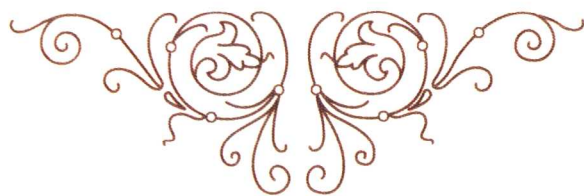


胡之德

科学论文选集(下)

《胡之德科学论文选集》编辑组 编



兰州大学出版社
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目 录

TABLE OF CONTENTS

第一部分 分离科学

- Rapid and ultrasensitive determination of ephedrine and pseudoephedrine derivatized with 5-(4,6-dichloro-s-triazin-2-ylamino) fluorescein by micellar electrokinetic chromatography with laser-induced fluorescence detection..... (1)
- Rapid and sensitive determination of ephedrine and pseudoephedrine by micellar electrokinetic chromatography with on-line regenerating covalent coating (13)
- Analysis of protoberberine alkaloids in several herbal drugs and related medicinal preparations by non-aqueous capillary electrophoresis..... (24)
- Non-aqueous capillary electrophoresis for simultaneous separation and determination of three major active components in traditional medicinal preparations..... (33)
- Determination of levodopa by capillary zone electrophoresis using an acidic phosphate buffer and its application in the analysis of beans..... (44)
- Application of nonaqueous micellar electrokinetic chromatography to the analysis of active components in *Radix Salviae miltiorrhizae* and its medicinal preparations..... (54)
- Separation and simultaneous determination of rutin, puerarin, daidzein, esculin and esculetin in medicinal preparations by non-aqueous capillary..... (62)
- Nonaqueous capillary electrophoresis for rapid and sensitive determination of fangchinoline and tetrandrine in *Radix Stephaniae tetrandrae* and its medicinal preparations..... (73)
- Quantification of glutathione and glutathione disulfide in human plasma and tobacco leave by capillary electrophoresis with laser-induced fluorescence detection (85)
- Separation and determination of gentiopicroside and swertiamarin in Tibetan medicines by micellar electrokinetic electrophoresis..... (93)

Determination of rhein, baicalin and berberine in traditional Chinese medicinal preparations by capillary electrophoresis with two-marker technique.....	(103)
Analysis of the aconitine alkaloids in traditional Chinese medicines by nonaqueous capillary electrophoresis using a new recording mode.....	(112)
Microemulsion electrokinetic chromatography with laser-induced fluorescence detection: as tested with amino acid derivatives	(122)
Simultaneous determination of some active ingredients in anti-viral preparations of traditional Chinese medicine by micellar electrokinetic chromatography	(135)
Separation and determination of two sesquiterpene lactones in <i>Radix inulae</i> and Liuwei Anxian San by microemulsion electrokinetic chromatography.....	(147)
Microemulsion electrokinetic chromatography with laser-induced fluorescence detection for sensitive determination of ephedrine and pseudoephedrine	(160)
Investigation of the components in RFCC gasoline affecting the accuracy of potentiometric titration by GC-MS and GC-IR.....	(169)
Identification of nitrogen compounds in RFCC diesel oil by mass spectrometry.....	(179)
A novel double coating for microemulsion electrokinetic chromatography with laser-induced fluorescence detection: as tested with amino acid derivatives	(189)
Separation and determination of active components in radix salviae miltiorrhizae and its medicinal preparations by nonaqueous capillary electrophoresis	(199)
Investigation of the factors that induce analyte peak splitting in capillary electrophoresis	(210)
Micellar electrokinetic chromatography with laser-induced fluorescence detection for rapid and sensitive analysis of two new bioactive reagents using dynamic covalent coating	(220)
Micellar electrokinetic chromatography with laser-induced fluorescence detection for sensitive determination of ephedrine and pseudoephedrine.....	(230)
用气相色谱质谱和气相色谱红外联用技术分析热裂解汽油C ₉ 馏分中的组分.....	(236)
Capillary electrophoresis with field-enhanced stacking for rapid and sensitive determination of strychnine and brucine	(245)
Quantification of neurotransmitter amino acids in human serums by capillary electrophoresis with laser-induced fluorescence detection.....	(252)
Quantification of noradrenaline and dopamine in <i>Portulaca oleracea</i> L by capillary electrophoresis with laser-induced fluorescence detection.....	(259)

