Use of Dipole Moment as a Parameter in Drug–Receptor Interaction and Quantitative Structure–Activity Relationship Studies

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Abstract □ The theoretical basis for using dipole moment as a free-energy related parameter in studying drug–receptor interaction and quantitative structure–activity relationship (QSAR) is presented. Over 300 group dipole moments for aromatic substituents were compiled using the dipole moments of monosubstituted benzene derivatives. Examples in the literature of using dipole moment in QSAR studies are also presented.

Keyphrases □ Dipole moment—parameter in drug–receptor interaction and quantitative structure–activity relationships, list of 300 for aromatic substituents □ Quantitative structure–activity relationships—dipole moment as a parameter, 300 dipole moments listed for aromatic substituents □ Drug–receptor interaction—dipole moment as a parameter, list of 300 dipole moments for aromatic substituents

It is generally accepted that most interactions between drugs and receptors are physicochemical processes. When an equilibrium between a drug–receptor complex (DR), a free drug (D), and unoccupied receptor (R) is established, the reversible process can be expressed as:

$$D + R \underset{k_2}{\overset{k_1}{\rightleftharpoons}} DR \qquad \text{(Eq. 1)}$$

Under equilibrium conditions the following holds:

$$\log K = -\Delta G°/2.303RT \qquad \text{(Eq. 2)}$$

where $K = (k_1/k_2)$ is the association constant of the complex DR, $\Delta G°$ is the change in standard free energy during the formation of DR, T is the absolute temperature, and R is the gas constant.

The ability of each member of a series of drugs to bind to the receptor is dependent on the difference in the standard free energy change ($\Delta G°$) under the same condition. Factors contributing to this variation in $\Delta G°$ can be divided into three major categories: lipophilic, electronic, and steric.

THEORETICAL

Based on linear free-energy relationships, Hansch and Fujita (1, 2) developed a general model to quantitatively describe the relationships between biological activities and molecular structures:

$$\log (1/C) = -a\pi^2 + b\pi + \rho\sigma + dE_s + c \qquad \text{(Eq. 3)}$$

where $\log (1/C)$ is the negative logarithm of the concentration or dosage of a drug producing a standard biological response, π is the hydrophobic constant of the substituent, σ is the Hammett substituent, and E_s is the steric constant.

This model was later extended to include differences in degree of ionization, molecular size, and dipole moment, as well as branching (3–5):

$$\log \text{biological response} = -a(\log P)^2 + b \log P + c\,(\text{pKa} - \text{pH}) + d \log MW + e\,\mu + f\,\chi + g \qquad \text{(Eq. 4)}$$

where pKa − pH equals the log (undissociated/dissociated) for acids, μ is the dipole moment, and χ is the branching or other steric factors.

The electronic effects in drug–receptor interactions are represented by the electric dipole moment, μ.

All forces between atoms or drug molecules and receptors or biomacromolecules are electrostatic in origin. Several types of noncovalent interactions between drugs and receptors can be described as interactions between charges (long-range force), between charge and a dipole, and between dipoles (short-range forces).

The potential energy of interaction of two oppositely charged ions relative to the magnitudes of the charges q_1 and q_2 and the distance between them r, is given by Coulomb's law:

$$E = \frac{-q_1 q_2}{Dr} \qquad \text{(Eq. 5)}$$

where D is the dielectric constant through which the charges interact. The energy of interactions between charges and receptors is much larger than that of noncharged electronic effects, hydrophobic effects, and others. A charged species also has quite different transport properties than a noncharged species. Therefore, the ionic member in a series of compounds often does not fit the regression line obtained from the series of noncharged compounds and is usually excluded from the series in quantitative structure–activity relationship (QSAR) analysis.

The energy of interaction between an ion and a dipole is given by the following (6):

$$E = \frac{-N_a e\,\mu\cos\theta}{D(r^2 - d^2)} \qquad \text{(Eq. 6)}$$

where N_a is Avogadro's number, e is the magnitude of the charge, θ is the angle between the line joining the charge and the middle of the dipole and the line between the ends of the dipole, D is the dielectric constant, r is the distance between the charge and the middle of the dipole, and d is the length of the dipole. It is obvious from this equation that the extent to which an ion and a dipole interact is related to the dipole orientation.

The energy of interaction between two dipoles in the most favorable alignment is given by:

$$E = \frac{-2\mu_a\mu_b}{Dr^3} \qquad \text{(Eq. 7)}$$

where μ_a and μ_b stand for the dipole moments (6):

The average interaction for all orientations is given by:

$$E = \frac{-2\mu_a^2\mu_b^2}{3\,KTDr^6} \qquad \text{(Eq. 8)}$$

The energy of dipole-induced dipole interactions (Debye forces) is:

$$E = \frac{-\mu_a^2\alpha_b + \mu_b^2\alpha_a}{D^2r^6} \qquad \text{(Eq. 9)}$$

where α_a and α_b are the polarizabilities.

The dispersion interactions (London forces) are governed by:

$$E = \frac{-3\alpha_a\alpha_b[I_aI_b/(I_a + I_b)]}{2r^6} \qquad \text{(Eq. 10)}$$

where I_a and I_b stand for the ionization potentials.

Note that the dipole–dipole (Keesom) interactions are not only dependent on the orientation of the dipoles but also inversely proportional to the third power of distance (Eq. 7) or the sixth power of distance for all orientations (Eq. 8).

In QSAR studies it it assumed that the receptor remains unchanged; therefore, only the properties of the drug molecule need to be considered (μ_a, α_a, I_a, *etc.*).

In most of the published QSAR studies, the electronic parameters most commonly used are the Hammett σ constant and Taft polar constant σ^*. The Hammett σ constants result from the comparison of the pKa of a series of substituted benzoic acids to that of benzoic acid. They describe the magnitude of electronic effects of substituents on the reactive center attached to the benzene ring, *i.e.*, the dissociation constants of substituted

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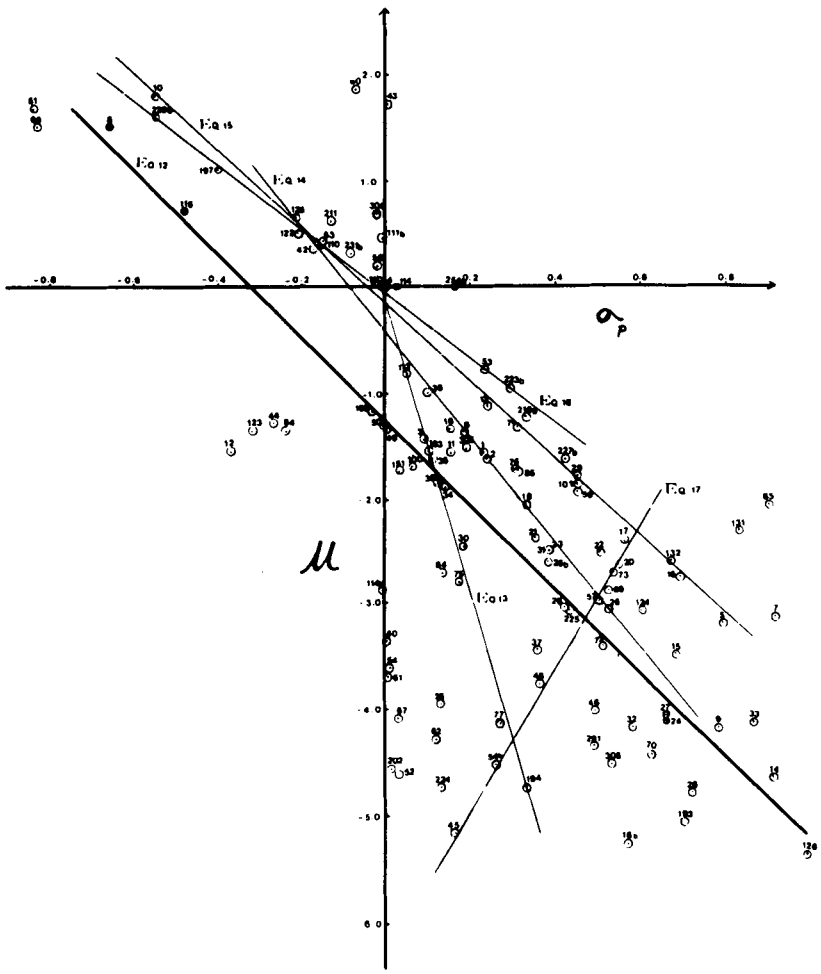


Figure 1—*A plot of* μ versus σ_p. *Note the scattering of the points, and the quite different slopes and intercepts for equations derived from various subsets.*

benzoic acids. In other words, σ constants are a measurement of substituent electronic effects on the reactivity of other parts of the same molecule. It is known that in using σ constants, the orientation and the rate or equilibrium of reactions can be predicted when aromatic compounds are substituted by various functional groups.

