Supporting Information for

On the Stereoselectivity of 4-Penten-1-oxyl Radical 5-*exo*-trig Cyclizations

Jens Hartung, Kristina Daniel,[a] Christian Rummey,[b] and Gerhard Bringmann[b]*

[a] Fachbereich Chemie, Organische Chemie, Technische Universität Kaiserslautern,

Erwin-Schrödinger-Straße, D-67663 Kaiserslautern, Germany

Fax: +49 631 205 3921

E-mail: hartung@chemie.uni-kl.de

[b] Institut für Organische Chemie, Universität Würzburg,

Am Hubland, D-97074 Würzburg, Germany

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1 General Remarks

(i) The compound numbering in this Supporting Information is consistent with that of the accompanying publication. (ii) The cited literature exclusively refers to this Supporting Information. The following abbreviations have been used: DABCO = 1,4-diazabicyclo[2.2.2]octane, DTA = differential thermoanalysis, E = envelope conformation MTB = *tert*-butyl methyl ether, T = twist conformation.

2 Experimental Procedure – Instrumentation and Reagents

Melting points [°C] were determined on a Koffler hot-plate melting point microscope (company *Reichert*) and are uncorrected. Differential-thermoanalysis (DTA) of substituted *N*-[(*tert*-butyl)pentenoxy)thiazole-2(3*H*)thiones **6d** and **6f** were performed on a Thermal-Analyzer 9000 (*Du Pont*). Photochemical reactions are performed using a Rayonet® Photoreactor equipped with sixteen RPR-350 nm light bulbs (*The Southern New England*). ^{1}H And ^{13}C spectra were recorded with a AC400 spectrometer (*Bruker*). Residual $CHCl_3$ in the applied solvent $CDCl_3$ served as internal standard (^{1}H NMR). Mass spectra were recorded with a Match 7 instrument (*Varian*) using electron impact techniques (EI, 70 eV ionization energy). Gas chromatography was performed using a Carlo Erba GC 6000 instrument (Vega Series 2, FID) using a DB-225 column (30 m × 0.32 mm, 0.25 μm layer) from *J&W Scientific* and a Spectra Physics Integrator 4290. Helium was used as carrier gas (flow rate of 3 mL/min, 80 kPa pressure). The retention times t_R refer to the following temperature program: 120 °C (5 min), 120 °C → 220 (10 °C min^{-1}), 220 °C (15 min); injector and detector temperature: 240 °C. *n*-$C_{14}H_{30}$ served as internal standard for quantitative GC analysis. Reaction progress was monitored via thin layer chromatography on aluminum plates coated with silica gel (60 F_{254}, *Merck*). The products were detected via UV-light (254 nm) or with Ekkert's reagent. Combustion analysis was performed using a Carlo Erba 1106 instrument. NEt_4OH (25% solution in MeOH) and Bu_3SnH were commercially available and were used as received (Fluka, Merck, Lancaster). *N*-(Hydroxy)-4-(*p*-chlorophenyl)thiazole-2(3*H*)thione,[1] 2-(1,1-dimethylethyl)-4-penten-1-yl *p*-toluenesulfonate (**5d**),[2] and 4,4-dimethyl-2-penten-1-ol[3] were prepared according to literature procedures.

3 Synthesis of 3-(1,1-dimethylethyl)-4-penten-1-yl *p*-toluenesulfonate (5f)

3.1 **Ethyl 3-(1,1-dimethylethyl)-4-pentenoate**.[4] A two-necked round-bottomed flask equipped with a reflux condenser and a magnetic stir bar was charged with 4,4-dimethyl-2-penten-1-ol (2.18 g, 19.35 mmol), ethyl orthoacetate (22 g, 135.4 mmol), and propionic acid (86 mg, 1.2 mmol). The reaction mixture was heated to 138 °C for 5 h, which led to a conversion of the starting alcohol of 95 %. An excess of ethyl orthoacetate was removed by distillation (60 °C, 20 mbar). The remaining liquid was purified by chromatography [SiO_2, petroleum ether/Et_2O = 1/1, (*v*/*v*)] to afford ethyl 3-(1,1-dimethylethyl)-4-pentenoate (1.92 g, 54 % yield) as colorless liquid [bp = 60 °C (20 mbar)].

3.2 **3-(1,1-Dimethylethyl)-4-penten-1-ol**.[5] To a stirred suspension of $LiAlH_4$ (290 mg, 7.6 mmol) in anhydrous Et_2O (20 mL) was added in drops a solution of ethyl 3-(1,1-dimethylethyl)-4-pentenoate (1.4 g, 7.6 mmol) in dry Et_2O (5 mL) at 0 °C. The mixture was heated in an oil bath (40 °C) for 1 h and was afterwards allowed to cool to 0 °C. H_2O was added until no further gas evolved. Salts, which formed upon hydrolysis, were dissolved by adding a satd. aqueous solution of NH_4Cl. The organic phase was separated. The aqueous layer was extracted with Et_2O (2 × 10 mL). The combined organic phases were washed with brine, dried ($MgSO_4$), and concentrated under reduced pressure. The residual yellow oil was purified by bulb-to-bulb distillation to furnish 604 mg (56 %) of 3-(1,1-dimethylethyl)-4-penten-1-ol as colorless oil. The ^{1}H NMR spectral data were in accord with the values reported in the literature.[5]

3.3 **3-(1,1-dimethyl)-4-penten-1-yl *p*-toluenesulfonate** (**5f**). A round-bottomed flask was charged with 3-(1,1-dimethylethyl)-4-penten-1-ol (324 mg, 2.28 mmol), CH_2Cl_2 (3 mL), and DABCO (510 mg, 4.56 mmol). The solution was stirred for 10 min at 0 ° and was afterwards treated in portions with *p*-toluenesulfonyl chloride (652 mg, 3.42 mmol), to afford a slurry, which was stirred for 2 h at 20 °C. The reaction mixture was poured into a mixture of MTB/H_2O [60 mL, 1/1 (*v*/*v*)]. The aqueous phase was separated and washed with MTB (3 × 30 mL). The combined organic phases were washed with 2M HCl, satd. aqueous $NaHCO_3$, and H_2O to afford a clear layer, which was dried ($MgSO_4$) and concentrated under reduced pressure. The remaining oil was purified by column chromatography [SiO_2, petroleum ether/Et_2O = 1/1 (*v*/*v*)] to yield 3-(1,1-dimethylethyl)-4-penten-1-yl *p*-toluenesulfonate (**5f**) as a colorless oil. Yield: 0.96 g (70 %). ^{1}H-NMR ($CDCl_3$, 250 MHz): δ = 0.81 [s, 9 H, $C(CH_3)_3$], 1.29–1.44 (m, 1 H, 5-H), 1.73 (ddd, *J* 11.9, 9.8, 2.4, 1 H, 6-H), 1.91 (m_c, 1 H, 5-H), 2.44 (s, 3 H, Ar-CH_3), 3.90 (dt, *J* 9.5, 6.4, 1 H, 4-H), 4.07 (ddd, *J* 9.5, 7.3, 6.4, 1 H, 4-H), 4.79 (dd, *J* 17.1, 2.1, 1 H, =CH_2), 4.97 (dd, *J* 10.4,

2.1, 1 H, =CH_2), 5.44 (dt, *J* 17.1, 10.1, 1 H, =CH), 7.34 (m_c, 2 H, Ar), 7.79 (m_c, 2 H, Ar). ^{13}C NMR (63 MHz; $CDCl_3$): δ = 22.0 (Ar-CH_3), 27.9 (CH_3), 28.5 [$C(CH_3)_3$], 32.7 (C-2), 51.2 (C-3), 70.1 (C-1), 117.9 (C-5), 128.3 (Ar), 130.2 (Ar), 138.6 (C-4). MS (70 eV, EI): *m*/*z* = 155 [$C_7H_7SO_2^+$] (5 %), 91 [$C_7H_7^+$] (19), 68 (100), 57 (68), 41 (39). Calcd. for $C_{16}H_{24}SO_3$ (296.42): C, 64.83; H, 8.16; S, 10.82. Found: C, 64.92, H, 7.80, S, 10.91.

4 Synthesis and Spectral Characterization of 4-*tert*-Butyl-2-methyltetrahydrofuran (3d) and 3-*tert*-Butyl-2-methyltetrahydrofuran (3f)

4.1 Synthesis of 2-(Iodomethyl)tetrahydrofurans

General procedure. A round-bottomed flask equipped with a magnetic stir bar was charged with I_2 (1.52 g, 6.0 mmol), MeCN (9 mL), and saturated aqueous solution of $NaHCO_3$ (4 mL). 2-(1,1-Dimethylethyl)-4-penten-1-ol or 3-(1,1-dimethylethyl)-4-penten-1-ol (475 mg, 3.3 mmol) was added in small portions at 0 °C and stirring was continued for 1 h at 0 °C and for 2–3 h at 20 °C. The organic solvent was removed under reduced pressure to afford a brown residue that was taken up in MTB (20 mL). The organic phase was successively washed with an aqueous solution of $Na_2S_2O_3$ [2 × 10 mL 10 % (w/w)], H_2O (15 mL), and brine (10 mL). The ethereal solution was dried ($MgSO_4$) and concentrated under reduced pressure to afford an oil, which was purified by chromatography (SiO_2).

4.2 **4-(*tert*-Butyl)-2-(iodomethyl)tetrahydrofuran**. Eluent used for chromatographic purification: petroleum ether/Et_2O = 5/1 (*v*/*v*), R_f = 0.45. Yield: 650 mg (73 %), colorless oil, *cis*:*trans* = 91:9 (GC). GC: t_r = 8.59 min (*cis*-isomer), 8.67 min (*trans*-isomer). Calcd. for $C_9H_{17}OI$ (268.14): C, 40.31; H, 6.39. Found: C, 40.43; H, 6.08. MS (70 eV, EI): *m*/*z* (%) = 268 [M^+] (2), 141 [$C_9H_{17}O^+$] (8), 127 [$C_8H_{15}O^+$] (100), 83 [$C_5H_7O^+$] (16), 57 [$C_4H_9^+$] (54). *cis*-Isomer: ^{1}H-NMR ($CDCl_3$, 250 MHz): δ = 0.89 [s, 9 H, $C(CH_3)_3$], 1.37 (m_c, 1 H, 3-H), 2.02–2.15 (m, 1 H, 3-H), 2.17–2.27 (m, 1 H, 4-H), 3.25 (dd, *J* 5.2, 6.1, 2 H, CH_2I), 3.69 (t, *J* 9.1, 1 H, 5-H), 3.87 (t, *J* 9.1, 1 H, 5-H), 3.89–4.01 (m, 1 H, 2-H). ^{13}C-NMR ($CDCl_3$, 63 MHz): δ = 10.7 (CH_2I), 28.0 (CH_3), 31.7 [$C(CH_3)_3$], 35.1 (3-C), 51.5 (4-C), 70.3 (5-C), 79.5 (2-C). *trans*-Isomer: ^{1}H-NMR ($CDCl_3$, 250 MHz): δ = 0.88 (s, 9 H, *t*Bu), 1.37 (m_c, 1 H, 3-H), 1.76 (m_c, 1 H, 3-H), 2.23 (m_c, 1 H, 4-H), 3.19 (dd, *J* 5.2, 2.8, 2 H, CH_2I), 3.54 (t, *J* 9.1, 1 H, 5-H), 3.69 (t, *J* 9.1, 1 H, 5-H), 3.92–4.05 (m, 1 H, 2-H). ^{13}C-NMR ($CDCl_3$, 63 MHz): δ = 11.2 (CH_2I), 26.2 [$C(CH_3)_3$], 31.3 (CH_3), 33.4 (3-C), 49.8 (4-C), 70.7 (5-C), 79.5 (2-C).

4.3 ***trans*-3-(*tert*-Butyl)-2-(iodomethyl)tetrahydrofuran**. Eluent used for chromatographic purification: petroleum ether/Et_2O = 9/1 (*v*/*v*), R_f = 0.30. Yield: 726 mg (2.95 mmol, 82 %). GC: t_r = 13.43 min. ^{1}H-NMR ($CDCl_3$, 250 MHz): δ = 0.90 [s, 9 H,C(CH_3)], 1.74–1.80 (m, 2 H, 4-H), 1.90–2.06 (m, 1 H, 3-H), 3.22 (dd, *J* 10.4, 6.7, 1 H, 6-H), 3.37 (dd, *J* 10.7, 3.7, 1 H, 6-H), 3.73–3.92 (m, 3 H, CHO, CH_2O). ^{13}C-NMR ($CDCl_3$, 63 MHz): δ = 13.5 (CH_2J), 28.2 (CH_3), 29.5 [C(CH_3)$_3$], 32.3 (C-3), 55.8 (C-4), 68.3 (C-5), 80.0 (C-2). MS (70 eV, EI): *m*/*z* (%) = 268 ($C_9H_{17}OI^+$, 2%), 141 ($C_9H_{17}O^+$, 6), 127 ($C_{15}H_8O^+$, 78), 57 ($C_4H_9^+$, 100), 41 ($C_3H_5^+$, 37). Calcd. for $C_9H_{17}OI$ (268.14: C, 40.31; H, 6.39. Found: C, 40.32; H, 6.10.

