

**EVALUATING THE EFFICIENCY OF ZEOLITE-BASED
ADSORBENTS FOR HYDROFLUOROCARBON
METHANE AND ETHANE DERIVATIVES USING
MOLECULAR DYNAMICS**

BY

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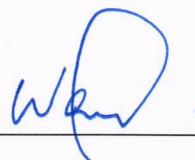
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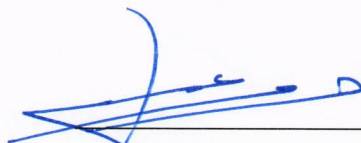
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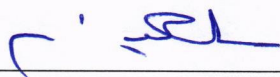
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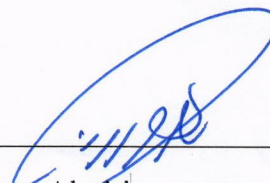
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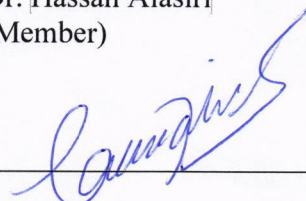
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Dedication:

This work is dedicated to my family, whose unwavering support, encouragement, and love have been my constant source of strength and motivation throughout this journey.

To my advisor and mentors, for their invaluable guidance and belief in my potential.

And finally, to all those striving to contribute to sustainable and innovative solutions for a better future. |

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TABLE OF CONTENTS

ACKNOWLEDGMENTS.....	iii
TABLE OF CONTENTS	iv
LIST OF TABLES	vi
LIST OF FIGURES	viii
LIST OF ABBREVIATIONS.....	ix
ABSTRACT	x
ملخص الرسالة	xi
Chapter 1.....	1
INTRODUCTION	1
1.1 Research Background.....	1
1.2 Research objective.....	7
Chapter 2.....	9
ADSORPTION OF REFRIGERANT IN ZEOLITE	9
2.1 Theory of adsorption	9
2.2 Determination of adsorption isotherms	12
2.2.1 Experimental methods	12
2.2.2 Langmuir-based models	13
2.3 Zeolites.....	16
2.3.1 Building Units	17
2.3.2 Composite Units	19
2.3.3 Topology	21
2.3.4 Key Considerations in the Selection of Zeolites for Gas Separation.....	24
2.4 Zeolite efficacy in the adsorption of natural refrigerants.....	25
2.4.1 Carbon Dioxide (CO ₂).....	26
2.4.2 Nitrogen.....	26
2.4.3 Methane	27
2.4.4 Ethane.....	27
2.4.5 Ethylene.....	28
2.4.6 Propane.....	28
2.4.7 Propylene.....	29
2.4.8 n-Butane	29
2.4.9 Ammonia.....	29
2.5 Zeolite efficacy in the adsorption of HFCs.....	30

Chapter 3.....	34
MOLECULAR DYNAMIC SIMULATION	34
3.1 Classical Molecular Dynamics Simulations	34
3.2 CVFF Forcefield.....	35
3.3 Metropolis Algorithm.....	38
3.4 Interaction Models in Molecular Simulations	41
3.4.1 Ewald Summation for Long-Range Electrostatics.....	41
3.4.2 Lennard-Jones Potential for Van der Waals Forces.....	42
3.4.3 Coulombic Interactions	42
3.4.4 Hydrogen Bonding	43
3.5 Simulation Framework and Methodology	43
3.5.1 Zeolite Framework Development	44
3.5.2 Molecular Dynamics and Grand Canonical Monte Carlo Simulations.....	44
3.6 Langmuir-Freundlich model.....	45
Chapter 4.....	47
RESULTS AND DISCUSSION.....	47
4.1 Model validation.....	47
4.2 Adsorption behavior of fluoromethane derivatives	48
4.3 Effect of HFC structure on adsorption behavior.....	55
4.4 Application of zeolites to HFC separation.....	57
4.5 Temperature dependence of HFC adsorption in zeolites	58
Chapter 5.....	60
CONCLUSION AND RECOMMENDATION.....	60
5.1 Conclusion.....	60
5.2 Recommendations for Future Research Directions	61
References	65
Appendix	75
Vitae.....	114

LIST OF TABLES

Table 1 Common applications, chemical properties, and GWP of HFCs	3
Table 2 Common HFC mixtures, their weight composition, and uses	5
Table 3 Selected zeolites for HFC adsorption	7
Table 4 Characteristics and properties of key industrial zeolites.....	22
Table 5 Overview of zeolite applications in gas adsorption and separation	30
Table 6 Dipole moments and normal boiling points of refrigerants	31
Table 7 Previous studies on the adsorption of HFCs in zeolites	33
Table 8 Langmuir-Freundlich isotherm model fitting parameters for various zeolites and refrigerants at 298 K.....	46
Table 9 Comparative Isotherm Analysis of R134a in Zeolite 13X at 293K, 313K, and 333K	75
Table 10 Comparative Isotherm Analysis of R32 in LTA zeolite	75
Table 11 Langmuir-Freundlich Adsorption Parameters for Methane Derivative Refrigerants in Zeolite 13X.....	76
Table 12 Adsorption Characteristics for R41in Zeolite 13x at Various Pressures and Temperatures	77
Table 13 Adsorption Characteristics for R32 in Zeolite 13x at Various Pressures and Temperatures.....	78
Table 14 Adsorption Characteristics for R23 in Zeolite 13x at Various Pressures and Temperatures.....	79
Table 15 Adsorption Characteristics for R14 in Zeolite 13x at Various Pressures and Temperatures.....	80
Table 16 Langmuir-Freundlich Adsorption Parameters for Methane Derivative Refrigerants in Zeolite 5A.....	81
Table 17 Adsorption Characteristics for R41 in Zeolite 5A at Various Pressures and Temperatures	82
Table 18 Adsorption Characteristics for R32 in Zeolite 5A at Various Pressures and Temperatures	83
Table 19 Adsorption Characteristics for R23 in Zeolite 5A at Various Pressures and Temperatures	84
Table 20 Adsorption Characteristics in Zeolite 5A for R14 at Various Pressures and Temperatures	85
Table 21 Langmuir-Freundlich Adsorption Parameters for Methane Derivative Refrigerants in Zeolite 4A.....	86
Table 22 Adsorption Characteristics for R41 in Zeolite 4A at Various Pressures and Temperatures	87
Table 23 Adsorption Characteristics for R32 in Zeolite 4A at Various Pressures and Temperatures	88
Table 24 Adsorption Characteristics for R23 in Zeolite 4A at Various Pressures and Temperatures	89
Table 25 Adsorption Characteristics for R14 in Zeolite 4A at Various Pressures and Temperatures	90
Table 26 Langmuir-Freundlich Adsorption Parameters for Methane Derivative Refrigerants in Zeolite 3A.....	91
Table 27 Adsorption Characteristics for R41in Zeolite 3A at Various Pressures and Temperatures	92
Table 28 Adsorption Characteristics for R32 in Zeolite 3A at Various Pressures and Temperatures	93

Table 29 Adsorption Characteristics for R23 in Zeolite 3A at Various Pressures and Temperatures	94
Table 30 Adsorption Characteristics for R14 in Zeolite 3A at Various Pressures and Temperatures	95
Table 31 Langmuir-Freundlich Adsorption Parameters for Ethane Derivative Refrigerants in Zeolite 13X.....	96
Table 32 Adsorption Characteristics for R152a in Zeolite 13x at Various Pressures and Temperatures.....	97
Table 33 Adsorption Characteristics for R152 in Zeolite 13x at Various Pressures and Temperatures.....	98
Table 34 Adsorption Characteristics for R143a in Zeolite 13x at Various Pressures and Temperatures.....	99
Table 35 Adsorption Characteristics for R143 in Zeolite 13x at Various Pressures and Temperatures.....	100
Table 36 Adsorption Characteristics for R134a in Zeolite 13x at Various Pressures and Temperatures.....	101
Table 37 Adsorption Characteristics for R134 in Zeolite 13x at Various Pressures and Temperatures.....	102
Table 38 Adsorption Characteristics for R125 in Zeolite 13x at Various Pressures and Temperatures.....	103
Table 39 Adsorption Characteristics for R116 in Zeolite 13x at Various Pressures and Temperatures.....	104
Table 40 Langmuir-Freundlich Adsorption Parameters for Ethane Derivative Refrigerants in Zeolite 5A.....	105
Table 41 Adsorption Characteristics for R152a in Zeolite 5A at Various Pressures and Temperatures.....	106
Table 42 Adsorption Characteristics for R152 in Zeolite 5A at Various Pressures and Temperatures.....	107
Table 43 Adsorption Characteristics for R143a in Zeolite 5A at Various Pressures and Temperatures.....	108
Table 44 Adsorption Characteristics for in Zeolite 5A R143at Various Pressures and Temperatures.....	109
Table 45 Adsorption Characteristics for R134a in Zeolite 5A at Various Pressures and Temperatures.....	110
Table 46 Adsorption Characteristics for R134 in Zeolite 5A at Various Pressures and Temperatures.....	111
Table 47 Adsorption Characteristics for R125 in Zeolite 5A at Various Pressures and Temperatures.....	112
Table 48 Adsorption Characteristics for R116 in Zeolite 5A at Various Pressures and Temperatures.....	113

LIST OF FIGURES

Figure 1 HFC Phase-down Schedule under the Kigali Amendment (source: conf.montreal-protocol.org).....	5
Figure 2 (a) Langmuir’s kinetic model of adsorption; (b,c) Plot of fractional adsorption site occupancy θ as a function of pressure, showing the effects of different Langmuir binding constants K	11
Figure 3 Different types of SBUs and their symbols. The number provided in brackets next to each refers to how often these units are found within zeolite structures.	18
Figure 4 Variations in the arrangement of Secondary Building Units (SBUs). Lines meet represent the central point of tetrahedral cations, either aluminum or silicon. a) Individual rings made of four or six members; b) pairs of interconnected four- or six-membered rings; c) partial cubo-octahedrons formed from four- and six-membered rings; d) a cluster of four partial cubo-octahedrons connected by a set of four doubled rings each comprising four members.....	18
Figure 5 Structural variants of zeolite frameworks	19
Figure 6 Composition and size of rings in the zeolitic framework.	21
Figure 7 Key zeolite frameworks: A) LTA, B) FAU Types X and Y, C) ZSM-5, D) MOR, E) FER, F) BEA I, II, and III- illustrating structural elements and exchangeable cation sites	22
Figure 8 Structural Overview of zeolite frameworks and pore orientations	23
Figure 9 Adsorption of R32 in LTA zeolites at 298.15 K and (b) Adsorption of R134a in 13X as a function of temperature. Open symbols represent experimental data [49,112] and filled symbols represent simulation results.	48
Figure 10 Adsorption isotherms of fluoromethane derivatives at 298.15 K in zeolites (a) 5A, (b) 4A, (c) 3A and (d) 13X.....	50
Figure 11 Density profiles for R41 and R23 in zeolites 13X and 5A at 298.15 K. (a) R41 in 13X, (b) R23 in 13X, (c) R41 in 5A and (d) R23 in 5A.	51
Figure 12 Molecular interactions between HFCs and zeolite 13X. (a) R41, (b) R32 and (c) R23.....	52
Figure 13 Molecular interactions between HFCs and zeolite 5A. (a) R41, (b) R32 and (c) R23.....	52
Figure 14 RDF analysis of cation–F interactions for R41, R23, and R32 in zeolites (a) 13X and (b) 5A.	54
Figure 15 RDF analysis of O–H interactions for R41, R23, and R32 in zeolites (a) 13X and (b) 5A.	54
Figure 16 Distribution of R32 at 1 am and 298 K in zeolite (a) 13X and (b) 5A.....	54
Figure 17 Adsorption isotherms of HFCs in zeolite 13X at 298.15 K. (a) R32/R152a, (b) R23/R143a and (c) R14/R134a.	56
Figure 18 Adsorption isotherms of structural isomers in zeolite 13X at 298.15 K. (a) difluoroethanes, (b) trifluoroethanes and (c) tetrafluoroethanes.	57
Figure 19 Adsorption isotherms of R32, R23, and R116 at 298.15 K in zeolites (a) 13X and (b) 5A.....	58
Figure 20 Effect of temperature on the adsorption of HFCs in zeolite 5A. (a) isotherms for R152a, (b) isosteric heat for R152a, (c) isotherms for R41 and (d) isosteric heat for R41.	58

LIST OF ABBREVIATIONS

HFC	:	Hydrofluorocarbon
GWP	:	Global Warming Potential
MD	:	Molecular Dynamics
GCMC	:	Grand Canonical Monte Carlo
Si/Al Ratio	:	Silicon-to-Aluminum Ratio
GWP	:	Global Warming Potential
FAU	:	Faujasite Framework
LTA	:	Linde Type A
HFC	:	Hydrofluorocarbon
CVFF	:	Consistent Valence Force Field
HFC	:	Hydrofluorocarbon
RDF	:	Radial Distribution Function
DFT	:	Density Functional Theory
MOF	:	Metal-Organic Framework
AI	:	Artificial Intelligence

ABSTRACT

Full Name : Abrar Elhaj Ahmed Elhussien
Thesis Title : [Evaluating the Efficiency of Zeolite-Based Adsorbents for Hydrofluorocarbon Methane and Ethane Derivatives Using Molecular Dynamics]
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Hydrofluorocarbons (HFCs) are widely used refrigerants with significant global warming potential (GWP), necessitating the development of efficient separation and recycling methods. This study explores the adsorption behavior of HFCs in zeolites 13X, 5A, 4A, and 3A using Molecular Dynamics (MD) and Grand Canonical Monte Carlo (GCMC) simulations, aiming to enhance understanding and optimization of zeolite-based materials for HFC separation. The simulations were validated against experimental data, confirming the accuracy of the employed computational models. The study investigated methane (R32, R23, R14, R41) and ethane derivatives (R152a, R134a, R143a, R125), examining their adsorption isotherms, isosteric heat, and molecular interactions within the zeolite frameworks. Zeolite 13X exhibited strong cation-fluorine interactions, favoring the adsorption of larger HFC molecules, while zeolite 5A demonstrated significant hydrogen bonding at low pressures and entropic effects at higher pressures. Selectivity patterns indicated zeolite 13X's effectiveness for separating R23 from R116 and zeolite 5A's selectivity for R32 over R23. Notably, the study also revealed that structural isomers, such as R134a and R143a, exhibit distinct adsorption capacities due to their molecular configurations. Temperature-dependent analyses showed exothermic adsorption processes for all HFCs studied, with adsorption capacity decreasing as temperature increased. The study highlighted the role of pore size, framework characteristics, and molecular properties—such as dipole moments and boiling points in influencing adsorption efficiency.

ملخص الرسالة

الاسم الكامل: ابرار الحاج احمد الحسين

عنوان الرسالة: تقييم كفاءة المواد الممتزة القائمة على الزيوليت لمشتقات الميثان والإيثان من الهيدروفلوروكربونات باستخدام الديناميكا الجزيئية

التخصص: الهندسة الكيميائية

تاريخ الدرجة العلمية: ديسمبر ٢٠٢٤

تُعتبر الهيدروفلوروكربونات (HFCs) مبردات مستخدمة على نطاق واسع ولكنها تمتلك تأثيرًا كبيرًا على الاحترار العالمي (GWP)، مما يستدعي تطوير طرق فعالة للفصل وإعادة التدوير. تستكشف هذه الدراسة سلوك الامتزاز للهيدروفلوروكربونات في الزيوليتات X13 وA5 وA4 وA3 باستخدام محاكاة الديناميكا الجزيئية (MD) ومحاكاة مونت كارلو ذات الإحداثيات الكبرى (GCMC)، بهدف تعزيز الفهم وتحسين المواد المعتمدة على الزيوليت لفصل الهيدروفلوروكربونات. تم التحقق من صحة المحاكاة باستخدام بيانات تجريبية، مما يؤكد دقة النماذج الحسابية المستخدمة. تناولت الدراسة مشتقات الميثان (R14، R23، R32)، (R41) ومشتقات الإيثان (R125، R143a، R134a، R152a)، حيث تم فحص منحنيات الامتزاز، الحرارة الإيزوستيرية، والتفاعلات الجزيئية داخل هياكل الزيوليت. أظهر الزيوليت X13 تفاعلات قوية بين الكاتيونات والفلور، مما يعزز امتزاز جزيئات HFC الأكبر، بينما أظهر الزيوليت A5 روابط هيدروجينية بارزة عند الضغوط المنخفضة وتأثيرات انتروبية عند الضغوط الأعلى. أشارت أنماط الانتقائية إلى فعالية الزيوليت X13 في فصل R23 عن R116 وانتقائية الزيوليت A5 لـ R32 على R23. كما كشفت الدراسة أن الأيزوميرات الهيكلية، مثل R134a وR143a، تظهر قدرات امتزاز مختلفة بسبب تكويناتها الجزيئية. أظهرت التحليلات المعتمدة على درجة الحرارة عمليات امتزاز طاردة للحرارة لجميع HFCs المدروسة، حيث انخفضت قدرة الامتزاز مع ارتفاع درجة الحرارة. سلطت الدراسة الضوء على دور حجم المسام، خصائص الهيكل، والخواص الجزيئية مثل العزوم ثنائية القطب ونقاط الغليان في التأثير على كفاءة الامتزاز.

Chapter 1

INTRODUCTION

1.1 Research Background

The development of refrigerants has evolved significantly over the past century, beginning with the use of natural refrigerants such as ammonia (NH_3), carbon dioxide (CO_2), and hydrocarbons (HCs) such as propane and butane. These early refrigerants, though effective, presented issues related to toxicity and flammability, which led to the search for safer alternatives [1,2]. However, natural refrigerants had minimal environmental impact, as they did not contribute to ozone depletion or global warming. In the 1930s, the invention of chlorofluorocarbons (CFCs) marked a new era in the refrigeration industry. CFCs were widely adopted for their stability, safety, and non-flammability[1,3]. However, by the 1970s, it became clear that CFCs posed a serious environmental threat. When released into the atmosphere, CFCs break down under ultraviolet radiation (UV), releasing chlorine atoms that destroy the ozone layer, which protects the Earth from harmful UV radiation [4,5]. This issue was initially outlined in the Refrigerant Report by DuPont, which highlighted the environmental implications of CFC emissions. The scientific basis for this phenomenon was later confirmed by researchers Mario J. Molina and F. Sherwood Rowland in their groundbreaking study published in *Nature* in 1974 [6,7]. They demonstrated the link between CFC emissions and ozone depletion through chlorine atom-catalyzed destruction of ozone molecules in the stratosphere. This discovery, along with subsequent studies, provided a clear understanding of the environmental damage caused by CFCs and ultimately led to global action to mitigate their impact[8]. The environmental impact of CFCs spurred global action, leading to the adoption of the Montreal Protocol in 1987, an

international treaty aimed at phasing out the production and consumption of ozone-depleting substances (ODS), including CFCs [9]. This agreement led to significant reductions in CFC use and a gradual recovery of the ozone layer [10]. As a temporary solution, hydrochlorofluorocarbons (HCFCs) were introduced to replace CFCs due to their lower ozone depletion potential. However, HCFCs were later recognized for their high global warming potential (GWP), prompting their scheduled phase-out under the same protocol.

Parallel to the Montreal Protocol, the Kyoto Protocol in 1997 was established to address greenhouse gas emissions and climate change. The Kyoto Protocol identified hydrofluorocarbons (HFCs), which replaced HCFCs, as potent greenhouse gases despite their ozone-friendliness [11]. HFCs are now commonly used in a wide range of applications, including refrigeration, air conditioning, fire suppression, and foam-blowing agents [12]. While HFCs do not harm the ozone layer, they have a significant impact on global warming due to their high GWP [13]. Table 1 presents the most common HFCs, their applications, and associated GWPs.

Table 1 Common applications, chemical properties, and GWP of HFCs

Common Name	ASHRAE Code	Application	Chemical Formula	Atmospheric Lifetime (years)	Global Warming Potential (100-year time horizon)	Reference
Difluoromethane	R32	Air conditioning systems, heat pumps	CH_2F_2	5.2	677	[14]
Trifluoromethane	R23	Ultra-low temperature refrigeration	CHF_3	270	14800	[15,16]
Tetrafluoromethane	R14	Electronics cooling, gas duster	CF_4	50000	7390	[17,18]
1,2-Difluoroethane	R152	Not commonly used as a single refrigerant	$\text{C}_2\text{H}_4\text{F}_2$	1.4	138	[18,19]
1,1-Difluoroethane	R152a	Foam blowing agent, aerosol propellants, refrigeration	$\text{C}_2\text{H}_4\text{F}_2$	1.4	138	[18,19]
1,1,1-Trifluoroethane	R143a	Air conditioning systems, and as a component in blends	$\text{C}_2\text{H}_3\text{F}_3$	52	4470	[14,17]
1,1,2-Trifluoroethane	R143	Not commonly used as a single refrigerant	$\text{C}_2\text{H}_3\text{F}_3$	13.4	1430	[20,21]
1,1,1,2-Tetrafluoroethane	R134a	Automotive air conditioning, refrigeration, chillers	$\text{C}_2\text{H}_2\text{F}_4$	13.4	1430	[22][21]
1,1,2,2-Tetrafluoroethane	R134	Not commonly used as a single refrigerant	$\text{C}_2\text{H}_2\text{F}_4$	13.4	1430	[16]
Pentafluoroethane	R125	Component in refrigerant blends	C_2HF_5	29.2	3500	[22,23]
Hexafluoroethane	R116	Gas-insulated switchgear, electronic cooling, and as a component in blends	C_2F_6	10000	12200	[24,25]

In response, the F-Gas Regulation in 2014 was introduced to control fluorinated gases, including HFCs. This regulation set stringent limits on the production and use of HFCs in refrigeration, air conditioning, and heat pump systems across the European Union, further accelerating the transition to low-GWP alternatives [26]. The F-Gas Regulation plays a key role in meeting the EU's climate goals, aligning with broader international efforts to mitigate

climate change. These developments have prompted renewed interest in natural refrigerants and hydrofluoroolefins (HFOs), which offer lower GWP and negligible ozone depletion potential [27,28]. HFOs are unsaturated organic compounds with lower GWP and a shorter atmospheric lifetime compared to HFCs, making them more environmental-friendly [29]. For instance, R1234yf, a common HFO, has a GWP of only 4, which makes it an attractive substitute for high-GWP HFCs like R134a [30]. However, HFOs also face challenges, including higher production costs and safety concerns related to their mild flammability, limiting their widespread adoption [1].

In addition, the Kigali Amendment to the Montreal Protocol in 2016 introduced a plan to phase down HFCs, which has been gradually implemented [28]. The global phase-down schedule is visually represented in Figure 1, which shows the timelines for different groups and highlights the HFC reduction milestones across various regions [31]. The Kigali Amendment establishes a phased reduction of HFC consumption, with A2 countries starting the process in 2019 and A5 countries, including Saudi Arabia, scheduled to begin between 2024 and 2028. Saudi Arabia, as part of Group 2 of the A5 countries, is expected to achieve an 85% reduction in HFC consumption by 2047.

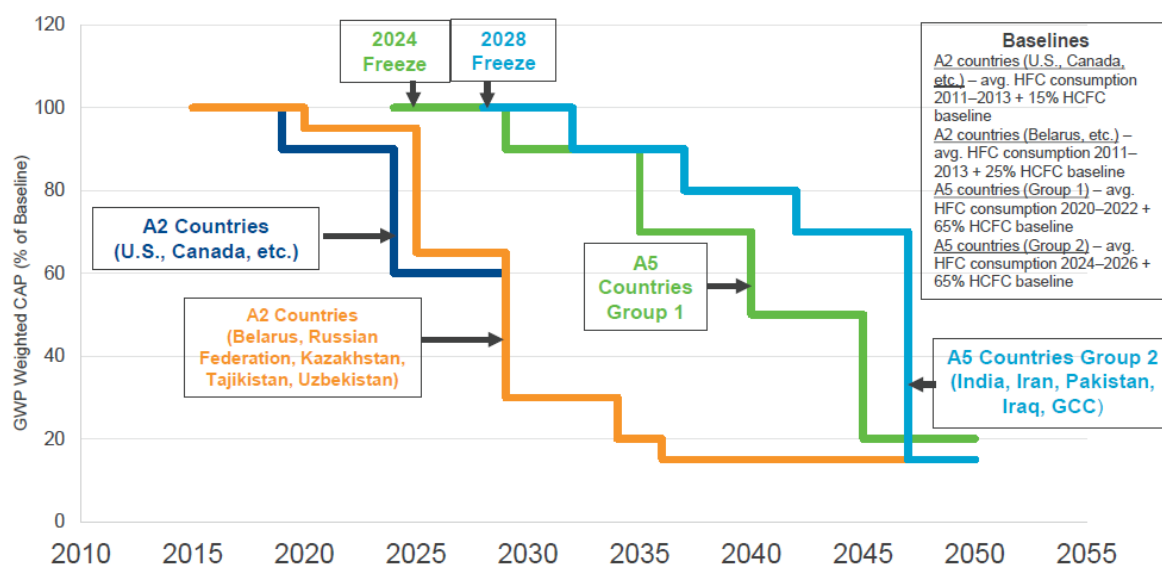


Figure 1 HFC Phase-down Schedule under the Kigali Amendment (source: conf.montreal-protocol.org)

Another way to mitigate the impact of HFCs is by recycling and reusing them. HFC mixtures such as R410A, which is composed of R32 and R125, are commonly used in air conditioning and heat pump systems [32]. Other common HFC mixtures and their compositions are listed in Table 2, which provides an overview of the different mixtures, their respective compositions, and their applications.

Table 2 Common HFC mixtures, their weight composition, and uses

HFC Mixture	Weight Composition (%)	Uses	Reference
R410A	R32 (50%) / R125 (50%)	Air conditioning and heat pump systems	[33]
R407C	R32 (23%) / R125 (25%) / R134a (52%)	Air conditioning, medium-temperature refrigeration	[34]
R404A	R125 (44%) / R143a (52%) / R134a (4%)	Commercial refrigeration, transport refrigeration	[35]
R507A	R125 (50%) / R143a (50%)	Low-temperature refrigeration	[36]
R422D	R125 (65%) / R134a (32%) / R600a (3%)	Retrofit for R22 systems in commercial refrigeration	[37]

To support ongoing sustainability efforts, the process of separating and recovering HFCs from industrial emissions has grown to be a critical area of research [38]. Traditional separation processes, such as cryogenic distillation, are often used for the separation of HFC mixtures. However, these methods face significant challenges due to the azeotropic nature of HFC mixtures which results in high energy consumption and operational costs. The latter limits their feasibility for widespread industrial applications [39]. To address these issues, adsorption has emerged as a promising alternative that is energy less intensive and suitable for the selective capture of individual HFCs based on their physical and chemical properties [40]. Consequently,

the development of efficient adsorbents is crucial to properly design and optimize adsorption processes [41].

Several materials were explored for the separation of HFCs, including metal-organic frameworks (MOFs), covalent organic frameworks (COFs), and zeolites. MOFs are characterized by their high surface area and tunable pore structure, which makes them excellent candidates for gas adsorption and separation [42]. Studies by Lee et al. [43] have demonstrated the successful adsorption of R32 and R125 in MOFs with specific pore sizes, achieving selectivity that surpasses conventional adsorbents [44]. COFs, on the other hand, provide a similar advantage with their well-defined pores and tunable chemistry, but they tend to be less stable under harsh industrial conditions compared to zeolites [45]. Zeolites, particularly types like 13X and 5A, have shown great promise for the separation of HFCs due to their high thermal stability, chemical robustness, and large surface area [46]. Among these porous materials, zeolites may be considered among the most suitable candidates due to their unique properties. For instance, zeolite 13X has a Faujasite (FAU) framework with large pores, making it ideal for adsorbing large HFC molecules like R134a and R125 [47,48]. On the other hand, zeolite 5A is efficient for smaller HFC molecules such as R32 [49,50]. The ion-exchangeable nature of zeolites allows them to be modified for specific separation requirements, thereby enhancing their adsorption capacity and selectivity for particular HFCs [38]. The usefulness of zeolites is not just a theory; a lot of research [48,51,52] supports their ability to be used on a large scale and shows they are a cost-effective way to recycle HFCs.

In the pursuit of optimized adsorption techniques, certain zeolites stand out due to their unique structural properties and compatibility with HFC molecules. This thesis focuses on zeolites such as 13X, 5A, 4A, and 3A which are chosen for their distinct pore sizes and framework structures. Table 3 details the choice of specific zeolites for HFC adsorption based on their structural properties and pore sizes.

Table 3 Selected zeolites for HFC adsorption

Zeolite	Total Volume (Å ³)	Occupied Volume (Å ³)	Free Volume (Å ³)	Surface Area (Å ²)	LCD	Density (g/cm ³)	MW (g/mol)
13X	15677.6	11403.66	4273.90	3548.01	10	1.425	13445.44
5A	14905.1	8363.15	6541.95	4206.85	5	1.498	13434.88
4A	14905.1	9737.23	5167.86	4016.37	4	1.519	13628.16
3A	14905.1	13007.59	1897.51	2605.9	3	1.623	14559.5

Molecular dynamics simulations have been employed to study the interactions between HFCs and different adsorbents at an atomic level and to provide insights for the optimization of separation processes [53]. This method allows researchers to test different scenarios and molecular arrangements more freely than in a physical lab and to speed up research. Additionally, these simulations play a key role in predicting how well zeolites can capture HFCs and the energy involved, which is crucial for making better zeolite-based separation methods [25,54].

1.2 Research objective

The primary objective of this thesis is to investigate the adsorption behavior of hydrofluorocarbons (HFCs), with a specific focus on methane derivatives (R32, R23, R14, R41) and ethane derivatives (R152, R152a, R143a, R143, R134a, R134, R125, and R116), using four distinct types of zeolites: the Faujasite (FAU) structure named 13X and Linde Type A (LTA) structures named 5A, 4A, and 3A. This research aims to:

1. Characterize the Adsorption Efficiency: determine the adsorption capacity of each zeolite type for the selected HFC molecules, identifying which zeolite demonstrates the most efficient adsorption properties for potential industrial applications. This will involve a detailed comparison of the adsorption performance across the four zeolite types to determine the most effective material for HFC capture.
2. Analyze Adsorption Isotherms: Construct adsorption isotherms for each HFC-zeolite pairing to study the relationship between the pressure (or concentration) of HFCs and the quantity adsorbed at constant different temperatures. This analysis will shed light on the underlying adsorption mechanisms and provide a foundational understanding of the adsorption process.
3. Investigate Molecular Interactions: Employ molecular simulation techniques to dissect the interactions between HFC molecules and zeolite surfaces at an atomic level. This investigation will offer crucial insights into the physical and chemical properties that influence adsorption, including the role of molecular size, shape, and polarity.
4. Examine the Influence of Fluorine Atoms: Study the pure behavior of methane and ethane derivatives separately to discern the effect of fluorine atom presence on the adsorption process. This examination will help correlate the physical and chemical properties of HFCs, and their interactions with zeolites, to identify which properties predominantly govern the adsorption process.

Chapter 2

ADSORPTION OF REFRIGERANT IN ZEOLITE

2.1 Theory of adsorption

Adsorption theory is a crucial concept in surface physics, which explains how atoms, ions, or molecules (the adsorbates) adhere to a solid or liquid surface (the adsorbent). Adsorption occurs due to various forces, including van der Waals forces, electrostatic interactions, and chemical bonding. Unlike absorption, where molecules diffuse into the bulk of a material, adsorption is confined to the surface, making it a surface phenomenon. Adsorption can be categorized into physical adsorption (physisorption) and chemical adsorption (chemisorption). Physisorption involves physical interactions such as van der Waals forces, and the process is usually reversible. In contrast, chemisorption involves the formation of stronger chemical bonds between the adsorbate and the surface, making it more specific and often irreversible. These two types of adsorption significantly influence material applications, including catalysis, gas storage, separation technologies, and environmental remediation [55,56].

