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QSPR STUDY FOR BOILING POINTS OF ALKANES

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KEYWORDS:

Derivatives of alkane, QSPR, Quantum Chemical Descriptors, Correlation Coefficient, PM3.

ABSTRACT

Quantitative structure activity relationship (QSPR) models of 75 alkane derivatives were created using quantum chemical descriptors.For molecular modelling and geometry optimization, the CACheprogramme was employed. Using the PM3 approach, MOPAC2002 estimated the values of several quantum chemical descriptors. The boiling points of alkane derivatives may be predicted very precisely throughout this investigation based on the cross validation coefficient and correlation coefficient results. Better results are obtained when total energy is combined with additional quantum chemical descriptors.

1. INTRODUCTION

QSPR study of molecules has been developed some thirty five years ago[1-2]. It has now developed into a tool for predicting the qualities of molecules. It relates the molecular properties to the molecular structure[3-4]. Molecular structural variations alter the molecular properties which can be predicted by QSPR study[5-6]. Determination of boiling points experimentally becomes technically challenging sometimes. If the boiling points are relatively higher the molecules start polymerizing before boiling points. Similarly if the boiling points are relatively lower there may occur explosion. Here lies the importance of

QSPR[7-11].Seventy five derivative of alkane have been chosen for the present study. QSPR models were created using the quantum chemical descriptors listed below.

S.No.	Quantum Chemical Descriptor	Symbol
1	Total Energy (Hartree)	TE
2	LUMO Energy (eV)	εLUMO
3	HOMO Energy (eV)	εHOMO
4	Heat of Formation (Kcal/mole)	ΔHf
5	Global Softness	S
6	Electronegativity	χ
7	Absolute Hardness	η
8	Molecular Weight	MW

Materials & Methods:

Seventy-five alkane derivatives were selected from the literature and employed as research materials. They are presented in table-1 along with their boiling points in degrees Celsius. CAChe software has been used to carry out the molecular modelling and geometry optimization of all the derivatives.[12-14]. MOPAC 2002 determined the values of different quantum chemical descriptors using the PM3 method as well as other well-known approaches.[15-22].

Results & Discussion:

QSPR models of derivatives of alkane for the prediction of boiling points have been carried out in the various combinations of quantum chemical descriptors.By use of multilinear regression, a total of 162 QSPR models (PB1-PB162) have been constructed. Most of the QSPR models were shown to have excellent prediction performance, with correlation coefficient and cross validation coefficient values more than 0.5 and 0.2, respectively. The best QSPR model is PB160. It uses Total Energy, HOMO Energy, Molecular Weight and Global Softness as the quantum chemical descriptors. The MLR equation for the best QSPR model is as follows-

PB160=-4.7517*TE+0.0441924*MW-15.2766*η-1731.21*S+80.1871

rCV^2=0.907049 , r^2=0.935849

Total energy alone is capable of producing QSPR model having good predicting power with MLR equation-

PB4=-4.77189*TE-147.317 (rCV^2=0.917029, r^2=0.930272)

Conclusion:

The best QSPR model for predicting boiling temperatures of alkane derivatives was constructed using the descriptors absolute hardness, total energy, molecular weight, and global softness. The correlation coefficient is 0.935849, indicating that this QSPR model has the greatest predictive capacity of all the models developed and can be used to forecast the boiling point of any alkane or its derivatives. With a correlation coefficient of 0.930272, total energy alone can build a solid QSPR model. A decent QSPR model may be created from any combination of descriptors with total energy.

Table-1: Derivatives of Alkane with their boiling points in ^{0}C

S. N.	Alkane	Exp. B.P.(^{0}C)	S. N.	Alkane	Exp. B.P.(^{0}C)
1	hexane	68.7	39	2,4-dimethylhexane	109.4
2	2-methylpentane	60.3	40	2,2-dimethylhexane	106.8
3	2,2-dimethylbutane	49.7	41	3-ethyl-2-methylpentane	115.6
4	isopropylcyclopropane	58.3	42	2,2,4-trimethylpentane	99.2
5	heptane	98.5	43	3-ethyl-3-methylpentane	118.2
6	1,1,2-trimethylcyclopropane	52.6	44	pentacyclopropane	128
7	ethylcyclobutane	70.7	45	(1-methylbutyl)cyclopropane	117.7
8	1,1-dimethylcyclobutane	53.6	46	1-butyl-2-methylcyclopropane	124
9	1-ethyl-2-methylcyclopropane	63	47	(1,2-dimethylpropyl)cyclopropane	115.5
10	2,4-dimethylpentane	80.5	48	1-isobytyl-2-methycyclopropane	110
11	bicyclo[2.2.0]hexane	83	49	bicyclo[3.3.0]octane	137
12	I-methylbicyclo[2.1.0]pentane	60.5	50	1,1,2,2,3-pentamethylcyclopropane	100.5
13	methylcyclopentane	71.8	51	sec-butylcyclobutane	123
14	2-methylhexane	90	52	1,2-diethylcyclobutane	119

15	1,1'-bi(cyclopropyl)	76	53	propylcyclopentane	131
16	2,3-dimethylpentane	89.8	54	isopropylcyclopentane	126.4
17	2,2,3-trimethylbutane	80.9	55	1,2,4-trimethylcyclopentane	115
18	butylcyclopropane	98	56	1-ethyl-1-methylcyclopentane	121.5
19	1,2-diethylcyclopropane	90	57	1,1,2-trimethylcyclopentane	114
20	1-methyl-1-propylcyclopropane	84.9	58	1-ethyl-cyclohexane	131.8
21	1,1-diethylcyclopropane	88.6	59	1,2-dimethylcyclohexane	126.6
22	1-isopropyl-1methylcyclopropane	81.5	60	1,1-dimethylcyclohexane	119.5
23	(cyclopropylmethyl)cyclopropane	102	61	(2-cyclopropylethyl)cyclopropane	129
24	1,1,2,2-tetramethylcyclopropane	78	62	2-ethyl-1,1,2-trimethylcyclopropane	104.5
25	isopropylcyclobutane	92.7	63	bicyclo[5.1.0]octane	141.0
26	1-ethyl-3-methylcyclobutane	89.5	64	2-methylbicyclo[2.2.1]heptane	125
27	1,3-dimethylcyclopentane	91.3	65	2-methylbicyclo[3.2.0]heptane	130.5
28	1,2-dimethylcyclopentane	95.6	66	1-methylbicyclo[2.2.1]heptane	117
29	cycloheptane	118.4	67	tricyclo[3.2.1.0]	136
30	1-ethyl-1,2 dimethylcyclopropane	85.2	68	3,3-dimethylbicyclo[3.1.0]hexane	115
31	bicyclo[3.2.0]heptane	110.5	69	2,2,4,4tetramethylbicycclo[1.1.0]butane	104
32	2-methylbicyclo[3.1.0]hexane	100	70	1,2,2,3-tetramethylbicycclo[1.1.0]	105
33	1,2-diethyl-3 methylcyclopropane	105.0	71	tricyclo[5.1.0.0]	142
34	1-methylbicyclo[3.1.0]hexane	92	72	1-methylbicyclo[4.1.0]heptane	125

35	tricyclo[4.1.0.0]	105	73	3-methyltetracyclo[2.2.1.0]heptane	120.5
36	2-methylpentane	117.6	74	1-methylcyclohexane	101
37	3-methylpentane	118.9	75	2,2,3-trimethylpentane	109.8
38	3-ethylhexane	118.5			

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