4.4 4-(*tert*-Butyl)-2-methyltetrahydrofuran (3d) and *trans*-3-(*tert*-Butyl)-2-methyltetrahydrofuran (3f)

General procedure for the conversion of 2-(iodomethyl)tetrahydrofurans into 2-methyltetrahydrofurans. A two-necked round-bottomed flask equipped with Ar inlet was charged with $LiAlH_4$ (0.25 g, 6.6 mmol), LiH (0.10 g, 12.6 mmol), and dry THF (25 mL). To this slurry was added at 20 °C in drops a solution of 0.56 g (2.1 mmol) of 4-(*tert*-butyl)-2-(iodomethyl)tetrahydrofuran (*cis*:*trans* = 91:9) or *trans*-3-(*tert*-butyl)-2-(iodomethyl)tetrahydrofuran in anhydrous THF (5 mL). Stirring was continued for 14 h at 20 °C. H_2O (5 mL) was added at 0°C to afford a colorless precipitate, which was dissolved with a minimum volume of 10% aq. H_2SO_4. The aqueous phase was separated and washed with MTB (3 × 20 mL). The combined organic phases were washed with brine (30 mL), dried ($MgSO_4$), and concentrated under reduced pressure. The residual oil was purified by column chromatography [SiO_2, petroleum ether/Et_2O = 2:1 (*v*/*v*)]

4-*tert*-Butyl-2-methyltetrahydrofuran (**3d**). Yield: 110 mg (1.64 mmol, 78 %); R_f = 0.55 [SiO_2, petroleum ether/Et_2O = 2:1 (*v*/*v*)]; colorless volatile oil; *cis*:*trans* = 91:9 (GC: t_r = 3.78 for *cis*-**3d** and 4.06 min for *trans*-**3d**). Calcd. for $C_9H_{18}O$ (142.24): C, 76.00; H, 12.76. Found: C, 76.09; H, 12.73. MS (70 eV, EI): *m*/*z* (%) = 142 [M^+] (4), 127 [$C_8H_{15}O^+$] (100), 83 [$C_5H_7O^+$] (38), 57 [$C_4H_9^+$] (92), 41 [$C_3H_5^+$] (47). *cis*-**3d**: ^{1}H-NMR ($CDCl_3$, 250 MHz): δ = 0.87 [s, 9 H, C(CH_3)$_3$], 1.25 (d, *J* 5.8, 3 H, CH_3), 1.54 (m_c, 1 H, 3-H), 1.90 (dt, J_d 13.4, J_t 6.7, 1 H, 3-H), 2.16 (m_c, 1 H, 4-H), 3.66 (t, *J* 8.6, 1 H, 5-H), 3.75 (t, *J* 8.6, 1 H, 5-H), 3.93 (m_c, 1 H, 2-H). ^{13}C-NMR ($CDCl_3$, 63 MHz): δ = 21.0 (CH_3), 28.0 [C(CH_3)$_3$], 36.3 (3-C), 51.4 (4-C), 69.3 (5-C), 76.5 (2-C). *trans*-**3d**: ^{1}H-NMR ($CDCl_3$, 250 MHz) δ = 0.84 [s, 9 H, C(CH_3)$_3$], 1.85 (d, 3 H, *J* = 5.8 Hz, CH_3), 1.44 (m, 1 H, *J* = 6.4,12.2 Hz, 3-H), 1.78 (dt, *J* = 7.3, 12.2 Hz, 1 H, 3-H), 2.16 (m_c, 1 H, 4-H), 3.44 (t, *J* = 8.9 Hz, 1 H, 5-H), 3.89 (t, *J* = 10.6

Hz, 1 H, 5-H), 3.96 (m, 1 H, 2-H). ^{13}C-NMR ($CDCl_3$, 63 MHz): δ = 20.8 (CH_3), 23.0 [$C(CH_3)_3$], 36.3 (3-C), 49.9 (4-C), 69.8 (5-C), 76.8 (2-C).

compound	*cis*-**3d**	*trans*-**3d**
Significant NOESY interactions	3-H – 2-CH_3	3-H – 2-H
	2-H – 4-H	3'-H – 2-CH_3
	3'-H – 4-H	3'-H – 4-H

***trans*-3-*tert*-Butyl-2-methyltetrahydrofuran** *trans*-(**3f**). Yield: 248 mg (85 %); R_f = 0.50 [SiO_2, petroleum ether/Et_2O = 2:1 (*v*/*v*)]; colorless volatile oil; diastereomerically pure [NMR, GC (t_r = 4.21 min)]. Calcd. for $C_9H_{18}O$ (142.24): C, 76.00; H, 12.76: Found: C, 76.38; H, 12.93. MS (70 eV, EI): *m*/*z* (%) = 142 [M^+] (1), 127 [$C_8H_{15}O^+$] (24), 83 [$C_5H_7O^+$] (26), 70 [$C_4H_6O^+$] (100), 57 [$C_4H_9^+$] (56). ^{1}H-NMR ($CDCl_3$, 250 MHz): δ = 0.88 [s, 9 H, $C(CH_3)_3$], 1.22 (d, *J* 6.1, 3 H, CH_3), 1.61 (m_c, 1 H, 4-H), 1.72 (dq, J_d 12.5, J_q 7.0, 1 H, 4-H), 1.82–1.96 (m, 1 H, 4-H), 3.62–3.78 (m, 2 H, 5-H), 3.84 (dq, *J* 12.2, 6.1, 1 H, 2-H). ^{13}C-NMR ($CDCl_3$, 63 MHz): δ = 15.7 (CH_3), 28.3 [$C(CH_3)_3$], 29.7 (4-C), 57.1 (3-C), 67.3 (5-C), 76.5 (2-C).

5 UHF-Calculated Energies of Radicals 1, *cis*-2, *trans*-2, and Transition Structures 7–10

Table 5.1. Computed energies (E), zero point vibrational energies (ZPVE), $\langle S^2 \rangle$ values, and relative heats of formation ($\Delta\Delta H_f$) of radicals **1**–**3** [a]

	parameter	**1**	*cis*-**2**	*trans*-**2**
1a → *cis*-**2a** + *trans*-**2a** ($R^1 = CH_3$)	E + ZPVE [b]	–308.251595	–308.260999	–308.261216
	ZPVE [c]	441430.5	443832.5	443370.3
	$\langle S^2 \rangle$	0.759	0.762	0.762
	$\Delta\Delta H_f$ [d]	≡ 0	–24.7	–25.3
	conformer [e]	– [f]	$^1T_5$	$_3T^4$
1b → *cis*-**2b** + *trans*-**2b** [$R^1 = C(CH_3)_3$]	E + ZPVE [b]	–425.261985	–425.271998	–425.272707
	ZPVE [c]	677237.8	680954.1	680918.6
	$\langle S^2 \rangle$	0.758777	0.762	0.762
	$\Delta\Delta H_f$ [d]	≡ 0	–26.3	–28.2
	conformer [e]	– [f]	$^1T_5$	$_3T^4$
1c → *cis*-**2c** + *trans*-**2c** ($R^2 = CH_3$)	E + ZPVE [b]	–308.248186	–308.256383	–308.256210
	ZPVE [c]	439708.0	444682.7	444515.6
	$\langle S^2 \rangle$	0.759	0.762	0.762
	$\Delta\Delta H_f$ [d]	≡ 0	–21.5	–21.1
	conformer [e]	– [f]	$_3T^4$	$_3T^4$
1d → *cis*-**2d** + *trans*-**2d** [$R^2 = C(CH_3)_3$]	E + ZPVE [b]	-425.248794	–425.265134	–425.264073
	ZPVE [c]	680242.0	681888.7	682482.0
	$\langle S^2 \rangle$	0. 772359	0.762	0.750
	$\Delta\Delta H_f$ [d]	≡ 0	–42.9	–40.1
	conformer [e]	– [f]	E_3	$_3T^4$
1e → *cis*-**2e** + *trans*-**2e** ($R^3 = CH_3$)	E + ZPVE [b]	–308.247471	–308.254008	–308.257112
	ZPVE [c]	440987.4	445135.1	443781.8
	$\langle S^2 \rangle$	0.759	0.762	0.762
	$\Delta\Delta H_f$ [d]	≡ 0	–17.2	–25.3
	conformer [e]	– [f]	$^3T_4$	$^3T_4$
1f → *cis*-**2f** + *trans*-**2f** [$R^3 = C(CH_3)_3$]	E + ZPVE [b]	–425.252956	–425.254563	–425.261936
	ZPVE [c]	678908.1	682872.7	683509.5
	$\langle S^2 \rangle$	0.75917	0.763	0.762
	$\Delta\Delta H_f$ [d]	≡ 0	–4.2	–23.6
	conformer [e]	– [f]	$^3T_4$	$_4T^5$

[a] UHF/6-31+G*//UHF/6-31+G*. [b] E (not temperature corrected) + ZPVE in a.u.; 1 a.u. = 2625.50 kJ mol^{-1}. [c] ZPVE in J mol^{-1}. [d] ΔH_f values (ZPVE-corrected) in kJ mol^{-1}, referenced versus the corresponding alkenoxyl radical **1**. [e] For cyclization products *cis*-**2** and *trans*-**3**. [f] Open chain conformation, see Figure 1 in the associated publication.

Table 5.2. UHF/6-31+G*//UHF/6-31+G*-calculated data, Boltzmann-weighted population P^a, and conformational details of transition structures **7**–**10**

7–**10**	data	**7**	**8**	**9**	**10**
a	E +ZPVE [a]	–308.223767	–308.222993	–308.225718	–308.221220
R^1 = Me	ZPVE [b]	439448.4	438673.2	439361.6	438732.0
	$\langle S^2 \rangle$	1.005	1.025	1.024	1.006
	$\Delta\Delta H_f$ [c]	73.1	75.1	67.9	79.7
	G [d]	–308.255222	–308.254934	–308.257265	–308.253258
	ΔG [e]	5.4	6.1	≡ 0.0	10.5
	P [%] [f]	9.28	6.99	82.55	1.18
	conf. [g]	${}_2T^3$	${}_2T^3$	${}^2T_3$	${}_2T^3$
	subst. [h]	*a*/*b*^{anticlinal}	*e*/*b*^{synclinal}	*e*/*b*^{anticlinal}	*a*/*b*^{synclinal}
b	E +ZPVE [a]	–425.230319	–425.233109	–425.235599	–425.229879
R^1 = *t*Bu	ZPVE [b]	676906.7	676083.5	676618.1	676970.3
	$\langle S^2 \rangle$	1.015	1.024	1.009	1.013
	$\Delta\Delta H_f$ [c]	83.1	75.8	69.3	84.3
	G [d]	–425.266453	–425.269829	–425.271960	–425.266463
	ΔG [e]	14.5	5.6	≡ 0.0	14.4
	P [%] [f]	0.25	9.43	90.06	0.27
	conf. [g]	${}^3T_4$	${}_3T^4$	${}^2T_3$	${}_4T^5$
	subst. [h]	*pa*/*pe*	*pe*/*pa*	*e*/*b*^{anticlinal}	*b*/*a*
c	E +ZPVE [a]	–308.222301	–308.216791	–308.220107	–308.219598
R^2 = Me	ZPVE [b]	439365.6	439539.6	439972.9	438771.3
	$\langle S^2 \rangle$	1.004	1.023	1.005	1.023
	$\Delta\Delta H_f$ [c]	68.0	82.4	73.7	75.1
	G [d]	–308.253860	–308.248450	–308.251540	–308.251475
	ΔG [e]	≡ 0.0	14.2	6.1	6.3
	P [%] [f]	85.55	0.28	7.33	6.84
	conf. [g]	${}^2T_3$	${}_2T^3$	${}_2T^3$	${}_3T^4$
	subst. [h]	*e*/*b*^{anticlinal}	*a*/*b*^{synclinal}	*a*/*b*^{anticlinal}	*e*/*pa*
d	E +ZPVE [a]	–425.228959	–425.222832	–425.223846	–425.226118
R^2 = *t*Bu	ZPVE [b]	677378.1	677031.3	678327.3	676688.6
	$\langle S^2 \rangle$	1.007	1.035	1.009	1.028
	$\Delta\Delta H_f$ [c]	52.1	68.2	65.5	59.5
	G [d]	–425.265552	–425.259396	–425.259780	–425.263285
	ΔG [e]	≡ 0.0	16.2	15.2	6.0
	P [%] [f]	91.38	0.13	0.20	8.28
	conf. [g]	${}^2T_3$	${}^1T_5$	${}_2T^3$	${}^2T_3$
	subst. [h]	*e*/*b*^{anticlinal}	*b*/*e*	*a*/*b*^{anticlinal}	*e*/*b*^{synclinal}
e	E +ZPVE [a]	–308.216807	–308.216459	–308.221074	–308.216912
R^3 = Me	ZPVE [b]	440869.6	439562.4	439706.2	439322.6
	$\langle S^2 \rangle$	1.002	1.020	1.005	1.023
	$\Delta\Delta H_f$ [c]	80.5	81.4	69.3	80.2
	G [d]	–308.248191	–308.248173	–308.252609	–308.249039
	ΔG [e]	11.6	11.6	≡ 0.0	9.4
	P [%] [f]	0.85	0.88	96.08	2.19
	conf. [g]	${}_2T^3$	${}_3T^4$	${}^2T_3$	${}_2T^3$
	subst. [h]	*pa*/*b*^{anticlinal}	*e*/*pa*	*pe*/*b*^{anticlinal}	*pa*/*b*^{synclinal}
f	E +ZPVE [a]	–425.213874	–425.221503	–425.227835	–425.222413
R^3 = *t*Bu	ZPVE [b]	678724.5	677999.6	677557.1	677538.4
	$\langle S^2 \rangle$	1.006	1.010	1.007	1.029
	$\Delta\Delta H_f$ [c]	102.6	82.6	66.0	80.2
	G [d]	–425.249976	–425.257746	–425.264133	–425.258472
	ΔG [e]	37.2	16.8	≡ 0.0	14.9
	P [%] [f]	3.1×10^{-5}	0.11	99.64	0.25
	conf. [g]	${}_2T^3$	${}_3T^4$	${}^2T_3$	${}^1T_2$
	subst. [h]	*pa*/*b*^{anticlinal}	*e*/*pa*	*pe*/*b*^{anticlinal}	*b*/*pe*

Footnotes for Table 5.2 (page 8):

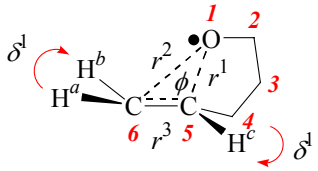
[a] *E* (not temperature corrected) + ZPVE in a.u.; 1 a.u. = 2625.50 kJ mol^{-1}. [b] ZPVE in J mol^{-1}. [c] $\Delta\Delta H_f$ values (ZPVE-corrected) in kJ mol^{-1}, referenced versus the associated alkenoxyl radical **1** (Table 5.1). [d] *G* (298.15) in a.u. [e] ΔG in kJ mol^{-1}, referenced versus the energetically lowest transition structure in each series of intermediates. [f] P^a [%] was calculated according to the to the following equation:

$$P^a = 100\,[\,\exp\{-\Delta G^a/RT\}/\sum_{i=1}^{4}\exp\{-\Delta G^i/RT\}\,]$$

where P^a denotes the percentage contribution of a transition structure *a* to the formation of cyclization products **2**. [h] Classification of transition structures as distorted conformers of tetrahydrofuran (T = twist; E = envelope). [i] Arrangement of substituents in tetrahydrofuran-derived transition structures: R^n / $=CH_2$ (*n* = 1, 2, or 3; *a* = *axial*, *b* = *bisectional*, *e* = *equatorial*, *pa* = *pseudoaxial*, *pe* = *pseudoequatorial* (see also Figures 5 and 6 of the associated publication). The notation $b^{anticlinal}$ = *anticlinal-bisectional*, $b^{synclinal}$ = *synclinal-bisectional* describes the spatial arrangement of the $=CH_2$ entity.

