Anexos

Anexo 1

TABLE 7
Hoy Group Molar Attraction Constants at 25°C

Group, z	Bond type	$F/J^{1/2}$ cm$^{3/2}$ mol^{-1}	$F_p/J^{1/2}$ cm$^{3/2}$ mol^{-1}	V cm^3 mol^{-1}
Base value		276.3	—	—
$-CH_3$	Saturated	303.4	0.0	21.548
$-CH_2-$	Saturated	269.0	0.0	15.553
$>CH-$	Saturated	175.9	0.0	9.557
$>C<$	Saturated	65.5	0.0	3.562
$CH_2=$	Alkene	258.8	66.9	19.173
$-CH=$	Alkene	248.5	59.5	13.178
$>C=$	Alkene	172.8	63.0	7.183
$-CH=$	Aromatic	239.9	62.2	13.417
$>C=$	Aromatic	200.7	64.8	7.422
$-O-$	Ether	235.2	216.0	6.462
$-O-$	Acetal	236.3	10.2	6.462
$-O-$	Epoxide	360.4	155.9	6.462
$-COO-$	Ester	668.1	524.1	23.728
$>C=O$	Ketone	538.0	525.7	17.265
$-CHO$	Aldehyde	598.6	531.6	23.261
$-(CO)_2O$	Anhydride	1160.4	1159.8	40.993
$-COOH$	Acid	564.8	415.6	26.102
$-OH\rightarrow$	H-bond OH	485.8	485.8	10.647
$-OH$	Primary (not H-bonded)	673.8	673.8	12.457
$-OH$	Secondary	591.6	591.6	12.457
$-OH$	Tertiary	798.6	798.6	12.457
$-OH$	Phenolic	349.8	349.8	12.457
$-NH_2$	Amino, primary	463.5	463.5	17.012
$-NH-$	Amino, secondary	368.2	368.2	11.017
$>N-$	Amino, tertiary	125.0	125.0	12.569
$-C\equiv N$	Nitrile	725.3	724.5	23.066
$-NCO$	Isocyanate	733.7	8.2	25.907
$HCON<$	Formamide	1017.0	724.1	35.830
$-CONH-$	Amide	1134.6	893.9	28.302
$-CONH_2$	Amide	1206.6	989.2	34.297
OCONH	Urethane	1261.9	892.2	34.784
$-S-$	Thioether	428.3	428.3	18.044
Cl	Primary	419.5	306.8	19.504
Cl	Secondary	426.1	315.0	19.504
Cl_2	Twinned	701.0	562.5	39.008
Cl	Aromatic	329.3	81.4	19.504
Br	Primary	527.5	122.7	25.305
Br	Aromatic	420.6	100.2	25.305
F	Primary	84.5	73.2	11.200
Conjugation		47.6	−19.8	—
Cis		−14.6	−14.5	—
Trans		−27.6	−27.6	—
4-Membered ring		159.1	200.5	—
5-Membered ring		42.9	84.9	—
6-Membered ring		−48.0	61.0	—
7-Membered ring		92.3	0.0	—
Bicycloheptane ring		46.2	—	—
Tricyclodecane ring		127.8	—	—
Ortho substitution		19.8	−13.3	—
Meta substitution		13.5	−24.3	—
Para substitution		82.4	−33.8	—

Adapted from Hoy, K. L., *The Hoy Tables of Solubility Parameters*, Union Carbide Corporation, 1975 and 1985; *J. Paint Technol.*, 42, 76, 1970.

Tabla tomada de (Hansen, 2007)

Anexo 2

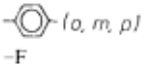
TABLE 13
Dispersion and Polar Group Molar Attraction Contributions

Structural group	^1F_d/J$^{1/2}$ cm$^{3/2}$ mol^{-1} Koenhen and Smolders[91]	^1F_d/J$^{1/2}$ cm$^{3/2}$ mol^{-1} van Krevelen[15]	^1F_p/J$^{1/2}$ cm$^{3/2}$ mol^{-1} van Krevelen[15]	$(^1F_p=^1V\ ^1\delta_p)$/J$^{1/2}$ cm$^{3/2}$ mol^{-1} Hansen and Beerbower[76]
–CH_3	411	420	0	—
–CH_2–	284	270	0	—
>C–	104	80	0	—
>C<	—	−70	0	—
=CH_2	—	400	0	—
=CH–	—	200	0	—
=C<	—	70	0	—
	—	1620	0	—
	1640	—	—	—
	1510	1430	110	—
 *(o, m, p)*	1350	1270	110	—
–F	—	(220)	—	460 ± 50
–Cl	—	450	550	610 ± 200
>Cl_2	—	—	—	360 ± 50
–Br	—	(550)	—	610 ± 50
–I	—	—	—	665 ± 50
–CN	446	430	1100	1070 ± 100
–OH	202	210	500	510 ± 60
(–OH)$_n$	—	—	—	n(350 ± 50)
–O–	—	100	400	410 ± 100
–COH	—	470	800	—
–C=O	325	—	—	—
–CO–	—	290	770	800 ± 30
–COOH	409	530	420	450 ± 20
–COO–	395	390	490	510 ± 50
HCOO–	—	530	—	—
–NH_2	—	280	—	610 ± 200
–NH–	143	160	210	205 ± 30
–N<	—	20	800	—
–NO_2	440	500	1070	1020 ± 100
–S–	—	440	—	—
=PO_4	—	740	1890	—
Ring	—	190	—	—
One plane of symmetry	—	—	0.50 ×	—
Two planes of symmetry	—	—	0.25 ×	—
More planes of symmetry	—	—	0 ×	—

Tabla tomada de (Hansen, 2007)

Anexo 3

TABLE 14
Hydrogen Bonding Parameter Group Contributions

Structural group, z	^zU_h/J mol^{-1} van Krevelen[15]	$-^zU_h = {}^zV^z\delta_h^2$/J mol^{-1} Hansen and Beerbower[76] Aliphatic	Aromatic
$-CH_3$	0	—	—
$-CH_2-$	0	—	—
$>CH-$	0	—	—
$>C<$	0	—	—
$=CH_2$	0	—	—
$=CH-$	0	—	—
$=C<$	0	—	—
	0	—	—
	0	—	—
 (o, m, p)	0	—	—
$-F$	—	~0	~0
$-Cl$	400	400 ± 80	400 ± 80
$>Cl_2$	—	690 ± 40	750 ± 40
$-Br$	—	2100 ± 400	2100 ± 400
$-I$	—	4000 ± 800	—
$-CN$	2500	2100 ± 800	2300 ± 800
$-OH$	20000	19500 ± 1700	19500 ± 2100
$-(OH)_n$	—	n(19500 ± 1700)	n(19500 ± 1700)
$-O-$	3000	4800 ± 1200	5200 ± 1200
$-COH$	4500	—	—
$-CO-$	2000	3300 ± 600	3300 ± 600
$-COOH$	10000	11500 ± 1000	9400 ± 1000
$-COO-$	7000	5200 ± 600	3300 ± 600
$-NH_2$	8400	5600 ± 800[a]	9400 ± 800[a]
$-NH-$	3100	3100 ± 800	—
$-N<$	5000	—	—
$-NO_2$	1500	1700 ± 200	1700 ± 200
$=PO_4$	13000	—	—

[a] Data from Bondi[8] corrected to 25°C and $V\delta_p^2$ subtracted. For important steric shielding effects, see his Tables 7.6 and 7.7.

Tabla tomada de (Hansen, 2007)