chloropropane (48.5 ml, 0.45 mol) in HEMPA-THF (200 ml of each) under nitrogen and kept at -20° with a Dry Ice-methanol bath. The bath was allowed to attain room temperature, and the mixture was kept overnight. The mixture was diluted with cold  $H_2O$  and worked up in the usual manner. Distillation (short path) provided 28.5 g of recovered 1 (36%) and 57.8 g of 2 (53%): bp 155–165° (0.8 mm);  $n^{25}$ D 1.4757; nmr  $\delta$  3.3–4.0 (m, 6, CH<sub>2</sub>O,  $CH_2Cl)$ , 4.50 (bs, 1, OCHO).

Anal. Calcd for C<sub>16</sub>H<sub>27</sub>ClO<sub>2</sub>: C, 66.99; H, 9.49; Cl, 12.36. Found: C, 66.97; H, 9.29; Cl, 12.28

(Z)-11-Hexadecen-7-yn-1-ol acetate (3a). Triphenylphosphine (43.3 g, 0.165 mol) and 2 (45 g, 0.157 mol) were heated at 145° under nitrogen for 16 hr. Magnetic stirring was required because the mixture became heterogenous for a time during the course of the reaction. The cooled mixture was agitated with ether several times. The ether washes, which contained unreacted starting materials, were stored for subsequent salt preparations. The oily salt (72.2 g, 84% yield) was dissolved in THF (260 ml) and transferred to a 1-l. three-neck round-bottom flask for the Wittig reaction. The solution was placed under nitrogen and cooled to  $\sim$ -5° (ice-methanol bath). Conversion to the ylide was effected by adding n-butyllithium (64.5 ml, 2.04 M) beyond the permanent coloration point. HMPA (130 ml) was added to this solution (no difference in product was noted if n-butyllithium was added to a salt solution in both solvents). Valeraldehyde (14.0 ml, 0.131 mol) was added to the mixture at one time. The bath was removed, and the mixture was stirred for 1 hr. The crude product was obtained by dilution of the mixture with H<sub>2</sub>O and extraction with petroleum ether. Replacement of the tetrahydropyranyl group by acetyl was effected by warming the crude product at 35-40° for 16 hr in a mixture of acetyl chloride (13.9 ml) and HOAc (140 ml). The presence of triphenylphosphine oxide (TPO) was not deleterious. The acetate, 3a, was isolated by dilution of the mixture (H<sub>2</sub>O) and extraction (petroleum ether). Filtration of the crude acetate through 85 g of alumina with petroleum ether removed most of the TPO. Distillation (short path) afforded 21 g (58%) of 3a: bp 145-150° (0.7 mm);  $n^{25}$  D 1.4628; ir 1740, 975 cm<sup>-1</sup> (trans, optical density extrapolatd to a 1.0 M solution, 0.12); nmr  $\delta$  1.93 (s, CH<sub>3</sub>CO), 3.97 (bt, 2, CH<sub>2</sub>O), 5.32 (bt, 2, CH=).

Anal. Calcd for C<sub>18</sub>H<sub>30</sub>O<sub>2</sub>: C, 77.65; H, 10.86. Found: C, 77.42 H, 10.70

(Z,Z)-7,11-Hexadecadien-1-ol Acetate (4a). Hydrogenation of 3a (5.6 g, 20 mmol) was carried out in pentane (60 ml) with 5% Pd on BaSO<sub>4</sub> (250 mg) and quinoline (0.25 ml).

The product was worked up in the usual manner and distilled (short path) giving 4a (4.7 g, 84%): bp 137-146° (0.5 mm); n<sup>25</sup>D 1.4578; ir 1740, 975 cm<sup>-1</sup> (trans, optical density extrapolated to a 1.0 M solution, 0.20); nmr δ 1.95 (s, CH<sub>3</sub>CO), 3.97 (bt, 2, CH<sub>2</sub>O), 5.28 (bt, 4, CH==); analysis by capillary glc discussed in text.