Field-amplified sample stacking in capillary electrophoresis for on-column concentration of alkaloids in <i>Sophora flavescens</i> Ait	(268)
Separation of diastereoisomers of podophyllum lignans by micellar electrokinetic chromatography	(278)
Separation and determination of podophyllum lignans by micellar electrokinetic chromatography	(286)
Identification and determination of active components in <i>Angelica dahurica</i> Benth and its medicinal preparation by capillary electrophoresis	(295)
Electrophoretic behavior study and determination of some active components in Chinese medicinal preparations by capillary electrophoresis	(304)
Identification and determination of active components in <i>gentiana rigescens</i> franch by micellar electrokinetic chromatography	(313)
Separation and determination of alantolactone and isoalantolactone in traditional Chinese herbs by capillary electrophoresis	(317)
一种新型毛细管区带电泳谱图记录模式的研究	(324)
Identification and determination of active components in <i>Gastrodia elata</i> Bl by capillary electrophoresis	(330)
Migration behavior and separation of active components in <i>Glycyrrhiza uralensis</i> Fisch and its commercial extract by micellar electrokinetic capillary chromatography	(338)
Kinetics studies on thermal isomerization of β -N-oxalyl-L-a, β -diaminopropionic acid by capillary zone electrophoresis	(349)
Analysis of ephedrine in ephedra callus by acetonitrile modified capillary zone electrophoresis	(355)
Separation and identification of active components in the extract of Rheum natural products by microemulsion electrokinetic chromatography	(363)
The mutual relationships between applied voltage, migration time and peak area in capillary zone electrophoresis	(374)
Identification and determination of aesculin and aesculetin in ash barks by capillary zone electrophoresis	(386)
Determination of three water-soluble active ingredients in Qiangli Yinqiao containing Vc tablets by capillary zone electrophoresis	(399)

Comments on a general theory of ion-exchange chromatographic separation processes	(407)
The measurement of average hydrodynamic velocity in capillary zone electrophoresis	(411)
Separation and determination of 10-hydroxy-2-decenoic acid in royal jelly by capillary electrophoresis	(420)
Determination of palladium(II) as a chloro complex by capillary zone electrophoresis	(429)
Influence of sample injection time of ions on migration time in capillary zone electrophoresis	(436)
氨性溶液中铜、铁离子作用机理的电镜研究	(449)
Rapid Reversed-Phase Chromatographic Separation and Determination of Selenium and Tellurium	(451)
Ion flotation behaviour of thirty-one metal ions in mixed hydrochloric/nitric acid solutions	(459)
P ₃₅₀ 反向萃取柱色层分离铟及矿石中微量铟的测定	(469)
Rapid ion chromatographic separation and determination of Arsenic(III) Arsenic(V) and Molybdenum(VI) - Chromium(VI)	(474)
硒、碲的快速反相萃取色谱分离及测定	(481)
P ₃₅₀ 作为气相色谱新固定液的研究	(485)
硒和碲的 HPIEC 分离和测定	(490)
分配色谱中的两相作用	(494)
高效离子交换色谱法分离稀土元素及镓、铋、铕的测定	(495)
高效离子交换色谱法分离和测定氯溴碘	(508)
硒和碲的反相薄层色谱和溶剂萃取的研究	(516)
Extraction separation of gallium with di-sec-octyl methyl-phosphonate	(525)
高速离子交换色谱法分离碱土金属及机油添加剂中钙、锌、钡的快速测定	(530)
5-Cl-PADAB 和钡的络合物萃取性能及萃取机构的初步研究	(539)
The paper chromatographic behaviours of selenium, tellurium, copper, cadmium, bismuth, and noble metals	(550)
Application of thin-layer chromatography in inorganic analysis the separation and determination of selenium and tellurium	(555)
Separation of niobium and tantalum by reversed-phase paper chromatography	(559)
硒和碲的反相纸色层分离	(561)

贵金属和硒、碲的反相纸色层分离·····	(563)
硒和碲的溴化物萃取性能及其分离·····	(568)

