Structure–Stability Relationships in Unsaturated Sulfur Compounds. III. A Thermodynamic and ^{13}C NMR Spectroscopic Study of the Conformations of Vinyl Sulfones

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The conformations of the stable rotamers of alkyl 1-propenyl sulfones have been studied in a thermodynamic and ^{13}C NMR spectroscopic study. The most stable rotamer of the E isomer was found to have the anticlinal conformation. The Z isomer will probably adopt a nearly anticlinal conformation.

The structural properties of unsaturated sulfur compounds have received much attention over the last 20 years.[1–20] In vinyl sulfides the lone pair electrons of the sulfur atom can conjugate with the π orbital of the double bond in the planar conformations (s-cis and s-trans), which stabilizes these conformations.[1] In vinyl sulfoxides and sulfones the S=O bonds can conjugate with the C=C bond when they are in the same plane. The conformations of the stable rotamers of vinyl sulfides have been studied widely.[1–6] All these studies agree in that the most stable rotamer has the planar s-cis conformation. The stable conformations of alkyl vinyl sulfoxides have not received much attention and only a few studies have been reported on this subject.[7–10] According to ab initio MO calculations the most stable rotamer has the anticlinal conformation (Fig. 1).[8,9] In a thermodynamic study the conclusion was drawn that in (E)-alkyl 1-propenyl sulfoxide the most stable rotamer has the anticlinal conformation.[10] The Z isomer probably has mainly the conformation in which the lone-pair electrons of the sulfur atom eclipse the double bond. The structural properties of vinyl sulfones have interested researchers more than the properties of vinyl sulfoxides.[7,9,11–18] The structural parameters of some vinyl sulfones have been determined both experimentally[11–14] and calculated theoretically[9] and the conformations of the stable rotamers have received some attention.[9,11–15] According to electron diffraction (ED) data the anticlinal conformation is the most stable one in both (E)- and (Z)-methyl cyanovinyl sulfone.[11] According to another ED study both the synperiplanar and anticlinal conformations are adopted in (E)-methyl chlorovinyl sulfone.[12,13] The Z isomer seems to be a mixture of the antiperiplanar and a nonplanar ($\theta = 80°$ from the synperiplanar) conformation. Two studies have been published concerning the stable rotamers of the
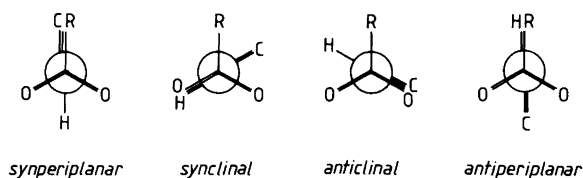

Fig. 1. Some conformations of vinyl sulfones.

unsubstituted methyl vinyl sulfone. According to IR data in the liquid phase this compound is a mixture of two conformations of which one is antiperiplanar. In the solid phase there is only one non-planar conformation present.[15] According to an ED study there are two conformers present.[14] One of them has the synperiplanar and the other an almost anticlinal conformation.

According to ab initio MO calculations the most stable rotamer of methyl vinyl sulfone has the anticlinal conformation.[9] Hence the results of the studies of the conformations of the stable rotamers of vinyl sulfones are contradictory and offer an interesting topic of study. In the present paper, a thermodynamic and ^{13}C NMR spectroscopic study is described, the aim of which was to acquire further knowledge of the conformations of vinyl sulfones.

Results and discussion

In this work the isomer equilibrium (1) was studied. The thermodynamic data for the $E \rightarrow Z$ reaction are summarized in Table 1. Sváta et al. have also equilibrated these isomers and $\Delta G^{\ominus}$ values acquired for the $E \rightarrow Z$ reaction are ca. 3 kJ mol^{-1} more positive than in the present study, but according to both studies $\Delta G^{\ominus}$ is independent of the size of the group R.[7] According to their

Table 1. The values of the thermodynamic functions for reactions $a \to E$ and $E \to Z$, eqn. (1), in Me_2SO at 298 K. The errors are twice the standard errors.

