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Research Letter

Spectral SAR Ecotoxicology of Ionic Liquids: The *Daphnia Magna* Case

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Aiming to provide a unified theory of ionic liquids ecotoxicity, the recent spectral structure activity relationship (S-SAR) algorithm is employed for testing the two additive models of anionic-cationic interaction containing ionic liquid activity: the causal and the endpoint, $|0+\rangle$ and $|1+\rangle$ models, respectively. As a working system, the *Daphnia magna* ecotoxicity was characterized through the formulated and applied spectral chemical-ecobiological interaction principles. Specific anionic-cationic-ionic-liquid rules of interaction along the developed mechanistic hypersurface map of the main ecotoxicity paths together with the so-called resonance limitation of the standard statistical correlation analysis were revealed.

1. INTRODUCTION

Since the reformulation of the classical quantitative structure activity relationship (QSAR) is modelled under the spectral SAR (S-SAR) analytical analysis [1–3], the ecotoxicological studies have been reinforced with new tools linking the molecular structure of the chemicals dispersed in environment over certain species with their recorded biological activities [4, 5]. Remarkably, the steps of an S-SAR analysis can be transposed into the driving principles of the associated spectral chemical ecostudies and biostudies:

(i) *principle 1* states that the "orthogonality" of assumed molecular factors which correlate with ecoeffects and bioeffects is assured by the spectral decomposition of the associate activity respecting them;
(ii) *principle 2* states that the "length" of the predicted (eco-) biological action follows the self-scalar product rule of the computed endpoint activity;
(iii) *principle 3* states that the "intensity" of the chemical eco-/biointeraction is determined by the ratio of the expected to measured activity norms;
(iv) *principle 4* states that the "selection" of the manifested chemical (eco-) biobond parallels the minimum distances of paths connecting all possible endpoints in the norm correlation hyperspace;
(v) *principle 5* states that the "validation" of the obtained mechanistic picture is done by constraining that the influential minimum paths are numbered by the cardinal of the input structural factors set so that, excepting the final endpoint which is always considered as the evolution target, all other endpoints are activated once and for one time only.

In the present study, the above algorithm is applied to the intriguing case of ionic liquids (*IL*) acting on the ecoparadigmatic *Daphnia magna* species within two different additive models of the Hansch expansion.

2. HANSCH S-SAR-IL $|0+\rangle \& |1+\rangle$ MODELS

Usually, when considering Hansch QSAR expansion, the hydrophobic, electronic, and steric factors have to be considered. The hydrophobicity index Log*P* describes at the best the quality of molecular transport through cellular membranes. For the electronic and steric contributions, we consider that the polarizability (POL) measures the inductive electronic effect reflecting the long range or van-der-Waals bonding whereas for the steric component, the total energy (E_{TOT}) is assumed as the representative index since it is calculated at the optimum molecular geometry where the stereospecificity is included. The recent ecotoxicological studies

Table 1: The studied ionic liquids actions on *Daphnia magna* species with the toxic activities $A_{\text{exp}} = \text{Log}(\text{EC}_{50})$ [9], while the marked values were taken from [10], along structural parameters Log*P*, POL, and E_{TOT} as accounting for the hydrophobicity, electronic (polarizability), and steric (total energy at optimized 3D geometry) effects, computed with HyperChem program [11], for each cation and anion fragment, as well as for the anionic-cationic $|0+\rangle$ composed state, by means of equations (2)–(4), respectively.

