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Article

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

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Abstract

In recent research works, an original method based on the London interaction equation was proposed for the determination of London dispersive and polar properties of solid surfaces. The published results showed an important deviation of the surface properties of materials compared to the classic methods. However, in the previous papers, the ionization energy and deformation polarizability were supposed as constants against the temperature. In this work, we studied the temperature effect of the above parameters on the various surface variables of the adsorption of organic solvents on solid surfaces as alumina, titania, and magnesium oxide. Inverse gas chromatography at infinite dilution was used to determine the net retention volume of the adsorbed solvents on solid surfaces allowing the determination of the free energy of adsorption, the London dispersive and polar energy, the Lewis acid-base parameters and the acid-base surface energies. The obtained results reflect the important role of the thermal effect on the values of the ionization energy and deformation polarizability of solvents and solid materials, and consequently on the surface properties of solid materials. The results showed that the small variations of the ionization energy and deformation polarizability of solvents against the temperature induced notable shifts in the surface thermodynamic parameters of alumina, titania, and magnesium oxide including changes in the London dispersive and polar components of the free energy of adsorption by up to 100% in many adsorbed solvents, and variations in the Lewis acid–base constants of solid surfaces reaching 200% in the case of MgO. The sensitivity of surface parameters to these molecular properties emphasizes the importance of considering temperature effects in surface–molecule interactions.

Keywords: thermal effect; London equation; molecular interaction; surface energy; Lewis acid-base parameters

1. Introduction

In a previous paper [1], an original method was proposed to determine the surface properties of solid surfaces using the London dispersion interaction energy between model organic solvents adsorbed on solid materials. This new method led to an accurate separation between the London dispersive and polar energies of the adsorbed molecules. This allowed to the correction of the Lewis acid-base parameters of solid surfaces relatively to the classic models or methods. The new separation of London dispersive and polar energy is of great importance to predicting the various surface physicochemical properties of materials and nanomaterials [1]. Inverse gas chromatography (IGC) technique at infinite dilution was used to quantify the dispersive and polar free energies using the

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retention volume of adsorbed solvents on solid materials [2–46]. The free energy of adsorption $\Delta G_a^0(T)$ was determined as a function of temperature. The proposed method using the London equation proved the highest superiority relative to the classic chromatographic methods based on various thermodynamic parameters such as the boiling point $T_{B.P.}$ [2], the vapor pressure P_0 [3,4], the London dispersive surface energy γ_l^d [8], the topological index the vapor pressure P_0 [6,7], enthalpy of vaporization $\Delta H_{vap.}^0$ or the deformation polarizability $\alpha_{0,L}$ [5] of organic solvents.

Several previous papers [1,8,13–17,26,27,34] were devoted to the correction of the surface properties of solid materials such as the London dispersive energy, the polar free energy, and the Lewis acid-base constants using the thermal model that proved the temperature effect on the surface area of organic molecules.

However, the recent paper [1] introducing the London equation to separate the London dispersive and polar energy used $\mathcal{P}_{SX}$ as a chromatographic parameter. This thermodynamic parameter was replaced by a new parameter given by:

$$\mathcal{P}_{SX} = \frac{3}{2}\frac{\alpha_{0S}\,\alpha_{0X}}{(4\pi\varepsilon_0)^2}\frac{\varepsilon_S\,\varepsilon_X}{(\varepsilon_S+\varepsilon_X)} \quad (1)$$

where α_{0S} and α_{0X} are the respective deformation polarizabilities of solid H and solvents X separated by a distance H, and ε_S and ε_X are the ionization energies of solid and solvent. The deformation polarizabilities and ionization energies of solid and solvents were supposed independent from the temperature.

We proposed in this work to determine the surface properties of solid materials such as alumina, titania, and magnesium oxide by studying the effect of temperature dependence of deformation polarizabilities and ionization energies of solids and solvents on the London dispersive and polar energy, the Lewis acid-base parameters of the above solid surfaces, and consequently on their Lewis acid and base surface energies.

