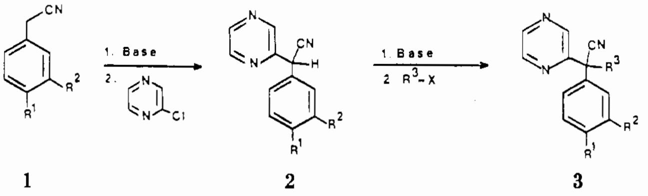
Scheme I



1a, $R^1 = R^2 = H$
1b, $R^1 = CH_3, R^2 = H$
1c, $R^1 = OCH_3, R^2 = H$
1d, $R^1 = R^2 = OCH_3$

2a, $R^1 = R^2 = H$
2b, $R^1 = CH_3, R^2 = H$
2c, $R^1 = OCH_3, R^2 = H$
2d, $R^1 = R^2 = OCH_3$

3a, $R^1 = R^2 = H, R^3 = (CH_2)_3CH_3$
3b, $R^1 = R^2 = H, R^3 = CH_2$-S-Ph
3c, $R^1 = R^2 = H, R^3 = CH_2-C_6H_4-(4-CH_3)$
3d, $R^1 = R^2 = H, R^3 = CH_2-C_6H_4-(4-NO_2)$
3e, $R^1 = R^2 = H, R^3 = CH_2COPh$
3f, $R^1 = R^2 = H, R^3 = (CH_2)_2-CN$
3g, $R^1 = R^2 = H, R^3 = CH_2CN$
3h, $R^1 = R^2 = H, R^3 = CH_2$-benzotriazol-1-yl
3i, $R^1 = R^2 = H, R^3 = CH_2$-2-pyridinyl
3j, $R^1 = R^2 = H, R^3 = (CH_2)_2Ph$
3k, $R^1 = R^2$, H, $R^3 = CH_2-C_6H_4-(4-OMe)$
3l, $R^1 = CH_3, R^2 = H, R^3 = CH_2Ph$
3m, $R^1 = CH_3, R^2 = H, R^3 = CH_2-C_6H_4-(4-CH_3)$
3n, $R^1 = OCH_3, R^2 = H, R^3 = CH_2Ph$
3o, $R^1 = OCH_3, R^2 = H, R^3 = CH_2-C_6H_4-(4-CH_3)$
3p, $R^1 = R^2 = OCH_3, R^3 = CH_3$
3q, $R^1 = R^2 = OCH_3, R^3 = CH_2-CH=CH_2$
3r, $R^1 = R^2 = OCH_3, R^3 = CH_2CO_2Et$
3s, $R^1 = R^2 = OCH_3, R^3 = CH_2Ph$
3t, $R^1 = R^2 = OCH_3, R^3 = CH_2CO_2H$
3u, $R^1 = R^2 = OCH_3, R^3 = CH_2CH_2CO_2H$

lapped with peaks due to aromatic protons of R^3 (Table I). In all cases where $R^1 = CH_3$, the protons appeared at $\delta \sim 2.2$, whereas the methoxy protons, for R^1 or R^2 = OMe, resonated at 4.0 ppm.