第二部分 化学信息学

基于启发式方法和支持向量机方法预测药物与人血浆蛋白结合率·····	(572)
Study of quantitative structure-mobility relationship of the peptides based on the structural descriptors and support vector machines ·····	(583)
Development of migration models for acids in capillary electrophoresis using heuristic and radial basis function neural network methods·····	(602)
The prediction of human oral absorption for diffusion rate-limited drugs based on heuristic method and support vector machine ·····	(618)
Study of probabilistic neural networks to classify the active compounds in medicinal plants ·····	(637)
3D QSAR studies on antimalarial alkoxylated and hydroxylated chalcones by CoMFA and CoMSIA·····	(653)
Study of quantitative structure-mobility relationship of carboxylic acids in capillary electrophoresis based on support vector machines ·····	(669)
Support vector machines-based quantitative structure-property relationship for the prediction of heat capacity ·····	(686)
QSAR Models for the prediction of binding affinities to human serum albumin using heuristic method and support vector machine ·····	(705)
Quantitative prediction of log <i>k</i> of peptides in high-performance liquid chromatography based on molecular descriptors by using the heuristic method and support vector machine ·····	(724)
An accurate QSPR study of O-H bond dissociation energy in substituted phenols based on support vector machines·····	(742)
Study of quantitative structure-mobility relationship of carboxylic and sulphonic acids in capillary electrophoresis ·····	(761)
Quantitative structure property relationship models for the prediction of liquid heat capacity ·····	(781)
Application of artificial neural networks in multivariable optimization of an on-line microwave FIA system for catalytic kinetic determination of iridium(III)·····	(816)

Radial basis function network based QSPR for the prediction of Henry's law constant	(827)
Radial basis function neural network based QSPR for the prediction of critical temperature	(849)
Radial basis function neural networks based QSPR for the prediction of LogP.....	(861)
Radial basis function neural network based QSPR for the prediction of critical pressures of substituted benzenes	(876)
Development of a quantitative structure-property relationship model for predicting the electrophoretic mobilities	(893)
Prediction of gas chromatographic retention indices by the use of radial basis function neural networks.....	(902)
Optimization of on-line microwave flow injection analysis system by artificial neural networks for the determination of ruthenium.....	(916)
Linear and non-linear modeling for the investigation of gas chromatography retention indices of alkylbenzenes on Cit.A-4, SE-30 and Carbowax 20M	(926)
Application of artificial neural networks for the simultaneous determination of a mixture of fluorescent dyes by synchronous fluorescence	(940)
Principal component analysis and artificial neural networks applied to the classification of Chinese pottery of neolithic age	(952)
Use of artificial neural networks to predict the gas chromatographic retention index data of alkylbenzenes on carbowax-20M	(966)
Application of artificial neural networks for prediction of the retention indices of alkylbenzenes	(981)
Neural network-topological indices approach to the prediction of properties of alkene	(991)
人工神经网络用于酸性染料分类	(1005)
微波吸收法计算弛豫过程的热力学参数.....	(1011)
人工神经网络用于预测离子交换分配系数.....	(1016)
Relationship between retention behavior and molecular structure in HPLC. correlation between solubility parameter molecular properties	(1021)
The use of β_2^H , α_2^H to measure hydrogen-bond terms in reversed phase liquid chromatography	(1041)
Prediction of gas chromatographic retention indices of alkenes from the total solubility parameters	(1047)

Study on the relationship between chromatographic retention behaviour and molecular structure	(1057)
溶解度参数在色谱中的应用	(1067)
色谱保留行为与溶质分子结构间的关系	(1076)
硝酸体系中阳离子交换平衡常数与离子势之间的定量关系	(1082)
分析化学中共沉淀离子和载体的统计分析	(1086)

第三部分 生命分析化学

Human serum albumin interaction with formononetin studied using fluorescence anisotropy, FT-IR spectroscopy and molecular modeling methods	(1089)
激光散射法研究蛋白质与氨比西林钠盐的相互作用	(1100)
Binding of the bioactive component jatrorrhizine to human serum albumin	(1109)
Effect of Chinese medicine alpinetin on the structure of human serum albumin	(1121)
Specific interaction of chalcone-protein: cardamonin binding site II on HSA molecule	(1140)
Binding of wogonin to human gamma globulin	(1157)
The effect of berberine on the secondary structure of human serum albumin	(1175)
Spectroscopic studies on binding of shikonin to human serum albumin	(1187)
Probing the binding of scutellarin to human serum albumin by circular dichroism, fluorescence spectroscopy, FT-IR, and molecular modeling method	(1203)
Interactions between 1-benzoyl-4-p-chlorophenyl thiosemicarbazide and serum albumin: investigation by fluorescence spectroscopy	(1215)
Interaction of isofraxidin with human serum albumin	(1226)
Binding of isofraxidin to bovine serum albumin	(1238)
Study of the interaction of kaempferol with bovine serum albumin	(1248)
Spectrofluorimetric study of the binding of daphnetin to bovine serum albumin	(1259)
Binding of wogonin to human serum albumin: a common binding site of wogonin in subdomain IIA	(1268)
Binding of the bioactive component daphnetin to human serum albumin demonstrated using tryptophan fluorescence quenching	(1281)
Interaction of magnolol with bovine serum albumin: a fluorescence-quenching study	(1291)