2. Materials and Methods

The solid materials and organic solvents were used in previous studies [1,16,17] applying chromatographic methods and models. The non-polar organic solvents were *n*-hexane, *n*-heptane, *n*-octane, and n-nonane, whereas the polar molecules were dichloromethane, chloroform, carbon tetrachloride, benzene, ethyl acetate, acetone, tetrahydrofuran, acetone, toluene, and acetonitrile. The solid materials were alumina (Al_2O_3), magnesium oxide (MgO), and titania (TiO_2) and previously characterized [1]. The net retention time of organic solvents adsorbed on the different solid surfaces was determined at different temperatures using inverse gas chromatography (IGC at infinite dilution with the help of a Focus GC gas chromatograph equipped with a flame ionization detector of high sensitivity (Sigma-Aldrich, Paris, France). A mass of 1 g of solid particles was packed into a stainless-steel column of a length of 30 cm and 2 mm internal diameter. Helium was used as carrier gas with a flow rate equal to 25 mL/min. The retention times of the different injected organic solvents were measured at infinite dilution, supposing that there is no interaction between the probe molecules themselves. The column temperatures varied from 30 to 200 °C. Average retention times and volumes were determined by repeating each solvent injection three times with a standard deviation less than 1% in all chromatographic measurements.

The IGC technique [2–46] allowed to characterize the surface properties of the various solid surfaces with the help of the net retention volume of the various solvents adsorbed on the solid materials. This allowed us to obtain the free energy of adsorption ΔG_a^0 of the adsorbed molecules by using the following fundamental equation of IGC:

$$\Delta G_a^0(T) = -RTlnVn + C(T) \quad (2)$$

Where V_n is the net retention volume of a probe, T the absolute temperature, R the perfect gas constant, and $C(T)$ a constant depending on the temperature and the parameters of interaction between the solid and the solvent given by:

$$C(T) = RT\ ln\left(\frac{sm\pi_0}{P_0}\right) \quad (3)$$

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where m the mass of the solid particles, s the specific surface area of solid surfaces, and P_0 the reference pressure and π_0 two-dimensional pressure given in the literature by one of the following reference states:

- Kemball and Rideal reference state [47] given for $T_0 = 0$ ºC by $P_0 = 1.013 \times 10^5\ Pa$ and $\pi_0 = 6.08 \times 10^{-5}\ N\ m^{-1}$.
- De Boer et al. reference state [48] given for $T_0 = 0$ ºC by $P_0 = 1.013 \times 10^5\ Pa$ and $\pi_0 = 3.38 \times 10^{-5}\ N\ m^{-1}$.

The total free energy of adsorption $\Delta G_a^0(T)$ is composed of the respective London dispersive energy $\Delta G_a^d(T)$ and polar energy $\Delta G_a^p(T)$:

$$\Delta G_a^0(T) = \Delta G_a^d(T) + \Delta G_a^p(T) \quad (4)$$

In a recent study, an original method based on the expression of the London dispersion interaction was proposed. The London dispersion equation [1] was used for the determination of the free dispersive energy $-\Delta G_a^d(T)$ and the fundamental equation is written as:

$$\Delta G_a^d(T) = -\frac{3}{2}\frac{\alpha_{01}\,\alpha_{02}}{(4\pi\varepsilon_0)^2\,H^6}\frac{\mathcal{N}\,\varepsilon_1\,\varepsilon_2}{(\varepsilon_1+\varepsilon_2)} \quad (5)$$

where α_{01} and α_{02} are the respective deformation polarizabilities of Molecules 1 and 2 separated by a distance H, ε_1 and ε_2 are the ionization energies of Molecules 1 and 2, and ν_1 and ν_2 are their characteristic electronic frequencies.

In the case of adsorption of organic solvents on solid materials, the solid molecule (Molecule 1) was denoted S and the probe molecule (Molecule 2) denoted by X and combining the previous equations. The free energy of adsorption $\Delta G_a^0(T)$ can be written as:

$$\Delta G_a^0(T) = -RTlnVn + C(T) = -\frac{\alpha_{0S}}{H^6}\left[\frac{3\mathcal{N}}{2(4\pi\varepsilon_0)^2}\left(\frac{\varepsilon_S\,\varepsilon_X}{(\varepsilon_S+\varepsilon_X)}\alpha_{0X}\right)\right] + \Delta G_a^{sp}(T) \quad (6)$$

A new thermodynamic parameter $\mathcal{P}_{SX}$ was proposed as new chromatographic indicator variable given by:

$$\mathcal{P}_{SX} = \frac{3}{2}\frac{\alpha_{0S}\,\alpha_{0X}}{(4\pi\varepsilon_0)^2}\frac{\varepsilon_S\,\varepsilon_X}{(\varepsilon_S+\,\varepsilon_X)}$$

In the previous studies [1,26,27], the ionization energy and deformation polarizability of solid and solvents were supposed constants independent from the temperature. Even if the variations of these variables slightly vary versus the temperature, the temperature effect of these parameters on the surface properties of solid materials was investigated in this paper.