Registry No. **2a**, 1080-87-1; **2b**, 1082-48-0; **2c**, 1084-83-9; **2d**, 1088-67-1; **3a**, 109929-53-5; **3b**, 109929-54-6; **3c**, 109929-55-7; **3d**, 109929-56-8; **3e**, 109929-57-9; **3f**, 4422-44-0; **3g**, 4190-80-1; **3h**, 109929-58-0; **3l**, 109929-59-1; **3j**, 109929-60-4; **3k**, 109929-61-5; **3l**, 109929-62-6; **3m**, 109929-63-7; **3n**, 109929-64-8; **3o**, 109929-65-9; **3p**, 109929-66-0; **3q**, 109929-67-1; **3r**, 109929-68-2; **3s**, 109929-69-3; **3t**, 109929-70-6; **3u**, 109929-71-7; $Me(CH_2)_3Br$, 109-65-9; $Br(CH_2)SPh$, 35572-08-8; 4-$MeC_6H_4CH_2Br$, 104-81-4; 4-$NO_2C_6H_4CH_2Br$, 100-11-8; $BrCH_2COPh$, 70-11-1; $Br(CH_2)_2CN$, 2417-90-5; $BrCH_2CN$, 590-17-0; $Br(CH_2)_2Ph$, 103-63-9; 4-$MeOC_6H_4CH_2Br$, 2746-25-0; $PhCH_2Br$, 100-39-0; MeBr, 74-83-9; $CH_2=CHCH_2Br$, 106-95-6; $MeCO_2Et$, 105-36-2; $Br(CH_2)_2CO_2H$, 590-92-1; 1-(chloromethyl)benzotriazole, 54187-96-1; 2-(bromomethyl)pyridine, 55401-97-3.

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Heterocycles. 14. Synthesis of 5*H*-Indenopyrimidines

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1-Indanone (I) was reacted with aryl aldehydes (II) to give the corresponding 2-arylidene-1-indanones (III). Condensation of the chalcones III with guanidine revealed the formation of the corresponding 5*H*-2-amino-4-arylidenopyrimidines (V). The structures of all products were substantiated by chemical and spectroscopic methods.

Various aromatic and heterocyclic aldehydes (IIa–k) were reacted with 1-indenone to give the corresponding 2-arylidene-1-indenones (IIIa–k) (Scheme I). The structures of these products were evident from the infrared (*1*, *2*), electronic (*3*, *4–7*), NMR spectra (*8*), and chemical analyses (Tables I and II). The infrared spectra of IIIa show absorption bands at 1625 and 1695 cm^{-1} attributed to $\nu_{C=C}$ and C=O, respectively. The chalcones (III a–k) were condensed with guanidine to yield the corresponding 5*H*-2-amino-4-arylindenopyrimidines (Va–k) (*3*, *9*, *10*) (Scheme I). The structures of these products were substantiated by spectroscopy (*3*, *8*) (Tables I and II). The IR spectrum of Va shows absorptions at 1600 cm^{-1} (C=C), 1640 cm^{-1} (C=N), and 3140, 3280, and 3460 cm^{-1} (NH_2).

Chemical evidence can be also adduced in favor of the structure of compounds V. Thus acetylation of Vf,h leads to the formation of the corresponding acetylamido derivatives (VIf,h) (Scheme I) (*3*, *9*). Their structures were established from their infrared (*11*), electronic (*12*), and mass spectra (Table I). The IR spectrum of VIf shows absorptions at 1720 cm^{-1} (C=O) and 3400 cm^{-1} (NH).

Treatment of the 2-aminopyrimidines (Vf,h,j) with nitrous acid revealed the formation of the corresponding 2(1*H*)-pyrimidinones (VIIf,h,j) (Scheme I). The lactam form of these products was inferred from their infrared (*9*), electronic and mass spectra (Table I). The IR spectrum of VIIf revealed absorptions at 1640 cm^{-1} (C=O) and 2990 and 3080 cm^{-1} (NH).

Experimental Section

Melting points were measured using a Bock-Monoscope (thermal microscope) and are uncorrected. Electronic and infrared spectra were run on Cary 17 and Perkin-Elmer 580B, respectively. The ^1H NMR and the mass spectra were measured with Varian T60A and Varian MAT 311A, respectively. Microanalyses were determined by A. Bernhardt Microanalytical Laboratory, GFR.