Anal. Calcd for C<sub>18</sub>H<sub>32</sub>O<sub>2</sub>: C, 77.09; H, 11.50. Found: C, 77.00; H, 11.32

Isomerization of 3a to 3b and Subsequent Reduction to 4b. Compound 3a (5.0 g, 17.9 mmol) was warmed under nitrogen to 70-75°. Aqueous NaNO<sub>2</sub> (1.25 ml of 2 M) and HNO<sub>3</sub> (0.85 ml of 6 M) were added. The mixture was stirred vigorously for 0.5 hr. The crude product was diluted with petroleum ether, washed with H<sub>2</sub>O, dried (MgSO<sub>4</sub>), and concentrated. Filtration through alumina (20 g) with petroleum ether was followed by distillation to give 3b (3.7) g, 74%): bp 150–160° (0.5 mm); n<sup>25</sup>D 1.4601; ir 1740, 975 cm<sup>-1</sup> (much more intense).

Hydrogenation of **3b** (5.6 g, 19.5 mmol) as described for **3a** gave **4b** (4.5 g, 80%): bp 125–135° (0.3 mm);  $n^{25}$ D 1.4564; ir 1740, 975  $cm^{-1}$  (trans, optical density extrapolated to a 1.0 M solution, 1.30); nmr, virtually identical with 3b; analysis by capillary glc discussed in text.

Registry No.-1, 16695-31-1; 2, 53042-77-6; 3a, 53042-80-1; 3b, 53042-78-7; (Z,Z)-4, 52207-99-5; (Z,E)-4, 51607-94-4; (E,Z)-4, 53042-79-8; (E,E)-4, 53042-81-2; 1-bromo-3-chloropropane, 109-70-6; triphenylphosphine, 603-35-0; valeraldehyde, 110-62-3.

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# **Proton Nuclear Magnetic Resonance Spectra** of 1,2-Disubstituted Acenaphthenes

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In conjunction with the study<sup>2</sup> of the nmr spectra of 1substituted acenaphthenes, and as an extension of our earlier examination<sup>3</sup> of the additivity of substituent effects on chemical shifts, we have analyzed the benzylic portions of the nmr spectra of several 1,2-disubstituted acenaphthenes. The results are shown in Table I. It can be seen that in the five-membered ring of acenaphthene chemical shift relationships are found to be similar to those observed previously<sup>5a</sup> in a limited range of compounds with threemembered rings and in several multiring structures. That is, where a substituent (e.g., Cl, CH<sub>3</sub>, OH, OAc) deshields a trans proton (dihedral angle  $\approx 120^{\circ}$ ) with respect to an eclipsed proton in the fragment 1, the signal resulting from



the trans isomer of the related 1,2-disubstituted compound is upfield of the signal resulting from the cis isomer. Where a substituent (e.g., COOH, COOMe) shields a trans proton with respect to an eclipsed proton in the fragment 1 the reverse applies. It follows that stereochemical assignments (i.e., cis-trans relationships) in a 1,2-disubstituted compound, incorporating a flat five-membered ring, may be made from chemical shift data alone, although it can be seen (Table I) that in most cases this relationship is of limited diagnostic utility because the actual differences of chemical shifts may be very small.

If  $\Delta \delta_x$  (gem),  $\Delta \delta_x$  (cis), and  $\Delta \delta_x$  (trans) are defined as the differences between the chemical shifts of the geminal, cisvicinal, and trans-vicinal protons, respectively, in a 1-substituted acenaphthene,<sup>2</sup> and the chemical shift of the corresponding proton in acenaphthene (X = H), then if the principle of simple additivity<sup>3</sup> applies, a value  $\Delta \delta_x$  (calcd) may be calculated for the benzylic protons in a cis-disubstituted acenaphthene by summing  $\Delta \delta_x$  (gem) and  $\Delta \delta_x$  (trans), and for a trans-disubstituted acenaphthene by summing  $\Delta \delta_x$  (gem) and  $\Delta \delta_x$  (cis).

It can be seen (Table II) that there is a fair additive relationship between data based on 1-substituted acenaphthenes<sup>2</sup> [ $\Delta \delta_x$  (calcd)] and experimental data obtained in this work for 1,2-disubstituted acenaphthenes ( $\Delta \delta_x$  (exptl)). In most cases, the predicted deshielding by the two substituents is slightly more than that observed.

An obvious source of discrepancy between the calculated and experimental results is the possibility of steric distortion in 1,2-disubstituted acenaphthenes.

