computational approach is as follows. First, we select the substructure whose contribution to the moments we would like to determine. Then we generate all the fragments (sub-graphs) which are contained in the corresponding substructure, and calculate the spectral moments for both, the substructure and all their fragments. The contribution of the substructure to the spectral moments is finally obtained as the difference between the spectral moments of the substructure and all those from their fragments. Having the contributions of the different structural fragments in which we are interested we only need to substitute these contributions into the quantitative model developed to describe the property studied, *e.g.*, model (1), and we obtain the quantitative contribution of the different fragments to *P*.

DATASETS AND COMPUTATIONAL STRATEGIES

In this study we have selected a data set of 43 nitrobenzene compounds for which the partition coefficient n-octanol/water and the toxicity to *Tetrahymena pyriformis* were reported in the literature [28]. The toxicity parameter studied here is the 50% growth inhibitory concentration of nitrobenzenes to *Tetrahymena pyriformis* strain GL-C ($\log IGC_{50}^{-1}$). The details of the determination of toxicity of nitrobenzene derivatives are given in the work of Cronin *et al.* [28]. The experimental values of $\log IGC_{50}^{-1}$ are given in Table I.

TABLE I Experimental and predicted values of toxicity to *Tetrahymena pyriformis* ($\log IGC_{50}^{-1}$) of nitrobenzenes

No.	*Compound*	$\log IGC_{50}^{-1}$ *Exp.*[a]	$\log IGC_{50}^{-1}$ *Cal.*[b]
1	2,6-Dimethylnitrobenzene	0.30	0.51
2	Pentachloronitrobenzene	NT	–[c]
3	2,3-Dimethylnitrobenzene	0.56	0.51
4	2-Methyl-3-chloronitrobenzene	0.68	0.74
5	2-Methylnitrobenzene	0.052	0.30
6	2-Chloronitrobenzene	0.68	0.52
7	2-Methyl-5-chloronitrobenzene	0.82	0.74
8	2,4,5-Trichloronitrobenzene	1.53	1.41
9	2,5-Dichloronitrobenzene	1.13	0.97
10	6-Chloro-1,3-dinitrobenzene	1.98	1.63
11	Nitrobenzene	0.14	0.08
12	3-Methylnitrobenzene	0.054	0.30
13	1,3-Dinitrobenzene	0.89	1.19
14	3,4-Dichloronitrobenzene	1.16	0.97
15	4-Methylnitrobenzene	0.17	0.30
16	1,4-Dinitrobenzene	1.30	1.19