17 |
| 9 | $Ph^+T\ T\ A^+CA^-TA^-$ | 21.8 | 177.6 | 175.1 | 90.0 | −1.8 | −95.5 | −175.9 | −116.8 | 3.05 | 2.46 | −0.47 |
| 10 | $Ph^+TG^-A^+T\ C\ TA^+$ | 26.3 | 171.4 | −84.9 | 119.7 | 177.4 | −2.3 | 177.6 | 116.0 | 3.20 | 2.54 | −1.07 |
| 11 | $Ph^+TG^-A^+CA^-TA^+$ | 26.5 | 171.7 | −83.9 | 117.7 | −0.7 | −120.6 | 172.9 | 111.1 | 2.31 | 2.60 | 1.51 |
| 12 | $Ph^-TG^-A^+T\ C\ TA^+$ | −26.2 | 176.3 | −87.5 | 119.3 | 177.1 | −2.3 | 177.9 | 117.0 | 3.32 | 2.65 | 0.30 |
| 13 | $Ph^+T\ T\ A^+CA^-TA^+$ | 22.2 | 178.7 | 176.0 | 92.0 | −1.9 | −92.0 | 179.3 | 116.7 | 3.97 | 3.08 | −2.53 |
| 14 | $Ph^-T\ T\ A^+CA^-TA^+$ | −23.3 | −176.6 | 176.9 | 109.2 | −1.9 | −93.0 | −180.0 | 116.4 | 4.36 | 3.56 | −3.02 |
| 15 | $Ph^-TG^+A^+CA^-TA^+$ | −26.9 | −176.0 | 74.1 | 89.4 | −1.5 | −91.0 | −179.5 | 117.3 | 3.85 | 3.91 | 1.56 |
| 16 | $Ph^-TG^-A^-CA^-TA^+$ | −26.2 | −178.5 | −80.6 | −112.9 | −0.3 | −97.4 | 179.9 | 116.7 | 4.33 | 4.10 | 0.01 |
| 17 | $Ph^+TG^+A^+CA^-TA^+$ | 26.1 | 177.1 | 78.3 | 101.3 | −1.6 | −93.8 | −179.8 | 117.7 | 4.65 | 4.38 | −0.02 |
| 18 | $Ph^+TG^-A^-CA^-TA^+$ | 25.2 | 177.6 | −77.5 | −108.9 | 0.0 | −98.1 | 179.6 | 117.4 | 4.83 | 4.50 | −0.86 |
| 19 | $Ph^+TG^+A^+CA^-GA^+$ | 24.4 | 176.0 | 74.5 | 95.1 | −1.6 | −124.3 | 59.4 | 129.6 | 7.28 | 7.75 | 7.05 |
| No. | Tetrazolone **15** (R) | A | | CN39 | | 1=234 | 2345 | 3456 | 456=7 | $\Delta E_{el}$ | $\Delta E_{ZPE}$ | $\Delta E_G$ |
| 1 | $T\ A^+\ T\ \ T\ A^+$ | −2.8 | | −170.1 | | 132.6 | 179.6 | 173.2 | 116.6 | −43.50 | −45.32 | −44.11 |
| 2 | $T\ \ C\ T\ \ T\ A^+$ | 1.4 | | −178.1 | | −4.1 | −179.2 | 172.0 | 117.3 | −43.55 | −44.68 | −41.78 |
| 3 | $G^+A^-T\ \ T\ A^+$ | 0.7 | | 49.4 | | −120.5 | 178.9 | 173.8 | 114.8 | −42.85 | −44.18 | −43.45 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | $G^-A^+G^+T\ A^+$ | −2.5 | −70.2 | | 93.8 | 50.8 | 175.0 | 112.5 | −41.80 | −43.56 | −42.66 |
| 5 | $T\ A^+\ T\ G^+A^-$ | 1.2 | −172.6 | | 134.2 | 174.9 | 71.6 | −128.9 | −40.00 | −41.21 | −36.91 |
| 6 | $T\ A^+\ T\ G^+A^+$ | −0.3 | −172.0 | | 132.5 | 171.2 | 62.1 | 85.4 | −37.93 | −38.52 | −30.80 |
| 7 | $C\ A^+\ T\ G^+A^+$ | 0.7 | 14.9 | | 119.6 | 167.9 | 59.9 | 91.0 | −31.57 | −32.45 | −29.90 |
| 8 | $A^-A^+G^+G^+A^+$ | 1.1 | −131.9 | | 110.2 | 47.7 | 61.9 | 93.5 | −32.18 | −32.39 | −29.20 |

| No. | Tetrazolone **18** | A | CN12 | N12=3 | 12=34 | 2=345 | 3456 | 456=7 | $\Delta E_{el}$ | $\Delta E_{ZPE}$ | $\Delta E_G$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $A^-\ A^+\ C\ A^-\ T\ A^-$ | −0.1 | −88.8 | 122.4 | −0.5 | −96.5 | −172.5 | −111.2 | −78.90 | −77.48 | −77.40 |
| 2 | $A^-\ A^+\ C\ A^-\ T\ A^+$ | 0.5 | −90.1 | 118.5 | −0.6 | −99.1 | −179.2 | 113.0 | −75.19 | −74.53 | −78.14 |
| 3 | $A^-\ A^+\ C\ A^+\ T\ A^-$ | 1.5 | −89.9 | 108.3 | 0.0 | 92.2 | 178.9 | −117.5 | −74.40 | −73.54 | −77.07 |
| 4 | $A^-\ A^+\ C\ A^+\ T\ A^+$ | 1.7 | −90.2 | 108.3 | −0.2 | 94.4 | 173.3 | 117.0 | −74.16 | −73.34 | −78.31 |
| 5 | $A^+\ A^-\ C\ A^-G^+\ A^-$ | −2.7 | 89.3 | −108.0 | 0.6 | −98.1 | 74.7 | −113.7 | −73.59 | −72.72 | −75.58 |
| 6 | $A^+\ A^+\ C\ A^-\ T\ A^+$ | 1.2 | 107.6 | 112.1 | −1.4 | −96.8 | 179.6 | 116.2 | −72.86 | −72.13 | −76.27 |
| 7 | $A^+\ A^+\ T\ A^+\ T\ A^+$ | 1.0 | 107.4 | 117.5 | 179.7 | 109.0 | 178.4 | 116.5 | −71.58 | −71.58 | −79.25 |
| 8 | $A^+\ A^+\ C\ A^+\ T\ A^+$ | −0.8 | 107.5 | 116.0 | −0.3 | 97.8 | 174.6 | 117.3 | −71.98 | −71.51 | −76.69 |
| 9 | $A^+\ A^+\ C\ A^+\ T\ A^-$ | 0.7 | 104.5 | 116.2 | 0.0 | 95.6 | 179.8 | −117.3 | −71.68 | −70.98 | −75.99 |
| 10 | $A^-\ A^+\ C\ A^+G^+A^+$ | 0.2 | −88.2 | 109.2 | 0.4 | 82.9 | 56.8 | 108.7 | −71.16 | −69.72 | −71.25 |

Definition of the geometric parameters (see also Figure 4 for the graphical representation). Compound "Ether **14**": dihedral angles A, B, C, are defined similar to the ethers derived from the carbocyclic allylic alcohols **9** and **10** (compare with Figure 1). The numbers from 1 to 7 in the names of the remaining dihedral angles correspond to the numbers of the carbon atoms of the side chain (as shown in Figure 4), e.g. "2=345" is defined as C(2)=C(3)C(4)C(5) dihedral angle. Compound "Tetrazolone **15** (R)" resulting from 3,3'-shift (R-enantiomer): A is defined as CCNC dihedral angle describing the mutual orientation of the phenyl and tetrazolone rings; dihedral angles "B" and "C" (analogous of ether) are not applicable; CN39 is defined as C(tetrazolone)−NC(3)C(9) dihedral angle. Compound "Tetrazolone **18**" resulting from 1,3'-shift: A is defined as CCNC dihedral angle in Tetrazolone **15**; dihedral angles "B" and "C" (analogous of ether) are not applicable; CN12 is defined as C(tetrazolone)−NC(1)C(2) dihedral angle. All relative energies are calculated with respect to $Ph^+TG^-A^+CA^-TA^-$ conformer (Nº1) of Ether **14**. $\Delta E_{el}$, $\Delta E_{ZPE}$, $\Delta E_G$ state for the relative electronic, zero-point-corrected and Gibbs free energy (at 298.15 K), respectively. The absolute values calculated for the most stable conformer of Ether **14** at the DFT(B3LYP)/6-31G(d,p) level are: $E_{el}$=−955.237317; $E_{ZPE}$=−954.868515, $E_G$=−954.923266 hartree.

**Table 4S.** Conformationally relevant geometric parameters and relative energies of conformers of (E)-5-(3,7-dimethylocta-2,6-dienyloxy)-1-phenyl-1*H*-tetrazole (**14**) [in brief: Ether **14**] and corresponding isomeric 1-(3,7-dimethylocta-1,6-dien-3-yl)-4-phenyl-1*H*-tetrazol-5(4*H*)-one (**15**) [in brief: Tetrazolone **15** (R)] and isomeric (E)-1-(3,7-dimethylocta-2,6-dienyl)-4-phenyl-1H-tetrazol-5(4*H*)-one (**18**) [in brief: Tetrazolone **18**] calculated at the MP2/6-31G(d,p) level of theory for selected structures.