 Table I

 Nmr Data<sup>a</sup> for 1,2-Disubstituted Acenaphthenes



	Registry no.	$E_x^b$	Chemical shift, ppm from TMS <sup>c</sup>			Coupling constants	
х			H1, 2	Others	Chemical shift from parent	J1, 2	<sup><i>J</i></sup> С13-Н1
cis-H	83-32-9	1.9	3.36		0.0	9.2	$129 \pm 1$
trans-H			3.36		0.0	3,8	$129\pm1$
<i>cis-</i> Me	18210-58-7	2.2	3.68	1.22 (CH <sub>3</sub> ), 7.0–7.6	0.32	7, 70 $\pm$ 0, 03 <sup>h</sup>	
trans-Me	51921-69-8		3.13	1.42 (CH <sub>3</sub> ), $6.9-7.7$	-0.23	$3,97 \pm 0,03^{h}$	
cis-COOMe	5673-22-3	2.6	4.82 (4.75)	3.7 (COOCH <sub>3</sub> ), $7.3-8.0$	1.46		
trans-COOMe	5673-04-1		5.10(5.04)	$3.7(COOCH_3), 7.5-8.0$	1.74		
cis-COOH <sup>d</sup>	5673-06-3	2.6	4.74	8.9 (COOH), 7.3-7.9	1.38		
trans-COOH <sup>d</sup>	5673-03-0		5.00	7.8 (COOH), 7.3-7.8	1,64		
cis-Ph	52522-93-7	2.8	5.22	6.5-7.8	1.86		$156 \pm 1$
trans-Br	25226-58-8	3.0	5,95(5,95)	7.4-7.8	2.59		$159 \pm 1$
cis-Cl	49601-80-1	3.2	5.70 (5.76)	7.2-7.8	2.34	6.3	$158 \pm 1$
trans-Cl	35468-33-8		5.66 (5.69)	7.2-7.7	2.30	$1.0 \pm 0.1$	$162 \pm 1$
$cis$ - $OH^e$	2963-86-2	3.4	5.32 (5.35)	4.12 (OH), 7.4-7.9	1,96	$6.20 \pm 0.05$	$156 \pm 1$
t rans -OH <sup>e</sup>	2963-87-3		5.32	3.33 (OH), 7.4-7.9	1.96	$1.2 \pm 0.1$	$154 \pm 1$
$cis$ -OB $z^{f}$	52522-94-8	$\sim 3.2$	6.50				
trans-OBz <sup>f</sup>	52522-95-9		6.46				
$cis$ -ONO $_2$	17668-54-1		6.73				
$trans-ONO_2$	17668-53-0		6.54				
cis-OAc	5810-80-0	3.7	6.62	2.1 (COCH <sub>2</sub> ), 7.3–7.8	3.26	6.2	156 + 1
trans-OAc	52522-96-0		6.60	2.1 (COCH <sub>2</sub> ), 7.4 $-7.9$	3.24	$1.40 \pm 0.03$	$158 \pm 1$
$cis - F^{g,i}$	6671-55-2	3.9				5 1	100 1 1
$trans$ - $\mathbf{F}^{g,i}$	6671-54-1					0.7	

<sup>*a*</sup> The data refer to 10% solutions in CDCl<sub>3</sub> unless otherwise indicated. Chemical shifts are in parts per million from TMS and are believed to be significant to  $\pm 0.2$  ppm and coupling constants to  $\pm 0.2$  Hz unless otherwise indicated. <sup>*b*</sup> See ref 2 for definition and data for acenaphthene (X = H). <sup>*c*</sup> Figures in parenthesis refer to chemical shifts in 1–3% solutions in CCl<sub>4</sub>. <sup>*d*</sup> Approximately 5% solution in CDCl<sub>3</sub> (90%) and DMSO (10%). <sup>*e*</sup> Approximately 10% solution in DMSO. <sup>*f*</sup> Ref 8. <sup>*s*</sup> Ref 4. <sup>*h*</sup>  $J_{CH_3,H}(cis) = 7.42 \pm 0.02$  Hz and  $J_{CH_3,H(trans)} = 7.15 \pm 0.02$  Hz. <sup>*i*</sup> Note Added in Proof. For new data on fluorinated acenaphthenes see L. D. Hall and D. L. Jones, *Can. J. Chem.*, **51**, 2902 (1973).