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Table I. Electronic and Nuclear Magnetic Resonance Spectral Data of Compounds III–VII

compd	electronic spectra (Ethanol)			NMR (DMSO-d_6) assignment
	λ_{max}, nm	ϵ	δ	(no. of protons)
IIIa	230	8025	3.95 (d)	(2) CH_2
	327	16735	7.33–7.87 (m)	(10) Ar-H + =CH
IIIb	247	8010	3.80 (s)	(3) OCH_3
	352	17975	3.93 (d)	(2) CH_2
			6.83–7.93 (m)	(9) Ar-H + =CH
IIIc	264	8130	3.83 (s)	(3) OCH_3
	313	17505	4.0 (d)	(2) CH_2
			6.87–7.93 (m)	(9) Ar-H + =CH
IIId	231	7955	4.20 (d)	(2) CH_2
	325	16865	7.80–8.40 (m)	(9) Ar-H + =CH
IIIe	241	4965	4.18 (d)	(2) CH_2
	312	17175	7.46–8.40 (m)	(9) Ar-H + =CH
IIIf	230	8165	3.96 (d)	(2) CH_2
	322	17920	7.17–7.87 (m)	(9) Ar-H + =CH
IIIg	225	8370	3.93 (d)	(2) CH_2
	279	11260	7.20–8.0 (m)	(9) Ar-H + =CH
	307	16745		
IIIh	270	11605	4.20 (d)	(2) CH_2
	398	5910	7.60–8.66 (m)	(12) Ar-H + =CH
IIIi	278	13130	4.34 (d)	(2) CH_2
	288	14630	766–8.60 (m)	(12) Ar-H + =CH
	333	16130		
IIIj	230	4710	3.90 (d)	(2) CH_2
	270	5025	6.97–7.77	(8) Ar-H + =CH
	353	18840		
IIIk	226	4520	4.0 (d)	(2) CH_2
	270	4670	6.40–7.87 (m)	(8) Ar-H + =CH
	354	17505		
Va	253	10605	2.72 (d)	(2) CH_2
	285	4335	6.10 (br)	(2) NH_2
	293	4060	7.07–7.70 (m)	(9) Ar-H
	342	5348		
Vb	260	11805	4.14 (d)	(2) CH_2
	283	3620	7.14 (br)	(2) NH_2
	345	6090	7.60–8.46 (m)	(8) Ar-H
Vc	250	12030	3.40 (d)	(2) CH_2
	286	3770	4.13 (s)	(3) OCH_3
	295	4370	7.20 (br)	(2) NH_2
	345	7890	7.60–8.62 (m)	(8) Ar-H
Vd	250	10670	4.26 (d)	(2) CH_2
	283	8000	6.94 (br)	(2) NH_2
	292	7275	7.40–8.30 (m)	(8) Ar-H
	345	9700		
Ve	255	11055	3.20 (d)	(2) CH_2
	285	3870	7.26 (br)	(2) NH_2
	294	3040	7.60–8.94 (m)	(8) Ar-H
	346	6080		
Vf	260	14565	3.06 (d)	(2) CH_2
	293	3350	6.20 (br)	(2) NH_2
	347	8130	7.0–8.46 (m)	(8) Ar-H
Vg	255	11140	4.34 (d)	(2) CH_2
	288	6320	7.14 (br)	(2) NH_2
	295	6620	7.86–8.6 (m)	(8) Ar-H
	353	8550		
Vh	250	10780	3.06 (d)	(2) CH_2
	283	7880	6.74 (br)	(2) NH_2
	292	7050	7.60–8.86 (m)	(11) Ar-H
	337	6220		
Vi	250	13170	3.14 (d)	(2) CH_2
	285	6825	7.14 (br)	(2) NH_2
	293	6070	7.86–8.34 (m)	(11) Ar-H
	348	7960		
Vj	265	12765	3.34 (d)	(2) CH_2
	285	8510	6.34 (br)	(2) NH_2
	292	8085	7.40–8.06 (m)	(7) Ar-H
	335	8510		
Vk	257	12595	3.34 (d)	(2) CH_2
	287	10335	7.26 (br)	(2) NH_2
	354	9040	7.40–8.60 (m)	(7) Ar-H
	366	8300		
VIf	255	13480		
	316	13480		
VIh	223	20475		
	245	7320		
	279 (sh)	4245		
VIIf	265	11440		
	312	9765		
	350	8080		
VIIh	222	25835		
	273	6135		
	340	3745		
VIIj	273	6575		
	304	4655		
	338	4460		