One of the most fundamental models in adsorption is the Langmuir adsorption theory, proposed by Irving Langmuir in 1918. The Langmuir model was the first to quantitatively describe the adsorption process by assuming that the adsorbate forms a monolayer on the surface of the adsorbent, with no further adsorption occurring once the surface is fully covered [57]. Langmuir's theory is based on few key assumptions:

1. Monolayer adsorption: adsorption occurs only at specific, localized sites on the surface, and each site can hold one molecule of adsorbate.

2. Homogeneous surface: all adsorption sites on the surface are equivalent, with the same energy of adsorption.
3. No interactions: there are no interactions between adjacent adsorbed molecules; each molecule adsorbs independently of others.
4. Dynamic equilibrium: adsorption and desorption occur simultaneously, and the process reaches equilibrium when the rates of adsorption and desorption are equal.

The Langmuir adsorption isotherm equation, which expresses the relationship between the amount of gas adsorbed on a surface and the pressure of the gas at a constant temperature, is given by:

$$\theta = \frac{KP}{1 + KP} \quad (1)$$

Where θ is the fractional coverage of the surface, K is the equilibrium constant related to the affinity of the adsorption sites for the adsorbate, and P is the pressure of the adsorbate gas.

At low pressures, the isotherm reduces to a linear relationship ($\theta \approx K$), whereas at high pressures, the surface becomes saturated, and no further adsorption occurs, leading to $\theta \approx 1$. Langmuir's model has proven effective in describing adsorption phenomena in a variety of systems, especially for gases on solid surfaces [58,59].

Figure 2 (a) illustrates the processes involved in Langmuir adsorption, namely: (1) incidence, (2) reflection, (3) adsorption, and (4) desorption. Figure 2 (b) also shows the relationship between fractional site occupancy and pressure, both in linear and logarithmic scales (Figure 2 b and Figure 2 c).

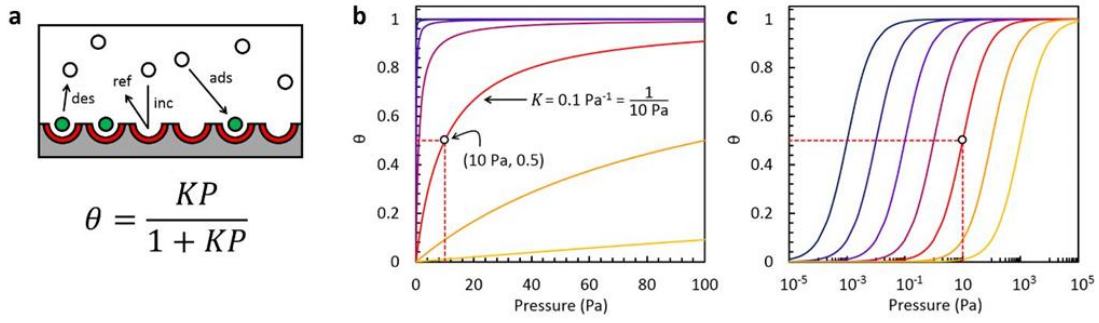


Figure 2 (a) Langmuir's kinetic model of adsorption; (b,c) Plot of fractional adsorption site occupancy θ as a function of pressure, showing the effects of different Langmuir binding constants K .

Enthalpy of adsorption

In the context of adsorption, as outlined in Langmuir's theory, the process involves the formation of a monolayer of adsorbate molecules on the surface of the adsorbent. While the Langmuir model provides a useful framework for understanding the relationship between pressure and adsorption capacity, the thermodynamic aspect of adsorption is further elucidated by examining the enthalpy of adsorption. Adsorption is typically an exothermic reaction, as energy is released when the adsorbate molecules interact with the surface of the adsorbent through van der Waals forces, hydrogen bonding, or electrostatic interactions. This exothermic nature highlights the tendency of the system to lose energy, stabilizing the adsorbed state. The enthalpy of adsorption represents the heat change that occurs when a substance is adsorbed onto a surface. It is a key thermodynamic parameter that provides insights into the strength of interaction between the adsorbate and the adsorbent. The enthalpy of adsorption is typically negative for exothermic processes, where heat is released as the molecules adhere to the surface [60]. The enthalpy of adsorption can be expressed as the difference in enthalpy between the adsorbed state and the gaseous state, as follows:

$$\Delta H_{ads} = H_a - H_g = T\Delta S_{ads} = \frac{-RT^2}{P} \left(\frac{dP}{dT} \right)_{Na} \quad (2)$$

Where H_a is the enthalpy of the adsorbed state, H_g is the enthalpy of the gas phase, T is the temperature, ΔS_{ads} is the entropy change during adsorption, R is the universal gas constant, P is the pressure, and $\left(\frac{dP}{dT}\right)_{Na}$ is the rate of change of pressure with respect to temperature at constant adsorbate amount Na . This equation can be derived from the Clausius-Clapeyron relation and is commonly used to calculate the enthalpy of adsorption by analyzing the temperature dependence of adsorption isotherms [61,62]. The magnitude of ΔH_{ads} provides information on the nature of the adsorption process. In physisorption, the values are typically low (ranging from 5 to 40 kJ/mol). whereas in chemisorption, the values are significantly higher (50–200 kJ/mol), reflecting the stronger interactions involved [63].

2.2 Determination of adsorption isotherms

Adsorption isotherms are crucial for understanding how adsorbate molecules interact with an adsorbent at a constant temperature. These isotherms depict the relationship between the amount of substance adsorbed and its equilibrium concentration or pressure. Determining adsorption isotherms helps in evaluating the adsorption capacity and optimizing conditions for industrial applications, such as gas separation and purification [62]. There are several approaches to determine adsorption isotherms, which can be broadly classified into experimental methods, molecular theory and simulation, as well as machine learning methods.

2.2.1 Experimental methods

Experimental methods for the determination of adsorption isotherms are divided into static and dynamic techniques. Static methods include volumetric and gravimetric approaches, where adsorption is assessed based on changes in either pressure or mass of the adsorbent, respectively [61]. Volumetric methods measure the adsorption by monitoring changes in the gas volume, typically using manometric setups. In these setups, the adsorbent is exposed to the adsorbate, and changes in pressure are used to determine the adsorbed quantity. These methods

are widely used due to their accuracy, although they require careful calibration and control of experimental parameters [64]. Gravimetric methods involve monitoring the change in weight of the adsorbent before and after adsorption. Highly sensitive balances are required for these measurements to detect small mass changes accurately. Although this method is highly precise, it requires sophisticated instruments, which can be cost-prohibitive [65]. Dynamic methods, such as chromatographic and flow techniques, are commonly employed to evaluate adsorption performance under continuous flow conditions. These methods provide rapid results but often lack the precision of static methods. Dynamic adsorption is widely used for industrial applications where adsorbents are required to work under continuous operating conditions [66].

In addition, the use of machine learning (ML) has gained traction in recent years as a powerful tool to predict adsorption isotherms, especially for complex systems where experimental data may be limited [67]. ML algorithms can model non-linear relationships between material properties (such as pore size, surface area, and chemical composition) and adsorption capacities, which are challenging to capture through traditional approaches. Common ML techniques applied in adsorption studies include neural networks, decision trees, and random forests. These models are trained on datasets generated from either experimental results or molecular simulations and can be used to predict adsorption behavior under different conditions. This approach not only reduces the time and cost associated with experimental studies but also provides a platform for screening new adsorbent materials more efficiently [68].

2.2.2 Langmuir-based models

Over the years, the Langmuir adsorption isotherm has been extensively modified to better fit experimental data in complex systems. In many practical applications, ideal conditions such as uniform adsorption sites and non-interacting adsorbates does not always apply. To account for

these deviations, several models have been developed based on Langmuir's original theory, enabling a more accurate description of the adsorption phenomena. While the classical Langmuir model is effective for systems that conform to ideal conditions, it often struggles to represent adsorption on heterogeneous surfaces where site diversity and interactions between adsorbed molecules are present. Despite these limitations, the classical Langmuir model remains widely used due to its simplicity and its practical application in gas-solid adsorption systems. The various Langmuir-based models that are commonly employed to describe adsorption isotherms include:

Extended Langmuir model

The Extended Langmuir model is used when more than one adsorbate species is present on the surface. This model assumes competitive adsorption among different molecules vying for the same adsorption sites. The model is expressed as:

$$\theta_i = \frac{K_i P_i}{1 + \sum_j K_j P_j} \quad (3)$$

Where θ_i is the surface coverage of species i , K_i is the adsorption constant for species i , P_i is the partial pressure of species i . This model is essential for systems involving multi-component adsorption, such as gas mixtures adsorbing onto a catalyst surface. It helps explain competition between different adsorbates and how this affects the adsorption equilibrium [59].

Modified Langmuir-Freundlich (Sips) isotherm

The Langmuir-Freundlich isotherm, also known as the Sips isotherm, introduces a correction factor to account for surface heterogeneity. While the classical Langmuir model assumes a homogeneous surface, real surfaces often have a distribution of adsorption energies due to varying site properties. The Sips isotherm combines features of both the Langmuir and Freundlich models:

$$\theta = \frac{KP^n}{1 + (KP)^n} \quad (4)$$

Where n is a heterogeneity parameter ($0 < n \leq 1$). When $n = 1$, the equation reduces to the classical Langmuir model. The Sips model is particularly useful for systems where the surface has a broad range of adsorption energies, which is common in materials like activated carbon and zeolites [69].

Temkin Langmuir model

The Temkin isotherm model considers the effects of adsorbate-adsorbate interactions on the adsorption process, which are ignored in the classical Langmuir model. In this model, the heat of adsorption decreases linearly with increasing coverage, reflecting the fact that as more molecules adsorb, the remaining adsorption sites may have different adsorption energies:

$$q_e = \frac{RT}{b} \ln (KP) \quad (5)$$

Where q_e is the amount adsorbed at equilibrium, R is the gas constant, T is the temperature, and b is the Temkin constant related to the heat of adsorption. This model is suitable for describing adsorption processes where lateral interactions between adsorbed molecules affect adsorption behavior [70].

Dual-site Langmuir model

In cases where two distinct types of adsorption sites are present on the surface, the dual-site Langmuir model can be applied. This model assumes two sets of adsorption sites with different energies, often represented as:

$$q = \frac{q_{max1}K_1P}{1 + K_1P} + \frac{q_{max2}K_2P}{1 + K_2P} \quad (6)$$

Where q_{max1} and q_{max2} are the maximum adsorption capacities of sites 1 and 2 respectively, K_1 and K_2 are the adsorption equilibrium constants for each type of site. This model is commonly used for heterogeneous materials like porous adsorbents, where different pores or functional groups create multiple adsorption environments [58].

Brunauer-Emmett-Teller (BET) model

Although the BET model is often seen as an extension of Langmuir's isotherm, it addresses multilayer adsorption rather than monolayer adsorption. The BET model assumes that after the first monolayer of adsorbate forms, additional layers can accumulate on top of the first layer, forming multilayers. The BET equation is given by:

$$q = \frac{q_m C P}{(P_0 - P)[1 + (C - 1)P/P_0]} \quad (7)$$

Where q_m is the monolayer adsorption capacity, C is the BET constant related to the energy of adsorption and P_0 is the saturation pressure of the adsorbate. The BET model is widely used for determining surface area, particularly in porous materials where multilayer adsorption occurs [71].

2.3 Zeolites

Adsorption processes rely heavily on the interaction between the adsorbent and the adsorbate, with the surface area, pore structure, and chemical composition of the adsorbent playing crucial roles in determining adsorption efficiency [55]. To optimize these interactions, materials that provide high surface area, selective adsorption capabilities, and tunable chemical properties are essential [72]. Among such materials, zeolites stand out due to their highly ordered microporous structures and exceptional versatility as molecular sieves [73].

Zeolites are crystalline aluminosilicates known for their unique adsorptive capabilities due to their microporous nature. They are composed of a framework of interconnected tetrahedra of silicon and aluminum, SiO_4 and AlO_4 , creating a three-dimensional network with cavities and channels. These features make them effective molecular sieves, facilitating selective adsorption based on molecular size [74].

The pores within the zeolite structure are usually occupied by water molecules and cations that can be exchanged. These channels are wide enough to allow other substances to move through. When the zeolites contain water, they typically lose this water when heated to temperatures below 400 °C, and this loss of water is generally reversible. The zeolite framework might also include (OH, F) groups, which are situated at the tip of a tetrahedron that does not join with the tetrahedra next to it [75].

2.3.1 Building Units

Zeolite crystals are generally classified by their basic and secondary structural components. The basic building blocks are the tetrahedrons of $(\text{SiO}_4)^{+4}$ and $(\text{AlO}_4)^{+5}$. These tetrahedrons connect at their oxygen corners to create a three-dimensional network of simple geometric shapes, known as the secondary building units (SBUs). SBUs can take various forms, including single and double rings, polyhedral shapes, and even more intricate structures. These are then assembled in different ways to form a unique network of channels and cavities within the zeolite. Each zeolite's smallest repetitive unit, or unit cell, comprises a whole number of these SBUs. Currently, scientists differentiate 23 kinds of SBUs, illustrated in Figures 3 and 4 [76].

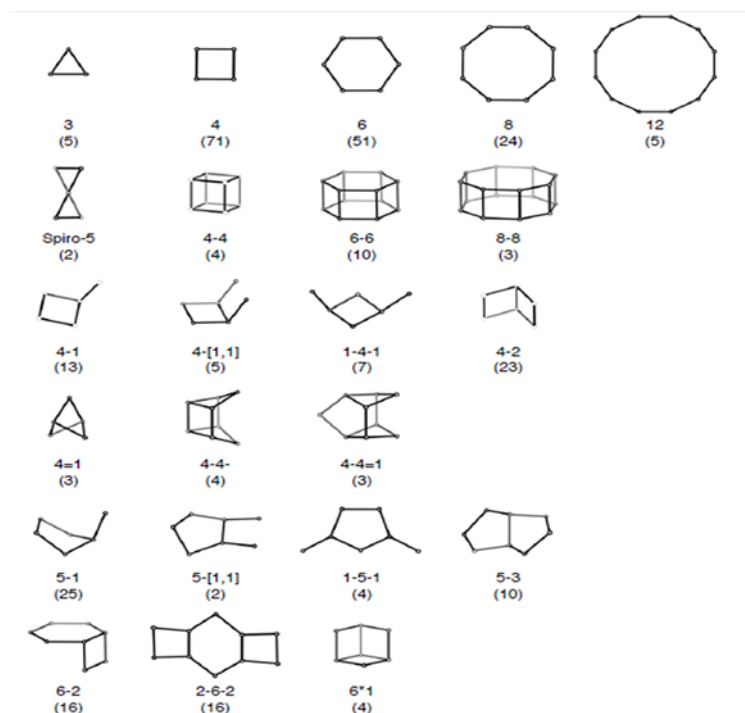


Figure 3 Different types of SBUs and their symbols. The number provided in brackets next to each refers to how often these units are found within zeolite structures.

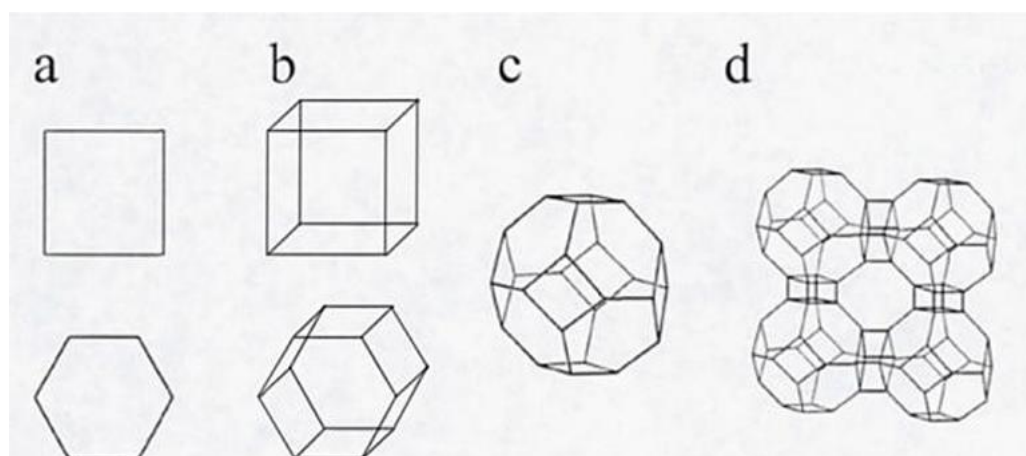


Figure 4 Variations in the arrangement of Secondary Building Units (SBUs). Lines meet represent the central point of tetrahedral cations, either aluminum or silicon. a) Individual rings made of four or six members; b) pairs of interconnected four- or six-membered rings; c) partial cubo-octahedrons formed from four- and six-membered rings; d) a cluster of four partial cubo-octahedrons connected by a set of four doubled rings each comprising four members.

The structural variety and specificity of zeolite types are further illustrated in Figure 5, which displays the unique configuration of Secondary Building Units (SBUs) in zeolites. These SBUs are foundational in forming the crystalline frameworks of zeolites, as shown by the different

structures of Type A, Sodalite, and Faujasite. Each type is characterized by distinct arrangements and shapes of rings ranging from 4-membered rings (4R) to 6-membered rings (6R) that coalesce into complex three-dimensional networks. These networks are crucial for determining the zeolite's pore size and connectivity, which in turn affect their adsorption properties and suitability for various applications in environmental management and industrial processes [77].

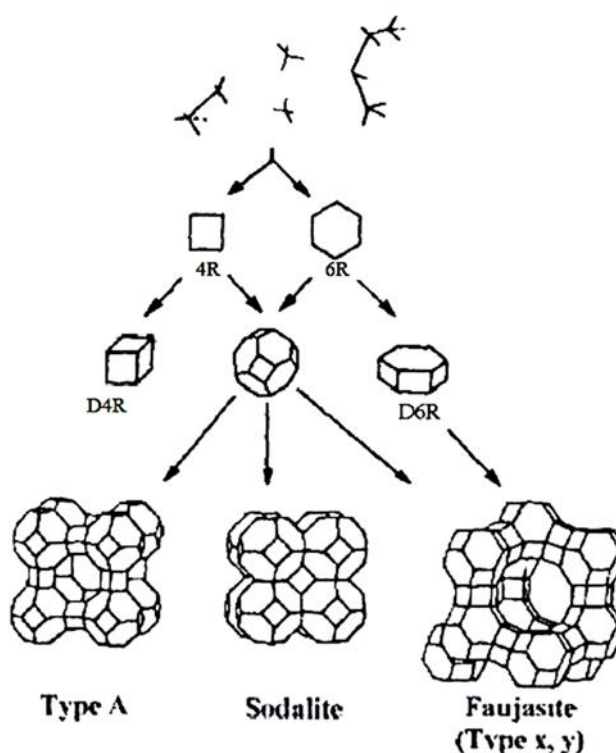


Figure 5 Structural variants of zeolite frameworks

Secondary building units are not chiral and can comprise as many as 16 T-atoms. Given that a unit cell consistently includes a whole number of these units, it's presumed that a single SBU type forms the complete framework.

2.3.2 Composite Units

Zeolites also consist of composite building units (CBUs) such as double rings, cages, and alpha cavities. CBUs, which can be chiral, don't form the zeolite framework alone but help identify

connections among framework types. Rings, a type of CBU defined by the number of tetrahedrons they enclose, are crucial for determining a zeolite's pore size [78].

Figure 6 illustrates the composition and size of various ring structures in the zeolitic framework, which describe the diversity and specificity of pore configurations across different zeolite types. These ring structures range from 4-rings to 12-rings, with their diameters increasing accordingly from 5.6 Å to more than 12 Å. The size and shape of these rings are critical as they determine the accessibility and size selectivity of the zeolite's pores, thereby influencing the types of molecules that can be adsorbed or catalytically processed. For instance, smaller rings, such as 4-rings and 5-rings, create more constrained environments suitable for smaller molecules or ions, whereas larger rings like 10-rings and 12-rings can accommodate larger molecules, making them ideal for applications requiring bulkier organic molecule processing [79]. These composite building units (CBUs), do more than structure the physical architecture of the zeolite; they also define its chemical and catalytic properties. For example, the ability of a zeolite to selectively adsorb hydrocarbons while excluding water can be attributed to the specific sizes and connectivity of these rings. Furthermore, the arrangement of these rings affects the thermal stability and hydrophobic or hydrophilic nature of the zeolite, which are essential considerations in their application in industrial catalysis and adsorption processes [80].

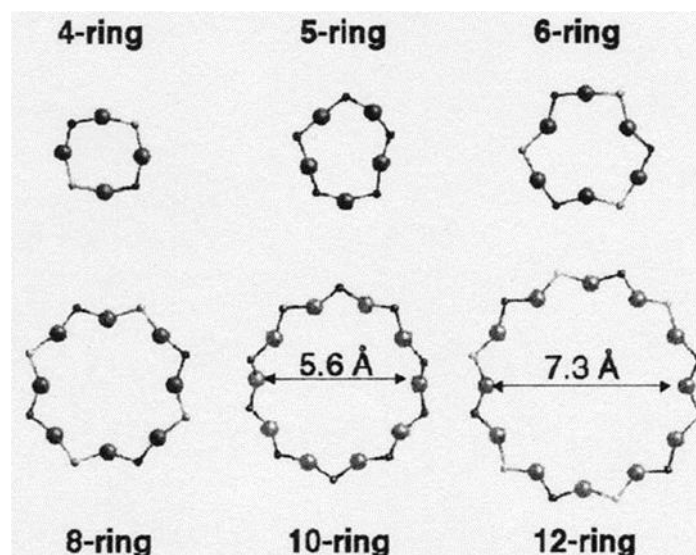


Figure 6 Composition and size of rings in the zeolitic framework.

2.3.3 Topology

Zeolites are highly structured microporous aluminosilicates renowned for their efficacy in molecular sieving and gas separation. These properties are facilitated by their well-defined pore systems, which can be precisely adjusted through techniques such as ion exchange. The ability of zeolites to act as molecular sieves stems directly from their structural organization, which is composed of building units and composite units (as discussed in sections 2.3.1 and 2.3.2). The arrangement and connectivity of these units determine the pore size, shape, and overall framework, allowing for selective adsorption based on molecular size. Table 4 shows zeolites such as LTA, FAU, MFI, and MOR listing their topology, Si/Al ratio, pore dimensions, and surface areas—critical factors that determine their suitability for different separation and catalytic processes [81]. For instance, Type A and Type X zeolites, known for their smaller and larger pore sizes respectively, are particularly effective at discriminating between molecules with minor size differences, making them essential in processes such as air separation and hydrocarbon processing [82,83].

Table 4 Characteristics and properties of key industrial zeolites

Name	Topology	Si/Al Ratio	Pore Diameter/Aperture (Å)	Surface Area (m ² /g)	References
Type A	LTA	1	11/4.2	~ 475	[84]
Chabazite	CHA	2-5	7.37/3.72	~	[84]
ZSM-5	MFI	10-15	6.4/4.7, 6.4/4.46	~ 420	[85]
Mordenite	MOR	2-5	(6.60 x 7.05), (4.82 x 3.92)	~ 425	[85]
Type X	FAU	1-1.5	11/7.4	~ 570	[86]
Type Y	FAU	1.5-3	11/7.4	~ 540	[86]

Figure 7 illustrates the most industrially important zeolite structures. Each structure is annotated with symbols indicating locations of exchangeable cation sites, which are crucial for their ion exchange capabilities. These illustrations also give information about the atomic framework, highlighting how the structural configuration influences their adsorptive and catalytic properties.

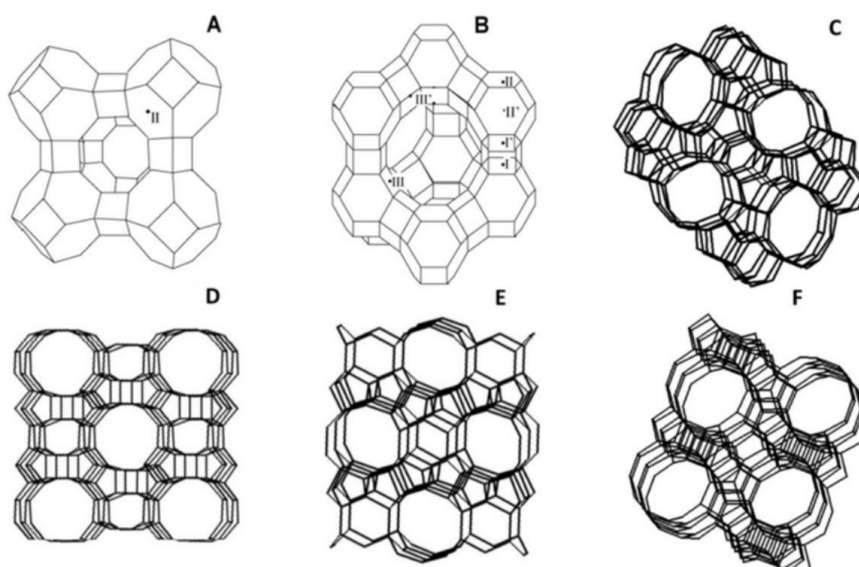


Figure 7 Key zeolite frameworks: A) LTA, B) FAU Types X and Y, C) ZSM-5, D) MOR, E) FER, F) BEA I, II, and III- illustrating structural elements and exchangeable cation sites

Figure 8 gives a detailed look at the diversity of zeolite structures. It details the various pore orientations and sizes such as 12-ring, 10-ring, and 8-ring, showcasing the geometric arrangements that are pivotal for understanding zeolite functionality in specific applications.

This figure emphasizes how the different pore sizes and arrangements allow for specialized molecular sieving capabilities tailored to distinct industrial needs [87].

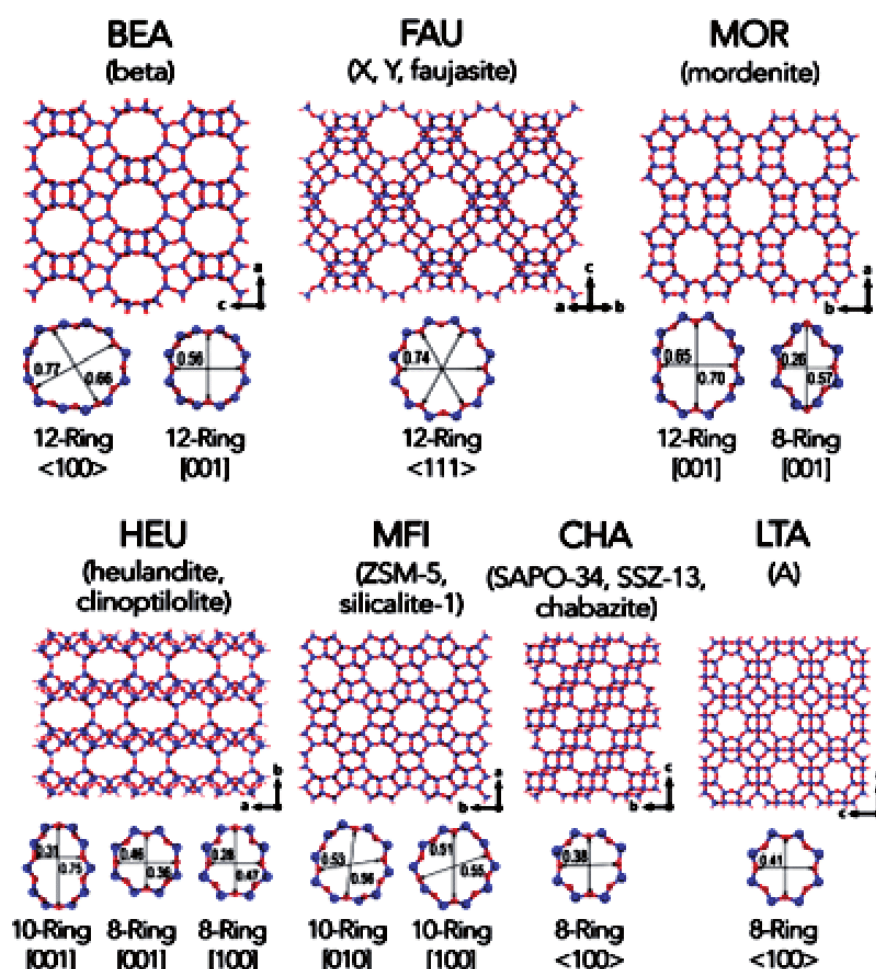


Figure 8 Structural Overview of zeolite frameworks and pore orientations

Additionally, the surface chemistry of zeolites can be modified to enhance their selectivity and affinity towards specific gases. For instance, silver-infused zeolite A optimizes the separation efficiency for ethylene from ethane, a critical step in the production of plastics and other synthetic materials. Recent advancements have explored the development of hierarchically structured zeolites, such as those depicted in the figure 8, which combine microporous and mesoporous structures to improve mass transfer and accessibility. This is particularly advantageous for processing larger molecules, which was previously challenging due to steric hindrance in the smaller microporous channels [88].

2.3.4 Key Considerations in the Selection of Zeolites for Gas Separation

The selection of appropriate zeolite materials for gas separation processes is critical for achieving high efficiency and specificity in industrial applications. Zeolites, with their well-defined pore structures and adjustable chemical properties, offer adaptable solutions for the separation of gases such as CO₂, N₂, NH₃, and various hydrocarbons. The most important key considerations that guide the selection of zeolites for these purposes are based on pore size, Si/Al ratio, cation presence, and thermal stability [89].

Pore size and structure

One of the primary factors in choosing a zeolite for gas separation is its pore size and structure. The molecular sieve properties of zeolites allow for the selective adsorption of molecules based on size exclusion. For instance, small-pore zeolites such as LTA with pore openings of approximately 4 Å are suitable for separating small molecules such as water or hydrogen sulfide, whereas larger-pore zeolites such as FAU with pore openings around 7.4 Å are effective for adsorbing larger molecules like nitrogen and methane [90].

Silica to alumina ratio

The silica to alumina (Si/Al) ratio in a zeolite framework affects its adsorption properties significantly. A higher Si/Al ratio increases the hydrophobicity of the zeolite, making it more suitable for adsorbing non-polar gases like nitrogen and methane. Conversely, a lower Si/Al ratio enhances the hydrophilicity, favoring the adsorption of polar molecules such as water and ammonia. This ratio also impacts the acidity of zeolites, influencing their catalytic activities in reactions that occur simultaneously with adsorption processes [91].

Cation exchange capacity

The ability to exchange cations in zeolite frameworks allows for the modification of adsorption characteristics to target specific gases. Cations such as sodium, potassium, calcium, and others impact the electrostatic forces within the pore channels, which can enhance the selectivity towards certain molecules. For example, calcium-exchanged zeolites have been shown to be particularly effective in CO₂ adsorption due to the formation of stronger electrostatic interactions with the polar CO₂ molecules [92].

Thermal and chemical stability

The operational environment of the zeolite significantly impacts its selection. Zeolites used in high-temperature processes must exhibit excellent thermal stability to prevent structural collapse. Similarly, chemical stability is crucial in environments where zeolites are exposed to corrosive gases or where they must withstand regular regeneration cycles without degradation. The choice of zeolite must consider both the nature of the gas being adsorbed and the conditions under which the adsorption will occur [89].

Regeneration capacity

For industrial applications where zeolites are regenerated for repeated use, their ability to withstand the regeneration process without loss of structural integrity or adsorption capacity is vital. Zeolites with high thermal stability and strong framework structures are preferred, as they can endure the thermal, pressure, and chemical stresses involved in regeneration processes [91].