Ionic liquid compound	A_{exp}	Log*P*			POL [Å^3]			E_{TOT} [kcal/mol]		
	$\lvert Y_{\text{exp}}\rangle$	$\lvert X_{1C}\rangle$	$\lvert X_{1A}\rangle$	$\lvert X_{1AC}\rangle$	$\lvert X_{2C}\rangle$	$\lvert X_{2A}\rangle$	$\lvert X_{2AC}\rangle$	$\lvert X_{3C}\rangle$	$\lvert X_{3A}\rangle$	$\lvert X_{3AC}\rangle$
1-n-octyl-3-methylpyridinium bromide	−2.60	4.90	0.94	4.92	26.69	3.01	87.08	−371060.81	−1596918.25	−1967840
1-n-hexyl-3-methylpyridinium bromide	−2.41	4.11	0.94	4.15	23.02	3.01	78.87	−322641.81	−1596918.25	−1919410
1-n-butyl-3-methylpyridinium bromide	−1.24	3.32	0.94	3.41	19.35	3.01	70.37	−274222.62	−1596918.25	−1870990
1-n-octyl-3-methylimidazolium bromide	−4.33	2.26	0.94	2.5	24.56	3.01	82.35	−357484.59	−1596918.25	−1954260
1-n-hexyl-3-methylimidazolium bromide	−2.22	1.47	0.94	1.93	20.89	3.01	73.98	−309065.84	−1596918.25	−1905830
1-n-butyl-3,5-dimethylpyridinium bromide	−1.01	3.78	0.94	3.84	21.18	3.01	74.65	−298437.03	−1596918.25	−1895210
1-n-hexyl-4-piperidino pyridinium bromide	−3.66	4.63	0.94	4.65	30.93	3.01	96.25	−452857.03	−1596918.25	−2049640
1-n-hexyl-4-dimethylamino pyridinium bromide	−3.28	3.91	0.94	3.96	26.2	3.01	86.00	−380945.12	−1596918.25	−1977720
1-n-hexyl-3-methyl-4-dimethylamino pyridinium bromide	−2.79	4.37	0.94	4.40	28.04	3.01	90.03	−405145.97	−1596918.25	−2001920
1-n-hexylpyridinium bromide	−1.93	3.64	0.94	3.71	21.18	3.01	74.65	−298427.37	−1596918.25	−1895200
1-n-hexyl-2,3-dimethylimidazolium bromide	−2.19	1.67	0.94	2.06	22.72	3.01	78.19	−333284.94	−1596918.25	−1930060
1-n-butyl-3-methylimidazolium chloride	−1.07*	0.68	0.63	1.34	17.22	2.32	59.60	−260646.64	−285190.78	−545677
1-n-butyl-3-methylimidazolium bromide	−1.43*	0.68	0.94	1.51	17.22	3.01	65.26	−260646.64	−1596918.25	−1857410
1-n-butyl-3-methylimidazolium tetrafluoroborate	−1.32*	0.68	1.37	1.78	17.22	2.46	60.80	−260646.64	−261310.59	−521798
1-n-butyl-3-methylimidazolium hexafluorophosphate	−1.15*	0.68	2.06	2.28	17.22	1.78	54.62	−260646.64	−580264.94	−840746
Tetrabutyl ammonium bromide	−1.53	4.51	0.94	4.54	30.91	3.01	96.21	−422421.97	−1596918.25	−2019200
Tetrabutyl phosphonium bromide	−2.05	2.89	0.94	3.02	30.91	3.01	96.21	−600149.625	−1596918.25	−2196930

based on these chemical descriptors have proved their reliability in providing the molecular mechanism based on which chemicals act upon certain species [3–5]. However, when the focus is on the ionic liquids, two different additive models for modelling anionic-cationic interaction can be considered.

The first one is based on the vectorial summation of the produced anionic and cationic biological effects. In other words, the so-called $|1+\rangle$ model is constructed on the superposition of the anionic (subscripted with *A*) and cationic (subscripted with *C*) activities. The analysis based on this model was recently reported for the *Vibrio fischeri* ecotoxicity [4].

