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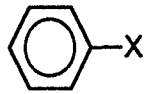
Table I: Calculatedβ vector components along the dipole moments for monosubstituted benzenes ($\times 10^{-36}$ esu)



X	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.
	AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
	PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00[a]
CH_3	0.01	0.04	0.05	0.20	0.27	0.25	0.35	0.45	0.34	0.45	<0.20[a]
OH	0.03	0.13	0.01	0.12	0.67	0.85	0.16	0.22	0.16	0.22	<0.20[a]
SH	1.44	1.59	1.29	1.30	1.86	0.87	0.54	0.54	0.46	0.48	<0.20[a]
OMe	0.05	0.45	0.07	0.02	0.90	1.03	0.10	0.09	0.09	0.13	<0.20[a]
SMe	0.19	0.54	0.79	0.74	3.55	1.37	0.33	0.47	0.26	0.45	<0.20[a]
NH_2	0.11	0.01	0.27	0.23	0.99	1.30	0.18	0.12	0.01	0.07	0.55[a]
NMe_2	0.85	0.44	1.05	0.91	1.70	1.81	0.59	0.62	0.29	0.30	1.10[a]
julolidine	2.23	0.75	1.66	1.30	2.28	1.36	2.81	2.49	1.02	0.82	1.30[b]
F	0.03	0.07	0.00	0.06	0.38	0.18	0.18	0.31	0.18	0.31	<0.20[a]
Cl	0.14	0.40	0.57	0.31	0.53	1.33	-	-	-	-	<0.20[a]
Br	0.22	0.68	0.01	0.73	0.49	0.35	-	-	-	-	<0.20[a]
I	0.20	0.84	1.22	0.19	0.51	0.86	-	-	-	-	<0.20[a]
SO_2CH_3	0.29	0.39	0.69	1.26	0.08	0.23	2.61	1.49	2.86	1.61	<0.20[b]

Table I: continued

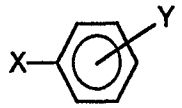
X	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.
	AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
	PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
SO_2F	0.73	0.08	0.03	0.75	0.02	0.22	0.96	0.86	1.05	0.99	0.30[a]
CN	1.09	0.04	0.82	0.06	0.23	0.17	0.66	0.31	0.67	0.32	0.36[a]
CHO	0.82	0.09	0.40	0.15	1.24	1.06	1.68	0.75	1.52	0.66	0.80[a]
$COCF_3$	1.48	0.94	1.41	0.68	0.66	0.66	2.53	1.72	2.26	1.54	1.30[b]
NO	1.62	0.68	1.27	0.12	0.35	0.37	3.02	1.98	3.33	2.13	1.70[b]
NO_2	0.03	0.29	0.19	0.17	0.03	0.08	2.06	1.62	2.23	1.78	1.90[a]
$C_2H(CN)_2$	0.48	0.96	0.67	0.80	4.03	3.43	0.26	1.14	0.06	0.82	3.10[b]

- experimental values measured in:

[a] neat

[b] p-dioxane

Table II: Calculated β vector components along the dipole moments ($\times 10^{-36}$ esu) for disubstituted benzenes; numbers in parenthesis refer to SCRF calculations, the solvent is indicated in the last column



X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.tl.
		AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
		PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
SO_2Me	OH	0.24	0.15	0.57	1.10	1.19	1.08	0.66	1.18	1.42	1.19	1.30[b]
CN	Me	0.80	0.23	1.13	0.30	0.82	0.75	1.42	0.96	1.41	0.92	0.70[a]
CN	Cl	0.12	0.44	0.34	0.21	1.16	2.70	-	-	-	-	0.80[b]
CN	Br	0.17	0.80	0.30	1.25	1.08	0.95	-	-	-	-	1.10[b]
CN	OPh	1.03	1.41	0.84	0.74	3.60	4.74	0.91	1.47	0.99	1.41	1.20[b]
CN	OMe	1.18	0.23	0.82	0.37	2.94	2.86	1.20	1.38	1.21	1.37	1.90[b]
CN	SMe	4.76	4.61	3.14	2.67	11.13	8.13	1.54	1.28	1.32	0.97	2.80[b]
CN	NH_2	1.35	0.40	2.12	1.42	2.99	4.38	2.28	2.40	2.17	2.22	3.10[b]
CN	NMe_2	2.15	1.81	4.60	3.99	4.54	5.66	3.82	3.52	3.53	3.21	5.00[b]
CHO	Me	1.03	0.50	0.53	0.08	2.68	2.30	2.49	1.46	2.25	1.30	1.70[a]
CHO	OPh	1.69	1.25	1.44	1.03	3.04	3.60	1.82	1.64	1.63	1.41	1.90[a]
CHO	OMe	1.47	0.97	1.33	0.59	3.21	3.11	3.10	2.27	2.88	2.11	2.20[a]
CHO	SMe	8.03	6.49	5.73	4.11	9.03	4.70	3.41	2.71	2.91	2.24	2.60[a]
CHO	NMe_2	4.26	3.34	6.24	5.51	9.78	10.44	4.76	4.26	4.07	3.65	6.30[b]