2.4 Zeolite efficacy in the adsorption of natural refrigerants

Zeolites play a vital role in adsorbing and separating gases due to their complex pore structures and adjustable surface properties. This section presents in-depth research on the interaction of various atmospheric and industrial gases with different zeolite frameworks. We emphasize

important research findings, particularly focusing on how specific zeolite traits such as pore size, Si/Al ratio, and cationic sites impact the effectiveness of adsorbing natural refrigerants like carbon dioxide, nitrogen, methane, ethane, ethylene, propane, propylene, n-butane, and ammonia.

2.4.1 Carbon Dioxide (CO₂)

The adsorption of CO₂ on zeolites, particularly those with high silicon-to-aluminum ratios such as Zeolite 13X and Zeolite 5A, has been extensively studied due to its relevance in climate change mitigation through carbon capture and storage (CCS) technologies. Zeolite 13X, known for its large pore size and substantial cation exchange capacity, has demonstrated particularly high CO₂ adsorption capacities. The work of Lee et al. [93] highlighted that ion-exchanged Zeolite A, particularly with lithium, enhances CO₂ adsorption due to increased electrostatic attractions within the zeolite framework. Furthermore, advancements in computational simulations have enabled the prediction of adsorption isotherms and optimization of zeolite structures for enhanced CO₂ capture, as explored by Siriwardane et al. [94] who utilized such technologies to significantly improve the efficiency of CO₂ adsorption at moderate temperatures. These studies collectively underline the importance of zeolite composition and structural characteristics in maximizing CO₂ adsorption efficiency, providing valuable insights for the development of targeted CCS technologies.

2.4.2 Nitrogen

The adsorption of nitrogen on zeolites is a crucial process, particularly for applications involving air separation and purification. Zeolites with specific pore characteristics, such as Zeolite 13X and 5A, are frequently studied due to their ability to selectively adsorb nitrogen over other atmospheric gases. Research has shown that the effectiveness of nitrogen adsorption is largely dependent on the zeolite's framework structure and the presence of specific cations

that enhance molecular sieving properties. For example, Villarreal et al. [95] demonstrated that the adsorption capacity of zeolites can be significantly influenced by their Si/Al ratio, which adjusts the size and connectivity of the pore system, directly affecting nitrogen uptake. Additionally, studies like those by Siriwardane et al. [94] utilized advanced adsorption models to predict the behavior of nitrogen in zeolite matrices under varying pressure and temperature conditions, providing a deeper understanding of the physicochemical interactions at play. These investigations underscore the potential of tailored zeolite applications for efficient nitrogen capture, which is essential for both industrial uses and environmental protection.

2.4.3 Methane

Methane is the main component of natural gas and a potent greenhouse gas. It is crucial to develop efficient methods for methane adsorption and storage. Studies have shown that zeolites can effectively adsorb methane due to their unique pore structure and affinity for hydrophobic molecules. The adsorption of methane on zeolites has been extensively studied, with researchers exploring various strategies to enhance adsorption capacity and selectivity [90]. These strategies include modifying the composition and structure of zeolites, as well as optimizing the operating conditions. The composition and structural characteristics of zeolites play a crucial role in maximizing methane adsorption efficiency [96]. However, the presence of water vapor in the gas mixture can limit methane adsorption by occupying adsorption sites and reducing the available surface area.

2.4.4 Ethane

Similar to methane, ethane can also be adsorbed by zeolites due to their hydrophobic nature and unique pore structure. Research has shown that zeolites with larger pore sizes tend to exhibit higher ethane adsorption capacities. In particular, zeolite Y has been found to have excellent ethane adsorption properties. The adsorption of ethane in zeolites has been

extensively studied, with researchers exploring ways to optimize the structural characteristics of zeolites to enhance adsorption capacity. In addition, studies have also investigated the effects of operating conditions, such as temperature and pressure, on ethane adsorption in zeolites [97].

2.4.5 Ethylene

Ethylene is an important industrial gas used in the production of various chemicals and plastics. Understanding the adsorption behavior of ethylene onto zeolites is crucial for its efficient storage and separation. Several studies have investigated the adsorption of ethylene onto zeolites and have found promising results. These studies have shown that zeolites can effectively adsorb ethylene due to their pore structure and affinity for hydrophobic molecules [97,98]. The adsorption capacity of zeolites for ethylene can be enhanced by modifying their composition and structure. For example, researchers have explored the use of different zeolite frameworks, such as ZSM-5 and Beta, and have found that larger pore sizes and increased framework flexibility can improve the adsorption capacity for ethylene [96]. Furthermore, the presence of ion-exchangeable cations in zeolites can also affect ethylene adsorption [90].

2.4.6 Propane

The adsorption of propane onto zeolites has also been investigated. Various studies have shown that zeolites can effectively adsorb propane due to their unique pore structure and affinity for hydrocarbon molecules. These studies have demonstrated that the adsorption capacity of zeolites for propane can be enhanced by adjusting their composition, structure, and operating conditions [96,97]. For example, Zeolite Beta has been found to have a high adsorption capacity for propane due to its large pore sizes and interconnected channel systems. Furthermore, research has shown that the Si/Al ratio of zeolites can also influence propane adsorption. When the Si/Al ratio is higher, the acidity of the zeolite increases, leading to stronger interactions between the zeolite and propane molecules [90].

2.4.7 Propylene

The adsorption of propylene onto zeolites has also been investigated and has shown promising results [96]. The unique pore structure and affinity of zeolites for hydrocarbon molecules make them effective adsorbents for propylene. These studies have demonstrated that zeolites, such as Zeolite Beta and ZSM-5, can effectively adsorb propylene due to their size-selective pore structure and hydrophobic nature [99]. Research has shown that the composition, structure, and operating conditions of zeolites can be adjusted to enhance their adsorption capacity for propane, ethylene, and propylene. Furthermore, studies have indicated that the Si/Al ratio of zeolites can also influence the adsorption of propylene.

2.4.8 n-Butane

The adsorption of n-butane onto zeolites has been extensively studied due to its importance in various industrial applications, such as natural gas storage and separation processes. The pore structure and composition of zeolites play a significant role in the adsorption of n-butane. Numerous studies have shown that zeolites can effectively adsorb n-butane due to their size-selective pore structure and affinity for hydrophobic molecules. These studies have demonstrated that zeolites with larger pore sizes, such as MFI and BEA frameworks, have higher adsorption capacities for n-butane compared to small pore zeolites like CHA and LTA. Zeolite Beta has been found to have a high adsorption capacity for propane due to its large pore sizes and interconnected channel systems [100].

2.4.9 Ammonia

The adsorption of ammonia onto zeolites has been widely studied due to its importance in various applications, such as gas separation and catalysis. The unique pore structure and strong acidic sites of zeolites make them highly effective adsorbents for ammonia. These studies have shown that zeolites, such as ZSM-5 and SSZ-13, exhibit high adsorption capacities for ammonia due to their size-selective

pore structure and ability to form strong hydrogen bonds with ammonia molecules. Furthermore, the surface modification of zeolites through ion exchange or functionalization can further enhance their adsorption capacity for ammonia. Zeolite LTA has also been shown to have good adsorption properties for ammonia [101]. Research has shown that 4A zeolite exhibits high adsorption capacities for ammonia due to its ability to exchange Na^+ ions with NH_4^+ ions and form strong electrostatic interactions with ammonia molecules. Furthermore, the operating conditions such as temperature and pressure can be optimized to enhance the adsorption capacity of 4A zeolite for ammonia. Several studies have also explored the potential of modifying the composition and structure of 4A zeolite to further improve its adsorption properties for ammonia. These modifications include controlling the Si/Al ratio, particle size, and surface area of the zeolite to maximize its adsorption capacity for ammonia. Additionally, functionalizing the surface of 4A zeolite with specific chemical groups has shown promising results in enhancing its ammonia adsorption efficiency [102].

Table 5 Overview of zeolite applications in gas adsorption and separation

Gas	Zeolite, Framework	Application	Ref
CO_2	13X and 5A	Carbon capture and storage and Enhanced CO_2 adsorption	[93]
N_2	13X and 5A	Air separation and purification	[94,95]
CH_4	13X, 5A and Y	Methane adsorption and storage	[96]
C_2H_6	Y	High ethane adsorption	[97]
C_2H_4	ZSM-5	Ethylene separation and storage	[90,97,98]
C_3H_6	Beta	Propylene adsorption	[96,97]
C_4H_{10}	MFI	n-Butane adsorption	[100]
NH_3	4A	Ammonia capture and separation	[101,102]

Table 5 provides a brief overview of different zeolites and natural refrigerants considered in the literature. It presents the specific types of zeolite frameworks used and their intended uses, demonstrating the wide-ranging applications of zeolites in environmental protection and industrial operations.

2.5 Zeolite efficacy in the adsorption of HFCs

HFCs are widely used in various applications due to their effective refrigerant properties. However, their environmental impact necessitates a deeper understanding of their molecular characteristics. Understanding their properties is crucial as they directly influence how these

molecules interact with adsorbent materials, like zeolites, which are used for separation and storage. The molecular size and dipole moment play significant roles in the adsorption process, affecting how these molecules are attracted to and held within the adsorbent material. Smaller molecules can access and diffuse into the micropores more readily, while larger molecules may face steric hindrance, impacting their adsorption capacity [103]. The presence of the highly electronegative fluorine atom and its orientation within the molecule contributes to the overall dipole moment. This characteristic governs the interaction of HFC molecules with adsorbent materials and influences the efficiency of adsorption processes [21]. Understanding these structural variations is essential for designing efficient adsorption processes and optimizing the performance of zeolite-based adsorbents for HFC adsorption [104]. Molecules with higher dipole moments often exhibit stronger intermolecular forces, which can contribute to an increase in boiling point. As the dipole moment strengthens gas-gas interactions, it correlates with higher boiling points, further affecting the attraction between HFC molecules and the adsorbent surface. Consequently, the boiling point of HFC molecules can provide insights into their adsorption affinity [20]. In reference to Table 6, the normal boiling points of refrigerants considered in this work were obtained from the literature [105–108] and their gas phase dipole moments were calculated using first-principles density functional theory (DFT) calculations performed with GAUSSIAN 16 software [109].

Table 6 Dipole moments and normal boiling points of refrigerants

Molecule	Dipole Moment (D)	Normal Boiling Point (K)
R41	1.896	131.26
R32	1.972	221.15
R23	1.594	191.15
R14	0.000	145.15
R152a	2.013	249.15
R152 (gauche, trans)	2.688, 0.000	249.15
R143a	2.562	225.55
R143 (gauche, trans)	3.156, 1.500	225.55
R134a	2.229	246.50
R134 (gauche, trans)	2.352, 0.000	246.50
R125	1.678	224.65
R116	0.000	194.95

Research has shown that different types of zeolites, such as 13X, 5A, and 4A, effectively separate HFC molecules based on their size and polar properties. Table 9 summarizes experimental efforts reported in the literature for the loading capacity of HFCs in zeolites. Shiflett et al. [110] reported that zeolite 5A exhibited the highest adsorption capacity for pure R23 compared to zeolites 13X, due to its optimal pore size and favorable interaction with the HFC molecules. Yancey et al. [40] found that R32 and R125 were adsorbed effectively by zeolite 5A. However, their work demonstrated that zeolites 4A and 3A showed negligible adsorption capacities for pure R125 due to steric hindrance. The low sorption of R125 on zeolites 4A and 3A is not surprising given that the pore diameters for these zeolites are approximately 4 Å and 3 Å, respectively, while the kinetic diameter of R125 is 4.4 Å [111]. Conversely, zeolite 4A exhibited substantial adsorption of pure R32, primarily due to its molecular sieving effect. However, while a similar effect was observed in zeolite 3A, the sorption process was significantly slower, rendering it less practical for commercial applications.

Additionally, Yancey et al. [112] found that zeolite 4A was particularly effective in separating mixtures of R32 and R125, due to the steric exclusion of R125 and preferential adsorption of R32, making it the best candidate for such separations. Wanigarathna et al. [50] demonstrated the separation of chlorodifluoromethane (R22), R32, and R125 using 4A and 5A zeolites, attributing the separation of R32 and R22 from R125 to steric effects. Their findings revealed that zeolite 5A exhibited a greater adsorption capacity for R32 and R125 than 4A. Based on measured pure gas adsorption isotherms of R134a, R125, and R143a on 4A and 5A zeolites, it was found that none of these gases could be adsorbed by 4A zeolite while all of them were adsorbed by 5A zeolite. Furthermore, Wanigarathna et al. [49] demonstrated enhanced separation capabilities for R134a, R125, and R143a using zeolites 13X and 5A under ambient conditions. They found that zeolite 13X exhibited the highest adsorption capacity for R134a

which is attributed to its optimal pore size and favorable interactions with the HFC molecules. Zeolite 5A also effectively adsorbed R134a, though to a slightly lesser extent than 13X, due to the molecular sieving effect. Bosch E et al. and Lim KH et al. [113,114] conducted nuclear magnetic resonance (NMR) measurements and molecular dynamic (MD) simulations on the HFC binding characteristics to NaX and NaY zeolites. Results indicated that R134a showed a higher binding affinity to NaX zeolite in comparison to R125 due to the stronger Na–F interactions and O–H hydrogen bonds with the framework. In addition, it was found that hydrogen bonds formed by the CFH₂ end group of R134a were more favorable than those formed by the CF₃ group. The studies are summarized in Table 7.

Table 7 Previous studies on the adsorption of HFCs in zeolites

HFC Compound	Zeolite Framework	Temperature Range (K)	Reference
R32	3A, 4A and 5A	293, 298, 323, 353	[40,50]
R-125	3A, 4A, 5A and 13X	293, 298, 313, 333	[40,49,50]
R-134a	13X	293, 313, 333	[49]
R-143a	13X	293, 313, 333	[49]
R-23	5A	298	[110]

Chapter 3

MOLECULAR DYNAMIC SIMULATION

3.1 Classical Molecular Dynamics Simulations

Molecular Dynamics (MD) simulations are a widely adopted computational technique that enables the study of the physical behavior of atoms and molecules over time by solving Newton's equations of motion. These simulations provide an atomistic view of molecular systems, offering valuable insights into structural, dynamical, and thermodynamic properties. MD simulations have become an indispensable tool in fields such as material science, biochemistry, and adsorption processes, allowing researchers to study complex systems at a level of detail that is inaccessible to experimental techniques [115–117]. The fundamental principle behind MD simulations is Newton's second law of motion, which states that the force F acting on a particle is equal to its mass m multiplied by its acceleration a [118,119]:

$$F = m \cdot a = m \frac{\partial^2 r}{\partial t^2} \quad (8)$$

Here, r represents the position vector of the particle, and $\frac{\partial^2 r}{\partial t^2}$ is the second derivative of the position with respect to time, denoting acceleration. The force acting on each particle in the system arises from interactions with other particles, which are described by the potential energy function U . The relationship between the force and the potential energy is given by:

$$F_i = -\nabla U(r_i) \quad (9)$$

This equation indicates that the force acting on a particle is the negative gradient of the potential energy with respect to its position. By numerically integrating these equations of motion over

discrete time steps, MD simulations provide a trajectory of the particles, describing how the system evolves over time [120,121]

In molecular simulations, the selection of an appropriate forcefield is crucial as it defines the potential energy surface of the system and governs the interactions between atoms and molecules. Forcefields such as COMPASS, Universal Force Field (UFF), CVFF, and DREIDING are frequently utilized, each tailored to specific types of materials and interactions [122–125].

In this study, the Consistent Valence Force Field (CVFF) was chosen for the MD simulations due to its proven reliability in accurately modeling molecular interactions. CVFF is well-suited for simulating systems with covalent bonds and van der Waals interactions, which are critical for capturing the behavior of HFCs in zeolite frameworks. The ability of CVFF to model both the flexibility of molecular structures and the complex interactions between HFC molecules and the zeolite surface makes it ideal for studying adsorption processes [126,127].

3.2 CVFF Forcefield

CVFF is a robust computational tool widely employed in molecular dynamics (MD) simulations to model molecular interactions. Developed to address the complexities of covalent and non-covalent interactions in organic and inorganic systems [128], CVFF is particularly effective for studying adsorption phenomena in materials such as zeolites. Its versatility and proven accuracy make it suitable for investigating the behavior of hydrofluorocarbons (HFCs) in zeolite frameworks.

The forcefield defines the potential energy surface (PES) of the system, which governs the motion of atoms and molecules during the simulation. The total potential energy E in CVFF is expressed as the sum of contributions from bonded and non-bonded interactions [129,130] :

$$E = E_{bond} + E_{non-bonded} \quad (10)$$

Bonded Interactions:

Bonded interactions account for the energies associated with bond stretching, angle bending, and torsional rotations. The relation is as follows.

$$E_{bond} = E_{stretching} + E_{angles} + E_{dihedral} + E_{improper} \quad (11)$$

These terms are expressed as follows:

1. Bond Stretching:

$$E_{stretching} = \sum_{bonds} k_b (r - r_0)^2 \quad (12)$$

Where k_b is the bond force constant, r is the actual bond length, and r_0 is the equilibrium bond length.

2. Angle Bending:

$$E_{angles} = \sum_{bonds} k_\theta (\theta - \theta_0)^2 \quad (13)$$

Where k_θ is the angle force constant, θ is the actual angle, and θ_0 is the equilibrium bond angle.

3. Dihedral (Torsional) Interaction:

$$E_{dihedral} = \sum_{dihedral} \frac{1}{2} V_n [1 + \cos (n\phi - \gamma)] \quad (14)$$

Where V_n dihedral force constant, ϕ dihedral angle, n periodicity, γ phase angle

4. Improper Torsion (to maintain planarity or chirality):

$$E_{improper} = \sum_{impropers} k_{\xi} (\xi - \xi_0)^2 \quad (15)$$

Where: k_{ξ} improper force constant, ξ Actual improper torsion angle, ξ_0 Equilibrium improper torsion angle.

Non-Bonded Interactions

Non-bonded interactions in CVFF encompass van der Waals forces and electrostatic interactions. These are critical for accurately modeling the adsorption of HFCs within zeolites, as they dominate host-guest interactions. The general expression for non-bonded interactions is:

$$E_{non-bonded} = E_{vdW} + E_{Coulmb} \quad (16)$$

Where:

1. Van der Waals Interactions: Van der Waals interactions are modeled using the Lennard-Jones (12-6) potential:

$$E_{vdW} = \sum_{i < j} 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] \quad (17)$$

Where: ϵ depth of the potential well, σ finite distance at which the interparticle potential is zero, r_{ij} distance between particles i and j .

2. Electrostatic Interactions: Electrostatic interactions are described by Coulomb's law:

$$E_{Coulmb} = \sum_{i < j} \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \quad (18)$$

Where: $q_i q_j$ are charges on particles i and j , ϵ_0 is permittivity of free space, r_{ij} is distance between charges i and j .

In this study, the CVFF forcefield was selected due to its capability to accurately model the interactions between HFC molecules and zeolite frameworks. The bonded terms in CVFF captured the flexibility of the HFC molecules, while the non-bonded terms represented the critical van der Waals and electrostatic interactions between the molecules and the zeolite surfaces. The ability of CVFF to describe these interactions reliably was validated against experimental data, demonstrating its predictive accuracy for adsorption processes.

The application of CVFF allowed for the detailed investigation of how molecular size, polarity, and structural conformation influence adsorption in zeolites.

3.3 Metropolis Algorithm

The Metropolis algorithm, introduced by Metropolis et al. in 1953 [131], is a cornerstone of Monte Carlo methods and plays a critical role in statistical mechanics and molecular simulations. It is particularly significant in Grand Canonical Monte Carlo (GCMC) simulations, which are widely employed to study adsorption phenomena in porous materials such as zeolites. The Metropolis algorithm enables the efficient sampling of configurational

space by probabilistically accepting or rejecting trial moves based on their contributions to the system's energy and statistical weight.

In GCMC simulations, the Metropolis algorithm governs particle insertions, deletions, and movements within the system to maintain equilibrium conditions. The algorithm evaluates the probability of transitioning between states using the Boltzmann distribution, ensuring that the system converges to the correct thermodynamic ensemble [132].

Key Steps of the Metropolis Algorithm

The Metropolis algorithm operates through the following steps:

1. Initialization:
 - Define the initial configuration of the system, including the positions of all particles, box dimensions, and thermodynamic parameters such as temperature (T) and chemical potential (μ).
 - Compute the initial energy $E_{initial}$ of the system.
2. Trial Move Generation:
 - A trial move is proposed, which could involve:
 - Adding a new particle to the system (insertion),
 - Removing an existing particle (deletion),
 - Displacing a particle to a new position (translation).
3. Energy Calculation:
 - Compute the energy of the system after the trial move E_{trial} using the defined forcefield (e.g., CVFF).

4. Acceptance Criterion:

- Calculate the change in energy using equation (19) and then evaluate the acceptance probability using the Metropolis criterion using equation (20):

$$\Delta E = E_{trial} - E_{initial} \quad (19)$$

$$P_{accept} = \min \left(1, e^{-\frac{\Delta E}{k_B T}} \right) \quad (20)$$

Where k_B is the Boltzmann constant, T is the absolute temperature

- For particle insertion or deletion, additional factors related to chemical potential and volume are included

$$P_{accept} = \min \left(1, \frac{V}{\Lambda^3 (N+1)} e^{-(\Delta E - \mu)/k_B T} \right) \quad (21)$$

- For insertion and

$$P_{accept} = \min \left(1, \frac{\Lambda^3 N}{V} e^{-(\Delta E + \mu)/k_B T} \right) \quad (22)$$

- For deletion, where: V : Volume of the simulation box, Λ : Thermal de Broglie wavelength, N : Number of particles.

5. Acceptance or Rejection:

- Generate a random number r uniformly distributed in $[0,1]$.

Accept the trial move if $r \leq P_{accept}$. If accepted, update the configuration to the trial state; otherwise, retain the current configuration.

6. Iterate:

- Repeat the process for a large number of steps to sample the configurational space and generate equilibrium ensemble averages.

In this study, the Metropolis algorithm was implemented within GCMC simulations to investigate the adsorption of HFCs in zeolite frameworks. The algorithm efficiently sampled particle insertions and deletions, allowing the calculation of adsorption isotherms and selectivity under various pressures and temperatures. Its probabilistic nature ensured that the simulations accurately captured the thermodynamic properties of the system while maintaining computational efficiency.

3.4 Interaction Models in Molecular Simulations

Accurate modeling of intermolecular interactions is critical for understanding adsorption processes in molecular simulations. This study employs various interaction models to capture the complexities of molecular behavior in zeolites, including Ewald summation for long-range electrostatics, Lennard-Jones potential for van der Waals forces, Coulombic interactions for electrostatics, and hydrogen bonding. Each interaction model plays a distinct role in accurately representing the physical and chemical interactions in the system [133].

3.4.1 Ewald Summation for Long-Range Electrostatics

In systems with charged particles, long-range Coulombic interactions significantly impact molecular behavior. The Ewald summation method is widely used to compute these interactions efficiently by splitting the potential into real-space and reciprocal-space components [134,135]:

$$E_{Coulomb} = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \frac{q_i q_j}{r_{i,j}} \cdot \text{erfc}(\alpha r_{i,j}) + \frac{1}{2V} \sum_{K \neq 1} \frac{4\pi}{k^2} [S(k)]^2 e^{-k^2/4\alpha^2} - \frac{\alpha}{\sqrt{\pi}} \sum_{i=1}^N q_i^2 \quad (23)$$

where q_i and q_j : Charges of particles i and j , $r_{i,j}$: Distance between charges, α

Ewald parameter controlling the split, $S(k)$: Structure factor in reciprocal

space, V : Volume of the simulation box.

Ewald summation ensures that both short-range and long-range contributions are efficiently calculated, maintaining accuracy and computational feasibility. This method is essential for modeling electrostatic interactions in systems like zeolites, where charged cations and polar molecules interact strongly [136].

3.4.2 Lennard-Jones Potential for Van der Waals Forces

Van der Waals interactions, which include attractive (dispersion) and repulsive forces, are described by the Lennard-Jones (12-6) potential

$$E_{vdW} = \sum_{i < j} 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] \quad (24)$$

Where: ϵ depth of the potential well, σ finite distance at which the interparticle potential is zero, r_{ij} distance between particles i and j .

The 12th power term models the strong repulsion at short distances, while the 6th power term accounts for the attractive dispersion forces. This potential is critical for capturing molecular packing and adsorption in zeolites, where van der Waals forces dominate non-bonded interactions [137,138].

3.4.3 Coulombic Interactions

Electrostatic interactions are represented by Coulomb's law:

$$E_{Coulmb} = \sum_{i < j} \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \quad (24)$$

Where: $q_i q_j$ are charges on particles i and j , ϵ_0 is permittivity of free space, r_{ij} is the distance between charges i and j [139,140].

These interactions play a significant role in adsorption processes involving polar molecules like HFCs and charged frameworks like zeolites. Coulombic interactions contribute to the strong cation-fluorine interactions observed in zeolite 13X.

3.4.4 Hydrogen Bonding

Hydrogen bonding, though typically weaker than covalent bonds, significantly impacts adsorption behavior in zeolites. Hydrogen bonding interactions are modeled using a combination of distance and angular criteria:

$$E_{HB} = -\varepsilon_{HB} \exp\left(-\frac{r_{OH} - r_0}{\sigma_{HB}}\right) \quad (25)$$

Where: ε_{HB} : Strength of the hydrogen bond, r_{OH} : Distance between the hydrogen donor and acceptor, r_0 : Equilibrium bond distance, σ_{HB} : Width of the interaction potential [137,140].

In zeolites, hydrogen bonding occurs between the hydrogen atoms in the polar HFC molecules and framework oxygen atoms. This interaction is particularly prominent at low pressures, where specific orientations of adsorbed molecules favor hydrogen bond formation.

In this study, these interaction models were applied within the framework of the CVFF forcefield to simulate the adsorption of HFCs in zeolites. Ewald summation was used to accurately capture long-range electrostatic interactions between charged sites in zeolites and polar HFCs a cutoff distance of 12.5 Å. The Lennard-Jones potential modeled van der Waals interactions between HFC molecules and zeolite pores. Coulombic interactions described the strong cation-fluorine interaction. Together, these interaction models provided a detailed understanding of the guest-host dynamics essential for optimizing HFC adsorption and separation.

3.5 Simulation Framework and Methodology

3.5.1 Zeolite Framework Development

The zeolite structures for this study, including 3A, 4A, 5A, and 13X, were meticulously developed using Material Studio 2023. These frameworks were constructed adhering to Löwenstein's rule, ensuring the absence of Al-O-Al bonds, and modeled as 2×2×2 supercells to ensure that their dimensions exceeded twice the radius of adsorbates, enhancing simulation accuracy.

For zeolite 13X, the Si/Al ratio of 1.18 was achieved by random substitution of Si with Al atoms, with charge balance maintained through the addition of Na⁺ ions. These Na⁺ ions were positioned using the "cation locator" tool in the Sorption module. The final structure for 13X was geometrically optimized and had a molecular formula of Na₈₈Al₈₈Si₁₀₄O₃₈₄ with lattice dimensions of 25.028 Å. Other zeolites, such as 5A, 4A, and 3A, were also developed with specific molecular formulas reflecting their optimized cation-exchange capacity and structural suitability for adsorption processes.

- **Zeolite 5A:** Molecular formula of Na₃₂Ca₃₂Al₉₆Si₉₆O₃₈₄ with a lattice length of 24.61 Å.
- **Zeolite 4A:** Molecular formula of Na₉₆Al₉₆Si₉₆O₃₈₄.
- **Zeolite 3A:** Molecular formula of K₅₈Na₃₈Al₉₆Si₉₆O₃₈₄.

These optimized frameworks allowed for precise modeling of guest-host interactions, essential for understanding the behavior of HFCs in zeolites.

3.5.2 Molecular Dynamics and Grand Canonical Monte Carlo Simulations

Molecular Dynamics (MD) and Grand Canonical Monte Carlo (GCMC) simulations were employed to study the adsorption behavior of HFCs within the zeolite frameworks. MD simulations were pivotal in capturing the dynamics and structural interactions over time, while

GCMC simulations provided adsorption isotherms and thermodynamic data under varying conditions.

GCMC simulations, which allow the exchange of particles between the system and a reservoir, were implemented under periodic boundary conditions. The chemical potential was linked to fugacity f using the following relationship:

$$\mu = \mu^0 + RT \ln \frac{f}{f^0} \quad (26)$$

Where μ^0 is the reference chemical potential, R is the gas constant, T is the temperature and f^0 is the reference fugacity. Assuming ideal gas behavior at low pressures (up to 100 kPa), the simplification facilitated computational efficiency.

Key parameters:

Equilibration: 1×10^6 steps, Production 1×10^7 steps and Temperature range: 293–333 K with 10 K increments.

3.6 Langmuir-Freundlich model

Adsorption isotherms obtained from the GCMC simulations were fitted against Langmuir-Freundlich model. Simulation results for all examined refrigerants in different zeolite structures are tabulated in the Appendix and the corresponding model parameters are presented in Table 8.

Table 8 Langmuir-Freundlich isotherm model fitting parameters for various zeolites and refrigerants at 298 K

Molecules		Zeolites			
		13X	5A	4A	3A
R41	q (mmol/g)	997.889	214.018	164.170	2.773
	K (kPa ⁻¹)	1.568e-05	1.068e-10	3.310e-10	0.525
	n	0.863	0.223	0.225	0.584
	R^2	0.999	0.999	0.999	1.000
R32	q (mmol/g)	6.110	8.895	5.235	3.902
	K (kPa ⁻¹)	0.046	0.024	0.353	8.601
	n	1.027	0.241	0.715	0.309
	R^2	1.000	0.999	1.000	1.000
R23	q (mmol/g)	3.832	3.752	2.958	2.375
	K (kPa ⁻¹)	0.071	0.053	0.442	4.126
	n	1.731	0.999	0.779	0.428
	R^2	0.999	1.000	1.000	1.000
R14	q (mmol/g)	2.792	3.245	3.624	2.774
	K (kPa ⁻¹)	0.052	0.098	0.140	0.525
	n	1.018	0.743	0.405	0.584
	R^2	1.000	0.998	1.000	1.000
R152a	q (mmol/g)	3.4723	3.333		
	K (kPa ⁻¹)	0.567	1.087	-	-
	n	0.566	0.538		
	R^2	1.000	1.000		
R143a	q (mmol/g)	4.350	2.961		
	K (kPa ⁻¹)	0.133	0.443	-	-
	n	0.224	0.684		
	R^2	0.999	1.000		
R134a	q (mmol/g)	2.774	3.343		
	K (kPa ⁻¹)	1.000	1.519	-	-
	n	0.746	0.287		
	R^2	1.000	0.999		
R125	q (mmol/g)	2.423	2.953		
	K (kPa ⁻¹)	5.533	2.408	-	-
	n	0.619	0.261		
	R^2	1.000	1.000		
R116	q (mmol/g)	2.078	2.388		
	K (kPa ⁻¹)	0.208	1.690	-	-
	n	6.80601	0.351		
	R^2	0.999	1.000		

Chapter 4

RESULTS AND DISCUSSION

4.1 Model validation

Figure 9 compares the adsorption isotherms of R32 in LTA zeolites and R134a in zeolite 13X against experimental data [49,112] found in the literature. Figure 9 (a) depicts that zeolites 3A, 4A, and 5A exhibit distinct adsorption capacities due to differences in their ion distribution and pore sizes. In zeolite 3A, the relatively large molecular size (1.38 Å) of the potassium (K^+) ions reduces the available pore size and limits the accommodation of larger molecules. In the case of zeolite 4A, the potassium ions are exchanged with sodium (Na^+) ions with smaller size (1.02 Å), resulting in a moderate pore size and reasonable adsorption capacity. In zeolite 4A, twelve Na^+ cations are present: eight in site I (SI), coordinated to the oxygen atoms of the 6-ring of the sodalite cage; three in site II (SII), partially obstructing the 8-ring windows of the α -cage and decreasing the effective pore diameter, coordinated with oxygen atoms of the 8-ring; and one in site III (SIII), coordinated with oxygens of the 4-ring. A similar arrangement exists in zeolite 3A, except with K^+ cations. When Na^+ ions in 4A are exchanged with calcium (Ca^{2+}) ions to form 5A zeolite, all Na^+ ions are removed from the 8-membered ring window, and Ca^{2+} ions (along with remaining Na^+ ions) occupy sites near the 6-membered ring window. This ion exchange significantly increases the accessibility of active sites on the zeolite pore surface which enhances the adsorption capacity for various gases. Consequently, zeolite 5A zeolite is usually expected to have the highest loading capacity.