The second S-SAR model can be advanced here when the additive stage is considered at the considered Hansch factors, which are firstly combined to produce the anionic-cationic (subscripted with *AC*) indices that are further used to produce the spectral mechanistic map of the concerned interaction. This way, the so-called $|0+\rangle$ model is produced:

$$|Y_{AC}\rangle^{0+} = \hat{O}_{\text{S-SAR}}\,|0+\rangle = \hat{O}_{\text{S-SAR}}\,f\left(\{|X_A\rangle\},\{|X_C\rangle\}\right) \tag{1}$$

with the particular specifications of the spectral vectors:

$$\begin{aligned} f\left(\text{Log}\,P_A, \text{Log}P_C\right) &\equiv \text{Log}P_{AC} \\ &= \log\left(e^{\text{Log}\,P_A} + e^{\text{Log}P_C}\right) \in \{|X_{1AC}\rangle\}, \end{aligned} \tag{2}$$

$$\begin{aligned} f\left(\text{POL}_A, \text{POL}_C\right) &\equiv \text{POL}_{AC} \\ &= \left(\text{POL}_A^{1/3} + \text{POL}_C^{1/3}\right)^3 \in \{|X_{2AC}\rangle\}[\text{Å}^3], \end{aligned} \tag{3}$$

$$\begin{aligned} f\left(E_A, E_C\right) &\equiv E_{AC} = E_A + E_C \\ &\quad - 627.71\frac{q_A q_C}{\text{POL}_{AC}^{1/3}} \in \{|X_{3AC}\rangle\}[\text{kcal/mol}]. \end{aligned} \tag{4}$$

The open issue addresses whether the $|0+\rangle\&|1+\rangle$ states yield the same results or in which aspects they might differ in the *IL* ecotoxicity upon certain species, here developed for the *Daphnia magna* case.

3. RESULTS ON *DAPHNIA MAGNA* SPECIES

Although many tests using *Daphnia magna* were established [6–8], the measured ionic liquids activity it remains rather unexplained in terms of molecular ways of action [9, 10]. To complete this, the above spectral-SAR ecotoxicological principles are systematically applied and interpreted for the observed toxicity of the ionic liquids of Table 1, with either $|0+\rangle$ and $|1+\rangle$ models.

In such case, when considering the principles of orthogonality, of the length, and of intensity of toxicological actions, Table 2 is produced, where, for comparison, the standard statistical factor was also added. First, it can be observed that

Table 2: Spectral structure activity relationships (S-SAR) of the ionic liquids toxicity of Table 1 against *Daphnia magna* species, with $|X_0\rangle = |1_1 \cdots 1_{17}\rangle$, together with the associated computed spectral norms and statistic and algebraic correlation factors [3, 4], throughout the possible correlation models considered from the *anionic, cationic,* and *ionic liquid* $|1+\rangle$ and $|0+\rangle$ states, respectively.