| Compound / Form | | Dihedral angle / degrees | | | | | | | | Energy |
|---|---|---|---|---|---|---|---|---|---|---|
| No. | Ether **14** | A | B | C | O12=3 | 12=34 | 2=345 | 3456 | 456=7 | $\Delta E_{el}$ |
| 1 | $Ph^+TG^+G^+CA^-G^+A^+$ | 32.7 | 172.8 | 67.2 | 60.9 | −3.4 | −118.6 | 53.8 | 138.7 | 0.0 |
| 2 | $Ph^+T\ T\ G^+\ CA^-TA^-$ | 31.1 | 176.1 | 171.4 | 73.9 | −1.7 | −97.7 | −175.7 | −85.9 | 10.7 |
| 3 | $Ph^+T\ G^-A^+CA^-TA^-$ | 35.5 | 162.3 | −72.0 | 118.6 | 2.3 | −123.6 | −173.3 | −107.7 | 11.6 |
| 4 | $Ph^+T\ G^-A^+CA^-TA^+$ | 35.7 | 160.7 | −78.4 | 111.6 | −1.2 | −118.9 | 166.3 | 95.1 | 13.8 |
| 5 | $Ph^-T\ G^-A^+CA^-TA^+$ | −36.4 | 165.8 | −81.0 | 111.2 | −1.1 | −118.2 | 166.4 | 95.0 | 14.3 |
| 6 | $Ph^+A^+G^-A^+TA^+TA^+$ | 31.4 | 125.1 | −64.2 | 101.7 | −168.0 | 90.9 | 179.9 | 89.8 | 14.4 |
| 7 | $Ph^-A^+G^-A^+TA^+TA^+$ | −16.8 | 122.3 | −64.1 | 98.8 | −167.1 | 100.0 | −178.1 | 110.6 | 17.2 |
| 8 | $Ph^-T\ G^+A^-CA^-TA^+$ | −35.7 | −164.3 | 76.5 | −120.5 | −1.7 | −86.1 | −178.5 | 106.0 | 18.8 |
| 9 | $Ph^+T\ G^+A^-CA^-TA^-$ | 36.3 | −170.4 | 79.2 | −120.7 | −1.6 | −86.0 | −178.5 | 106.0 | 19.4 |
| 10 | $Ph^+T\ G^-A^+TA^-TA^+$ | 35.7 | 164.5 | −76.1 | 120.5 | 177.3 | −113.9 | 177.6 | 96.3 | 19.7 |
| 11 | $Ph^-T\ G^-A^+TA^-TA^+$ | −36.3 | 170.5 | −78.8 | 120.7 | 177.2 | −113.9 | 177.6 | 96.1 | 20.2 |
| 12 | $Ph^-T\ G^-A^+TA^+TA^+$ | −36.4 | 168.0 | −75.9 | 117.3 | −177.1 | 99.5 | 176.7 | 101.6 | 20.7 |
| 13 | $Ph^+T\ G^-A^+TC\ TA^+$ | 35.6 | 163.5 | −75.7 | 119.9 | 178.4 | −1.2 | 177.8 | 101.8 | 22.7 |
| 14 | $Ph^-T\ G^-A^+TC\ TA^+$ | −36.4 | 169.3 | −78.3 | 120.1 | 178.4 | −1.1 | 177.7 | 101.7 | 23.2 |
| No. | Tetrazolone **15** (R) | A | | CN39 | | 1=234 | 2345 | 3456 | 456=7 | $\Delta E_{el}$ |
| 1 | $Ph^+T\ A^+\ T\ G^+\ A^-$ | 20.1 | | −174.9 | | 135.0 | −178.4 | 70.7 | −124.3 | −70.1 |
| 2 | $Ph^-T\ A^+\ T\ G^+\ G^+$ | −20.5 | | −174.6 | | 134.3 | 177.3 | 61.8 | 80.0 | −67.1 |
| 3 | $Ph^+T\ A^+\ T\ G^+\ G^+$ | 10.6 | | −175.2 | | 134.4 | 175.6 | 59.4 | 81.0 | −66.4 |
| 4 | $Ph^+A^-A^+G^+G^+\ A^-$ | 26.6 | | −125.2 | | 111.3 | 50.6 | 59.0 | −124.4 | −64.8 |
| 5 | $Ph^-A^-A^+G^+G^+G^+$ | −22.1 | | −129.5 | | 113.2 | 53.1 | 56.6 | 77.2 | −60.7 |
| 6 | $Ph^-C\ A^+\ T\ G^+G^+$ | −22.9 | | −3.9 | | 125.6 | 173.4 | 54.6 | 79.8 | −60.2 |
| 7 | $Ph^-T\ A^+\ T\ T\ \ A^+$ | −25.5 | | −165.4 | | 128.3 | −175.1 | 173.1 | 105.3 | −50.8 |
| 8 | $Ph^+T\ A^+\ T\ T\ \ A^+$ | 26.0 | | −164.6 | | 127.1 | −175.4 | 172.2 | 106.2 | −50.7 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 9 | $Ph^{-}$ T C T $A^{+}$ | −24.6 | −177.2 | | −1.0 | −176.4 | 171.2 | 105.0 | −49.1 |
| 10 | $Ph^{+}$ T C T $A^{+}$ | 24.4 | −177.1 | | −1.2 | −176.2 | 171.4 | 105.0 | −48.9 |
| 11 | $Ph^{-}G^{-}G^{+}G^{+}G^{+}$ | −24.3 | −70.7 | | 88.1 | 51.9 | −179.3 | 89.6 | −48.7 |
| 12 | $Ph^{+}G^{-}G^{+}G^{+}G^{+}$ | 22.6 | −71.1 | | 87.6 | 52.1 | −179.1 | 89.6 | −48.6 |
| 13 | $Ph^{+}G^{+}A^{-}$ T $A^{+}$ | 24.2 | 52.8 | | −123.6 | 178.8 | 173.8 | 169.4 | −47.9 |
| 14 | $Ph^{-}G^{+}A^{-}$ T $A^{+}$ | −25.6 | 52.7 | | −123.4 | 178.9 | 169.5 | 100.8 | −47.8 |

| No. | Tetrazolone **18** | A | CN12 | N12=3 | 12=34 | 2=345 | 3456 | 456=7 | $\Delta E_{el}$ |
|---|---|---|---|---|---|---|---|---|---|
| 1 | $Ph^{-}$ $A^{+}$ $A^{-}$ C $A^{-}G^{+}A^{-}$ | −23.0 | 90.0 | −105.9 | −2.1 | −93.1 | 70.0 | −97.4 | −63.2 |
| 2 | $Ph^{+}$ $A^{-}$ $G^{+}$ C $A^{-}$T $A^{+}$ | 39.0 | −110.9 | 73.9 | −1.8 | −99.3 | 173.5 | 133.5 | −62.0 |
| 3 | $Ph^{+}$ $A^{-}$ $A^{+}$ C $A^{-}$T $A^{-}$ | 24.7 | −92.2 | 123.0 | −0.7 | −93.2 | −172.1 | −99.4 | −61.5 |
| 4 | $Ph^{+}$ $A^{-}$ $A^{+}$ C $A^{+}$T $A^{+}$ | 24.7 | −101.1 | 99.5 | 0.5 | 89.9 | 180.0 | 83.9 | −57.6 |
| 5 | $Ph^{+}$ $A^{-}$ $A^{+}$ C $A^{+}G^{+}A^{+}$ | 23.3 | −87.7 | 108.0 | 1.8 | 81.4 | 54.6 | 95.7 | −55.1 |
| 6 | $Ph^{+}$ $A^{-}$ $A^{+}$ C $A^{+}$T $A^{-}$ | 23.4 | −92.2 | 104.9 | 1.4 | 88.3 | 178.7 | −105.9 | −53.8 |
| 7 | $Ph^{+}$ $G^{+}$ $A^{+}$ C $A^{-}$T $A^{+}$ | 23.0 | 75.1 | 106.7 | −1.6 | −90.5 | −178.9 | 93.4 | −51.9 |
| 8 | $Ph^{-}$ $G^{+}$ $A^{+}$ C $A^{+}$T $A^{+}$ | −22.5 | 68.4 | 85.8 | 0.9 | 92.3 | 178.9 | 83.6 | −50.8 |
| 9 | $Ph^{+}$ $G^{+}$ $A^{+}$ C $A^{+}$T $A^{-}$ | 22.9 | 80.2 | 96.9 | 1.8 | 91.2 | 178.9 | −101.2 | −49.2 |
| 10 | $Ph^{+}$ $A^{+}$ $A^{+}$ T $A^{+}$ T $A^{+}$ | 23.4 | 107.7 | 90.9 | −176.2 | 112.4 | −179.4 | 100.6 | −48.1 |

For the definition of the geometric parameters see caption of Table 3S and also Figure 4 for the graphical representation. All relative electronic energies ($\Delta E_{el}$, in kJ $mol^{-1}$) are calculated with respect to $Ph^{+}TG^{+}G^{+}CA^{-}G^{+}A^{+}$ conformer (Nº1) of Ether **14**. The absolute value calculated for $Ph^{+}TG^{+}G^{+}CA^{-}G^{+}A^{+}$ conformer at the MP2/6-31G(d,p) level is $E_{el}$=−952.323974 hartree.

This Section of Supplementary information contains Cartesian coordinates for optimized structures of the transition states for the sigmatropic isomerisation of 5-allyloxytetrazoles to the corresponding tetrazolones. For brevity, before each structure, the theoretical methods are specified briefly as DFT or MP2, which correspond to DFT(B3LYP)/6-31G(d,p) and MP2/6-31G(d,p), respectively. The theory level is followed by a short name of the structure: TS1a, TS1a', TS1b, TS1b', TS2a, TS2a', TS2b, TS2b', TS3a, TS3a', TS3a'', TS3b and TS3b'.

In these names "TS" designates "Transition State". Numbers 1, 2 and 3 correspond to the tetrazoles derived from the carbocyclic allylic alcohols (1) cyclohex-2-enol; (2) 3-methylcyclohex-2-enol; (3) natural terpene alcohol nerol.

Some names finish with one or two apostrophes, which designate transition states occurring on alternative "parallel" pathways. These structures have relative energies slightly higher than the base structure (without apostrophe). The calculated electronic energies (in hartree) and total dipole moments (debye) are also shown.

DFT, TS1a, -797.93481127 hartree, 7.7 debye

| | | | |
|---|---|---|---|
| N | 0.80257800 | 1.92563300 | -0.04402300 |
| N | -0.47814500 | 1.97239800 | -0.13656600 |
| N | -1.02000200 | 0.74216900 | -0.22650200 |
| C | -0.00998300 | -0.16931700 | -0.19803100 |
| N | 1.14675600 | 0.58658900 | -0.07568000 |
| C | 2.49971700 | 0.17943400 | -0.01058800 |
| C | 3.50476300 | 1.15147300 | 0.09605800 |
| C | 4.83796600 | 0.75503200 | 0.16159600 |
| C | 5.18330200 | -0.59746600 | 0.12187200 |
| C | 4.17532400 | -1.55591600 | 0.01532500 |
| C | 2.83382300 | -1.18111900 | -0.05156500 |
| H | 3.22862300 | 2.19782100 | 0.12528600 |
| H | 5.61186700 | 1.51292400 | 0.24373400 |
| H | 6.22512200 | -0.89940800 | 0.17264900 |
| H | 4.42994800 | -2.61158900 | -0.01749100 |
| H | 2.04383600 | -1.91639800 | -0.13633000 |
| O | -0.11580300 | -1.41770400 | -0.26978400 |
| C | -2.75530200 | -1.26885200 | -0.57084800 |
| C | -2.92029900 | -1.45559100 | 0.81195400 |
| C | -3.56082800 | -0.48570400 | 1.53670500 |
| C | -4.02201300 | 0.76650000 | 0.89063700 |
| C | -4.57671800 | 0.49813200 | -0.51866200 |
| C | -3.59523000 | -0.33330100 | -1.36552000 |
| H | -2.07931000 | -1.92875000 | -1.10034200 |
| H | -2.42181900 | -2.28807900 | 1.29581400 |
| H | -4.73831100 | 1.30683200 | 1.51534800 |
| H | -3.10726400 | 1.38666600 | 0.80297200 |
| H | -5.52645400 | -0.04145400 | -0.42457800 |
| H | -4.79482400 | 1.44494500 | -1.01927000 |
| H | -2.91411800 | 0.29703100 | -1.94465700 |
| H | -4.13211500 | -0.94475000 | -2.10791400 |
| H | -3.62419700 | -0.58152100 | 2.61884100 |