If interactions between drugs and receptors are controlled by the electronic nature of the substituents on the benzene ring, σ constants are suitable descriptors of electronic effects for QSAR analysis. However, not all the electronic effects of a series of drugs in drug–receptor complexes work by varying the electronic properties of another reactive center. Different substituents in a series of drugs may directly interact with receptors, *i.e.*, *via* charge–dipole, dipole–dipole, dipole–induced dipole, and induced dipole–induced dipole interactions between the substituent of a drug and a part of receptor. These interactions could affect the binding force of the drug with the receptor. Therefore, dipole moments, which are the quantitative measurements of separation of charge, should be useful in describing direct drug–receptor interactions through noncovalent bonding.

Group dipole moments of substituents are thermodynamically linear free-energy related functions. They are vectors with additive and constitutive properties. For congeneric series of compounds, dipole moments have been frequently found to correlate well with σ or other linear free-energy related parameters. For example, the dipole moments of substituted anilines have been correlated with the melting points, N–H stretching frequency in infrared spectra, as well as σ_p constants (7). Colinese *et al.*, also have found linear correlation between the dipole moments and $\nu_{(O-H)}$ of a series of 4′-substituted-4-hydroxyazobenzenes (8). It was also reported that for *N*-(4-substituted benzylidene)-4-hydroxyanilines that $\nu_{(O-H)}$ and $\mu_{(O-H)}$ are linearly related to Hammett's σ constant (9). A linear relationship between $\mu_{(O-H)}$ and the relative frequency shift ($\Delta\nu$) in dioxane has been used as an evidence of the dependence of $\mu_{(O-H)}$ on the strength of hydrogen bonding (9). Van Beek (10) also reported some linear relationships between dipole moments and σ constants in a few disubstituted benzene systems. Apparent correlation has also been reported between the N–H chemical shift and the dipole moment of lactams and thiolactams (11).

Despite successful correlation within limited series, the correlation between μ and σ may vary drastically or fail completely if noncongeneric groups are lumped together (Figs. 1 and 2).

Since Hammett's substituent constants (σ) are more readily available for a wide variety of substituents (12, 13) than dipole moments, the use of dipole moments in QSAR has only been reported by a few groups in spite of the direct relationship with interaction energy. The present report reviews the reported cases of QSAR using dipole moment as an independent electronic parameter, and compiles a table of group dipole moments for future use.

Method—More than 300 group dipole moments were collected (Appendix I), most of which were taken from McClellan's book (14). The magnitudes of the group dipole moments of substituents are equal to those of the corresponding monosubstituted benzene. The sign is taken by comparison of the electronegativities between the substituent and the aromatic carbon to which the group is connected. A negative sign stands for a negative end pointing away from the benzene ring.

A total of 114 substituent groups (for which both μ and σ are available) were analyzed to examine the interrelationship between μ and σ. Hammett's σ constants were taken from Hansch and Leo's book (13). All the regression lines were derived by computer[1] *via* the method of nonweighted least-squares fit.

RESULTS AND DISCUSSION

The overall correlations between Hammett σ constants and the group dipole moments of 114 substituents are shown in Eqs. 11 and 12:

$$\mu = -5.99\,\sigma_m - 0.53 \qquad \text{(Eq. 11)}$$
$$n = 114,\ r = 0.749,\ s = 1.279$$

[1] IBM 370/185 computer.

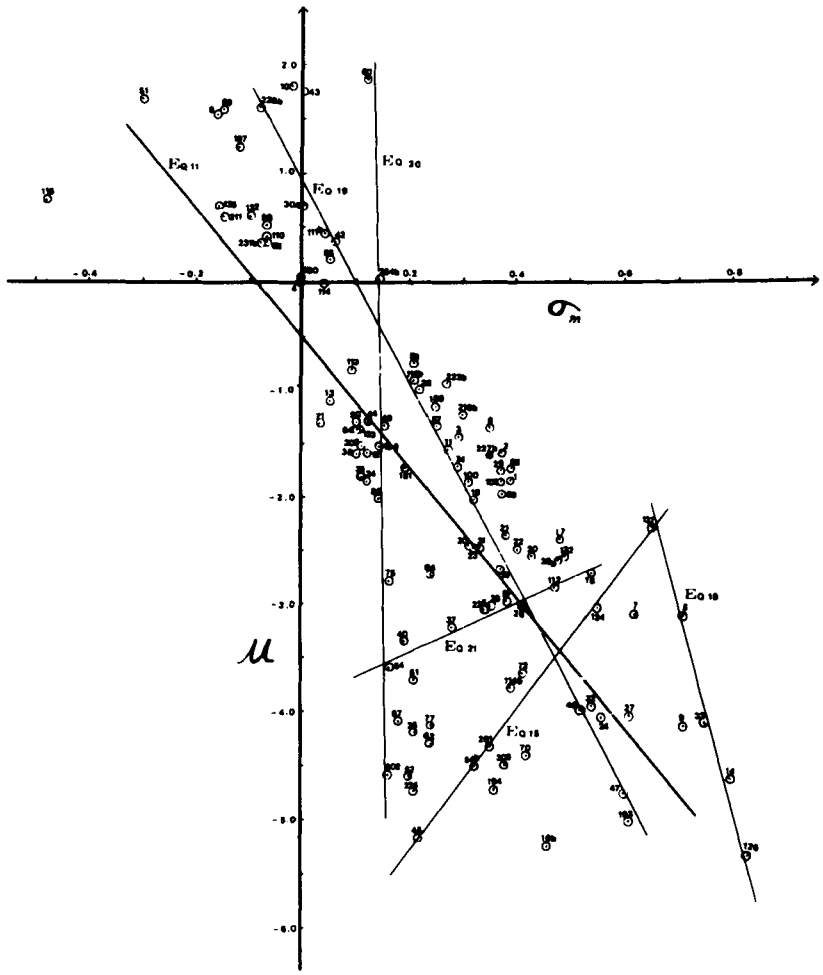


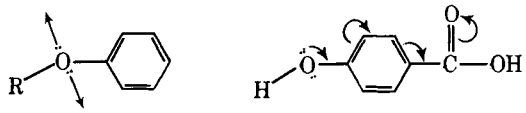
Figure 2—*A plot of* μ versus σ_m. *Note the scattering of the points, and the quite different slopes and intercepts for equations derived from various subsets.*

$$\mu = -3.65\,\sigma_p - 1.27$$
$$n = 114, r = 0.706, s = 1.367 \qquad \text{(Eq. 12)}$$

where μ is the group dipole moment of the substituent, and σ_m and σ_p are *meta*- and *para*-substituent constants, respectively.

Equations 11 and 12 indicate that the correlations between σ constants and dipole moments are not very good, and only 56 and 50%, respectively, ($r^2 \times 100$) of the variance in the data can be explained by these equations. In other words, about half of the variance in the data cannot be accounted for by these linear relationships. Comparison of Eqs. 11 and 12 shows that the correlation between σ_m and μ is better than that of σ_p and μ. This is probably due to the delocalization of π electrons between *para*-substituents and the benzene ring. The σ_m value is mainly a measure of inductive effect of the substituent and hence is more comparable to the group dipole moment.