3. Results

The new method was based on the temperature effect on the chromatographic parameter $\mathcal{P}_{SX}$ of alumina, titania, and magnesium oxide. Table 1 gave the variations of $\mathcal{P}_{SX}(T)$ as a function of temperature of the adsorbed organic molecules on solid materials. It was observed a slight variation of $\mathcal{P}_{SX}(T)$ versus the temperature. However, there is an important variation of $\mathcal{P}_{SX}(T)$ depending on both solvents and solid surfaces. This was more elucidated in Table 2 giving the equations $\mathcal{P}_{SX}(T)$ of the different solvents with the extrapolated values of $\mathcal{P}_{SX}(0\text{K})$ at 0K. $\mathcal{P}_{SX}(0\text{K})$ largely varied from solvent to another and from solid to solid. The slope $d\mathcal{P}_{SX}(T)/dT$ which is equal to the derivative of $\mathcal{P}_{SX}$ with respect of temperature represents a thermal expansion coefficient.

Table 1. Values of parameter $\mathcal{P}_{SX}(T)$ of solvents adsorbed on of the solid materials as a function of temperature.

Parameter $\mathcal{P}_{SX}(T)$ (in 10^{-54} SI) of alumina				
Temperature (K)	323.15	343.15	363.15	383.15
n-Hexane	34.885	35.073	35.261	35.450
n-Heptane	39.639	39.862	40.086	40.309
n-Octane	46.084	46.354	46.624	46.896
n-Nonane	50.093	50.393	50.693	50.993

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CCl_4	33.196	33.351	33.505	33.660
CH_2Cl_2	21.941	22.029	22.118	22.206
Chloroform	27.036	27.157	27.278	27.399
Ether	27.060	27.196	27.332	27.468
THF	23.367	23.483	23.599	23.715
Ethyl acetate	26.756	26.914	27.073	27.231
Toluene	32.751	32.904	33.058	33.212
Parameter $\mathcal{P}_{SX}(T)$ (in 10^{-54} SI) of titania				
Temperature (K)	323.15	343.15	363.15	383.15
n-Hexane	60.648	61.029	61.411	61.793
n-Heptane	68.759	69.207	69.656	70.107
n-Octane	79.819	80.358	80.899	81.441
n-Nonane	86.674	87.269	87.866	88.464
CH_2Cl_2	38.621	38.810	39.000	39.190
Chloroform	47.612	47.867	48.122	48.379
THF	40.272	40.508	40.744	40.981
Ethyl acetate	46.454	46.770	47.087	47.405
Acetone	31.743	31.902	32.062	32.222
Benzene	50.392	50.672	50.953	51.234
Nitromethane	39.167	39.365	39.565	39.765
Acetonitrile	24.545	24.661	24.778	24.895
Parameter $\mathcal{P}_{SX}(T)$ (in 10^{-54} SI) of MgO				
Temperature (K)	323.15	343.15	363.15	383.15
n-Hexane	41.560	41.701	41.842	41.982
n-Heptane	47.169	47.340	47.511	47.681
n-Octane	54.795	55.007	55.219	55.429
n-Nonane	59.530	59.767	60.004	60.240
CH_2Cl_2	26.309	26.362	26.415	26.468
Chloroform	32.426	32.506	32.586	32.666
Diethyl ether	32.118	32.215	32.312	32.408
THF	27.712	27.794	27.877	27.958
Ethyl acetate	31.854	31.979	32.103	32.227
Acetone	21.803	21.850	21.896	21.942
Acetonitrile	16.654	16.685	16.716	16.747
Toluene	38.700	38.804	38.908	39.012

Table 2. Equations $\mathcal{P}_{SX}(T)$ of the different solvents adsorbed on solid materials with the extrapolated values of $\mathcal{P}_{SX}(0\text{K})$ at 0K and the corresponding slopes $d\mathcal{P}_{SX}(T)/dT$.