Table II: continued

X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.
		AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
		PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
$iSO_2C_3F_7$	OMe	1.18 (1.73)	1.73	2.20	1.29	0.13	1.22	0.10	0.15	0.23	0.48	3.30[c]
$COCF_3$	OMe	2.75	1.25	2.71	1.95	2.51	2.01	3.66	3.20	3.34	2.95	3.60[b]
$COCF_3$	OPh	6.71	3.81	4.14	1.49	9.61	6.60	4.93	3.70	3.70	2.47	3.60[b]
$COCF_3$	NMe_2	6.98	5.85	8.82	7.99	0.50	1.48	6.76	6.38	4.62	4.39	10.00[b]
NO	NMe_2	6.46	4.75	8.58	7.46	4.11	4.73	7.61	7.12	7.53	6.91	12.00[b]
NO_2	Me	0.32	0.49	0.52	0.20	0.85	0.77	3.14	2.66	3.37	2.85	2.10[b]
NO_2	Br	2.38	0.16	2.08	0.71	1.04	0.90	-	-	-	-	3.30[b]
NO_2	OH	0.36	0.43	0.68	0.31	1.95	1.88	3.20	2.74	3.53	3.04	3.00[b]
NO_2	OPh	5.01	2.82	2.10	0.77	5.26	5.25	7.41	3.66	5.52	3.87	4.00[b]
NO_2	OMe	0.82	0.97	1.12	0.59	3.02	2.81	3.49	3.27	3.84	3.57	5.10[b]
NO_2	SMe	9.54	7.02	6.43	4.80	12.28	8.36	4.08	2.95	3.99	2.78	6.10[b]
NO_2	N_2H_3	5.86	4.89	5.45	4.67	7.45	9.75	6.49	6.08	4.70	4.32	7.60[b]
NO_2	NH_2	1.41 (5.09)	1.86	3.65	2.75	3.45	4.33	5.50	5.04	5.55	4.93	9.20[d]
NO_2	NMe_2	4.15 (8.89)	3.39	6.07	5.07	5.69	5.97	6.95	6.52	6.72	6.29	12.00[d]
NO_2	CN	0.55	0.03	0.12	0.48	0.03	0.29	2.32	2.26	2.52	2.40	0.60[b]

Table II: continued

X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.
		AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
		PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
NO_2	CHO	0.22	0.25	0.21	0.24	0.34	0.23	0.75	0.69	0.92	0.84	0.20[b]
$CHC(CN)_2$	OMe	3.28	3.37	3.16	3.10	9.82	7.73	2.73	3.80	2.30	3.24	9.80[b]
$CHC(CN)_2$	NMe_2	7.46 (10.67)	8.10	10.01	9.46	26.01	24.40	6.53	7.44	5.08	5.98	32.00[c]
$CHC(CN)_2$	julolidine	10.32 (14.79)	11.18	9.27	10.12	29.85	22.78	9.14	10.18	5.72	6.37	44.00[c]
$C_2(CN)_3$	NH_2	8.81 (17.68)	9.33	6.39	7.14	5.58	2.65	7.63	8.83	3.54	4.39	39.00[c]
$C_2(CN)_3$	NMe_2	10.93 (21.35)	12.52	8.50	9.36	17.67	20.66	10.11	11.96	4.96	6.33	50.00[c]
$C_2(CN)_3$	julolidine	14.02 (23.81)	16.17	7.81	8.83	25.23	20.44	13.96	15.80	6.10	7.63	60.00[c]
NO_2	o-Me	0.31	0.1	0.35	0.45	0.58	0.89	2.15	1.83	0.45	0.49	1.00[a]
NO_2	o-Br	0.97	0.47	0.49	0.21	1.93	1.49	-	-	-	-	0.40[b]
NO_2	o-OH	0.06	0.17	0.52	0.42	0.98	1.77	1.79	1.50	0.62	0.42	1.20[b]
NO_2	o-OMe	0.13	0.20	0.06	0.11	0.59	0.62	1.82	1.49	2.00	1.66	1.40[a]
NO_2	o-NH_2	0.68	0.79	0.49	0.01	1.12	2.60	2.42	2.04	2.43	2.04	2.50[b]
NO_2	o-CN	0.05	0.26	0.07	0.01	0.03	0.31	2.09	1.51	1.45	1.10	1.20[b]