The signs of the dipole moments of hydroxy and alkoxy groups are negative, *i.e.*, the oxygen atom is at the negative end of the dipoles in phenol and alkoxybenzene molecules. This can be explained in terms of the high electronegativity of oxygen in spite of the resonance effect in benzoic acid:



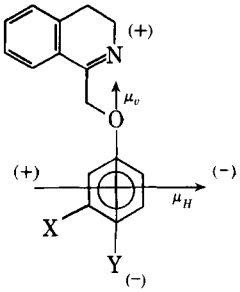
By dividing 11 substituents into subgroups graphically, there are quite different equations correlating dipole moments and σ constants as shown in Table I. In each subgroup no distinct structural relationship is found. The slopes range from −161 to +6.62, while the intercept ranges from +17.46 to −6.63.

Table I—Correlations Between Group Dipole Moment and σ Constants for Selected Subgroups from Table I, Showing Different Slopes and Intercepts [a]

	n	*r*	*SD*	*Equation*
$\mu = -6.82\,\sigma_p - 0.05$	13	0.965	0.459	(13)
$\mu = -4.83\,\sigma_p - 0.49$	15	0.999	0.079	(14)
$\mu = -3.68\,\sigma_p - 0.18$	14	0.999	0.065	(15)
$\mu = -2.99\,\sigma_p - 0.06$	10	0.999	0.036	(16)
$\mu = 6.42\,\sigma_p - 6.16$	8	0.995	0.097	(17)
$\mu = -16.52\,\sigma_m + 8.48$	5	0.994	0.147	(18)
$\mu = -8.57\,\sigma_m + 0.42$	14	0.954	0.603	(19)
$\mu = -161\,\sigma_m + 17.46$	8	0.910	0.909	(20)
$\mu = 2.20\,\sigma_m - 3.87$	9	0.946	0.099	(21)
$\mu = 6.62\,\sigma_m - 6.63$	5	0.999	0.041	(22)

[a] n = number of data points; r = correlation coefficient; and SD = standard deviation.

Although the application of dipole moment in QSAR is not as common as that of σ constants, in some cases it can play an important role in drug–receptor interactions. For example, Tute's results (15) on the inhibition of viral neuraminidase by 1-phenoxymethyl-3,4-dihydroquinolidines was reexamined. Using group dipole moment values instead of the components along the vertical axis μ_v, Eq. 23 was derived, which is slightly better than Tute's result using μ_v (Eq. 24):



$$\log 1/C = 0.258\pi + 0.094\mu + 0.034\mu^2 + 2.596$$
$$n = 16, r = 0.956, s = 0.062 \qquad \text{(Eq. 23)}$$

Table II—Examples of the Application of Dipole Moment and Polarizability in QSAR [a]

Compounds	Biological Activity and Correlations Reported	Reference
1-Decylnipecotamides	Chlorinesterase inhibition. Inhibitory activity parallels the increase in dipole moment	16
Local anesthetics	Minimum blocking concentration (MBC) is a function of polarizability and ionization potential I_p $\log MBC = -a\alpha I_p + b$	17
Chloramphenicol analogs	Antimicrobial activity is a function of electronic polarization (P_e) $k_I = 2.76\,P_e - 6.55$ $n = 10, r = 0.991$	18
Cyclic ureas and thioureas	Respiratory stimulant activity is dependent on the dipole moment of three series of the compounds, while the acute lethal toxicity is a function of molecular weight	19
1-Decyl-3-carbamoylpiperidines	Butyrylcholinesterase $pI_{50} = -0.058\pi^2 + 0.923\pi - 0.456\mu + 5.589$ $n = 6, r^2 = 0.998$ (more data needed)	20
Anticonvulsants	Antielectroshock in mice $\log 1/C = 0.720 \log P - 0.396\mu + 3.144$ $n = 11, r = 0.967, SD = 0.189$	21
Sulfonamides	Antimicrobial activity measured as minimum inhibitory concentration (MIC) $\log 1/MIC = -0.11\ pKa + 0.041\mu^2 + 5.31$ $n = 10, r^2 = 0.91, SD = 0.18$	22
Nitroanilines	Sweetening potency $\log$ relative sweetness $= 1.31\pi - 1.08\sigma_0 + 0.45\mu^2 + 0.052(\alpha_R - \alpha_H) + 1.66$ $n = 9, r^2 = 0.976, SD = 0.149$ (too many parameters for too few data points)	22
Miscellaneous anticonvulsants	Antielectroshock activity $\log 1/C = -0.222(\log P)^2 + 1.153 \log P - 0.368\mu + 2.994$ $n = 18, r = 0.092, SD = 0.24$	23
Barbiturates, hydantoins, and imides	Antipentylenetetrazol seizures $\log 1/C = -0.123(\log P)^2 + 0.588 \log P - 0.597\mu + 0.825$ $n = 10, r = 0.99, SD = 0.12$	23
	Acute lethal toxicity $\log 1/C = -0.226(\log P)^2 + 0.800 \log P - 0.361\mu + 0.175$ $n = 10, r = 0.99, SD = 0.11$	2
Convulsants (lactams, thiolactams, ureas, and thioureas)	Acute lethal toxicity $\log 1/C = -0.364(\log P)^2 + 1.005 \log P + 0.247\mu + 1.298$ $n = 20, r = 0.89, SD = 0.24$	23
7-Substituted-1,4-benzodiazepinones	Antipentylenetetrazol seizures $\log 1/C = -0.301(\log P)^2 + 0.852 \log P - 0.629\mu + 4.139$ $n = 12, r = 0.915, SD = 0.227$	24
	Rotorod Ataxia log 1/C = 15.939 log Molecular Weight − 0.972 log P + 0.549μ − 33.187 $n = 16, r = 0.933, SD = 0.388$	24
Carbamates and aromatic compounds	Acetylcholinesterase inhibition $\log 1/K_d = -1.340 \log MR - 2.340\Sigma\pi + 2.404\Sigma\sigma - 0.478\,D + 0.338\mu + 4.818$ $n = 32, r = 0.945, SD = 0.594$	25
Quaternary ammonium compounds	Affinity for Acetylcholine Receptors $\log K = 0.784\pi_R - 0.353\,(\pi^{\oplus}_{-N\equiv})^2 - 0.171\,\pi^{\oplus}_{-N\equiv} + 0.736\mu_R + 2.309\,n_{OH} + 2.173$ $n = 128, r = 0.961, SD = 0.441$	26
N–$SCCl_3$ containing fungicides	Inhibition of spore germination *versus Stemphylium sarcinaeforme* $\log 1/C = -0.314\,(\log P)^2 + 2.385 \log P + 0.683\mu - 1.666$ $n = 14, r = 0.951, SD = 0.411$	27

[a] n = number of data points used in the regression, r = correlation coefficient, SD = standard deviation.

$$\log 1/C = 0.271\pi + 0.062\mu_v + 0.030\mu_v^2 + 2.552 \quad n = 16, r = 0.937, s = 0.074 \qquad \text{(Eq. 24)}$$

It seems that the substituent effect in the drug–receptor interaction depends more directly on the separation of charge μ than on the electronic distribution of the benzene ring (σ). Although the difference in the regressions obtained is small, this example illustrates the usefulness of the aromatic group dipole moment in QSAR.

Other examples of QSAR using dipole moment as an independent variable are shown in Table II. The examples presented and the theoretical relationships between dipole moment and intermolecular interaction energies with receptors, strongly suggest that dipole moment may be a parameter worth considering in QSAR, especially if σ or other electronic parameters fail to give meaningful correlation.