Alumina			
Solvents	Equation $\mathcal{P}_{SX}(T)$ (in 10^{-54} SI)	$d\mathcal{P}_{SX}(T)/dT$ (10^{-3})	$\mathcal{P}_{SX}(0K)$ (in 10^{-54} SI)
n-Hexane	$\mathcal{P}_{SX}(T) = 0.0094\ T + 31.843$	9.4	31.843

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n-Heptane	$\mathcal{P}_{SX}(T)$ = 0.0112 T + 36.031	11.2	36.031
n-Octane	$\mathcal{P}_{SX}(T)$ = 0.0135 T + 41.711	13.5	41.711
n-Nonane	$\mathcal{P}_{SX}(T)$ = 0.015 T + 45.247	15	45.247
CCl_4	$\mathcal{P}_{SX}(T)$ = 0.0077 T + 30.696	7.7	30.696
CH_2Cl_2	$\mathcal{P}_{SX}(T)$ = 0.0044 T + 20.517	4.4	20.517
Chloroform	$\mathcal{P}_{SX}(T)$ = 0.006 T + 25.083	6	25.083
Ether	$\mathcal{P}_{SX}(T)$ = 0.0068 T + 24.866	6.8	24.866
THF	$\mathcal{P}_{SX}(T)$ = 0.0058 T + 21.491	5.8	21.491
Ethyl acetate	$\mathcal{P}_{SX}(T)$ = 0.0079 T + 24.196	7.9	24.196
Toluene	$\mathcal{P}_{SX}(T)$ = 0.0077 T + 30.27	7.7	30.27
	Titania		
Solvents	Equation $\mathcal{P}_{SX}(T)$ (in 10^{-54} SI)	$d\mathcal{P}_{SX}(T)/dT$ (10^{-3})	$\mathcal{P}_{SX}(0K)$
n-Hexane	$\mathcal{P}_{SX}(T)$ = 0.0191 T + 54.481	19.1	54.481
n-Heptane	$\mathcal{P}_{SX}(T)$ = 0.0225 T + 61.502	22.5	61.502
n-Octane	$\mathcal{P}_{SX}(T)$ = 0.027 T + 71.085	27	71.085
n-Nonane	$\mathcal{P}_{SX}(T)$ = 0.0298 T + 77.028	29.8	77.028
CH_2Cl_2	$\mathcal{P}_{SX}(T)$ = 0.0095 T + 35.556	9.5	35.556
Chloroform	$\mathcal{P}_{SX}(T)$ = 0.0128 T + 43.483	12.8	43.483
THF	$\mathcal{P}_{SX}(T)$ = 0.0118 T + 36.454	11.8	36.454
Ethyl acetate	$\mathcal{P}_{SX}(T)$ = 0.0158 T + 41.333	15.8	41.333
Acetone	$\mathcal{P}_{SX}(T)$ = 0.008 T + 29.164	8	29.164
Benzene	$\mathcal{P}_{SX}(T)$ = 0.014 T + 45.856	14	45.856
Nitromethane	$\mathcal{P}_{SX}(T)$ = 0.01 T + 35.947	10	35.947
Acetonitrile	$\mathcal{P}_{SX}(T)$ = 0.0058 T + 22.658	5.8	22.658
	MgO		
Solvents	Equation $\mathcal{P}_{SX}(T)$ (in 10^{-54} SI)	$d\mathcal{P}_{SX}(T)/dT$ (10^{-3})	$\mathcal{P}_{SX}(0K)$
n-Hexane	$\mathcal{P}_{SX}(T)$ = 0.007 T + 39.287	7	39.287
n-Heptane	$\mathcal{P}_{SX}(T)$ = 0.0085 T + 44.409	8.5	44.409
n-Octane	$\mathcal{P}_{SX}(T)$ = 0.0106 T + 51.378	10.6	51.378
n-Nonane	$\mathcal{P}_{SX}(T)$ = 0.0118 T + 55.708	11.8	55.708
CH_2Cl_2	$\mathcal{P}_{SX}(T)$ = 0.0027 T + 25.452	2.7	25.452
Chloroform	$\mathcal{P}_{SX}(T)$ = 0.004 T + 31.134	4	31.134
Diethyl ether	$\mathcal{P}_{SX}(T)$ = 0.0048 T + 30.556	4.8	30.556
THF	$\mathcal{P}_{SX}(T)$ = 0.0041 T + 26.386	4.1	26.386
Ethyl acetate	$\mathcal{P}_{SX}(T)$ = 0.0062 T + 29.842	6.2	29.842
Acetone	$\mathcal{P}_{SX}(T)$ = 0.0023 T + 21.053	2.3	21.053
Acetonitrile	$\mathcal{P}_{SX}(T)$ = 0.0016 T + 16.153	1.6	16.153
Toluene	$\mathcal{P}_{SX}(T)$ = 0.0052 T + 37.023	5.2	37.023