DFT, TS1a', -797.93427933 hartree, 8.6 debye

| | | | |
|---|---|---|---|
| N | -1.41384700 | 2.31525400 | 0.00450300 |
| N | -0.23227900 | 2.82370500 | -0.05032500 |
| N | 0.71852200 | 1.87674600 | -0.11240100 |
| C | 0.10658600 | 0.66522000 | -0.12705600 |
| N | -1.24900300 | 0.94411000 | -0.02522200 |
| C | -2.36486000 | 0.07595900 | 0.00268700 |
| C | -3.65182900 | 0.61717900 | 0.13601500 |
| C | -4.75385600 | -0.23315100 | 0.16883000 |
| C | -4.59172800 | -1.61675200 | 0.07051100 |
| C | -3.30743400 | -2.14474400 | -0.06211500 |
| C | -2.19013300 | -1.31111200 | -0.09806500 |
| H | -3.76895200 | 1.69075100 | 0.21108200 |
| H | -5.74772500 | 0.19291300 | 0.27231400 |
| H | -5.45593700 | -2.27370000 | 0.09590600 |
| H | -3.16681200 | -3.21921600 | -0.14115200 |
| H | -1.18949500 | -1.70959100 | -0.20334900 |
| O | 0.65688600 | -0.46351200 | -0.22016600 |
| C | 3.09952100 | 0.70177600 | -0.62980200 |
| C | 3.42013900 | 0.81564800 | 0.73442300 |
| C | 3.57535700 | -0.32199800 | 1.47921900 |
| C | 3.34373100 | -1.66405000 | 0.88447700 |
| C | 3.83209200 | -1.71734000 | -0.57370400 |
| C | 3.25686400 | -0.55514400 | -1.40018900 |
| H | 2.82189100 | 1.60203800 | -1.16444300 |
| H | 3.42725300 | 1.79770100 | 1.19358700 |
| H | 3.79035000 | -2.45572800 | 1.49244900 |
| H | 2.24581800 | -1.79666100 | 0.90203700 |
| H | 4.92769500 | -1.66442100 | -0.58050700 |
| H | 3.55535300 | -2.67321300 | -1.02629100 |
| H | 2.25381000 | -0.79276200 | -1.78024100 |
| H | 3.87371400 | -0.33817200 | -2.28445400 |
| H | 3.76750000 | -0.23950900 | 2.54713200 |

DFT, TS1b, -797.95473353 hartree, 5.2 debye

| | | | |
|---|---|---|---|
| N | 0.89407200 | 2.17726300 | -0.17393700 |
| N | -0.34542100 | 2.48115000 | -0.35645600 |
| N | -1.08874900 | 1.38186200 | -0.63944900 |
| C | -0.25378000 | 0.30815300 | -0.59786300 |
| N | 1.00440800 | 0.82254400 | -0.29588100 |
| C | 2.25128400 | 0.16937800 | -0.11846800 |
| C | 3.33197500 | 0.89030100 | 0.40676200 |
| C | 4.55883400 | 0.25496100 | 0.58019600 |
| C | 4.71775200 | -1.09074000 | 0.24282800 |
| C | 3.63428000 | -1.79870000 | -0.27729500 |
| C | 2.39880100 | -1.17965500 | -0.46528500 |
| H | 3.19940600 | 1.93332000 | 0.66551200 |
| H | 5.39453000 | 0.81811500 | 0.98503500 |
| H | 5.67640100 | -1.58078500 | 0.38292000 |
| H | 3.74680300 | -2.84470600 | -0.54734800 |
| H | 1.55453700 | -1.72238400 | -0.86904000 |
| O | -0.56316300 | -0.90604100 | -0.73144600 |
| C | -2.14080300 | -1.45801100 | 0.76055200 |
| C | -2.17034500 | -0.24856100 | 1.44943000 |
| C | -2.84820000 | 0.81662900 | 0.87830300 |
| C | -3.92809700 | 0.60921400 | -0.14335800 |
| C | -4.38507900 | -0.85500200 | -0.20031000 |
| C | -3.18724800 | -1.81375500 | -0.25406500 |
| H | -1.47584100 | -2.24447300 | 1.10060300 |
| H | -1.45632100 | -0.06657100 | 2.24670300 |
| H | -4.77029200 | 1.27233700 | 0.08948600 |
| H | -3.53202900 | 0.94276200 | -1.10889800 |
| H | -4.97968800 | -1.07811100 | 0.69411900 |
| H | -5.03679400 | -1.01504100 | -1.06452500 |
| H | -2.70501800 | -1.79303200 | -1.23849600 |
| H | -3.50964100 | -2.84919100 | -0.08850000 |
| H | -2.72717100 | 1.81107600 | 1.29550400 |

DFT, TS1b', -797.95167216 hartree, 5.8 debye

| | | | |
|---|---|---|---|
| N | -0.25351300 | 2.14655400 | 0.32602800 |
| N | 0.93772000 | 2.48635600 | -0.05218200 |
| N | 1.45061900 | 1.60842300 | -0.94460800 |
| C | 0.51599300 | 0.62755900 | -1.12657900 |
| N | -0.56433100 | 0.98493000 | -0.30931300 |
| C | -1.82175200 | 0.35560800 | -0.11298500 |
| C | -2.65460200 | 0.79824800 | 0.92371700 |
| C | -3.89026600 | 0.18629100 | 1.11765700 |
| C | -4.30164200 | -0.86466300 | 0.29513900 |
| C | -3.46429800 | -1.29740700 | -0.73300600 |
| C | -2.22510400 | -0.69456400 | -0.94873200 |
| H | -2.32970100 | 1.61615400 | 1.55457100 |
| H | -4.53413100 | 0.53524500 | 1.91956900 |
| H | -5.26554800 | -1.33853600 | 0.45321400 |
| H | -3.77561000 | -2.10963600 | -1.38335200 |
| H | -1.57226700 | -1.02261800 | -1.74670200 |
| O | 0.62318200 | -0.42219700 | -1.80462400 |
| C | 2.14491100 | -1.70088000 | -0.63722400 |
| C | 3.12521200 | -0.72657000 | -0.75722900 |
| C | 3.18015100 | 0.29226700 | 0.18158200 |
| C | 2.58264500 | 0.15111300 | 1.54899600 |
| C | 2.16397800 | -1.29675700 | 1.84618600 |
| C | 1.42368700 | -1.93110400 | 0.65866000 |
| H | 2.00330600 | -2.41607300 | -1.43931400 |
| H | 3.64809300 | -0.61210800 | -1.70026500 |
| H | 3.31699700 | 0.49900700 | 2.28677400 |
| H | 1.73923200 | 0.85050700 | 1.64635800 |
| H | 3.06486600 | -1.88704500 | 2.05286800 |
| H | 1.54170100 | -1.33706900 | 2.74495300 |
| H | 0.40825100 | -1.52430800 | 0.56864100 |
| H | 1.29317800 | -3.00891000 | 0.81225800 |
| H | 3.80923600 | 1.15426600 | -0.00914100 |

MP2, TS1a, -795.54103565 hartree, 9.0 debye

| | | | |
|---|---|---|---|
| N | 0.75323400 | 1.90374800 | -0.38207600 |
| N | -0.55928200 | 1.94111000 | -0.54112700 |
| N | -1.08146100 | 0.69039000 | -0.54089600 |
| C | -0.06642500 | -0.20146900 | -0.37716700 |
| N | 1.08099200 | 0.58463100 | -0.27567000 |
| C | 2.42521300 | 0.19010100 | -0.08280900 |
| C | 3.37656600 | 1.15612700 | 0.26937800 |
| C | 4.70227400 | 0.76902500 | 0.45105600 |
| C | 5.08099800 | -0.56725100 | 0.30009900 |
| C | 4.11992000 | -1.51874700 | -0.04324100 |
| C | 2.78842400 | -1.15249900 | -0.24229900 |
| H | 3.06890400 | 2.18519300 | 0.38352000 |
| H | 5.43971300 | 1.51542500 | 0.71866700 |
| H | 6.11218500 | -0.86147600 | 0.44794400 |
| H | 4.40457300 | -2.55652800 | -0.16478000 |
| H | 2.03069300 | -1.87556300 | -0.50347500 |
| O | -0.14999600 | -1.46167600 | -0.30684400 |
| C | -2.76140200 | -1.38312000 | -0.36294800 |
| C | -2.62735300 | -1.30360400 | 1.02642400 |
| C | -3.11203500 | -0.18080600 | 1.65405300 |
| C | -3.78130600 | 0.90205000 | 0.90464200 |
| C | -4.58877000 | 0.33428900 | -0.26045000 |
| C | -3.71400700 | -0.55811100 | -1.13670700 |
| H | -2.18435000 | -2.13313700 | -0.88518100 |
| H | -2.00140400 | -2.01664700 | 1.54055400 |
| H | -4.38997900 | 1.51845000 | 1.56517800 |
| H | -2.95320400 | 1.51996000 | 0.51596200 |
| H | -5.41890600 | -0.25261500 | 0.14038300 |
| H | -5.01666700 | 1.14111700 | -0.85367100 |
| H | -3.09682400 | 0.02643200 | -1.82311000 |
| H | -4.30996400 | -1.23733100 | -1.75586000 |
| H | -2.89177800 | -0.03493000 | 2.70681500 |

MP2, TS1a', -795.53941160 hartree, 10.2 debye

| | | | |
|---|---|---|---|
| N | -1.35155200 | 2.32906000 | -0.02859100 |
| N | -0.14476900 | 2.86016800 | -0.12657800 |
| N | 0.79159300 | 1.89822100 | -0.31216900 |
| C | 0.16771300 | 0.69307900 | -0.33933700 |
| N | -1.18152700 | 0.98229900 | -0.15571500 |
| C | -2.28516500 | 0.10423300 | -0.07011400 |
| C | -3.48615400 | 0.56901300 | 0.48057200 |
| C | -4.57792400 | -0.29304600 | 0.55486700 |
| C | -4.47601300 | -1.61124100 | 0.10331300 |
| C | -3.27008100 | -2.06196000 | -0.43519700 |
| C | -2.16825000 | -1.21178000 | -0.53301400 |
| H | -3.54829900 | 1.59054200 | 0.82641900 |
| H | -5.50889500 | 0.06620300 | 0.97525800 |
| H | -5.32680500 | -2.27722400 | 0.16970100 |
| H | -3.18393400 | -3.08094900 | -0.79187200 |
| H | -1.22664600 | -1.54226400 | -0.94414800 |
| O | 0.69322400 | -0.45318600 | -0.49062200 |
| C | 3.14852800 | 0.70205000 | -0.44670900 |
| C | 3.08203400 | 0.73321100 | 0.95100300 |
| C | 2.99956900 | -0.46337500 | 1.61860600 |
| C | 3.00830600 | -1.76177500 | 0.90583100 |
| C | 3.88495700 | -1.68721400 | -0.34212600 |
| C | 3.46075900 | -0.51463600 | -1.22000200 |
| H | 3.00332800 | 1.63252300 | -0.97794800 |
| H | 2.93712500 | 1.67701700 | 1.45413100 |
| H | 3.31173900 | -2.56833400 | 1.57250100 |
| H | 1.95945600 | -1.92104700 | 0.61469500 |
| H | 4.92557600 | -1.55304600 | -0.03583000 |
| H | 3.82800300 | -2.61914700 | -0.90303400 |
| H | 2.52763200 | -0.73113100 | -1.75258800 |
| H | 4.20973600 | -0.26201900 | -1.97612600 |
| H | 2.82028500 | -0.45322700 | 2.68904000 |