McFarland (22) has reported that in some cases μ^2 gives better correlation than μ; this may be due to the relatively narrow range of μ examined. When μ^2 is used, a wider range of values and a better correlation are obtained. Another report (28) found high degrees of intercorrelation between log molar refraction ($MR = P_e$) and log molar volume (MV), and between log molar refraction and log molecular mass (M):

$$\log MR = -0.290 + 0.981 \log MV \quad n = 213, r = 0.943, s = 0.086 \qquad \text{(Eq. 25)}$$

$$\log MR = -0.358 + 0.884 \log M \quad n = 213, r = 0.917, s = 0.104 \qquad \text{(Eq. 26)}$$

This is easily understandable from the following equations:

$$MR = \frac{n^2 - 1}{n^2 + 2}\frac{M}{d} \qquad \text{(Eq. 27)}$$

$$MV = \frac{M}{d} \qquad \text{(Eq. 28)}$$

The only substituent groups which will not fit Eqs. 27 and 28 are the ones with unusually high densities (d), such as heavy metals and polyhalogenated groups (28).

Furthermore, because of the interrelationship between MR (P_e) (29) and α, one would also expect similar relationship between α and M:

$$MR = P_e, P_e = (4/3)\pi N_a \alpha \qquad \text{(Eq. 29)}$$

where N_a is Avogadro's number.

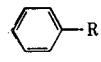
It was recently reported (25) that charge-transfer effects of various carbamates and aromatic compounds can be separated into steric, electronic (μ and σ), and indicator variables (the number of lone pair electrons). They have also shown that the binding of these acetylcholinesterase inhibitors to the enzyme is well correlated with substituent constants like log MR, $\Sigma\pi$, $\Sigma\sigma$, and D (indicator variable, Table II).

The affinity constants of 128 quarternary ammonium compounds were correlated linearly with the hydrophobicity constant of the side chain (π_R), the dipole moment (μ_R), and the number of hydroxy group (n_{OH}). The dependence on the hydrophobicity constant of the quaternary ammonium head (π-$^{+}_{N\equiv}$) is parabolic (26).

The dipole moment of the heterocyclic ring bearing N-$SCCl_3$ group has also been shown to be important in determining the antifungal activity of these fungicides (27). This is true in the spore germination test against a single organism *S. sarcinaeforme* in QSAR as well as in a test using mixed organisms. In the latter case, discriminant analysis has indicated the important roles of both μ and log P (27).

It is hoped that the compilation of Table I will make it easier for medicinal chemists to use dipole moment as an independent electronic parameter in future QSAR work.

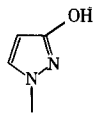
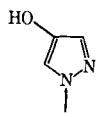
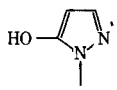
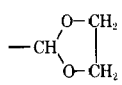
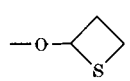
Appendix I—Aromatic Group Dipole Moments [a]



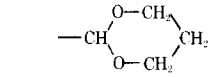
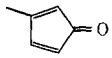
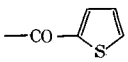
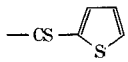
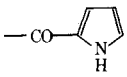
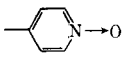
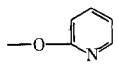
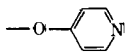
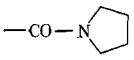
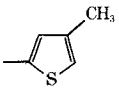
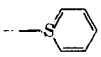
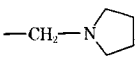
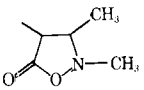
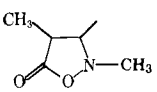
No.	Formula	R	μ_R (Debye)	WLN[b]	Solvent[c]	Temperature, °C
1	Br	—Br	−1.57	*E	cHx	20
2	Cl	—Cl	−1.59	*G	B	25
3	F	—F	−1.43	*F	B	30
4	H	—H	0.03	*H	L	25
5	$GeCl_3$	—$GeCl_3$	−3.15	*-GE-GGG	B	25
6	I	—I	−1.36	*I	B	30
7	NO	—NO	−3.09[d]	*NO	B	25
8	NH_2	—NH_2	1.53	*Z	B	25
9	NO_2	—NO_2	−4.13	*NW	B	25
10	N_2H_3	—$NHNH_2$	1.80	*MZ	D	25
11	N_3	—N=N=N	−1.56	*NNN	B	25
12	OH	—OH	−1.59	*Q	B	25
13	PH_2	—PH_2	−1.11	*PHH	Hx	20
14	SFO_2	—SO_2F	−4.59	*SWF	B	25
15	SF_5	—SF_5	−3.44	*SFFFFF	B	25
16	SH	—SH	−1.33	*SH	D	25
17	$SiCl_3$	—$SiCl_3$	−2.40	*-SI-GGG	B	25
18	SiF_3	—SiF_3	−2.72	*-SI-FFF	B	25
19	CCl_3	—CCl_3	−2.03	*XGGG	CCl_4	25
20	CF_3	—CF_3	−2.61	*XFFF	B	25
21	CF_3O	—OCF_3	−2.36	*OXFFF	B	25
22	CF_3S	—SCF_3	−2.50	*SXFFF	B	ns
23	CF_3Se	—$SeCF_3$	−2.48	*-SE-XFFF	B	ns
24	CN	—CN	−4.08	*CN	D	35
25	CNO	—N=C=O	−3.93	*NCO	B	20
26a	CNS	—SCN	−3.01	*SCN	B	25
26b	CNS	—NCS	−2.91	*NCS	B	20
27	CNSe	—SeCN	−4.01	*-SE-CN	B	25
28	CHO	—CHO	−3.02	*VH	B	25
29	CHO_2	—COOH	−1.30	*VQ	B	25
30	CHF_2O	—$OCHF_2$	−2.46	*OYFF	B	25
31	CHF_2S	—$SCHF_2$	−2.48	*SYFF	B	25
32	CHF_2OS	—$SOCHF_2$	−3.93	*SO&YFF	B	25
33	CHF_2O_2S	—SO_2CHF_2	−4.08	*SWYFF	B	25
34	CH_2Br	—CH_2Br	−1.87	*1E	B	25
35	CH_2Cl	—CH_2Cl	−1.83	*1G	B	20
36	CH_2I	—CH_2I	−1.60	*1I	CCl_4	25
37	CH_2NO	—$CONH_2$	−3.42	*VZ	B	25
38	CH_2NO	—CH=NOH(*trans*)	−0.87	*1UNQ-T	B	25
39	CH_2NO	—CH=NOH(*cis*)	−0.85	*1UNQ-C	B	25
40	CH_2NO	—NHCHO	−3.35	*MVH	CCl_4	ns
41	CH_2NO_2	—CH_2ONO	−2.10	*1ONO	ns	ns
42	CH_3	—CH_3	0.36	*1	B	25
43	CH_3O	—CH_2OH	1.73	*1Q	B	25
44	CH_3O	—OCH_3	−1.30	*O1	B	25
45	CH_3NS	—$NHCSNH_2$	−5.16	*MYZUS	D	25
46	CH_3OS	—$SOCH_3$	−3.98	*SO&1	B	20
47	CH_3O_2S	—SO_2CH_3	−4.75	*SW1	B	25
48	CH_3O_3S	—OSO_2CH_3	−3.77	*OSW1	B	25
49	CH_3S	—SCH_3	−1.34	*S1	B	ns
50	CH_3Se	—$SeCH_3$	−1.31	*-SE-1	ns	ns
51	CH_4N	—$NHCH_3$	1.69	*M1	B	25
52	CH_4NSO_2	—$NHSO_2CH_3$	−4.60	*MSW1	D	30
53	C_2H	—C≡CH	−0.77	*1UU1	B	25
54	C_2H_2N	—CH_2CN	−3.60	*1CN	D	25
55	$C_2H_2N_2O_2$		−6.63	*AT5NNVOJ	B	30
56	C_2H_3	—CH=CH_2	0.20	*1U1	B	25
57	C_2H_3O	—$COCH_3$	−2.90	*V1	B	25
58	$C_2H_3O_2$	—$OCOCH_3$	−1.72	*OV1	B	25
59	$C_2H_3O_2$	—$COOCH_3$	−1.92	*VO1	B	25
60	$C_2H_3O_2$	—CH_2COOH	1.86	*IVQ	D	25
61	C_2H_4NO	—$NHCOCH_3$	−3.65	*MV1	B	25
62	C_2H_4NS	—$NHCSCH_3$	−4.28	*MYUS	B	25
63	C_2H_5	—CH_2CH_3	0.39	*2	cHx	25
64	C_2H_5O	—OC_2H_5	−1.38	*O2	B	25
65	$C_2H_5O_2S$	—$SO_2C_2H_5$	−3.48	*SW2	B	25
66	$C_2H_5O_3S$	—$SO_3C_2H_5$	−4.99	*SW02	D	25
67	C_2H_5S	—CH_2SCH_3	1.46	*1S1	D	25
68	C_2H_5S	—SC_2H_5	−4.08	*S2	B	25
69	C_2H_6N	—$N(CH_3)_2$	1.61	*N1&1	B	25
70	C_2H_6OP	—$PO(CH_3)_2$	−4.39	*PO&1&1	B	20
71	C_2H_6P	—$P(CH_3)_2$	−1.31	*P1&1	B	20
72	C_3F_3	—C≡CCF_3	−3.38	*1UU1XFFF	B	ns
73	C_3F_7	—$CF(CF_3)_2$	−2.68	*XFXFFFXFFF	B	25
74	C_3HF_6O	—$C(OH)(CF_3)_2$	−1.71	*XQXFFFXFFF	L	25

