LOGARITHMS OF SUBCOOLED VAPOR PRESSURES FOR 399 CHLOROAZOXYBENZENE CONGENERS DETERMINED BY THE RM1 SEMI-EMPIRICAL METHOD AND NEURAL NETWORK

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Abstract

Computationally predicted data on logarithm of subcooled liquid vapor pressure (log P_L) for all 399 congeners of *trans*-chloroazoxybenzene are presented. We used descriptors get from semi-empirical method RM1 using MOPAC program. The values of log P_L ranged between -6.59 and -0.93.

Introduction

*C*hloroazoxybenzenes in *trans* configuration consist a group of 399 theoretically possible congeners, which are toxicologically and environmentally relevant compounds[1]. Some of *t*-CAOBs have been identified as by-side impurity in technical grade 3,4-dichloroaniline (3,4-DCA), and also in derived of this chemical pesticides such as Diuron, Linuron or Propanil[2,3].

Materials and Methods

Initially a set of structural descriptors was computed for each of 399 CAOB congeners and based on the semi-empirical method (RM1) in the MOPAC program[4].

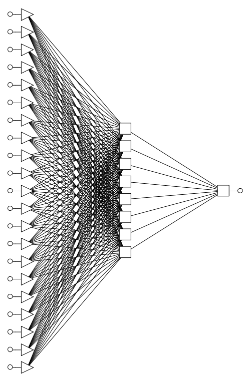

Figure 1. The architecture of the network 21-8-1.

The values on subcooled liquid vapor pressure for *t*-chloroazoxybenzene congeners from semi-empirical method were estimated using the neural network based on twenty one topological and quantum chemical descriptors such as: number of chlorine atoms in molecule (NCL), number of chlorine atoms present in the first aromatic ring (NCLP1), number of chlorine atoms present in the second aromatic ring (NCLP2), core-core repulsion (CC_REP), the solvent accessible molecular surface area in the water (CAR), the solvent accessible molecular volume in the water (CVO), the dipole moment (DIP), point group (PG), distance (D1, D2, D3), electronic energy (EE), heat of formation (HF), energy of the highest occupied molecular orbital (HO), energy of the lowest unoccupied molecular orbital (LU), ionization potential (IP), molecular weight of molecule (MW), total energy (TE), the molecular hardness (HA), the molecular softness (SO) and chemical potential (CP). These descriptors were calculated using the RM1 method and the MOPAC program. The architecture of the network used was 21-8-1 (Fig. 1).

Table 1. Characteristics of used neural network

Characterictics of neural networks:	**RM1**
Complexity of the model	21:8:1
RMSEP for the training set	0.475
RMSEP for the validation set	0.428
RMSEP for the test set	0.537
Correlation coefficient for the training set	0.939
Correlation coefficient for the validation set	0.947
Correlation coefficient for the test set	0.914
Numbers of backpropagation (BP) learning epochs	50
Numbers of conjugate gradient descent (CG) learning epochs	77

The neural networks with variable selection using a genetic algorithm (GA-NN) were applied. For each property, a set of congeners, for which experimental data are available, was divided into training and validation subsets. The models were compared taking into account their predictive ability, measured by means of the root mean square error of prediction (RMSEP) for the validation set, and the complexity of the model, expressed as the number of independent variables (descriptors) used.

Results and Discussion

The results obtained using a semi-empirical method of neural network together with calculated log P_L are presented in Table 2.