MP2, TS1b, -795.57454659 hartree, 6.0 debye

| | | | |
|---|---|---|---|
| N | -0.06026300 | 2.13455100 | 0.34940800 |
| N | 1.19081100 | 2.42634000 | -0.00707000 |
| N | 1.65810100 | 1.51187700 | -0.89788100 |
| C | 0.64906700 | 0.60519200 | -1.13289600 |
| N | -0.40552900 | 1.01217900 | -0.30451500 |
| C | -1.68773700 | 0.43060800 | -0.13005200 |
| C | -2.38552000 | 0.67885500 | 1.05708400 |
| C | -3.64713900 | 0.11299700 | 1.22710600 |
| C | -4.19152700 | -0.71476200 | 0.24183400 |
| C | -3.47418300 | -0.96263900 | -0.92959700 |
| C | -2.21681700 | -0.39232400 | -1.12983000 |
| H | -1.94884700 | 1.32249500 | 1.80761100 |
| H | -4.19842900 | 0.30866500 | 2.13779700 |
| H | -5.16875000 | -1.15738300 | 0.38413100 |
| H | -3.89376600 | -1.59899200 | -1.69811800 |
| H | -1.65148400 | -0.57444000 | -2.03130700 |
| O | 0.69460500 | -0.43975500 | -1.83475300 |
| C | 1.92670000 | -1.74879200 | -0.64326000 |
| C | 2.99585600 | -0.86790300 | -0.64021200 |
| C | 2.98135700 | 0.18554900 | 0.26990400 |
| C | 2.25654300 | 0.06039800 | 1.57989400 |
| C | 1.77912400 | -1.37052500 | 1.81564700 |
| C | 1.06862100 | -1.91371800 | 0.57835500 |
| H | 1.85834000 | -2.49593600 | -1.42337000 |
| H | 3.64489600 | -0.81635100 | -1.50339400 |
| H | 2.93511500 | 0.37576700 | 2.37624000 |
| H | 1.42075600 | 0.76725100 | 1.62396600 |
| H | 2.64380100 | -2.00266800 | 2.03076000 |
| H | 1.11796900 | -1.41224200 | 2.68221900 |
| H | 0.11670700 | -1.39578200 | 0.43417800 |
| H | 0.82157400 | -2.97002500 | 0.70314500 |
| H | 3.73737000 | 0.95545200 | 0.19069500 |

MP2, TS1b', -795.57201317 hartree, 4.9 debye

| | | | |
|---|---|---|---|
| N | 0.80281800 | 2.19570400 | -0.21368500 |
| N | -0.47474700 | 2.49579900 | -0.40753100 |
| N | -1.18169600 | 1.36851800 | -0.70163200 |
| C | -0.31792900 | 0.31358600 | -0.67290100 |
| N | 0.91742900 | 0.85842100 | -0.34235100 |
| C | 2.15918800 | 0.20363000 | -0.14281900 |
| C | 3.12674700 | 0.81866100 | 0.65788900 |
| C | 4.34950600 | 0.17836600 | 0.84700300 |
| C | 4.59388300 | -1.06863000 | 0.26627400 |
| C | 3.61111800 | -1.67221700 | -0.51997800 |
| C | 2.38720900 | -1.03999700 | -0.73925400 |
| H | 2.91725500 | 1.78115500 | 1.10243400 |
| H | 5.10719600 | 0.65060200 | 1.45887300 |
| H | 5.54288500 | -1.56417600 | 0.42436200 |
| H | 3.79771200 | -2.63589800 | -0.97614600 |
| H | 1.61913700 | -1.49506200 | -1.34629700 |
| O | -0.60822200 | -0.92076200 | -0.75015800 |
| C | -1.86733700 | -1.37191700 | 0.79779000 |
| C | -1.97646900 | -0.12072700 | 1.40563300 |
| C | -2.69323200 | 0.85332200 | 0.72162200 |
| C | -3.80245200 | 0.45460900 | -0.21828900 |
| C | -4.21205800 | -0.99566000 | 0.02100800 |
| C | -2.99423700 | -1.91270700 | -0.04085100 |
| H | -1.17120500 | -2.09078800 | 1.21342900 |
| H | -1.25625700 | 0.17738400 | 2.15718800 |
| H | -4.65005700 | 1.12688400 | -0.07013100 |
| H | -3.46420700 | 0.59315600 | -1.24544900 |
| H | -4.67102600 | -1.07768600 | 1.00884200 |
| H | -4.95780300 | -1.30499800 | -0.71235300 |
| H | -2.64352500 | -2.02487500 | -1.06815100 |
| H | -3.24977300 | -2.91213400 | 0.32018300 |
| H | -2.68480200 | 1.87151200 | 1.09211800 |

DFT, TS2a, -837.26441743 hartree, 8.8 debye

| | | | |
|---|---|---|---|
| N | 1.06105700 | 1.92976500 | 0.26993900 |
| N | -0.20804900 | 2.03400400 | 0.09476300 |
| N | -0.75515300 | 0.87751500 | -0.33187600 |
| C | 0.24092400 | -0.04475700 | -0.44683400 |
| N | 1.39373100 | 0.62917300 | -0.05896100 |
| C | 2.73106900 | 0.17845500 | 0.01617200 |
| C | 3.73268000 | 1.06430200 | 0.43993800 |
| C | 5.05110900 | 0.62333000 | 0.51845800 |
| C | 5.38667300 | -0.68932700 | 0.18001200 |
| C | 4.38294400 | -1.56195200 | -0.24105000 |
| C | 3.05613000 | -1.14148600 | -0.32690400 |
| H | 3.46468100 | 2.08046100 | 0.69995300 |
| H | 5.82157300 | 1.31511500 | 0.84728600 |
| H | 6.41713600 | -1.02608900 | 0.24303600 |
| H | 4.62955700 | -2.58566800 | -0.50892300 |
| H | 2.26907000 | -1.80899700 | -0.65359600 |
| O | 0.13552300 | -1.23790800 | -0.81737500 |
| C | -2.54122300 | -0.96579900 | -1.17258900 |
| C | -2.75144200 | -1.43092200 | 0.12639300 |
| C | -3.41120700 | -0.63505900 | 1.04123200 |
| C | -3.85230700 | 0.72633300 | 0.62176200 |
| C | -4.37163100 | 0.73873500 | -0.82378700 |
| C | -3.33541200 | 0.13323600 | -1.78337100 |
| H | -1.83067800 | -1.49849000 | -1.79382700 |
| H | -2.25386100 | -2.34097300 | 0.44507300 |
| H | -4.58244500 | 1.14410600 | 1.32136800 |
| H | -2.93380600 | 1.34234900 | 0.67533400 |
| H | -5.30324500 | 0.16206600 | -0.87338900 |
| H | -4.61221000 | 1.76196700 | -1.12410700 |
| H | -2.61780400 | 0.88186400 | -2.13384000 |
| H | -3.81336000 | -0.27043000 | -2.68867200 |
| C | -3.55088600 | -1.03179900 | 2.47001500 |
| H | -3.03387900 | -0.30027300 | 3.10549900 |
| H | -4.60608400 | -1.00250700 | 2.77039500 |
| H | -3.14446300 | -2.02416800 | 2.67367000 |

DFT, TS2a', -837.26395925 hartree, 9.8 debye

| | | | |
|---|---|---|---|
| N | -1.68982700 | 2.32227200 | 0.06953300 |
| N | -0.52727300 | 2.85938500 | -0.06213000 |
| N | 0.43300400 | 1.94018000 | -0.26905600 |
| C | -0.15643800 | 0.71799600 | -0.29465000 |
| N | -1.50435900 | 0.95963000 | -0.05844600 |
| C | -2.59606100 | 0.06639500 | 0.02295400 |
| C | -3.87320800 | 0.56712800 | 0.31656500 |
| C | -4.95200300 | -0.30895400 | 0.40177900 |
| C | -4.77731900 | -1.67965700 | 0.19884900 |
| C | -3.50360100 | -2.16765800 | -0.09338800 |
| C | -2.40973100 | -1.30762900 | -0.18478600 |
| H | -4.00048900 | 1.63093500 | 0.47169700 |
| H | -5.93785300 | 0.08666500 | 0.62931800 |
| H | -5.62347800 | -2.35690100 | 0.26629200 |
| H | -3.35333800 | -3.23143600 | -0.25638600 |
| H | -1.41772700 | -1.67397300 | -0.41447200 |
| O | 0.39774500 | -0.39609900 | -0.49332000 |
| C | 2.83683200 | 0.80800400 | -0.97727000 |
| C | 3.22409900 | 0.82615700 | 0.36410300 |
| C | 3.41957200 | -0.35844100 | 1.04368600 |
| C | 3.15152800 | -1.64700500 | 0.33759600 |
| C | 3.58457300 | -1.59129800 | -1.13602600 |
| C | 2.94628800 | -0.38881900 | -1.84619600 |
| H | 2.51209400 | 1.74115900 | -1.42261800 |
| H | 3.23927900 | 1.77341800 | 0.89287600 |
| H | 3.60689100 | -2.49111300 | 0.86449400 |
| H | 2.05319800 | -1.76285800 | 0.38131000 |
| H | 4.67787900 | -1.51340400 | -1.18608300 |
| H | 3.30683000 | -2.52021000 | -1.64139100 |
| H | 1.91835500 | -0.61351500 | -2.16220200 |
| H | 3.49575600 | -0.10883100 | -2.75608600 |
| C | 3.74964200 | -0.38592700 | 2.49564000 |
| H | 2.96209400 | -0.92088600 | 3.04313200 |
| H | 4.67352000 | -0.95502700 | 2.66216200 |
| H | 3.85917100 | 0.61276700 | 2.92207800 |

DFT, TS2b, -837.28137234 hartree, 5.5 debye

| | | | |
|---|---|---|---|
| N | 0.96944900 | 2.02639500 | -0.44243900 |
| N | -0.28357600 | 2.21201200 | -0.68312400 |
| N | -0.93979500 | 1.03755000 | -0.83980400 |
| C | -0.03451200 | 0.03356800 | -0.65100000 |
| N | 1.17965000 | 0.67788100 | -0.39959700 |
| C | 2.46760500 | 0.14713500 | -0.13562700 |
| C | 3.51789300 | 1.02066700 | 0.17889800 |
| C | 4.78450600 | 0.50390000 | 0.43831900 |
| C | 5.01630700 | -0.87237800 | 0.39163500 |
| C | 3.96364400 | -1.73205600 | 0.07813700 |
| C | 2.68802200 | -1.23558500 | -0.18881700 |
| H | 3.33048600 | 2.08643700 | 0.21224900 |
| H | 5.59503800 | 1.18547200 | 0.67950900 |
| H | 6.00636300 | -1.26860100 | 0.59578800 |
| H | 4.13133800 | -2.80443800 | 0.03529600 |
| H | 1.86640000 | -1.89486100 | -0.43488900 |
| O | -0.25171000 | -1.20018000 | -0.65308400 |
| C | -2.04969500 | -1.61548200 | 0.87816600 |
| C | -2.15043800 | -0.32249500 | 1.34608400 |
| C | -2.83253000 | 0.64738600 | 0.59857400 |
| C | -3.77767500 | 0.21829300 | -0.49684000 |
| C | -4.17622600 | -1.25984200 | -0.39468300 |
| C | -2.94568400 | -2.15237800 | -0.19281300 |
| H | -1.38541800 | -2.30858100 | 1.38389400 |
| H | -1.52555600 | 0.00048500 | 2.17395500 |
| H | -4.66413300 | 0.86385600 | -0.47343800 |
| H | -3.26914700 | 0.42283100 | -1.44495600 |
| H | -4.85869400 | -1.39264900 | 0.45420900 |
| H | -4.72338800 | -1.56174600 | -1.29303500 |
| H | -2.34301600 | -2.21104100 | -1.10819100 |
| H | -3.23916400 | -3.17941700 | 0.05559600 |
| C | -2.89967200 | 2.06804400 | 1.05432800 |
| H | -2.90087300 | 2.75182300 | 0.20284200 |
| H | -3.84394900 | 2.20963300 | 1.60023800 |
| H | -2.07196500 | 2.33272500 | 1.71418400 |