- Determination of nucleic acids with crystal violet by a resonance light-scattering technique
..... (1299)
- Study of the interaction of protein and dibromomethyl-Arsenazo-Al(III) by Rayleigh
light-scattering technique..... (1310)
- Homogeneous time-resolved fluorescence DNA hybridization assay by DNA-mediated formation
of an EDTA-Eu(III)- β -diketonate ternary complex..... (1320)
- The high-sensitivity determination of protein concentrations by the enhancement of Rayleigh light
scattering of Arsenazo-DBN..... (1327)
- Microdetermination of proteins using m-carboxychlorophosphonazo as detection probe by
enhanced resonance light scattering spectroscopy..... (1335)
- Determination of proteins at nanogram levels based on their enhancement effects of Rayleigh light
scattering on dibromomethylchlorophosphonazo..... (1344)

第四部分 荧光分析及其它

- Sensitive determination of sulfate in drinks and vegetables digests by Rayleigh light scattering
technique..... (1352)
- The fluorescence study of the inclusion coordinated compound of β -cyclodextrin and
p-hydroxyphenolacetamide and its analytical applications..... (1364)
- Fluorescence characteristic study of the ternary complex of fluoroquinolone antibiotics and
cobalt (II) with ATP..... (1376)
- Two sensitive fluorescence methods for the determination of cobaltous in food and hair samples
..... (1385)
- On-line microwave FIA technique and its application to determination of rhodium and sequential
determination of palladium and rhodium..... (1394)
- The synthesis and application of 1- (o -nitrophenyl) -3 -(2-thiazolyl) triazene for the determination
of palladium(II) by the resonance enhanced Rayleigh light-scattering technique (1404)
- Study on the mechanism and applications of the fluorescence reactions among cobalt (II), H_2O_2
and two new derivatives of 8-sulfonamidoquinoline..... (1416)
- Synthesis of a new triazene reagent and its application for the determination of silver(I) by the
Rayleigh light-scattering..... (1427)

Sequential fluorescent determination of copper (II) and cobalt (II) in food samples by flow injection analysis	(1436)
Highly sensitive spectrophotometric determination of trace amounts of tellurium(IV) with the tungstate-basic dyes-poly (vinyl alcohol) system	(1445)
Direct spectrophotometric determination of chromium by microwave-oven induced flow-injection analysis.....	(1452)
Spectrofluorimetric determination of palladium(II) using 4,4'-bis (8-aminoquinoline -5-azo) -biphenyl	(1461)
Syntheses of three new derivatives of 8-aminoquinoline and its applications for fluorimetric determination of copper(II)	(1466)
Calculation of thermodynamic parameters of relaxation process using a microwave attenuation method	(1476)
微波炉在流动注射体系中的在线应用.....	(1483)
Effect of solvent properties on the dispersion coefficient in an on-line microwave flow-injection system	(1490)
Spectrophotometric determination of uranium(VI) with chlorophosphonazo-mn by flow injection analysis.....	(1499)
Dispersion behaviour of chromogenic reagents in a microwave field in a flow system. Application to the spectrophotometric flow-injection determination of palladium and rhodium	(1507)
有机溶剂和二元体系溶液在 9590 兆赫的微波吸收分析应用.....	(1520)
Application of three chromogenic reagents to the determination of Palladium using a laboratory-made optical fibre detector for flow-injection analysis.....	(1525)
DCB-偶氮胂作显色剂流动注射分光光度法测定钯.....	(1533)
Studies on flow injection analysis of platinum metals.....	(1537)
以十二烷基苯磺酸钠浮选铈 (III) 水和阳离子及其与钯 (II)、铂 (IV) 分离的研究	(1544)
微量钯的新的直接分光光度法和流动注射分光光度法.....	(1548)
The spectrophotometric determination of Sc in eriochrome cyanine R(chromeazurol s)-phosphatidyl choline system.....	(1552)
硝酸铈酰及硝酸钍与 5-Br-PADAP 固体配合物的合成及性质研究.....	(1558)