Table II: continued

X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.
		AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
		PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
NO_2	o-CHO	0.78	0.04	0.60	0.01	0.18	0.21	2.55	1.83	2.03	1.48	0.80[b]
NO_2	m-Me	0.20	0.34	0.07	0.14	0.09	0.14	2.37	1.95	2.55	2.11	1.50[a]
NO_2	m-Br	0.76	0.24	0.59	0.62	0.41	0.37	-	-	-	-	1.00[b]
NO_2	m-OH	0.05	0.01	0.06	0.22	0.31	0.19	2.18	1.75	2.36	1.91	0.80[b]
NO_2	m-OMe	0.24	0.29	0.08	0.02	0.31	0.46	2.28	1.95	2.47	2.10	1.60[b]
NO_2	m-NH_2	0.93	0.78	1.52	0.92	0.79	0.80	2.74	2.30	2.68	2.24	1.90[b]
NO_2	m-CN	0.33	0.19	0.41	0.36	0.29	0.25	1.15	0.90	1.27	1.02	0.80[b]
NO_2	m-CHO	0.50	0.12	0.02	0.56	0.06	0.51	1.61	1.47	1.55	1.02	1.70[b]

- experimental values measured in:

[a] neat

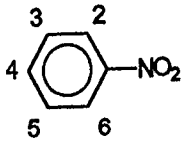
[b] p-dioxane

[c] $CHCl_3$

[d] Acetone

[e] CH_2Cl_2

Table III: Calculated β vector components along the dipole moments ($\times 10^{-36}$ esu) for heteraromatic and polysubstituted benzenes; the number in parenthesis refers to a SCRF calculations in acetone.



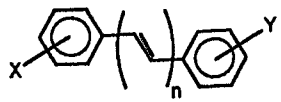
Substitution	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.
	AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
	PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
3-aza 4-NH_2	1.98 (3.45)	1.63	1.56	1.04	1.60	2.03	3.91	3.82	4.22	4.00	3.70[d]
2-aza 4-OMe	1.31	0.40	0.77	0.10	2.29	2.00	2.78	2.47	2.32	2.11	2.20[b]
3-Me 4-NH_2	1.97	2.46	3.37	3.10	4.99	6.25	6.16	5.68	6.21	5.58	8.70[b]
2-Cl 4-NH_2	0.99	0.68	4.03	2.52	1.14	1.41	-	-	-	-	6.80[b]
3-OMe 4-NH_2	2.76	2.67	5.16	4.00	7.71	9.36	6.82	6.32	6.78	6.16	8.70[b]
2-F 4-OMe	0.61	0.79	0.77	0.42	3.20	3.03	2.87	2.70	3.15	2.92	2.50[b]
2,5-F 4-OMe	1.18	1.03	0.68	0.38	3.51	2.77	3.39	2.99	2.85	2.61	2.60[b]
2,3,5,6-F 4-OMe	0.78	0.79	0.50	0.02	3.24	2.14	3.07	2.66	1.79	1.68	1.70[b]

- experimental values measured in:

[b] p-dioxane

[d] Acetone

Table IV: Calculated β vector components along the dipole moments ($\times 10^{-36}$ esu) for mono- and disubstitued stilbenes; numbers in parenthesis refer to SCRF calculations, the solvent is indicated in the last column.