DFT, TS2b', -837.27860054 hartree, 5.7 debye

| | | | |
|---|---|---|---|
| N | 0.38022600 | -2.04148500 | 0.32097400 |
| N | -0.83304300 | -2.27637800 | -0.06344300 |
| N | -1.26516600 | -1.35838200 | -0.95627400 |
| C | -0.24960300 | -0.45630700 | -1.13954800 |
| N | 0.79488200 | -0.91192600 | -0.31712600 |
| C | 2.09963700 | -0.39395200 | -0.11273500 |
| C | 2.93261900 | -0.98882600 | 0.84542600 |
| C | 4.21323000 | -0.48168000 | 1.04925500 |
| C | 4.67242000 | 0.61262100 | 0.31298200 |
| C | 3.83572600 | 1.19575100 | -0.63838300 |
| C | 2.55049300 | 0.70180400 | -0.86176300 |
| H | 2.57100600 | -1.83906500 | 1.40981000 |
| H | 4.85553400 | -0.94821400 | 1.79046300 |
| H | 5.67185800 | 1.00331900 | 0.47802700 |
| H | 4.18290800 | 2.04359300 | -1.22183500 |
| H | 1.89716400 | 1.14393300 | -1.60220800 |
| O | -0.26523500 | 0.58569500 | -1.82406300 |
| C | -1.89253400 | 1.95112900 | -0.58543400 |
| C | -2.85653000 | 0.98657000 | -0.75880700 |
| C | -2.99006300 | -0.06647700 | 0.15943000 |
| C | -2.38048700 | 0.05156800 | 1.53305600 |
| C | -1.93340100 | 1.48012200 | 1.87392400 |
| C | -1.16472300 | 2.12450300 | 0.71274300 |
| H | -1.71435300 | 2.66968100 | -1.37780700 |
| H | -3.36823700 | 0.91057200 | -1.71273000 |
| H | -3.11415400 | -0.30548300 | 2.26691000 |
| H | -1.54599900 | -0.66047800 | 1.60504500 |
| H | -2.82098600 | 2.08813600 | 2.08752300 |
| H | -1.32219800 | 1.47661500 | 2.78131100 |
| H | -0.16534300 | 1.67986300 | 0.61076900 |
| H | -0.99455000 | 3.19137300 | 0.89870400 |
| C | -3.97703900 | -1.16606200 | -0.05987100 |
| H | -3.59444100 | -2.10857500 | 0.33926400 |
| H | -4.90091100 | -0.92159800 | 0.48520300 |
| H | -4.21218400 | -1.29661500 | -1.11651000 |

MP2, TS2a, -834.74626254 hartree, 9.0 debye

| | | | |
|---|---|---|---|
| N | -0.16131800 | 1.30122100 | 1.40781600 |
| N | 1.05079600 | 0.98257400 | 1.87593300 |
| N | 1.26829500 | -0.35038500 | 1.83657000 |
| C | 0.17107200 | -0.94185100 | 1.28518500 |
| N | -0.72972100 | 0.12263500 | 1.05576600 |
| C | -1.96425800 | 0.09221400 | 0.37383100 |
| C | -2.48660200 | 1.28164200 | -0.15653100 |
| C | -3.70103000 | 1.24873200 | -0.83919300 |
| C | -4.38259600 | 0.04242400 | -1.01828000 |
| C | -3.84933100 | -1.13388000 | -0.48900800 |
| C | -2.64217600 | -1.12380600 | 0.21085100 |
| H | -1.95876900 | 2.21047900 | 0.00759100 |
| H | -4.11048900 | 2.16838700 | -1.23824500 |
| H | -5.32282700 | 0.02254700 | -1.55409800 |
| H | -4.37697900 | -2.07117700 | -0.61392700 |
| H | -2.21470400 | -2.02438400 | 0.62452300 |
| O | 0.00091500 | -2.13502500 | 0.92039300 |
| C | 1.14751700 | -1.07124400 | -1.24339700 |
| C | 1.05365900 | 0.30982600 | -1.21284100 |
| C | 2.11117800 | 1.06741500 | -0.70573200 |
| C | 3.38321400 | 0.41233800 | -0.30157000 |
| C | 3.61665600 | -0.90736700 | -1.02823600 |
| C | 2.38676900 | -1.79587500 | -0.88996500 |
| H | 0.27154400 | -1.64752400 | -1.51443100 |
| H | 0.12492600 | 0.79503300 | -1.48250100 |
| H | 4.21258400 | 1.11073000 | -0.42605400 |
| H | 3.25957100 | 0.22530700 | 0.77463800 |
| H | 3.81215200 | -0.71424300 | -2.08663400 |
| H | 4.49423000 | -1.40775700 | -0.62022500 |
| H | 2.22749700 | -2.11241400 | 0.15071700 |
| H | 2.45821500 | -2.70933700 | -1.48244300 |
| C | 2.00670900 | 2.53985400 | -0.57328400 |
| H | 2.33802200 | 2.82620100 | 0.42390600 |
| H | 2.68376200 | 2.99769900 | -1.30134600 |
| H | 0.99288900 | 2.89580400 | -0.72819700 |

MP2, TS2a', -834.73903699 hartree, 10.3 debye

| | | | |
|---|---|---|---|
| N | -1.23362300 | 2.45921400 | 0.31699700 |
| N | -0.07549900 | 3.09294800 | 0.21374200 |
| N | 0.84755800 | 2.33603800 | -0.43099000 |
| C | 0.26312100 | 1.15663500 | -0.76286200 |
| N | -1.04648900 | 1.24994300 | -0.28249800 |
| C | -2.05247400 | 0.26317500 | -0.26121800 |
| C | -3.10439500 | 0.37488400 | 0.65960000 |
| C | -4.09219900 | -0.60699800 | 0.68713100 |
| C | -4.02529800 | -1.70870600 | -0.17021000 |
| C | -2.96851200 | -1.81215100 | -1.07583400 |
| C | -1.97593900 | -0.83237600 | -1.13303100 |
| H | -3.14196500 | 1.23450800 | 1.31334200 |
| H | -4.91068100 | -0.51572500 | 1.39020800 |
| H | -4.79381100 | -2.47036500 | -0.13932000 |
| H | -2.91608800 | -2.65631200 | -1.75235200 |
| H | -1.15726600 | -0.88759500 | -1.83462000 |
| O | 0.78774700 | 0.13214100 | -1.29893600 |
| C | 3.10796900 | 0.62147200 | -0.07930800 |
| C | 2.40388800 | 0.38732000 | 1.09116000 |
| C | 1.77405700 | -0.84576700 | 1.18636100 |
| C | 2.17801100 | -1.99024000 | 0.32216300 |
| C | 3.57378600 | -1.80691300 | -0.25489900 |
| C | 3.65810400 | -0.44929600 | -0.93478300 |
| H | 3.22014600 | 1.65359700 | -0.39141900 |
| H | 2.05965100 | 1.22492900 | 1.68047300 |
| H | 2.08627800 | -2.91869300 | 0.88998900 |
| H | 1.42687200 | -2.01423500 | -0.47627100 |
| H | 4.30703900 | -1.85504400 | 0.55392600 |
| H | 3.80630400 | -2.60667000 | -0.95684900 |
| H | 3.05278100 | -0.41405600 | -1.84682200 |
| H | 4.68028200 | -0.18300600 | -1.21802900 |
| C | 0.56381300 | -0.99864700 | 2.02955100 |
| H | -0.29748000 | -0.98983300 | 1.35143600 |
| H | 0.56100400 | -1.95815700 | 2.54643700 |
| H | 0.44772900 | -0.18183000 | 2.73767000 |

MP2, TS2b, -834.76908917 hartree, 5.8 debye

| | | | |
|---|---|---|---|
| N | 0.17028500 | -2.07420000 | 0.25558000 |
| N | -1.09295600 | -2.25921300 | -0.13154000 |
| N | -1.47774400 | -1.28121700 | -0.99178200 |
| C | -0.40276100 | -0.44428600 | -1.18367500 |
| N | 0.60709100 | -0.95881000 | -0.35510600 |
| C | 1.92360700 | -0.47724900 | -0.13945900 |
| C | 2.59101800 | -0.83739200 | 1.03678100 |
| C | 3.88598500 | -0.36897900 | 1.24708800 |
| C | 4.49603600 | 0.47298100 | 0.31364200 |
| C | 3.80948800 | 0.83328200 | -0.84689300 |
| C | 2.51845500 | 0.36224300 | -1.08749100 |
| H | 2.10408200 | -1.49020000 | 1.74730400 |
| H | 4.41274500 | -0.65188200 | 2.14939700 |
| H | 5.49941000 | 0.83939100 | 0.48731700 |
| H | 4.27915500 | 1.48126500 | -1.57576300 |
| H | 1.97587300 | 0.63198000 | -1.98086800 |
| O | -0.35850300 | 0.61866200 | -1.85251500 |
| C | -1.57700900 | 1.96481200 | -0.59521900 |
| C | -2.68290000 | 1.13944700 | -0.64309600 |
| C | -2.78048600 | 0.05609600 | 0.23599400 |
| C | -2.03017900 | 0.09796600 | 1.54247800 |
| C | -1.46546500 | 1.48391300 | 1.84049100 |
| C | -0.71463300 | 2.02994600 | 0.63005900 |
| H | -1.45488200 | 2.72680500 | -1.35394100 |
| H | -3.32410100 | 1.16256500 | -1.51485500 |
| H | -2.71817400 | -0.21236600 | 2.33391600 |
| H | -1.23817500 | -0.65902600 | 1.54311700 |
| H | -2.28937200 | 2.16051800 | 2.08000400 |
| H | -0.80919800 | 1.44528300 | 2.71117100 |
| H | 0.20213500 | 1.45677500 | 0.46662000 |
| H | -0.40100000 | 3.06258000 | 0.79638300 |
| C | -3.93073100 | -0.89558700 | 0.15588500 |
| H | -3.62503300 | -1.87871300 | 0.50869500 |
| H | -4.73322900 | -0.53031700 | 0.80392500 |
| H | -4.30148900 | -0.98303300 | -0.86187800 |