Reaction	R	$\Delta G^{\ominus}/kJ \, mol^{-1}$	$\Delta H^{\ominus}/kJ \, mol^{-1}$	$\Delta S^{\ominus}/J \, K^{-1} \, mol^{-1}$
$a \to E$	Me	−1.9(1)	−2.5(2)	−2(1)
$a \to E$	Et	−3.6(1)	−4.3(4)	−2(1)
$a \to E$	i-Pr	−5.7(2)	−7.4(15)	−5(4)
$a \to E$	t-Bu	−8.4(1)	−9.9(2)	−5(1)
$a \to E$	Ph	−3.2(1)	−4.1(8)	−3(3)
$a \to E$	all	−3.0(2)[a,b]		
$a \to E$	E-pr	−2.5(2)[a,b]		
$E \to Z$	Me	+11.0(2)	+11.3(8)	+1(2)
$E \to Z$	Et	+10.8(2)	+9.8(7)	−4(2)
$E \to Z$	i-Pr	+11.3(2)	+11.0(11)	−1(3)
$E \to Z$	t-Bu	+11.3(1)	+10.7(5)	−2(2)
$E \to Z$	Ph	+11.0(4)	+11.2(27)	+1(8)
$E \to Z$	all	+8.6(3)[a]		
$E \to Z$	E-pr	+9.2(5)[a,b]		
$E \to Z$	Z-pr	+4.0(6)[a,b]		

[a] The temperature dependence of K could not be measured sufficiently accurately to obtain reliable values for $\Delta H^{\ominus}$ and $\Delta S^{\ominus}$.
[b] $\Delta G^{\ominus}$ values are statistically corrected.

study, however, the temperature dependence of K is not reasonable. O'Connor and Lyness have equilibrated the isomers $a \to E + Z$ in the case R = Me. $\Delta G^{\ominus}$ of this reaction was +0.6 kJ mol^{-1}, which is 2.5 kJ mol^{-1} more positive than the value determined by us.[18] Sataty and Meyers have equilibrated isomers $a \to E$ and $E \to Z$ with

$$RSO_2CH_2CH=CH_2$$

$$a$$

$$E$$

(1)

$$Z$$
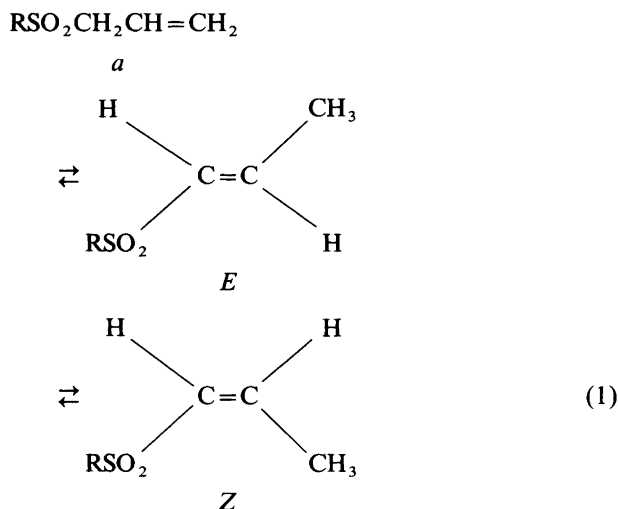
1 R = Me, **2** R = Et, **3** R = i-Pr, **4** R = t-Bu, **5** R = Ph, **6** R = CH_2=$CHCH_2$-, **7** R = (E)-CH_3CH=CH-, **8** R = (Z)-CH_3CH=CH-

R = Ph.[16] $\Delta G^{\ominus}$ of the former reaction was −2.2 kJ mol^{-1}, which is quite near the value found in this study (−3.2 kJ mol^{-1}). $\Delta G^{\ominus}$ of the latter reaction was +7.8 kJ mol^{-1}, which is 3 kJ mol^{-1} smaller than the present value.