 Table II

 Comparison of  $\Delta \delta_x$  (calcd)<sup>a</sup> and  $\Delta \delta_x$  (exptl)<sup>a</sup> for 1,2-Disubstituted Acenaphthenes

x	$\Delta \delta_x$ (gem) <sup>b</sup>	$\Delta \delta_x$ (trans) <sup>b</sup>	$\Delta \delta_x$ (cis) <sup>b</sup>	$\Delta \delta_{\chi}$ (calcd)	Δδ <sub>χ</sub> (exptl)
cis-Me	-0.17	-0.09		-0.26	-0.32
trans-Me	-0.17		0.62	0.45	0.23
cis- COOMe	-1.13	-0.16		-1.29	-1.46
trans- COOMe	-1.13		-0.46	-1.59	-1.74
cis- COOH	-1.19	-0.21		-1.40	-1.38
trans- COOH	-1.19		-0.46	-1.65	-1.64
cis-Ph	-1.35	-0.46		-1.81	-1.86
<i>trans-</i> Br	-2.35		-0.29	-2.64	-2.59
cis-Cl	-2.31	-0.46		-2.77	-2.34
trans-Cl	-2.31		-0.16	-2.47	-2.30
cis-OH	-2.23	-0.28		-2.51	-1.96
trans-OH	-2.23		0.25	-1.98	-1.96
cis-OAc	-3.14	-0.32		-3.46	-3.26
trans - OAc	-3.14		0.18	-2.96	-3.24

<sup>*a*</sup> In parts per million.  $\Delta \delta_x(\text{calcd}) = \Delta \delta_x(\text{gem}) + \Delta \delta_x(\text{trans})$  for cis isomer and  $\Delta \delta_x(\text{calcd}) = \Delta \delta_x(\text{gem}) + \Delta \delta_x(\text{cis})$  for trans isomer.  $\Delta \delta_x(\text{exptl}) = \delta_x - \delta_H$  where  $\delta_x$  and  $\delta_H$  are the chemical shifts of the benzylic protons in the 1,2-disubstituted acenaphthene and acenaphthene, respectively. <sup>*b*</sup> See text for definition. Negative sign indicates deshielding with respect to unsubstituted case. Data are derived from ref 2. However, the agreement between  $\Delta \delta_x$  (calcd) and  $\Delta \delta_x$  (exptl) in the cis isomer, where such distortions are more likely is much the same as in the trans isomer (except for the dichloro and diol cases). Some of the above discrepancies may result from the spectra of several 1,2-disubstituted acenaphthenes being recorded in a different solvent than that used for the corresponding 1-substituted derivative.

The results in Table I show that, as in the case of 1-substituted acenaphthenes,<sup>2</sup> and as predicted by the Karplus rule,<sup>6</sup>  $J_{\rm cis}$  is always significantly larger than  $J_{\rm trans}$ . Firm stereochemical assignments (cis-trans relationships) are therefore possible, on the basis of coupling constant in 1,2disubstituted acenaphthenes, and presumably also in other five-membered rings which do not deviate appreciably from planarity.

A decrease in both  $J_{\rm cis}$  and  $J_{\rm trans}$  in 1,2-disubstituted acenaphthenes is observed as the electronegativity of the substituent increases, a result also noted for 1-substituted acenaphthenes,<sup>2</sup> although here the decrease is more dramatic ( $J_{\rm trans} = 3.8-0.7$  Hz and  $J_{\rm cis} = 9.2-5.1$  Hz).

If  $\Delta J_x(\text{cis})$  and  $\Delta J_x(\text{trans})$  are the decreases, respectively, that occur in  $J_{\text{cis}}$  and  $J_{\text{trans}}$  on monosubstitution of acenaphthene at the 1-position, then  $\Delta J_x(\text{cis})(\text{calcd})$  and  $\Delta J_x(\text{trans})(\text{calcd})$  may be determined for 1,2-disubstituted acenaphthenes by doubling  $\Delta J_x(\text{cis})$  and  $\Delta J_x(\text{trans})$ , respectively. These calculated values and the experimentally determined  $\Delta J$  values for the 1,2-disubstituted compounds are compared in Table III. It can be seen that there is good agreement between  $\Delta J_x(\text{trans})(\text{calcd})$  and  $\Delta J_x(\text{trans})(\text{calcd})$  and  $\Delta J_x(\text{trans})(\text{exptl})$  in all cases except X = F (unless  $J_{\text{trans}}$  for fluorine