MP2, TS2b', -834.76579356 hartree, 5.1 debye

| | | | |
|---|---|---|---|
| N | 0.87139900 | 2.06979900 | -0.50458500 |
| N | -0.41879800 | 2.25886700 | -0.75550500 |
| N | -1.04836500 | 1.06226800 | -0.91245300 |
| C | -0.12240500 | 0.07430700 | -0.74105700 |
| N | 1.07122100 | 0.73755300 | -0.46563900 |
| C | 2.34666900 | 0.19494700 | -0.16893700 |
| C | 3.26177300 | 0.97128900 | 0.54957800 |
| C | 4.51846200 | 0.44119700 | 0.83325700 |
| C | 4.84940300 | -0.85422900 | 0.42783400 |
| C | 3.91874400 | -1.61846500 | -0.27783500 |
| C | 2.66172000 | -1.10052600 | -0.59017300 |
| H | 2.98612100 | 1.96948800 | 0.85855400 |
| H | 5.23514600 | 1.03844600 | 1.38213800 |
| H | 5.82451800 | -1.26287000 | 0.65892800 |
| H | 4.17192500 | -2.62086200 | -0.59848600 |
| H | 1.93253000 | -1.68025300 | -1.13558400 |
| O | -0.32412000 | -1.17510800 | -0.69153900 |
| C | -1.66620900 | -1.51783000 | 0.89504800 |
| C | -1.89132300 | -0.21017000 | 1.30478300 |
| C | -2.65931700 | 0.62544500 | 0.49247500 |
| C | -3.62831700 | -0.00738800 | -0.48030200 |
| C | -3.96162700 | -1.43880400 | -0.07194700 |
| C | -2.68363400 | -2.25757800 | 0.07370900 |
| H | -0.93385900 | -2.10911000 | 1.43169900 |
| H | -1.24602400 | 0.23792100 | 2.05147900 |
| H | -4.53236900 | 0.60476900 | -0.52377900 |
| H | -3.18254500 | 0.01094800 | -1.47509900 |
| H | -4.49163400 | -1.42499300 | 0.88346900 |
| H | -4.62597900 | -1.89581900 | -0.80669600 |
| H | -2.25068700 | -2.47888000 | -0.90330700 |
| H | -2.89309800 | -3.21587600 | 0.55595600 |
| C | -2.90633400 | 2.05023100 | 0.87229700 |
| H | -3.05528400 | 2.66146000 | -0.01467300 |
| H | -3.81773800 | 2.08689900 | 1.47606200 |
| H | -2.08189900 | 2.46563100 | 1.44654200 |

DFT, TS3a, -955.18072885 hartree, 7.8 debye

| | | | |
|---|---|---|---|
| N | 2.37017500 | -1.16957200 | -1.70231000 |
| N | 1.46656600 | -2.08055700 | -1.63850800 |
| N | 0.91412500 | -2.14403000 | -0.41332700 |
| C | 1.50696900 | -1.20943800 | 0.37976800 |
| N | 2.42948100 | -0.58832500 | -0.44717200 |
| C | 3.33976500 | 0.45852800 | -0.17044300 |
| C | 4.18929000 | 0.91645200 | -1.18758200 |
| C | 5.08321400 | 1.95006700 | -0.92009000 |
| C | 5.14207900 | 2.53292800 | 0.34754700 |
| C | 4.29304200 | 2.06823800 | 1.35216900 |
| C | 3.39012000 | 1.03437900 | 1.10619600 |
| H | 4.13799500 | 0.45870300 | -2.16728500 |
| H | 5.73907200 | 2.30035300 | -1.71203300 |
| H | 5.84214000 | 3.33815900 | 0.54902400 |
| H | 4.32968300 | 2.51131700 | 2.34343800 |
| H | 2.72833000 | 0.66480600 | 1.87921300 |
| O | 1.25736100 | -0.97983000 | 1.58476200 |
| C | -0.49873700 | -2.88657300 | 1.55220100 |
| C | -1.61925800 | -2.06773700 | 1.46422900 |
| C | -2.47621700 | -2.07019300 | 0.37659200 |
| C | -3.60412700 | -1.09113400 | 0.32227200 |
| C | -3.25301800 | 0.13231400 | -0.59020700 |
| H | 0.16824400 | -2.80921700 | 2.39845500 |
| H | -1.78281800 | -1.33738900 | 2.25184500 |
| H | -4.49830900 | -1.57906400 | -0.08543800 |
| H | -3.84527300 | -0.72100600 | 1.32301300 |
| H | -2.99820700 | -0.24020200 | -1.59023800 |
| C | -2.21945400 | -2.92681100 | -0.81654400 |
| H | -2.23483100 | -3.99125000 | -0.55592200 |
| H | -2.94878800 | -2.75791800 | -1.61033100 |
| H | -1.19984900 | -2.71817600 | -1.18335900 |
| H | -0.34453200 | -3.71059800 | 0.87184500 |
| H | -2.35315600 | 0.61202800 | -0.19829000 |
| C | -4.40620100 | 1.09124100 | -0.68610800 |
| H | -5.28243400 | 0.69600900 | -1.20193600 |
| C | -4.48020300 | 2.34545600 | -0.21254400 |
| C | -5.73031000 | 3.16758800 | -0.41370600 |
| H | -6.15172100 | 3.48325400 | 0.54960500 |
| H | -5.50972800 | 4.08683600 | -0.97147300 |
| H | -6.50100000 | 2.61621900 | -0.95870700 |
| C | -3.37758100 | 3.05709200 | 0.53103900 |
| H | -2.48982700 | 2.44386300 | 0.69314200 |
| H | -3.06706300 | 3.95790700 | -0.01334000 |
| H | -3.73549700 | 3.39700700 | 1.51116900 |

DFT, TS3a', -955.17940164 hartree, 8.1 debye

| | | | |
|---|---|---|---|
| N | 1.88538300 | -1.88034700 | 0.06183600 |
| N | 0.65159900 | -1.71157800 | -0.25586100 |
| N | 0.42151900 | -0.46110100 | -0.69050800 |
| C | 1.58922600 | 0.23283900 | -0.65692600 |
| N | 2.51918000 | -0.67109100 | -0.17482400 |
| C | 3.90390100 | -0.51162400 | 0.06689500 |
| C | 4.63763300 | -1.58565500 | 0.58983500 |
| C | 6.00070500 | -1.43150400 | 0.82951400 |
| C | 6.64137800 | -0.22139600 | 0.55532000 |
| C | 5.90104800 | 0.84028500 | 0.03490800 |
| C | 4.53523300 | 0.70759600 | -0.21316400 |
| H | 4.13334900 | -2.52058700 | 0.79863300 |
| H | 6.56445200 | -2.26709900 | 1.23444100 |
| H | 7.70462800 | -0.10860200 | 0.74463600 |
| H | 6.38714000 | 1.78680500 | -0.18421600 |
| H | 3.95173300 | 1.52499400 | -0.61776700 |
| O | 1.75422500 | 1.42981800 | -0.99220000 |
| C | -0.72721800 | 1.58811100 | -1.55840600 |
| C | -1.06660400 | 2.33374100 | -0.42777900 |
| C | -1.95929400 | 1.90244200 | 0.53288600 |
| C | -2.61385500 | 0.55737700 | 0.48508900 |
| C | -3.89694800 | 0.53311800 | -0.40875100 |
| H | -1.27082200 | 0.69940400 | -1.83619700 |
| H | -0.55869300 | 3.28222000 | -0.27796300 |
| H | -1.89221400 | -0.18232600 | 0.11546100 |
| H | -2.90595100 | 0.26219000 | 1.49806700 |
| H | -3.61105100 | 0.82015800 | -1.42906600 |
| C | -2.27622100 | 2.77578600 | 1.70434600 |
| H | -3.36171700 | 2.85283600 | 1.84419000 |
| H | -1.88552400 | 2.31288400 | 2.62090700 |
| H | -1.85266000 | 3.77803600 | 1.61417300 |
| H | -0.02858200 | 1.98735400 | -2.27906200 |
| H | -4.59839800 | 1.29647400 | -0.05880300 |
| C | -4.52426500 | -0.83205200 | -0.42292000 |
| H | -3.88920900 | -1.61271200 | -0.84259100 |
| C | -5.73695000 | -1.19407200 | 0.02520600 |
| C | -6.19368300 | -2.62949800 | -0.07509400 |
| H | -6.42850800 | -3.03639100 | 0.91712400 |
| H | -7.11376000 | -2.70905000 | -0.66868600 |
| H | -5.43573600 | -3.26927600 | -0.53392300 |
| C | -6.74652000 | -0.26141700 | 0.64710500 |
| H | -6.39693100 | 0.76901700 | 0.73286000 |
| H | -7.67432000 | -0.25221600 | 0.06080000 |
| H | -7.02020000 | -0.60829600 | 1.65170300 |

DFT, TS3a'', -955.17905429 hartree, 7.5 debye

| | | | |
|---|---|---|---|
| N | -1.32575600 | -1.56439200 | -0.80763100 |
| N | -0.19357100 | -1.14421800 | -1.24927800 |
| N | -0.12571100 | 0.19782800 | -1.24441000 |
| C | -1.29977900 | 0.68555500 | -0.77026100 |
| N | -2.06177800 | -0.43537200 | -0.48910000 |
| C | -3.37616800 | -0.53926400 | 0.02394300 |
| C | -3.94301700 | -1.80767700 | 0.21115400 |
| C | -5.23603100 | -1.91173700 | 0.71768000 |
| C | -5.97095900 | -0.76871200 | 1.03911100 |
| C | -5.39666200 | 0.48817400 | 0.84803900 |
| C | -4.10335100 | 0.61536600 | 0.34243800 |
| H | -3.36693500 | -2.68868800 | -0.04179800 |
| H | -5.67052200 | -2.89704700 | 0.86035000 |
| H | -6.97896300 | -0.85762300 | 1.43288000 |
| H | -5.95762600 | 1.38563200 | 1.09315900 |
| H | -3.64880800 | 1.58609300 | 0.18931800 |
| O | -1.59512300 | 1.89675300 | -0.62360600 |
| C | 0.68498700 | 2.57625900 | -1.51867900 |
| C | 1.20948600 | 2.97810000 | -0.28883500 |
| C | 2.33205600 | 2.43136000 | 0.30284100 |
| C | 3.03843100 | 1.22145300 | -0.21940500 |
| C | 2.78076800 | -0.03231500 | 0.68980000 |
| H | -0.18239300 | 3.07825700 | -1.92103300 |
| H | 0.67896800 | 3.76208500 | 0.24479700 |
| H | 2.71725800 | 0.97230900 | -1.22995800 |
| H | 4.11910100 | 1.40696100 | -0.24523200 |
| H | 1.70310200 | -0.10233400 | 0.86500900 |
| C | 2.83146800 | 3.00459800 | 1.59293200 |
| H | 2.69198100 | 2.27981600 | 2.40572100 |
| H | 3.90951600 | 3.19727600 | 1.53729100 |
| H | 2.31558000 | 3.92694200 | 1.86646600 |
| H | 1.21663100 | 1.90510400 | -2.17419400 |
| H | 3.26777500 | 0.11808900 | 1.65763600 |
| C | 3.24121000 | -1.29580100 | 0.01647900 |
| H | 2.54243200 | -1.67939600 | -0.72584300 |
| C | 4.38161700 | -1.97065200 | 0.23171800 |
| C | 4.67926200 | -3.23889800 | -0.53071000 |
| H | 5.61518200 | -3.14813100 | -1.09816300 |
| H | 4.81300400 | -4.08700600 | 0.15373900 |
| H | 3.87817000 | -3.49006800 | -1.23012700 |
| C | 5.44822700 | -1.56740600 | 1.21994800 |
| H | 5.21469400 | -0.64846700 | 1.76188300 |
| H | 5.61186200 | -2.36110800 | 1.96044900 |
| H | 6.40942500 | -1.42007600 | 0.71027700 |