Mode	S-SAR equations	$\Vert\, \vert Y\rangle^{\text{Mode}} \Vert$	*STATISTIC* $r_{\text{S-SAR}}$	*ALGEBRAIC* $r_{\text{S-SAR}}$
Ia	$\vert Y_{A\text{-Ia}}\rangle = -2.91325\vert X_0\rangle + 0.773243\vert X_{1A}\rangle$	8.83127	0.266552	0.920421
	$\vert Y_{C\text{-Ia}}\rangle = -1.41993\vert X_0\rangle - 0.250543\vert X_{1C}\rangle$	8.92169	0.420761	0.929845
	$\vert Y_{AC\text{-Ia}}\rangle^{0+} = -1.21571\vert X_0\rangle - 0.287831\vert X_{1AC}\rangle$	8.89048	0.374616	0.926593
	$\vert Y_{AC\text{-Ia}}\rangle^{1+} = \vert Y_{A\text{-Ia}}\rangle + \vert Y_{C\text{-a}}\rangle$	17.6883	2.21964 $\boldsymbol{i}$	1.84353
Ib	$\vert Y_{A\text{-Ib}}\rangle = 1.40126\vert X_0\rangle - 1.23268\vert X_{2A}\rangle$	8.94784	0.455964	0.932572
	$\vert Y_{C\text{-Ib}}\rangle = 0.502967\vert X_0\rangle - 0.113186\vert X_{2C}\rangle$	9.06691	0.59121	0.944981
	$\vert Y_{AC\text{-Ib}}\rangle^{0+} = 1.35675\vert X_0\rangle - 0.0447316\vert X_{2AC}\rangle$	*9.08979*	*0.613973*	*0.947366*
	$\vert Y_{AC\text{-Ib}}\rangle^{1+} = \vert Y_{A\text{-b}}\rangle + \vert Y_{C\text{-Ib}}\rangle$	17.9079	2.19638 $\boldsymbol{i}$	1.86641
Ic	$\vert Y_{A\text{-Ic}}\rangle = -0.851715\vert X_0\rangle + 9.25362\cdot 10^{-7}\vert X_{3A}\rangle$	8.96309	0.475327	0.934161
	$\vert Y_{C\text{-Ic}}\rangle = -0.426598\vert X_0\rangle + 4.93426\cdot 10^{-6}\vert X_{3C}\rangle$	8.95817	0.469161	0.933648
	$\vert Y_{AC\text{-Ic}}\rangle^{0+} = -0.555261\vert X_0\rangle + 9.12119\cdot 10^{-7}\vert X_{3AC}\rangle$	*8.99267*	*0.510889*	*0.937244*
	$\vert Y_{AC\text{-Ic}}\rangle^{1+} = \vert Y_{A\text{-Ic}}\rangle + \vert Y_{C\text{-Ic}}\rangle$	17.8233	2.20167 $\boldsymbol{i}$	1.8576
IIa	$\vert Y_{A\text{-IIa}}\rangle = 3.01778\vert X_0\rangle - 0.572955\vert X_{1A}\rangle - 1.59437\vert X_{2A}\rangle$	8.96021	0.47173	0.933861
	$\vert Y_{C\text{-IIa}}\rangle = 0.624239\vert X_0\rangle + 0.0453509\vert X_{1C}\rangle - 0.123924\vert X_{2C}\rangle$	9.06885	0.59317	0.945183
	$\vert Y_{AC\text{-IIa}}\rangle^{0+} = 1.63496\vert X_0\rangle + 0.138794\vert X_{1AC}\rangle - 0.0539568\vert X_{2AC}\rangle$	*9.1014*	*0.62522*	*0.948575*
	$\vert Y_{AC\text{-IIa}}\rangle^{1+} = \vert Y_{A\text{-a}}\rangle + \vert Y_{C\text{-IIa}}\rangle$	17.9161	2.1931 $\boldsymbol{i}$	1.86727
IIb	$\vert Y_{A\text{-IIb}}\rangle = -1.03967\vert X_0\rangle + 0.134654\vert X_{1A}\rangle + 8.88035\cdot 10^{-7}\vert X_{3A}\rangle$	8.96426	0.476781	0.934283
	$\vert Y_{C\text{-IIb}}\rangle = -0.468198\vert X_0\rangle - 0.143221\vert X_{1C}\rangle + 3.63796\cdot 10^{-6}\vert X_{3C}\rangle$	8.99112	0.50908	0.937082
	$\vert Y_{AC\text{-IIb}}\rangle^{0+} = -0.48744\ \vert X_0\rangle - 0.0777712\vert X_{1AC}\rangle + 8.08314\cdot 10^{-7}\vert X_{3AC}\rangle$	*8.99774*	*0.51675*	*0.937772*
	$\vert Y_{AC\text{-IIb}}\rangle^{1+} = \vert Y_{A\text{-Ib}}\rangle + \vert Y_{C\text{-IIb}}\rangle$	17.8793	2.21324 $\boldsymbol{i}$	1.86343
IIc	$\vert Y_{A\text{-IIc}}\rangle = 0.0383859\vert X_0\rangle - 0.445991\vert X_{2A}\rangle + 6.44823\cdot 10^{-7}\vert X_{3A}\rangle$	8.96808	0.481497	0.93468
	$\vert Y_{C\text{-IIc}}\rangle = 0.657036\vert X_0\rangle - 0.185992\vert X_{2C}\rangle - 4.45973\cdot 10^{-6}\vert X_{3C}\rangle$	9.09155	0.615686	0.947549
	$\vert Y_{AC\text{-IIc}}\rangle^{0+} = 1.26793\vert X_0\rangle - 0.040945\vert X_{2AC}\rangle + 1.19517\cdot 10^{-7}\vert X_{3AC}\rangle$	9.09116	0.615307	0.947508
	$\vert Y_{AC\text{-IIc}}\rangle^{1+} = \vert Y_{A\text{-IIc}}\rangle + \vert Y_{C\text{-Ic}}\rangle$	17.9586	2.19937 $\boldsymbol{i}$	1.8717
III	$\vert Y_{A\text{-III}}\rangle = 0.893032\vert X_0\rangle - 0.218536\vert X_{1A}\rangle - 0.721371\vert X_{2A}\rangle + 5.32183\cdot 10^{-7}\vert X_{3A}\rangle$	8.96926	0.482946	0.934803
	$\vert Y_{C\text{-III}}\rangle = 1.38233\vert X_0\rangle + 0.223392\vert X_{1C}\rangle - 0.299344\vert X_{2C}\rangle - 8.16291\cdot 10^{-6}\vert X_{3C}\rangle$	9.12145	0.644232	0.950666
	$\vert Y_{AC\text{-III}}\rangle^{0+} = 1.53849\vert X_0\rangle + 0.141501\vert X_{1AC}\rangle - 0.0497924\vert X_{2AC}\rangle + 1.37119\cdot 10^{-7}\vert X_{3AC}\rangle$	9.10319	0.62694	0.948762
	$\vert Y_{AC\text{-III}}\rangle^{1+} = \vert Y_{A\text{-III}}\rangle + \vert Y_{C\text{-III}}\rangle$	17.9531	2.17933 $\boldsymbol{i}$	1.87113