X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.
		AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
		PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
H	H(trans)	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00[c]
H	H (cis)	0.36	0.31	0.12	0.16	0.03	0.13	1.01	0.37	1.21	0.28	0.00[c]
NH_2	H	6.93	3.84	3.46	1.43	4.40	2.86	6.20	5.26	5.40	4.43	7.40[b]
NMe_2	H	9.96	5.40	12.71	3.07	26.04	11.73	9.14	7.08	7.97	5.89	10.00[b]
NO_2	H	9.79	5.86	8.22	4.50	6.60	5.66	18.85	12.81	21.40	15.39	11.00[b]
$COCF_3$	OMe	19.57	12.39	16.00	8.82	30.71	26.24	22.57	18.46	15.88	12.42	16.40[b]
CN	OH	6.32	5.06	7.22	4.44	1.19	1.69	9.88	9.28	9.63	8.92	13.00[b]
CN	OMe	8.24 (14.87)	6.26	8.49	5.26	1.23	1.97	11.20	10.21	10.80	9.72	19.00[c]
CN	NMe_2	20.35 (35.13)	14.15	22.58	14.07	49.99	47.07	21.40	17.08	18.94	14.80	36.00[c]
NO_2	Me	12.85	7.68	10.89	6.19	8.74	7.53	-	-	-	-	15.00[b]
NO_2	Br	11.90 (19.43)	6.50	11.12	4.04	7.43	7.70	-	-	-	-	14.00[b] (18.00)[c]

Table IV: continued

X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.
		AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
		PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
NO_2	OH	15.87	10.13	14.10	8.95	5.90	5.40	25.67	18.90	26.64	19.60	17.00[b]
NO_2	OPh	23.25	10.48	19.04	9.06	36.07	35.16	33.35	20.94	34.21	21.43	18.00[b]
NO_2	OMe	17.47 (33.67)	11.32	15.26	9.46	5.91	5.62	27.13	20.03	27.48	20.57	28.00[b] (34.00)[e]
NO_2	SME	26.10 (46.18)	17.55	21.50	10.84	7.39	1.87	24.23	17.87	23.31	16.94	26.00[b] (34.00)[e]
NO_2	NH_2	25.86	17.07	20.98	13.28	18.23	14.06	34.37	25.94	28.48	21.10	40.00[e]
NO_2	NMe_2	27.04 (83.68)	17.22	27.53	18.31	64.03	62.97	35.34	26.16	35.40	26.65	73.00[e] (93.00)[f]
NO_2	julolidine	34.51 (47.25)	24.24	12.96	7.50	26.12	11.37	42.06	33.30	16.72	11.62	96.00[e]
NO_2	COOMe	4.12 (4.01)	1.58	3.50	1.26	5.30	5.87	7.21	5.94	9.56	8.29	4.00[e]
NO_2	CHO	3.59	1.14	3.25	0.77	5.88	6.12	6.33	5.42	7.71	6.73	6.00[b]
Br	OMe	0.59	1.56	2.37	1.15	1.77	1.72	-	-	-	-	2.50[b]
2 OMe	2' NO_2	3.16 (5.58)	1.61	1.73	0.82	9.86	0.90	6.46	4.36	2.81	1.49	4.40[e]
3 OMe	2' NO_2	0.01 (0.13)	0.49	1.18	0.43	4.98	3.32	0.48	0.20	1.01	0.78	1.60[e]

Table IV: continued

X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.
		AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
		PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
4 OMe	2' NO_2	1.31 (2.71)	0.82	0.62	0.71	13.39	5.52	1.43	0.92	1.23	1.19	3.80[c]
2 OMe	3' NO_2	3.75 (7.36)	2.31	3.19	1.59	10.07	9.29	5.26	4.30	5.08	4.32	5.50[c]
3 OMe	3' NO_2	5.02 (5.74)	2.25	4.09	2.63	3.93	7.97	6.88	5.00	6.27	3.75	4.50[c]
4 OMe	3' NO_2	7.96	4.19	6.85	3.60	19.66	17.22	-	-	-	-	5.30[b]
2 OMe	4' NO_2	9.77 (19.42)	6.91	8.64	5.72	3.30	2.32	20.68	15.64	21.63	16.51	22.00[c]
3 OMe	4' NO_2	12.86 (19.51)	7.92	11.25	6.81	18.68	0.59?	20.90	15.61	21.27	16.14	21.00[c]
2 Br	4' NO_2	6.71 (10.38)	3.91	7.29	3.10	2.66	2.17	-	-	-	-	12.00[c]
3 Br	4' NO_2	7.46 (11.66)	3.57	7.67	2.92	4.40	2.89	-	-	-	-	14.00[c]