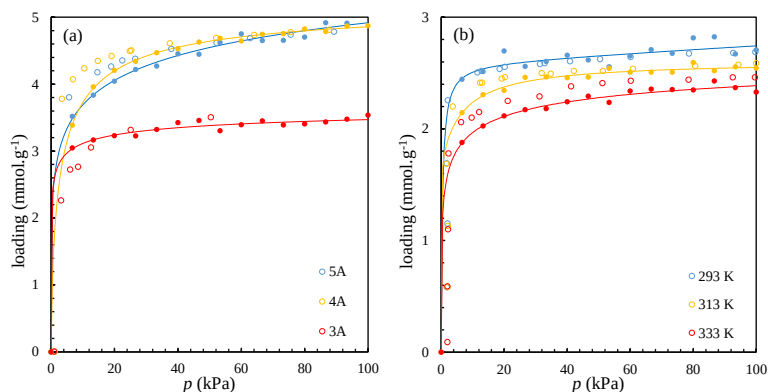


Figure 9 Adsorption of R32 in LTA zeolites at 298.15 K and (b) Adsorption of R134a in 13X as a function of temperature.

Open symbols represent experimental data [49,112] and filled symbols represent simulation results.

However, both experimental and simulation data show that the loading capacity of R32 in zeolite 4A is higher than that in zeolite 5A at low pressures below 60 kPa. This can be attributed to the similarity in values between the pore diameter of zeolite 4A and the kinetic diameter of R32 (3.9 Å). The pore size is slightly larger enough to allow R32 molecules to enter but the tight fit results in them being effectively trapped within the pores. This trapping effect maximizes the number of R32 molecules that can be adsorbed within the available pore space, leading to a higher adsorption capacity compared to zeolite 5A. Furthermore, Figure 9 (b) represents the temperature-dependent adsorption isotherm of R134a in zeolite 13X. The observed decrease in adsorption capacity with increasing temperature reflects the exothermic nature of the adsorption process. The close alignment between the experimental [49,112] and simulation data in Figure 9 indicates the accuracy of the force field used in this work which ensures the reliability of the computational models employed.

4.2 Adsorption behavior of fluoromethane derivatives

Previous studies [114,141] have established that hydrogen bonding between hydrofluorocarbons (HFCs) and zeolite framework oxygen atoms, as well as F–M⁺ (M⁺ = cations) interactions at non-framework Lewis acid sites, are critical factors in adsorption. In zeolites with low Si/Al ratios, such as type A zeolite (Si/Al = 1), the increased charge on the

framework oxygen atoms enhances the strength of hydrogen bonding, making it the dominant binding mechanism. This is because the oxygen atoms carry a more negative charge, increasing the Lewis basicity of the zeolite and strengthening hydrogen bonding [142]. In reference to Figure 10 (a-c), R32 (CF_2H_2) exhibits the highest adsorption capacity among all fluoromethane derivatives due to its symmetrical molecular structure which includes two fluorine atoms and two hydrogen atoms. The hydrogen atoms facilitate stronger hydrogen bonds with the oxygen sites. These hydrogen bonds are particularly crucial in zeolites with low Si/Al ratios, where hydrogen bonding is the dominant interaction mechanism. The presence of fluorine atoms also contributes to stronger electrostatic interactions with non-framework cations due to their high electronegativity. In reference to Table 6, R32's high dipole moment (1.972 D) further supports this argument, justifying its superior adsorption capacity. In comparison, R41 (CH_3F) has a slightly lower dipole moment (1.896 D) but still benefits from the electrostatic interaction of its single fluorine atom with the zeolite's active sites. Despite having more hydrogen atoms than R32, the lack of multiple fluorine atoms reduces the molecule's electron-accepting capability (positive partial charges) which weakens the strength of any hydrogen bonds. The moderate adsorption capacity exhibited by R23 (CF_3H) can be attributed to its asymmetrical structure which leads to a lower dipole moment (1.594 D) and a limited number of possible hydrogen bonds. R14 (CF_4), with tetrahedral symmetry and no dipole moment, relies solely on van der Waals forces, resulting in the lowest adsorption capacity.

It is worth noting that the boiling points of these refrigerants correlate well with the strength of their interactions. Higher boiling points indicate stronger gas-gas interactions and, consequently, stronger host-gas interactions. According to Table 6, R32, with the highest boiling point, exhibits the strongest interactions with the zeolite, followed by R41, R23, and R14. All LTA types of zeolites display consistent adsorption behavior, with 5A being the most effective due to its highest pore size and ion distribution.

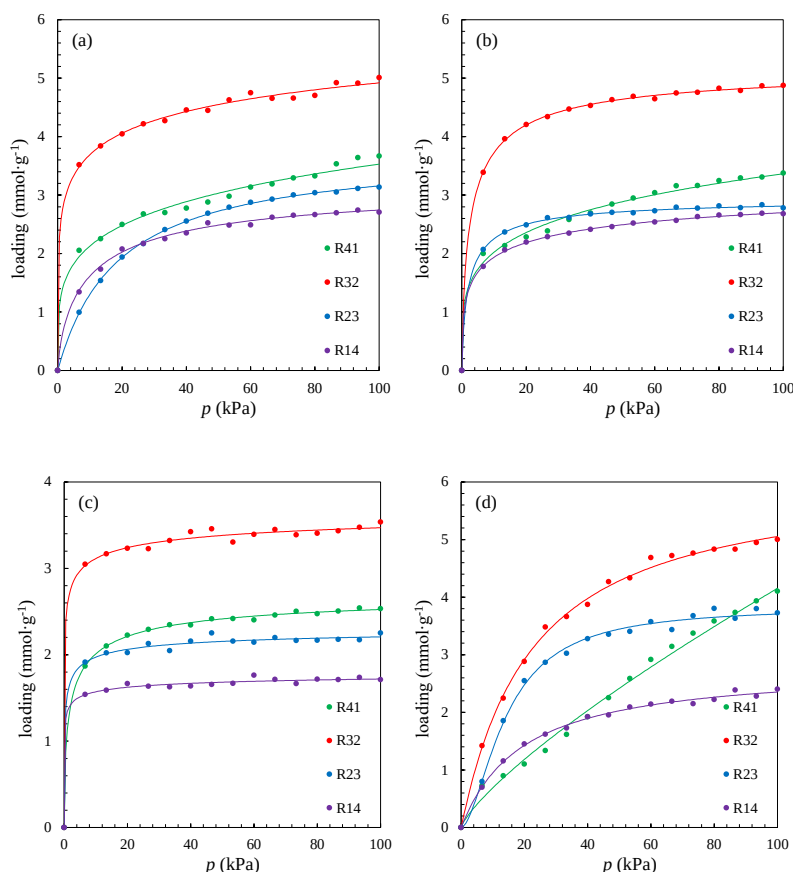


Figure 10 Adsorption isotherms of fluoromethane derivatives at 298.15 K in zeolites (a) 5A, (b) 4A, (c) 3A and (d) 13X.

To examine the effect of the framework, a comparison between zeolites 5A and 13X is shown in Figures 10 (a) and (d), respectively. At low pressures, zeolite 5A shows a steeper initial rise in adsorption which indicates a stronger initial affinity for refrigerants. This pronounced initial adsorption in zeolite 5A is particularly noticeable for R41 and can be attributed to the presence of calcium (Ca^{2+}) ions which create stronger electrostatic interactions with the adsorbates. Conversely, zeolite 13X, which primarily contains sodium (Na^+) ions, starts with a lower capacity but eventually surpasses zeolite 5A at higher pressures due to its larger pore size and enhanced packing efficiency. These observations are consistent with previous findings [143] which suggest that the sorption of HFCs is dominated at lower pressures by enthalpic interactions at Lewis acid sites and at high pressures by entropic effects and the packing efficiency of the sorbate within the zeolite framework.

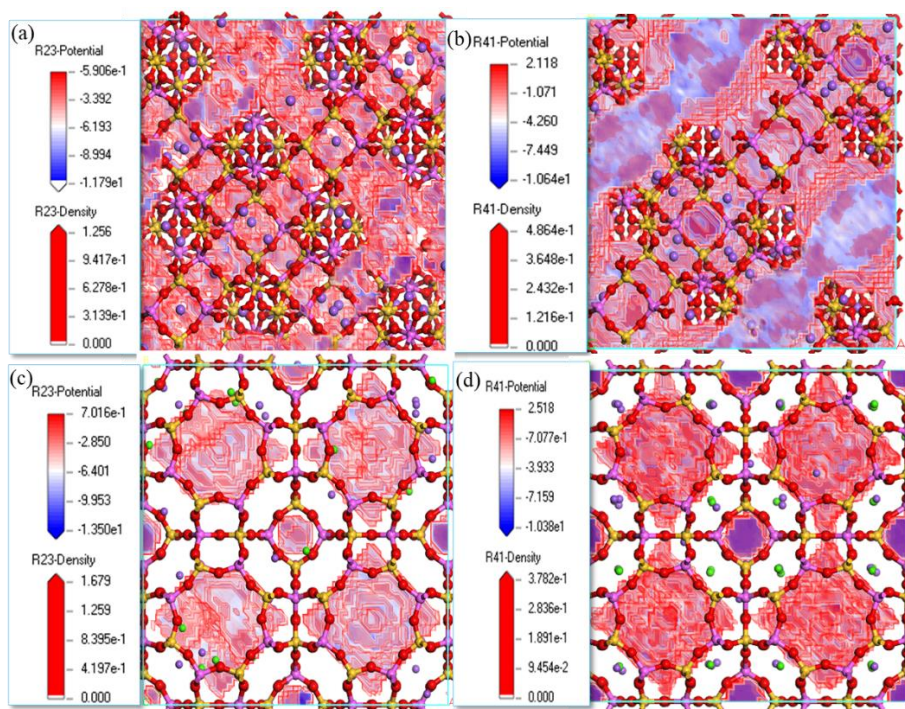


Figure 11 Density profiles for R41 and R23 in zeolites 13X and 5A at 298.15 K. (a) R41 in 13X, (b) R23 in 13X, (c) R41 in 5A and (d) R23 in 5A.

Figure 11 provides further support for the discussions of Figures 10 (a) and (d) by illustrating the density profiles and potential maps of R41 and R23 within zeolites 13X and 5A at 298.15 K. In these maps, red regions indicate higher density and stronger adsorption potential, while blue regions indicate lower density and weaker adsorption potential. The maps in Figures 11 (a) and 11 (b) reveal higher densities and stronger interaction potentials for R23 compared to R41, which aligns with the higher adsorption capacity of R23 in zeolite 13X as described in Figure 10 (d). Conversely, Figures 11 (c) and 11 (d) depict higher densities and stronger interaction potentials for R41 compared to R23, which aligns with the higher adsorption capacity of R41 in zeolite 13X as described in Figure 10 (a).

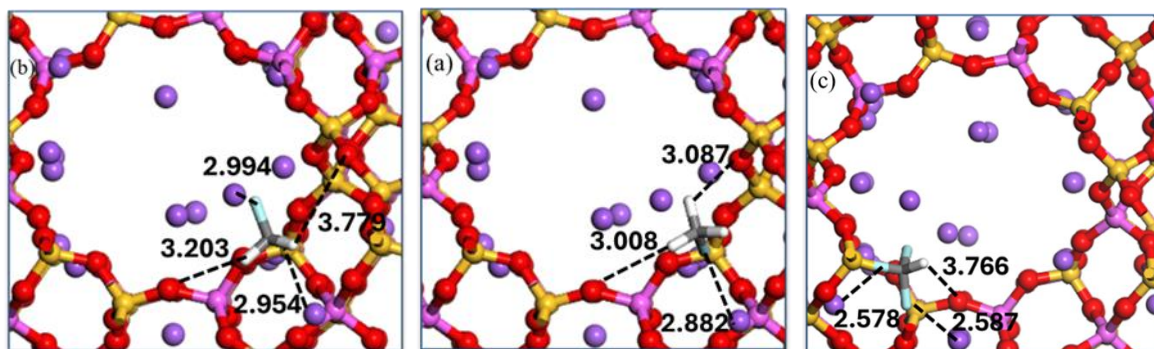


Figure 12 Molecular interactions between HFCs and zeolite 13X. (a) R41, (b) R32 and (c) R23.

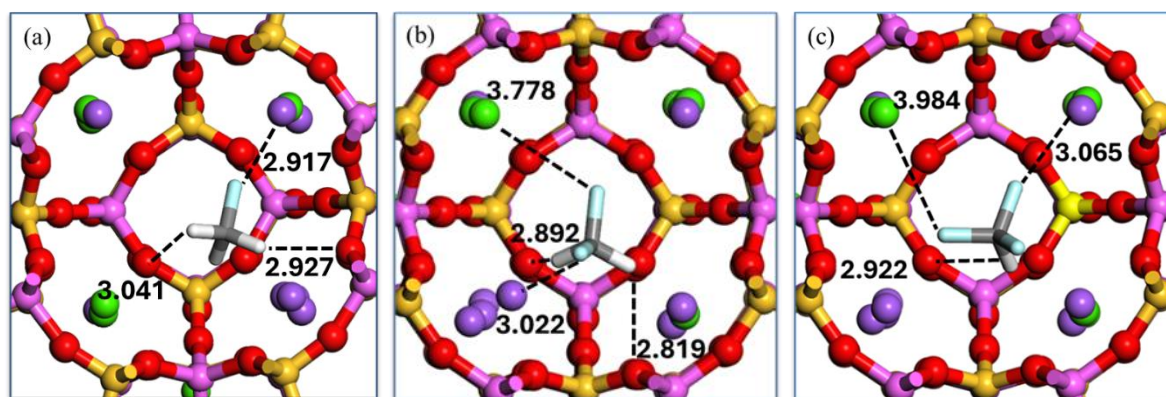


Figure 13 Molecular interactions between HFCs and zeolite 5A. (a) R41, (b) R32 and (c) R23.

Figures 12 and 13 illustrate the distances of various electrostatic interactions at low loading occurring within the zeolite 13X and 5A frameworks, respectively. In reference to Figure 12, the dominant interaction in zeolite 13X appears to be Na–F, as these distances are shorter than the O–H distances. In reference to Figure 12 (a), R41 forms two hydrogen bonds with the zeolite framework at a distance of around 3 Å. In addition, the single fluorine atom in R41 is electrostatically interacting with the Na ion at distance of 2.882 Å. On the other hand, R32 in Figure 12 (b) is coordinated between two Na ions at distance of 3 Å and can form one hydrogen bond only at a distance of 3.208 Å. The latter explains why R32 has the highest adsorption capacity among all studied fluoromethane derivatives in this work. In comparison to R32, Figure 12 (c) shows that R23 is coordinated by two Na ions at a shorter distance of 2.578 Å but forms a weaker hydrogen bond at a larger distance of 3.766 Å. Hence, it can be concluded that the main reason behind which R23 is showing a greater adsorption capacity in zeolite 13X

in comparison to R41 is the presence of more fluorine atoms which facilitates more Na–F interactions.

In reference to Figure 13, the dominant interaction in zeolite 5A appears to be hydrogen bonding, as these distances are shorter than the M–F distances. It seems that R41, R32 and R23 form hydrogen bonds and Na–F interactions with the zeolite framework at a similar approximate distance of 2.9 Å. R41 and R32 have the ability to form two hydrogen bonds while R23 can form only one. For R32 and R23, electrostatic interactions Ca^{2+} occur at a greater distance of 3.777 Å for R32 and 3.984 Å for R23. Hence, it can be concluded that the main reason behind which R41 is showing a greater adsorption capacity in zeolite 5A in comparison to R23 is the presence of more hydrogen atoms which facilitates more O–H interactions.

Figures 14 and 15 present the radial distribution functions (RDFs) for R41, R23, and R32 in zeolites 13X and 5A. In Figure 14 (a), the strong peak at around 2 Å reinforces the significance of Na–F interactions as the primary driver of adsorption in zeolite 13X. On the other hand, Figure 14 (b) shows a weaker intensity for the first peak which supports the notion that zeolite 5A relies more on hydrogen bonding interactions rather than cation–F interactions. Moreover, the O–H RDF peaks shown in Figure 15 at around 3 Å suggest that all refrigerants exhibit strong hydrogen bonding interactions in both zeolite frameworks. Thus, the RDF results corroborate the conclusion that Na–F interactions primarily drive adsorption in zeolite 13X, while hydrogen bonding plays a more significant role in zeolite 5A.

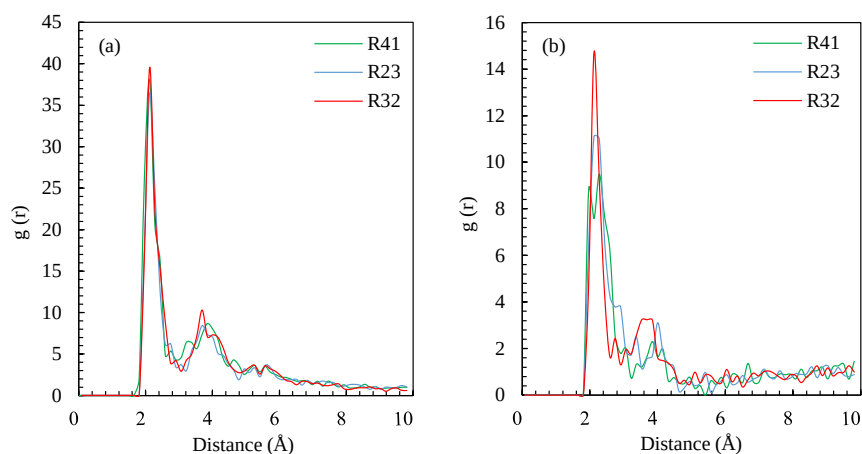


Figure 14 RDF analysis of cation–F interactions for R41, R23, and R32 in zeolites (a) 13X and (b) 5A.

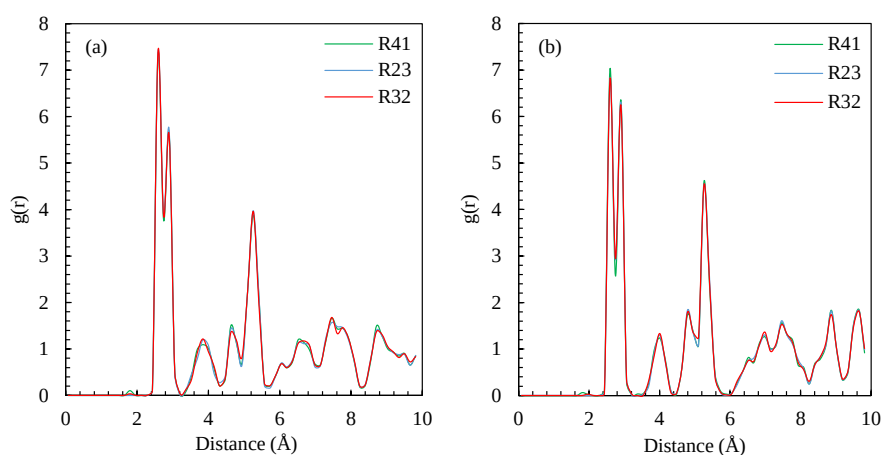


Figure 15 RDF analysis of O–H interactions for R41, R23, and R32 in zeolites (a) 13X and (b) 5A.

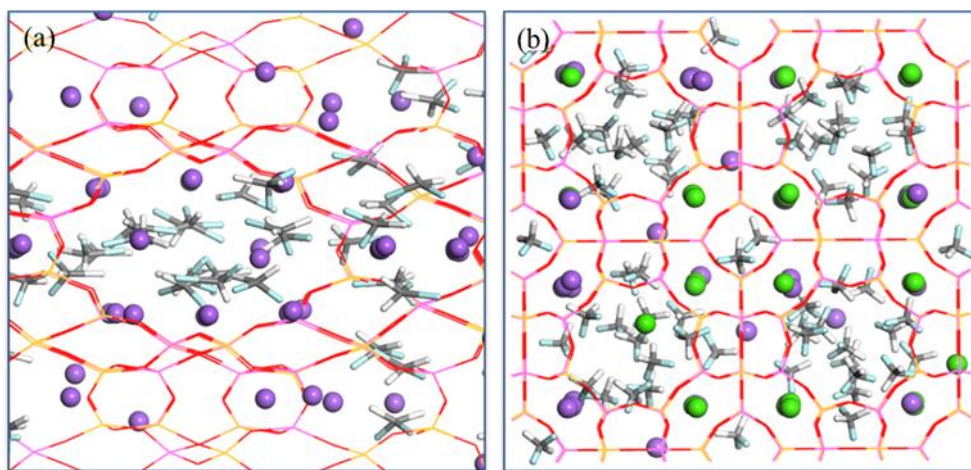


Figure 16 Distribution of R32 at 1 atm and 298 K in zeolite (a) 13X and (b) 5A.

Figure 16 demonstrates that R32 exhibits different molecular placements (adsorption locations) depending on the type of zeolite used. In 13X, R32 molecules are more concentrated within

the 12-membered ring windows, indicating that 13X provides a higher pore size for sorption. Conversely, molecules in zeolite 5A are more evenly distributed but primarily occupy the 8-membered ring windows, reflecting its smaller pore size. This observation underscores that zeolite 13X offers larger pore sizes which facilitates better accommodation and adsorption of HFCs. On the other hand, more restricted adsorption sites are shown by zeolite 5A due to its with its smaller pore size.

4.3 Effect of HFC structure on adsorption behavior

Figure 17 presents adsorption isotherms for pairs of refrigerants on zeolite 13X at 298.15K. The compared pairs have the same fluorine number but differ in their carbon number. Despite R152a and R143a having a higher dipole moment due to the presence of an extra methyl (CH_3) group in both molecules, Figures 17 (a-b) show that R32 and R23 exhibit better interactions with the zeolite at higher pressures due to their smaller molecular size and better packing efficiency. However, at lower pressures, adsorption is driven enthalpically by the larger dipole moments of R152a and R143a which leads to their higher adsorption capacities. Figure 17 (c) shows that R134a exhibits higher adsorption capacity in zeolite 13X in comparison to R14. The presence of the CH_2F group in R134a allows for hydrogen bonding and stronger electrostatic interactions with the non-framework cations which consistently results in higher adsorption capacity. In contrast, R14 relies solely on van der Waals forces due to the absence of hydrogen atoms and a zero-dipole moment which results in significantly lower adsorption capacity. These observations are consistent with the general trend that ethane-based refrigerants with higher dipole moments exhibit higher adsorption capacities at low pressures due to enthalpically driven sorption, while methane-based refrigerants with their smaller sizes, achieve higher capacities at high pressures due to entropic effects and packing efficiency.

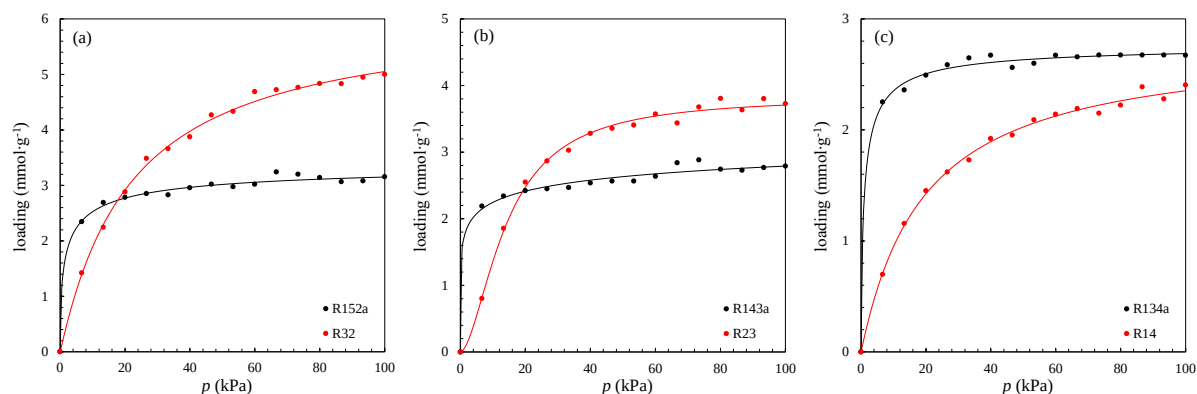


Figure 17 Adsorption isotherms of HFCs in zeolite 13X at 298.15 K. (a) R32/R152a, (b) R23/R143a and (c) R14/R134a.

Figure 18 illustrates the adsorption isotherms of various HFC isomers on 13X zeolite at 298.15 K. The latter would demonstrate how molecular conformations and end-group interactions impact the adsorption behavior. In Figure 18 (a), 1,2-difluoroethane (R152) exhibits greater adsorption capacity than R152a. This difference is primarily due to the presence of the CH_3 group in R152a, which reduces its ability to form strong hydrogen bonds and electrostatic interactions with the zeolite framework. Although the dipole moment of the trans conformer for R152 is zero, previous efforts [144] shows that R152 prefers the gauche conformer which has a higher dipole moment than that of R152a. Similarly, 1,1,2-trifluoroethane (R143) outperforms R143a in Figure 18 (b). While the C_1 (trans) conformer of R143 has a lower dipole moment than R143a, the higher adsorption of R143 suggests that it predominantly exists in the C_s (gauche) conformer which has a dipole moment higher than R143a [145]. The higher adsorption capacity shown by 1,1,1,2-tetrafluoroethane (R134) in Figure 18 (c) can also be attributed to the presence of the gauche conformer which has a higher dipole moment compared to R134a. Despite the trans conformer being more thermodynamically stable in the gas phase, previous research efforts [146] have shown that the gauche conformer of R134 is the dominant form in the sorbed phase of Faujasite zeolites.

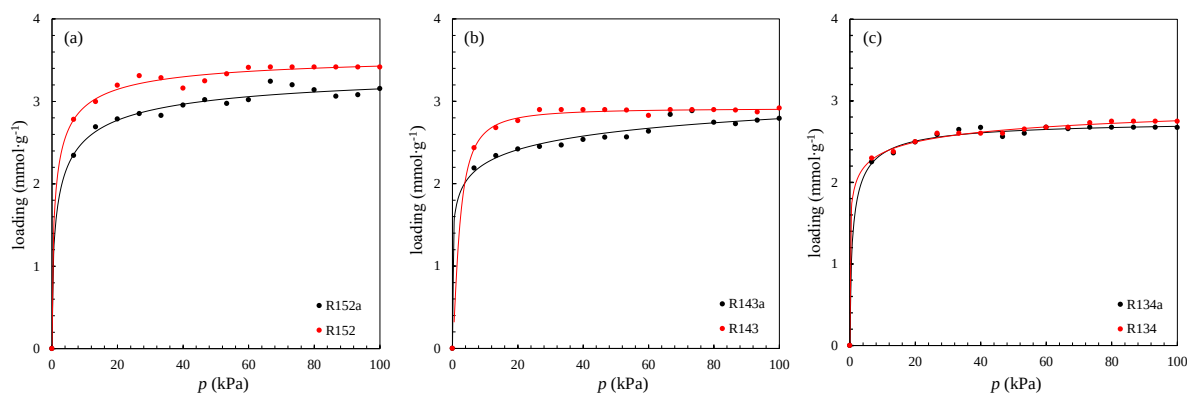


Figure 18 Adsorption isotherms of structural isomers in zeolite 13X at 298.15 K. (a) difluoroethanes, (b) trifluoroethanes and (c) tetrafluoroethanes.

4.4 Application of zeolites to HFC separation

Previous efforts [40,49,50,112] have shown that zeolites 13X and 5A are effective in separating azeotropic HFC mixtures. Wanigarathna et al. [49,50,112] demonstrated the potential of these zeolites for separating components in R410A, R404A, R407C, and R417A mixtures. Superior separation capabilities were shown by zeolite 5A, with R-32 being successfully separated from both R410A and R407C due to its optimal pore size and specific interactions. Additionally, zeolite 13X also showed promise, especially for the separation of R134a from R404A and R417A. Yancey et al. [40] found that zeolite 5A effectively adsorbed R32 from R125, due to the molecular sieving effect. These studies highlight the suitability of 5A and 13X for industrial HFC separation applications.

Building on these previous studies, Figure 19 examines the potential of zeolites for separating R-23 + R-32 and R23 + R116 (R508) binary mixtures. Zeolite 13X demonstrated higher selectivity for R23 compared to zeolite 5A when separating R23 from R116. As shown in Figure 12, Na–F electrostatic interactions dominate the adsorption behavior of HFC molecules in zeolite 13X. The presence of three fluorine atoms and one highly acidic hydrogen atom in R23 results in a higher adsorption capacity in zeolite 13X, making it better suited for separating R23 from R508 blends. In contrast, zeolite 5A showed higher selectivity for R32 compared to

zeolite 13X when separating R23 from R32. The difference in molecular structure between R23 and R32 is a single fluorine atom. As shown in Figure 13, O–H interactions (hydrogen bonding) dominate the adsorption behavior in zeolite 5A, leading to a higher adsorption capacity for R32 due to the presence of two hydrogen atoms.

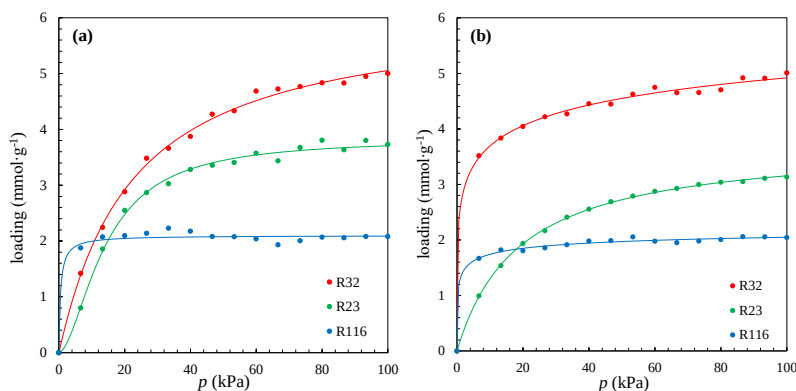


Figure 19 Adsorption isotherms of R32, R23, and R116 at 298.15 K in zeolites (a) 13X and (b) 5A.

4.5 Temperature dependence of HFC adsorption in zeolites

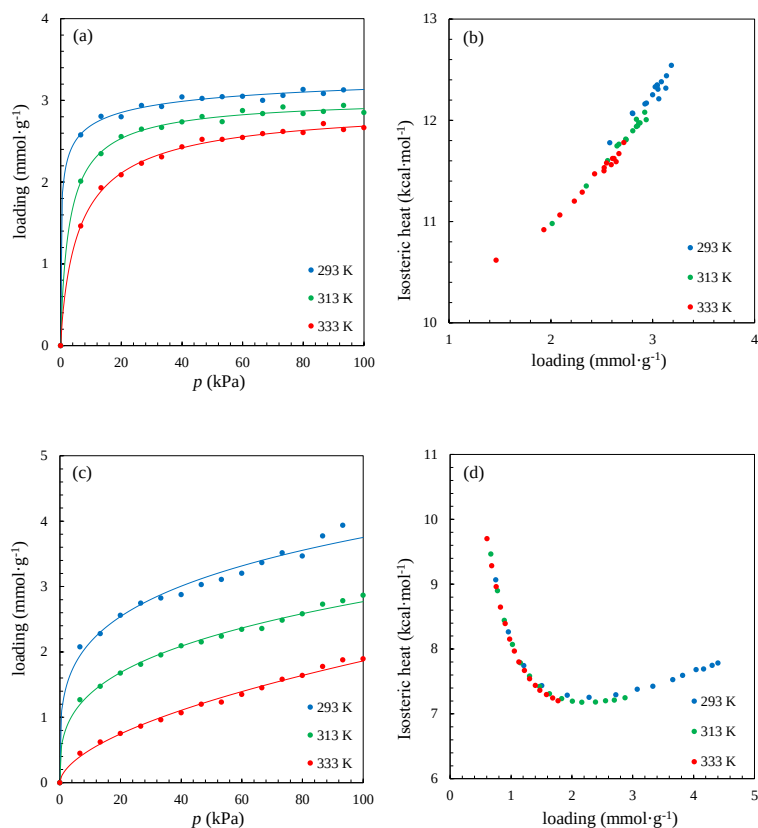


Figure 20 Effect of temperature on the adsorption of HFCs in zeolite 5A. (a) isotherms for R152a, (b) isosteric heat for R152a, (c) isotherms for R41 and (d) isosteric heat for R41.