continued

Appendix I—*Continued*

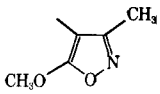
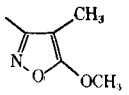
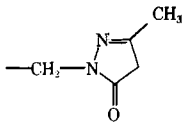
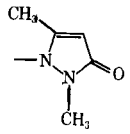
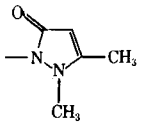
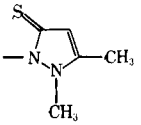
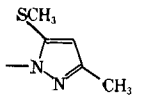
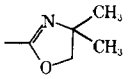
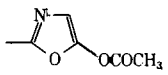
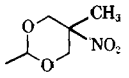
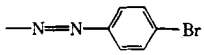
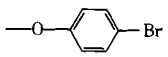
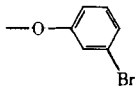
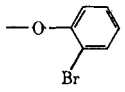
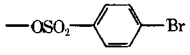
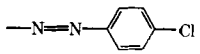
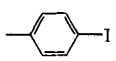
No.	Formula	R	μ_R (Debye)	WLN[b]	Solvent[c]	Temperature, °C
75	$C_3H_2F_3$	—CH=CHCF$_3$	−2.79	*1U1XFFF	B	ns
76	$C_3H_2F_3$	—C(CF$_3$)=CH$_2$	−2.25	*YU1&XFFF	B	20
77	C_3H_2N	—CH=CHCN(*trans*)	−4.12	*1U1CN -T	B	20
78	C_3H_2N	—CH=CHCN(*cis*)	−3.54	*1U1CN -C	B	20
79	C_3H_2NS		−1.21	*BT5N CSJ	CCl_4	20
80	C_3H_2NS		−1.33	*ET5N CSJ	CCl_4	20
81	C_3H_2NS		−1.89	*DT5N CSJ	CCl_4	20
82	$C_3H_2O_2$	—COCH$_2$CO—	−2.73	*V1V*	D	25
83	$C_3H_2O_2$	—OCOCH=CH—	−4.63	*OV1U1*	D	25
84	C_3H_3O	—CH=CHCHO	−2.71	*1U1VH	B	25
85	$C_3H_3O_2$	—CH=CHCOOH	−2.04	*1U1VQ	B	ns
86	$C_3H_3O_2$	—COCOCH$_3$	−2.44	*VV1	B	25
87	$C_3H_3N_2$		3.14	*AT5N CNJ	B	25
88	$C_3H_3N_2$		2.00	*AT5NNJ	B	25
89	$C_3H_3N_2$		2.26	*CT5MNJ	B	25
90	$C_3H_3N_2O$		2.18	*AT5NNJ CQ	D	25
91	$C_3H_3N_2O$		2.43	*AT5NNJ DQ	D	25
92	$C_3H_3N_2O$		3.41	*AT5NNJ EQ	D	25
93	C_3H_3Se	—SeC≡CCH$_3$	−1.31	*-SE-1UU2	B	25
94	$C_3H_3O_2Se$	—SeCH=CHCOOH(*trans*)	−2.27	*SE-1U1VQ -T	B	25
95	$C_3H_3O_2Se$	—SeCH=CHCOOH(*cis*)	−1.69	*-SE-1U1VQ -C	B	25
96	C_3H_4	—CH=CHCH$_2$—	0.62	*1U2*	B	25
97	$C_3H_4O_2$	—CH$_2$CH$_2$COO—	−3.85	*2VO*	B	25
98	C_3H_5		0.51	*AL3TJ	B	25
99	C_3H_5O	—COC$_2$H$_5$	−2.90	*V2	B	30
100	$C_3H_5O_2$	—CH$_2$OCOCH$_3$	−1.68	*1OV1	L	25
101	$C_3H_5O_2$	—COOC$_2$H$_5$	−1.85	*VO2	B	25
102	$C_3H_5O_2$	—CH$_2$COOCH$_3$	−1.81	*1VO1	B	24
103	$C_3H_5O_2$		1.97[e]	*BT5O COTJ	B	20
104	C_3H_5OS		1.30	*O- CT4STJ	ns	ns
105	C_3H_5OS	—COSC$_2$H$_5$	−1.55	*VS2	B	25
106	C_3H_5OS	—CSOC$_2$H$_5$	−2.24	*YUS&O2	B	25
107	C_3H_6	—CH$_2$CH$_2$CH$_2$—	0.55	*3*	cHx	25
108	C_3H_6	—C(CH$_3$)=CH$_2$	0.77	*YU1	B	25
109	C_3H_6NO	—N(CH$_3$)COCH$_3$	−3.60	*N1&V1	B	25
110	C_3H_7	—CH(CH$_3$)$_2$	0.40	*Y	cHx	25
111	$C_3H_7O_2$	—CH(OCH$_3$)$_2$	1.06[e]	*Y01&01	B	20
112	C_4F_9	—(CF$_2$)$_3$CF$_3$	−2.86	*/XFF/4F	B	25
113	C_4H_3S		0.81	*BT5SJ	B	25