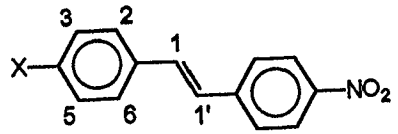
- experimental values measured in:

[a] neat [d] Acetone

[b] p-dioxane [e] CH_2Cl_2

[c] $CHCl_3$ [f] NMP

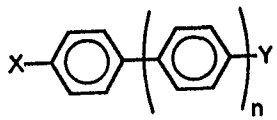
Table V: Calculated β vector components along the dipole moments ($\times 10^{-36}$ esu) for heteroaromatic and trisubstituted stilbenes

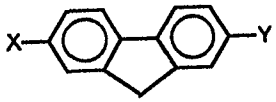


X	Substitution	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.[b]
		AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
		PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
H	1-aza	9.19	5.57	7.38	3.11	10.22	3.06	15.17	11.06	13.63	9.43	4.90
Me	1-aza	10.95	5.69	10.38	4.97	7.20	12.53	20.00	15.44	17.55	12.96	15.00
OMe	1-aza	13.95	8.46	12.54	7.16	20.87	8.91	23.80	18.98	25.83	20.87	14.00
OMe	1'-aza	13.73	8.94	13.83	8.38	1.95	1.43	13.14	9.27	13.50	10.10	6.60
NH_2	1,1'-azo	23.94	14.89	24.65	14.30	15.78	41.36	27.68	21.70	25.64	18.18	29.00
OMe	3-Me	18.17	11.51	15.99	9.98	17.07	13.81	28.18	20.89	28.68	21.30	26.00
OMe	3-OMe	19.60	13.21	12.16	7.45	5.00	21.30	27.68	21.22	25.53	18.29	23.00
OMe	3-F	16.09	10.09	13.96	8.30	8.26	7.59	25.01	18.24	25.76	18.84	18.00
OMe	2-OMe	15.16	9.99	14.50	9.57	32.32	12.90	24.52	18.23	27.52	21.35	32.00
OMe	1'-CN	14.11	7.25	10.92	4.88	15.50	10.10	15.77	9.76	14.57	8.02	21.00
Br	1'-CN	10.21	4.38	9.17	2.32	1.92	3.12	-	-	-	-	8.00
Br	1-aza 1'CN	11.84	5.29	1.42	0.53	2.58	0.58	-	-	-	-	2.10
OMe	2'-NO_2	18.91	9.55	11.72	6.90	34.36	18.30	24.68	15.13	23.28	13.42	22.00

[b] measured in p-dioxane

Table VI : Calculated β vector components along the dipole moments ($\times 10^{-36}$ esu) for 4,4'-substituted biphenyls, polyphenyls and fluorenes; numbers in parenthesis refer to SCRF calculations in chloroform.





X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.
		AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
		PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
H	H	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00[b]
CN	H	0.85	1.64	0.78	1.17	1.45	1.11	1.75	2.31	1.46	1.97	1.90[b]
$COCH_3$	H	2.10	1.43	1.76	0.93	3.99	2.99	2.61	2.11	2.14	1.72	2.00[b]
NO_2	H	4.75	2.77	3.39	1.96	2.28	1.75	9.35	6.13	9.25	5.86	4.10[b]
$SO_2C_6H_{12}OH$	NMe_2	12.87 (8.87)	6.73	10.61	5.60	15.30	4.45	4.01	2.69	3.31	1.60	13.00[c]
CN	OH	3.06	3.30	3.18	2.82	5.58	4.52	3.20	3.71	2.68	3.16	6.30[b]
$COCH_3$	OMe	5.23	3.23	4.25	2.39	6.74	5.34	4.67	4.00	3.74	3.20	4.90[b]
NO_2	Br	6.93	3.32	5.59	2.18	3.10	2.59	-	-	-	-	4.40[b]
NO_2	OH	7.00	3.98	5.28	3.12	3.12	2.51	11.97	8.07	11.82	7.63	7.70[b]
NO_2	OMe	7.96	4.39	5.86	3.34	3.18	2.66	12.72	8.58	12.42	8.06	9.20[b]
NO_2	NH_2	12.29 (19.03)	7.28	11.53	6.62	9.34	8.97	16.40	11.38	14.84	9.84	24.00[c] (24.00)[f]
NO_2	NMe_2	15.65 (23.80)	9.09	14.23	8.26	13.19	25.27	18.82	13.25	16.59	11.20	50.00[c]

