Supplementary Information

Effect of Temperature Dependence of Deformation Polarizability and Ionization energy of Solvents on Surface Properties of Solid Materials

Tayssir Hamieh [a,b,c*]

[a] Faculty of Science and Engineering, Maastricht University, P.O. Box 616, 6200 MD Maastricht, The Netherlands, Email: t.hamieh@maastrichtuniversity.nl

[b] Institut de Science des Matériaux de Mulhouse, Université de Haute-Alsace, CNRS, IS2M UMR 7361, F-68100 Mulhouse, France

[c] Laboratory of Materials, Catalysis, Environment and Analytical Methods Laboratory (MCEMA), Faculty of Sciences, Lebanese University, Hadath, Lebanon

Table S1. Corrected donor *DN* and acceptor *DN'* electron numbers and dipole moment μ (in D) of organic solvents with the different Lewis acid-base character.

Probe	*DN*	*AN*	Lewis character	μ (D)	Comment
CCl_4	0.00	2.3	weak acid	0	no permanent dipole
Chloroform	0	18.7	Stronger acid	1.04	Moderately polar
Benzene	0.25	0.6	Weaker amphoteric	0	Perfectly symmetric aromatic molecule
Dichloromethane	3	13.5	More acid	1.6	Polar due to asymmetric C–Cl bonds
Nitromethane	6.75	14.8	Amphoteric more acid	3.46	Strongly polar nitro group
Toluene	9.75	3.3	Amphoteric	0.37	Very weak permanent dipole; π-electron donor
Acetonitrile	35.25	16.3	Amphoteric more basic	3.92	Highly polar nitrile
Acetone	42.5	8.7	Amphoteric more basic	2.88	Strong dipole from C=O group
Ethyl acetate	42.75	5.3	Strong base	1.78	Polar aprotic solvent
Diethyl ether	48	4.9	Strong base	1.15	Polar; oxygen lone pairs dominate
THF	50	1.9	Strongest base	1.75	Strongly polar ether

Table S2. Variations of the deformation polarizability α_0 (in 10^{-40} C m² V⁻¹) of solvents and solid materials as a function of temperature.

Temperature (K)	323.15	343.15	363.15	383.15
n-Hexane	13.315	13.373	13.431	13.489
n-Heptane	15.243	15.313	15.383	15.453
n-Octane	17.810	17.896	17.982	18.068
n-Nonane	19.427	19.523	19.619	19.715
CCl_4	12.121	12.165	12.209	12.253
Nitromethane	8.242	8.268	8.294	8.320
CH_2Cl_2	8.048	8.072	8.096	8.120
Chloroform	9.901	9.935	9.969	10.003
Diethyl ether	10.579	10.621	10.663	10.705
THF	9.184	9.220	9.256	9.292
Ethyl acetate	10.258	10.308	10.358	10.408
Acetone	7.117	7.139	7.161	7.183
Acetonitrile	4.946	4.960	4.974	4.988
Toluene	13.186	13.234	13.282	13.330
Benzene	11.577	11.619	11.661	11.703
Alumina	5.957	5.963	5.969	5.975
Titania	7.948	7.963	7.978	7.993
MgO	6.128	6.122	6.116	6.110

Table S3. Variations of the ionization energy $\varepsilon(T)$ (in J/mol) of solvents and solid materials as a function of temperature.

Temperature (K)	323.15	343.15	363.15	383.15
n-Hexane	977328	977378	977428	977478
n-Heptane	958034	958084	958134	958184
n-Octane	945497	945551	945605	945659
n-Nonane	936817	936873	936929	936985
CCl_4	1106589	1106629	1106669	1106709
Nitromethane	1068995	1069059	1069123	1069187
CH_2Cl_2	1092143	1092203	1092263	1092323
Chloroform	1096969	1097031	1097093	1097155
Diethyl ether	917535	917601	917667	917733
THF	904996	905064	905132	905200
Ethyl acetate	965769	965833	965897	965961
Acetone	936147	936207	936267	936327

Acetonitrile	1177041	1177103	1177165	1177227
Toluene	851695	851755	851815	851875
Benzene	891847	891907	891967	892027
Alumina	577465	577465	577465	577465
Titania	916488	916488	916488	916488
MgO	737648	737648	737648	737648

Table S4. Variations of the free energy of adsorption $(-\Delta G_a^0)(T)$ (in kJ/mol) of solvents on alumina as a function of temperature *T*.