Figure 20 analyzes the temperature dependence of the adsorption isotherms and isosteric heat of adsorption for R152a and R41 in zeolite 5A. For both refrigerants, the adsorption capacity decreases with increasing temperature, indicative of an exothermic process. For R152a, the isosteric heat increases with loading, which indicates stronger interactions with the zeolite framework as more sites become occupied. In contrast, R41 exhibits a distinct isosteric heat trend due to its smaller molecular size. Initially, R41 molecules occupy the high-energy adsorption sites near the cations in the zeolite framework, resulting in higher isosteric heat. As the loading increases, these high-energy sites become saturated, and entropic effects dominate due to molecular rearrangements and the occupation of less favorable sites, causing a dip in the isosteric heat. At higher loadings, intermolecular (dipole-dipole) interactions among R41 molecules become significant, leading to an increase in isosteric heat as the adsorbate approaches saturation. This interplay between framework interactions, entropic contributions, and intermolecular forces explains the observed minimum in the isosteric heat of R41.

Chapter 5

CONCLUSION AND RECOMMENDATION

5.1 Conclusion

Nations are legally bound to phase down the production and consumption of HFCs by 85% by the year 2048 due to their high GWPs. The effective recovery and recycling of HFCs represents a short to medium-term solution to mitigate their negative environmental impact. The latter creates the need for advanced materials that can selectively adsorb and recycle these refrigerants. Zeolites, with their unique microporous structures and properties, represent a promising class of materials for this application.

In this thesis, zeolites 13X, 5A, 4A, and 3A were chosen for their advantageous properties, high surface area, and exceptional selective adsorption capabilities. The work focused on utilizing Molecular Dynamics (MD) and Grand Canonical Monte Carlo (GCMC) simulations to provide insights into the guest-host interactions and adsorption trends for various HFCs. The CVFF forcefield used in these simulations exhibited strong agreement with experimental data, underscoring its reliability as a predictive tool for HFC adsorption behavior.

Distinct adsorption trends were observed for each zeolite type, with zeolite 13X generally exhibiting higher adsorption capacities due to its larger pore size and strong cation-fluorine interactions. In contrast, zeolite 5A showed higher selectivity at lower pressures due to dominant hydrogen bonding interactions, which became less significant at higher pressures where entropic effects took precedence. The tighter pore sizes of zeolites 4A and 3A restricted access for fluoromethane derivatives, favoring the adsorption of fluoromethane derivatives, as steric hindrance limited the accessibility of the pores. These trends underscore the importance of aligning refrigerant molecular properties with zeolite framework characteristics to maximize the adsorption capacity.

The adsorption behavior of individual HFCs, such as R32, R41, and R14, further highlighted the effect of molecular size and structure on adsorption trends. R32 a small and polar molecule displayed high selectivity in smaller-pore zeolites like 5A and 4A due to its ability to establish hydrogen bonds and fit effectively within the restricted pore spaces. R41, with a less polarity,

showed moderate adsorption in both 13X and 5A, this reflects its balanced interaction between pore accessibility and molecular structure. In contrast, R14 a larger and less polar molecule exhibited lower adsorption in smaller-pore zeolites due to steric hindrance but showed better adsorption affinity in the larger pore windows of zeolite 13X.

The analysis also highlighted the significant impact of carbon number on adsorption behavior with HFCs that contain higher carbon content demonstrating lower adsorption due to steric hindrance within smaller pore windows. Additionally, structural isomerism influenced adsorption capacities; for instance, R143 showed a preference for the Cs conformer over the C1 conformer, while both R152 and R134 favored the gauche conformer over the trans conformer, underscoring the role of molecular structure in adsorption efficiency.

In addition to these structural considerations, this thesis also highlighted the relevance of specific HFC mixtures, such as R410A and R507, which are widely used in refrigeration and air conditioning applications. The ability to selectively adsorb and separate components within these HFC blends is crucial for recycling efforts, as it enables the reuse of refrigerants and contributes to reducing greenhouse gas emissions.

Finally, the thesis identified distinct selectivity patterns across different HFCs, with R23 demonstrating higher selectivity over R116 in zeolite 13X, while R32 exhibited higher selectivity over R23 in zeolite 5A. These findings underscore the influence of both molecular structure and zeolite framework characteristics on adsorption efficiency. The insights from this thesis can guide the optimization of zeolite-based materials for selective HFC separation.

In summary, this thesis provides valuable insights into the selective adsorption capabilities of various zeolites, for the capture and separation of HFCs. The results highlight the importance of factors such as pore size, framework structure, carbon content, and molecular conformer in determining adsorption performance. By advancing the understanding of guest-host interactions in zeolite-based systems, this work contributes to the development of advanced adsorbent materials, supporting global efforts to reduce the environmental impact of HFCs

5.2 Recommendations for Future Research Directions

While this study provides valuable insights into the adsorption behavior of HFCs in various zeolite structures, several opportunities exist for further investigation to expand the

understanding and practical applications of this thesis. The following recommendations are proposed for future research:

1. **Adsorption of other pure HFCs and HFOs:** Expanding the study to include additional hydrofluorocarbons (HFCs) and hydrofluoroolefins (HFOs) could provide a more comprehensive understanding of the adsorption properties of various refrigerants in zeolites. HFOs, as a newer class of low-GWP refrigerants, present different molecular structures and physical properties compared to traditional HFCs, making it valuable to investigate their adsorption behavior. For instance, we expect that the presence of a double bond in 2,3,3,3-tetrafluoropropene (R1234yf) and trans-1,3,3,3-tetrafluoropropene (R1234ze(E)) would introduce interesting adsorption characteristics.
2. **Adsorption of pure HFCs in MOFs:** Investigating the adsorption behavior of pure hydrofluorocarbons (HFCs) in metal-organic frameworks (MOFs) offers a promising research direction for developing efficient and selective materials for refrigerant capture and recycling. MOFs are highly tunable materials with extensive porosity and diverse structural compositions, allowing for precise adjustments in pore size, shape, and surface chemistry to target specific molecules. Unlike zeolites, MOFs can be engineered with various organic linkers and metal clusters, providing tailored environments that could optimize adsorption for specific HFCs based on their molecular characteristics. Exploring the adsorption of HFCs, such as R32 and R125, in MOFs could help to identify materials with enhanced selectivity and capacity, advancing the development of efficient separation technologies for refrigerant gases. This research could further inform how MOFs compare to traditional zeolites in terms of stability, adsorption strength, and recyclability, contributing valuable insights for future industrial applications focused on mitigating the environmental impact of HFCs.

3. **Adsorption of HFC blends:** Investigating the adsorption behavior of HFC blends, rather than pure components, would offer insights into how these zeolites perform in realistic, mixed-refrigerant scenarios. Studying blends such as R410A (a mixture of R32 and R125) and R508 (a mixture of R23 and R116) is particularly relevant due to their extensive use in refrigeration and air conditioning. These azeotropic mixtures are challenging to separate using conventional methods, making them ideal candidates for adsorption using zeolites. Understanding how zeolites interact with these complex mixtures could reveal selective adsorption patterns and identify materials optimized for separating azeotropic components, advancing the potential for recycling and reuse. This line of investigation addresses the limitations of traditional separation processes and could lead to more efficient methods for recovering valuable refrigerants from industrial mixtures.
4. **Kinetic and dynamic studies:** While this study primarily focuses on equilibrium adsorption behavior, investigating the adsorption kinetics and dynamic diffusion processes of HFCs in zeolites would provide valuable insights into the rate-controlling steps and overall efficiency of adsorption in real-world applications. Future research could incorporate breakthrough curve analysis to measure the adsorption and desorption rates. This would help to assess the performance of zeolites in continuous-flow conditions typical of industrial applications. Breakthrough curves, which track the concentration of HFCs exiting the adsorbent bed over time, could be obtained experimentally to reflect practical adsorption dynamics. Additionally, molecular dynamics simulations can complement experimental findings by providing detailed insights into diffusion pathways and interaction energies within zeolite frameworks. Combining experimental breakthrough studies with simulation-based kinetic modeling

would create a comprehensive understanding of the adsorption process, highlighting zeolite materials optimized for rapid and efficient HFC separation.

5. **Development of enhanced forcefields:** Continued refinement of forcefields tailored specifically for HFC- and HFO-zeolite interactions could improve the predictive accuracy of molecular simulations. This would enable more reliable predictions for novel HFO molecules and adsorbents that have yet to be experimentally tested.

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Appendix

Table 9 Comparative Isotherm Analysis of R134a in Zeolite 13X at 293K, 313K, and 333K

13X/R134a											
293K				313K				333K			
Exp.		Sim.		Exp.		Sim		Exp.		Sim	
P	L	P	L	P	L	P	L	P	L		
99.67	2.69	0	0.00	100.00	2.59	0	0.00	99.6	2.46	0	0.00
92.65	2.68	6.67	2.44	94.31	2.58	6.67	2.14	92.6	2.46	6.67	1.88
78.63	2.67	13.33	2.51	80.60	2.56	13.33	2.31	78.5	2.44	13.33	2.02
60.10	2.64	20	2.70	60.87	2.54	20	2.34	60.2	2.43	20	2.12
50.42	2.62	26.67	2.56	51.34	2.52	26.67	2.46	51.2	2.41	26.67	2.17
40.90	2.61	33.33	2.60	42.14	2.52	33.33	2.46	41.3	2.38	33.33	2.18
32.89	2.59	40	2.66	34.78	2.49	40	2.46	31.2	2.29	40	2.24
31.39	2.58	46.67	2.62	31.94	2.50	46.67	2.46	21.1	2.25	46.67	2.29
20.20	2.56	53.33	2.56	20.23	2.46	53.33	2.54	12.08	2.15	53.33	2.24
18.53	2.54	60	2.65	19.23	2.45	60	2.51	9.73	2.1	60	2.34
12.85	2.52	66.67	2.71	12.37	2.41	66.67	2.51	6.38	2.06	66.67	2.36
11.52	2.51	73.33	2.68	13.04	2.41	73.33	2.51	2.35	1.78	73.33	2.35
2.17	2.25	80	2.81	3.68	2.20	80	2.59	2.18	1.1	80	2.35
1.84	1.69	86.67	2.82	1.67	1.69	86.67	2.52	2.01	0.59	86.67	2.43
2.00	1.15	93.33	2.67	2.17	1.13	93.33	2.55	2.01	0.09	93.33	2.37
1.84	0.58	100	2.71	2.01	0.58	100	2.54			100	2.33
P≡ Pressure (kPa), L≡ loading (mmol/g)											

Table 10 Comparative Isotherm Analysis of R32 in LTA zeolite

5A/R32				4A/R32				3A/ R32			
298K				298K							
Exp.		Sim.		Exp.		Sim.		Exp.		Sim.	
P	L	P	L	P	L	P	L	P	L	P	L
1.11	0.01	0.00	0.00	1.13	0.01	0.00	0.00	0.96	0.01	0.00	0.00
5.68	3.80	6.67	3.52	3.46	3.78	6.67	3.39	3.18	2.26	6.67	3.05
14.61	4.18	13.33	3.84	6.86	4.07	13.33	3.96	6.04	2.72	13.33	3.17
18.96	4.27	20.00	4.05	10.46	4.24	20.00	4.21	8.54	2.77	20.00	3.23
22.45	4.36	26.67	4.22	14.77	4.35	26.67	4.34	12.56	3.05	26.67	3.23
26.54	4.38	33.33	4.27	19.10	4.42	33.33	4.47	25.15	3.32	33.33	3.32
37.95	4.53	40.00	4.45	24.88	4.49	40.00	4.53	50.39	3.51	40.00	3.42
52.21	4.62	46.67	4.45	25.30	4.51	46.67	4.63	100.21	3.71	46.67	3.46
62.80	4.69	53.33	4.62	37.44	4.61	53.33	4.69			53.33	3.30
75.59	4.74	60.00	4.75	52.12	4.69	60.00	4.65			60.00	3.39
89.28	4.78	66.67	4.65	64.10	4.73	66.67	4.75			66.67	3.45
101.16	4.82	73.33	4.66	75.57	4.78	73.33	4.75			73.33	3.39
		80.00	4.70	87.75	4.81	80.00	4.82			80.00	3.41
		86.67	4.92	102.59	4.83	86.67	4.79			86.67	3.43
		93.33	4.91			93.33	4.87			93.33	3.48
		100.0	5.01			100.0	4.87			100.0	3.54
P≡ Pressure (kPa), L≡ loading (mmol/g)											

Table 11 Langmuir-Freundlich Adsorption Parameters for Methane Derivative Refrigerants in Zeolite 13X

Molecules		Temperatures (K)					
		293	298	303	313	323	333
R41	q(mmol/g)	14.803	997.889	3594.660	4911.500	2523.160	1101.450
	K(kPa ⁻¹)	0.004	1.56e-05	3.68e-06	1.49e-06	1.38e-06	2.60e-06
	n	0.976	0.863	0.883	0.864	0.813	0.806
	R ²	0.998	0.999	0.999	0.998	0.999	0.999
R32	q(mmol/g)	5.327	6.111	6.175	8.318	1764.830	1122.450
	K(kPa ⁻¹)	0.082	0.046	0.036	0.011	3.91e-08	9.86e-09
	n	1.394	1.027	0.964	0.717	0.494	0.429
	R ²	0.999	1.000	0.999	0.999	0.999	0.999
R23	q(mmol/g)	4.015	3.832	3.711	3.574	3.613	3.676
	K(kPa ⁻¹)	0.077	0.071	0.057	0.042	0.028	0.019
	n	1.580	1.730	1.700	1.632	1.491	1.427
	R ²	0.999	0.999	0.999	1.000	1.000	0.999
R14	q(mmol/g)	2.818	2.791	2.720	2.630	2.572	2.266
	K(kPa ⁻¹)	0.061	0.052	0.045	0.033	0.025	0.023
	n	1.023	1.017	1.039	1.068	1.082	1.138
	R ²	1.000	1.000	1.000	1.000	1.000	1.000

Table 12 Adsorption Characteristics for R41in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R41	0.00	0.00	0.00	0.0	0.0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0
	6.67	0.49	8.06	-45.5	0.43	8.10	-40.0	0.38	8.15	-35.6	0.32	8.27	-30.1	0.23	8.19	-22.1	0.18	8.18	-17.0
	13.33	0.77	7.66	-66.5	0.67	7.64	-57.1	0.57	7.64	-49.0	0.50	7.88	-44.3	0.37	7.87	-33.5	0.28	7.77	-24.4
	20	1.04	7.22	-81.1	0.90	7.33	-72.2	0.82	7.44	-66.9	0.59	7.39	-48.1	0.51	7.66	-44.0	0.36	7.50	-30.6
	26.67	1.29	7.06	-96.3	1.14	7.15	-87.6	0.95	7.12	-72.9	0.74	7.25	-58.7	0.63	7.44	-51.6	0.52	7.61	-44.3
	33.33	1.65	7.07	-120.4	1.39	7.04	-102.1	1.24	7.11	-93.2	0.86	7.05	-65.2	0.73	7.31	-58.1	0.56	7.27	-44.6
	40	1.97	7.13	-140.8	1.65	7.02	-118.7	1.43	7.03	-104.3	1.08	7.06	-81.0	0.84	7.29	-66.7	0.70	7.32	-55.8
	46.67	2.64	7.33	-188.6	1.97	7.07	-140.1	1.65	6.98	-117.8	1.18	7.00	-87.5	0.88	6.98	-66.0	0.77	7.14	-59.7
	53.33	2.71	7.29	-192.7	2.25	7.12	-158.6	1.83	6.98	-129.3	1.34	6.92	-96.0	1.12	7.13	-85.0	0.82	7.01	-61.8
	60	2.95	7.41	-210.3	2.51	7.21	-177.4	2.27	7.15	-161.1	1.56	6.94	-111.0	1.24	7.00	-91.4	0.88	6.96	-65.6
	66.67	3.15	7.42	-223.5	2.73	7.26	-192.3	2.39	7.16	-168.5	1.60	6.94	-113.8	1.30	6.93	-93.9	1.01	6.96	-74.7
	73.33	3.37	7.52	-240.4	3.00	7.36	-211.7	2.61	7.23	-183.3	1.89	6.98	-132.4	1.39	6.93	-99.4	1.10	6.92	-79.9
	80	3.57	7.59	-256.1	3.22	7.46	-228.9	2.71	7.24	-190.1	2.03	6.99	-142.1	1.51	6.88	-105.8	1.20	6.96	-87.3
	86.67	3.79	7.70	-273.8	3.36	7.52	-239.9	2.99	7.34	-211.0	2.28	7.08	-158.7	1.67	6.95	-118.1	1.26	6.83	-89.3
	93.33	3.82	7.70	-275.7	3.45	7.53	-245.7	3.02	7.31	-211.6	2.41	7.12	-168.2	1.77	6.98	-125.3	1.37	6.86	-96.9
	100.00	4.02	7.82	-293.9	3.61	7.61	-259.2	3.39	7.57	-242.8	2.37	7.06	-163.4	1.88	6.94	-130.8	1.43	6.81	-99.8
M $\equiv$ Molecules type, P $\equiv$ Pressure kPa, L $\equiv$ loading (mmol/g), I.H $\equiv$ Isosteric heats (kcal/mol), T.H $\equiv$ Overall system energies (kcal/mol)																			

Table 13 Adsorption Characteristics for R32 in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R32	0.00	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0
	6.67	1.54	6.47	-28.1	1.42	6.21	-21.5	1.29	5.92	-15.2	1.19	5.71	-10.1	1.12	5.47	-6.7	1.08	5.34	-4.9
	13.33	2.93	7.93	-110.6	2.24	7.13	-66.2	1.84	6.70	-43.5	1.53	6.19	-26.4	1.34	5.90	-17.1	1.22	5.64	-11.5
	20	3.80	8.97	-204.7	2.88	8.26	-149.3	2.80	7.90	-113.3	1.96	6.75	-49.3	1.61	6.29	-30.2	1.39	5.81	-18.9
	26.67	4.03	9.48	-260.7	3.48	9.05	-216.7	3.05	8.55	-174.5	2.67	7.44	-90.7	1.92	6.61	-46.5	1.59	6.13	-28.8
	33.33	4.02	9.43	-258.3	3.66	8.98	-225.2	3.36	8.88	-204.9	2.68	8.29	-149.2	2.28	6.93	-66.2	1.85	6.50	-42.5
	40	4.12	9.31	-261.5	3.87	9.22	-242.7	3.84	9.17	-240.2	3.04	8.66	-181.9	2.34	7.63	-105.2	1.95	6.77	-57.9
	46.67	4.61	9.92	-309.7	4.27	9.61	-278.6	3.79	9.06	-234.5	3.23	8.62	-191.8	2.39	8.00	-133.5	2.15	7.20	-76.0
	53.33	4.65	9.87	-310.3	4.33	9.54	-280.5	3.97	9.21	-249.3	3.27	8.61	-194.1	2.61	8.12	-147.1	2.28	7.44	-94.9
	60	4.93	10.10	-336.0	4.68	9.89	-312.6	4.07	9.27	-256.6	3.48	8.81	-209.9	3.12	8.59	-184.2	2.38	7.54	-106.0
	66.67	4.74	9.85	-316.6	4.72	9.85	-313.7	4.17	9.34	-266.1	3.80	9.14	-236.4	3.07	8.47	-178.4	2.46	7.82	-128.9
	73.33	4.77	9.95	-320.6	4.76	9.99	-320.8	4.52	9.71	-297.2	3.88	9.14	-242.3	3.18	8.48	-185.7	2.64	8.14	-149.2
	80	5.10	10.26	-352.5	4.83	9.99	-326.0	4.46	9.75	-294.1	4.02	9.33	-253.8	3.53	8.83	-213.4	2.66	8.06	-148.8
	86.67	5.06	10.23	-349.5	4.83	10.02	-325.9	4.62	9.85	-307.5	4.07	9.36	-257.9	3.70	8.98	-225.9	2.70	8.05	-150.7
	93.33	5.22	10.27	-361.0	4.94	10.03	-334.5	4.78	9.90	-318.7	4.15	9.36	-264.1	3.50	8.76	-209.6	2.95	8.35	-169.8
	100.00	5.21	10.31	-361.1	5.00	10.09	-339.7	4.85	9.90	-325.1	4.17	9.35	-265.1	3.80	9.05	-233.9	3.13	8.51	-183.0
M ≡ Molecules type, P≡ Pressure (kPa,) L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol) , T.H ≡ Overall system energies (kcal/mol)																			

Table 14 Adsorption Characteristics for R23 in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R23	0.00	0	0.00	0	0	0.00	0	0	0.00	0	0	0.00	0	0	0.00	0	0	0.00	0
	6.67	1.00	6.93	1523.3	0.8	6.74	1215.4	0.60	6.51	916.0	0.40	6.28	614.4	0.28	6.05	429.7	0.20	5.93	309.2
	13.33	2.13	7.94	3223.6	1.85	7.66	2805.8	1.35	7.18	2045.1	0.97	6.85	1475.9	0.65	6.48	992.6	0.45	6.22	687.6
	20	2.63	8.24	3970.1	2.54	8.26	3842.4	2.19	7.93	3312.6	1.50	7.32	2282.3	1.04	6.85	1584.1	0.70	6.46	1076
	26.67	3.04	8.61	4578.1	2.86	8.53	4317.6	2.49	8.14	3766.9	1.95	7.66	2958.3	1.38	7.13	2100.9	1.00	6.81	1529.1
	33.33	3.18	8.77	4792.9	3.02	8.63	4553.9	2.77	8.38	4180.4	2.23	7.89	3374.8	1.72	7.41	2615.0	1.26	7.01	1914.6
	40	3.50	9.11	5258.6	3.28	8.90	4928.9	2.88	8.42	4350.5	2.58	8.24	3904.6	1.91	7.53	2901.3	1.51	7.20	2289.2
	46.67	3.47	9.02	5221.7	3.35	8.98	5041.5	3.00	8.62	4518.6	2.60	8.19	3930.7	2.11	7.78	3202.8	1.62	7.24	2467.8
	53.33	3.61	9.29	5415.8	3.40	9.01	5115.6	3.46	9.13	5207.8	2.82	8.35	4259.5	2.36	7.93	3578.7	1.87	7.49	2835.8
	60	3.57	9.16	5370.4	3.57	9.19	5360.8	3.15	8.69	4739.3	2.90	8.49	4373.7	2.53	8.06	3820.5	1.97	7.54	2986.6
	66.67	3.76	9.34	5649.2	3.43	8.95	5163.9	3.33	8.85	5015.2	3.06	8.63	4612.2	2.59	8.18	3912.1	2.15	7.77	3254.9
	73.33	3.66	9.23	5500.5	3.67	9.23	5515.9	3.32	8.84	5004.3	3.01	8.55	4546.7	2.67	8.19	4035.5	2.40	7.99	3624.9
	80	3.72	9.29	5591.6	3.80	9.34	5704.8	3.39	8.92	5108.5	3.05	8.49	4597.3	2.63	8.11	3981.4	2.33	7.86	3531.6
	86.67	3.88	9.41	5819.6	3.63	9.20	5452.5	3.49	9.04	5245.9	3.28	8.79	4932.7	2.83	8.37	4271.4	2.47	8.01	3731.4
	93.33	4.04	9.60	6056.9	3.80	9.27	5702.6	3.61	9.17	5425.6	3.21	8.72	4835.7	2.88	8.36	4348.0	2.54	8.09	3837.8
	100.00	3.91	9.46	5867.6	3.72	9.16	5598.3	3.61	9.16	5428.4	3.24	8.74	4882.8	3.02	8.56	4555.5	2.55	8.07	3859.4
M ≡ Molecules type, P ≡ Pressure (kPa,) L≡ loading (mmol/g), I.H ≡ Isosteric heats(kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 15 Adsorption Characteristics for R14 in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R14	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0
	6.67	0.75	9.07	-78.9	0.73	9.19	-77.4	0.71	9.30	-76.2	0.67	9.46	-73.7	0.63	9.60	-70.9	0.61	9.70	-68.4
	13.33	0.96	8.26	-89.6	0.90	8.44	-86.1	0.85	8.62	-83.7	0.78	8.90	-79.5	0.73	9.11	-76.7	0.68	9.28	-73.3
	20	1.21	7.74	-103.0	1.10	7.92	-96.7	1.01	8.11	-91.8	0.89	8.44	-85.3	0.82	8.72	-81.1	0.76	8.96	-77.8
	26.67	1.51	7.43	-119.5	1.34	7.58	-109.5	1.20	7.74	-101.8	1.02	8.07	-92.1	0.91	8.38	-85.7	0.83	8.64	-81.2
	33.33	1.93	7.29	-144.6	1.62	7.38	-125.6	1.43	7.49	-114.5	1.16	7.79	-99.0	1.00	8.10	-90.6	0.91	8.39	-85.5
	40	2.29	7.25	-166.9	1.92	7.25	-143.5	1.66	7.34	-127.5	1.31	7.58	-107.1	1.11	7.87	-96.0	0.98	8.15	-89.0
	46.67	2.72	7.30	-195.1	2.25	7.24	-164.2	1.91	7.25	-142.4	1.47	7.42	-116.1	1.22	7.68	-101.6	1.06	7.97	-93.1
	53.33	3.08	7.38	-219.4	2.59	7.26	-185.6	2.18	7.22	-159.2	1.64	7.31	-125.4	1.33	7.53	-107.6	1.13	7.80	-96.6
	60	3.33	7.43	-236.8	2.92	7.33	-207.7	2.41	7.20	-172.7	1.84	7.24	-137.0	1.45	7.42	-114.1	1.22	7.67	-101.6
	66.67	3.66	7.53	-260.6	3.14	7.35	-222.4	2.69	7.25	-191.6	2.01	7.19	-147.3	1.57	7.33	-121.1	1.31	7.54	-106.0
	73.33	3.82	7.59	-272.5	3.37	7.43	-239.0	2.98	7.32	-210.9	2.17	7.18	-156.9	1.70	7.26	-128.4	1.40	7.44	-111.1
	80	4.05	7.68	-290.0	3.59	7.48	-253.8	3.17	7.35	-223.9	2.39	7.18	-170.9	1.84	7.21	-136.3	1.48	7.36	-115.0
	86.67	4.17	7.69	-298.1	3.74	7.53	-264.8	3.31	7.37	-232.9	2.56	7.20	-181.4	1.94	7.18	-142.4	1.58	7.30	-121.1
	93.33	4.31	7.75	-309.0	3.93	7.60	-279.6	3.51	7.44	-247.4	2.70	7.21	-190.6	2.09	7.16	-151.3	1.69	7.25	-126.9
	100.00	4.40	7.79	-316.5	4.11	7.68	-293.5	3.67	7.49	-259.1	2.88	7.25	-202.4	2.23	7.14	-159.6	1.78	7.20	-131.9
M $\equiv$ Molecules type, P $\equiv$ Pressure (kPa), L $\equiv$ loading (mmol/g), I.H $\equiv$ Isotheric heats (kcal/mol), T.H $\equiv$ Overall system energies (kcal/mol)																			

Table 16 Langmuir-Freundlich Adsorption Parameters for Methane Derivative Refrigerants in Zeolite 5A

Molecules		Temperatures (K)					
		293	298	303	313	323	333
R41	q(mmol/g)	313.908	214.018	77.623	328.411	414.428	1229.41
	K(kPa ⁻¹)	1.42e-10	1.06e-10	3.73e-09	2.17e-09	3.28e-08	1.09e-07
	n	0.244	0.223	0.211	0.310	0.410	0.568
	R ²	0.999	0.999	1.000	0.999	0.999	0.999
R32	q(mmol/g)	9.368	8.894	19.037	7.590	7.477	46.205
	K(kPa ⁻¹)	0.020	0.024	5.46e-05	0.033	0.032	6.81e-08
	n	0.235	0.242	0.205	0.307	0.239	0.192
	R ²	0.999	1.000	1.000	1.000	1.000	1.000
R23	q(mmol/g)	3.662	3.751	3.798	3.920	4.852	8.479
	K(kPa ⁻¹)	0.068	0.053	0.042	0.026	0.010	0.001
	n	1.088	0.999	0.968	0.893	0.756	0.640
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R14	q(mmol/g)	2.941	3.245	3.148	2.626	10.487	3.185
	K(kPa ⁻¹)	0.136	0.099	0.073	0.087	0.001	0.025
	n	0.937	0.743	0.803	1.148	0.402	0.653
	R ²	0.999	0.998	0.999	0.998	0.999	0.999