Vinyl sulfones. $\Delta H^{\ominus}$ of the $E \to Z$ reaction, according to our study, is the same with all groups R (except with R = allyl or propenyl group). In the corresponding vinyl

sulfoxides the size of the alkyl group also had no effect on $\Delta H^{\ominus}$ (≈ 7 kJ mol^{-1}).[10] In alkyl 1-propenyl sulfides $\Delta H^{\ominus}$ of the $E \to Z$ isomerization increases, when the size of the alkyl group decreases, which was explained by changes in the spatial orientation of the alkylthio group when the alkyl group is small.[1] Because the size of the alkyl group has no effect on $\Delta H^{\ominus}$ of the $E \to Z$ reaction of alkyl 1-propenyl sulfones, it can be concluded that the size of the alkyl group has no effect on the spatial orientation of the RSO_2 group in either of the geometric isomers. Thus either there are no conformational changes in $E \to Z$ reaction or the change is the same for all alkyl groups R. One may therefore conclude that under these circumstances the synperiplanar conformation, Fig. 1, which is the most stable in methyl vinyl sulfide, is unlikely to be the most stable in vinyl sulfones, even for small alkyl groups. Steric strain makes this conformation energetically highly unfavourable for large alkyl groups even in the E isomer.[1] The same conclusion was reached in the study of vinyl sulfoxides.[10]

According to *ab initio* calculations the anticlinal conformation is the most stable in methyl vinyl sulfone.[9] In this conformation the S=O bond can conjugate with the C=C bond and thereby stabilize the molecule. That is why this conformation is the most probable choice for the most stable rotamer of (E)-alkyl 1-propenyl sulfone. In the Z isomer, however, this conformation is energetically unfavourable because of the steric strain between the S=O group and the Me group.[10] $\Delta H^{\ominus}$ of the $E \to Z$ reaction is ca. 10.5 kJ mol^{-1}. This shows that the Z isomer is energetically less favourable than the E isomer. The present data do not reveal whether this is due to the steric strain between these two groups or whether the Z isomer adopts a conformation with diminished conjugation. If this is the case, there has to be a change in the spatial orientation of the RSO_2 group in the $E \to Z$ isomerization, but this change will apparently be the same for all

Table 2. Chemical shifts (ppm from Me_4Si) from the ^{13}C NMR spectra recorded.

Compound	Isomer	δ(a)	δ(b)	δ(c)	δ(d)	δ(e)
$CH_3SO_2CH=CHCH_3$	E	42.67	130.74	143.89	17.08	
a b c d	Z	43.49	130.34	143.13	13.95	
$CH_2SO_2CH_2CH=CH_2$		38.97	59.16	125.19	124.61	
a b c d						
$CH_3CH_2SO_2CH=CHCH_3$	E	7.03	48.78	128.53	145.22	17.36
a b c d e	Z	6.82	49.75	128.07	144.34	14.11
$CH_3CH_2SO_2CH_2CH=CH_2$		6.31	45.53	56.64	125.04	124.31
a b c d e						
$(CH_3)_2CHSO_2CH=CHCH_3$	E	14.77	53.33	126.43	145.28	16.87
a b c d e	Z	14.47	54.18	125.89	144.47	13.59
$(CH_3)_2CHSO_2CH_2CH=CH_2$		14.56	51.05	54.00	124.46	123.73
a b c d e						
$(CH_3)_3CSO_2CH=CHCH_3$	E	22.61	57.43	124.61	145.98	17.02
a b c d e	Z	22.27	58.52	123.64	145.32	13.62
$(CH_3)_3CSO_2CH_2CH=CH_2$		23.06	59.28	51.02	124.06	123.64
a b c d e						
$C_6H_5SO_2CH_2CH=CH_2$		124–138	60.22	124–138		
a b c d						
$SO_2(CH_2CH=CH_2)_2$		55.70	124.49	124.49		
a b c						
$SO_2(CH=CHCH_3)_2$	E, E	130.68	142.58	16.87		
a b c	Z, Z	130.99	141.49	14.23		
	E, Z	130.11	142.16	16.60 (E)		
		131.20	141.82	13.47 (Z)		

alkyl groups R. This is consistent with the conclusion drawn earlier in this paper.