Appendix I—*Continued*

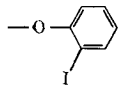
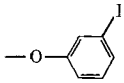
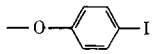
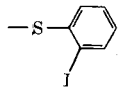
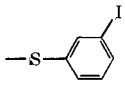
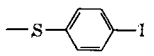
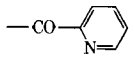
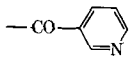
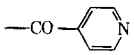
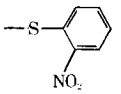
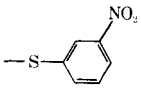
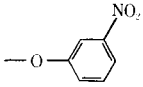
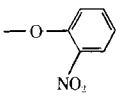
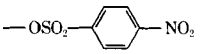
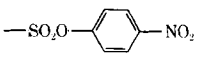
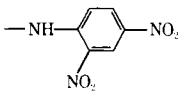
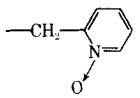
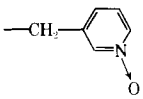
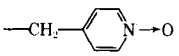
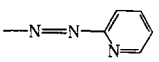
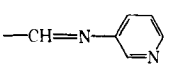
No.	Formula	R	μ_R (Debye)	WLN[b]	Solvent[c]	Temperature, °C
114a	C_4H_4	—(CH)$_4$—	0.00	*R A*B*	B	25
114b	C_4H_5O	—CH=CHCOCH$_3$	−2.89	*1U1V1	B	25
115	C_4H_8	—(CH$_2$)$_4$—	0.73	*4*	B	25
116	$C_4H_7O_2$	—CH$_2$OCOC$_2$H$_5$	−1.80	*1OV2	L	28
117	$C_4H_7O_2$	—CH$_2$COOC$_2$H$_5$	−1.85	*1VO$_2$	B	24
118	$C_4H_7O_2$	—COOCH(CH$_3$)$_2$	−1.82	*VOY	B	25
119	$C_4H_7O_2$	—CH$_2$CH$_2$OCOCH$_3$	−1.86	*2OV1	B	25
120	$C_4H_7O_2$	—CH=CHCOOCH$_3$	−2.13	*1U1VO1	B	30
121	$C_4H_7O_2$		1.47[e]	*BT6O COTJ	B	20
122	C_4H_9	—C(CH$_3$)$_3$	0.52	*X	B	25
123	C_4H_9O	—O(CH$_2$)$_3$CH$_3$	−1.19	*O4	B	20
124	$C_4H_{10}O_3P$	—PO(OC$_2$H$_5$)$_2$	−3.04	*PO&O2&O2	CCl_4	25
125	$C_4H_{11}Si$	—CH$_2$Si(CH$_3$)$_3$	0.68	*1-SI-1&1&1	B	25
126	C_5N_3	—C(CN)=C(CN)$_2$	−5.30	*YCN&UYCN&CN	B	30
127	C_5H_3O		−4.10	* CL5VJ	B	30
128	C_5H_3OS		−3.45	*V- BT5SJ	B	25
129	$C_5H_3S_2$		−3.15	*YUS- BT5SJ	B	ns
130	C_5H_4N		−1.94	* BT6NJ	B	25
131	C_5H_4N		−2.28	* CT6NJ	B	25
132	C_5H_4N		−2.57	* DT6NJ	B	25
133	C_5H_4NO		−1.64	*V- BT5MJ	B	25
134	C_5H_4NO		−4.52	* DT6NJ AO	ns	ns
135	C_5H_5NO		−1.96	*O- BT6NJ	B	20
136	C_5H_4NO		−2.46	*O- DT6NJ	B	20
137	$C_5H_4NO_3$		−4.10	*V- AT5NTJ	D	30
138	C_5H_5S		−1.10	* BT5SJ Cl	B	25
139	C_5H_5S		−0.88	* BT5SJ D1	B	25
140	C_5H_5S		−0.79	* AT6SJ &5	B	30
141	$C_5H_6NO_2$		1.80	*1- AT5NTJ	D	25
142	$C_5H_6NO_2$		−5.65	* DT5NOVTJ A1 E1	B	ns
143	$C_5H_6NO_2$		−5.70	* ET5NOVTJ A1 D1	B	ns

continued

Appendix I—*Continued*

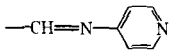
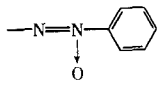
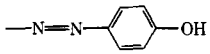
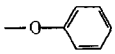
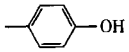
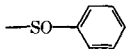
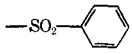
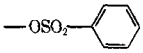
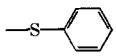
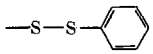
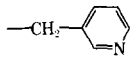
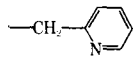
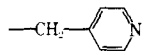
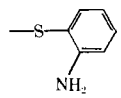
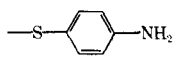
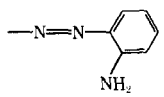
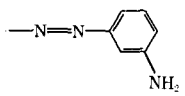
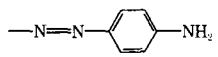
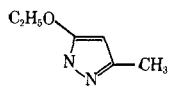
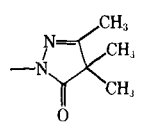
No.	Formula	R	μ_R (Debye)	WLN[b]	Solvent[c]	Temperature, °C
144	$C_5H_6NO_2$		−2.32	* DT5NOJ CO1 E1	D	ns
145	$C_5H_6NO_2$		−2.83	* ET5NOJ CO1 D1	D	ns
146	$C_5H_7N_2O$		−3.10	*1- BT5NNV DHJ E1	D	25
147	$C_5H_7N_2O$		−5.47	* AT5NNVJ B1 E1	D	25
148	$C_5H_7N_2O$		−5.47	* BT5NNVJ A1 E1	B	25
149	$C_5H_7N_2S$		−7.60	* BT5NNYJ A1 CUS E1	D	25
150	$C_5H_7N_2S$		−2.80	* BT5NNJ CS1 E1	B	25
151	$C_5H_7O_2$	—CH=CHCOOC$_2$H$_5$	−1.73	*1U1VO2	L	26
152	C_5H_8NO		−1.11	* BT5N CO AUTJ E1 E1	B	25
153	C_5H_8NO		−3.96	* AT6NVTJ	B	25
154	$C_5H_8NO_3$		−2.95	* BT5N COJ DOV1	B	ns
155	$C_5H_8NO_4$		−4.47	* BT6O COTJ ENW E1	B	ns
156	$C_5H_{11}O_2$	—CH(OC$_2$H$_5$)$_2$	1.23[e]	*YO2 &O2	B	20
157	$C_6H_4N_2Br$		−1.47	*NUNR DE	B	25
158	C_6H_4BrO		−1.59	*OR DE	B	20
159	C_6H_4BrO		−1.78	*DR CE	B	20
160	C_6H_4BrO		−2.20	*OR BE	B	20
161	$C_6H_4BrO_3S$		−3.82	*OSWR DE	B	25
162	$C_6H_4N_2Cl$		1.56	*NUNR DG	B	25
163	C_6H_4I		1.55	*R DI	B	25

Appendix I—*Continued*

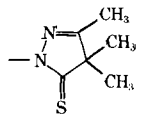
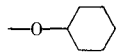
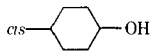
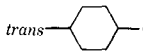
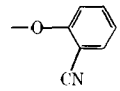
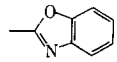
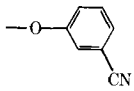
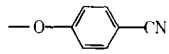
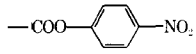
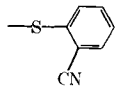
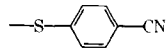
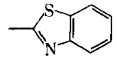
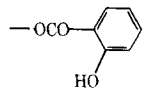
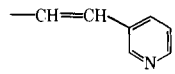
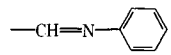
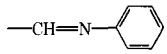
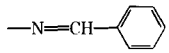
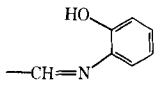
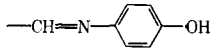
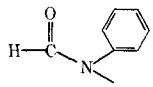
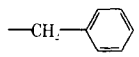
No.	Formula	R	μ_R (Debye)	WLN[b]	Solvent[c]	Temperature, °C
164	C_6H_4IO		2.06	*OR BI	B	20
165	C_6H_4IO		1.68	*OR CI	B	20
166	C_6H_4IO		1.47	*OR DI	B	20
167	C_6H_4IS		2.38	*SR BI	B	20
168	C_6H_4IS		1.80	*SR CI	B	20
169	C_6H_4IS		1.50	*SR DI	B	20
170	C_6H_4NO		−2.95	*V- BT6NJ	B	25
171	C_6H_4NO		−3.01	*V- CT6NJ	B	25
172	C_6H_4NO		−3.06	*V- DT6NJ	B	25
173	$C_6H_4NO_2S$		−5.22	*SR BNW	B	20
174	$C_6H_4NO_2S$		−4.04	*SR CNW	B	20
175	$C_6H_4NO_3$		−4.04	*OR CNW	B	20
176	$C_6H_4NO_3$		−4.60	*OR BNW	B	20
177	$C_6H_4NO_5S$		−4.72	*OSWR DNW	B	25
178	$C_6H_4NO_5S$		−2.76	*SWOR DNW	B	ns
179	$C_6H_4N_3O_4$		−6.36	*MR BNW DNW	B	ns
180	C_6H_5		0.00	*R	L	ns
181	C_6H_5NO		−4.13	*1- BT6NJ AO	B	25
182	C_6H_5NO		−4.61	*1- CT6NJ AO	B	25
183	C_6H_5NO		−4.63	*1- DT6NJ AO	D	25
184	$C_6H_5N_2$		−1.36	*1UN- BT6NJ	B	25
185	$C_6H_5N_2$		−2.98	*1UN- CT6NJ	B	25