Table 17 Adsorption Characteristics for R41 in Zeolite 5A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R41	0.00	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0
	6.67	2.07	7.53	-65.7	2.05	7.62	-64.5	1.89	7.67	-59.8	1.26	7.81	-53.7	0.79	7.90	-47.9	0.40	7.96	-40.2
	13.33	2.28	7.13	-85.8	2.25	7.21	-80.2	2.07	7.28	-74.1	1.47	7.44	-66.1	1.00	7.57	-60.1	0.61	7.67	-52.9
	20	2.55	7.00	-107.5	2.49	7.02	-98.8	2.34	7.07	-89.6	1.67	7.23	-78.2	1.20	7.35	-69.4	0.81	7.49	-62.1
	26.67	2.74	7.01	-133.4	2.67	6.98	-114.0	2.53	6.99	-105.7	1.81	7.07	-89.2	1.34	7.17	-76.1	0.94	7.30	-68.6
	33.33	2.82	6.99	-147.2	2.69	6.97	-134.5	2.60	6.97	-118.9	1.95	6.99	-99.1	1.48	7.07	-83.5	1.08	7.19	-74.4
	40	2.87	7.08	-171.2	2.77	7.04	-154.5	2.67	6.98	-137.5	2.09	6.94	-111.0	1.62	7.00	-95.0	1.23	7.08	-80.7
	46.67	3.02	7.13	-186.2	2.87	7.11	-171.5	2.76	7.00	-148.1	2.15	6.93	-119.3	1.68	6.96	-101.0	1.28	7.01	-88.7
	53.33	3.10	7.29	-208.9	2.97	7.14	-183.0	2.82	7.01	-161.0	2.24	6.97	-134.6	1.77	6.94	-110.8	1.37	6.96	-90.4
	60	3.20	7.30	-215.2	3.13	7.20	-194.0	2.83	7.12	-178.4	2.34	6.93	-140.2	1.87	6.94	-118.3	1.48	6.95	-97.8
	66.67	3.36	7.35	-226.3	3.18	7.21	-202.2	2.87	7.13	-185.6	2.35	6.99	-151.4	1.87	6.93	-125.7	1.48	6.90	-103.7
	73.33	3.51	7.42	-237.4	3.29	7.35	-221.4	2.96	7.17	-197.4	2.48	7.04	-164.5	1.96	6.88	-130.3	1.66	6.91	-112.1
	80	3.46	7.36	-232.8	3.32	7.29	-222.4	3.07	7.22	-204.4	2.58	7.07	-170.8	2.10	6.94	-139.3	1.72	6.88	-115.6
	86.67	3.77	7.55	-257.0	3.53	7.41	-237.8	3.21	7.28	-214.7	2.73	7.09	-180.3	2.23	6.98	-148.3	1.86	6.91	-124.1
	93.33	3.93	7.64	-270.6	3.64	7.48	-246.4	3.25	7.27	-217.2	2.78	7.08	-182.8	2.31	6.96	-152.2	1.97	6.91	-130.7
	100.00	3.91	7.61	-267.8	3.66	7.49	-248.0	3.33	7.27	-221.0	2.86	7.12	-189.3	2.40	6.98	-158.4	1.98	6.90	-131.5
M ≡ Molecules type, P ≡ Pressure(kPa), L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 18 Adsorption Characteristics for R32 in Zeolite 5A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R32	0.00	0	0.00	0	0	0.00	0	0	0.00	0	0	0.0	0	0	0.00	0	0	0.00	0
	6.67	3.74	8.20	1748.9	3.51	8.14	1418.1	3.24	8.19	1262.7	2.94	8.34	969.5	3.08	8.54	813.2	2.69	8.70	721.0
	13.33	3.83	8.68	3079.2	3.83	8.39	2569.0	3.43	8.24	2177.8	3.27	8.10	1583.4	3.38	8.09	1249.3	2.98	8.26	1007.2
	20	4.04	8.88	3497.6	4.04	8.84	3346.1	3.68	8.55	2930.1	3.47	8.18	2145.4	3.50	8.03	1666.8	3.26	8.04	1283.7
	26.67	4.38	9.04	3825.3	4.21	8.96	3665.5	3.92	8.79	3386.1	3.82	8.44	2703.4	3.66	8.18	2111.2	3.37	8.05	1687.2
	33.33	4.46	9.06	3898.9	4.27	8.97	3717.1	4.20	8.95	3650.6	3.95	8.62	3123.9	3.79	8.20	2388.5	3.40	8.03	1936.5
	40	4.57	9.31	4146.5	4.45	9.22	4031.8	4.18	8.99	3777.9	3.94	8.66	3257.5	3.84	8.34	2728.3	3.47	8.12	2236.6
	46.67	4.62	9.27	4203.4	4.44	9.15	4028.1	4.32	9.13	3909.8	4.00	8.93	3601.0	3.95	8.32	2837.8	3.65	8.18	2404.1
	53.33	4.74	9.34	4311.6	4.62	9.31	4197.0	4.28	9.06	3877.1	4.14	9.00	3739.3	3.97	8.62	3222.5	3.79	8.37	2758.1
	60	4.76	9.45	4327.9	4.75	9.46	4315.0	4.41	9.15	3999.3	4.13	8.97	3733.2	4.00	8.60	3245.6	3.91	8.39	2803.2
	66.67	4.77	9.37	4345.7	4.65	9.33	4224.6	4.56	9.26	4136.6	4.21	8.97	3807.7	3.97	8.65	3438.1	4.01	8.49	3039.3
	73.33	5.20	9.80	4744.0	4.65	9.37	4226.2	4.61	9.32	4191.1	4.33	9.07	3926.6	4.16	8.89	3619.8	4.07	8.60	3242.9
	80	4.96	9.59	4520.3	4.70	9.32	4274.9	4.64	9.29	4218.2	4.31	9.04	3907.4	4.14	8.86	3601.1	4.11	8.55	3214.9
	86.67	4.99	9.51	4554.1	4.91	9.55	4476.3	4.82	9.47	4389.1	4.36	9.06	3952.8	4.11	8.75	3573.2	4.15	8.53	3255.1
	93.33	4.94	9.58	4497.4	4.91	9.42	4473.5	4.86	9.43	4425.3	4.48	9.18	4067.0	4.31	8.91	3766.3	4.21	8.64	3383.6
	100.00	4.99	9.57	4551	5.00	9.63	4560.2	4.94	9.52	4505.2	4.50	9.15	4086.9	4.35	8.95	3804.2	4.34	8.71	3505.5
M $\equiv$ Molecules type, P $\equiv$ Pressure (kPa,) L $\equiv$ loading (mmol/g), I.H $\equiv$ Isosteric heats (kcal/mol) , T.H $\equiv$ Overall system energies (kcal/mol)																			

Table 19 Adsorption Characteristics for R23 in Zeolite 5A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R23	0.00	0	0.00	0.0	0	0.00	0.00	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0
	6.67	1.88	8.28	-96.7	1.77	8.36	-88.7	1.64	8.40	-78.5	1.49	8.63	-66.8	1.46	8.89	-59.0	1.36	9.01	-50.7
	13.33	2.03	8.26	-144.7	2.00	8.24	-130.6	1.91	8.19	-116.5	1.75	8.23	-92.2	1.56	8.36	-77.3	1.49	8.52	-66.3
	20	2.30	8.43	-181.3	2.24	8.33	-162.9	2.04	8.23	-145.1	1.91	8.16	-115.6	1.88	8.20	-95.3	1.69	8.30	-80.5
	26.67	2.45	8.59	-208.9	2.32	8.40	-181.4	2.14	8.31	-166.5	2.09	8.19	-136.2	1.91	8.12	-109.1	1.70	8.18	-92.3
	33.33	2.60	8.65	-220.9	2.40	8.52	-202.6	2.19	8.41	-184.2	2.16	8.24	-154.6	1.96	8.12	-125.1	1.77	8.11	-103.5
	40	2.73	8.70	-232.8	2.55	8.57	-215.6	2.37	8.52	-200.0	2.21	8.35	-172.1	2.05	8.14	-137.8	1.83	8.09	-114.5
	46.67	2.89	8.84	-249.0	2.68	8.68	-228.8	2.51	8.58	-213.2	2.23	8.35	-179.5	2.05	8.20	-150.7	1.87	8.07	-122.6
	53.33	2.90	8.82	-249.5	2.79	8.76	-238.4	2.66	8.67	-227.0	2.31	8.39	-185.7	2.06	8.21	-157.6	1.91	8.09	-131.9
	60	2.99	8.89	-257.7	2.87	8.80	-246.2	2.70	8.69	-229.9	2.41	8.42	-195.0	2.21	8.22	-163.0	1.94	8.11	-140.9
	66.67	3.05	8.92	-264.0	2.92	8.83	-251.7	2.75	8.70	-233.6	2.53	8.51	-206.1	2.32	8.36	-180.0	2.02	8.16	-147.0
	73.33	3.13	9.01	-272.4	3.00	8.88	-258.5	2.84	8.75	-242.2	2.59	8.53	-210.7	2.35	8.35	-182.7	2.05	8.19	-155.7
	80	3.13	9.01	-271.8	3.03	8.91	-261.9	2.88	8.83	-247.1	2.64	8.55	-215.2	2.44	8.42	-190.6	2.05	8.22	-161.9
	86.67	3.22	9.04	-280.6	3.05	8.92	-263.0	2.88	8.77	-246.1	2.73	8.62	-223.6	2.64	8.40	-191.6	2.08	8.19	-163.9
	93.33	3.24	9.05	-282.7	3.11	8.95	-269.5	3.05	8.90	-263.5	2.75	8.63	-225.0	2.65	8.39	-194.1	2.17	8.26	-172.2
	100.00	3.27	9.06	-286.0	3.13	8.96	-270.7	3.02	8.87	-259.8	2.86	8.64	-228.7	2.72	8.43	-200.1	2.28	8.27	-174.7
M ≡ Molecules type, P≡ Pressure (kPa) L≡ loading(mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 20 Adsorption Characteristics in Zeolite 5A for R14 at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R14	0.00	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0
	6.67	1.47	9.47	-259.5	1.34	9.48	-245.9	1.26	9.51	-234.7	1.05	9.61	-211.2	0.90	9.78	-187.9	0.79	10.00	-169.8
	13.33	1.89	9.48	-292.3	1.73	9.47	-281.1	1.62	9.46	-268.8	1.40	9.48	-246.2	1.20	9.53	-225.7	1.05	9.63	-205.0
	20	2.15	9.52	-311.4	2.07	9.48	-298.0	1.90	9.47	-287.4	1.64	9.46	-267.2	1.42	9.47	-246.2	1.25	9.52	-227.5
	26.67	2.28	9.52	-319.1	2.16	9.50	-310.5	2.04	9.48	-300.4	1.80	9.45	-278.4	1.58	9.46	-261.3	1.40	9.48	-241.1
	33.33	2.40	9.57	-332.7	2.25	9.53	-318.9	2.11	9.50	-309.4	1.93	9.46	-289.6	1.71	9.45	-270.1	1.51	9.46	-251.3
	40	2.46	9.57	-336.0	2.35	9.55	-327.4	2.26	9.53	-320.9	2.03	9.48	-297.6	1.82	9.46	-278.7	1.62	9.45	-258.6
	46.67	2.55	9.63	-352.2	2.52	9.56	-333.6	2.28	9.54	-323.0	2.12	9.49	-303.1	1.90	9.46	-286.0	1.69	9.45	-267.5
	53.33	2.57	9.62	-350.6	2.48	9.60	-342.2	2.41	9.54	-328.7	2.18	9.50	-308.9	1.99	9.46	-289.2	1.78	9.44	-272.0
	60	2.69	9.65	-358.3	2.48	9.59	-344.5	2.49	9.57	-334.0	2.25	9.50	-312.1	2.03	9.47	-295.7	1.84	9.45	-277.3
	66.67	2.67	9.70	-371.0	2.62	9.60	-348.2	2.49	9.57	-337.9	2.30	9.51	-315.3	2.10	9.47	-298.5	1.91	9.45	-282.1
	73.33	2.62	9.66	-364.2	2.65	9.65	-357.8	2.51	9.60	-345.9	2.35	9.52	-320.1	2.17	9.47	-301.4	1.96	9.45	-284.9
	80	2.74	9.67	-365.0	2.66	9.65	-361.4	2.57	9.59	-345.2	2.39	9.54	-327.2	2.20	9.48	-304.0	2.00	9.46	-289.7
	86.67	2.72	9.70	-371.5	2.69	9.66	-362.6	2.57	9.62	-351.3	2.42	9.54	-327.6	2.22	9.49	-309.5	2.05	9.47	-294.5
	93.33	2.75	9.71	-375.4	2.74	9.66	-365.4	2.66	9.63	-355.4	2.46	9.53	-328.0	2.27	9.50	-312.2	2.08	9.46	-295.2
	100.00	2.79	9.75	-384.9	2.70	9.66	-364.5	2.61	9.61	-350.4	2.48	9.57	-336.2	2.29	9.52	-317.8	2.11	9.46	-297.3
M ≡ Molecules type, P≡ Pressure (kPa) L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 21 Langmuir-Freundlich Adsorption Parameters for Methane Derivative Refrigerants in Zeolite 4A

Molecules		Temperatures (K)					
		293	298	303	313	323	333
R41	q(mmol/g)	114.207	164.17	233.626	443.185	707.830	1113.890
	K(kPa ⁻¹)	4.73e-10	3.31e-10	7.19e-10	3.24e-10	6.96e-10	2.96e-09
	n	0.204	0.224	0.259	0.291	0.341	0.413
	R ²	1.000	0.999	0.999	0.999	0.999	0.998
R32	q(mmol/g)	5.333	5.235	5.094	4.814	4.839	4.951
	K(kPa ⁻¹)	0.432	0.354	0.255	0.168	0.113	0.076
	n	0.688	0.715	0.832	1.002	0.916	0.825
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R23	q(mmol/g)	3.073	2.958	2.926	2.962	2.843	2.796
	K(kPa ⁻¹)	0.729	0.442	0.349	0.222	0.145	0.101
	n	0.598	0.779	0.805	0.721	0.831	0.826
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R14	q(mmol/g)	3.685	3.624	3.118	2.860	2.636	2.592
	K(kPa ⁻¹)	0.134	0.140	0.174	0.150	0.126	0.092
	n	0.364	0.405	0.484	0.562	0.663	0.664
	R ²	1.000	1.000	1.000	1.000	1.000	1.000

Table 22 Adsorption Characteristics for R41 in Zeolite 4A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R41	0.00	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0
	6.67	2.16	7.75	-106.5	1.99	7.84	-97.1	1.79	7.94	-89.9	1.50	8.16	-80.1	1.17	8.34	-72.3	0.86	8.50	-66.2
	13.33	2.35	7.65	-166.2	2.13	7.61	-145.4	1.88	7.61	-127.4	1.58	7.71	-104.8	1.25	7.87	-91.4	0.94	8.05	-81.7
	20	2.44	7.82	-216.0	2.28	7.72	-193.1	2.02	7.64	-168.0	1.73	7.59	-133.8	1.40	7.65	-109.3	1.09	7.78	-95.3
	26.67	2.57	7.99	-253.6	2.38	7.85	-226.7	2.19	7.73	-201.0	1.90	7.58	-158.5	1.57	7.56	-127.7	1.26	7.63	-108.4
	33.33	2.74	8.10	-277.7	2.57	7.97	-252.9	2.31	7.86	-230.8	2.01	7.65	-182.8	1.69	7.57	-149.4	1.38	7.56	-122.8
	40	2.92	8.23	-299.1	2.69	8.06	-271.2	2.49	7.95	-249.3	2.15	7.70	-201.8	1.78	7.58	-165.4	1.47	7.53	-136.2
	46.67	2.99	8.24	-305.7	2.84	8.15	-288.5	2.64	8.02	-265.1	2.23	7.79	-221.5	1.82	7.61	-179.9	1.50	7.53	-149.7
	53.33	3.12	8.34	-321.6	2.94	8.21	-299.9	2.76	8.09	-279.1	2.41	7.88	-239.5	1.99	7.67	-196.1	1.63	7.55	-161.4
	60	3.20	8.40	-331.1	3.03	8.27	-310.4	2.85	8.14	-288.4	2.49	7.92	-248.1	2.11	7.72	-207.9	1.76	7.57	-173.5
	66.67	3.24	8.41	-335.3	3.15	8.37	-325.0	2.94	8.18	-298.0	2.60	7.97	-259.6	2.19	7.74	-216.3	1.87	7.62	-184.4
	73.33	3.36	8.50	-349.8	3.16	8.34	-324.1	3.04	8.26	-310.1	2.69	8.02	-269.6	2.33	7.81	-230.8	1.99	7.66	-195.2
	80	3.38	8.50	-351.1	3.24	8.40	-334.4	3.09	8.29	-316.1	2.77	8.08	-278.3	2.40	7.84	-238.1	2.06	7.67	-202.1
	86.67	3.42	8.54	-356.7	3.29	8.44	-340.3	3.12	8.31	-319.8	2.83	8.11	-285.2	2.47	7.89	-245.3	2.14	7.71	-210.1
	93.33	3.45	8.57	-361.3	3.30	8.43	-341.2	3.17	8.34	-325.2	2.89	8.14	-291.7	2.56	7.93	-254.2	2.23	7.75	-219.3
	100.00	3.50	8.59	-366.4	3.37	8.50	-350.3	3.24	8.39	-333.2	2.94	8.18	-297.3	2.60	7.94	-258.7	2.29	7.77	-225.1
M ≡ Molecules type, P≡ Pressure (kPa) L≡ loading(mmol/g), I.H≡ Isosteric heats(kcal/mol) T.H ≡ Overall system energies(kcal/mol)																			

Table 23 Adsorption Characteristics for R32 in Zeolite 4A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R32	0.00	0	0.00	0	0	0.00	0	0	0.00	0	0	0.00	0	0	0.00	0	0	0.00	0
	6.67	3.59	9.69	2948.2	3.38	9.54	2716.9	3.08	9.40	2421.6	2.52	9.19	1877.5	2.10	9.18	1472.2	1.82	9.28	1189.3
	13.33	4.12	10.01	3444.8	3.96	9.87	3271.4	3.80	9.77	3119.1	3.37	9.49	2706.2	2.86	9.24	2214.2	2.44	9.12	1805.2
	20	4.31	10.15	3617.1	4.20	10.05	3506.3	4.06	9.95	3370.5	3.74	9.72	3065.7	3.27	9.39	2612.3	2.86	9.22	2219.1
	26.67	4.51	10.30	3807.3	4.34	10.12	3634.4	4.19	10.02	3496.3	3.92	9.81	3239.5	3.55	9.54	2882.5	3.18	9.33	2524.2
	33.33	4.58	10.35	3872.5	4.46	10.25	3755.0	4.34	10.13	3638.6	4.05	9.88	3360.6	3.73	9.65	3062.1	3.41	9.43	2748.3
	40	4.68	10.43	3962.6	4.53	10.30	3814.5	4.43	10.22	3729.2	4.16	9.95	3465.1	3.86	9.74	3184.0	3.56	9.52	2896.0
	46.67	4.74	10.45	4017.2	4.63	10.39	3909.4	4.54	10.31	3827.6	4.24	10.04	3547.1	3.95	9.77	3269.5	3.68	9.59	3007.9
	53.33	4.74	10.47	4019.4	4.68	10.43	3963.9	4.56	10.32	3846.7	4.34	10.12	3644.1	4.06	9.88	3374.7	3.82	9.70	3143.7
	60	4.77	10.50	4045.1	4.64	10.35	3925.4	4.57	10.29	3857.1	4.34	10.07	3644.4	4.12	9.92	3431.3	3.84	9.69	3169.4
	66.67	4.88	10.57	4147.2	4.74	10.45	4019.6	4.60	10.34	3890.3	4.39	10.13	3684.4	4.20	9.97	3511.9	3.90	9.71	3223.8
	73.33	4.92	10.58	4177.0	4.75	10.46	4027.8	4.67	10.37	3952.4	4.45	10.18	3748.1	4.20	9.96	3505.4	3.96	9.76	3280.2
	80	4.87	10.55	4132.4	4.82	10.48	4094.6	4.71	10.41	3995.1	4.46	10.18	3748.5	4.26	10.01	3567.1	4.02	9.83	3340.3
	86.67	4.93	10.59	4191.2	4.78	10.51	4056.5	4.73	10.44	4010.6	4.49	10.21	3784.1	4.34	10.07	3638.8	4.10	9.85	3411.0
	93.33	4.95	10.63	4253.5	4.86	10.52	4135.7	4.82	10.50	4097.4	4.54	10.26	3836.4	4.35	10.08	3642.5	4.12	9.89	3437.1
	100.00	4.95	10.61	4205.5	4.87	10.53	4140.6	4.78	10.44	4056.8	4.64	10.35	3923.3	4.33	10.03	3632.5	4.13	9.88	3445.7
M ≡ Molecules type P≡ Pressure (kPa) L≡ loading(mmol/g) I.H≡ Isosteric heats (kcal/mol) T.H ≡ Overall system energies (kcal/mol)																			

Table 24 Adsorption Characteristics for R23 in Zeolite 4A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R23	0.00	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0
	6.67	2.21	10.35	-315.6	2.06	10.22	-292.3	1.93	10.15	-274.1	1.69	10.05	-239.7	1.40	9.99	-201.0	1.16	10.07	-170.9
	13.33	2.42	10.48	-345.9	2.36	10.45	-337.1	2.26	10.36	-321.7	2.02	10.13	-283.3	1.78	10.01	-250.0	1.57	9.95	-222.0
	20	2.56	10.60	-367.6	2.49	10.52	-355.2	2.43	10.51	-347.8	2.21	10.26	-311.4	2.01	10.13	-282.6	1.81	10.00	-253.8
	26.67	2.61	10.62	-374.9	2.61	10.65	-374.5	2.51	10.56	-358.7	2.33	10.36	-329.1	2.13	10.21	-299.2	1.93	10.04	-268.6
	33.33	2.67	10.70	-385.1	2.61	10.64	-374.9	2.56	10.59	-366.4	2.38	10.39	-336.6	2.23	10.28	-314.3	2.04	10.11	-284.3
	40	2.73	10.80	-395.6	2.67	10.75	-385.8	2.61	10.66	-374.2	2.45	10.46	-347.7	2.32	10.34	-326.7	2.10	10.13	-292.7
	46.67	2.75	10.79	-397.8	2.70	10.73	-389.1	2.63	10.65	-377.0	2.51	10.52	-357.1	2.35	10.36	-331.2	2.17	10.20	-303.8
	53.33	2.76	10.79	-399.1	2.69	10.70	-387.1	2.66	10.67	-381.3	2.50	10.51	-355.2	2.39	10.38	-337.3	2.25	10.25	-314.9
	60	2.80	10.84	-406.4	2.72	10.74	-392.7	2.68	10.68	-385.8	2.56	10.56	-365.2	2.47	10.48	-349.6	2.29	10.31	-321.3
	66.67	2.81	10.84	-407.1	2.78	10.82	-403.2	2.70	10.72	-389.3	2.58	10.58	-368.3	2.44	10.42	-343.8	2.32	10.32	-325.2
	73.33	2.79	10.80	-404.0	2.77	10.75	-399.1	2.71	10.69	-389.1	2.62	10.60	-373.3	2.48	10.46	-351.3	2.32	10.26	-323.6
	80	2.80	10.80	-405.4	2.81	10.85	-408.1	2.72	10.69	-390.3	2.62	10.58	-373.2	2.49	10.46	-350.8	2.35	10.32	-329.2
	86.67	2.82	10.82	-409.1	2.78	10.79	-401.4	2.75	10.75	-396.3	2.65	10.62	-378.9	2.54	10.52	-360.3	2.40	10.38	-337.7
	93.33	2.79	10.77	-403.7	2.83	10.86	-411.0	2.76	10.74	-398.3	2.66	10.65	-378.6	2.55	10.53	-361.0	2.42	10.39	-340.9
	100.00	2.90	10.90	-422.5	2.77	10.76	-400.2	2.78	10.78	-401.9	2.67	10.65	-381.8	2.57	10.52	-363.4	2.45	10.44	-345.9
M ≡ Molecules type, P≡ Pressure (kPa) L≡ loading(mmol/g) I.H≡ Isosteric heats(kcal/mol) T.H ≡ Overall system energies (kcal/mol)																			

Table 25 Adsorption Characteristics for R14 in Zeolite 4A at Various Pressures and Temperatures

M	P	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R14	0.00	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0
	6.67	1.80	9.47	-259.5	1.77	9.48	-245.9	1.61	9.51	-234.7	1.42	9.61	-211.2	1.23	9.78	-187.9	1.08	10.00	-169.8
	13.33	2.04	9.48	-292.3	2.06	9.47	-281.1	1.87	9.46	-268.8	1.70	9.48	-246.2	1.54	9.53	-225.7	1.38	9.63	-205.0
	20	2.18	9.52	-311.4	2.19	9.48	-298.0	2.01	9.47	-287.4	1.87	9.46	-267.2	1.71	9.47	-246.2	1.56	9.52	-227.5
	26.67	2.24	9.53	-319.1	2.28	9.50	-310.5	2.11	9.48	-300.4	1.95	9.45	-278.4	1.82	9.46	-261.3	1.67	9.48	-241.1
	33.33	2.33	9.57	-332.7	2.34	9.53	-318.9	2.17	9.50	-309.4	2.03	9.46	-289.6	1.89	9.45	-270.1	1.75	9.46	-251.3
	40	2.36	9.57	-336.0	2.41	9.55	-327.4	2.25	9.53	-320.9	2.09	9.48	-297.6	1.96	9.46	-278.7	1.81	9.45	-258.6
	46.67	2.46	9.63	-352.2	2.45	9.57	-333.6	2.27	9.54	-323.0	2.13	9.49	-303.1	2.01	9.46	-286.0	1.88	9.45	-267.5
	53.33	2.46	9.62	-350.6	2.51	9.60	-342.2	2.31	9.54	-328.7	2.18	9.50	-308.9	2.04	9.46	-289.2	1.91	9.44	-272.0
	60	2.51	9.65	-358.3	2.53	9.59	-344.5	2.35	9.57	-334.0	2.20	9.50	-312.1	2.08	9.473	-295.7	1.95	9.45	-277.3
	66.67	2.59	9.70	-371.0	2.56	9.60	-348.2	2.38	9.57	-337.9	2.22	9.51	-315.3	2.11	9.47	-298.5	1.99	9.45	-282.1
	73.33	2.55	9.66	-364.2	2.63	9.65	-357.8	2.43	9.60	-345.9	2.26	9.52	-320.1	2.13	9.47	-301.4	2.01	9.45	-284.9
	80	2.56	9.67	-365.0	2.65	9.65	-361.4	2.42	9.59	-345.2	2.31	9.54	-327.2	2.15	9.48	-304.0	2.05	9.46	-289.7
	86.67	2.60	9.70	-371.5	2.66	9.66	-362.6	2.47	9.62	-351.3	2.31	9.54	-327.6	2.19	9.49	-309.5	2.08	9.47	-294.5
	93.33	2.63	9.71	-375.4	2.68	9.66	-365.4	2.49	9.63	-355.4	2.31	9.53	-328.0	2.21	9.50	-312.2	2.09	9.46	-295.2
	100.00	2.69	9.75	-384.9	2.68	9.66	-364.5	2.46	9.61	-350.4	2.37	9.57	-336.2	2.24	9.52	-317.8	2.10	9.46	-297.3
M ≡ Molecules type, P≡ Pressure (kPa) L≡ loading (mmol/g) I.H≡ Isosteric heats(kcal/mol) T.H ≡ Overall system energies (kcal/mol)																			

Table 26 Langmuir-Freundlich Adsorption Parameters for Methane Derivative Refrigerants in Zeolite 3A

Molecules		Temperatures (K)					
		293	298	303	313	323	333
R41	q(mmol/g)	2.840	2.773	2.681	2.698	2.542	2.440
	K(kPa ⁻¹)	0.633	0.525	0.454	0.280	0.116	0.823
	n	0.548	0.584	0.642	0.602	0.716	0.328
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R32	q(mmol/g)	4.119	3.902	3.823	3.677	4.358	3.550
	K(kPa ⁻¹)	6.542	8.601	3.785	1.656	0.585	0.561
	n	0.282	0.308	0.368	0.451	0.277	0.516
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R23	q(mmol/g)	2.281	2.375	2.639	2.486	2.224	2.440
	K(kPa ⁻¹)	1.200	4.126	3.121	2.459	0.818	0.824
	n	0.738	0.427	0.280	0.310	0.558	0.328
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R14	q(mmol/g)	2.840	2.773	2.680	2.698	2.542	2.440
	K(kPa ⁻¹)	0.633	0.524	0.454	0.280	0.116	0.823
	n	0.548	0.584	0.642	0.602	0.716	0.328
	R ²	1.000	1.000	1.000	1.000	1.000	1.000

Table 27 Adsorption Characteristics for R41in Zeolite 3A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R41	0.00	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0
	6.67	1.94	10.41	-236.3	1.86	10.36	-226.9	1.79	10.29	-217.0	1.60	10.16	-192.0	1.15	9.97	-161.0	1.55	9.80	-134.6
	13.33	2.19	10.57	-268.8	2.10	10.48	-256.2	2.03	10.42	-247.0	1.83	10.24	-220.0	1.47	10.17	-203.3	1.68	9.97	-173.4
	20	2.28	10.56	-279.2	2.22	10.54	-272.4	2.16	10.50	-264.1	2.01	10.39	-243.1	1.65	10.23	-217.2	1.71	10.08	-195.5
	26.67	2.35	10.63	-289.2	2.29	10.61	-281.5	2.25	10.54	-274.7	2.11	10.43	-255.9	1.79	10.22	-226.3	1.80	10.18	-213.0
	33.33	2.37	10.65	-292.9	2.34	10.65	-288.5	2.28	10.56	-278.5	2.12	10.44	-257.0	1.84	10.33	-242.7	1.81	10.15	-218.6
	40	2.44	10.69	-301.0	2.34	10.57	-286.3	2.31	10.55	-281.7	2.20	10.45	-267.0	1.88	10.38	-249.3	1.82	10.19	-223.8
	46.67	2.40	10.68	-296.2	2.41	10.66	-296.9	2.33	10.56	-284.6	2.22	10.43	-269.0	1.96	10.35	-252.5	1.90	10.24	-233.9
	53.33	2.46	10.68	-302.5	2.41	10.63	-296.2	2.36	10.57	-287.9	2.22	10.48	-269.5	1.98	10.42	-256.7	1.88	10.27	-237.0
	60	2.53	10.74	-312.2	2.40	10.61	-293.4	2.38	10.59	-291.0	2.24	10.49	-272.3	2.01	10.39	-260.7	1.92	10.24	-239.8
	66.67	2.47	10.69	-304.8	2.46	10.66	-301.8	2.44	10.63	-298.5	2.31	10.59	-282.7	2.04	10.40	-261.9	1.96	10.24	-242.8
	73.33	2.49	10.69	-306.8	2.50	10.69	-306.9	2.38	10.59	-290.7	2.31	10.51	-280.4	2.09	10.43	-266.8	1.90	10.30	-249.9
	80	2.576	10.77	-318.1	2.47	10.65	-303.1	2.43	10.60	-296.8	2.34	10.59	-285.9	2.11	10.44	-269.6	1.96	10.32	-252.8
	86.67	2.60	10.79	-322.9	2.50	10.67	-307.2	2.48	10.68	-305.3	2.35	10.56	-285.9	2.12	10.48	-275.3	1.94	10.34	-254.1
	93.33	2.55	10.75	-314.5	2.54	10.74	-312.9	2.45	10.60	-300.0	2.38	10.57	-289.7	2.16	10.42	-270.5	1.95	10.36	-259.5
	100.00	2.58	10.74	-318.7	2.53	10.69	-311.1	2.47	10.63	-301.9	2.384	10.58	-290.0	2.20	10.47	-278.5	1.97	10.40	-264.3
M ≡ Molecules type P≡ Pressure (kPa) L≡ loading (mmol/g) I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 28 Adsorption Characteristics for R32 in Zeolite 3A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R32	0.00	0	0.00	0	0	0.00	0	0	0.00	0	0	0.00	0	0	0.00	0	0	0.00	0
	6.67	3.06	12.39	2398.8	3.04	12.35	2388.3	2.92	12.19	2295.2	2.75	12.06	2160.0	2.59	11.97	2040.9	2.35	11.77	1852.9
	13.33	3.27	12.60	2565.5	3.16	12.44	2480.4	3.12	12.41	2444.9	2.92	12.19	2298.6	2.77	12.05	2184.1	2.62	11.87	2063.3
	20	3.29	12.49	2582.6	3.23	12.43	2531.9	3.17	12.44	2485.5	3.07	12.35	2410.8	2.87	12.11	2255.7	2.77	12.05	2178.9
	26.67	3.34	12.54	2622.4	3.22	12.47	2527.0	3.22	12.42	2526.5	3.09	12.33	2424.6	2.97	12.20	2337.4	2.86	12.04	2248.3
	33.33	3.34	12.53	2615.7	3.32	12.51	2601.5	3.23	12.42	2535.4	3.20	12.35	2516.3	3.05	12.24	2399.3	2.91	12.11	2290.9
	40	3.43	12.57	2685.3	3.42	12.59	2680.2	3.33	12.51	2611.0	3.19	12.34	2504.0	3.10	12.30	2437.9	2.94	12.05	2312.7
	46.67	3.32	12.59	2602.0	3.45	12.58	2706.2	3.28	12.43	2572.9	3.18	12.30	2500.2	3.02	12.18	2376.2	2.97	12.12	2338.3
	53.33	3.37	12.49	2641.1	3.30	12.42	2588.1	3.32	12.51	2606.1	3.23	12.37	2534.2	3.14	12.30	2471.7	3.01	12.21	2365.2
	60	3.42	12.56	2684.8	3.39	12.60	2656.1	3.43	12.63	2691.4	3.27	12.428	2563.5	3.16	12.30	2481.7	3.02	12.22	2377.3
	66.67	3.50	12.64	2739.8	3.45	12.52	2702.8	3.47	12.49	2724.2	3.27	12.42	2566.7	3.26	12.32	2560.3	3.05	12.18	2403.6
	73.33	3.51	12.64	2753.7	3.38	12.54	2653.5	3.37	12.48	2648.0	3.30	12.47	2586.8	3.20	12.24	2519.2	3.12	12.28	2451.9
	80	3.55	12.70	2781.2	3.40	12.56	2667.3	3.37	12.52	2644.5	3.29	12.38	2586.9	3.26	12.45	2559.0	3.14	12.21	2468.9
	86.67	3.63	12.66	2848.9	3.43	12.57	2689.2	3.41	12.54	2674.7	3.40	12.48	2672.5	3.21	12.30	2523.2	3.17	12.17	2492.5
	93.33	3.52	12.58	2756.8	3.47	12.57	2722.1	3.32	12.46	2607.7	3.31	12.41	2601.9	3.33	12.40	2619.0	3.14	12.30	2467.1
	100.00	3.61	12.64	2827.5	3.53	12.65	2767.8	3.51	12.60	2755.0	3.31	12.43	2599.6	3.26	12.32	2563.5	3.12	12.20	2453.1
M ≡ Molecules type P ≡ Pressure (kPa), L≡ loading (mmol/g), I.H ≡ Isosteric heats(kcal/mol) T.H ≡ Overall system energies (kcal/mol)																			