Table 3: The values of the cosines of the anion-cationic vectorial angles [4], for all considered modes of action of Table 2, for the $|1+\rangle$ states of the ionic liquids of Table 1.

Mode	Ia	Ib	Ic	IIa	IIb	IIc	III
$\cos\theta_{AC}$	0.985468	0.976338	0.978196	0.975018	0.983081	0.97768	0.969683

both anionic and cationic fragments have quite important contribution to the "length" and "intensity" of ionic liquids ecotoxicity through the computed spectral norms and algebraic correlation factors, respectively, very close to the experimental one, that is, to 9.59481. Then, in all cases, the mode of action in which all three Hansch factors were considered (mode III with Log$P$ + POL + E_{TOT}) records the best norm and correlations being the closest description of the ionic liquids *Daphnia magna* chemical-biological interaction.

As well, the cationic influence is found with the dominant contribution over the anionic effects in ecotoxicity, in all considered Hansch modes of action. Nevertheless, the statistical correlation factors always yield lower values than the corresponding algebraically ones. Moreover, with the $|1+\rangle$ model, there are even recorded imaginary statistical correlations of the computed endpoints $|Y_{AC\text{-Mode}}\rangle^{1+}$; whereas the algebraical outputs give almost the sum of the anionic and cationic length and intensity endpoint activity. This can be phenomenologically explained by the so-called resonance effect when almost zero angles between the anionic and cationic endpoint vectors, for all molecular modes of actions of Table 2, are obtained as clearly evidenced by the

Table 4: Synopsis of the statistic and algebraic values of the paths connecting the S-SAR models of Table 2, in the norm correlation spectral space, for *Daphnia magna* species against the ionic liquids toxicity of Table 1; the primary (α), secondary (β), and tertiary (γ) paths are indicated according to the "selection" and "validation" principles in norm correlation spectral space when the statistic and algebraic variants of the correlation factors are, respectively, used.