Further evidence for the stable conformations was acquired from the ^{13}C NMR shifts of the α and β carbons of the (E)- and (Z)-alkyl 1-propenyl sulfones presented in Table 2. These data show that the ^{13}C signals of the α carbons in both of the isomers shift upfield when the size of the alkyl group increases. This is caused by the increased shielding effect due to the bulkier alkyl groups. Fig. 2 shows that there is a reasonably linear relationship between the ^{13}C shifts of the α carbons of E and Z isomers with a slope of 1.09(2).

The effect of the size of the alkyl group on the ^{13}C signal of the β carbon in the (E)- and (Z)-alkyl 1-propenyl sulfones is smaller than on the signal of the α carbon and shifts downfield when the size of the alkyl group increases in both isomers. Once more a satisfactory linear relationship between the ^{13}C shifts of the β carbons of the E and Z isomers is observed, Fig. 3; slope = 1.03(1).

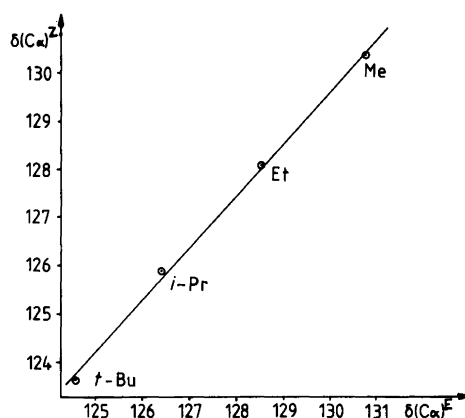In alkyl 1-propenyl sulfides the ^{13}C signal of the β carbon of the E isomer shifts ca. 10 ppm downfield when

Fig. 2. $\delta(C_\alpha)^Z$ vs. $\delta(C_\alpha)^E$ for alkyl 1-propenyl sulfones.

R is changed from Me to t-Bu. This reflects the change in the spatial orientation of the alkyl group since small alkyl groups will adopt the synperiplanar conformation and shield the β carbon whereas the t-BuS group in the
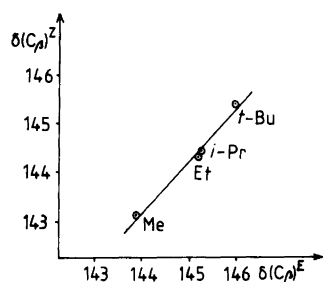
Fig. 3. $\delta(C_\beta)^Z$ vs. $\delta(C_\beta)^E$ for alkyl 1-propenyl sulfones.

antiperiplanar conformation will have no shielding effect on the β carbon atom.[1]

The ^{13}C signals of the β carbon of (Z)-alkyl 1-propenyl sulfides shift only ca. 3 ppm downfield when R is changed from Me to *t*-Bu. The reason for this is that in the Z isomer the alkyl group is far enough from the β carbon so that it has no shielding effect on it.[1] The change in the ^{13}C shift of the β carbon in both (E)- and (Z)-alkyl 1-propenyl sulfones when the size of the alkyl group increases is of the same magnitude as in the (Z)-alkyl 1-propenyl sulfides. This seems to indicate that the shielding effect of the alkyl group on the β carbon does not change in alkyl 1-propenyl sulfones when the size of the alkyl group increases, i.e., the distance between R and the β carbon is large enough for the alkyl group to have no shielding effect on the β carbon. Therefore the synperiplanar conformation will not be possible in any of the geometric isomers of alkyl 1-propenyl sulfones. On the same basis the synclinal conformation is out of question, even though the S = O and C = C bonds are in the same plane and can conjugate with each other. In alkyl 1-propenyl sulfoxides the conformation in which the lone-pair electrons of the sulfur atom eclipse the C = C bond, were concluded to be the most probable choice for the Z isomer because there is no steric strain present there; however, in sulfones there exists no such conformation. $\Delta H^\ominus$ of the $E \rightarrow Z$ reaction is 3–4 kJ mol^{-1} larger in sulfones than in sulfoxides, which shows that the Z isomers of 1-propenyl sulfones are of higher energy than the Z isomers of the corresponding sulfoxides (compared with the E isomers).