6 Selected Parameter of UHF/6-31+G*-Calculated Transition Structures 7–10

Table 6.1. Geometrical parameter for the description of transition structures **7–10** [a]

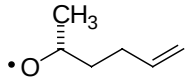


7–10

7–10	parameter	**7**	**8**	**9**	**10**
a	r^1 [Å]	1.916	1.931	1.916	1.932
R^1 = Me	r^2 [Å]	2.649	2.633	2.641	2.631
	r^3 [Å]	1.403	1.403	1.402	1.404
	ϕ [°]	104.87	103.19	104.43	102.97
	δ^1 [°]	–170.35	–170.22	–170.13	–170.14
	δ^2 [°]	151.03	152.15	151.36	152.25
b	r^1 [Å]	1.927	1.936	1.924	1.930
R^1 = *t*Bu	r^2 [Å]	2.661	2.641	2.645	2.670
	r^3 [Å]	1.401	1.402	1.401	1.397
	ϕ [°]	105.08	103.41	104.34	105.66
	δ^1 [°]	–171.05	–170.70	–170.38	–172.02
	δ^2 [°]	151.66	153.2	151.99	156.00
c	r^1 [Å]	1.913	1.922	1.914	1.929
R^2 = Me	r^2 [Å]	2.637	2.649	2.638	2.633
	r^3 [Å]	1.403	1.404	1.402	1.404
	ϕ [°]	104.30	104.45	104.3	103.27
	δ^1 [°]	–170.09	–170.87	–170.20	–170.21
	δ^2 [°]	151.24	150.47	151.16	152.04
d	r^1 [Å]	1.918	1.935	1.923	1.934
R^2 = *t*Bu	r^2 [Å]	2.64	2.672	2.641	2.637
	r^3 [Å]	1.401	1.399	1.400	1.403
	ϕ [°]	104.30	105.40	104.18	103.29
	δ^1 [°]	–170.24	–173.13	–170.59	–170.35
	δ^2 [°]	151.51	152.70	151.86	152.11
e	r^1 [Å]	1.913	1.929	1.912	1.930
R^3 = Me	r^2 [Å]	2.629	2.615	2.635	2.628
	r^3 [Å]	1.404	1.403	1.403	1.404
	ϕ [°]	103.81	102.21	104.21	102.93
	δ^1 [°]	–169.13	–169.41	–169.92	–170.02
	δ^2 [°]	150.40	152.76	150.42	151.57
f	r^1 [Å]	1.912	1.924	1.913	1.928
R^3 = *t*Bu	r^2 [Å]	2.568	2.590	2.613	2.631
	r^3 [Å]	1.404	1.402	1.403	1.402
	ϕ [°]	100.42	101.15	102.91	103.22
	δ^1 [°]	–167.85	–168.30	–169.83	–169.92
	δ^2 [°]	151.86	155.42	151.95	150.87

[a] r^1 = O1–C5, r^2 = O1–C6, r^3 = C5–C6, ϕ = O1–C5–C6, δ^1 = C5–C6–H^a–H^b, δ^2 = C6–C5–C4–H^c

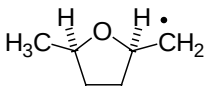
7 Atomic Coordinates of UB3LYP/6-31+G*-Calculated Geometries of Alkoxyl Radicals 1, Cyclized Radicals 2, and Transition Structures 7–10



1a

Standard orientation:

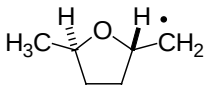
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.886679	1.284646	-0.155816
2	6	0	1.517385	0.060520	0.351543
3	6	0	0.175762	-0.442833	-0.204935
4	6	0	-0.994960	0.494453	0.150749
5	6	0	-2.301752	0.038679	-0.437707
6	6	0	-3.392702	-0.291095	0.261709
7	6	0	2.693067	-0.894883	-0.021555
8	1	0	1.485693	0.108325	1.457056
9	1	0	0.262830	-0.533450	-1.296324
10	1	0	-0.023243	-1.447586	0.192570
11	1	0	-1.087856	0.574940	1.242652
12	1	0	-0.753682	1.500072	-0.224691
13	1	0	-2.334572	-0.025262	-1.527640
14	1	0	-4.308522	-0.615427	-0.226232
15	1	0	-3.410429	-0.243094	1.349606
16	1	0	2.473388	-1.884974	0.391875
17	1	0	2.788265	-0.970636	-1.108769
18	1	0	3.633898	-0.529116	0.397610



cis-**2a**

Standard orientation:

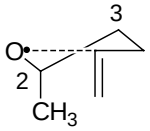
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.028835	-0.930727	0.080495
2	6	0	1.197194	-0.151735	0.359553
3	6	0	0.838247	1.267236	-0.183895
4	6	0	-0.705513	1.318199	-0.069921
5	6	0	-1.101041	-0.107568	0.393759
6	6	0	2.391135	-0.788071	-0.245839
7	1	0	1.325296	-0.080128	1.455874
8	1	0	3.380268	-0.610454	0.162908
9	1	0	2.290792	-1.350669	-1.168493
10	1	0	1.158868	1.352866	-1.227082
11	1	0	1.344540	2.052515	0.386903
12	1	0	-1.161693	1.546153	-1.040051
13	1	0	-1.050339	2.076277	0.641944
14	6	0	-2.340530	-0.691334	-0.263330
15	1	0	-1.231464	-0.109686	1.490328
16	1	0	-2.224250	-0.707854	-1.353421
17	1	0	-2.517339	-1.715840	0.081355
18	1	0	-3.222315	-0.087725	-0.016182



trans-**2a**

Standard orientation:

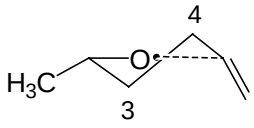
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.023019	-0.956550	0.008443
2	6	0	1.166293	-0.167930	0.406502
3	6	0	0.840715	1.272943	-0.070812
4	6	0	-0.688079	1.302857	0.034378
5	6	0	-1.071547	-0.115048	-0.413199
6	6	0	2.414182	-0.756939	-0.140565
7	1	0	1.213809	-0.168933	1.508378
8	1	0	2.407221	-1.213861	-1.125410
9	1	0	3.350074	-0.690176	0.405093
10	1	0	1.162114	1.403298	-1.111542
11	1	0	1.345556	2.029431	0.538294
12	1	0	-1.152381	2.077225	-0.586199
13	1	0	-1.000379	1.467840	1.074442
14	1	0	-1.116734	-0.151393	-1.513972
15	6	0	-2.374781	-0.656077	0.157467
16	1	0	-3.223862	-0.053289	-0.189253
17	1	0	-2.535785	-1.690874	-0.163397
18	1	0	-2.354482	-0.635702	1.253389



7a

Standard orientation:

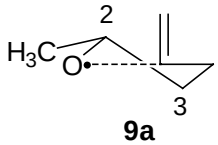
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.142509	-0.769011	-1.083277
2	6	0	-1.206110	-0.120346	-0.447834
3	6	0	-0.749641	1.319236	-0.132937
4	6	0	0.644034	1.204564	0.516185
5	6	0	1.463813	0.183823	-0.232626
6	6	0	2.072442	-0.883204	0.387596
7	1	0	-2.005059	-0.072171	-1.212707
8	1	0	-1.455246	1.857267	0.512936
9	1	0	-0.668600	1.874272	-1.075570
10	1	0	0.558443	0.909723	1.568827
11	1	0	1.151812	2.178220	0.495708
12	1	0	1.811109	0.468274	-1.222157
13	1	0	1.838243	-1.145573	1.416342
14	1	0	2.732708	-1.551420	-0.156920
15	6	0	-1.750922	-0.887871	0.765237
16	1	0	-1.007380	-0.945259	1.568671
17	1	0	-2.653143	-0.406523	1.165393
18	1	0	-2.004517	-1.911936	0.471970



8a

Standard orientation:

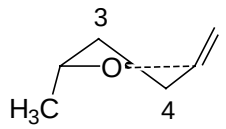
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.289466	-1.017797	-0.629575
2	6	0	-1.149919	0.058462	-0.377528
3	6	0	-0.367540	1.121768	0.423222
4	6	0	1.021863	1.239835	-0.221155
5	6	0	1.598680	-0.149522	-0.385618
6	6	0	2.022275	-0.903348	0.679217
7	1	0	-1.439566	0.520938	-1.342063
8	1	0	-0.272284	0.781987	1.462866
9	1	0	-0.899717	2.081329	0.433095
10	1	0	1.681424	1.863478	0.396803
11	1	0	0.939851	1.726391	-1.200027
12	1	0	1.887315	-0.462254	-1.384433
13	1	0	1.855809	-0.585021	1.705674
14	1	0	2.464916	-1.883639	0.532899
15	6	0	-2.411796	-0.415752	0.353295
16	1	0	-2.148664	-0.858348	1.321037
17	1	0	-3.100405	0.423094	0.521218
18	1	0	-2.934337	-1.174238	-0.239068



9a

Standard orientation:

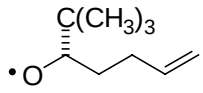
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.231051	-1.091617	-0.290604
2	6	0	-1.040899	-0.154616	0.363930
3	6	0	-0.593118	1.243755	-0.083935
4	6	0	0.936842	1.268627	0.081694
5	6	0	1.521466	-0.019231	-0.446635
6	6	0	2.337583	-0.831873	0.303392
7	1	0	-0.929368	-0.238175	1.461921
8	1	0	-1.075804	2.043794	0.492551
9	1	0	-0.860262	1.380061	-1.140598
10	1	0	1.198519	1.380937	1.142022
11	1	0	1.372738	2.123961	-0.452050
12	1	0	1.514158	-0.152135	-1.525254
13	1	0	2.450443	-0.681616	1.374431
14	1	0	2.817606	-1.704556	-0.129003
15	6	0	-2.502931	-0.469969	0.005516
16	1	0	-2.766237	-1.483030	0.325372
17	1	0	-3.171470	0.239848	0.508570
18	1	0	-2.655584	-0.396312	-1.076894



10a

Standard orientation:

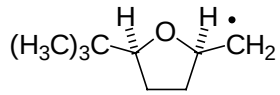
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.183614	-1.261721	0.086115
2	6	0	-1.108443	-0.306771	0.528338
3	6	0	-0.363564	1.042343	0.694312
4	6	0	0.608308	1.194128	-0.489044
5	6	0	1.393330	-0.088749	-0.640376
6	6	0	2.348700	-0.482524	0.261260
7	1	0	-1.482910	-0.607778	1.522868
8	1	0	0.205335	1.016469	1.631444
9	1	0	-1.067555	1.881485	0.758241
10	1	0	1.282425	2.042859	-0.313471
11	1	0	0.059308	1.406603	-1.412223
12	1	0	1.349036	-0.598588	-1.598011
13	1	0	2.507504	0.052767	1.194481
14	1	0	2.922438	-1.391686	0.111067
15	6	0	-2.296953	-0.212268	-0.442604
16	1	0	-2.745175	-1.201774	-0.582022
17	1	0	-3.068122	0.461765	-0.046346
18	1	0	-1.981646	0.154686	-1.426260



1b

Standard orientation:

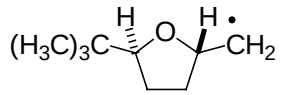
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.584819	-1.826832	-0.037254
2	6	0	0.525777	-0.501699	-0.377588
3	6	0	-0.796571	0.018350	0.302804
4	6	0	-2.075068	-0.557689	-0.329887
5	6	0	-3.313206	-0.060049	0.366974
6	6	0	-4.268443	0.687576	-0.195967
7	6	0	1.819035	0.293579	-0.004303
8	6	0	2.036261	0.323862	1.519141
9	6	0	3.003280	-0.435928	-0.675025
10	6	0	1.740267	1.726878	-0.563661
11	1	0	0.351960	-0.409557	-1.469070
12	1	0	-0.757953	-0.223310	1.370487
13	1	0	-0.794563	1.110116	0.212863
14	1	0	-2.115724	-0.288458	-1.393660
15	1	0	-2.034365	-1.653355	-0.276905
16	1	0	-3.413236	-0.340044	1.417850
17	1	0	-5.140762	1.016658	0.363253
18	1	0	-4.215599	0.991353	-1.240450
19	1	0	3.008134	0.774405	1.756003
20	1	0	1.268017	0.915592	2.031268
21	1	0	2.024055	-0.689493	1.936110
22	1	0	3.946033	0.083922	-0.464448
23	1	0	3.089719	-1.464039	-0.306091
24	1	0	2.879864	-0.476118	-1.765499
25	1	0	2.701322	2.238083	-0.427289
26	1	0	1.519261	1.726410	-1.639519
27	1	0	0.977289	2.333216	-0.061797



cis-**2b**

Standard orientation:

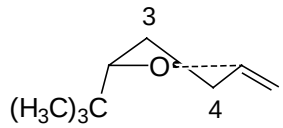
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.788641	-0.782518	-0.232074
2	6	0	-0.173189	0.233281	-0.549608
3	6	0	0.466210	1.573498	-0.082046
4	6	0	1.935983	1.208476	0.229325
5	6	0	2.089336	-0.208560	-0.392279
6	6	0	-1.553114	-0.152021	0.035289
7	6	0	-1.991668	-1.496366	-0.582670
8	6	0	-2.572778	0.936864	-0.356252
9	6	0	-1.500096	-0.295594	1.568469
10	1	0	-0.279081	0.262659	-1.648729
11	1	0	-0.031366	1.981075	0.802656
12	1	0	0.391763	2.328769	-0.871657
13	1	0	2.104812	1.147375	1.309809
14	1	0	2.659954	1.917195	-0.185872
15	6	0	3.111748	-1.079697	0.234387
16	1	0	2.302611	-0.094902	-1.471963
17	1	0	-2.987386	-1.779797	-0.218364
18	1	0	-2.042299	-1.430329	-1.677412
19	1	0	-1.290120	-2.296209	-0.326170
20	1	0	-3.576735	0.658335	-0.013205
21	1	0	-2.329139	1.908554	0.090321
22	1	0	-2.619598	1.068111	-1.445474
23	1	0	-2.483274	-0.594160	1.953266
24	1	0	-0.772029	-1.057362	1.864742
25	1	0	-1.229553	0.645181	2.062937
26	1	0	4.138191	-1.070618	-0.116810
27	1	0	2.859533	-1.653026	1.120827



trans-**2b**

Standard orientation:

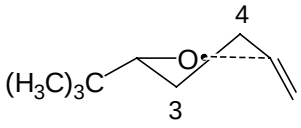
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.795109	-0.812544	-0.135769
2	6	0	-0.147635	0.204610	-0.513974
3	6	0	0.476647	1.537517	-0.049190
4	6	0	1.980505	1.229819	-0.106945
5	6	0	2.015207	-0.247162	0.358823
6	6	0	-1.566177	-0.143486	0.007127
7	6	0	-2.008041	-1.475989	-0.636584
8	6	0	-2.540189	0.973086	-0.422039
9	6	0	-1.587479	-0.296585	1.540858
10	1	0	-0.204396	0.213796	-1.615874
11	1	0	0.178674	1.778865	0.978076
12	1	0	0.185258	2.376521	-0.688795
13	1	0	2.591959	1.881540	0.525660
14	1	0	2.354142	1.305035	-1.135714
15	1	0	1.995729	-0.262607	1.463444
16	6	0	3.183686	-1.040264	-0.111263
17	1	0	-3.020044	-1.746077	-0.309185
18	1	0	-2.020063	-1.401383	-1.731980
19	1	0	-1.328965	-2.289540	-0.361670
20	1	0	-3.568291	0.710600	-0.144016
21	1	0	-2.301534	1.930121	0.058104
22	1	0	-2.520493	1.126198	-1.509334
23	1	0	-2.588956	-0.594838	1.875427
24	1	0	-0.878920	-1.065590	1.866829
25	1	0	-1.339516	0.639873	2.054970
26	1	0	4.121109	-1.017465	0.436961
27	1	0	3.144292	-1.533968	-1.077639



7b

Standard orientation:

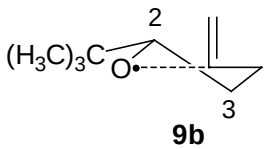
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.641305	-0.606561	-1.174437
2	6	0	-0.278616	0.373566	-0.795507
3	6	0	0.529706	1.603301	-0.296537
4	6	0	1.752767	1.110211	0.500362
5	6	0	2.373974	-0.074310	-0.189374
6	6	0	2.682009	-1.243148	0.464772
7	1	0	-0.761370	0.683795	-1.744851
8	1	0	-0.076157	2.301791	0.291155
9	1	0	0.882859	2.151218	-1.178728
10	1	0	1.476342	0.837257	1.524028
11	1	0	2.490906	1.921369	0.573939
12	1	0	2.844665	0.113658	-1.150641
13	1	0	2.325740	-1.436194	1.473315
14	1	0	3.217957	-2.045143	-0.034186
15	6	0	-1.448556	-0.148735	0.105806
16	6	0	-0.985448	-0.555165	1.516187
17	1	0	-1.818281	-1.002355	2.073983
18	1	0	-0.181416	-1.297374	1.467807
19	1	0	-0.632812	0.305469	2.097313
20	6	0	-2.534303	0.941280	0.216840
21	1	0	-3.410641	0.553653	0.751484
22	1	0	-2.183631	1.824379	0.764086
23	1	0	-2.873088	1.272059	-0.774045
24	6	0	-2.056634	-1.382286	-0.593354
25	1	0	-2.904053	-1.773047	-0.015503
26	1	0	-2.424242	-1.128869	-1.596692
27	1	0	-1.312615	-2.177468	-0.702137



8b

Standard orientation:

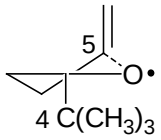
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.578704	-0.838177	-0.822249
2	6	0	-0.182100	0.302127	-0.543815
3	6	0	0.678952	1.251358	0.326036
4	6	0	2.108300	1.202656	-0.234222
5	6	0	2.535711	-0.241593	-0.363453
6	6	0	2.750323	-1.052956	0.720015
7	1	0	-0.368510	0.836969	-1.498316
8	1	0	0.677130	0.903689	1.365430
9	1	0	0.280110	2.271943	0.315595
10	1	0	2.794556	1.754035	0.422511
11	1	0	2.141371	1.687278	-1.216812
12	1	0	2.882677	-0.580278	-1.334983
13	1	0	2.516199	-0.730394	1.731736
14	1	0	3.092437	-2.075798	0.596410
15	6	0	-1.579664	-0.072450	0.053929
16	6	0	-1.444233	-0.864759	1.366458
17	1	0	-2.431367	-1.203185	1.706045
18	1	0	-0.810400	-1.745878	1.223375
19	1	0	-1.014094	-0.259899	2.173983
20	6	0	-2.397605	1.211842	0.292392
21	1	0	-3.424894	0.960351	0.584789
22	1	0	-1.970278	1.829702	1.091248
23	1	0	-2.455761	1.825676	-0.616744
24	6	0	-2.310637	-0.947266	-0.986484
25	1	0	-3.313894	-1.214890	-0.631013
26	1	0	-2.423665	-0.416113	-1.940907
27	1	0	-1.755532	-1.871544	-1.179490



9b

Standard orientation:

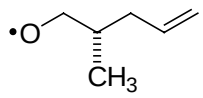
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.608987	-0.956320	0.297487
2	6	0	0.095012	0.062624	-0.348199
3	6	0	-0.537696	1.399758	0.072749
4	6	0	-2.052786	1.223607	-0.140276
5	6	0	-2.492138	-0.111939	0.405854
6	6	0	-3.184556	-1.034478	-0.339972
7	1	0	0.001828	-0.035771	-1.448183
8	1	0	-0.157218	2.251689	-0.503239
9	1	0	-0.334176	1.589381	1.133378
10	1	0	-2.290785	1.277398	-1.210719
11	1	0	-2.608304	2.031332	0.355829
12	1	0	-2.489553	-0.221763	1.487188
13	1	0	-3.289483	-0.922670	-1.416507
14	1	0	-3.565996	-1.949069	0.103862
15	6	0	1.628976	-0.111216	-0.034162
16	6	0	2.079952	-1.476805	-0.591644
17	1	0	3.157222	-1.616306	-0.433614
18	1	0	1.549003	-2.298760	-0.101996
19	1	0	1.887775	-1.546731	-1.670228
20	6	0	2.412893	1.007073	-0.748660
21	1	0	3.491350	0.836251	-0.638948
22	1	0	2.189362	1.031759	-1.823281
23	1	0	2.192466	1.996638	-0.331735
24	6	0	1.910585	-0.061937	1.479069
25	1	0	2.977476	-0.239335	1.665559
26	1	0	1.661823	0.913767	1.912399
27	1	0	1.337655	-0.827375	2.011785



10b

Standard orientation:

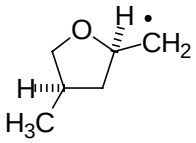
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.591993	1.151158	0.075541
2	6	0	-0.132195	0.178940	-0.616471
3	6	0	0.689678	-1.150249	-0.627681
4	6	0	1.720049	-1.137740	0.513274
5	6	0	2.438448	0.190155	0.544891
6	6	0	3.187305	0.676090	-0.487333
7	1	0	-0.283452	0.494499	-1.664597
8	1	0	1.213908	-1.216496	-1.588808
9	1	0	0.048040	-2.035817	-0.564660
10	1	0	2.434161	-1.961630	0.374456
11	1	0	1.226803	-1.301566	1.475702
12	1	0	2.490380	0.705736	1.500085
13	1	0	3.235146	0.173411	-1.450608
14	1	0	3.714125	1.621520	-0.401493
15	6	0	-1.575406	0.067789	0.010410
16	6	0	-2.190566	1.482977	0.034812
17	1	0	-3.225125	1.444636	0.399724
18	1	0	-1.619016	2.151502	0.686559
19	1	0	-2.204435	1.925211	-0.969769
20	6	0	-2.445167	-0.830981	-0.890500
21	1	0	-3.478989	-0.841512	-0.522548
22	1	0	-2.465580	-0.461165	-1.923721
23	1	0	-2.095504	-1.869934	-0.910663
24	6	0	-1.541490	-0.496892	1.440703
25	1	0	-2.550806	-0.492052	1.872216
26	1	0	-1.183570	-1.533381	1.464273
27	1	0	-0.895970	0.107243	2.086898



1c

Standard orientation:

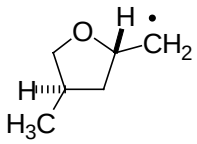
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.442545	-1.196900	-0.091623
2	6	0	-1.952488	0.044870	0.216194
3	6	0	-0.549520	0.374805	-0.316976
4	6	0	0.485264	-0.615697	0.266735
5	6	0	1.833839	-0.544989	-0.395126
6	6	0	2.990910	-0.280490	0.220990
7	6	0	-0.197166	1.839093	-0.022522
8	1	0	-2.703805	0.774602	-0.156784
9	1	0	-2.006567	0.166955	1.319846
10	1	0	-0.582824	0.229884	-1.407182
11	1	0	0.590745	-0.441840	1.347876
12	1	0	0.079148	-1.630634	0.142585
13	1	0	1.841973	-0.737273	-1.470439
14	1	0	3.934086	-0.257951	-0.319504
15	1	0	3.037331	-0.083804	1.290972
16	1	0	0.798772	2.088957	-0.402052
17	1	0	-0.916835	2.525544	-0.486836
18	1	0	-0.196711	2.035211	1.058736



cis-**2c**

Standard orientation:

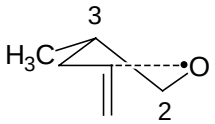
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.836320	1.184469	-0.030105
2	6	0	0.589589	1.240775	0.116187
3	6	0	1.145612	-0.107596	-0.370900
4	6	0	-0.030492	-1.042676	-0.048161
5	6	0	-1.257094	-0.155519	-0.374050
6	1	0	0.833577	1.405186	1.177149
7	6	0	2.484752	-0.498016	0.256270
8	1	0	1.262633	-0.063428	-1.463564
9	1	0	-0.030939	-1.303358	1.018754
10	1	0	-0.027175	-1.972045	-0.627579
11	6	0	-2.508995	-0.496936	0.345149
12	1	0	-1.436762	-0.192525	-1.462298
13	1	0	2.400610	-0.573671	1.348122
14	1	0	2.833054	-1.466458	-0.122041
15	1	0	3.261533	0.243566	0.030543
16	1	0	0.967389	2.094432	-0.459390
17	1	0	-2.665394	-0.133812	1.356192
18	1	0	-3.248198	-1.153825	-0.102012



trans-**2c**

Standard orientation:

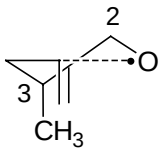
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.871035	1.203360	0.172816
2	6	0	0.541529	1.257574	-0.037061
3	6	0	0.985062	-0.172091	-0.377905
4	6	0	0.019447	-0.987150	0.500784
5	6	0	-1.284470	-0.148723	0.448990
6	1	0	1.042834	1.612289	0.880133
7	6	0	2.469961	-0.447945	-0.140820
8	1	0	0.743572	-0.365404	-1.432994
9	1	0	0.400331	-1.033971	1.530394
10	1	0	-0.127490	-2.012726	0.146346
11	1	0	-1.768374	-0.146860	1.443399
12	6	0	-2.268868	-0.602234	-0.577675
13	1	0	2.741474	-0.274282	0.909125
14	1	0	2.723659	-1.486743	-0.385209
15	1	0	3.100628	0.201270	-0.761888
16	1	0	0.738977	1.979239	-0.838229
17	1	0	-2.636526	-1.625512	-0.564702
18	1	0	-2.766774	0.129241	-1.206783



7c

Standard orientation:

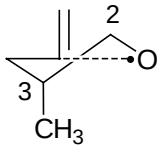
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.752870	1.447430	-0.213969
2	6	0	0.537031	1.231330	0.266098
3	6	0	1.099272	-0.061833	-0.345193
4	6	0	-0.018994	-1.103460	-0.120269
5	6	0	-1.364136	-0.498385	-0.434663
6	6	0	-2.408747	-0.498184	0.460819
7	1	0	0.573858	1.184938	1.371312
8	1	0	1.141096	2.102070	-0.045444
9	1	0	1.198365	0.106113	-1.427161
10	1	0	-0.001814	-1.441471	0.925214
11	1	0	0.151493	-1.987347	-0.750380
12	1	0	-1.587207	-0.320915	-1.483310
13	1	0	-2.255098	-0.762218	1.504218
14	1	0	-3.394403	-0.141583	0.178248
15	6	0	2.452800	-0.489282	0.225902
16	1	0	2.392975	-0.648816	1.310703
17	1	0	2.800547	-1.424473	-0.229815
18	1	0	3.219798	0.273151	0.042001



8c

Standard orientation:

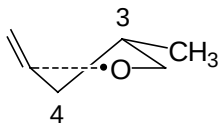
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.211700	1.415992	-0.612622
2	6	0	-0.988520	1.228492	0.067069
3	6	0	-1.135532	-0.260014	0.447219
4	6	0	0.210556	-0.615423	1.137616
5	6	0	1.367713	0.061155	0.430530
6	6	0	2.081768	-0.541091	-0.580770
7	1	0	-1.811359	1.526067	-0.605969
8	1	0	-1.046836	1.850282	0.980480
9	1	0	-1.955018	-0.369442	1.171586
10	1	0	0.351824	-1.703538	1.148403
11	1	0	0.181564	-0.283178	2.182062
12	1	0	1.825041	0.908801	0.932486
13	1	0	1.762733	-1.482987	-1.019899
14	1	0	2.941693	-0.051409	-1.027894
15	6	0	-1.434588	-1.143144	-0.770644
16	1	0	-0.678994	-1.012340	-1.552164
17	1	0	-1.463318	-2.203636	-0.490681
18	1	0	-2.409314	-0.886418	-1.203554