Table II. Mass Spectra of Compounds V–VII Indicating the Molecular Ions

compd	MS	
	m/e	% of base peak
Va	259	28.33
Vf	309	100
Vi	292	100
Vk	249	100
VIf	355	73.88
VIIf	294	100
VIIh	310	91.31

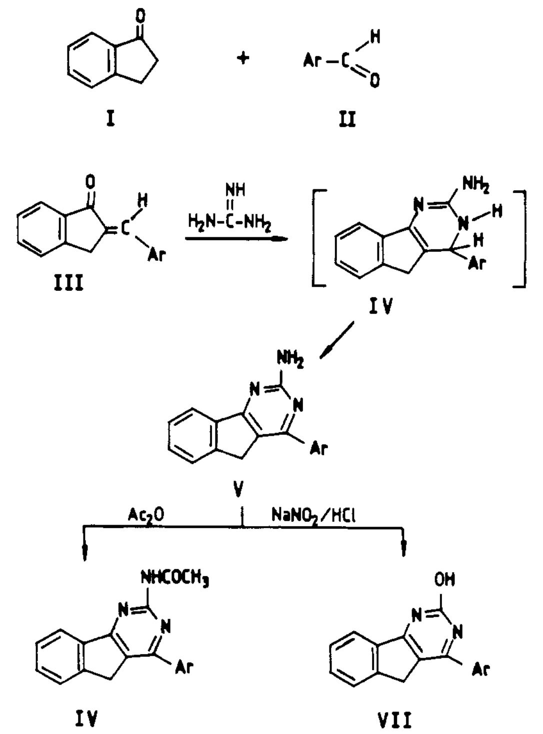
Table III. Yields and Melting Points of Compounds III, V–VII

compd	yield, %	mp, °C	compd	yield, %	mp, °C
IIIa	88	108	Vd	79	218–219
IIIb	90	134	Ve	78	188–189
IIIc	91	138	Vf	87	245–246
IIId	89	185–186	Vg	84	215–216
IIIe	92	140–141	Vh	82	193–194
IIIf	87	174–175	Vi	80	230–231
IIIg	84	155–156	Vj	88	251–252
IIIh	89	118–119	Vk	78	280–281
IIIi	83	177–178	VIf	92	200–201
IIIj	84	152–153	VIh	94	189–190
IIIk	80	113	VIIf	90	274–175
Va	81	190–191	VIIh	89	>360
Vb	83	240–241	VIIj	88	>360
Vc	85	197–198			

Preparation of 2-Arylidene-1-indanones (IIIa–k). General Procedure. Equimolar amounts of the aldehydes (0.1 mol) and 1-indanone (0.1 mol) in ethanol (100 mL) were treated with an aqueous solution of sodium hydroxide (5 g/10 mL of water). Addition of the base was carried out during 20 min and the mixture was stirred for a further 3 h. The precipitated product was filtered off and crystallized from hexane or cyclohexane to give the indanone product III.

Condensation of 2-Arylidene-1-indanones (III) with Guanidine. General Procedure. To a solution of 0.02 mol (1.9 g) of guanidine hydrochloride in 20 mL of ethanol was added 0.02 mol (0.8 g) of sodium hydroxide. The solution was stirred for 15 min and the precipitated sodium chloride was filtered. The filtrate was added to an ethanolic solution of 0.004 mol of the chalcone III, and the mixture was refluxed for 6 h and then concentrated and water added. After acidification the precip-

Scheme I



Compound	Ar	Compound	Ar
II-VIIa	C_6H_5	II-VIIf	$p-ClC_6H_4$
b	$p-OCH_3-C_6H_4$	g	$o-ClC_6H_4$
c	$m-OCH_3C_6H_4$	h	$1-C_{10}H_7$
d	$p-Br-C_6H_4$	i	$2-C_{10}H_7$
e	$m-Br-C_6H_4$	j	$2-C_4H_3S$
		k	$2-C_4H_3O$

itated material was filtered, washed with water, and dried. Crystallization from benzene gave 5*H*-2-amino-4-arylindeno-[1,2-*d*]pyrimidines (V).