It therefore seems reasonable that (Z)-alkyl 1-propenyl sulfones adopt a conformation in which the alkylsulfonyl groups deviate somewhat from the anticlinal conformation to relieve the steric strain even though this also decreases the conjugation.

Di-1-propenyl sulfones. When $\Delta G^\ominus$-values of the $E \rightarrow Z$ reaction of di-1-propenyl sulfones are considered, the fact that the E, Z isomer is statistically favoured by a factor of two must be taken into account. To eliminate the effect of this statistical factor, the term $RT\ln 2$ (1.7 kJ mol^{-1} at 298 K) must be added to $\Delta G^\ominus$ of the reaction:

(E, E)-di-1-propenyl sulfone

$\rightarrow$ (E, Z)-di-1-propenyl sulfone

and the same factor must be subtracted from $\Delta G^\ominus$ of the reaction:

(E, Z)-di-1-propenyl sulfone

$\rightarrow$ (Z, Z)-di-1-propenyl sulfone.

$\Delta G^\ominus$-values given in Table 1 for these reactions are statistically corrected. It can be seen that when R = allyl or E-propenyl, $\Delta G^\ominus$ is quite near the value for saturated alkyl groups. Thus it can be concluded that the possible changes in the spatial orientation of the allyl or propenyl groups in these $E \rightarrow Z$ reactions are approximately the same as in the case of saturated alkyl groups. In contrast, $\Delta G^\ominus$ of the reaction, where the second methyl group is transferred from the E to the Z position, i.e., $8E \rightarrow 8Z$ is ca. 5 kJ mol^{-1} smaller than that of reaction $7E \rightarrow 7Z$. A possible explanation for this is that when the first methyl group is transferred to the Z position, the spatial orientation of the 1-propenyl group changes in a way that diminishes the conjugation in the molecule. Thus the transfer of the second methyl group from the E to the Z position does not exert as large on effect on the conjugation and $\Delta G^\ominus$ of this reaction is smaller than in the reaction in which the first methyl group is transferred to the Z position. In di-1-propenyl sulfides $\Delta H^\ominus$ of $E, E \rightarrow E, Z$ and $E, Z \rightarrow Z, Z$ reactions are, to within experimental error, the same and it was concluded that there are no conformational changes in these reactions.[1] The most stable conformation was considered to be the s-*trans*, s-*trans* conformation. According to *ab initio* calculations divinyl sulfone adopts a conformation in which the S = O groups are *cis* to the double bonds.[19] In (E, E)-di-1-propenyl sulfone this conformation is possible, but in the Z isomers steric strain makes this conformation energetically unfavourable as was also the case in alkyl 1-propenyl sulfones.