Table VI: continued

X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.
		AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
		PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
NO_2 [1)]	NH_2	23.69	8.02	18.69	5.86	15.74	12.90	27.69	14.02	23.16	11.17	16.00[f]
NO_2 [2)]	NH_2	29.16	10.84	20.22	6.85	10.32	3.70	33.75	15.81	25.37	14.00	11.00[f]
NO_2 [3)]	OMe	19.92	6.18	15.91	4.42	20.57	15.43	-	-	-	-	11.00[b]
Fluorene												
H	H	0.37	0.31	0.34	0.35	0.43	0.44	0.65	0.73	0.63	0.70	0.00[b]
CN	H	0.99	1.58	1.06	1.01	3.76	3.56	2.65	3.35	2.52	3.20	3.00[b]
NO_2	H	4.90	2.63	4.12	2.32	6.38	6.11	11.29	8.47	11.84	8.96	5.10[b]
NO_2	Br	7.23	3.22	6.09	1.62	8.43	7.98	-	-	-	-	6.00[b]
NO_2	OMe	10.20	6.34	8.86	5.78	12.62	12.01	15.64	11.97	16.30	12.53	11.00[b]
NO_2	NMe_2	19.87 (36.29)	13.25	20.03	14.10	31.16	36.30	22.36	17.41	21.52	16.68	40.00[b] (55.00)[c]

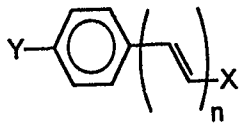
- experimental values measured in p-dioxane[b], $CHCl_3$ [c] and NMP f

[1)] n=2

[2)] n=3

[3)] n=2

VII: Calculated β vector components along the dipole moments ($\times 10^{-36}$ esu) for substituted styrenes and α-phenylpolyene; numbers in parenthesis refer to SCRF calculations, the solvent is chloroform.



n	X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.[a]
			AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
			PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
1	CN	OMe	2.62 (3.93)	2.32	2.94	2.32	6.01	5.03	3.55	4.23	3.59	4.20	7.00
1	CN	NMe_2	5.53 (10.21)	5.93	8.63	8.43	23.00	24.70	8.34	8.12	7.54	7.15	23.00
1	CHO	Br	3.11 (4.34)	0.57	2.57	0.28	4.72	3.87	-	-	-	-	6.50
1	CHO	NMe_2	10.95 (18.83)	7.51	12.43	8.94	25.48	23.49	10.44	9.30	8.64	7.73	30.00
1	COMe	OMe	3.62 (5.03)	2.36	3.26	2.25	3.03	1.49	5.30	4.55	4.77	4.04	8.90
1	NMe_2	NO_2	14.13 (24.19)	9.70	16.67	12.55	30.67	33.86	13.88	13.03	14.89	13.88	35.00
1	NO_2	NMe_2	13.87 (31.47)	10.20	15.74	12.25	7.35	32.74	15.85	15.13	15.13	14.26	50.00
1	NO_2	OH	5.04 (8.68)	3.35	3.81	3.04	4.51	2.85	8.70	8.48	9.48	9.22	18.00
1	NO_2	OMe	6.27 (10.43)	4.62	4.72	3.86	7.06	4.74	-	-	-	-	17.00

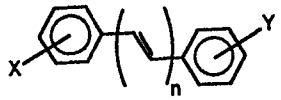
Table VII: continued

n	X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.°
			AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
			PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
2	CHO	OMe	6.68 (10.47)	5.36	5.99	4.69	8.80	3.62	11.97	11.66	10.59	10.33	28.00
3	CHO	OMe	9.58 (29.31)	7.00	8.40	5.77	37.45	7.47	20.28	19.20	17.76	16.78	42.00
2	CHO	NMe_2	17.14 (39.94)	12.58	20.26	12.58	46.18	39.67	18.05	16.54	14.90	13.41	52.00
3	CHO	NMe_2	21.87 (80.87)	17.45	20.47	16.27	70.46	57.56	27.21	25.82	22.09	20.78	88.00
1	$CHC(CN)_2$	OMe	7.89 (11.86)	8.87	8.65	9.03	6.47	10.60	9.73	11.98	9.66	11.64	32.00
1	$CHC(CN)_2$	NMe_2	17.25 (39.21)	17.92	19.77	19.10	22.95	67.59	17.11	13.38	14.72	16.69	82.00
2	$CHC(CN)_2$	NMe_2	26.79 (*)	24.88	26.52	24.61	113.41	100.96	31.39	33.41	27.14	28.80	163.00