DFT, TS3b, -955.19733638 hartree, 4.5 debye

| | | | |
|---|---|---|---|
| N | -1.06364400 | -0.85350000 | -1.52797400 |
| N | -0.07486300 | -0.08925000 | -1.84624900 |
| N | -0.22505800 | 1.15411200 | -1.32620200 |
| C | -1.37627900 | 1.15656000 | -0.60233400 |
| N | -1.89984300 | -0.12795000 | -0.73177200 |
| C | -3.08186900 | -0.70266700 | -0.19547100 |
| C | -3.30016000 | -2.07889900 | -0.34277400 |
| C | -4.45913100 | -2.64733300 | 0.17913700 |
| C | -5.39818600 | -1.86117500 | 0.85003300 |
| C | -5.16876300 | -0.49276400 | 0.99214600 |
| C | -4.01732100 | 0.09787300 | 0.47214000 |
| H | -2.56725100 | -2.68110700 | -0.86471300 |
| H | -4.62565400 | -3.71392800 | 0.06058000 |
| H | -6.29900200 | -2.31112200 | 1.25603100 |
| H | -5.89326600 | 0.12985700 | 1.50894000 |
| H | -3.83358000 | 1.15882600 | 0.57695000 |
| O | -1.84009800 | 2.09933300 | 0.09334400 |
| C | -0.31594600 | 2.65224700 | 1.56326300 |
| C | 0.74250000 | 1.83924100 | 1.21825100 |
| C | 1.46990900 | 2.00619200 | 0.02893900 |
| C | 2.56312800 | 1.04666200 | -0.36386700 |
| C | 2.64568700 | -0.30081700 | 0.37436500 |
| H | -0.91970000 | 2.42374200 | 2.43403300 |
| H | 0.86415300 | 0.90724800 | 1.76001200 |
| H | 2.46600300 | 0.86827300 | -1.44034800 |
| H | 3.51455600 | 1.58904000 | -0.24299500 |
| H | 1.67255900 | -0.80123900 | 0.29087000 |
| C | 1.48538000 | 3.31330700 | -0.71605600 |
| H | 2.20854000 | 3.98447500 | -0.23249800 |
| H | 1.80075500 | 3.15978500 | -1.74885100 |
| H | 0.51078400 | 3.79847400 | -0.72908300 |
| H | -0.44954700 | 3.63920900 | 1.14574200 |
| H | 2.83265700 | -0.13580600 | 1.43955800 |
| C | 3.69919200 | -1.19080000 | -0.23019900 |
| H | 3.48650800 | -1.49743100 | -1.25489000 |
| C | 4.83740500 | -1.63427300 | 0.32487200 |
| C | 5.77234400 | -2.53197800 | -0.45011400 |
| H | 6.76926800 | -2.08047300 | -0.54065000 |
| H | 5.91319100 | -3.49213700 | 0.06377500 |
| H | 5.39946000 | -2.73802200 | -1.45681700 |
| C | 5.30022500 | -1.31475500 | 1.72530200 |
| H | 4.62604300 | -0.64782700 | 2.26582500 |
| H | 5.40749500 | -2.23364400 | 2.31640800 |
| H | 6.29197600 | -0.84446400 | 1.70495600 |

DFT, TS3b', -955.19685072 hartree, 4.4 debye

| | | | |
|---|---|---|---|
| N | 1.78123700 | 1.46002100 | -1.20802800 |
| N | 0.49645600 | 1.52927700 | -1.12631400 |
| N | -0.01655400 | 0.44601300 | -0.49362700 |
| C | 1.02676700 | -0.34439300 | -0.12604000 |
| N | 2.16799100 | 0.31350300 | -0.57874800 |
| C | 3.53886100 | -0.04043500 | -0.47767800 |
| C | 4.51471100 | 0.89190700 | -0.85426200 |
| C | 5.86090400 | 0.54900500 | -0.75992300 |
| C | 6.24414600 | -0.70850100 | -0.28901200 |
| C | 5.26364400 | -1.62738400 | 0.08480200 |
| C | 3.90953200 | -1.30674500 | -0.00791700 |
| H | 4.20886000 | 1.86469600 | -1.21818900 |
| H | 6.61398900 | 1.27357600 | -1.05535700 |
| H | 7.29568400 | -0.96871500 | -0.21615000 |
| H | 5.54896100 | -2.61007900 | 0.44886200 |
| H | 3.14365500 | -2.01530600 | 0.27806400 |
| O | 0.98018700 | -1.41484100 | 0.53722800 |
| C | 0.00130600 | -0.97346900 | 2.44058400 |
| C | -0.34326900 | 0.35311900 | 2.29939100 |
| C | -1.34167500 | 0.80613400 | 1.41977800 |
| C | -2.44171500 | -0.10509100 | 0.92992700 |
| C | -3.23613800 | 0.37043300 | -0.30324500 |
| H | 0.84618300 | -1.25480600 | 3.05845700 |
| H | 0.32953700 | 1.10330300 | 2.70778300 |
| H | -2.03043500 | -1.09586400 | 0.72710100 |
| H | -3.13925200 | -0.22278000 | 1.77470500 |
| H | -2.51422900 | 0.56325900 | -1.10508400 |
| C | -1.54641200 | 2.28393800 | 1.27187500 |
| H | -1.62405800 | 2.56310800 | 0.21883300 |
| H | -2.48823700 | 2.56949100 | 1.75988500 |
| H | -0.73300800 | 2.85463500 | 1.72359800 |
| H | -0.65778500 | -1.77882600 | 2.15191800 |
| H | -3.74009000 | 1.31621700 | -0.08692800 |
| C | -4.21951900 | -0.67563500 | -0.75500800 |
| H | -3.75863200 | -1.60514300 | -1.09313400 |
| C | -5.55927300 | -0.60767800 | -0.79202500 |
| C | -6.37649300 | -1.77499400 | -1.29219300 |
| H | -7.07466700 | -2.12791200 | -0.52144200 |
| H | -6.98993600 | -1.48607800 | -2.15594200 |
| H | -5.74623700 | -2.61677800 | -1.59109100 |
| C | -6.37756700 | 0.58730600 | -0.36806700 |
| H | -5.77542000 | 1.41508500 | 0.01066100 |
| H | -6.97393800 | 0.96512000 | -1.20873000 |
| H | -7.09320000 | 0.30572300 | 0.41546100 |

MP2, TS3a, -952.24896144 hartree, 7.7 debye

| | | | |
|---|---|---|---|
| N | -0.33396400 | -1.63861700 | -1.88482000 |
| N | -1.65666700 | -1.73330200 | -1.80942800 |
| N | -2.07120100 | -1.75934300 | -0.51758200 |
| C | -0.97600200 | -1.65913600 | 0.28731400 |
| N | 0.10384400 | -1.60869400 | -0.59694700 |
| C | 1.46661600 | -1.40952000 | -0.29309100 |
| C | 2.28515700 | -0.74226400 | -1.21274700 |
| C | 3.63215400 | -0.55266400 | -0.90817300 |
| C | 4.15499300 | -1.00134100 | 0.30862300 |
| C | 3.32133900 | -1.65250100 | 1.22109000 |
| C | 1.97436100 | -1.86726000 | 0.92810700 |
| H | 1.86311000 | -0.40383900 | -2.14839100 |
| H | 4.27300700 | -0.04968100 | -1.62188200 |
| H | 5.20177300 | -0.84955900 | 0.53979300 |
| H | 3.72153400 | -2.00658000 | 2.16295100 |
| H | 1.31157200 | -2.35823200 | 1.62527900 |
| O | -0.92829400 | -1.53694400 | 1.54253600 |
| C | -3.46086500 | -0.86157100 | 1.53724600 |
| C | -2.99440200 | 0.43029000 | 1.45465900 |
| C | -3.08372300 | 1.14467000 | 0.25925200 |
| C | -2.09427200 | 2.22126500 | 0.04305300 |
| C | -0.79998300 | 1.49805300 | -0.47205100 |
| H | -3.20558100 | -1.48081400 | 2.38219700 |
| H | -2.33426700 | 0.79506600 | 2.22917100 |
| H | -2.42909900 | 2.95295600 | -0.69147400 |
| H | -1.84447200 | 2.72546500 | 0.97711700 |
| H | -1.02859200 | 0.97626600 | -1.40464600 |
| C | -3.91846400 | 0.71085200 | -0.88487300 |
| H | -4.87637400 | 0.30314400 | -0.57203600 |
| H | -4.07570800 | 1.52728300 | -1.58465200 |
| H | -3.36676300 | -0.09833400 | -1.38734100 |
| H | -4.09737400 | -1.28676900 | 0.77810300 |
| H | -0.53669300 | 0.73970100 | 0.25979600 |
| C | 0.32788100 | 2.45679200 | -0.66813400 |
| H | 0.25860100 | 3.11130800 | -1.53281700 |
| C | 1.41501500 | 2.55260100 | 0.12278200 |
| C | 2.52171300 | 3.51090200 | -0.21817500 |
| H | 2.70932800 | 4.20076600 | 0.60734800 |
| H | 3.44985500 | 2.96224100 | -0.39304600 |
| H | 2.29291000 | 4.09287200 | -1.10975900 |
| C | 1.66160100 | 1.72978200 | 1.35595200 |
| H | 0.84753200 | 1.05539300 | 1.61060400 |
| H | 2.55863500 | 1.12336900 | 1.22139500 |
| H | 1.84062700 | 2.38952300 | 2.20843000 |