Table 2. The values of log P_L for all 399 *t*-chloroazoxybenzene congeners

Substitution pattern	log P_L	Substitution pattern	log P_L	Substitution pattern	log P_L	Substitution pattern	log P_L
2	-1.03	2,2´,6,6´	-3.13	2´,3,3´,4,4´	-3.37	2,3,3´,4,4´,6	-3.89
2´	-0.93	2,3,3´,4	-4.08	2,3,3´,4,5	-4.83	2´,3,3´,4,4´,6´	-4.81
3	-1.02	2,3,3´,4´	-4.10	2,3,3´,4´,5	-4.73	2,3,3´,4,5,5´	-5.33
3´	-1.75	2´,3,3´,4	-2.72	2,3,3´,4,5´	-4.58	2,3,3´,4´,5,5´	-2.95
4	-1.48	2´,3,3´,4´	-3.01	2,3,3´,4´,5´	-4.42	2´,3,3´,4,5,5´	-3.77
4´	-1.98	2,3,3´,5	-3.91	2´,3,3´,4,5	-3.07	2´,3,3´,4´,5,5´	-3.65
2,2´	-146	2,3,3´,5´	-3.75	2´,3,3´,4´,5	-3.25	2,3,3´,4,5,6	-5.48
2,3	-1.98	2´,3,3´,5	-2.68	2´,3,3´,4,5´	-3.40	2,3,3´,4´,5,6	-4.73
2,3´	-2.47	2´,3,3´,5´	-2.84	2´,3,3´,4´,5´	-3.36	2,3,3´,4,5´,6	-5.22
2´,3	-1.68	2,3,3´,6	-3.92	2,3,3´,4,6	-4.82	2,3,3´,4´,5´,6	-4.72
2´,3´	-2.16	2´,3,3´,6´	-3.15	2,3,3´,4´,6	-4.69	2´,3,3´,4,5,6´	-4.88
2,4	-2.22	2,3,4,4´	-4.37	2´,3,3´,4,6´	-4.15	2´,3,3´,4´,5,6´	-3.91
2,4´	-2.62	2,3´,4,4´	-4.33	2´,3,3´,4´,6´	-3.72	2´,3,3´,4,5´,6´	-4.90
2´,4	-1.60	2´,3,4,4´	-2.91	2,3,3´,5,5´	-4.61	2´,3,3´,4´,5´,6´	-4.17
2´,4´	-2.23	2´,3´,4,4´	-3.03	2´,3,3´,5,5´	-3.18	2,3,3´,5,5´,6	-4.76
2,5	-1.81	2,3,4,5	-4.02	2,3,3´,5,6	-4.19	2´,3,3´,5,5´,6´	-3.08
2´,5´	-1.93	2´,3,4,5	-2.59	2,3,3´,5´,6	-4.41	2,3´,4,4´,5,5´	-5.31
2,6	-1.88	2,3´,4,5	-4.11	2´,3,3´,5,6´	-3.35	2´,3,4,4´,5,5´	-3.91
2´,6´	-2.05	2,3,4´,5	-4.10	2´,3,3´,5´,6´	-2.84	2,3,4,4´,5,6	-5.59
3,3´	-2.20	2,3´,4´,5	-4.04	2,3,4,4´,5	-5.07	2,3´,4,4´,5´,6	-5.10
3,4	-2.56	2,3´,4,5´	-3.94	2,3´,4,4´,5	-4.94	2´,3,4,4´,5,6´	-5.15
3,4´	-2.49	2,3´,4´,5´	-3.86	2,3´,4,4´,5´	-4.63	2´,3´,4,4´,5´,6´	-4.78
3´,4	-2.78	2´,3,4´,5	-2.48	2´,3,4,4´,5	-3.44	3,3´,4,4´,5,5´	-5.82
3´,4´	-3.11	2´,3,4,5´	-2.63	2´,3,4,4´,5´	-3.27	2,2´,3,3´,4,4´,5	-4.05
3,5	-1.78	2´,3´,4,5´	-3.04	2´,3´,4,4´,5´	-3.35	2,2´,3,3´,4,4´,5´	-4.00
3´,5´	-2.69	2´,3,4´,5´	-2.82	2,3,4,4´,6	-5.09	2,2´,3,3´,4,4´,6	-5.11
4,4´	-3.12	2´,3´,4´,5´	-3.41	2,3´,4,4´,6	-4.94	2,2´,3,3´,4,4´,6´	-4.77
2,2´,3	-2.18	2,3,4,6	-4.01	2´,3,4,4´,6´	-4.38	2,2´,3,3´,4,5,5´	-3.79
2,2´,3´	-2.39	2,3´,4,6	-4.13	2´,3´,4,4´,6´	-4.29	2,2´,3,3´,4´,5,5´	-3.95
2,2´,4	-2.11	2,3,4´,6	-4.10	2,3´,4,5,5´	-4.72	2,2´,3,3´,4,5,6	-4.98
2,2´,4´	-2.46	2,3´,4´,6	-4.07	2,3´,4´,5,5´	-4.51	2,2´,3,3´,4,5´,6	-4.39
2,2´,5	-1.69	2´,3,4,6´	-3.52	2´,3,4,5,5´	-3.35	2,2´,3,3´,4,5,6´	-4.99
2,2´,5´	-2.26	2´,3´,4,6´	-2.79	2´,3,4´,5,5´	-3.41	2,2´,3,3´,4,5´,6´	-4.88
2,2´,6	-2.25	2´,3,4´,6´	-3.43	2,3,4,5,6	-4.70	2,2´,3,3´,4´,5,6	-5.19
2,2´,6´	-2.01	2´,3´,4´,6´	-3.19	2,3,4´,5,6	-4.53	2,2´,3,3´,4´,5´,6	-3.97
2,3,3´	-3.21	2,3´,5,5´	-3.83	2,3´,4,5´,6	-4.56	2,2´,3,3´,4´,5,6´	-4.92
2´,3,3´	-2.30	2´,3,5,5´	-2.72	2,3´,4´,5´,6	-4.31	2,2´,3,3´,4´,5´,6´	-4.64
2,3,4	-3.16	2,3,5,6	-3.48	2´,3,4,5,6´	-4.11	2,2´,3,3´,4,6,6´	-4.09
2,3´,4	-3.35	2,3´,5´,6	-3.75	2´,3,4´,5,6´	-3.76	2,2´,3,3´,4´,6,6´	-4.78
2,3,4´	-3.35	2´,3,5,6´	-2.96	2´,3´,4,5,6´	-4.27	2,2´,3,3´,5,5´,6	-5.19
2,3´,4´	-3.51	2´,3´,5´,6´	-3.78	2´,3´,4´,5´,6´	-4.29	2,2´,3,3´,5,5´,6´	-3.24
2´,3,4	-2.04	2,4,4´,5	-4.41	3,3´,4,4´,5	-5.37	2,2´,3,3´,5,6,6´	-4.91
2´,3´,4	-2.32	2´,4,4´,5´	-2.91	3,3´,4,4´,5´	-5.13	2,2´,3,3´,5´,6,6´	-4.74
2´,3,4´	-2.33	2,4,4´,6	-4.40	3,3´,4,5,5´	-5.16	2,2´,3,4,4´,5,5´	-4.07