Temperature (K)	323.15	343.15	363.15	383.15
n-Hexane	28.716	28.776	28.827	28.878
n-Heptane	31.857	31.774	31.692	31.609
n-Octane	35.117	34.813	34.510	34.207
n-Nonane	38.467	37.716	37.163	36.611
CCl_4	34.514	34.449	34.435	34.420
CH_2Cl_2	59.637	57.919	56.367	54.442
$CHCl_3$	42.524	40.448	38.512	36.838
Ether	65.062	63.377	61.763	60.317
THF	62.228	60.464	58.838	57.449
Ethyl acetate	66.680	64.899	62.986	61.085
Toluene	46.302	45.020	44.028	43.511

Table S5. Variations of the free energy of adsorption $(-\Delta G_a^0)(T)$ (in kJ/mol) of solvents on titania as a function of temperature *T*.

Temperature (K)	323.15	343.15	363.15	383.15
n-Hexane	12.233	11.145	10.061	8.981
n-Heptane	16.137	15.048	13.963	12.882
n-Octane	18.889	17.739	16.593	15.451
n-Nonane	21.792	20.513	19.239	17.968
CH_2Cl_2	10.867	9.570	8.377	6.987
CHCl3	10.667	8.570	6.477	4.387
THF	25.570	24.453	23.341	22.232
Ethyl Acetate	10.834	8.311	5.792	3.278
Acetone	7.440	4.874	2.312	-0.246
Benzene	13.915	11.560	9.210	6.863
Nitromethane	14.816	12.536	10.261	7.989
Acetonitrile	3.591	0.691	-2.205	-5.098

Table S6. Variations of the free energy of adsorption $(-\Delta G_a^0)(T)$ (in kJ/mol) of solvents on MgO as a function of temperature *T*.

Temperature T (K)	323.15	343.15	363.15	383.15
n-Hexane	28.716	28.776	28.827	28.878
n-Heptane	31.857	31.774	31.692	31.609
n-Octane	35.117	34.813	34.510	34.207
n-Nonane	38.467	37.716	37.163	36.611
CH_2Cl_2	60.663	60.381	59.917	59.450
Chloroform	34.514	34.449	34.435	34.420
Diethyl ether	59.637	57.919	56.367	54.442
THF	42.524	40.448	38.512	36.838
Ethyl Acetate	53.277	51.481	49.553	47.618
Acetone	65.062	63.377	61.763	60.317
Acetonitrile	62.228	60.464	58.838	57.449
Toluene	46.302	45.020	44.028	43.511

List of abbreviations

AN': corrected acceptor number of solvent

C5: n-pentane

C6: n-hexane

C7: n-heptane

C5: n-octane

C9: n-nonane

DN': corrected donor number of solvent

H: separation distance (in Å)

IGC: inverse gas chromatography

K_A: Lewis acid constant of solid

K_D: Lewis base constant of solid

m: solid mass (in g)

$\mathcal{N}$*:* Avogadro's number,

P_0: standard pressure (in Pa)

$\mathcal{P}_{SX}$: chromatographic index (in $J \cdot Å^6 \cdot mol^{-1}$)

T: temperature (in K)

s: specific surface area of the solid (in m^2/g)

THF: tetrahydrofuran

α_0: deformation polarizability (in C m^2 V^{-1})

ε: ionization energy (in J/mol)

ε_0: permittivity of vacuum (in F/m)

$(-\Delta G_a^0)$: standard Gibbs free energy of adsorption (in J/mol)

$(-\Delta G_a^0)(Ref.)$: reference free energy of adsorption (in J/mol)

$(-\Delta G_a^d(T))$: London dispersive energy of adsorption (in J/mol)

$\left(-\Delta G_a^p(T)\right)$: polar energy of adsorption (in J/mol)

$(-\Delta H_a^p)$: polar adsorption enthalpy (in J/mol)

$(-\Delta S_a^p)$: polar adsorption entropy (in J K^{-1} mol^{-1})

π_0: two-dimensional pressure (N/m)

ω_A: entropic Lewis acid constant of solid

ω_D: entropic Lewis base constant of solid.