Table 29 Adsorption Characteristics for R23 in Zeolite 3A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R23	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0
	6.67	1.89	12.62	-290.9	1.91	12.68	-295.7	1.83	12.52	-281.8	1.78	12.48	-271.8	1.61	12.26	-242.9	1.55	12.22	-233.7
	13.33	1.98	12.69	-307.1	2.02	12.77	-314.1	2.00	12.70	-309.5	1.83	12.50	-279.0	1.76	12.41	-266.9	1.69	12.34	-255.0
	20	2.10	12.81	-326.0	2.02	12.68	-312.0	2.03	12.70	-313.4	1.88	12.54	-288.3	1.81	12.46	-276.1	1.72	12.36	-259.9
	26.67	2.15	12.81	-334.4	2.13	12.80	-330.1	2.03	12.82	-316.0	1.90	12.57	-291.8	1.87	12.53	-286.6	1.81	12.44	-274.4
	33.33	2.11	12.82	-327.5	2.05	12.74	-317.4	2.04	12.79	-316.0	1.99	12.69	-306.5	1.97	12.63	-301.5	1.82	12.36	-274.5
	40	2.17	12.82	-336.6	2.16	12.95	-337.5	2.09	12.76	-323.8	2.02	12.78	-311.8	1.93	12.58	-295.7	1.82	12.42	-275.7
	46.67	2.12	12.83	-330.6	2.25	12.95	-351.4	2.11	12.87	-328.6	2.05	12.68	-315.1	2.00	12.54	-304.3	1.91	12.52	-290.2
	53.33	2.19	12.88	-341.0	2.16	12.85	-334.9	2.15	12.89	-334.7	2.08	12.71	-320.5	1.97	12.57	-300.5	1.88	12.50	-286.6
	60	2.23	12.96	-349.4	2.14	12.79	-333.1	2.11	12.73	-325.4	2.07	12.79	-320.9	2.01	12.62	-308.4	1.93	12.53	-293.5
	66.67	2.20	12.87	-343.1	2.20	12.84	-341.0	2.16	12.83	-334.9	2.10	12.75	-324.0	2.03	12.65	-310.8	1.96	12.61	-299.4
	73.33	2.22	12.84	-344.1	2.17	12.86	-337.5	2.08	12.74	-322.2	2.14	12.91	-332.3	2.04	12.64	-312.4	1.90	12.50	-289.0
	80	2.25	12.98	-351.9	2.17	12.89	-338.2	2.19	12.94	-341.2	2.08	12.77	-321.9	1.98	12.60	-302.4	1.96	12.55	-299.0
	86.67	2.17	12.88	-338.1	2.18	12.84	-338.0	2.20	12.86	-341.2	2.05	12.71	-315.9	2.06	12.70	-316.7	1.95	12.52	-296.4
	93.33	2.20	12.88	-343.0	2.17	12.84	-337.8	2.25	12.97	-351.3	2.08	12.71	-320.9	2.00	12.64	-307.0	1.96	12.61	-299.1
	100.00	2.19	12.92	-342.8	2.25	12.94	-351.8	2.22	12.90	-344.8	2.04	12.62	-311.7	2.07	12.61	-316.4	1.97	12.58	-301.0
M ≡ Molecules type P≡ Pressure (kPa) L≡ loading(mmol/g) I.H≡ Isosteric heats(kcal/mol),T.H ≡ Overall system energies (kcal/mol)																			

Table 30 Adsorption Characteristics for R14 in Zeolite 3A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R14	0.00	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0	0	0.00	0.0
	6.67	1.54	12.14	-243.5	1.54	12.14	-242.4	1.49	12.09	-226.7	1.44	12.09	-226.7	1.31	11.97	-203.7	1.23	11.94	-191.4
	13.33	1.61	12.16	-254.2	1.58	12.13	-249.5	1.57	12.07	-230.9	1.47	12.07	-230.9	1.45	12.03	-226.3	1.36	11.99	-211.2
	20	1.68	12.14	-264.2	1.66	12.13	-261.2	1.59	12.08	-241.3	1.54	12.08	-241.3	1.48	12.04	-230.6	1.44	12.04	-224.4
	26.67	1.66	12.14	-260.2	1.63	12.12	-256.1	1.63	12.10	-246.3	1.57	12.10	-246.3	1.53	12.05	-238.5	1.45	12.00	-224.1
	33.33	1.66	12.15	-262.0	1.62	12.11	-254.9	1.64	12.11	-250.5	1.60	12.11	-250.5	1.54	12.06	-240.8	1.49	12.02	-231.3
	40	1.68	12.13	-263.7	1.63	12.15	-257.5	1.61	12.08	-249.0	1.59	12.08	-249.0	1.56	12.07	-243.9	1.53	12.02	-237.6
	46.67	1.68	12.12	-263.9	1.65	12.11	-259.3	1.65	12.09	-252.5	1.61	12.09	-252.5	1.57	12.07	-244.9	1.53	12.03	-236.9
	53.33	1.66	12.14	-261.2	1.66	12.14	-261.8	1.72	12.07	-252.5	1.62	12.07	-252.5	1.58	12.06	-246.6	1.54	12.05	-240.2
	60	1.71	12.13	-268.6	1.76	12.11	-275.4	1.67	12.08	-255.6	1.64	12.08	-255.6	1.59	12.06	-248.3	1.56	12.04	-242.4
	66.67	1.67	12.10	-260.8	1.71	12.12	-268.3	1.67	12.07	-261.4	1.68	12.07	-261.4	1.60	12.07	-249.1	1.56	12.04	-243.0
	73.33	1.70	12.14	-267.8	1.66	12.13	-261.0	1.68	12.07	-253.0	1.62	12.07	-253.0	1.61	12.06	-251.3	1.55	12.05	-241.3
	80	1.74	12.12	-272.5	1.71	12.12	-269.1	1.67	12.10	-255.2	1.63	12.10	-255.2	1.603	12.05	-248.7	1.57	12.03	-244.1
	86.67	1.76	12.07	-276.0	1.71	12.13	-268.0	1.76	12.10	-258.9	1.66	12.10	-258.9	1.61	12.07	-250.3	1.59	12.03	-246.3
	93.33	1.76	12.06	-274.7	1.73	12.11	-271.5	1.74	12.06	-262.0	1.68	12.06	-262.0	1.62	12.06	-252.7	1.56	12.04	-242.3
	100.00	1.80	12.10	-282.5	1.71	12.10	-267.7	1.73	12.09	-263.3	1.69	12.09	-263.3	1.64	12.06	-254.7	1.59	12.04	-246.9
M ≡ Molecules type P≡ Pressure(kPa) L≡ loading (mmol/g) I.H≡ Isosteric heats (kcal/mol) T.H ≡ Overall system energies (kcal/mol)																			

Table 31 Langmuir-Freundlich Adsorption Parameters for Ethane Derivative Refrigerants in Zeolite 13X

Molecules		Temperatures (K)					
		293	298	303	313	323	333
R152a	q(mmol/g)	3.822	3.472	3.297	3.082	3.152	2.668
	K(kPa ⁻¹)	1.228	0.567	0.860	0.373	0.262	0.173
	n	0.313	0.566	0.511	0.765	0.608	1.214
	R ²	0.999	1.000	1.000	0.999	1.000	0.999
R152	q(mmol/g)	4.226	3.604	3.357	4.519	4.144	3.056
	K(kPa ⁻¹)	0.811	0.987	0.621	0.780	1.020	0.682
	n	0.321	0.645	0.845	0.243	0.273	0.825
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R143a	q(mmol/g)	2.971	4.351	3.479	3.305	2.673	2.553
	K(kPa ⁻¹)	0.992	0.133	1.018	0.448	0.418	0.228
	n	0.588	0.224	0.277	0.373	0.698	0.808
	R ²	0.999	0.999	1.000	0.999	1.000	0.999
R143	q(mmol/g)	3.854	2.915	3.194	2.972	3.098	3.225
	K(kPa ⁻¹)	1.693	0.462	2.915	1.569	1.603	8.827
	n	0.263	1.427	0.418	0.661	0.592	0.276
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R134a	q(mmol/g)	3.215	2.773	2.626	2.926	2.737	2.851
	K(kPa ⁻¹)	3.886	1.000	0.459	1.965	0.746	0.807
	n	0.287	0.745	1.167	0.328	0.543	0.374
	R ²	1.000	1.000	1.000	1.000	0.999	1.000
R134	q(mmol/g)	3.294	3.354	2.902	2.755	2.866	3.491
	K(kPa ⁻¹)	1.195	2.033	0.873	5.334	0.447	0.616
	n	0.333	0.287	0.613	0.464	1.005	0.271
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R125	q(mmol/g)	2.569	2.423	3.131	2.379	2.765	2.584
	K(kPa ⁻¹)	14.538	5.533	1.695	0.901	2.469	0.767
	n	0.427	0.618	0.229	0.722	0.259	0.418
	R ²	1.000	1.000	0.999	0.999	0.999	0.999
R116	q(mmol/g)	2.186	2.077	2.208	2.100	2.197	2.208
	K(kPa ⁻¹)	0.369	0.208	54.116	1.120	16.842	5.28197
	n	1.771	6.806	0.300	0.787	0.291	0.307
	R ²	0.999	0.999	1.000	0.998	0.999	0.999

Table 32 Adsorption Characteristics for R152a in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R152a	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.51	11.42	-815.9	2.34	11.11	-754.4	2.35	11.08	-757.6	2.09	10.59	-664.4	1.83	10.24	-577.5	1.42	9.58	-442.7
	13.33	2.76	11.96	-908.6	2.69	11.62	-876.8	2.52	11.40	-818.6	2.33	11.06	-750.1	2.12	10.59	-675.9	2.01	10.47	-637.4
	20	2.76	11.92	-909.5	2.78	11.85	-913.0	2.72	11.78	-891.5	2.45	11.17	-791.8	2.36	11.07	-760.4	2.27	10.92	-727.5
	26.67	2.75	11.98	-905.2	2.85	11.97	-937.3	2.64	11.57	-859.1	2.56	11.56	-833.5	2.44	11.27	-789.2	2.32	11.01	-745.5
	33.33	2.86	11.91	-940.2	2.82	11.98	-928.9	2.78	11.97	-917.0	2.67	11.65	-870.5	2.55	11.44	-826.2	2.30	10.91	-738.1
	40	3.02	12.35	-1003.3	2.9	12.31	-977.3	2.80	11.98	-920.5	2.95	12.14	-975.4	2.50	11.35	-808.2	2.33	10.95	-748.0
	46.67	2.95	12.40	-980.6	3.01	12.46	-1003.3	2.90	12.13	-958.7	2.98	12.24	-986.0	2.51	11.29	-812.2	2.37	10.97	-761.7
	53.33	3.03	12.33	-1006.9	2.97	12.30	-984.9	2.97	12.37	-985.4	2.76	11.91	-906.7	2.56	11.42	-830.0	2.46	11.16	-791.6
	60	3.09	12.50	-1030.8	3.01	12.44	-1003.7	2.91	12.19	-963.7	2.79	12.02	-918.0	2.57	11.38	-834.6	2.45	11.19	-791.6
	66.67	3.12	12.78	-1046.5	3.24	12.79	-1087.7	2.94	12.21	-971.6	2.90	12.02	-955.3	2.74	11.78	-895.7	2.62	11.52	-852.7
	73.33	3.18	12.74	-1066.5	3.20	12.69	-1070.0	3.04	12.40	-1010.0	2.78	11.82	-913.6	2.75	11.81	-899.8	2.58	11.45	-835.1
	80	3.04	12.37	-1009.3	3.14	12.56	-1047.0	2.98	12.19	-985.3	2.89	12.17	-954.3	2.71	11.81	-884.6	2.65	11.45	-859.3
	86.67	3.01	12.44	-1002.5	3.06	12.45	-1018.6	2.95	12.15	-974.9	2.79	11.85	-915.6	2.70	11.65	-881.6	2.52	11.35	-814.2
	93.33	3.04	12.43	-1011.7	3.07	12.39	-1023.5	2.93	12.21	-970.1	2.76	11.89	-903.6	2.75	11.83	-901.2	2.74	11.78	-895.1
	100.00	3.14	12.54	-1046.8	3.15	12.57	-1051.1	2.89	12.05	-952.6	2.97	12.13	-978.6	2.85	11.84	-936.2	2.54	11.29	-820.3
M ≡ Molecules type P≡ Pressure (kPa) L≡ loading(mmol/g) I.H≡ Isosteric heats(kcal/mol) T.H ≡ Overall system energies (kcal/mol)																			

Table 33 Adsorption Characteristics for R152 in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R152	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.62	14.01	-287.5	2.78	14.20	-308.06	2.60	13.89	-280.39	2.72	14.15	-299.8	2.58	13.79	-277.6	2.38	13.47	-248.1
	13.33	2.97	14.82	-342.9	2.99	14.94	-346.97	2.80	14.63	-319.07	2.95	14.56	-333.8	2.79	14.39	-312.3	2.58	13.67	-275.0
	20	3.08	15.35	-370.1	3.19	15.05	-374.63	3.01	14.99	-351.93	2.99	14.64	-340.3	2.87	14.59	-325.4	2.81	14.50	-314.7
	26.67	3.12	15.33	-372.8	3.30	15.59	-402.09	3.06	15.07	-358.62	3.11	15.04	-363.2	3.10	14.93	-360.1	2.87	14.39	-319.7
	33.33	3.13	15.20	-372.5	3.28	15.45	-395.35	3.14	15.20	-372.99	3.08	15.10	-361.0	3.02	14.80	-348.1	2.76	14.05	-300.3
	40	3.11	15.07	-367.5	3.15	15.40	-378.84	3.19	15.23	-378.00	3.05	15.10	-358.0	3.01	14.52	-340.6	2.81	14.19	-308.6
	46.67	3.07	15.03	-360.4	3.24	15.52	-392.11	3.19	15.27	-381.08	3.11	15.21	-368.4	3.03	14.64	-344.2	2.91	14.33	-322.9
	53.33	3.19	15.29	-380.8	3.33	15.70	-405.28	3.19	15.09	-375.79	3.12	15.27	-369.9	2.99	14.96	-346.8	2.86	14.25	-317.5
	60	3.27	15.49	-394.9	3.41	15.69	-416.83	3.19	15.37	-382.00	3.17	15.23	-374.8	3.08	14.81	-354.0	2.96	14.47	-334.0
	66.67	3.33	15.49	-403.7	3.41	15.91	-424.54	3.23	15.38	-386.41	3.29	15.52	-396.5	3.04	14.85	-349.2	2.93	14.53	-329.9
	73.33	3.34	15.75	-410.8	3.41	15.78	-420.90	3.26	15.30	-390.04	3.30	15.65	-400.1	3.10	14.77	-355.0	3.00	14.52	-338.5
	80	3.38	15.79	-416.5	3.41	16.00	-425.45	3.19	15.10	-375.25	3.34	15.50	-402.0	3.19	15.29	-378.3	2.86	14.35	-318.4
	86.67	3.41	15.66	-417.6	3.41	15.78	-420.60	3.22	15.18	-378.61	3.40	15.82	-417.1	3.26	15.41	-390.7	2.93	14.59	-331.4
	93.33	3.41	15.81	-422.2	3.417	15.92	-423.98	3.27	15.31	-390.10	3.41	15.87	-420.7	3.41	15.69	-415.5	2.97	14.64	-337.3
	100.00	3.41	15.73	-420.5	3.417	15.89	-422.19	3.21	15.13	-378.64	3.41	15.79	-418.6	3.23	15.17	-381.7	2.99	14.53	-337.6

M ≡ Molecules type, P≡ Pressure (kPa) L≡ loading (mmol/g) I.H≡ Isosteric heats (kcal/mol) T.H ≡ Overall system energies (kcal/mol)

Table 34 Adsorption Characteristics for R143a in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R143a	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.44	10.96	-949.14	2.17	10.81	-910.4	2.07	10.77	-903.6	1.87	10.53	-834.7	1.66	10.12	-733.0	1.40	9.58	-592.8
	13.33	2.51	11.18	-994.19	2.36	11.07	-976.9	2.24	11.16	-995.2	2.12	10.56	-862.9	1.95	10.66	-871.0	1.75	10.28	-782.0
	20	2.69	11.35	-1047.08	2.37	11.22	-1014.1	2.40	11.35	-1026.4	2.23	11.06	-972.5	2.03	10.64	-889.2	1.91	10.43	-823.3
	26.67	2.55	11.57	-1109.65	2.50	11.17	-1025.3	2.41	11.36	-1059.6	2.31	10.99	-969.4	2.13	10.93	-945.7	2.00	10.52	-863.2
	33.33	2.60	11.55	-1085.39	2.56	11.23	-1034.1	2.46	11.35	-1044.2	2.40	11.25	-1029.3	2.22	10.75	-917.9	2.09	10.42	-850.9
	40	2.65	11.36	-1072.34	2.58	11.46	-1067.9	2.51	11.32	-1050.6	2.38	11.42	-1071.8	2.25	11.04	-982.5	2.10	10.66	-889.9
	46.67	2.61	11.82	-1161.23	2.65	11.41	-1078.7	2.56	11.56	-1085.5	2.43	11.51	-1090.2	2.32	11.22	-1011.6	2.18	10.69	-900.1
	53.33	2.55	11.98	-1220.14	2.60	11.42	-1079.4	2.53	11.51	-1100.3	2.40	11.26	-1032.3	2.30	11.06	-989.4	2.18	10.84	-942.2
	60	2.65	12.20	-1234.78	2.67	11.56	-1111.3	2.59	11.44	-1080.6	2.42	11.55	-1083.2	2.32	11.27	-1024.2	2.19	10.78	-930.9
	66.67	2.70	12.12	-1233.64	2.61	12.01	-1208.4	2.63	11.55	-1116.8	2.50	11.56	-1098.5	2.35	11.35	-1052.6	2.28	10.89	-959.4
	73.33	2.67	11.86	-1193.32	2.65	12.08	-1228.2	2.57	11.58	-1117.6	2.51	11.55	-1109.4	2.39	11.28	-1056.5	2.24	11.03	-985.6
	80	2.81	11.79	-1140.79	2.66	11.82	-1162.1	2.60	11.79	-1163.9	2.52	11.17	-1013.5	2.38	11.17	-1018.5	2.25	10.84	-947.9
	86.67	2.82	11.76	-1122.80	2.69	11.95	-1157.9	2.67	11.95	-1180.7	2.54	11.38	-1070.0	2.35	11.06	-987.5	2.28	10.87	-956.7
	93.33	2.67	11.72	-1153.63	2.71	12.01	-1177.8	2.62	11.84	-1189.5	2.57	11.59	-1138.7	2.43	11.36	-1054.2	2.33	11.14	-1000.2
	100.00	2.70	11.64	-1140.20	2.65	11.84	-1183.2	2.68	11.59	-1103.9	2.58	11.82	-1173.0	2.46	11.16	-1035.3	2.35	11.17	-1023.9
M ≡ Molecules type, P≡ Pressure (kPa), L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 35 Adsorption Characteristics for R143 in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R143	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.56	18.04	-187.1	2.43	17.82	-173.8	2.48	17.54	-171.9	2.46	17.48	-169.5	2.45	17.12	-164.1	2.47	17.31	-166.0
	13.33	2.67	18.60	-207.5	2.67	18.42	-203.6	2.59	18.41	-196.2	2.59	18.09	-190.1	2.74	18.49	-209.9	2.55	17.91	-181.3
	20	2.67	18.92	-213.4	2.76	18.68	-216.1	2.71	18.53	-206.3	2.68	18.44	-203.2	2.74	18.61	-211.9	2.56	17.98	-182.9
	26.67	2.82	19.02	-228.9	2.89	18.81	-231.6	2.74	18.80	-215.3	2.74	18.60	-212.6	2.77	18.73	-216.5	2.59	18.04	-188.2
	33.33	2.89	19.04	-236.0	2.89	18.62	-228.2	2.75	18.80	-215.9	2.74	18.70	-214.2	2.82	18.61	-219.5	2.67	18.30	-199.4
	40	2.89	19.08	-235.2	2.89	18.98	-234.0	2.82	18.78	-221.9	2.82	18.74	-222.4	2.86	18.76	-225.1	2.67	18.23	-197.9
	46.67	2.89	19.23	-238.4	2.89	18.95	-234.7	2.82	18.92	-225.3	2.82	18.60	-219.2	2.89	18.56	-224.3	2.71	18.42	-203.6
	53.33	2.91	19.35	-241.5	2.89	18.91	-233.1	2.88	18.83	-229.0	2.84	18.63	-220.6	2.86	18.53	-221.0	2.73	18.59	-209.0
	60	2.97	19.21	-245.1	2.82	18.91	-226.9	2.89	18.89	-231.3	2.86	18.72	-224.6	2.82	18.43	-215.3	2.67	18.34	-199.9
	66.67	3.01	19.33	-252.0	2.89	19.27	-239.1	2.89	18.90	-232.5	2.82	18.93	-224.2	2.87	18.54	-221.8	2.77	18.40	-209.4
	73.33	3.04	19.32	-254.5	2.89	19.24	-237.8	2.89	18.89	-232.8	2.82	18.59	-217.9	2.89	18.66	-225.8	2.82	18.39	-215.6
	80	3.04	19.30	-255.0	2.89	19.28	-239.5	2.89	18.76	-229.5	2.89	18.74	-227.2	2.92	18.73	-229.9	2.82	18.48	-214.6
	86.67	3.04	19.27	-255.4	2.89	19.29	-239.9	2.89	18.88	-232.2	2.89	18.73	-228.5	2.97	18.92	-237.7	2.78	18.44	-212.2
	93.33	3.04	19.06	-250.5	2.86	18.99	-231.1	2.89	18.82	-232.1	2.83	18.86	-225.9	2.97	18.92	-239.2	2.82	18.67	-219.5
	100.00	3.04	19.19	-252.7	2.91	18.86	-233.5	2.89	18.84	-232.7	2.82	18.85	-224.2	3.02	18.53	-235.0	2.74	18.41	-207.7
M ≡ Molecules type, P≡ Pressure (kPa), L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 36 Adsorption Characteristics for R134a in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R134a	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.44	12.71	-82.6	2.42	12.43	-75.23	2.29	12.05	-62.5	2.14	11.91	-59.4	1.97	11.70	-52.87	1.87	11.52	-47.1
	13.33	2.51	12.96	-91.3	2.44	12.75	-85.07	2.37	12.52	-77.5	2.30	12.22	-68.2	2.15	11.78	-54.79	2.02	11.77	-53.8
	20	2.69	13.03	-94.0	2.51	13.16	-97.15	2.57	13.05	-93.7	2.34	12.18	-67.5	2.22	12.38	-72.72	2.11	12.09	-63.3
	26.67	2.55	13.15	-96.2	2.48	13.20	-101.50	2.50	13.27	-102.7	2.46	12.27	-71.6	2.27	12.45	-76.25	2.17	12.28	-68.3
	33.33	2.60	13.51	-110.7	2.52	13.60	-112.5	2.51	13.17	-97.8	2.46	12.80	-86.0	2.49	12.91	-89.59	2.17	12.54	-76.6
	40	2.65	13.51	-111.9	2.58	13.64	-113.8	2.51	13.06	-96.0	2.45	12.90	-90.8	2.35	12.51	-78.27	2.24	12.47	-75.2
	46.67	2.61	13.36	-109.4	2.59	13.31	-102.7	2.41	13.38	-103.3	2.46	12.91	-90.0	2.46	12.68	-80.49	2.29	11.91	-59.2
	53.33	2.55	13.51	-110.8	2.69	13.40	-105.5	2.58	13.21	-101.0	2.54	12.58	-79.4	2.32	12.84	-86.10	2.23	12.24	-69.0
	60	2.65	13.35	-105.4	2.68	13.61	-112.7	2.64	12.98	-94.3	2.50	12.78	-85.6	2.49	12.89	-89.62	2.33	12.58	-79.6
	66.67	2.70	13.51	-108.7	2.61	13.40	-108.5	2.67	13.14	-102.0	2.50	13.11	-93.3	2.41	12.85	-88.16	2.35	12.59	-79.9
	73.33	2.67	13.37	-106.3	2.73	13.57	-111.9	2.66	13.43	-106.4	2.50	13.09	-92.8	2.46	13.13	-97.27	2.35	12.64	-79.3
	80	2.81	13.58	-113.9	2.66	13.47	-110.5	2.60	13.37	-106.0	2.59	12.97	-91.0	2.39	13.15	-96.86	2.34	12.56	-77.5
	86.67	2.82	13.79	-121.4	2.69	13.28	-106.8	2.60	13.48	-107.0	2.52	12.99	-91.8	2.45	13.11	-98.28	2.42	12.79	-84.8
	93.33	2.67	13.76	-120.2	2.70	13.41	-110.2	2.50	13.22	-102.9	2.55	13.16	-95.8	2.40	12.81	-84.86	2.36	12.57	-80.3
	100.00	2.70	13.80	-121.2	2.76	13.52	-111.9	2.66	13.27	-103.6	2.54	12.92	-89.3	2.45	12.73	-83.76	2.32	12.68	-82.8
M ≡ Molecules type, P≡ Pressure (kPa), L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 37 Adsorption Characteristics for R134 in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R134	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.18	15.10	393.6	2.29	15.31	410.2	2.16	14.62	396.5	2.31	15.25	415.0	2.15	14.55	397.5	2.08	14.26	389.2
	13.33	2.35	15.94	412.0	2.37	15.39	420.5	2.37	15.55	419.8	2.42	15.78	424.1	2.44	15.80	428.6	2.26	14.87	413.0
	20	2.43	16.14	419.8	2.49	16.42	425.7	2.47	15.93	432.2	2.44	16.15	425.1	2.59	16.24	444.5	2.29	14.99	417.4
	26.67	2.53	16.31	433.0	2.59	16.70	438.8	2.59	16.14	447.2	2.52	16.74	426.3	2.64	16.42	450.5	2.34	15.43	419.7
	33.33	2.59	16.44	440.5	2.59	16.68	438.8	2.59	16.15	447.7	2.52	16.32	433.5	2.69	16.32	461.0	2.43	15.66	430.5
	40	2.59	16.78	435.4	2.60	16.75	438.4	2.59	16.47	442.9	2.52	16.30	433.9	2.74	16.11	472.4	2.39	15.58	424.4
	46.67	2.59	16.71	436.3	2.60	16.94	434.0	2.59	16.35	444.1	2.54	16.14	439.8	2.73	16.12	470.4	2.36	15.55	420.9
	53.33	2.59	16.94	432.7	2.65	16.58	447.8	2.59	16.35	444.8	2.59	16.32	443.9	2.74	16.60	464.4	2.56	15.99	444.7
	60	2.59	16.71	436.4	2.67	16.91	445.9	2.59	16.45	442.1	2.59	16.33	445.2	2.74	16.83	459.3	2.67	16.13	461.6
	66.67	2.59	16.62	438.3	2.67	17.00	445.1	2.67	16.62	450.8	2.59	16.17	444.8	2.74	16.81	459.6	2.67	16.09	462.5
	73.33	2.68	16.92	444.8	2.72	16.60	460.3	2.67	16.30	456.5	2.59	16.51	442.9	2.74	16.67	461.1	2.67	16.43	456.7
	80	2.74	17.17	451.2	2.74	16.54	463.4	2.72	16.56	460.1	2.59	16.58	440.9	2.77	16.45	471.7	2.58	16.12	446.7
	86.67	2.74	17.14	451.0	2.74	16.64	461.1	2.74	16.75	460.8	2.59	16.36	443.4	2.82	16.89	469.5	2.52	15.96	439.9
	93.33	2.74	16.97	454.5	2.74	16.65	462.2	2.74	16.75	460.7	2.59	16.43	442.1	2.82	16.80	472.6	2.57	16.20	444.4
	100.00	2.75	16.90	456.6	2.74	16.62	462.3	2.74	16.89	458.0	2.59	16.37	443.0	2.81	16.81	470.1	2.59	16.43	445.1
M ≡ Molecules type, P≡ Pressure (kPa), L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 38 Adsorption Characteristics for R125 in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R125	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.16	12.80	986.3	2.177	12.59	953.3	2.04	12.16	896.3	1.83	11.58	816.2	1.87	11.82	830.8	1.73	11.29	774.9
	13.33	2.25	12.68	969.3	2.28	12.80	983.3	2.18	12.58	951.1	2.16	12.34	949.1	1.94	11.98	859.2	1.84	11.61	820.1
	20	2.26	12.98	1028.6	2.18	12.90	1004.5	2.19	12.52	959.0	2.05	12.14	905.3	2.10	12.39	921.7	1.89	11.79	841.1
	26.67	2.35	13.35	1085.25	2.26	12.76	984.7	2.13	12.39	931.9	2.16	12.44	948.5	2.03	12.08	894.0	2.07	12.21	909.7
	33.33	2.31	13.02	1030.4	2.26	12.96	1011.1	2.06	12.29	905.3	2.14	12.27	942.7	2.08	12.19	915.3	2.10	12.22	923.8
	40	2.33	13.12	1039.5	2.25	13.04	1025.5	2.16	12.43	945.2	2.13	12.36	936.5	2.05	12.06	903.5	2.07	12.09	911.2
	46.67	2.41	13.32	1046.2	2.35	12.90	1007.1	2.34	12.89	1015.1	2.29	12.84	997.4	2.14	12.31	938.1	2.11	12.27	929.7
	53.33	2.35	12.95	1010.2	2.38	12.98	1011.1	2.39	13.01	1034.5	2.29	12.76	998.9	2.18	12.43	953.6	2.08	12.13	916.5
	60	2.38	13.07	1038.5	2.44	13.07	1041.2	2.27	12.75	986.2	2.21	12.64	966.1	2.17	12.47	952.7	2.16	12.36	950.9
	66.67	2.31	13.45	1099.0	2.48	13.09	1043.7	2.30	12.81	998.7	2.23	12.65	974.2	2.20	12.51	961.8	2.18	12.49	957.6
	73.33	2.33	13.06	1023.2	2.36	12.93	1007.3	2.36	13.05	1019.9	2.26	12.61	989.0	2.20	12.44	961.9	2.16	12.40	949.4
	80	2.43	13.18	1048.6	2.44	12.94	1010.0	2.45	13.30	1054.9	2.24	12.81	977.0	2.21	12.52	967.9	2.22	12.50	973.4
	86.67	2.49	13.20	1044.5	2.52	13.03	1025.8	2.45	13.30	1055.5	2.26	12.69	984.3	2.14	12.33	941.8	2.27	12.67	993.0
	93.33	2.47	13.25	1062.3	2.49	12.95	1014.9	2.45	13.11	1058.7	2.33	12.80	1012.3	2.24	12.57	980.8	2.21	12.53	968.0
	100.00	2.51	13.35	1077.8	2.37	13.11	1038.0	2.38	13.00	1032.4	2.34	12.95	1012.7	2.28	12.87	993.9	2.13	12.21	936.5
M ≡ Molecules type, P≡ Pressure (kPa), L≡ loading (mmol/g), I.H≡ Isosteric heats(kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 39 Adsorption Characteristics for R116 in Zeolite 13x at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R116	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	1.82	11.51	1656.9	1.87	11.57	1706.27	1.89	11.68	1720.2	1.75	11.34	1597.4	1.77	11.39	1616.5	1.63	11.07	1493.9
	13.33	2.01	11.91	1825.3	2.07	12.05	1877.14	1.95	11.78	1779.8	1.87	11.60	1701.9	1.80	11.41	1646.7	1.79	11.45	1633.2
	20	2.21	12.27	2003.0	2.09	12.05	1898.77	1.99	11.86	1813.0	1.90	11.65	1735.9	1.87	11.61	1704.2	1.74	11.25	1597.8
	26.67	2.22	12.35	2010.3	2.13	12.14	1935.08	2.01	11.91	1826.5	2.00	11.85	1818.6	1.86	11.54	1700.9	1.84	11.47	1685.7
	33.33	2.15	12.17	1948.3	2.22	12.32	2012.45	1.91	11.65	1744.2	1.89	11.63	1724.3	1.87	11.56	1707.6	1.90	11.62	1738.1
	40	2.15	12.22	1946.8	2.17	12.27	1966.04	1.94	11.68	1765.1	1.95	11.77	1775.9	1.85	11.53	1690.0	1.80	11.48	1648.5
	46.67	2.07	12.04	1877.2	2.07	12.07	1883.68	1.96	11.75	1785.0	1.96	11.75	1782.1	1.89	11.56	1726.9	1.83	11.40	1670.5
	53.33	2.07	12.06	1884.0	2.07	12.10	1880.94	2.07	12.05	1880.3	2.15	12.19	1954.9	1.93	11.70	1760.2	1.87	11.58	1706.3
	60	2.12	12.16	1921.9	2.03	11.98	1849.36	2.06	12.01	1875.8	2.17	12.13	1973.5	1.93	11.71	1758.1	1.80	11.39	1650.9
	66.67	2.15	12.19	1949.2	1.93	11.70	1755.54	2.05	12.00	1865.3	2.09	12.06	1900.4	1.97	11.80	1797.3	1.86	11.49	1703.3
	73.33	2.19	12.31	1984.3	2.00	11.86	1820.37	1.99	11.86	1814.6	2.12	12.11	1921.8	2.07	12.01	1881.9	1.82	11.40	1665.1
	80	2.22	12.33	2013.9	2.06	11.95	1874.92	2.04	12.00	1852.5	2.05	11.94	1867.6	2.04	11.90	1853.7	1.99	11.72	1811.6
	86.67	2.22	12.37	2013.0	2.05	11.94	1867.37	2.05	12.01	1858.4	1.95	11.72	1773.4	1.95	11.71	1782.1	1.98	11.84	1807.4
	93.33	2.22	12.41	2012.1	2.07	11.99	1886.27	2.07	12.00	1885.2	1.94	11.76	1765.0	1.91	11.64	1740.2	1.93	11.67	1756.6
	100.00	2.22	12.36	2011.3	2.07	12.01	1885.11	2.07	12.04	1885.0	2.01	11.89	1833.0	1.90	11.64	1734.0	1.94	11.74	1767.7
M ≡ Molecules type, P≡ Pressure (kPa), L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 40 Langmuir-Freundlich Adsorption Parameters for Ethane Derivative Refrigerants in Zeolite 5A