Isomerization allyl $\rightarrow$ 1-propenyl. Table 1 shows that the $\Delta H^\ominus$-values of the isomerization reactions in which the double bond migrates from the β, γ-position to the α, β-position, are negative and decrease when the size of the alkyl group increases. This shows that large alkylsulfonyl groups stabilize the double bond more than do small alkylsulfonyl groups or that large alkyl groups destabilize the allylic isomer more than do small alkyl groups. It is notable that the effect of the $PhSO_2$ group attached to the double bond is as large as that of the $EtSO_2$ group. This is astonishing, because a Ph group is much larger than an Et group. When considering $\Delta G^\ominus$-values of the $a \rightarrow E$ reaction of dipropenyl sulfones, the fact that (E)-1-propenyl 2-propenyl sulfone is statistically favoured by factor of two must be taken into account. Thus 1.7 kJ mol^{-1} (at 298 K) must be added to $\Delta G^\ominus$ of reaction $6a \rightarrow 6E$ and the same factor must be subtracted from $\Delta G^\ominus$ of reaction $7a \rightarrow 7E$. $\Delta G^\ominus$-values in Table 1 for these reactions are statistically corrected. It can be seen that the corrected $\Delta G^\ominus$ values for these reactions are as large as that of an $MeSO_2$ or $EtSO_2$ group, which is quite

Table 3. The boiling points and yields of the synthesized compounds.

Compound	Yield (%)	B.p./°C/Pa[a]	B.p. (lit.)[7]
Methyl 2-propenyl sulfone	23	53–58/35	65–67/13
(Z)-Methyl 1-propenyl sulfone	22	55–62/40	55–56/6.5
(E)-Methyl 1-propenyl sulfone	19	54–58/40	56–57/6,5
Ethyl 2-propenyl sulfone	18	75–78/55	73–75/20
(Z)-Ethyl 1-propenyl sulfone	19	75–80/55	70–71/6.5[b]
(E)-Ethyl 1-propenyl sulfone	21	81–86/60	70–71/6.5[b]
Isopropyl 2-propenyl sulfone	25	73–77/55	75–76/20
Isopropyl 1-propenyl sulfones	24	72–79/50	77–78/20
tert-Butyl 2-propenyl sulfone	22	61–63/15	66–68/6.5
tert-Butyl 1-propenyl sulfones	19	57–60/15	68–70/9
Diallyl sulfone	23	78–79/55	
Di-1-propenyl sulfones	19	72–78/50	

[a]The pressures may be somewhat erroneous because it was afterwards found out that values that the pressure apparatus gave, were somewhat too small. [b]The b.p. of a mixture of the E and Z isomers.

reasonable, because these groups are approximately equal in size.

The results for the corresponding propenyl sulfoxides and sulfides are much the same.[10,20]

Experimental

Materials. Alkyl 1-propenyl, alkyl 2-propenyl and dipropenyl sulfones were prepared by the method described by Sváta et al.[7] The products, their boiling points and yields are summarized in Table 3. Allyl phenyl sulfone was from Lancaster Synthesis (98 %).

NMR spectra. ^{1}H NMR spectra, 80 MHz and ^{13}C NMR spectra, 15 MHz, were recorded for 10–20 % solutions in $CDCl_3$. The recorded ^{1}H NMR spectra are summarized in Table 4 and the ^{13}C NMR spectra in Table 2. All results are relative to Me_4Si.

Table 4. Chemical shifts (ppm from Me_4Si) and coupling constants from the ^{1}H NMR spectra.