三元络合物光度法测定铬(VI)	(1564)
金的简易、快速测定	(1568)
锆的间接极谱测定	(1574)
后记	(1576)

Quantitative structure property relationship models for the prediction of liquid heat capacity

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Abstract: Quantitative Structure-Property Relationship (QSPR) models based on molecular descriptors derived from molecular structures have been developed for the prediction of liquid heat capacity at 25 °C using a diverse set of 871 organic compounds. The molecular descriptors used to represent molecular structures include constitutional and topological indices and quantum chemical parameters. Forward stepwise regression and radial basis function neural networks (RBFNNs) were used to construct the QSPR models. The root mean square errors in liquid heat capacity predictions for the training, test and overall data sets are 16.857, 18.744 and 17.141 heat capacity units, respectively. The prediction results are in agreement with the experimental values, but the RBFNN model seems to be better than stepwise regression method.

1. Introduction

The study of the quantitative relationship between property/activity and molecular structure (QSPR/QSAR) is an important research area in computational chemistry and has been widely used in the prediction of physicochemical properties and biological activities of organic compounds^[1-2]. This kind of study can not only develop a method for the prediction of the property under investigation of new compounds that have not been synthesized but also can identify and describe important structural features of molecules that are relevant to variations in molecular properties, thus gain some insight into structural factors affecting molecular properties. To develop a QSPR model, the following steps are usually involved: data collection, molecular geometry optimization, molecular descriptors generation, descriptors selection, model development and finally model performance evaluation.

One of the important problems in QSPR is the description of molecular structures using molecular descriptors, which can include structural information as much as possible. At present, there exists a great number of molecular descriptors that encode constitutional, topological, geometry and electronic features of organic compounds^[3-5]. Among various structure descriptors,

those derived from molecular structure alone have a particular advantage of the possibility to calculate them based only on molecular structural feature and to be applicable to different families of compounds^[6-7]. After the calculation of molecular descriptors, linear methods, such as multiple linear regression (MLR), principal component regression (PCR) and partial least squares (PLS) or non-linear methods, such as many types of artificial neural networks, can be used in the development of a mathematical relationship between the structural descriptors and the property to be predicted.

Physical and thermodynamic property data of organic compounds such as liquid heat capacity are important in the engineering design and operation of industrial chemical processes^[8]. In liquid phase reactions, the liquid heat capacity is often required to evaluate the energy variation for the liquid chemical reactants involved in the reaction. The heat capacity of a compound is defined as the amount of energy needed to raise a unit of the substance in question by one unit of temperature. The liquid heat capacity data is also needed in the heat exchanger and energy balance design calculations. Since the experimental determination of heat capacity is both time-consuming and expensive, and there is increased need of reliable physical and thermodynamic data for the optimization of chemical processes, it would be very useful to develop predictive models that can be used to predict these properties of organic compounds that are not synthesized or their properties are unknown.

Although many reported QSPR methods have been successfully used to predict a diverse set of physicochemical properties, their use in predicting heat capacity is rather limited^[9-10]. Gakh et al obtained a QSPR model for heat capacity of alkanes using graph theory descriptors and neural networks with a RMS of 4.04 heat capacity unit^[9]. Liu et al developed several QSPR models of alkanes using their molecular electronic edge vectors (MEDV). The RMS for the heat capacity of 134 alkanes was 3.81 heat capacity unit^[10]. The works reported are only limited to the investigations of alkanes. In our previous works we have successfully developed several QSPR models based on RBFNNs for the prediction of physicochemical properties^[11-15] and HPLC retention indices of N-Benzylideneanilines^[16]. The goal of the present study is to extend our previous investigations in order to, for the first time, establish a QSPR model that can predict the liquid heat capacity at 25°C for a diverse set of organic compounds dependent only upon their molecular structures. MLR and RBFNNs are applied to establish quantitative linear and non-linear relationships between heat capacity and molecular descriptors respectively. The data set used in our work is more diverse and the models developed are more general and practical with respect to the models reported early by other authors.

2. Materials and methods

2.1 Data set

The data used in this investigation were collected from literature^[8]. The set consists of 871

organic compounds. The data set includes hydrocarbons, fluorocarbons, chlorocarbons, bromocarbons, iodocarbons, alcohols, acids, ketones, aldehydes, ethers, esters, amines, nitriles, etc. A complete list of the compound names and their corresponding experimental liquid heat capacities at 25°C is given in Table 1. The data were randomly separated into two subsets: a training set of 746 compounds and a test set of 125 compounds. The training set was used to adjust the parameters of RBFNNs and the test set was used to evaluate the predictive ability of RBFNNs.