The results given in Tables 1 and 2 were used to determine the polar free energy $\Delta G_a^p(T)$ of the adsorbed organic solvents on solid materials. The new values of $\Delta G_a^p(T)$ of the various solvents adsorbed on alumina, titania, and MgO were given in Table 3 as a function of temperature.

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Table 3 showed that the lowest values of free polar interaction $\Delta G_a^p(T)$ were obtained with the titanium dioxide, whereas MgO gave the highest $\Delta G_a^p(T)$. However, the values of $\Delta G_a^p(T)$ relative alumina are not so far from the those of magnesium oxide.

Table 3. Variations of polar free energy $\Delta G_a^p(T)$ of adsorbed solvents on solid surfaces as a function of temperature.

Alumina				
Temperature (K)	323.15	343.15	363.15	383.15
CCl_4	6.848	6.591	6.442	6.291
CH_2Cl_2	38.946	36.464	34.334	31.831
Chloroform	18.676	16.093	13.779	11.726
Ether	41.199	39.000	37.001	35.171
THF	40.653	38.187	36.030	34.111
Ethyl acetate	43.013	40.705	38.397	36.089
Toluene	18.913	17.415	16.269	15.598
Titania				
Temperature (K)	323.15	343.15	363.15	383.15
CH_2Cl_2	5.965	5.575	5.287	4.801
Chloroform	2.622	1.497	0.374	0.000
THF	4.122	2.800	1.480	0.167
Ethyl acetate	3.193	1.611	0.032	0.000
Acetone	4.943	3.228	1.515	0.000
Benzene	0.580	0.529	0.481	0.440
Nitromethane	9.723	8.353	6.985	5.619
Acetonitrile	3.610	1.506	0.000	0.000
MgO				
Temperature (K)	323.15	343.15	363.15	383.15
CH_2Cl_2	39.945	38.903	37.861	36.819
Chloroform	10.589	10.026	9.635	9.248
Diethyl ether	35.873	33.635	31.689	29.375
THF	21.071	18.283	15.806	13.596
Ethyl Acetate	29.652	27.310	24.968	22.626
Acetone	46.707	44.062	41.716	39.541
Acetonitrile	46.573	43.625	41.094	38.803
Toluene	19.088	17.577	16.417	15.737

The determined free energy of adsorption of the polar solvents in Table 3 showed closest values for MgO and alumina very larger than those of titania then proving higher polar interaction for alumina and MgO.

The results showed in Table 3 were compared to those previously obtained without considering the thermal effect on the ionization energy and deformation polarizability [1]. It was observed in Table 4 an important deviation between the results of the two methods varying from 7% to 2665% (in the case of THF adsorbed on titania).

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Table 4. Error percentage committed when the thermal effect of the chromatographic parameters is neglected in adsorbed solvents on alumina, titania and MgO.

Alumina				
Temperature (K)	323.15	343.15	363.15	383.15
CCl4	95.1	97.5	98.7	
CH2Cl2	82.7	81.8	80.8	79.1
Chloroform	107.8	127.7	151.6	178.1
Ether	55.0	58.4	62.1	65.0
THF	1.1	2.5	3.4	4.9
Ethyl acetate	73.0	76.8	79.5	83.0
Toluene	114.3	120.4	123.6	123.6
Titania				
Temperature (K)	323.15	343.15	363.15	383.15
CH2Cl2	57.3	65.5	76.3	84.9
Chloroform	20.0	34.9	138.5	
THF	84.9	136.5	279.7	2665.2
Ethyl acetate	24.6	50.0	2544.8	
Acetone	16.9	26.0	55.9	
Benzene	859.4	693.7	489.8	232.6
Nitromethane	6.9	8.0	9.6	11.8
Acetonitrile	27.8	67.6		
MgO				
Temperature (K)	323.15	343.15	363.15	383.15
CH2Cl2	91.7	90.3	88.0	85.8
TCM	44.9	73.1	83.8	76.5
Diethyl ether	59.8	50.8	41.1	29.5
THF	9.4	36.8	70.4	111.8
Ethyl Acetate	79.0	72.1	63.5	53.5
Acetone	66.3	53.4	39.2	23.5