2´,3´,4´	-2.85	2´,4,4´,6´	-3.76	3,3´,4´,5,5´	-4.20	2,2´,3,4,4´,5,6	-5.37
2,3,5	-1.39	3,3´,4,4´	-4.74	2,2´,3,3´,4,4´	-3.67	2,2´,3,4,4´,5´,6	-4.42
2,3´,5	-3.08	3,3´,4,5	-4.46	2,2´,3,3´,4,5	-3.21	2,2´,3,4,4´,5,6´	-5.15
2,3´,5´	-3.13	3,3´,4´,5	-3.65	2,2´,3,3´,4´,5	-3.58	2,2´,3´,4,4´,5,5´	-3.69
2´,3,5	-1.62	3,3´,4,5´	-4.34	2,2´,3,3´,4,5´	-3.62	2,2´,3´,4,4´,5,6´	-5.17
2´,3,5´	-2.52	3,3´,4´,5´	-3.74	2,2´,3,3´,4´,5´	-3.75	2,2´,3´,4,4´,5´,6	-4.47
2´,3´,5´	-2.83	3,3´,5,5´	-3.52	2,2´,3,3´,4,6	-3.76	2,2´,3´,4,4´,5´,6´	-4.90
2,3,6	-2.85	3,4,4´,5	-4.75	2,2´,3,3´,4´,6	-3.74	2,2´,3,4,4´,6,6´	-5.06
2,3´,6	-3.17	3´,4,4´,5´	-4.48	2,2´,3,3´,4,6´	-4.23	2,2´,3´,4,4´,6,6´	-5.04
2´,3,6´	-2.59	2,2´,3,3´,4	-3.15	2,2´,3,3´,4´,6´	-4.18	2,2´,3,4,5,5´,6	-4.62
2´,3´,6´	-3.01	2,2´,3,3´,4´	-3.52	2,2´,3,3´,5,5´	-2.88	2,2´,3,4,5,6,6´	-4.73
2,4,4´	-3.67	2,2´,3,3´,5	-3.08	2,2´,3,3´,5,6	-4.54	2,2´,3,4´,5,5´,6	-4.47
2´,4,4´	-2.46	2,2´,3,3´,5´	-3.34	2,2´,3,3´,5´,6	-3.49	2,2´,3,4´,5,6,6´	-5.10
2,4,5	-3.12	2,2´,3,3´,6	-3.82	2,2´,3,3´,5,6´	-4.67	2,2´,3´,4,5,5´,6´	-5.21
2,4´,5	-3.29	2,2´,3,3´,6´	-3.70	2,2´,3,3´,5´,6´	-3.50	2,2´,3´,4,5´,6,6´	-4.08
2´,4,5´	-2.36	2,2´,3,4,4´	-3.16	2,2´,3,3´,6,6´	-4.21	2,2´,3´,4´,5,5´,6´	-5.02
2´,4´,5´	-2.67	2,2´,3´,4,4´	-3.35	2,2´,3,4,4´,5	-3.75	2,2´,3´,4´,5´,6,6´	-4.65
2,4,6	-1.89	2,2´,3,4,5	-2.81	2,2´,3,4,4´,5´	-4.34	2,3,3´,4,4´,5,5´	-5.88
2,4´,6	-3.33	2,2´,3´,4,5	-2.81	2,2´,3,4,4´,6	-4.86	2,3,3´,4,4´,5,6	-4.04
2´,4,6´	-2.86	2,2´,3,4´,5	-3.28	2,2´,3,4,4´,6´	-4.92	2,3,3´,4,4´,5´,6	-5.70
2´,4´,6´	-3.15	2,2´,3,4,5´	-3.10	2,2´,3´,4,4´,5	-3.32	2´,3,3´,4,4´,5,5´	-4.16
3,3´,4	-3.68	2,2´,3´,4´,5	-3.00	2,2´,3´,4,4´,5´	-3.61	2´,3,3´,4,4´,5,6´	-5.26
3,3´,4´	-3.15	2,2´,3´,4,5´	-3.21	2,2´,3´,4,4´,6	-3.99	2´,3,3´,4,4´,5´,6´	-4.26
3,3´,5	-2.75	2,2´,3,4´,5´	-3.35	2,2´,3´,4,4´,6´	-4.48	2,3,3´,4,5,5´,6	-5.86
3,3´,5´	-2.96	2,2´,3´,4´,5´	-3.42	2,2´,3,4,5,5´	-3.52	2,3,3´,4´,5,5´,6	-5.19