9c

Standard orientation:

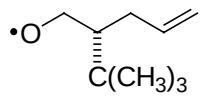
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.350121	1.349958	-0.484694
2	6	0	0.590697	1.216031	0.536008
3	6	0	1.130822	-0.225790	0.545667
4	6	0	-0.151881	-1.094852	0.539078
5	6	0	-1.164534	-0.534015	-0.430820
6	6	0	-2.445531	-0.201673	-0.055492
7	1	0	0.174040	1.482989	1.524126
8	1	0	1.397986	1.937143	0.315454
9	1	0	1.690573	-0.411692	1.473697
10	1	0	-0.589139	-1.115403	1.545502
11	1	0	0.090716	-2.131667	0.268740
12	1	0	-0.961812	-0.665943	-1.489748
13	1	0	-2.730521	-0.152397	0.992740
14	1	0	-3.184159	0.113684	-0.786055
15	6	0	2.048600	-0.511390	-0.650881
16	1	0	2.962601	0.092500	-0.593179
17	1	0	2.348451	-1.566508	-0.676610
18	1	0	1.553195	-0.272241	-1.598478



10c

Standard orientation:

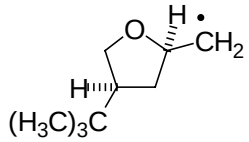
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.756964	1.499020	0.093401
2	6	0	-0.618943	1.300038	0.015540
3	6	0	-0.917136	-0.177818	-0.328516
4	6	0	0.023332	-1.001071	0.575069
5	6	0	1.423467	-0.438281	0.488340
6	6	0	2.218028	-0.608096	-0.618442
7	1	0	-1.047131	1.948753	-0.767041
8	1	0	-1.106362	1.540305	0.979750
9	1	0	-0.612312	-0.334163	-1.372756
10	1	0	0.010034	-2.055996	0.270111
11	1	0	-0.335332	-0.958077	1.611206
12	1	0	1.889575	-0.096891	1.407428
13	1	0	1.832867	-1.051151	-1.533870
14	1	0	3.234538	-0.227862	-0.644062
15	6	0	-2.394145	-0.546378	-0.178210
16	1	0	-3.025911	0.075707	-0.824021
17	1	0	-2.569576	-1.593667	-0.453163
18	1	0	-2.733715	-0.409483	0.856525



1d

Standard orientation:

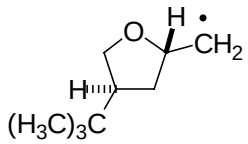
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.724896	1.776035	-0.288750
2	6	0	-0.523751	1.409650	0.275052
3	6	0	0.073052	0.126557	-0.352421
4	6	0	-0.886971	-1.047278	-0.016129
5	6	0	-2.298349	-0.778619	-0.457046
6	6	0	-3.357438	-0.699384	0.363574
7	1	0	0.141363	2.269268	0.059962
8	1	0	-0.594970	1.334176	1.374475
9	1	0	0.030849	0.280433	-1.441087
10	6	0	1.577345	-0.133550	0.004207
11	1	0	-0.529750	-1.956245	-0.516953
12	1	0	-0.874977	-1.248563	1.062938
13	1	0	-2.451013	-0.644303	-1.527827
14	1	0	-4.355979	-0.496400	-0.013621
15	1	0	-3.256116	-0.819368	1.440799
16	6	0	2.067108	-1.416061	-0.705365
17	6	0	2.441147	1.039784	-0.513091
18	6	0	1.809932	-0.287782	1.523037
19	1	0	3.150472	-1.529898	-0.575273
20	1	0	1.596977	-2.319858	-0.303281
21	1	0	1.863865	-1.378879	-1.783709
22	1	0	3.506522	0.818008	-0.374434
23	1	0	2.274205	1.216708	-1.583511
24	1	0	2.237991	1.976294	0.019108
25	1	0	2.870896	-0.484535	1.722544
26	1	0	1.537224	0.618828	2.075578
27	1	0	1.239158	-1.123847	1.943391



cis - **2d**

Standard orientation:

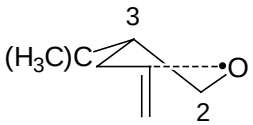
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.207815	-0.185347	-0.392097
2	8	0	-1.927416	1.156432	0.048389
3	6	0	-0.516682	1.415933	-0.017157
4	6	0	0.171557	0.110425	-0.483034
5	6	0	-0.889015	-0.948502	-0.127093
6	6	0	1.624538	-0.123597	0.027365
7	6	0	-3.405724	-0.704970	0.311175
8	1	0	-0.189683	1.731881	0.981170
9	1	0	0.234699	0.147397	-1.581399
10	1	0	-0.841530	-1.229598	0.931286
11	1	0	-0.816361	-1.859735	-0.729011
12	1	0	-2.394051	-0.175695	-1.481348
13	6	0	1.706624	-0.280528	1.559865
14	6	0	2.185417	-1.401712	-0.630660
15	6	0	2.498715	1.075716	-0.400716
16	1	0	-0.339485	2.246613	-0.711564
17	1	0	-3.596461	-0.409467	1.338010
18	1	0	-4.055561	-1.434208	-0.161670
19	1	0	2.753685	-0.395066	1.867096
20	1	0	1.305994	0.591095	2.089945
21	1	0	1.166080	-1.166352	1.911870
22	1	0	3.230428	-1.562543	-0.336768
23	1	0	1.617746	-2.291627	-0.333824
24	1	0	2.154373	-1.331891	-1.725797
25	1	0	3.547550	0.908261	-0.125488
26	1	0	2.459646	1.228381	-1.487147
27	1	0	2.176568	2.006593	0.081632



trans-**2d**

Standard orientation:

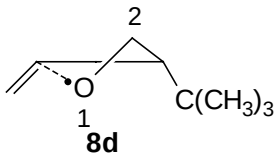
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.117920	-0.187141	0.354117
2	8	0	-1.926321	1.156370	-0.109468
3	6	0	-0.528182	1.413753	-0.022336
4	6	0	0.169206	0.125308	-0.520027
5	6	0	-0.888864	-0.974481	-0.209968
6	6	0	1.616490	-0.119874	0.002997
7	6	0	-3.447876	-0.684518	-0.071030
8	1	0	-0.257972	1.647889	1.020157
9	1	0	0.248373	0.208628	-1.612196
10	1	0	-0.545445	-1.715379	0.518323
11	1	0	-1.169163	-1.515530	-1.118797
12	1	0	-2.053406	-0.191923	1.457522
13	6	0	1.680484	-0.321421	1.531640
14	6	0	2.191446	-1.373807	-0.688772
15	6	0	2.492540	1.094426	-0.375804
16	1	0	-0.320402	2.292298	-0.638481
17	1	0	-3.951173	-1.466407	0.488048
18	1	0	-3.874516	-0.343577	-1.009138
19	1	0	3.229555	-1.547275	-0.377735
20	1	0	1.616595	-2.274014	-0.440810
21	1	0	2.184256	-1.261902	-1.780730
22	1	0	3.538025	0.922635	-0.090676
23	1	0	2.468341	1.278628	-1.457769
24	1	0	2.160481	2.009772	0.129023
25	1	0	2.718730	-0.491254	1.843168
26	1	0	1.315969	0.553640	2.081544
27	1	0	1.098378	-1.190676	1.859393



7d

Standard orientation:

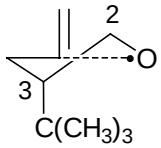
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.886650	1.440425	-0.258605
2	6	0	-0.579933	1.371123	0.220490
3	6	0	0.124863	0.150081	-0.406293
4	6	0	-0.861022	-1.018225	-0.153844
5	6	0	-2.272217	-0.582937	-0.457016
6	6	0	-3.297939	-0.686824	0.449753
7	1	0	-0.546475	1.336073	1.323426
8	1	0	-0.093157	2.309867	-0.093928
9	1	0	0.134731	0.333483	-1.491662
10	1	0	-0.801551	-1.351992	0.889454
11	1	0	-0.607303	-1.878113	-0.786353
12	1	0	-2.523496	-0.436287	-1.504044
13	1	0	-3.105284	-0.918572	1.494557
14	1	0	-4.321359	-0.451551	0.174065
15	6	0	1.604617	-0.104230	0.017829
16	6	0	1.762752	-0.346971	1.534508
17	6	0	2.151271	-1.333620	-0.740419
18	6	0	2.459429	1.120960	-0.377339
19	1	0	2.818530	-0.522543	1.776982
20	1	0	1.202657	-1.226192	1.873506
21	1	0	1.430507	0.513402	2.126428
22	1	0	2.032066	-1.218026	-1.825791
23	1	0	1.645299	-2.258912	-0.441653
24	1	0	3.221243	-1.465695	-0.535474
25	1	0	2.360400	1.346853	-1.446970
26	1	0	3.520564	0.930253	-0.173695
27	1	0	2.174901	2.018405	0.183973



8d

Standard orientation:

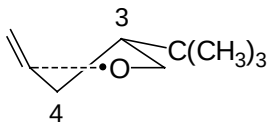
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.427953	1.378375	0.576635
2	6	0	-0.471657	1.607945	-0.403840
3	6	0	0.240122	0.298621	-0.820716
4	6	0	-0.911272	-0.752328	-0.996077
5	6	0	-2.221650	-0.303889	-0.387225
6	6	0	-2.852108	-0.977059	0.625820
7	1	0	-0.912797	2.078615	-1.303886
8	1	0	0.243868	2.332390	0.016423
9	1	0	0.698273	0.483381	-1.803433
10	6	0	1.416410	-0.174646	0.099825
11	1	0	-1.073634	-0.934063	-2.066228
12	1	0	-0.629394	-1.715151	-0.560187
13	1	0	-2.815086	0.398564	-0.968054
14	1	0	-3.835478	-0.676303	0.974959
15	1	0	-2.357432	-1.779493	1.167921
16	6	0	0.958773	-0.545467	1.525152
17	6	0	2.479011	0.943872	0.196711
18	6	0	2.099809	-1.398985	-0.551760
19	1	0	0.266685	-1.395619	1.524057
20	1	0	0.451429	0.290128	2.015797
21	1	0	1.826447	-0.833130	2.133221
22	1	0	2.123548	1.805783	0.772134
23	1	0	2.780144	1.299729	-0.797665
24	1	0	3.378246	0.569201	0.701174
25	1	0	2.483615	-1.155204	-1.551358
26	1	0	1.421404	-2.253688	-0.653886
27	1	0	2.949158	-1.730515	0.058589



9d

Standard orientation:

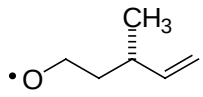
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.238141	1.281372	0.476232
2	6	0	0.461617	1.427513	-0.673167
3	6	0	-0.260214	0.108970	-0.934835
4	6	0	0.865976	-0.931538	-0.817063
5	6	0	1.770824	-0.551974	0.337235
6	6	0	3.163019	-0.496952	0.176697
7	1	0	1.078490	1.703437	-1.527131
8	1	0	-0.228236	2.244589	-0.476417
9	1	0	-0.668096	0.101045	-1.943131
10	1	0	1.445688	-0.946555	-1.735507
11	1	0	0.468620	-1.932622	-0.673401
12	1	0	1.413433	-0.790949	1.321866
13	1	0	3.606302	-0.420627	-0.800555
14	1	0	3.809746	-0.367396	1.024809
15	6	0	-1.390890	-0.143358	0.079960
16	6	0	-1.996797	-1.537775	-0.165153
17	6	0	-0.820350	-0.074666	1.508616
18	6	0	-2.482889	0.929315	-0.089802
19	1	0	-1.484014	-2.277253	0.467307
20	1	0	-1.869762	-1.808836	-1.223637
21	1	0	-3.068638	-1.511898	0.081234
22	1	0	-1.544804	-0.506985	2.214496
23	1	0	-0.630263	0.975612	1.774666
24	1	0	0.122891	-0.639373	1.546069
25	1	0	-3.356958	0.663580	0.522710
26	1	0	-2.778678	0.983222	-1.147811
27	1	0	-2.082624	1.902833	0.229651



10d

Standard orientation:

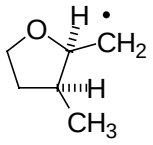
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.931584	1.467873	0.024134
2	6	0	0.539800	1.486576	0.001138
3	6	0	-0.002846	0.044678	-0.214886
4	6	0	0.864125	-0.851783	0.698468
5	6	0	2.326054	-0.565334	0.449434
6	6	0	2.963235	-0.899713	-0.714956
7	1	0	0.194614	2.132987	-0.819898
8	1	0	0.149510	1.882375	0.956148
9	1	0	0.242691	-0.212736	-1.255775
10	1	0	0.651167	-1.910995	0.509553
11	1	0	0.630041	-0.655518	1.750412
12	1	0	2.932314	-0.269022	1.299832
13	1	0	2.420869	-1.292630	-1.571886
14	1	0	4.024534	-0.713391	-0.847899
15	6	0	-1.547970	-0.123207	-0.067398
16	6	0	-1.952117	-1.529960	-0.563355
17	6	0	-2.031720	0.046121	1.388417
18	6	0	-2.264401	0.918506	-0.955248
19	1	0	-1.635848	-1.691709	-1.602092
20	1	0	-3.042066	-1.649904	-0.525004
21	1	0	-1.514760	-2.325742	0.050377
22	1	0	-1.630176	-0.732265	2.047274
23	1	0	-3.125811	-0.024517	1.431112
24	1	0	-1.750303	1.019998	1.805052
25	1	0	-3.344843	0.728629	-0.970055
26	1	0	-1.904080	0.875709	-1.991347
27	1	0	-2.115488	1.940444	-0.588554



1e

Standard orientation:

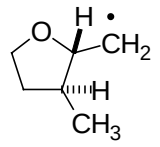
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.990727	0.198508	0.170637
2	6	0	-1.703436	0.369488	-0.260200
3	6	0	-0.731795	-0.751221	0.136124
4	6	0	0.729694	-0.470631	-0.281989
5	6	0	1.285046	0.727992	0.448819
6	6	0	1.721644	1.856917	-0.119995
7	6	0	1.608866	-1.712515	-0.033755
8	1	0	-1.674538	0.580740	-1.346981
9	1	0	-1.383666	1.325359	0.214902
10	1	0	-0.792511	-0.901111	1.222654
11	1	0	-1.071203	-1.684604	-0.332066
12	1	0	0.745016	-0.251672	-1.360480
13	1	0	1.328423	0.633254	1.537243
14	1	0	2.119585	2.678121	0.471181
15	1	0	1.702029	1.998668	-1.199552
16	1	0	2.639480	-1.536175	-0.360984
17	1	0	1.633587	-1.969436	1.033168
18	1	0	1.219497	-2.581388	-0.578202



cis-**2e**

Standard orientation:

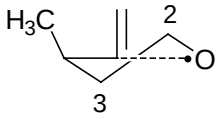
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.388195	0.738663	-0.262009
2	6	0	0.031805	0.870207	-0.475693
3	6	0	0.595291	-0.592113	-0.423469
4	6	0	-0.421874	-1.279261	0.500837
5	6	0	-1.729242	-0.615287	0.072265
6	1	0	0.183787	1.269343	-1.492324
7	6	0	2.060303	-0.734034	-0.012751
8	1	0	0.472843	-1.014410	-1.431661
9	1	0	-0.195537	-1.052315	1.551014
10	1	0	-0.438010	-2.368569	0.381905
11	1	0	-2.492716	-0.586000	0.856798
12	1	0	-2.157819	-1.114654	-0.810558
13	1	0	2.228550	-0.358157	1.003154
14	1	0	2.366707	-1.786804	-0.040362
15	1	0	2.723070	-0.180147	-0.689682
16	6	0	0.599451	1.831260	0.510897
17	1	0	0.036080	2.098451	1.398231
18	1	0	1.564196	2.299331	0.337041



trans-**2e**

Standard orientation:

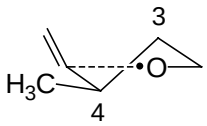
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.281458	0.845007	-0.200147
2	6	0	-0.151041	0.810230	-0.347718
3	6	0	-0.593420	-0.511035	0.346005
4	6	0	0.595859	-1.426125	0.012523
5	6	0	1.790624	-0.467916	0.093073
6	6	0	-0.742243	2.055645	0.198824
7	6	0	-1.959739	-1.029524	-0.098170
8	1	0	-0.608756	-0.327565	1.429880
9	1	0	0.484488	-1.826220	-1.004337
10	1	0	0.688509	-2.275442	0.698871
11	1	0	2.583626	-0.706074	-0.625773
12	1	0	2.231688	-0.451719	1.099334
13	1	0	-1.980532	-1.210545	-1.181047
14	1	0	-2.203149	-1.974251	0.402605
15	1	0	-2.755090	-0.313071	0.139830
16	1	0	-0.396575	0.726235	-1.422432
17	1	0	-0.286109	2.535209	1.059087
18	1	0	-1.650009	2.475742	-0.222056



7e

Standard orientation:

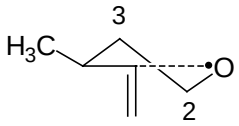
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.908479	-1.433244	-0.215325
2	6	0	1.588831	-0.258955	-0.539404
3	6	0	1.218897	0.815209	0.489128
4	6	0	-0.328591	0.813682	0.573730
5	6	0	-0.765552	-0.639872	0.640943
6	6	0	-1.717767	-1.215295	-0.172112
7	1	0	1.375093	0.078467	-1.569153
8	1	0	2.667303	-0.490703	-0.489923
9	1	0	1.608324	1.808241	0.228246
10	1	0	1.641827	0.531576	1.461110
11	6	0	-0.973692	1.625207	-0.559250
12	1	0	-0.526264	-1.150460	1.569781
13	1	0	-2.086213	-0.723968	-1.066700
14	1	0	-2.051871	-2.233057	0.003519
15	1	0	-0.618339	1.277688	1.528636
16	1	0	-2.066234	1.635307	-0.474114
17	1	0	-0.626689	2.664022	-0.518411
18	1	0	-0.717527	1.228973	-1.548600



8e

Standard orientation:

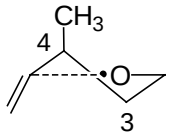
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.753935	0.504284	-0.275901
2	6	0	1.675299	-0.852624	0.054217
3	6	0	0.243933	-1.185083	0.515270
4	6	0	-0.715175	-0.449126	-0.438226
5	6	0	-0.262362	0.999359	-0.507661
6	6	0	-0.331177	1.864461	0.554353
7	1	0	2.395247	-1.093559	0.853122
8	1	0	1.914356	-1.467385	-0.832942
9	1	0	0.096570	-0.826426	1.542418
10	1	0	0.067357	-2.268589	0.514273
11	6	0	-2.192241	-0.608867	-0.034716
12	1	0	-0.086638	1.417680	-1.494555
13	1	0	-0.590177	1.531462	1.555826
14	1	0	-0.042122	2.905071	0.445314
15	1	0	-0.587109	-0.881838	-1.439756
16	1	0	-2.376699	-0.211329	0.970069
17	1	0	-2.854384	-0.080172	-0.729730
18	1	0	-2.477538	-1.667911	-0.036258



9e

Standard orientation:

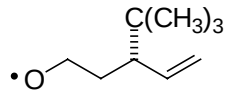
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.720482	0.109597	-0.484772
2	6	0	1.469564	-1.046233	0.257730
3	6	0	0.009518	-1.451727	0.050596
4	6	0	-0.822199	-0.177895	0.313705
5	6	0	-0.124733	0.990430	-0.352465
6	6	0	0.235256	2.130697	0.327389
7	1	0	1.693179	-0.909171	1.331461
8	1	0	2.158232	-1.820634	-0.123160
9	1	0	-0.300948	-2.275339	0.707510
10	1	0	-0.132094	-1.776692	-0.989138
11	1	0	-0.825311	0.007652	1.397837
12	1	0	-0.194480	1.037557	-1.436803
13	1	0	0.225958	2.164559	1.414221
14	1	0	0.633556	2.996555	-0.192602
15	6	0	-2.279172	-0.316945	-0.160832
16	1	0	-2.324796	-0.476884	-1.245757
17	1	0	-2.762196	-1.173759	0.324026
18	1	0	-2.864365	0.579421	0.073848



10e

Standard orientation:

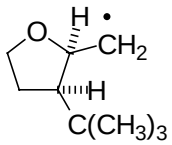
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.835361	1.146911	-0.839178
2	6	0	0.221165	1.678264	-0.098720
3	6	0	0.609851	0.686158	1.017160
4	6	0	0.576764	-0.736294	0.415544
5	6	0	-0.740970	-0.879564	-0.322660
6	6	0	-1.950870	-0.964508	0.317819
7	1	0	-0.071655	2.640160	0.353275
8	1	0	1.093614	1.851816	-0.753757
9	1	0	-0.127642	0.759176	1.825297
10	1	0	1.593092	0.927103	1.442350
11	1	0	0.591138	-1.454032	1.248866
12	1	0	-0.695450	-1.152106	-1.373849
13	1	0	-2.042434	-0.810409	1.390445
14	1	0	-2.871359	-1.109704	-0.239089
15	6	0	1.777047	-1.032491	-0.495142
16	1	0	2.720543	-0.913652	0.050556
17	1	0	1.736581	-2.061370	-0.872953
18	1	0	1.798550	-0.361665	-1.361725



1f

Standard orientation:

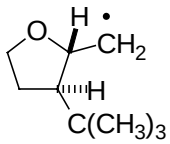
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.438775	2.711202	-0.168484
2	6	0	-0.146231	1.559986	0.446901
3	6	0	0.017385	0.218065	-0.230079
4	6	0	1.450922	-0.406294	-0.033065
5	6	0	2.516271	0.630947	-0.445569
6	6	0	-1.135690	-0.714549	0.221992
7	6	0	-2.501086	-0.269241	-0.325515
8	8	0	-3.566921	-0.997341	0.124987
9	6	0	1.701418	-0.830691	1.428736
10	6	0	1.612868	-1.638680	-0.949354
11	1	0	-2.503835	-0.202347	-1.431164
12	1	0	-2.718313	0.768941	0.016435
13	1	0	-1.201051	-0.747196	1.316333
14	1	0	-0.089567	0.383088	-1.314245
15	1	0	-0.047500	1.562441	1.534420
16	1	0	-0.566013	3.638534	0.385084
17	1	0	-0.554566	2.770005	-1.249859
18	1	0	-0.959657	-1.740791	-0.117852
19	1	0	1.004830	-1.611759	1.754198
20	1	0	1.612430	0.013899	2.122406
21	1	0	2.716811	-1.232588	1.534720
22	1	0	0.940407	-2.459029	-0.676390
23	1	0	2.637240	-2.025854	-0.883616
24	1	0	1.423544	-1.380684	-1.999526
25	1	0	2.507127	1.509472	0.208097
26	1	0	2.352768	0.981660	-1.472947
27	1	0	3.518222	0.186459	-0.399365



cis - **2f**

Standard orientation:

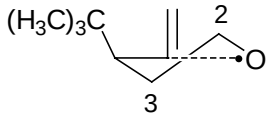
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.397187	0.237203	-0.455836
2	6	0	2.308363	-1.122981	-0.000260
3	6	0	0.884645	-1.306109	0.527530
4	6	0	0.094070	-0.343857	-0.376437
5	6	0	1.091586	0.864577	-0.474866
6	6	0	-1.403181	-0.082871	-0.042977
7	6	0	-1.647982	0.339097	1.420127
8	6	0	-1.953131	1.008204	-0.987363
9	6	0	-2.191241	-1.386776	-0.307074
10	1	0	3.082273	-1.284948	0.758634
11	1	0	2.509496	-1.795175	-0.847618
12	1	0	0.819274	-1.002458	1.579001
13	1	0	0.547428	-2.345074	0.452792
14	1	0	0.101232	-0.784199	-1.386240
15	6	0	1.041613	1.914543	0.581055
16	1	0	0.980867	1.341696	-1.457391
17	1	0	-2.717394	0.527504	1.580261
18	1	0	-1.346164	-0.444096	2.125345
19	1	0	-1.104699	1.254195	1.678872
20	1	0	-3.033871	1.132257	-0.843773
21	1	0	-1.482567	1.980801	-0.804685
22	1	0	-1.785934	0.744410	-2.039960
23	1	0	-3.262595	-1.230386	-0.129380
24	1	0	-2.071103	-1.723252	-1.344949
25	1	0	-1.863436	-2.199746	0.351414
26	1	0	1.541189	1.756265	1.531559
27	1	0	0.560053	2.871613	0.404399



trans-**2f**

Standard orientation:

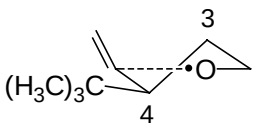
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.269149	-0.005506	0.600317
2	6	0	2.205856	-1.192783	-0.189879
3	6	0	0.719777	-1.528763	-0.268236
4	6	0	0.075970	-0.130822	-0.412358
5	6	0	1.083535	0.808639	0.327388
6	6	0	-1.418235	-0.003769	0.015721
7	6	0	-1.652119	-0.354728	1.500171
8	6	0	-1.900699	1.440873	-0.236385
9	6	0	-2.263544	-0.958401	-0.855304
10	1	0	2.630140	-1.015869	-1.192302
11	1	0	2.813661	-1.951704	0.312440
12	1	0	0.479051	-2.191905	-1.106076
13	1	0	0.403136	-2.019899	0.658632
14	1	0	0.109616	0.136314	-1.479310
15	1	0	0.709994	1.102989	1.312943
16	6	0	1.477133	2.019186	-0.446089
17	1	0	-1.382822	-1.392287	1.727130
18	1	0	-2.713900	-0.232406	1.748173
19	1	0	-1.084270	0.294851	2.175887
20	1	0	-1.755901	1.731730	-1.284584
21	1	0	-1.362219	2.165467	0.385610
22	1	0	-2.969611	1.535018	-0.006017
23	1	0	-2.003661	-2.008551	-0.677151
24	1	0	-2.121484	-0.751981	-1.924226
25	1	0	-3.331564	-0.839775	-0.632711
26	1	0	1.667598	2.965823	0.050681
27	1	0	1.792991	1.919640	-1.481832



7f

Standard orientation:

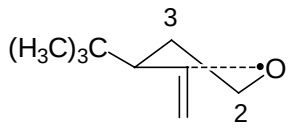
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.617573	0.003812	0.055187
2	6	0	1.945291	-1.134262	0.499858
3	6	0	0.820011	-1.454080	-0.485760
4	6	0	0.003844	-0.144772	-0.745681
5	6	0	1.003159	1.014377	-0.686182
6	6	0	1.078397	2.040138	0.228945
7	1	0	1.569283	-1.018893	1.530244
8	1	0	2.686267	-1.953004	0.517662
9	1	0	0.185738	-2.277694	-0.139154
10	1	0	1.278359	-1.774626	-1.428998
11	6	0	-1.351769	-0.038676	0.046524
12	1	0	1.537027	1.170743	-1.619815
13	1	0	0.546464	2.033636	1.172401
14	1	0	1.783866	2.850814	0.074468
15	1	0	-0.307680	-0.179606	-1.799759
16	6	0	-2.296736	-1.146056	-0.482179
17	6	0	-1.207705	-0.230538	1.571060
18	6	0	-2.046308	1.309758	-0.249457
19	1	0	-2.466332	-1.041401	-1.561637
20	1	0	-3.272263	-1.078440	0.014556
21	1	0	-1.908167	-2.153695	-0.300131
22	1	0	-0.555912	0.514985	2.035795
23	1	0	-0.807757	-1.220419	1.817946
24	1	0	-2.191431	-0.149656	2.050903
25	1	0	-2.142945	1.471845	-1.330916
26	1	0	-1.507178	2.165594	0.164708
27	1	0	-3.057034	1.313981	0.177464



8f

Standard orientation:

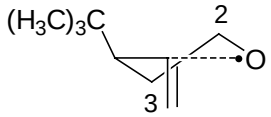
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.665412	0.064414	-0.505343
2	6	0	2.310988	-1.196473	-0.006034
3	6	0	0.878590	-1.151457	0.568279
4	6	0	0.070809	-0.229854	-0.364815
5	6	0	0.850670	1.071451	-0.467995
6	6	0	1.200052	1.873589	0.589096
7	1	0	3.022023	-1.526280	0.768033
8	1	0	2.335820	-1.925017	-0.836608
9	1	0	0.908424	-0.746195	1.586271
10	1	0	0.458049	-2.161246	0.630005
11	6	0	-1.460802	-0.081430	-0.046819
12	1	0	0.968425	1.485702	-1.465498
13	1	0	1.070734	1.567559	1.622189
14	1	0	1.716987	2.813393	0.420251
15	1	0	0.112923	-0.682317	-1.366126
16	6	0	-2.140734	-1.457692	-0.217334
17	6	0	-1.738456	0.434772	1.378464
18	6	0	-2.088834	0.895673	-1.064061
19	1	0	-3.227408	-1.360913	-0.101563
20	1	0	-1.796729	-2.184173	0.527424
21	1	0	-1.948831	-1.877176	-1.213402
22	1	0	-1.324732	1.436247	1.537657
23	1	0	-1.326034	-0.233428	2.143794
24	1	0	-2.820737	0.496735	1.548452
25	1	0	-1.913006	0.564117	-2.095933
26	1	0	-1.678845	1.906607	-0.958529
27	1	0	-3.174065	0.959601	-0.916361



9f

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.621721	-0.081191	0.489791
2	6	0	-2.256035	-1.181003	-0.287811
3	6	0	-0.759835	-1.438611	-0.107366
4	6	0	-0.062171	-0.079061	-0.360309
5	6	0	-0.887875	1.000170	0.317419
6	6	0	-1.412153	2.074165	-0.362907
7	1	0	-2.506578	-1.038674	-1.354994
8	1	0	-2.852751	-2.036380	0.074843
9	1	0	-0.394077	-2.214229	-0.790864
10	1	0	-0.579594	-1.778603	0.919605
11	1	0	-0.116396	0.110868	-1.443651
12	1	0	-0.823591	1.066890	1.399159
13	1	0	-1.419690	2.105328	-1.449834
14	1	0	-1.922343	2.877726	0.159754
15	6	0	1.464439	-0.036223	0.011418
16	6	0	1.713433	-0.207813	1.524803
17	6	0	2.199903	-1.164401	-0.743113
18	6	0	2.060826	1.313738	-0.440599
19	1	0	1.308127	-1.151559	1.906706
20	1	0	1.277943	0.609326	2.111002
21	1	0	2.791991	-0.210674	1.725634
22	1	0	3.283290	-1.076618	-0.594135
23	1	0	2.007993	-1.113996	-1.822934
24	1	0	1.900086	-2.157962	-0.391994
25	1	0	1.598515	2.159120	0.081086
26	1	0	1.918766	1.469247	-1.518105
27	1	0	3.138888	1.343961	-0.238814



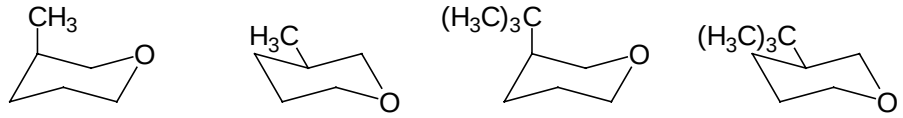
10f

Standard orientation:

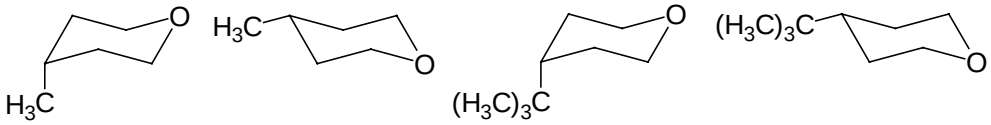
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.468037	-0.337680	0.548008
2	6	0	-1.753600	-1.483710	0.206884
3	6	0	-0.773709	-1.147964	-0.928117
4	6	0	-0.018423	0.172867	-0.585626
5	6	0	-0.964858	1.050155	0.219400
6	6	0	-1.714806	2.042919	-0.364060
7	1	0	-2.470842	-2.243762	-0.149067
8	1	0	-1.216046	-1.901766	1.074694
9	1	0	-1.359009	-0.980691	-1.839883
10	1	0	-0.093214	-1.983870	-1.127173
11	1	0	0.157923	0.690807	-1.539210
12	1	0	-0.833524	1.081479	1.296772
13	1	0	-1.770760	2.147144	-1.445207
14	1	0	-2.352966	2.689563	0.230552
15	6	0	1.402464	0.013640	0.061235
16	6	0	1.385863	-0.812304	1.363392
17	6	0	2.346918	-0.671158	-0.950502
18	6	0	1.975769	1.416211	0.363132
19	1	0	0.713877	-0.386373	2.117640
20	1	0	2.391885	-0.840889	1.800621
21	1	0	1.078213	-1.848757	1.185416
22	1	0	2.401855	-0.104783	-1.889313
23	1	0	2.030252	-1.691751	-1.192272
24	1	0	3.362699	-0.733542	-0.540714
25	1	0	3.006708	1.336521	0.730098
26	1	0	1.394351	1.945471	1.126567
27	1	0	1.989178	2.042709	-0.538004

8 B3LYP/6-31+G*-Calculated Data of Methyl- and *tert*-Butyl-substituted Tetrahydropyrans – *A*-Value Analysis

11a(ax) **11a**(eq) **11b**(ax) **11b**(eq)



11c(ax) **11c**(eq) **11d**(ax) **11d**(eq)

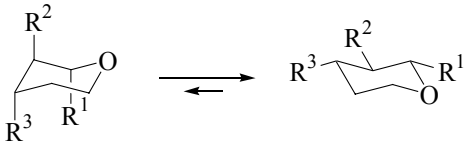


11e(ax) **11e**(eq) **11f**(ax) **11f**(eq)

Table 8.1. B3LYP/6-31+G*//B3LYP/6-31+G*-calculated data for substituted tetrahydropyrans **11**

11	data	**11**(ax)	**11**(eq)
a	E +ZPVE [a]	–310.920809	–310.926521
R^1 = Me	ZPVE [b]	459107.6	458168.3
	G [d]	–310.951148	–310.956932
	ΔG [e]	15.16	≡ 0
b	E +ZPVE [a]	-428.770279	–428.781759
R^1 = *t*Bu	ZPVE [b]	681770.1	680572.6
	G [d]	–428.805572	-428.817129
	ΔG [e]	30.34	≡ 0
c	E +ZPVE [a]	–310.919279	-310.922356
R^2 = Me	ZPVE [b]	459303.8	458438.3
	G [d]	–310.949651	–310.952822
	ΔG [e]	8.32	≡ 0
d	E +ZPVE [a]	–428.768024	–428.773941
R^2 = *t*Bu	ZPVE [b]	682402.0	681109.1
	G [d]	–428.803804	–428.809968
	ΔG [e]	16.18	≡ 0
e	E +ZPVE [a]	–310.918157	–310.922578
R^3 = Me	ZPVE [b]	459439.4	458557.8
	G [d]	–310.948524	–310.952995
	ΔG [e]	11.74	≡ 0
f	E +ZPVE [a]	–428.765212	–428.775089
R^3 = *t*Bu	ZPVE [b]	682449.1	680919.8
	G [d]	–428.801116	–428.811703
	ΔG [e]	27.79	≡ 0

Table 8.2 *A*-value analysis of 2-, 3-, and 4- alkyl-substituted tetrahydropyrans **11**.



11 *axial* **11** *equatorial*

11	R^1	R^2	R^3	A^{calcd}[kJ mol^{-1}] [a]	A^{exp} [kJ mol^{-1}] [b]
a	CH_3	H	H	15.2	12.0 ± 0.8
b	$C(CH_3)_3$	H	H	30.3	– [c]
c	H	CH_3	H	8.3	6.0 ± 0.2
d	H	$C(CH_3)_3$	H	16.2	– [c]
e	H	H	CH_3	11.7	8.2 ± 0.2
f	H	H	$C(CH_3)_3$	27.8	– [c]

[a] $A^{calcd} = -\Delta G^{298} = G^{298}_{ax} - G^{298}_{eq}$ (B3LYP/6-31+G*// B3LYP/6-31+G*). [b] Refers to the temperature range of 188–173 K.[6] [c] Hitherto not reported.

11a^{ax}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.288673	-1.151218	-0.686337
2	6	0	1.075337	0.039648	-0.502157
3	6	0	0.183922	1.294400	-0.563812
4	6	0	-1.018748	1.199990	0.390160
5	6	0	-1.772384	-0.116908	0.150561
6	6	0	-0.804446	-1.299514	0.220177
7	1	0	1.739530	0.038034	-1.373953
8	6	0	1.952541	-0.039723	0.754495
9	1	0	-0.186553	1.400617	-1.592491
10	1	0	0.787100	2.185930	-0.346172
11	1	0	-1.684321	2.060109	0.243416
12	1	0	-0.680387	1.244566	1.435419
13	1	0	-2.242515	-0.099413	-0.842636
14	1	0	-2.574091	-0.253750	0.889127
15	1	0	-1.293063	-2.234172	-0.072337
16	1	0	-0.432729	-1.426487	1.250403
17	1	0	2.521596	-0.975844	0.754495
18	1	0	2.664650	0.794690	0.765486
19	1	0	1.374062	0.008108	1.683402

11a^{eq}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.352190	-1.160228	-0.200728
2	6	0	-0.977182	0.018802	0.324260
3	6	0	-0.239262	1.278809	-0.150100
4	6	0	1.255988	1.210985	0.200462
5	6	0	1.858870	-0.111790	-0.295975
6	6	0	1.013125	-1.291160	0.188419
7	1	0	-0.919388	-0.028396	1.428235
8	6	0	-2.437483	-0.022870	-0.103612
9	1	0	-0.702752	2.166122	0.302150
10	1	0	-0.363908	1.366064	-1.239131
11	1	0	1.377224	1.278705	1.292393
12	1	0	1.791334	2.067680	-0.228230
13	1	0	2.892730	-0.229892	0.056256
14	1	0	1.884569	-0.121214	-1.394321
15	1	0	1.073930	-1.375027	1.288592
16	1	0	1.355055	-2.237270	-0.242610
17	1	0	-2.916168	-0.941168	0.252761
18	1	0	-2.982519	0.836040	0.305712
19	1	0	-2.516916	0.003520	-1.196715

11b^{ax}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.646499	1.156473	-0.782546
2	6	0	-0.137830	-0.051128	-0.809760
3	6	0	0.763317	-1.302987	-0.687341
4	6	0	1.870712	-1.195625	0.375856
5	6	0	2.635159	0.123383	0.212802
6	6	0	1.649234	1.288954	0.223779
7	1	0	-0.531401	-0.037523	-1.833558
8	6	0	-1.418506	0.001812	0.096459
9	1	0	1.247295	-1.452160	-1.662294
10	1	0	0.148081	-2.192996	-0.510488
11	1	0	2.550803	-2.051966	0.279619
12	1	0	1.447328	-1.245852	1.386832
13	1	0	3.182737	0.125643	-0.740167
14	1	0	3.373142	0.255734	1.015615
15	1	0	2.148427	2.236793	-0.003002
16	1	0	1.190909	1.386321	1.220492
17	6	0	-2.051091	1.402911	-0.028091
18	6	0	-2.427358	-1.034449	-0.452246
19	6	0	-1.180996	-0.312555	1.589175
20	1	0	-3.011998	1.432367	0.501382
21	1	0	-1.402490	2.177103	0.392550
22	1	0	-2.234872	1.664303	-1.077658
23	1	0	-3.363483	-0.989600	0.117880
24	1	0	-2.670481	-0.838672	-1.504425
25	1	0	-2.050303	-2.061613	-0.379497
26	1	0	-2.133674	-0.260139	2.132232
27	1	0	-0.778861	-1.321340	1.737112
28	1	0	-0.498994	0.399915	2.063958

11b^{eq}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.559202	-1.125565	0.182633
2	6	0	0.051093	0.059238	-0.349025
3	6	0	-0.716879	1.302238	0.131144
4	6	0	-2.207235	1.196793	-0.237374
5	6	0	-2.792667	-0.134122	0.254911
6	6	0	-1.915792	-1.294232	-0.217419
7	1	0	-0.033634	0.015257	-1.452370
8	6	0	1.565827	0.004432	-0.005878
9	1	0	-0.287067	2.206072	-0.316358
10	1	0	-0.614994	1.395351	1.220196
11	1	0	-2.315901	1.258963	-1.331037
12	1	0	-2.764025	2.044796	0.181341
13	1	0	-3.819550	-0.272928	-0.109985
14	1	0	-2.831327	-0.142053	1.352882
15	1	0	-1.965082	-1.384298	-1.317682
16	1	0	-2.236917	-2.247188	0.215243
17	6	0	2.168020	-1.261389	-0.652729
18	6	0	2.274753	1.241633	-0.594564
19	6	0	1.799619	-0.049128	1.517418
20	1	0	3.244963	-1.318044	-0.450251
21	1	0	1.695585	-2.167767	-0.263288
22	1	0	2.033488	-1.250299	-1.742671
23	1	0	3.360776	1.142762	-0.476413
24	1	0	2.068237	1.352116	-1.667622
25	1	0	1.975072	2.169417	-0.094315
26	1	0	2.871913	-0.144889	1.730218
27	1	0	1.446907	0.860209	2.018406
28	1	0	1.284743	-0.905733	1.963736

11c^{ax}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.828837	-1.241065	-0.376813
2	6	0	0.221730	-1.237026	0.588052
3	6	0	1.095125	0.026197	0.500872
4	6	0	0.184081	1.267707	0.633129
5	6	0	-1.011377	1.199091	-0.332733
6	6	0	-1.726653	-0.147447	-0.197218
7	1	0	0.807707	-2.141238	0.392895
8	1	0	-0.214622	-1.322364	1.599491
9	6	0	1.949346	0.043096	-0.776676
10	1	0	1.777118	0.006655	1.364542
11	1	0	0.763184	2.185499	0.466120
12	1	0	-0.196291	1.320348	1.664470
13	1	0	-0.674171	1.321081	-1.369984
14	1	0	-1.719164	2.013883	-0.127958
15	1	0	-2.504841	-0.271185	-0.956685
16	1	0	-2.202622	-0.227164	0.797287
17	1	0	1.331272	-0.013976	-1.678845
18	1	0	2.551766	0.958393	-0.833989
19	1	0	2.637857	-0.811117	-0.795399