Serious consequences resulted from the above results leading to a higher disparity in the values of other surface thermodynamic parameters, particularly on the polar enthalpy and entropy of adsorption, and Lewis acid-base parameters of the solid substrates.

The polar enthalpy $\left(-\Delta H_a^p\right)$ and entropy $\left(-\Delta S_a^p\right)$ of solvents adsorbed on solid surfaces were obtained from the variations of the free energy of adsorption against the temperature using the following relation:

$$\Delta G_a^p(T) = \Delta H_a^p - T\,\Delta S_a^p \qquad (7)$$

The values of the above thermodynamic variables were given in Table 5 compared to the previous results obtained without taking into account the thermal effect on the ionization energy and deformation polarizability of solvents.

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Table 5. Comparison between the values of polar enthalpy ($-\Delta H_a^p$ *in* kJ mol^{-1}) and entropy ($-\Delta S_a^p$ *in* J K^{-1}mol^{-1}) of the various polar solvents adsorbed on the various solid obtained using the previous method [1] and the new method, with the error percentages of the previous method.

Alumina						
	Previous results		New results		Error (%) on	Error (%) on
Solvents	$-\Delta S_a^p$(J K^{-1}mol^{-1})	$-\Delta H_a^p$(kJ mol^{-1})	$-\Delta S_a^p$(J K^{-1}mol^{-1})	$-\Delta H_a^p$(kJ mol^{-1})	($-\Delta S_a^p$)	($-\Delta H_a^p$)
CCl_4	6.2	2.314	9.1	9.7553	31.9	76.3
CH_2Cl_2	1.9	7.3421	117.4	76.843	98.4	90.4
$CHCl_3$	102.8	71.989	115.8	55.971	11.2	28.6
Diethyl ether	104.6	52.207	100.4	73.55	4.2	29.0
THF	88.8	69.683	108.9	75.711	18.5	8.0
Ethyl acetate	90.4	40.683	115.4	80.305	21.7	49.3
Toluene	94.9	71.036	55.4	36.628	71.3	93.9
Titanium dioxide						
	Previous results		New results		Error (%) on	Error (%) on
Solvents	$-\Delta S_a^p$(J K^{-1}mol^{-1})	$-\Delta H_a^p$(kJ mol^{-1})	$-\Delta S_a^p$(J K^{-1}mol^{-1})	$-\Delta H_a^p$(kJ mol^{-1})	($-\Delta S_a^p$)	($-\Delta H_a^p$)
CH_2Cl_2	30.7	12.146	18.9	12.084	62.4	0.5
$CHCl_3$	56.4	20.818	56.2	20.780	0.4	0.2
THF	10	23.277	65.9	25.423	84.8	8.4
Ethyl Acetate	78.1	28.448	79	28.729	1.1	1.0
Acetone	85.4	32.518	85.7	32.635	0.4	0.4
Benzene	68.3	26.965	2.3	1.335	2869.6	1920.0
Nitromethane	68.5	31.846	68.4	31.829	0.1	0.1
Acetonitrile	104.6	37.37	105.1	37.586	0.5	0.6
MgO						
	Previous results		New results		Error (%) on	Error (%) on
Solvents	$-\Delta S_a^p$(J K^{-1}mol^{-1})	$-\Delta H_a^p$(kJ mol^{-1})	$-\Delta S_a^p$(J K^{-1}mol^{-1})	$-\Delta H_a^p$(kJ mol^{-1})	($-\Delta S_a^p$)	($-\Delta H_a^p$)
CH_2Cl_2	32.2	7.1665	52.100	56.781	38.2	87.4
$CHCl_3$	-60.5	-24.435	22.1	17.665	373.8	238.3
Diethyl ether	105.1	19.543	107.2	70.503	2.0	72.3