3,4,4´	-4.02	2,2´,3,4,6	-2.98	2,2´,3´,4,5,5´	-3.30	2´,3,3´,4,5,5´,6´	-4.24
3´,4,4´	-4.03	2,2´,3´,4,6	-3.36	2,2´,3,4´,5,5´	-3.17	2´,3,3´,4´,5,5´,6´	-4.30
3,4,5	-3.45	2,2´,3,4´,6	-4.01	2,2´,3´,4´,5,5´	-4.46	2,2´,3,3´,4,4´,5,5´	-4.33
3,4´,5	-3.17	2,2´,3,4,6´	-2.94	2,2´,3,4,5,6	-4.41	2,2´,3,3´,4,4´,5,6	-5.73
3´,4,5´	-3.58	2,2´,3´,4´,6	-3.57	2,2´,3,4´,5,6	-4.78	2,2´,3,3´,4,4´,5´,6	-4.95
3´,4´,5´	-3.67	2,2´,3´,4,6´	-3.94	2,2´,3,4,5´,6	-4.16	2,2´,3,3´,4,4´,5,6´	-5.56
2,2´,3,3´	-2.89	2,2´,3,4´,6´	-3.75	2,2´,3,4,5,6´	-4.34	2,2´,3,3´,4,4´,5´,6´	-5.22
2,2´,3,4	-2.63	2,2´,3´,4´,6´	-3.94	2,2´,3´,4,5´,6	-3.54	2,2',3,3´,4,4´,6,6´	-5.43
2,2´,3´,4	-2.73	2,2´,3,5,5´	-2.71	2,2´,3´,4,5,6´	-4.70	2,2´,3,3´,4,5,5´,6	-5.01
2,2´,3,4´	-2.59	2,2´,3´,5,5´	-3.02	2,2´,3,4´,5´,6	-3.59	2,2´,3,3´,4,5,5´,6´	-5.71
2,2´,3´,4´	-3.06	2,2´,3,5,6	-2.59	2,2´,3,4´,5,6´	-4.50	2,2´,3,3´,4´,5,5´,6	-4.72
2,2´,3,5	-2.33	2,2´,3,5´,6	-3.44	2,2´,3´,4´,5´,6	-4.01	2,2´,3,3´,4´,5,5´,6´	-5.35
2,2´,3´,5	-2.54	2,2´,3,5,6´	-3.78	2,2´,3´,4´,5,6´	-4.45	2,2´,3,3´,4,5,6,6´	-4.80
2,2´,3,5´	-2.53	2,2´,3´,5´,6	-3.34	2,2´,3´,4,5´,6´	-3.79	2,2´,3,3´,4,5´,6,6´	-4.52
2,2´,3´,5´	-2.93	2,2´,3´,5,6´	-3.93	2,2´,3´,4´,5´,6´	-4.30	2,2´,3,3´,4´,5,6,6´	-5.49
2,2´,3,6	-3.25	2,2´,3´,5´,6´	-3.44	2,2´,3,4,6,6´	-4.15	2,2´,3,3´,4´,5´,6,6´	-5.18
2,2´,3´,6	-3.00	2,2´,3,6,6´	-3.66	2,2´,3,4´,6,6´	-4.35	2,2´,3,3´,5,5´,6,6´	-5.63
2,2´,3,6´	-3.04	2,2´,3´,6,6´	-3.20	2,2´,3´,4,6,6´	-3.74	2,2´,3,4,4´,5,5´,6	-5.06
2,2´,3´,6´	-3.36	2,2´,4,4´,5	-3.17	2,2´,3´,4´,6,6´	-4.29	2,2´,3,4,4´,5,6,6´	-5.63
2,2´,4,4´	-2.92	2,2´,4,4´,5´	-3.25	2,2´,3,5,5´,6	-4.57	2,2´,3´,4,4´,5,5´,6´	-5.53
2,2´,4,5	-2.48	2,2´,4,4´,6	-3.68	2,2´,3,5,6,6´	-4.30	2,2´,3´,4,4´,5´,6,6´	-5.39
2,2´,4´,5	-2.54	2,2´,4,4´,6´	-4.05	2,2´,3´,5,5´,6´	-2.94	2,3,3´,4,4´,5,5´,6	-6.28
2,2´,4,5´	-2.66	2,2´,4,5,5´	-2.94	2,2´,3´,5´,6,6´	-3.44	2´,3,3´,4,4´,5,5´,6´	-6.08