11c^{eq}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.108700	-1.245626	-0.262267
2	6	0	-0.261364	-1.229847	0.129205
3	6	0	-0.994247	0.033329	-0.345037
4	6	0	-0.240030	1.277039	0.159791
5	6	0	1.253759	1.195837	-0.192472
6	6	0	1.837114	-0.141244	0.269364
7	1	0	-0.330373	-1.310253	1.230219
8	1	0	-0.705456	-2.131830	-0.304499
9	6	0	-2.462364	0.021592	0.095500
10	1	0	-0.957114	0.033619	-1.445058
11	1	0	-0.354167	1.344340	1.253703
12	1	0	-0.687643	2.188908	-0.258000
13	1	0	1.810437	2.021225	0.272008
14	1	0	1.386525	1.284501	-1.279377
15	1	0	1.831726	-0.197184	1.373123
16	1	0	2.868301	-0.272322	-0.072539
17	1	0	-2.549097	0.005131	1.190272
18	1	0	-2.987261	0.914913	-0.264655
19	1	0	-2.992687	-0.856274	-0.295160

11d^{ax}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.636130	-1.228062	0.372326
2	6	0	0.755406	-1.230580	-0.749215
3	6	0	-0.152313	0.015296	-0.837052
4	6	0	0.769115	1.265639	-0.771055
5	6	0	1.841326	1.201398	0.333597
6	6	0	2.561781	-0.146603	0.313852
7	1	0	0.184643	-2.158154	-0.675377
8	1	0	1.360047	-1.286829	-1.672515
9	6	0	-1.417103	0.012350	0.095568
10	1	0	-0.570034	-0.008404	-1.856394
11	1	0	0.184050	2.186484	-0.675381
12	1	0	1.286704	1.339261	-1.739449
13	1	0	1.394015	1.348278	1.322099
14	1	0	2.572771	2.008991	0.190206
15	1	0	3.222875	-0.266104	1.177788
16	1	0	3.172957	-0.242051	-0.602282
17	6	0	-1.094722	0.104728	1.602267
18	6	0	-2.329413	1.200509	-0.287301
19	6	0	-2.227919	-1.283072	-0.145124
20	1	0	-2.016164	-0.015453	2.187328
21	1	0	-0.387801	-0.670421	1.913673
22	1	0	-0.670365	1.079158	1.868903
23	1	0	-3.254480	1.174475	0.302136
24	1	0	-1.853779	2.169121	-0.097971
25	1	0	-2.610527	1.164486	-1.348316
26	1	0	-3.201772	-1.216857	0.355563
27	1	0	-2.416163	-1.449381	-1.214388
28	1	0	-1.722967	-2.170093	0.252549

11d^{eq}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.065721	-1.233614	-0.295935
2	6	0	0.705018	-1.232130	0.134503
3	6	0	-0.053808	0.022440	-0.343656
4	6	0	0.708112	1.268145	0.161061
5	6	0	2.193851	1.199800	-0.230435
6	6	0	2.803968	-0.128341	0.214645
7	1	0	0.675342	-1.307728	1.235365
8	1	0	0.278523	-2.147108	-0.281587
9	6	0	-1.587051	0.007416	-0.013386
10	1	0	0.021173	0.018049	-1.442806
11	1	0	0.632069	1.330313	1.256546
12	1	0	0.265252	2.187408	-0.238232
13	1	0	2.750417	2.033218	0.219891
14	1	0	2.296618	1.290308	-1.320434
15	1	0	2.832809	-0.183932	1.318130
16	1	0	3.825228	-0.252274	-0.158753
17	6	0	-1.871543	0.046866	1.504051
18	6	0	-2.266273	1.227654	-0.673995
19	6	0	-2.237946	-1.264689	-0.603462
20	1	0	-2.953835	0.020041	1.683742
21	1	0	-1.433693	-0.810181	2.029101
22	1	0	-1.487157	0.960737	1.971213
23	1	0	-3.352962	1.183118	-0.528808
24	1	0	-1.920762	2.176298	-0.249289
25	1	0	-2.075528	1.251674	-1.754841
26	1	0	-3.329509	-1.213467	-0.505013
27	1	0	-2.005119	-1.373877	-1.670699
28	1	0	-1.910606	-2.176658	-0.091995

11e^{ax}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.763669	0.000000	-0.115167
2	6	0	-0.995871	1.182551	-0.332806
3	6	0	0.209961	1.255942	0.608902
4	6	0	1.105568	0.000000	0.506686
5	6	0	0.209961	-1.255942	0.608902
6	6	0	-0.995871	-1.182551	-0.332806
7	1	0	-1.680685	2.018503	-0.160451
8	1	0	-0.676697	1.221541	-1.388598
9	1	0	-0.165037	1.350071	1.637063
10	1	0	0.790658	2.163664	0.392187
11	1	0	1.784093	0.000000	1.371483
12	6	0	1.986467	0.000000	-0.754846
13	1	0	-0.165037	-1.350071	1.637063
14	1	0	0.790658	-2.163664	0.392187
15	1	0	-1.680685	-2.018503	-0.160451
16	1	0	-0.676697	-1.221541	-1.388598
17	1	0	2.633863	0.885719	-0.777063
18	1	0	2.633863	-0.885719	-0.777062
19	1	0	1.399752	0.000000	-1.680616

11e^{eq}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.836263	0.000000	-0.338730
2	6	0	1.229397	-1.182753	0.175942
3	6	0	-0.261909	-1.252834	-0.163273
4	6	0	-1.004484	0.000000	0.336452
5	6	0	-0.261909	1.252834	-0.163273
6	6	0	1.229397	1.182753	0.175942
7	1	0	1.371961	-1.219754	1.271117
8	1	0	1.781273	-2.017834	-0.266140
9	1	0	-0.696314	-2.161084	0.278324
10	1	0	-0.375376	-1.335756	-1.253915
11	1	0	-0.954575	0.000000	1.438254
12	1	0	-0.696314	2.161084	0.278324
13	1	0	-0.375376	1.335756	-1.253915
14	1	0	1.371961	1.219754	1.271117
15	1	0	1.781273	2.017834	-0.266140
16	6	0	-2.481922	0.000000	-0.070730
17	1	0	-3.000830	-0.886787	0.315050
18	1	0	-3.000830	0.886787	0.315050
19	1	0	-2.588386	0.000000	-1.163642

11f^{ax}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.647428	-0.004786	0.201822
2	6	0	1.859469	1.174007	0.344368
3	6	0	0.770085	1.257564	-0.728320
4	6	0	-0.154373	0.010602	-0.813683
5	6	0	0.748665	-1.251912	-0.730782
6	6	0	1.850780	-1.179268	0.333530
7	1	0	2.557054	2.012167	0.247287
8	1	0	1.433644	1.208318	1.360251
9	1	0	1.282402	1.354410	-1.695521
10	1	0	0.195782	2.180473	-0.592351
11	1	0	-0.565489	0.023093	-1.833851
12	6	0	-1.445053	0.003079	0.088416
13	1	0	1.245073	-1.375063	-1.702974
14	1	0	0.158209	-2.161829	-0.569964
15	1	0	2.541795	-2.021057	0.222171
16	1	0	1.433025	-1.220003	1.351449
17	6	0	-2.214840	1.331309	-0.093333
18	6	0	-2.377626	-1.132609	-0.396785
19	6	0	-1.187624	-0.202746	1.596174
20	1	0	-3.205700	1.261833	0.372727
21	1	0	-1.699449	2.178816	0.371779
22	1	0	-2.363700	1.567259	-1.155333
23	1	0	-3.314228	-1.127210	0.174522
24	1	0	-2.634457	-1.010992	-1.457110
25	1	0	-1.929018	-2.124326	-0.272397
26	1	0	-2.139830	-0.173359	2.141832
27	1	0	-0.724387	-1.173055	1.806696
28	1	0	-0.547057	0.578654	2.018705

11f^{eq}

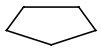
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.810288	-0.000009	0.282802
2	6	0	2.182157	1.177607	-0.212829
3	6	0	0.700257	1.247989	0.168318
4	6	0	-0.061633	0.000010	-0.329172
5	6	0	0.700251	-1.247967	0.168329
6	6	0	2.182145	-1.177612	-0.212842
7	1	0	2.292873	1.216169	-1.311840
8	1	0	2.740582	2.016740	0.213368
9	1	0	0.278705	2.167197	-0.256625
10	1	0	0.626312	1.329302	1.260781
11	1	0	0.015193	0.000015	-1.430668
12	1	0	0.278668	-2.167188	-0.256559
13	1	0	0.626339	-1.329231	1.260796
14	1	0	2.292852	-1.216165	-1.311854
15	1	0	2.740562	-2.016756	0.213345
16	6	0	-1.598420	-0.000002	-0.017402
17	6	0	-2.255876	1.247129	-0.649212
18	6	0	-2.255952	-1.246747	-0.649894
19	6	0	-1.895596	-0.000400	1.497002
20	1	0	-3.346220	1.202524	-0.535411
21	1	0	-1.918934	2.177376	-0.178924
22	1	0	-2.036585	1.312612	-1.723220
23	1	0	-3.346268	-1.202319	-0.535753
24	1	0	-2.036955	-1.311448	-1.724009
25	1	0	-1.918798	-2.177301	-0.180365
26	1	0	-2.979647	-0.000171	1.667755
27	1	0	-1.487723	-0.886882	1.996212
28	1	0	-1.487258	0.885557	1.996768

9 B3LYP/6-31+G*-Calculated Data of Distinguished Conformers of Cyclopentane and the Chair Conformation of Cyclohexane

9.1 Cyclopentane

(A) Planar conformer (D_{5h}-symmetry): E + ZPVE = –196.414753 Hartree, ZPVE = 370047.9 J mol^{-1}, G^{298} = –196.441562 Hartree, i = – 203 and – 201 cm^{-1}.



Standard orientation:

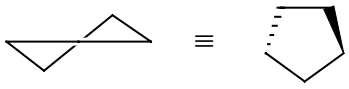
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.776827	-1.069161	0.000000
2	6	0.776986	-1.069138	0.000000
3	6	1.257095	0.408265	0.000000
4	6	0.000000	1.321568	0.000000
5	6	-1.257163	0.408424	0.000000
6	1	-1.164407	-1.602134	0.876192
7	1	-1.164407	-1.602134	-0.876192
8	1	1.164428	-1.602238	-0.876169
9	1	1.164428	-1.602238	0.876169
10	1	1.883850	0.611890	-0.876182
11	1	1.883850	0.611890	0.876182
12	1	-0.000182	1.980548	-0.876199
13	1	-0.000182	1.980548	0.876199
14	1	-1.883964	0.612056	-0.876191
15	1	-1.883964	0.612056	0.876191

(B) Envelope conformer (C_s-symmetry): E + ZPVE = –196.421850 Hartree, ZPVE = 369950.9 J mol^{-1}, G^{298} = –196.451165 Hartree, no imaginary vibrational mode.

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.239249	-0.302683	-0.201659
2	6	0.676147	1.115042	0.069966
3	6	-0.877594	0.964624	0.070438
4	6	-1.158088	-0.534815	-0.202061
5	6	0.121240	-1.252342	0.263076
6	1	2.196356	-0.481989	0.302057
7	1	1.410013	-0.442160	-1.278297
8	1	1.021828	1.838925	-0.676774
9	1	1.022496	1.480712	1.044415
10	1	-1.356580	1.609333	-0.675213
11	1	-1.287056	1.255795	1.045516
12	1	-1.298242	-0.703810	-1.278869
13	1	-2.063261	-0.894696	0.301039
14	1	0.219681	-2.266559	-0.142293
15	1	0.129040	-1.334515	1.359862

(C) Twist conformer (C_2-symmetry): E + ZPVE = –196.421908 Hartree, ZPVE = 369810.3 J mol^{-1}, G^{298} = –196.449017 Hartree, i = –12 cm^{-1}.

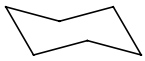


Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.012681	-0.754531	0.247120
2	6	-0.404195	-1.226012	-0.139678
3	6	-1.308983	0.033872	0.000231
4	6	-0.340108	1.245615	0.139148
5	6	1.050774	0.700869	-0.246748
6	1	1.803447	-1.380550	-0.183328
7	1	1.135549	-0.777271	1.339616
8	1	-0.752517	-2.064826	0.473862
9	1	-0.401619	-1.573680	-1.181180
10	1	-1.966156	-0.042195	0.874295
11	1	-1.963049	0.143232	-0.872615
12	1	-0.320350	1.594135	1.180146
13	1	-0.644135	2.100519	-0.475706
14	1	1.872831	1.285236	0.183659
15	1	1.174981	0.716517	-1.339187

9.2 Cyclohexane

Chair conformer: E + ZPVE = –235.715869 Hartree, ZPVE = 447819.2 J mol^{-1}, G^{298} = –235.744664 Hartree, no imaginary vibrational mode.



Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.360189	1.423627	0.227885
2	6	1.413545	0.400098	-0.227922
3	6	1.053286	-1.023710	0.227903
4	6	-0.360188	-1.423628	-0.227885
5	6	-1.413545	-0.400098	0.227920
6	6	-1.053286	1.023710	-0.227901
7	1	0.377976	1.494376	1.326546
8	1	0.612474	2.422583	-0.152746
9	1	1.485441	0.420386	-1.326487
10	1	2.404378	0.681011	0.153882
11	1	1.791647	-1.741837	-0.153606
12	1	1.106683	-1.075413	1.326559
13	1	-0.377974	-1.494377	-1.326546
14	1	-0.612473	-2.422583	0.152747
15	1	-2.404377	-0.681011	-0.153889
16	1	-1.485446	-0.420388	1.326484
17	1	-1.106686	1.075418	-1.326557
18	1	-1.791646	1.741836	0.153612

10 References

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