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Ethyl acetate	71.9	17.038	124.5	61.159	42.2	72.1
THF	95.8	7.8791	117.100	67.493	18.2	88.3
Acetone	242	62.489	119.2	85.107	103.0	26.6
Acetonitrile	81.6	2.0138	129.2	88.148	36.8	97.7
Toluene	-13.8	15.211	56.1	37.003	124.6	58.9

The results in Table 5 led to the Lewis enthalpic acid–base constants K_A and K_D using the empirical relation (8):

$$-\Delta H^p = K_A \times DN + K_D \times AN \quad (8)$$

where AN and DN are, respectively, the electron donor and acceptor numbers of the polar molecule [45,46].

The values of K_A and K_D of solids were deduced by drawing the variations of $\left(\frac{-\Delta H^{Sp}}{AN}\right)$ versus $\left(\frac{DN}{AN}\right)$ of polar solvents using Equation (9):

$$\left(-\frac{\Delta H^{Sp}}{AN}\right) = K_A\left(\frac{DN}{AN}\right) + K_D \quad (9)$$

The same procedure was used for the determination of the Lewis entropic acidic ω_A and basic ω_D constants of the various solid surfaces using Equations (10) or 11.

$$\left(-\Delta S_a^{sp}\right) = \omega_A\, DN' + \omega_D\, AN' \quad (10)$$

$$\left(\frac{-\Delta S_a^{sp}}{AN'}\right) = \omega_A\left(\frac{DN'}{AN'}\right) + \omega_D \quad (11)$$

The Lewis enthalpic and entropic acid-base parameters were shown in Table 6 and compared to the previous results.

Table 6. Values of the enthalpic acid–base constants K_A and K_D and the entropic acid base constants ω_A and ω_D of the various solid surfaces with the corresponding acid–base ratios, using the new thermal method compared to the results of the previous method [1].

	Previous results			**This work**		
Lewis parameter	Alumina	Titania	MgO	Alumina	Titania	MgO
K_A	0.71	0.25	0.08	0.79	0.27	0.65
K_D	2.21	0.87	1.13	2.69	0.89	2.37
K_D/K_A	3.1	3.5	14	3.41	3.26	3.65
R^2	0.7301	0.9874	0.1722	0.9827	0.9895	0.9585
$10^3.\omega_A$	0.92	0.86	1.16	1.13	0.73	1.39
$10^3.\omega_D$	4.21	1.8	0.57	3.92	2.03	2.00
ω_D / ω_A	4.58	2.09	0.49	3.48	2.79	1.44
R^2	0.7739	0.9804	0.8126	0.973	0.9885	0.9754

The results obtained showed the three solid materials exhibited an amphoteric character with higher basicity. Alumina proved the highest enthalpic and entropic Lewis basic and acidic constants followed by MgO while titania had the lowest Lewis acid and basic constants. It was observed that the Lewis acid-base parameters of MgO and alumina were very close, whereas titania presented K_A and K_D three times lower than those of alumina and MgO. The comparison with the previous results [1] showed comparable values of K_A and K_D in the case of alumina and titania but very different values for MgO surfaces. However, this deviation increased for the entropic acid-base constants ω_A and ω_D between the two methods. The new method gave more accurate quantification of the surface properties of solid materials.

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4. Discussion

The temperature effect on the ionization energy and deformation polarizability of solvents adsorbed on alumina, titania, and MgO led to important variations in the surface thermodynamic properties, and especially, in polar energy and Lewis acid-base constants of solid surfaces. A correction of the surface properties of these materials relative to the previous method was carried out highlighting the effect of temperature on the thermodynamic parameters strongly affecting the Lewis acid-base properties of solid surfaces.