Compound	Isomer	δ(a)	δ(b)	δ(c)	δ(d)	δ(e)	J/Hz
$CH_3SO_2CH=CHCH_3$	E	2.93	6.1–7.1		1.97		J(cd) = 5.5
a b c d	Z	2.60	6.1–7.1		2.18		J(cd) = 5.5
$CH_3SO_2CH_2CH=CH_2$		2.86	3.73	5.3–6.3			J(bc) = 7.5
a b c d							
$CH_3CH_2SO_2CH=CHCH_3$	E	1.27	2.98	6.0–7.1		1.97	J(ab) = 7.5
a b c d e							J(de) = 7.0
	Z	1.32	3.03	6.0–7.1		2.15	J(ab) = 7.9
							J(de) = 8.1
$CH_3CH_2SO_2CH_2CH=CH_2$		1.28	3.01	3.784		5.2–6.2	J(ab) = 7.7
a b c d e							J(cd) = 6.9
$(CH_3)_2CHSO_2CH=CHCH_3$	E	1.31	2.96	6.0–7.1		2.08	J(ab) = 6.9
a b c d e	Z	1.41	2.99	6.0–7.1		2.08	J(de) = 7.0
$(CH_3)_2CHSO_2CH_2CH=CH_2$		1.36	3.20	3.73		5.2–6.2	J(ab) = 7.0
a b c d e							J(cd) = 7.0
$(CH_3)_3CSO_2CH=CHCH_3$	E	1.43	6.0–7.2		2.09		J(cd) = 7.0
a b c d	Z	1.46	6.0–7.2		2.29		J(cd) = 7.0
$(CH_3)_3CSO_2CH_2CH=CH_2$		1.49	3.84	5.2–6.2			J(bc) = 7.0
a b c d							
$C_6H_5SO_2CH_2CH=CH_2$		7.1–8.0	3.78	4.9–6.1			J(bc) = 7.0
a b c d							
$SO_2(CH_2CH=CH_2)_2$		3.74	5.4–6.1				J(ab) = 7.0
a b c							
$SO_2(CH=CHCH_3)_2$	E, E	6.0–7.2		1.89			J(bc) = 7.0
a b c	Z, Z	6.0–7.2		2.11			J(bc) = 7.0
	E, Z	6.0–7.2		a.92(E)			J(bc) = 7.0
				2.11 (Z)			

Table 5. Equilibrium constants for reactions $a \rightarrow E$ in eqn. (1).[a]

T/K	K(1E/1a)	K(2E/2a)	K(3E/3a)	K(4E/4a)	K(5E/5a)
298	2.13	4.13	9.27[b]	29.6	3.55
323	2.00	3.73	8.72	21.8	3.25
348	1.85	3.36	6.35	16.6	2.87
373	1.72	2.95	5.59	13.1	2.55
398	1.66	2.76	4.81	10.9	
423	1.59	2.49		9.1	

[a]The following equilibrium constants were determined at one temperature only (298 K), because the temperature dependence of K could not be determined with reasonable accuracy. The errors are estimated, based upon the results in the equilibrium experiments: $K(6E/6a) = 6.5(3)$, $K(7E/7a) = 1.4(1)$. [b]$T = 303$ K.

Equilibrations. The equilibration experiments were carried out in *tert*-butyl alcohol solution with potassium *tert*-butoxide as the catalyst.[7,21] The samples were analysed by gas chromatography using NB-20M (compounds **1**, **2** and **4**), NB-9C (**3**), NB-30 (**5**) and SE-30 (**6–8**) as the stationary phases. The values of the

Table 6. Equilibrium constants for reactions $E \rightarrow Z$ in eqn. (1).[a]

T/K	K(1Z/1E)	K(2Z/2E)	K(3Z/3E)	K(4Z/4E)	K(5Z/5E)
298	0.0125	0.0131	0.0116[b]	0.0102	0.0127
323	0.0160	0.0170	0.0144	0.0151	0.0155
348	0.0230	0.0220	0.0205	0.0199	0.0237
373	0.0300	0.0293	0.0246	0.0253	0.0303
398	0.0380	0.0331	0.0330	0.0308	
423	0.0460	0.0420		0.0368	

[a]The following equilibrium constants were determined at one temperature only, because the temperature dependence of K could not be determined with reasonable accuracy. The errors are estimated, based upon the results in the equilibrium experiments: $K(6Z/6E) = 0.032(4)$, $K(7Z/7E) = 0.05(1)$, $K(8Z/8E) = 0.10(2)$. [b]$T = 303$ K.

thermodynamic parameters were evaluated by linear least-squares treatment of ln K versus T^{-1}. The values of the equilibrium constant K are given in Tables 5 and 6.

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