Table III Comparison of  $\Delta J_x$  (calcd)<sup>*a*</sup> with  $\Delta J_x$  (exptl)<sup>*a*</sup> for 1,2-Disubstituted Acenaphthenes

 X	$\Delta J_x^b$	$\Delta J_X$ (calcd)	$\Delta J_x$ (exptl)	$\Delta J_{\chi}(calcd)\Delta J_{\chi}(exptl)$	
 cis-Me	1.1	2,2	1.5	0.7	
trans-Me	0.0	0.0	-0.2	0.2	
cis-Cl	1.8	3,6	2.9	0.7	
trans-Cl	1.36	2.7	2.8	0.1	
cis-OH	2.1	4.2	3.0	1.2	
trans -OH	1.2	2.4	2.6	-0.2	
cis-OAc	1.95	3.9	3.0	0.9	
trans-OAc	1.3	2.6	2.4	0.2	
$cis$ - $F^b$	2.5	5.0	4.1	0.9	
$trans$ - $\mathbf{F}^{b}$	2.3	4.6	3.1	1.5	

<sup>a</sup> In hertz.  $\Delta J_x$ (calcd) =  $2\Delta J_x$ . <sup>b</sup>  $\Delta J_x$  is the difference between  $J_{1,2}$  in acenaphthene and the corresponding coupling constant in 1-X substituted acenaphthene.<sup>2</sup> <sup>b</sup> See footnote in Table I.

is negative,<sup>5c</sup> in which case the agreement is exact), but a much poorer agreement between  $\Delta J_x(\text{cis})(\text{calcd})$  and  $\Delta J_x(\operatorname{cis})(\operatorname{exptl})$  in every compound. This cannot be easily rationalized in terms of distortions of the expected type 2 because X-ray diffraction studies7 on cis-1,2-acenaphthenediol (where  $J_{cis}$  shows a very large deviation from additivity) showed that distortions from perfect eclipsing due to nonbonded interactions between the cis-vicinal oxygen atoms was of the order of 10°. The nature of the Karplus curve indicates that a change of 10° in the interproton dihedral angle in a 1,2-disubstituted acenaphthene would only cause a small change in the value of  $J_{\rm cis}$  (~0.3).

Distortion of the type 3 would, however, cause a diminution in the H-C-C angles resulting in an increase in  $J_{cis}^{5d}$ .



#### **Experimental Section**

Analyses of Nmr Spectra. The nmr spectra (100 MHz) of several 1,2-disubstituted acenaphthenes consisted of a singlet between  $\delta$  4.7 and 6.7, and a broad multiplet at  $\delta$  7.0–8.0. The <sup>13</sup>C satellites of the resonance assigned to the benzylic protons ( $\delta$  4.7-6.7) were analyzed as an AX system with  $\nu_{AX} = \frac{1}{2}J_{13CH}$  after decoupling of the aromatic protons. Each satellite was a doublet with splitting  $J_{AX}$ . cis-1,2-Diphenylacenaphthene, cis-1,2-acenaphthenediol, and cis- and trans 1,2-acenaphthenedicarboxylic acid were too insoluble in chloroform or dimethyl sulfoxide to give observable satellite resonances. However satisfactory satellite spectra of the first two compounds were obtained using multiple scans (CAT)

Analyses were not carried out for the signals assigned to the aromatic protons ( $\delta$  7.0–8.0) although several of these multiplets have been analyzed previously as ABC systems by Hayward and Csizmadia.8 The methyl and benzylic proton regions of the nmr spectra of cis- and trans-1,2-dimethylacenaphthene were analyzed as  $X_3AA'X_3'$  spin systems ( $J_{XX'} = 0$ ) according to the method of Anet.<sup>9</sup> Analyses were performed using the iterative computer program LAME<sup>10</sup> executed on an IBM 7040/1401 in the Basser Computing Laboratory, School of Physics, University of Sydney. Trial parameters were calculated by the use of interval rules<sup>9</sup> for the X<sub>3</sub>AA'X<sub>3</sub>' spin system as well as estimates from related compounds whose nmr spectra had been analyzed previously.