Acetylation of the 2-Aminopyrimidines (Vf,h). A mixture of the pyrimidine derivatives (1 g) and acetic anhydride (5 mL) was refluxed for 2 h. The product was poured in 30 mL of water–ethanol mixture (1:1) and cooled. The precipitated solid was filtered off. Crystallization from ethanol–water gave the corresponding 5*H*-2-acetamido-4-arylindeno[1,2-*d*]pyrimidines (VIf,h).

Reaction of 2-Aminopyrimidines Vf,h,j with Nitrous Acid. A solution of sodium nitrite (1.5 g) in water (10 mL) was added dropwise to a solution of the pyrimidine derivative (1.0 g) in glacial acetic acid (15 mL). The precipitated solid was crystallized from benzene to give the corresponding 5*H*-4-aryl-indeno[1,2-*d*]-2(1*H*)-pyrimidinone (VII).

Registry No. I, 83-33-0; IIa, 100-52-7; IIb, 123-11-5; IIc, 591-31-1; IId, 1122-91-4; IIe, 3132-99-8; IIf, 104-88-1; IIg, 89-98-5; IIh, 66-77-3; IIi, 66-99-9; IIj, 98-03-3; IIk, 98-01-1; IIIa, 5706-12-7; IIIb, 5706-14-9; IIIc, 110117-34-5; IIId, 5706-19-4; IIIe, 81975-58-8; IIIf, 5706-17-2; IIIg, 5706-16-1; IIIh, 92882-96-7; IIIi, 92882-97-8; IIIj, 5706-21-8; IIIk, 6072-51-1; Va, 110117-35-6; Vb, 110117-36-7; Vc, 110117-37-8; Vd, 110117-38-9; Ve, 110117-39-0; Vf, 110117-40-3; Vg, 110117-41-4; Vh, 110117-42-5; Vi, 110117-43-6; Vj, 110117-44-7; Vk, 110117-45-8; VIf, 110117-46-9; VIh, 110117-47-0; VIIf, 110117-48-1; VIIh, 110117-49-2; VIIj, 110117-50-5; guanidine hydrochloride, 50-01-1.

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Synthesis and Spectral Studies of Some New Sulfides, Sulfoxides, and Sulfones. 2

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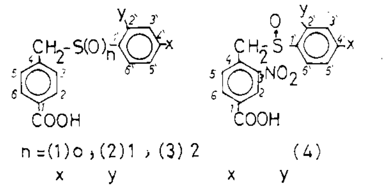
New substituted benzylphenyl sulfides, sulfoxides, and sulfones have been synthesized. Their structures were confirmed by IR, ^{1}H NMR, and mass spectra.

As a continuation of our interest in substituted benzylphenyl sulfides, sulfones, and sulfoxides, a new series has been synthesized. Sulfides (**1a–h**) and sulfones (**3a–h**) have been prepared by conventional procedures (*1–3*). The sulfoxides were prepared as described in the literature (*6*, *7*). The structures of the synthesized compounds were investigated by IR, ^{1}H NMR, and mass spectra.



n =(1)o , (2)1 , (3) 2 (4)

	x	y		x	y
a	H	H	e	Cl	H
b	CH_3	H	f	Br	H
c	OCH_3	H	g	NO_2	H
d	NH_2	H	h	H	COOH

The mass spectra (*9*, *10*) of **1a**, **1c**, **3a**, and **4b** were studied. The relative intensities of the most prominent peaks in their