Path	Cationic		Anionic		Ionic liquid			
					State $\|0+\rangle$		State $\|1+\rangle$	
	Statistic	*Algebraic*	*Statistic*	*Algebraic*	*Statistic*	*Algebraic*	*Statistic*	*Algebraic*
Ia-IIa-III	0.299988	0.200851	**0.256742** γ	0.13874	0.330033	**0.213862** γ	0.260535	0.266181
Ia-IIb-III	**0.300103** γ	0.200851	0.2567	0.13874	**0.330581** γ	0.213862	**0.25639** γ	**0.266181** γ
Ia-IIc-III	0.299895	**0.200851** γ	0.25666	**0.13874** γ	0.33011	0.213862	0.269477+ R* ***i***	0.277223
Ib-IIa-III	**0.07607** α	**0.0548409** α	0.034447	**0.0215298** β	0.0186427	0.0134673	**0.0418672** α	**0.0454552** α
Ib-IIb-III	0.299514	0.207241	0.0344468	0.0215298	0.286398	0.198562	0.0886683	0.102966
Ib-IIc-III	0.0760732	0.0548409	**0.0344464** β	0.0215298	**0.0186427** α	**0.0134673** α	0.0506137+ R* ***i***	0.0564973
Ic-IIa-III	0.23953	0.16417	0.0190146	0.0119873	**0.160257** β	0.111113	0.126723	0.130484
Ic-IIb-III	0.23952	**0.16417** β	**0.00980164** α	**0.00619966** α	0.160264	**0.111113** β	**0.120323** β	**0.130484** β
Ic-IIc-III	**0.239484** β	0.16417	0.00980164	0.00619966	0.16027	0.111113	0.135252+ R* ***i***	0.141526

[*] R = 0.0192723.

cosines values of Table 3 [4]. Instead, within $|0+\rangle$ model, all the lengths and intensities of the endpoints $|Y_{AC\text{-Mode}}\rangle^{0+}$ approach a kind of average of anionic and cationic ecotoxicological effects with a smooth increase over the individual cationic effects for the modes Ib (POL), Ic (E_{TOT}), IIa (Log$P$ + POL), and IIb (Log$P$ + E_{TOT}). However, to further decide which of these modes is further selected by the binding mechanism, the remaining spectral ecotoxicological principles, namely, the selection and validation principles are finally employed with the results collected in Table 4. It is interesting that although different in their analytical formulations, the $|0+\rangle$ and $|1+\rangle$ models furnish the same hierarchies of the paths for the chemical-biological actions (see Table 4). Worth mentioning that the statistical imaginary correlation values for the ionic liquids $|1+\rangle$ states in Table 2 extend their behavior in Table 4 too; however, these paths are excluded from the validation principle. It is observed that if the alpha (α) path starts with *Ib* (on POL) molecular mode of action in the ionic liquid $|0+\rangle$ state, the alpha path in ionic liquid $|1+\rangle$ state begins with the same molecular mode of action even following different intermediate mode until the common final *III* endpoint mode.

The same happens also with the beta (β) and gamma (γ) paths of considered ionic liquids *Daphnia magna* ecotoxicity. However, this rule is not met at the cationic and anionic fragments, while the dominant cationic effects can be noted also at the least paths level since the nature of cationic mechanism is preserved to the ionic liquids nature according with the spectral path equations: $\alpha_c + \beta_A = \alpha_{IL}$, $\beta_c + \alpha_A = \beta_{IL}$, and $\gamma_c + \gamma_A = \gamma_{IL}$.

Finally, the results of all spectral SAR ecotoxicological principles applied to ionic liquids *Daphnia magna* case of chemical ecobiological interaction can be unitarily presented in Figure 1, where the spectral hypersurface was generated by the 3D interpolation of all lengths (norms) for all the endpoint modes of Table 2, and for all cationic, anionic, $|0+\rangle$, and $|1+\rangle$ states of ionic liquids of Table 1.