MP2, TS3a', -952.24252078 hartree, 8.3 debye

| | | | |
|---|---|---|---|
| N | -1.02983800 | -1.42897100 | -1.10388400 |
| N | 0.05535000 | -0.88315800 | -1.63123100 |
| N | -0.01386100 | 0.46689700 | -1.56713800 |
| C | -1.18467900 | 0.81617900 | -0.97771200 |
| N | -1.81185300 | -0.38967500 | -0.69016800 |
| C | -3.05748900 | -0.62624000 | -0.06150700 |
| C | -3.36391900 | -1.91847600 | 0.38208900 |
| C | -4.59379400 | -2.15003600 | 0.99393500 |
| C | -5.50482200 | -1.10696400 | 1.17824600 |
| C | -5.18000300 | 0.17641000 | 0.73722300 |
| C | -3.95943700 | 0.42975500 | 0.11069000 |
| H | -2.64900300 | -2.71442300 | 0.23315000 |
| H | -4.83629500 | -3.14908300 | 1.33362600 |
| H | -6.45641200 | -1.29385900 | 1.65901200 |
| H | -5.88141400 | 0.98999300 | 0.87351200 |
| H | -3.69001400 | 1.41705100 | -0.23374700 |
| O | -1.57759100 | 1.99363300 | -0.73046200 |
| C | 0.60932600 | 2.83463100 | -1.38281400 |
| C | 0.88622800 | 2.99546900 | -0.02537600 |
| C | 1.89896200 | 2.32000300 | 0.62286300 |
| C | 2.69193500 | 1.22016100 | 0.00968600 |
| C | 2.36975100 | -0.13211000 | 0.70524000 |
| H | -0.17998900 | 3.40839100 | -1.83926300 |
| H | 0.24419300 | 3.65365500 | 0.54476700 |
| H | 2.48525900 | 1.10501100 | -1.05015800 |
| H | 3.75876700 | 1.42374000 | 0.13940900 |
| H | 1.28680700 | -0.26169400 | 0.71812600 |
| C | 2.13479700 | 2.59088400 | 2.07347000 |
| H | 1.65691600 | 1.80833000 | 2.66812200 |
| H | 3.19969200 | 2.56500000 | 2.30411500 |
| H | 1.71822900 | 3.54840400 | 2.37838300 |
| H | 1.29096200 | 2.32329500 | -2.03890100 |
| H | 2.71681200 | -0.10474600 | 1.73841900 |
| C | 2.98627700 | -1.26461600 | -0.05952800 |
| H | 2.38601300 | -1.62449900 | -0.88860900 |
| C | 4.19325400 | -1.81549800 | 0.16950200 |
| C | 4.69408700 | -2.94300800 | -0.68975500 |
| H | 5.63650800 | -2.67536600 | -1.17320600 |
| H | 4.88867300 | -3.83274400 | -0.08663000 |
| H | 3.97267000 | -3.20336500 | -1.46199600 |
| C | 5.13016600 | -1.39366300 | 1.26741600 |
| H | 4.75226900 | -0.55874500 | 1.85363200 |
| H | 5.32226000 | -2.22585100 | 1.94822700 |
| H | 6.09540600 | -1.10049200 | 0.84865000 |

MP2, TS3a'', -952.23962938 hartree, 9.1 debye

| | | | |
|---|---|---|---|
| N | 1.74110400 | -1.90293000 | -0.13424800 |
| N | 0.49399700 | -1.72512300 | -0.53514300 |
| N | 0.31533500 | -0.45193600 | -0.95931900 |
| C | 1.48128700 | 0.22726100 | -0.82225200 |
| N | 2.37074300 | -0.70218800 | -0.30335500 |
| C | 3.73283600 | -0.54345000 | 0.04666600 |
| C | 4.36486200 | -1.54004900 | 0.80019200 |
| C | 5.70780500 | -1.38494700 | 1.13649100 |
| C | 6.41378700 | -0.24585200 | 0.74174200 |
| C | 5.76642600 | 0.74115000 | -0.00238500 |
| C | 4.42534000 | 0.60218700 | -0.36105700 |
| H | 3.80567000 | -2.41449200 | 1.09904900 |
| H | 6.20086400 | -2.15582700 | 1.71523700 |
| H | 7.45576100 | -0.13044700 | 1.01114400 |
| H | 6.30649100 | 1.62622300 | -0.31457500 |
| H | 3.90773800 | 1.35758300 | -0.93331100 |
| O | 1.67309700 | 1.44681900 | -1.10044800 |
| C | -0.69107100 | 1.67024100 | -1.59124100 |
| C | -0.88218500 | 2.29852600 | -0.35842800 |
| C | -1.71761300 | 1.77968600 | 0.60657400 |
| C | -2.44349000 | 0.48993100 | 0.43514700 |
| C | -3.76969600 | 0.66353700 | -0.34940200 |
| H | -1.31881700 | 0.85303500 | -1.89920400 |
| H | -0.30891800 | 3.19057600 | -0.14616600 |
| H | -1.79075800 | -0.22519300 | -0.07590900 |
| H | -2.68628600 | 0.08297700 | 1.41813400 |
| H | -3.54517800 | 1.08975000 | -1.33074100 |
| C | -1.89858700 | 2.49559600 | 1.90238600 |
| H | -2.96179600 | 2.58538700 | 2.13330800 |
| H | -1.45278500 | 1.90000200 | 2.70297000 |
| H | -1.44221600 | 3.48271600 | 1.90236400 |
| H | -0.07218100 | 2.13092100 | -2.34281200 |
| H | -4.40529000 | 1.38536500 | 0.16488900 |
| C | -4.45410000 | -0.65801100 | -0.51245700 |
| H | -3.93268700 | -1.36370400 | -1.15352500 |
| C | -5.59549600 | -1.06771300 | 0.07226600 |
| C | -6.13077000 | -2.44876300 | -0.18825700 |
| H | -6.21522200 | -3.01200600 | 0.74341000 |
| H | -7.13177800 | -2.39975200 | -0.62210100 |
| H | -5.48868200 | -3.00617400 | -0.86776300 |
| C | -6.43451100 | -0.23942800 | 1.00501500 |
| H | -6.01759800 | 0.74466700 | 1.20309100 |
| H | -7.43722800 | -0.10556300 | 0.59411600 |
| H | -6.55109200 | -0.75477700 | 1.96042900 |

MP2, TS3b, -952.27651013 hartree, 4.2 debye

| | | | |
|---|---|---|---|
| N | -0.86315400 | -0.79764700 | -1.52363900 |
| N | 0.13396100 | 0.03410700 | -1.80789800 |
| N | -0.11148000 | 1.26019900 | -1.26795500 |
| C | -1.30697100 | 1.20069100 | -0.61457900 |
| N | -1.73877200 | -0.11314800 | -0.76301900 |
| C | -2.90513800 | -0.73365300 | -0.24723400 |
| C | -2.89800600 | -2.11685900 | -0.04245200 |
| C | -4.04578700 | -2.72832800 | 0.45693700 |
| C | -5.17420300 | -1.96683500 | 0.77162400 |
| C | -5.15726500 | -0.58540400 | 0.57226200 |
| C | -4.02610700 | 0.04509600 | 0.05376900 |
| H | -2.01308300 | -2.68740000 | -0.28642500 |
| H | -4.05273100 | -3.79952900 | 0.61162700 |
| H | -6.05942300 | -2.44719900 | 1.16761600 |
| H | -6.03087500 | 0.00760100 | 0.81032600 |
| H | -3.99961000 | 1.11232100 | -0.10705100 |
| O | -1.84749300 | 2.10112100 | 0.10117600 |
| C | -0.55148900 | 2.53927300 | 1.58373400 |
| C | 0.55474900 | 1.75773000 | 1.28933300 |
| C | 1.31267800 | 1.98704200 | 0.13738200 |
| C | 2.45582900 | 1.07445100 | -0.21766400 |
| C | 2.42561100 | -0.33344600 | 0.38171500 |
| H | -1.18904000 | 2.27001500 | 2.41519700 |
| H | 0.62900600 | 0.78941400 | 1.76545100 |
| H | 2.50035900 | 1.00517300 | -1.30608300 |
| H | 3.37839000 | 1.58034200 | 0.09422800 |
| H | 1.44223400 | -0.77235200 | 0.20142500 |
| C | 1.38970400 | 3.35520200 | -0.48369000 |
| H | 2.06895600 | 3.97473000 | 0.10778600 |
| H | 1.77876100 | 3.27774900 | -1.49547800 |
| H | 0.41863300 | 3.83804600 | -0.53200800 |
| H | -0.60329300 | 3.57168600 | 1.27839100 |
| H | 2.56736200 | -0.28495300 | 1.46188300 |
| C | 3.46299500 | -1.20080000 | -0.26557600 |
| H | 3.22110800 | -1.51018500 | -1.27888600 |
| C | 4.64400600 | -1.59200400 | 0.24794200 |
| C | 5.58039100 | -2.45398700 | -0.55353800 |
| H | 6.54397300 | -1.95826600 | -0.69133400 |
| H | 5.77971600 | -3.39534100 | -0.03640300 |
| H | 5.17002300 | -2.68385000 | -1.53542500 |
| C | 5.14169000 | -1.23590900 | 1.62139400 |
| H | 4.46456900 | -0.58170000 | 2.16479300 |
| H | 5.29498800 | -2.13797200 | 2.21786500 |
| H | 6.10990600 | -0.73543300 | 1.55252500 |

MP2, TS3b', -952.27503700 hartree, 4.1 debye

| | | | |
|---|---|---|---|
| N | 1.81398300 | 1.34726300 | -1.39240800 |
| N | 0.49229600 | 1.47560100 | -1.37445000 |
| N | -0.06551600 | 0.46374500 | -0.65481400 |
| C | 0.94136200 | -0.33034000 | -0.19470100 |
| N | 2.11226400 | 0.26490100 | -0.64755200 |
| C | 3.45741100 | -0.12608100 | -0.42507500 |
| C | 4.46219300 | 0.84360900 | -0.49728900 |
| C | 5.78440900 | 0.45858200 | -0.28676500 |
| C | 6.09589800 | -0.86925600 | 0.01633100 |
| C | 5.07733700 | -1.82034600 | 0.09614500 |
| C | 3.74877100 | -1.46123500 | -0.13128100 |
| H | 4.20024200 | 1.86650100 | -0.72762600 |
| H | 6.57000500 | 1.20055200 | -0.34818200 |
| H | 7.12428200 | -1.15968700 | 0.18733500 |
| H | 5.31461900 | -2.85110000 | 0.32584800 |
| H | 2.95139200 | -2.18683100 | -0.07436700 |
| O | 0.85035300 | -1.31324600 | 0.60923400 |
| C | 0.07160900 | -0.60418200 | 2.30888400 |
| C | -0.24648800 | 0.71254200 | 2.00802700 |
| C | -1.22113400 | 1.02735900 | 1.05753300 |
| C | -2.34805300 | 0.06677200 | 0.75968500 |
| C | -3.17658600 | 0.38233100 | -0.48972500 |
| H | 0.91107700 | -0.81181200 | 2.95912400 |
| H | 0.47275100 | 1.48431800 | 2.25747400 |
| H | -1.94724900 | -0.94213800 | 0.66957400 |
| H | -3.01437300 | 0.07108500 | 1.63153700 |
| H | -2.49261900 | 0.49080100 | -1.33329400 |
| C | -1.45317300 | 2.47039200 | 0.72341800 |
| H | -1.68560200 | 2.59935900 | -0.32991000 |
| H | -2.30138100 | 2.83296100 | 1.31104300 |
| H | -0.58025900 | 3.07497800 | 0.96006100 |
| H | -0.67373300 | -1.38144400 | 2.25819900 |
| H | -3.69605800 | 1.33251700 | -0.36863200 |
| C | -4.14735400 | -0.72652300 | -0.76818000 |
| H | -3.70833000 | -1.62444900 | -1.19602300 |
| C | -5.46945000 | -0.74239400 | -0.51483900 |
| C | -6.30100800 | -1.95152000 | -0.84443600 |
| H | -6.78761300 | -2.34548300 | 0.05069000 |
| H | -7.09497100 | -1.69570800 | -1.54969700 |
| H | -5.69755500 | -2.74456000 | -1.28319900 |
| C | -6.23760000 | 0.39904100 | 0.09180300 |
| H | -5.60660500 | 1.24182900 | 0.36233200 |
| H | -7.00293600 | 0.75574200 | -0.60097100 |
| H | -6.75796900 | 0.06545200 | 0.99216000 |