The original consequence of this new approach was the determination of the intermolecular distance $H(T)$ between the organic solvents and the solid materials as a function of temperature. Indeed, using Equation (4) the London dispersive free energy $-\Delta G_a^p(T)$ of adsorption of solvents on the different solid surfaces was obtained against the temperature and led to the values of the intermolecular distance from the following Equation:

$$\left(-\Delta G_a^d(T)\right) = \frac{\mathcal{P}_{SX}(T)}{H(T)^6} \quad (12)$$

And $H(T)$ was determined as a function of temperature from Equation (13):

$$H(T) = \left[\frac{\mathcal{P}_{SX}(T)}{\left(-\Delta G_a^d(T)\right)}\right]^{1/6} \quad (13)$$

The variations of $H(T)$ between the solvents and the solid substrates shown in Table 7 highlighted an effect of temperature on the intermolecular distance with increasing tendency of $H(T)$ as the temperature increased for n-alkanes while a decrease of $H(T)$ was observed for polar solvents. The results in Table 7 also showed large differences of the values of the intermolecular distance strongly depending on the polarity of solid surfaces. Indeed, $H(T)$ of different solvents was the lowest with alumina followed by MgO, while the highest values were observed with titania then confirming the results obtained with the Lewis acid-base properties of solid materials where alumina was proved to have the highest acid-base constants leading to lowest values of $H(T)$ due to the strong van der Waals interaction.

Table 7. Variations of the intermolecular distance $H(T)$ (in Å) of the different solvents adsorbed on solid as a function of temperature.

Alumina				
Temperature T(K)	323.15	343.15	363.15	383.15
n-Hexane	3.267	3.268	3.270	3.272
n-Heptane	3.280	3.284	3.289	3.293
n-Octane	3.309	3.317	3.325	3.333
n-Nonane	3.305	3.319	3.330	3.342
CCl_4	3.260	3.259	3.258	3.258
CH_2Cl_2	3.193	3.176	3.164	3.153
Chloroform	3.229	3.220	3.214	3.209
Ether	3.229	3.220	3.215	3.209
THF	3.205	3.190	3.180	3.171
Ethyl acetate	3.227	3.218	3.213	3.207
Toluene	2.871	2.877	2.887	2.903
Titania				
Temperature T(K)	323.15	343.15	363.15	383.15
n-Hexane	4.129	4.198	4.275	4.361
n-Heptane	4.026	4.078	4.134	4.194

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n-Octane	4.021	4.068	4.118	4.172
n-Nonane	3.980	4.025	4.073	4.125
CH_2Cl_2	4.461	4.619	4.825	5.116
Chloroform	4.253	4.349	4.461	4.596
THF	4.409	4.549	4.724	4.957
Ethyl acetate	4.272	4.372	4.488	4.629
Acetone	4.831	5.183	5.853	-
Benzene	4.213	4.299	4.398	4.515
Nitromethane	4.443	4.595	4.790	5.060
		MgO		
Temperature T(K)	323.15	343.15	363.15	383.15
n-Hexane	3.363	3.364	3.365	3.366
n-Heptane	3.376	3.380	3.383	3.387
n-Octane	3.406	3.413	3.420	3.427
n-Nonane	3.401	3.414	3.425	3.436
CH_2Cl_2	3.291	3.246	3.068	3.066
Chloroform	3.327	3.308	3.133	3.135
Diethyl ether	3.325	3.272	2.882	2.900
THF	3.300	3.226	2.996	3.020
Ethyl acetate	3.324	3.263	2.802	2.817
Acetone	3.254	3.167	2.660	2.672
Acetonitrile	3.195	3.085	2.564	2.575
Toluene	3.353	3.327	3.098	3.105

5. Conclusions

The surface properties of solid surfaces such as alumina, titania, and magnesium oxide were determined using a new method based on the effect temperature on ionization energy and deformation polarizability of solvents and consequently on the different surface thermodynamic parameters of solid materials. Even if a slight variation of ionization energy and deformation polarizability of organic molecules was observed, however, an important difference in the surface properties of oxides was shown leading to different Lewis acid-base constants between the new thermal method and the previous method which supposed a neglected temperature effect on the polar and dispersive energy of adsorption of solvents on the solid surfaces. The large differences proved between the values of the intermolecular distance between the solvents and the various solid substrates confirmed the superiority of the new method.

These findings highlight the critical need to account for temperature-dependent electronic and polarizability effects when evaluating surface reactivity, adhesion, and interfacial interactions. From a broader materials science perspective, this work establishes a foundational link between molecular-scale properties of probe molecules and macroscopic surface behaviors, offering new insights for the rational design of functional materials, surface coatings, and nanostructured interfaces with tailored thermodynamic and interfacial properties.

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