continued

Appendix I—*Continued*

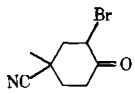
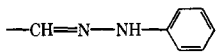
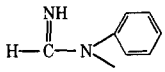
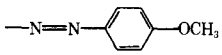
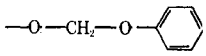
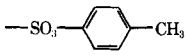
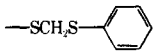
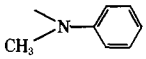
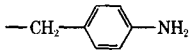
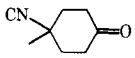
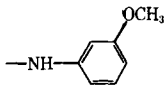
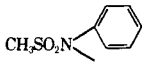
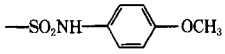
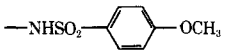
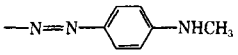
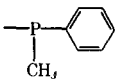
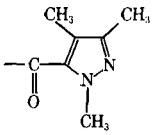
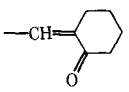
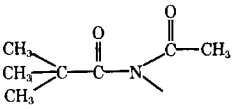
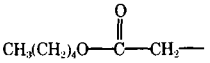
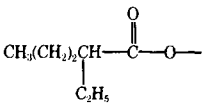
No.	Formula	R	μ_R (Debye)	WLN[b]	Solvent[c]	Temperature, °C
186	$C_6H_5N_2$		−4.16	*1UN- DT6NJ	B	25
187	$C_6H_5N_2O$		−1.73	*NUNO&R	B	25
188	$C_6H_5N_2O$		1.66	*NUNR DQ	B	25
189	C_6H_5O		1.16	*OR	B	25
190	C_6H_5O		1.34	*R DQ	B	20
191	C_6H_5O		1.63	*R BQ	B	25
192	C_6H_5OS		−4.07	*SO&R	B	25
193	$C_6H_5O_2S$		−5.05	*SWR	B	25
194	$C_6H_5O_3S$		−4.72	*OSWR	B	25
195	C_6H_5S		1.55[e]	*SR	B	25
196	$C_6H_5S_2$		1.79	*SSR	B	25
197	C_6H_6N		1.11	*MR	B	25
198	C_6H_6N		1.45	*R BZ	B	25
199	C_6H_6N		−2.18	*1- CT6NJ	B	25
200	C_6H_6N		−1.89	*1- BT6NJ	B	25
201	C_6H_6N		−2.65	*1- DT6NJ	B	25
202	$C_6H_6NO_2S$		−4.58	*MSWR	B	25
203	C_6H_6NS		1.87	*SR BZ	B	20
204	C_6H_6NS		2.44	*SR DZ	B	20
205	$C_6H_6N_3$		1.49	*NUNR BZ	B	20
206	$C_6H_6N_3$		1.71	*NUNR CZ	B	20
207	$C_6H_6N_3$		2.50	*NUNR DZ	B	20
208	$C_6H_9N_2O$		−2.65	* AT5NNJ C1 EO2	D	25
209	$C_6H_9N_2O$		−2.83	* BT5NNV DHJ D1 D1 E1	D	25

Appendix I—*Continued*

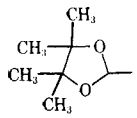
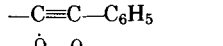
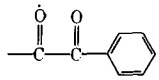
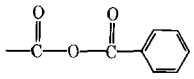
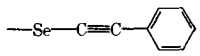
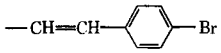
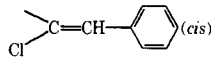
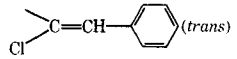
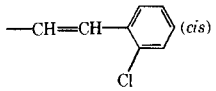
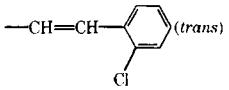
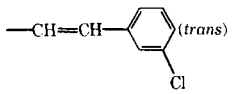
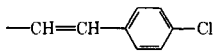
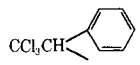
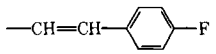
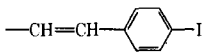
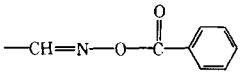
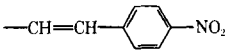
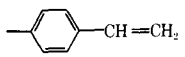
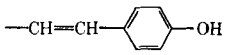
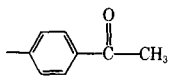
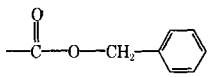
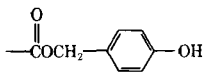
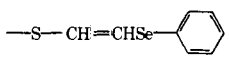
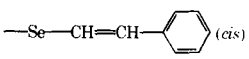
No.	Formula	R	μ_R (Debye)	WLN[b]	Solvent[c]	Temperature, °C
210	$C_6H_9N_2S$		−3.16	* BT5NNY DHJ CUS D1 D1 E1	D	25
211	C_6H_{11}		0.62	*AL6TJ	B	30
212	$C_6H_{11}N_2$		−1.55	*O- AL6TJ	B	20
213	$C_6H_{11}O$		1.87	* AL6TJ DQ -C	B	25
214	$C_6H_{11}O$		1.56	* AL6TJ DQ -T	B	25
215	$C_6H_{11}O_2$	$-CH_2CH_2OCOC_3H_7$	1.85	*2OV3	L	25
216	$C_6H_{11}O_2$	$-COOC_5H_{11}-n$	−1.99	*VO5	L	25
217	$C_6H_{11}N$	$-N(i-C_3H_7)_2$	1.53	*NY&&Y	B	25
218a	C_7H_4NO		−4.88	*OR BCN	B	20
218b	C_7H_4NO		−1.22	* CT56 BN DOJ	B	25
219	C_7H_4NO		−4.01	*OR CCN	B	20
220	C_7H_4NO		−4.23	*OR DCN	B	20
221	$C_7H_4NO_4$		−4.43	*VOR DNW	B	40
222	C_7H_4NS		−5.04	*SR BCN	B	20
223a	C_7H_4NS		−4.14	*SR DCN	B	20
223b	C_7H_4NS		−0.94	* CT56 BN DSJ	B	20
224	$C_7H_5O_2$	$-OCOC_6H_5$	−1.90	*OVR	B	25
225	C_7H_5O	$-COC_6H_5$	−3.04	*VR	B	25
226	$C_7H_5O_3$		−1.92	*OVR BQ	B	25
227a	C_7H_6N		−2.90	*1U1- CT6NJ	B	25
227b	C_7H_6N		−1.61	*YUNR	B	25
228a	C_7H_6N		−2.70	*1U1- DT6NJ	B	25
228b	C_7H_6N		1.61	*NUYR	B	25
229	C_7H_6NO		−2.73	*1UNR BQ	B	25
230	C_7H_6NO		1.94	*NUCUNR DQ	B	25
231a	C_7H_6NO		−3.44	*NR&VH	B	25
231b	C_7H_7		0.36	*1R	B	20