2,2´,4´,5´	-2.97	2,2´,4´,5,5´	-3.00	2,2´,4,4´,5,5´	-3.48	2,2´,3,3´,4,4´,5,5´,6	-6.25
2,2´,4,6	-3.15	2,2´,4,5´,6	-3.49	2,2´,4,4´,5´,6	-4.04	2,2´,3,3´,4,4´,5,5´,6´	-6.54
2,2´,4´,6	-3.06	2,2´,4,5,6´	-3.93	2,2´,4,4´,5,6´	-4.73	2,2´,3,3´,4,4´,5,6,6´	-6.06
2,2´,4,6´	-3.31	2,2´,4´,5´,6	-3.52	2,2´,4,4´,6,6´	-4.68	2,2´,3,3´,4,4´,5´,6,6´	-5.91
2,2´,4´,6´	-3.40	2,2´,4´,5,6´	-3.89	2,3,3´,4,4´,5	-5.53	2,2´,3,3´,4,5,5´,6,6´	-5.28
2,2´,5,5´	-2.42	2,2´,4,6,6´	-3.77	2,3,3´,4,4´,5´	-3.29	2,2´,3,3´,4´,5,5´,6,6´	-6.08
2,2´,5´,6	-2.78	2,2´,4´,6,6´	-3.83	2´,3,3´,4,4´,5	-3.54	2,2´,3,3´,4,4´,5,5´,6,6´	-6.59
2,2´,5,6´	-3.17	2,3,3´,4,4´	-4.92	2´,3,3´,4,4´,5´	-3.66		

T-chloroazoxybenzenes might be divided into three main classes of volatility based on values of log P_L. Monochloroazoxybenzenes might be classified as relatively easily volatile, because the values of log P_L ranged from -2 to 0. Few of di- and trichloroazoxybenzenes might be classified as relatively easily volatile, and other might be classified as relatively low volatile. All isomers of octa- and nona-*t*-CAOB and decachloroazoxybenzene might be classified as low volatile because their values of logarithm of subcooled liquid vapor pressure are below -4.

Acknowledgements

Computations were carried out using computers in the TASK - Academic Computer Center in Gdańsk. Financial support under grant no. DS/8250-4-0092-9.

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