The alpha dominant paths are easily identified, according with Table 4, as originating in the *Ib* , that is, on Polarizability or on van-der-Waals molecular mode of action, while the beta and gamma ones start with the steric (*Ic* : E_{TOT}) and hydrophobic (*Ia* : Log P) specific chemical-biological binding, respectively.

4. CONCLUSIONS

In the context of quantitative structure-activity relationship ecotoxicological studies, the spectral SAR model is firstly employed to produce the so-called spectral ecotoxicological principles. The particular case of *Daphnia magna* was presented respecting a selected series of 17-ionic-liquid ecotoxicity, within the introduced cationic-anionic Hansch models by the additive factors and endpoints, the $|0+\rangle\&|1+\rangle$ S-SAR-IL states, respectively. The application of the spectral ecotoxicological principles on this chemical-biological coupled system revealed that the cationic fragments clearly dominate the anionic effects by driving the containing ionic-liquid-specific interaction paths. Moreover, it was found that the $|0+\rangle$ state may be identically transformed into $|1+\rangle$ state respecting the origin of specific interaction while producing different intermediate paths through the recorded endpoints. The resonance effect, manifested when the anionic and cationic endpoint vectors are almost parallel in the additive $|1+\rangle$ state of ionic liquids, was also met for the *Daphnia magna* case; whereas with the model $|0+\rangle$, the associate imaginary statistical correlations and activity paths are avoided. Overall, it resulted that the primary path of bonding between the working ionic liquids and *Daphnia magna* species occurs via molecular polarizability, thus emphasizing on the long-range chemical-biological interaction, followed by the steric and the hydrophobic Hansch mechanisms through the beta and gamma manifested paths. Nevertheless, the presented methodology leaves with the possibility of analytical characterization of bio-and ecoactivity of other species against

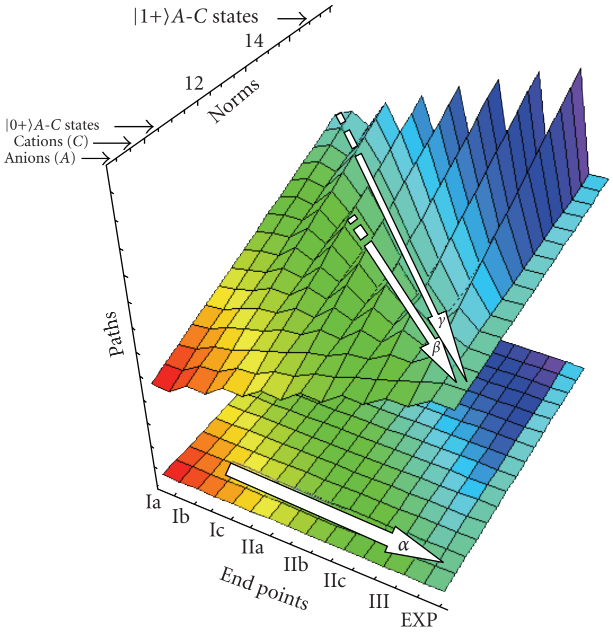

Figure 1: The spectral hypersurface of the structural hierarchical paths towards the recorded (EXP) ecotoxicological activity (in the extreme right hypersurface region) of the ionic liquids of Table 1 on *Daphnia magna* species: the alpha path (α) initiates on the polarizability (POL) anionic-cationic interaction (in the left-bottom hypersurface region), being followed by the beta path (β) which originates on the steric (*Ic*) anionic-cationic interaction (in the left-top hypersurface region hypersurface region), and successively by the gamma path (γ) based on the hydrophobic (*Ia*) anionic-cationic interaction (in the extreme left-top hypersurface region) of the norm correlation spectral space of Table 2, with the decaying order of the thickness of the connecting arrows, respectively.

given set of trained or new synthesized chemicals as well as for the interspecies correlations.

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