Preparation of Compounds. cis- and trans -1,2-dichloroacenaphthene,<sup>11</sup> trans -1,2-dibromoacenaphthene,<sup>12</sup> cis- and trans -1,2-acenaphthenediol,<sup>12</sup> cis- and trans -1,2-diacetoxyacenaphthene,<sup>8</sup> cis-1,2-diphenylacenaphthene,<sup>13</sup> cis- and trans-acenaphthenedicarboxylic acid,<sup>14</sup> dimethyl cis- and trans-1,2-acenaphthenedicarboxylate,  $^{14}$  and cis -1,2-dimethylacenaphthene  $^{15}$ 

were prepared as described previously. Physical constants and spectral data were consistent with those reported.

cis- and trans-1,2-Dimethyl-1,2-acenaphthenediol. Acenaphthenequinone (15.0 g) was added in small portions to the Grignard reagent prepared from magnesium (8 g), methyl iodide (50 g) and diethyl ether (100 ml). The reaction mixture was heated under reflux for 3 hr, cooled, and poured into a mixture of ice (200 g) and 3N sulfuric acid (100 ml). Extraction with diethylether (50 ml) left a large amount of the diol as a suspension in the aqueous phase. This was filtered and the crystals obtained were washed with water and recrystallized from ethanol to give 3.1 g (18%) of cis-1,2-dimethyl-1,2-acenaphthenediol: mp 202-203° (lit.<sup>16,17</sup> 187–189°); nmr (CDCl<sub>3</sub>/ $d_6$ -DMSO)  $\delta$  1.58 (s, 6, CH<sub>3</sub>), 4.63 (br s exch, 2, OH), 5.32 (s, 2, benzylic), 7.40-7.85 (m, 6, aromatic). The ether extract was washed with saturated NaHCO<sub>3</sub> solution (20 ml), dried, and the solvent evaporated to give a solid product of mp 156-165°. Successive recrystallizations from methanol and chloroform yielded 6.3 g (36%) of trans-1,2-dimethyl-1,2-acenaph-thenediol: mp 182–183° (lit.<sup>16,17</sup> 182–183°); nmr ( $CDCl_3/d_6$ -DMSO) & 1.61 (s, 6, CH<sub>3</sub>), 4.36 (br s, exch, 2, OH), 5.32 (s, 2, benzylic), 7.30-7.80 (brm, 6, aromatics).

cis-1,2-Dimethylacenaphthene. A suspension of cis-1,2-dimethyl-1,2-acenaphthenediol (1.0 g) in ethanol (10 ml) was shaken at room temperature, under 4 atmospheres of hydrogen for 3 hr with 10% palladium/charcoal (200 mg) and 10 N hydrochloric acid (0.3 ml). The reaction mixture was filtered and the solvent evaporated. The crystalline product was washed with light petroleum (2  $\times$  5 ml) and the washing chromatographed on neutral alumina. The first component eluted by light petroleum was rechromatographed. cis-1,2-Dimethylacenaphthene (0.120 g, 14%) was obtained as a colorless oil which became crystalline when cooled with a few milliliters of ethanol, mp 52–54° (lit.<sup>15</sup> 53–54°).

trans-1,2-Dimethylacenaphthene. A solution of trans-1,2dimethyl-1,2-acenaphthenediol (2.0 g) in ethanol (15 ml) was shaken at room temperature under 4 atmospheres of hydrogen for 3 hours with 10% palladium/charcoal (400 mg) and 10 N hydrochloric acid (0.4 ml). The mixture was filtered and the solvent evaporated to give a solid product. This was washed with light petroleum  $(3 \times 5 \text{ ml})$  and the washings were chromatographed on neutral alumina. Light petroleum eluted a colorless liquid which was distilled under reduced pressure to yield *trans* -1,2-dimethyl-acenaphthene (0.14 g, 17%): bp 92–94° (0.6 mm); ir (CHCl<sub>3</sub>) 3010, 2970, 2940, 2876, 1603, 1448, 1371, 820 cm<sup>-1</sup>; uv (ethanol)  $\lambda_{max}$  228 (52,000), 288 (4400) nm.

Anal. Calcd for C14H14: C, 92.3; H, 7.7. Found: C, 91.9; H, 8.0.

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Registry No.-cis-1,2-Dimethyl-1,2-acenaphthenediol, 6566-38-7; trans-1,2-dimethyl-1,2-acenaphthenediol, 6566-39-8; acenaphthenequinone, 82-86-0.

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