Table 1 The compounds and the predicted results of liquid heat capacities: (J/mol.K)

Number	NAME	HEATCAP	MLR	RBFNNs
1	Bromochlorodifluoromethane	127.81	106.55	127.23
2*	Bromotrichloromethane	130.65	108.16	130.03
3	Bromotrifluoromethane	143.25	104.50	126.00
4	dibromodifluoromethane	129.94	109.53	129.03
5	dichlorodifluoromethane	121.07	105.12	125.43
6	phosgene	112.03	118.18	117.02
7	trichlorofluoromethane	68.65	108.15	128.95
8	carbontetrachloride	130.72	100.65	126.01
9*	tribromomethane	129.94	141.93	136.20
10	chlorodifluoromethane	111.66	100.40	105.96
11	dichlorofluoromethane	107.20	104.37	106.08
12	chloroform	112.49	97.81	99.01
13	bromochloromethane	100.75	113.78	100.37
14	dibromomethane	105.11	129.51	116.57
15	dichloromethane	101.98	95.29	82.05
16*	difluoromethane	107.05	101.92	94.33
17	diiodomethane	135.45	145.06	141.58
18	formic acid	98.40	98.60	106.48
19	methylbromide	85.16	119.67	81.05
20	methylchloride	82.33	104.69	61.86
21	methyliodide	82.91	128.28	98.97
22	nitromethane	104.22	111.55	127.14
23*	methanol	79.93	123.08	94.04
24	methylmercaptan	96.39	131.43	92.57
25	methylamine	114.19	120.29	99.43
26	bromotrifluoroethylene	135.33	135.29	140.92
27	1,2-dibromotetrafluoroethane	184.03	153.13	179.99
28	chlorotrifluoroethylene	150.36	135.29	140.92
29	chloropentafluoroethane	174.61	150.71	173.07

Table 1 (continued)

Number	NAME	HEATCAP	MLR	RBFNNs
30*	1,2-dichlorotetrafluoroethan	110.13	150.31	174.06
31	1,1,2-trichlorotrifluoroetha	169.44	153.97	177.66
32	tetrachloroethylene	146.93	134.64	140.24
33	trichloroacetylchloride	168.81	161.40	169.97
34	2-chloro-1,1-difluoroethylen	126.95	140.04	138.28
35	trichloroethylene	123.67	130.81	128.04
36	dichloroacetyl chloride	154.23	152.81	152.72
37*	trichloroacetaldehyde	153.22	150.51	154.35
38	pentachloroethane	190.91	146.28	163.41
39	trifluoroacetic acid	170.15	155.99	160.88
40	pentafluoroethane	168.85	143.59	157.87
41	1,1,2,2-tetrabromoethane	168.43	157.56	156.62
42	1,1-dichloroethylene	112.43	122.69	121.29
43	cis-1,2-dichloroethylene	117.88	116.74	110.47
44*	trans-1,2-dichloroethylene	118.37	115.54	109.88
45	chloroacetyl chloride	142.92	138.03	137.11
46	dichloroacetaldehyde	134.07	141.23	138.66
47	dichloroacetic acid	172.72	164.08	161.64
48	1,1,1-trichlorofluoroethane	151.42	147.95	154.60
49	1,1,1,2-tetrachloroethane	154.63	144.61	151.58
50	1,1,2,2-tetrachloroethane	159.39	133.99	139.18
51*	1,1,1,2-tetrafluoroethane	141.80	135.99	145.90
52	vinyl bromide	103.13	109.82	106.96
53	vinyl chloride	86.01	106.30	101.32
54	1-chloro-1,1-difluoroethane	132.37	127.27	140.17
55	acetyl chloride	115.02	114.12	121.16
56	chloroacetaldehyde	115.19	124.99	124.32
57	methyl chloroformate	141.03	114.12	121.16
58*	1,1,1-trichloroethane	145.56	137.87	147.19
59	1,1,2-trichloroethane	151.46	131.14	130.57
60	1,1,1-trifluoroethane	139.86	122.51	137.18
61	acetonitrile	91.94	99.29	88.93
62	1,1-dibromoethane	133.61	127.47	128.10
63	1,2-dibromoethane	131.75	125.05	122.86
64	1,1-dichloroethane	131.00	128.86	128.18