continued

Appendix I—*Continued*

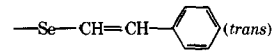
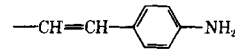
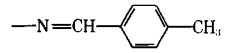
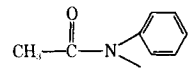
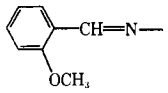
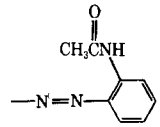
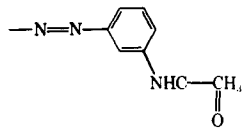
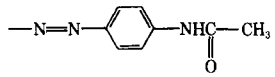
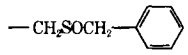
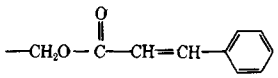
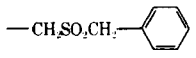
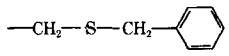
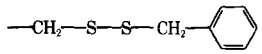
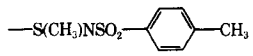
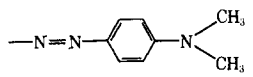
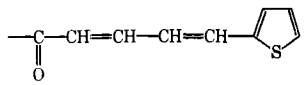
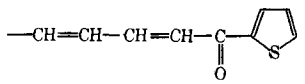
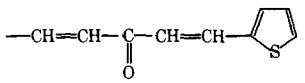
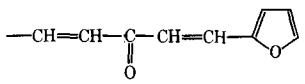
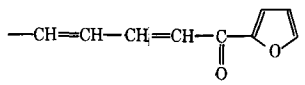
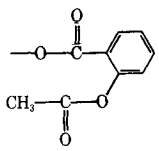
No.	Formula	R	μ_R (Debye)	WLN[b]	Solvent[c]	Temperature, °C
232	C_7H_7BrNO		4.21	* DL6NTJ BE DCN	B	25
233	$C_7H_7N_2$		−2.03	*1UNMR	B	25
234	$C_7H_7N_2$		−2.20	*NR&YUM	D	25
235	$C_7H_7N_2O$		1.54	*NUNR DO1	B	20
236	C_7H_7O		1.38	*R BO1	B	35
237	$C_7H_7O_2$		1.16	*O1OR	B	25
238	$C_7H_7O_3S$		−5.29	*OSWR D1	B	ns
239	$C_7H_7S_2$		1.34	*S1SR	B	25
240	C_7H_8N		1.24	*N1&R	B	20
241	C_7H_8N		1.84	*1R DZ	B	ns
242	C_7H_8NO		3.63	* DL6VTJ DCN	B	30
243	C_7H_8NO		1.79	*MR C01	B	25
244	$C_7H_8NO_2S$		−4.41	*NR&SW1	D	30
245	$C_7H_8NO_3S$		−5.08 −5.44	*SWMR DO1	B D	ns 25
246	$C_7H_8NO_3S$		5.21 5.65	*MSWR DM1	B D	ns 25
247	$C_7H_8N_3$		2.91	*NUNR DM1	B	20
248	C_7H_8P		1.39	*P1&R	B	20
249	$C_7H_9N_2O$		−2.80	*V- CT5NNJ B1 D1 E1	B	25
250	C_7H_9O		−3.23	*1U BL6VYTJ	B	25
251	$C_7H_{12}NO_2$		−3.59	*NV1&VX	B	20
252	$C_7H_{13}O_2$		−2.13	*1VO5	B	25
253	$C_7H_{13}O_2$		−2.05	*OVY2&3	B	25

Appendix I—*Continued*

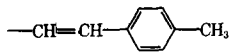
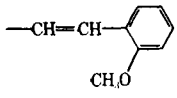
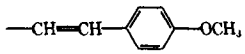
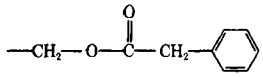
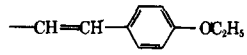
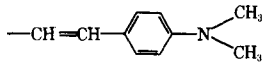
No.	Formula	R	μ_R (Debye)	WLN[b]	Solvent[c]	Temperature, °C
254a	$C_7H_{13}O_2$		−1.70	*BT5O COTJ D1 D1 E1 E1	B	25
254b	C_8H_5		0.00	*1UU1R	CCl_4	25
255	$C_8H_5O_2$		−3.71	*VVR	B	25
256	$C_8H_5O_3$		−3.30	*VOVR	B	25
257	C_8H_5Se		1.32	*-SE-1UU1R	B	25
258	C_8H_6Br		1.85	*1U1R DE	B	25
259	C_8H_6Cl		−1.68	*YGU1R -C	B	25
260	C_8H_6Cl		−1.29	*YGU1R -T	B	25
261	C_8H_6Cl		1.56	*1U1R BG -C	B	25
262	C_8H_6Cl		1.34	*1U1R BG -T	B	25
263	C_8H_6Cl		1.66	*1U1R CG -T	B	25
264	C_8H_6Cl		1.73	*1U1R DG	B	25
265	$C_8H_6Cl_3$		1.82	*YR&XGGG	B	17
266	C_8H_6F		1.49	*1U1R DF	B	25
267	C_8H_6F		1.80	*1U1R DI	B	25
268	$C_8H_6NO_2$		−3.32	*1UNOVR	B	25
269	$C_8H_6NO_2$		−4.74	*1U1R DNW	B	25
270	C_8H_7		0.64	*R D1U1	B	ns
271	C_8H_7O		1.64	*1U1R DQ	B	25
272	C_8H_7O		−3.11	*R DV1	B	20–60
273	$C_8H_7O_2$		−2.06	*VO1R	B	30
274	$C_8H_7O_3$		−2.56	*VO1R DQ	B	30
275	C_8H_7SSe		1.81	*S1U1-SE-R	B	25
276	C_8H_7Se		1.17	*-SE-1U1R -C	B	25

continued

Appendix I–*Continued*

No.	Formula	R	μ_R (Debye)	WLN[b]	Solvent[c]	Temperature, °C
277	C_8H_7Se		1.06	*-SE-1U1R -T	B	25
278	C_8H_8N		2.06	*1U1R DZ	B	25
279	C_8H_8N		1.93	*NU1R D1	B	25
280	C_8H_8NO		−3.61	*NR&V1	B	25
281	C_8H_8NO		2.87	*NU1R BO1	B	25
282	$C_8H_8N_3O$		3.47	*NUNR BMV1	B	20
283	$C_8H_8N_3O$		3.71	*NUNR CMV1	B	20
284	$C_8H_8N_3O$		3.72	*NUNR DMV1	B	20
285	C_8H_9OS		−3.76	*1SO&1R	B	25
286	$C_8H_9O_2$		−2.27	*1OV1U1R	B	30
287	$C_8H_9O_2S$		−4.25	*1SW1R	B	25
288	C_8H_9S		1.34	*1S1R	B	25
289a	$C_8H_9S_2$		1.87	*1SS1R	B	25
289b	$C_8H_{10}NO_2S_2$		−7.46	*S1&UNSWR D1	B	20
290	$C_8H_{10}N_3$		2.82	*NUNR DN1&1	B	20
291	$C_8H_{18}PO$	$PO(C_4H_9)_2$	−4.31	*PO&4&4	B	25
292	C_9H_7OS		−3.25	*V1U2U1- BT5SJ	B	25
293	C_9H_7OS		−3.50	*1U2U1V- BT5SJ	B	25
294	C_9H_7OS		−3.21	*1U1V1U1- BT5SJ	B	25
295	$C_9H_7O_2$		−3.29	*1U1V1U1-BT5OJ	B	25
296	$C_9H_7O_2$		−3.27	*1U2U1V-BT5OJ	B	25
297	$C_9H_7O_4$		−2.54	*OVR BOV1	B	25

Appendix I—*Continued*

No.	Formula	R	μ_R (Debye)	WLN[b]	Solvent[c]	Temperature, °C
298	C_9H_9		0.59	*1U1R D1	B	25
299	C_9H_9O		1.05	*1U1R DO1	B	25
300	C_9H_9O		1.45 1.13	*1U1R DO1	B	25
301	$C_9H_9O_2$		1.97	*1OV1R	B	24
302	$C_{10}H_{11}O_2$		1.66	*1U1R DO2	B	25
303	$C_{10}H_{12}N$		2.27	*1U1R DN1&1	B	25
304	$C_{12}H_{10}N$	$-N(C_6H_5)_2$	0.70	*NR&R	B	25
305	$C_{12}H_{10}P$	$-P(C_6H_5)_2$	−1.52	*PR&R	B	25
306	$C_{12}H_{10}PO$	$-PO(C_6H_5)_2$	−4.49	*PO&R&R	B	25

[a] Taken from Ref. 14 unless stated otherwise. [b] From E. G. Smith, "The Wiswesser Line—Formula Chemical Notation," McGraw-Hill, New York, N.Y., 1968. [c] Solvents: cHx = Cyclohexane, Hx = hexane, B = benzene, D = 1,4-dioxane, L = liquid state, ns = not stated. [d] V. I. Minkin, O. A. Osipov, and Y. A. Zhdanov "Dipole Moments in Organic Chemistry," English Translation by B. J. Hazzard, Plenum, New York, N.Y., 1970. [e] O. Exner, V. Jehlieka, and B. Uchytil, *Coll. Czech. Chem. Commun.*, **33**, 2862 (1968).

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