° measured in $CHCl_3$

(*) Excitation energy is near half of the calculated absorption maxima, therefore the calculated β values are not printed (SOS problem)

Table VIII: Calculated β vector components along the dipole moments ($\times 10^{-36}$ esu) for disubstituted diphenylpolyene oligomers; numbers in parenthesis refer to SCRF calculations in chloroform.



n	X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.[a]
			AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
			PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
2	CN	OMe	13.46 (30.42)	7.05	14.17	6.88	34.63	2.10	20.77	16.40	19.77	15.25	27.00
3	CN	OMe	21.60 (23.13)	8.77	11.00	8.36	47.64	40.73	34.39	22.91	32.47	20.86	40.00
2	NO_2	Br	16.85 (25.43)	7.67	16.97	5.73	31.21	9.82	-	-	-	-	21.00
3	NO_2	Br	16.71 (11.24)	10.33	24.26	8.28	44.07	38.50	-	-	-	-	35.00
2	NO_2	OMe	23.78 (54.83)	13.88	21.37	11.93	5.44	4.46	36.54	30.77	36.86	30.71	47.00
3	NO_2	OMe	29.12 (*)	17.35	26.62	14.29	3.90	2.27	52.84	42.87	52.36	41.73	76.00
4	NO_2	OMe	40.72 (*)	22.08	36.21	17.81	99.26	80.83	68.35	55.39	65.95	52.86	101.00
2	NO_2	SMe	30.88 (*)	20.26	26.65	13.43	81.47	18.80	33.03	26.96	31.22	24.94	55.00

Table VIII: continued

n	X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.°
			AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
			PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
2	NO_2	NMe_2	34.64 (98.81)	22.87	36.74	23.27	94.74	88.57	48.39	38.55	48.41	38.77	107.00
3	NO_2	NMe_2	48.26 (*)	26.74	46.69	26.56	122.60	110.84	61.66	51.06	62.62	50.77	131.00
4	NO_2	NMe_2	55.72 (*)	30.77	52.60	29.70	151.05	130.96	79.13	64.52	76.84	62.79	190.00 (±50)
2	2'-CN	2-OMe	2.26 (4.60)	2.76	2.25	2.25	17.77	16.94	3.75	4.97	3.71	4.49	4.50
3	2'-CN	2-OMe	4.40 (*)	3.61	4.33	3.55	29.03	26.74	7.26	7.69	7.11	7.47	7.10
2	2'-CN	4-OMe	0.28 (0.07)	1.65	0.10	0.95	28.57	25.33	0.13	1.71	0.17	2.03	2.60
3	2'-CN	4-OMe	0.82 (10.63)	2.03	0.21	1.67	40.22	35.03	1.21	3.05	1.71	3.55	4.30
2	4'-CN	2-OMe	5.04 (14.21)	4.57	6.47	4.51	-	-	12.13	11.99	11.60	11.10	16.00
2	2'-NO_2	2-OMe	5.19 (10.99)	3.62	2.68	1.30	11.25	14.50	9.52	6.71	4.00	2.37	6.40
3	2'-NO_2	2-OMe	9.22 (*)	5.17	5.22	1.83	19.22	13.86	14.24	9.98	7.14	3.80	11.00

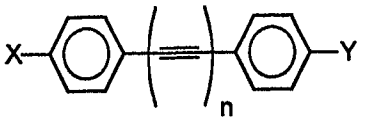
Table VIII: continued

n	X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.°
			AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
			PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
2	2'-NO_2	4-OMe	2.53 (4.82)	1.62	0.97	0.11	7.14	11.99	4.51	3.32	0.17	0.19	4.90
3	2'-NO_2	4-OMe	3.60 (*)	2.53	1.29	0.67	12.64	19.12	6.23	5.23	0.27	0.64	11.00
2	4'-NO_2	2-OMe	17.56 (*)	10.90	15.78	9.42	2.69	5.60	29.58	25.70	30.11	25.84	17.00
3	4'-NO_2	2-OMe	19.74 (61.26)	15.86	19.25	12.80	-	-	43.12	37.68	43.05	36.80	56.00

°Solvent $CHCl_3$

(*) Excitation energy is near half of the calculated absorption maxima, therefore the calculated β values are not printed (SOS problem)