Molecules		Temperatures (K)					
		293	298	303	313	323	333
R152a	q(mmol/g)	3.551	3.333	3.452	3.046	3.159	2.968
	K(kPa ⁻¹)	2.062	1.087	0.969	0.323	0.231	0.146
	n	0.378	0.538	0.439	0.859	0.678	0.838
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R152	q(mmol/g)	3.608	3.234	3.691	3.340	3.734	3.299
	K(kPa ⁻¹)	2.845	0.842	10.392	1.414	1.642	0.673
	n	0.498	1.434	0.293	0.632	0.330	0.557
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R143a	q(mmol/g)	2.896	2.961	3.021	2.845	3.308	3.331
	K(kPa ⁻¹)	0.633	0.442	0.397	0.311	0.106	0.064
	n	0.722	0.683	0.580	0.621	0.461	0.446
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R143	q(mmol/g)	3.450	3.382	3.185	3.593	3.402	3.148
	K(kPa ⁻¹)	1.650	7.667	8.036	3.109	3.293	2.307
	n	0.654	0.445	0.566	0.407	0.437	0.659
	R ²	1.000	1.000	1.000	1.000	1.000	1.000
R134a	q(mmol/g)	3.677	3.343	3.775	3.791	4.561	2.715
	K(kPa ⁻¹)	1.091	1.519	0.488	0.212	0.0234	0.322
	n	0.247	0.286	0.221	0.251	0.245	0.480
	R ²	1.000	0.999	0.999	0.999	0.999	1.000
R134	q(mmol/g)	3.525	3.472	2.951	2.812	2.773	3.435
	K(kPa ⁻¹)	11.956	3.109	2.161	1.160	0.889	0.627
	n	0.261	0.278	0.559	0.788	0.721	0.272
	R ²	0.999	1.000	1.000	1.000	1.000	0.999
R125	q(mmol/g)	2.891	2.953	2.458	2.926	2.524	2.242
	K(kPa ⁻¹)	3.080	2.408	0.687	1.109	0.874	0.410
	n	0.284	0.262	0.733	0.241	0.394	0.654
	R ²	0.999	1.000	0.999	0.999	1.000	1.000
R116	q(mmol/g)	2.302	2.386	2.229	2.897	2.438	2.900
	K(kPa ⁻¹)	1.853	1.691	1.570	0.229	0.405	0.068
	n	0.420	0.351	0.417	0.225	0.313	0.227
	R ²	1.000	1.000	1.000	1.000	1.000	1.000

Table 41 Adsorption Characteristics for R152a in Zeolite 5A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R152a	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.57	11.77	-865.5	2.48	11.63	-829.3	2.40	11.52	-803.3	2.01	10.97	-663.7	1.80	10.92	-597.1	1.46	10.61	-482.3
	13.33	2.80	12.06	-945.8	2.69	11.91	-906.4	2.53	11.57	-845.5	2.34	11.35	-779.8	2.18	11.24	-725.4	1.93	10.91	-637.6
	20	2.79	12.07	-943.9	2.78	11.94	-936.7	2.79	12.06	-940.8	2.55	11.60	-853.6	2.29	11.29	-760.4	2.08	11.06	-690.6
	26.67	2.93	12.16	-992.5	2.87	12.10	-970.9	2.83	12.11	-956.0	2.64	11.74	-886.3	2.47	11.52	-825.1	2.23	11.20	-738.6
	33.33	2.92	12.16	-988.0	2.87	12.09	-970.9	2.84	12.10	-959.7	2.66	11.76	-893.0	2.53	11.60	-844.0	2.30	11.28	-765.6
	40	3.04	12.34	-1031.7	2.91	12.12	-985.5	2.83	11.93	-951.3	2.73	11.81	-916.4	2.55	11.62	-853.1	2.43	11.46	-808.5
	46.67	3.02	12.32	-1025.3	3.04	12.30	-1032.4	2.91	12.11	-982.7	2.80	11.89	-940.7	2.62	11.73	-876.3	2.52	11.53	-840.2
	53.33	3.04	12.34	-1032.2	3.01	12.24	-1018.1	2.87	12.08	-969.8	2.74	11.80	-917.2	2.68	11.73	-896.8	2.52	11.49	-838.2
	60	3.05	12.30	-1033.4	2.93	12.11	-991.4	3.03	12.26	-1025.3	2.87	11.97	-966.2	2.67	11.73	-892.6	2.54	11.57	-848.1
	66.67	3.00	12.25	-1015.0	3.02	12.26	-1021.9	2.94	12.23	-997.1	2.83	12.00	-954.4	2.75	11.82	-921.2	2.59	11.56	-862.6
	73.33	3.06	12.21	-1034.4	3.19	12.37	-1083.6	2.90	12.07	-979.7	2.92	12.07	-982.9	2.81	11.93	-946.2	2.61	11.62	-872.7
	80	3.13	12.43	-1065.0	3.04	12.33	-1032.6	2.98	12.20	-1006.4	2.83	11.93	-953.0	2.79	11.91	-935.6	2.60	11.62	-868.1
	86.67	3.08	12.38	-1046.6	3.05	12.30	-1033.3	2.99	12.21	-1011.6	2.86	11.97	-961.7	2.79	11.88	-937.5	2.71	11.77	-907.9
	93.33	3.12	12.31	-1060.5	2.97	12.15	-1004.6	3.17	12.38	-1076.0	2.93	12.00	-986.3	2.78	11.83	-931.5	2.64	11.59	-879.2
	100.00	3.18	12.54	-1083.3	3.12	12.39	-1061.4	3.03	12.17	-1022.8	2.85	11.94	-957.0	2.80	11.80	-938.5	2.66	11.67	-889.4
M ≡ Molecules type, P ≡ Pressure (kPa), L≡ loading(mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 42 Adsorption Characteristics for R152 in Zeolite 5A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R152	0.00	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.95	14.06	-348.1	2.98	14.28	-356.8	2.86	14.02	-335.6	2.69	13.59	-308.1	2.55	13.43	-289.4	2.30	12.94	-253.4
	13.33	3.05	14.38	-367.3	3.11	14.41	-373.5	3.07	14.43	-370.5	2.89	13.99	-338.2	2.76	13.79	-319.2	2.54	13.29	-285.2
	20	3.14	14.65	-383.5	3.18	14.65	-388.8	3.01	14.24	-357.7	2.95	14.10	-347.4	2.85	13.94	-332.5	2.67	13.47	-302.2
	26.67	3.26	14.81	-401.5	3.23	14.56	-391.4	3.11	14.39	-372.6	3.00	14.27	-357.1	2.90	13.98	-339.4	2.79	13.69	-320.6
	33.33	3.23	14.80	-397.7	3.23	14.56	-390.7	3.10	14.28	-368.5	3.16	14.41	-378.7	3.01	14.10	-353.1	2.82	13.72	-323.6
	40	3.28	14.79	-403.5	3.21	14.63	-390.2	3.01	14.33	-360.5	3.09	14.31	-368.5	3.01	14.13	-353.8	2.75	13.60	-313.8
	46.67	3.30	14.76	-404.7	3.23	14.64	-392.8	3.18	14.63	-387.3	3.05	14.25	-362.4	2.94	13.96	-342.7	2.91	13.95	-338.3
	53.33	3.35	14.77	-411.5	3.16	14.45	-380.2	3.17	14.53	-383.5	3.16	14.45	-379.5	3.01	14.16	-355.3	2.93	13.96	-340.7
	60	3.41	15.06	-425.1	3.21	14.58	-389.5	3.36	14.89	-413.6	3.17	14.50	-382.2	2.97	14.06	-347.8	2.90	13.96	-337.5
	66.67	3.43	15.08	-427.5	3.19	14.65	-388.4	3.19	14.54	-386.4	3.16	14.40	-379.6	3.07	14.19	-362.0	2.95	13.89	-341.0
	73.33	3.49	15.10	-433.7	3.16	14.54	-382.7	3.16	14.54	-383.2	3.18	14.53	-383.9	3.12	14.38	-372.6	2.91	13.87	-336.9
	80	3.38	15.09	-421.3	3.21	14.73	-392.9	3.25	14.77	-399.2	3.19	14.44	-383.1	3.08	14.22	-364.0	2.90	13.86	-335.4
	86.67	3.33	14.95	-412.6	3.26	14.87	-401.8	3.26	14.65	-395.7	3.17	14.38	-379.1	3.13	14.27	-370.8	3.03	14.19	-357.8
	93.33	3.35	14.81	-412.6	3.30	14.83	-406.2	3.28	14.55	-396.7	3.15	14.39	-376.5	3.15	14.38	-375.9	3.04	14.02	-355.3
	100.00	3.30	14.77	-405.5	3.22	14.56	-390.7	3.29	14.72	-401.4	3.21	14.48	-385.7	3.23	14.43	-385.1	3.02	14.04	-352.2
M $\equiv$ Molecules type, P $\equiv$ Pressure (kPa), L $\equiv$ loading (mmol/g), I.H $\equiv$ Isosteric heats (kcal/mol), T.H $\equiv$ Overall system energies (kcal/mol)																			

Table 43 Adsorption Characteristics for R143a in Zeolite 5A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R143a	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.14	11.14	-1089.6	2.00	10.98	-1018.2	1.91	10.87	-972.4	1.74	10.74	-881.0	1.51	10.58	-766.8	1.35	10.58	-687.0
	13.33	2.37	11.40	-1210.2	2.25	11.24	-1146.1	2.20	11.21	-1122.6	1.99	10.93	-1010.2	1.78	10.70	-901.2	1.60	10.55	-806.9
	20	2.48	11.45	-1267.9	2.42	11.44	-1236.9	2.32	11.33	-1182.1	2.19	11.15	-1113.9	1.99	10.92	-1009.2	1.78	10.70	-900.1
	26.67	2.52	11.49	-1289.2	2.59	11.65	-1327.9	2.41	11.36	-1230.0	2.22	11.18	-1131.5	2.04	10.93	-1033.4	1.83	10.70	-925.2
	33.33	2.69	11.68	-1376.6	2.46	11.41	-1258.6	2.47	11.44	-1264.0	2.31	11.26	-1177.1	2.07	10.93	-1047.9	1.91	10.75	-967.0
	40	2.65	11.65	-1357.1	2.65	11.69	-1357.2	2.49	11.44	-1272.1	2.37	11.32	-1209.2	2.20	11.10	-1115.9	1.98	10.81	-1001.0
	46.67	2.66	11.65	-1361.6	2.62	11.63	-1342.2	2.52	11.50	-1290.1	2.44	11.39	-1243.4	2.25	11.17	-1147.2	2.09	10.98	-1056.7
	53.33	2.68	11.62	-1375.1	2.67	11.70	-1369.9	2.58	11.53	-1318.1	2.41	11.37	-1231.3	2.28	11.18	-1161.8	2.11	11.00	-1071.8
	60	2.69	11.71	-1378.8	2.67	11.65	-1365.0	2.65	11.62	-1357.1	2.35	11.26	-1197.0	2.30	11.24	-1170.8	2.16	11.07	-1099.1
	66.67	2.65	11.59	-1356.1	2.61	11.59	-1333.7	2.62	11.57	-1340.1	2.41	11.36	-1228.6	2.33	11.23	-1184.6	2.22	11.10	-1126.6
	73.33	2.72	11.70	-1396.9	2.71	11.70	-1390.6	2.62	11.57	-1338.5	2.52	11.43	-1284.5	2.39	11.34	-1217.2	2.27	11.17	-1156.9
	80	2.74	11.73	-1403.3	2.70	11.70	-1385.5	2.61	11.57	-1337.1	2.50	11.45	-1275.4	2.38	11.25	-1212.0	2.25	11.13	-1142.3
	86.67	2.78	11.82	-1427.6	2.74	11.73	-1404.0	2.67	11.65	-1367.8	2.55	11.54	-1304.2	2.44	11.37	-1245.7	2.25	11.12	-1141.7
	93.33	2.70	11.72	-1385.3	2.70	11.71	-1381.8	2.73	11.75	-1399.4	2.55	11.48	-1300.3	2.46	11.40	-1256.5	2.26	11.13	-1148.7
	100.00	2.78	11.70	-1424.3	2.85	11.87	-1463.7	2.72	11.71	-1391.0	2.56	11.51	-1302.2	2.49	11.43	-1273.1	2.29	11.20	-1162.1
M ≡ Molecules type, P≡ Pressure (kPa), L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 44 Adsorption Characteristics for in Zeolite 5A R143at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R143	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.84	17.00	-213.8	2.87	17.06	-217.0	2.88	16.71	-211.0	2.80	16.96	-208.1	2.45	16.64	-194.6	2.68	16.35	-186.7
	13.33	3.03	17.33	-236.0	3.03	17.25	-234.3	2.96	17.13	-226.4	2.89	17.05	-217.9	2.74	16.79	-197.6	2.88	16.84	-212.2
	20	3.21	17.62	-255.5	3.05	17.16	-233.7	3.02	17.24	-232.9	2.99	17.24	-229.1	2.74	17.15	-228.9	2.98	17.00	-222.5
	26.67	3.22	17.76	-260.1	3.11	17.26	-239.8	3.03	17.31	-233.7	3.11	17.50	-242.9	2.77	17.15	-235.6	2.92	17.04	-219.6
	33.33	3.20	17.82	-260.1	3.04	17.32	-237.3	3.04	17.29	-235.1	3.17	17.39	-246.0	2.82	16.96	-226.3	2.92	17.04	-220.1
	40	3.17	17.79	-257.7	3.08	17.41	-240.8	3.04	17.33	-236.1	3.19	17.53	-251.2	2.86	16.79	-214.6	2.97	17.13	-225.6
	46.67	3.16	17.85	-256.9	3.17	17.73	-254.9	3.05	17.16	-233.3	3.19	17.54	-250.0	2.89	17.06	-227.5	3.03	17.11	-228.2
	53.33	3.25	17.86	-262.9	3.19	17.88	-259.5	3.12	17.50	-244.6	3.19	17.67	-253.7	2.86	16.99	-228.6	2.97	16.91	-220.5
	60	3.27	17.95	-266.6	3.19	17.62	-254.4	3.13	17.36	-241.9	3.19	17.59	-252.1	2.82	17.09	-230.9	2.98	17.04	-224.2
	66.67	3.33	17.82	-267.8	3.19	17.62	-254.2	3.17	17.61	-251.7	3.19	17.65	-251.8	2.87	17.18	-240.6	3.08	17.17	-234.1
	73.33	3.36	17.81	-270.6	3.19	17.67	-255.3	3.12	17.41	-243.8	3.16	17.43	-244.1	2.89	17.19	-238.8	3.06	17.28	-234.7
	80	3.36	17.75	-268.0	3.19	17.61	-254.0	2.98	17.17	-228.8	3.26	17.66	-256.6	2.92	17.22	-239.5	3.02	17.22	-231.3
	86.67	3.38	17.60	-266.0	3.20	17.51	-252.9	3.08	17.36	-239.3	3.27	17.71	-259.0	2.97	17.44	-242.9	3.05	17.33	-235.2
	93.33	3.31	17.62	-262.7	3.19	17.69	-255.0	3.11	17.29	-239.6	3.27	17.62	-257.6	2.98	17.38	-244.8	3.05	17.10	-230.5
	100.00	3.27	17.55	-257.1	3.21	17.77	-258.9	3.13	17.46	-244.6	3.30	17.74	-262.4	3.02	17.22	-237.2	3.11	17.32	-239.7
M ≡ Molecules type, P≡ Pressure (kPa), L≡ loading (mmol/g), I.H≡ Isosteric heats(kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 45 Adsorption Characteristics for R134a in Zeolite 5A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R134a	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.29	12.76	-102.8	2.23	12.75	-99.5	2.20	12.73	-98.1	1.96	12.25	-80.9	1.74	11.83	-67.1	1.61	11.68	-61.5
	13.33	2.47	12.95	-114.0	2.35	12.92	-107.3	2.32	12.80	-104.0	2.14	12.47	-91.5	2.03	12.32	-83.8	1.79	11.84	-68.2
	20	2.53	13.14	-119.9	2.37	12.89	-106.9	2.30	12.71	-101.8	2.31	12.67	-102.2	1.99	12.17	-80.0	1.91	11.99	-74.1
	26.67	2.51	13.10	-119.9	2.36	12.84	-106.1	2.41	12.87	-108.4	2.31	12.72	-102.6	2.15	12.41	-89.4	1.98	12.09	-77.9
	33.33	2.58	13.08	-122.4	2.56	13.32	-123.7	2.49	13.01	-115.2	2.29	12.70	-100.4	2.32	12.69	-100.4	2.09	12.32	-85.5
	40	2.60	13.09	-122.7	2.49	13.19	-118.2	2.35	12.78	-104.6	2.43	12.86	-109.3	2.22	12.44	-92.6	2.11	12.31	-85.9
	46.67	2.63	13.25	-127.2	2.78	13.43	-137.3	2.37	12.90	-107.3	2.35	12.77	-103.8	2.28	12.53	-96.7	2.16	12.46	-89.8
	53.33	2.68	13.49	-134.0	2.75	13.45	-136.2	2.43	12.93	-109.8	2.33	12.75	-102.4	2.30	12.73	-100.0	2.17	12.41	-89.1
	60	2.60	13.19	-124.5	2.54	13.19	-119.9	2.59	13.25	-124.3	2.42	12.98	-111.1	2.38	12.94	-107.0	2.14	12.33	-87.1
	66.67	2.77	13.43	-137.5	2.59	13.23	-122.4	2.57	13.16	-122.4	2.63	13.24	-126.4	2.34	12.74	-102.3	2.15	12.34	-87.8
	73.33	2.81	13.57	-142.8	2.74	13.31	-131.8	2.64	13.38	-130.6	2.60	13.22	-124.3	2.40	12.76	-105.9	2.19	12.50	-91.6
	80	2.69	13.37	-132.6	2.68	13.44	-132.1	2.73	13.50	-136.6	2.53	13.08	-118.9	2.43	12.83	-107.6	2.31	12.57	-98.5
	86.67	2.77	13.46	-139.2	2.66	13.41	-130.3	2.74	13.35	-133.7	2.55	13.03	-118.1	2.58	13.12	-120.1	2.31	12.53	-98.4
	93.33	2.83	13.65	-146.1	2.66	13.35	-129.0	2.68	13.30	-130.3	2.58	13.09	-120.6	2.48	12.88	-112.6	2.26	12.51	-94.5
	100.00	2.87	13.56	-145.3	2.63	13.31	-126.8	2.64	13.28	-127.5	2.59	13.10	-121.5	2.55	12.98	-117.0	2.24	12.38	-91.5
M ≡ Molecules type, P≡ Pressure (kPa), L≡ loading (mmol/g), I.H ≡ Isosteric heats(kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 46 Adsorption Characteristics for R134 in Zeolite 5A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R134	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.77	15.56	464.4	2.42	14.70	419.9	2.39	14.56	415.5	2.34	14.52	409.7	2.15	14.06	382.8	2.02	13.77	364.1
	13.33	2.76	15.54	463.9	2.58	14.99	444.1	2.59	14.79	447.3	2.50	14.96	430.5	2.46	14.70	428.5	2.21	14.14	393.7
	20	2.84	15.51	477.6	2.66	15.22	453.6	2.70	15.22	458.5	2.60	15.13	445.3	2.44	14.61	425.8	2.39	14.58	418.7
	26.67	2.89	15.78	480.2	2.75	15.42	464.4	2.64	14.99	452.8	2.64	15.12	452.3	2.46	14.63	430.5	2.35	14.51	412.6
	33.33	2.82	15.59	470.5	2.60	15.15	443.4	2.54	14.91	437.5	2.66	15.32	450.5	2.50	14.68	435.9	2.35	14.31	416.1
	40	2.83	15.53	473.9	2.70	15.17	459.1	2.68	15.40	453.3	2.69	15.12	460.3	2.55	14.90	441.0	2.38	14.39	419.9
	46.67	2.84	15.43	476.1	2.80	15.59	467.7	2.80	15.65	469.7	2.67	15.09	457.7	2.61	14.84	452.3	2.36	14.46	415.0
	53.33	2.91	15.61	486.3	2.74	15.31	463.9	2.82	15.67	469.8	2.62	15.17	448.1	2.59	14.93	447.6	2.59	14.91	448.9
	60	3.03	15.89	502.0	2.80	15.34	472.2	2.86	15.56	478.9	2.74	15.40	464.7	2.66	15.17	455.3	2.45	14.75	427.9
	66.67	3.09	15.88	512.7	2.81	15.46	472.7	2.73	15.38	462.7	2.70	15.18	461.7	2.68	15.22	457.7	2.45	14.56	431.6
	73.33	3.10	15.87	514.1	2.84	15.37	478.3	2.74	15.33	464.7	2.83	15.23	482.1	2.67	15.11	457.0	2.49	14.69	434.4
	80	3.00	15.71	500.2	2.93	15.64	489.8	2.84	15.68	475.8	2.78	15.19	473.5	2.63	14.94	454.6	2.53	14.80	440.2
	86.67	3.07	15.85	509.0	2.88	15.72	479.0	2.81	15.73	469.7	2.73	15.22	465.6	2.70	15.31	460.2	2.56	14.63	449.1
	93.33	3.04	15.74	505.9	2.89	15.44	487.0	2.75	15.43	464.1	2.68	15.08	459.4	2.61	14.94	450.3	2.67	14.99	461.0
	100.00	3.12	16.04	513.8	2.87	15.42	481.7	2.80	15.37	472.4	2.73	15.20	465.4	2.64	15.06	453.5	2.63	14.90	454.7
M ≡ Molecules type, P ≡ Pressure (kPa), L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 47 Adsorption Characteristics for R125 in Zeolite 5A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R125	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	2.03	12.72	865.6	2.01	12.70	856.3	1.89	12.43	809.2	1.79	12.33	768.1	1.68	12.18	722.6	1.47	11.85	634.6
	13.33	2.13	12.84	910.7	2.05	12.64	874.6	1.98	12.51	845.8	2.02	12.64	861.5	1.83	12.30	784.4	1.69	12.09	727.4
	20	2.14	12.82	908.9	2.24	12.95	949.3	2.17	12.85	924.7	1.97	12.51	841.7	1.88	12.34	809.6	1.79	12.24	769.8
	26.67	2.21	12.85	937.3	2.16	12.75	919.2	2.20	12.98	934.5	1.98	12.46	846.9	1.89	12.37	810.7	1.85	12.33	792.5
	33.33	2.26	13.08	958.6	2.21	12.83	939.5	2.29	13.09	968.8	2.07	12.68	881.3	2.04	12.63	870.8	1.88	12.40	806.8
	40	2.31	13.23	977.4	2.20	12.80	935.0	2.34	13.20	990.2	2.11	12.78	896.5	2.04	12.58	871.9	1.96	12.49	840.7
	46.67	2.36	13.33	994.9	2.32	13.09	981.4	2.30	13.13	972.9	2.02	12.52	863.8	2.02	12.49	865.4	1.88	12.26	809.4
	53.33	2.40	13.29	1012.5	2.30	13.17	972.8	2.30	13.14	973.1	2.08	12.72	888.6	2.06	12.61	879.7	1.96	12.47	838.8
	60	2.27	13.07	962.4	2.32	13.20	980.4	2.29	13.16	969.3	2.10	12.61	894.9	2.10	12.73	894.5	1.99	12.47	851.8
	66.67	2.41	13.22	1018.1	2.34	13.13	987.4	2.33	13.12	988.5	2.15	12.83	915.3	2.09	12.67	894.2	2.08	12.70	887.4
	73.33	2.32	13.17	981.7	2.38	13.22	1007.0	2.32	13.12	983.1	2.19	12.87	932.4	2.15	12.71	915.4	2.06	12.57	882.6
	80	2.34	13.22	987.1	2.28	13.08	963.7	2.45	13.23	1033.6	2.16	12.75	919.0	2.12	12.67	907.2	2.02	12.54	865.2
	86.67	2.41	13.09	1020.3	2.37	13.25	1001.1	2.43	13.21	1027.9	2.20	12.78	935.0	2.15	12.74	915.0	2.02	12.51	864.9
	93.33	2.35	13.17	993.5	2.42	13.22	1023.3	2.34	13.09	991.2	2.24	12.92	951.5	2.11	12.70	901.6	2.05	12.55	878.9
	100.00	2.45	13.17	1038.2	2.38	13.25	1004.1	2.24	13.04	951.0	2.30	13.00	978.1	2.11	12.61	902.8	2.03	12.51	869.8
M ≡ Molecules type, P≡ Pressure (kPa,) L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

Table 48 Adsorption Characteristics for R116 in Zeolite 5A at Various Pressures and Temperatures

M	p	Temperatures (K)																	
		293			298			303			313			323			333		
		L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H	L	I.H	T.H
R116	0.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6.67	1.70	12.20	1522.7	1.66	12.14	1493.4	1.64	12.06	1472.9	1.54	12.01	1380.1	1.40	11.88	1257.1	1.32	11.86	1190.4
	13.33	1.84	12.32	1645.9	1.81	12.28	1626.2	1.68	12.14	1509.2	1.63	12.09	1460.5	1.53	11.97	1374.5	1.44	11.91	1298.4
	20	1.87	12.32	1679.5	1.80	12.26	1614.0	1.80	12.27	1614.9	1.70	12.15	1525.7	1.61	12.05	1451.1	1.48	11.89	1333.4
	26.67	1.93	12.42	1729.6	1.85	12.29	1660.8	1.84	12.31	1653.3	1.72	12.15	1540.9	1.67	12.08	1496.2	1.55	11.97	1394.3
	33.33	1.96	12.41	1753.8	1.91	12.36	1711.6	1.85	12.29	1658.1	1.73	12.14	1553.8	1.68	12.11	1511.7	1.58	12.00	1424.1
	40	1.97	12.44	1760.3	1.98	12.41	1770.6	1.90	12.33	1701.2	1.76	12.16	1583.4	1.71	12.10	1533.1	1.61	12.02	1446.3
	46.67	1.91	12.39	1707.8	1.98	12.44	1774.9	1.88	12.32	1689.5	1.84	12.29	1652.9	1.67	12.08	1502.8	1.63	12.03	1469.8
	53.33	2.04	12.48	1825.0	2.05	12.47	1836.6	2.00	12.46	1787.5	1.86	12.25	1664.7	1.78	12.19	1596.5	1.63	12.00	1462.3
	60	2.08	12.51	1861.3	1.97	12.40	1765.9	1.97	12.42	1760.2	1.84	12.25	1635.8	1.81	12.22	1622.5	1.69	12.08	1519.3
	66.67	2.01	12.48	1797.1	1.95	12.39	1743.9	1.98	12.47	1772.0	1.88	12.30	1686.8	1.85	12.23	1656.3	1.71	12.11	1539.8
	73.33	2.08	12.53	1859.6	1.97	12.41	1768.7	1.97	12.43	1763.0	1.90	12.33	1702.3	1.76	12.16	1577.1	1.68	12.06	1512.7
	80	2.03	12.48	1815.7	2.00	12.44	1792.3	1.91	12.33	1707.3	1.90	12.31	1708.1	1.79	12.16	1603.2	1.72	12.13	1541.1
	86.67	2.01	12.43	1797.3	2.05	12.54	1837.3	1.96	12.40	1755.0	1.93	12.34	1728.2	1.84	12.26	1655.3	1.70	12.08	1525.6
	93.33	2.12	12.52	1897.2	2.05	12.50	1836.3	1.98	12.45	1772.3	1.91	12.33	1707.2	1.86	12.28	1668.4	1.78	12.16	1596.9
	100.00	2.04	12.44	1825.6	2.04	12.53	1823.1	1.96	12.34	1753.1	1.98	12.42	1774.3	1.87	12.24	1667.4	1.80	12.20	1617.1
M ≡ Molecules type, P≡ Pressure (kPa), L≡ loading (mmol/g), I.H≡ Isosteric heats (kcal/mol), T.H ≡ Overall system energies (kcal/mol)																			

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384, 2025, Article 113442. DOI: 10.1016/j.micromeso.2024.113442.
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2. ACS Qatar Chapter & RSC Joint Conference, Doha, 2024 Presented: From Molecular Dynamics to AI-Enhanced Prediction: Optimizing Zeolites for HFC Separation.

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