Table IX: Calculated β components along the dipole moment for 4,4'-disubstituted tolans and diphenylpolyynes; numbers in parenthesis refer to SCRF calculations for chloroform.



n	X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.[a]
			AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
			PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
1	SO_2Me	NH_2	13.85 (*)	9.64	11.88	7.07	32.99	22.24	6.88	7.13	7.47	6.34	13.00
1	COOMe	SMe	13.73 (*)	8.77	7.43	3.70	13.23	13.45	8.03	3.79	5.31	1.89	8.00
1	COOMe	NH_2	13.44 (29.57)	9.19	10.91	6.93	33.65	23.14	14.23	13.48	11.46	10.81	15.00
1	COMe	SMe	12.71 (*)	7.52	7.37	3.41	17.31	13.94	7.40	3.65	6.06	2.42	9.80 (± 2)
1	COMe	NH_2	12.33 (27.64)	7.67	10.38	5.94	23.49	17.34	10.16	9.69	9.74	9.02	12.00
1	COPh	NH_2	20.34 (*)	9.40	18.54	8.31	30.39	9.80	15.40	9.10	11.42	5.80	19.00
1	CN	SMe	18.43 (*)	11.64	15.11	6.20	5.75	1.07	8.99	8.19	7.19	6.34	15.00
1	CN	NH_2	12.91 (27.83)	9.95	15.60	9.99	31.59	32.15	14.68	13.50	12.83	11.63	20.00
1	CN	NHMe	14.94 (34.99)	10.55	17.22	10.74	36.58	35.14	16.85	14.68	14.67	12.51	27.00

Table IX: continued

n	X	Y	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.[c]
			AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
			PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
1	CN	NMe_2	16.86 (37.80)	10.96	18.55	11.32	41.06	37.82	19.27	15.77	16.75	13.37	29.00
1	NO_2	OMe	14.58 (23.18)	8.73	11.73	7.54	8.41	7.67	27.57	18.99	28.04	18.77	14.00[b]
1	NO_2	SMe	23.45 (*)	14.06	16.34	8.85	13.38	6.26	24.32	16.93	23.07	15.13	20.00
1	NO_2	NH_2	20.79 (37.50)	12.03	20.19	12.12	20.72	41.53	33.83	24.07	28.39	19.19	24.00 (40)[f]
1	NO_2	NHMe	23.01 (42.78)	13.34	22.01	13.13	21.89	45.33	36.22	25.82	33.93	23.18	46.00
1	NO_2	NMe_2	24.90 (44.29)	14.26	23.18	13.77	25.97	48.66	38.56	27.32	35.68	24.28	46.00
2	CN	SMe	28.62 (*)	12.03	19.56	7.15	33.03	21.14	13.99	11.01	10.96	8.53	17.00 (± 2)
2	NO_2	SMe	38.26 (*)	15.09	23.05	9.39	39.12	25.63	28.25	22.98	25.54	20.45	17.00 (± 2)
3	NO_2	NH_2	35.72 (*)	14.19	28.42	12.48	25.16	48.85	37.93	31.44	34.13	27.77	28.00 (± 2)

° Solvent $CHCl_3$

(*) Excitation energy is near half of the calculated absorption maxima, therefore the calculated β values are not printed (SOS problem)

Table X: Calculated β vector components along the dipole moments ($\times 10^{-36}$ esu) on heteropentacyclic arene derivatives

Structure[1]	VAMP (PECI-SOS)				MOPAC (TDHF)		CNDO/S (SCI-SOS)				exptl.tl.[2]
	AM1		PM3		AM1	PM3	AM1 geometry		PM3-geometry		
	PECI=8	PECI=20	PECI=8	PECI=20			CI= 4 4	CI=10 10	CI= 4 4	CI=10 10	
4	24.22	17.75	20.27	17.57	63.04	54.86	30.76	26.72	29.56	25.32	83.00
5	33.88	22.79	41.77	25.21	79.39	81.54	41.21	36.62	39.16	34.56	98.00
6	31.77	23.19	25.08	21.33	91.66	75.80	42.27	37.65	39.95	34.84	113.00
7	20.44	11.39	18.93	10.18	20.85	20.32	33.41	27.46	34.18	27.94	40.00

[1] Structures **4** - **7** are shown in scheme 1

[2] Unknown solvent