



NATIONAL UNIVERSITY OF SCIENCE AND TECHNOLOGY

FACULTY OF INDUSTRIAL TECHNOLOGY

DEPARTMENT OF CHEMICAL ENGINEERING

Separation Processes

ECE 3204

Final Examination Paper

March 2025

This examination paper consists of 4 pages

Time Allowed: 3 hours

Total Marks: 100

INSTRUCTIONS

1. Answer **Question A1** and **any other three (3)** questions
2. Each question carries 25 marks
3. Use of calculators is permissible

MARK ALLOCATION

QUESTION	MARKS
A1	25
B1	25
B2	25
B3	25
B4	25
TOTAL ATTAINABLE	100

SECTION A

Answer all questions

QUESTION A1

- a) What is the importance of separation processes in chemical and biochemical industries? [8]
- b) Describe and explain two mechanisms by which material transfer from liquid phase to the solid phase in crystallisation. [6]
- c) What is fouling in membrane separation processes, and what methods can be used to prevent it? [5]
- d) Compare and contrast between chemisorption and physisorption [6]

SECTION B

Answer any 3 questions

QUESTION B1

- a) Discuss any two mechanisms by for creating supersaturation in crystallization. [5]
- b) Describe how the Ion exchange process occurs. [4]
- c) Acetone(1)-cyclohexane (2) form an azeotrope at 25°C and 262 Torr where $x_1 = 0.7390$. Using the van Laar model predict the P-x-y data at 25°C.

$$\ln \gamma_1 = \frac{A}{\left(1 + \frac{A x_1}{B x_2}\right)^2}$$

$$\ln \gamma_2 = \frac{B}{\left(1 + \frac{B x_2}{A x_1}\right)^2}$$

[15]

QUESTION B2

a) You have been tasked with designing a water treatment process for your community. The water source has been characterised, and you need to ensure that the treated water meets environmental standards for safe consumption and ecological protection.

Water Characteristics

The following table summarizes the characteristics of the raw water sourced from the local river:

Water Characteristic	Measured Value	Environmental Standard Limit
pH	6.5	6.5 - 8.5
Turbidity (NTU)	15	< 5
Total Dissolved Solids (TDS) (mg/L)	800	< 500
E. coli (CFU/100 mL)	200	0
Nitrate (NO ₃ ⁻) (mg/L)	10	< 10

1. Based on the above characteristics, outline a series of steps necessary for treating this water to meet environmental standards.
2. Justify each step in your treatment process and the mechanism of separation and how it addresses specific contaminants or characteristics that exceed the environmental limits.

[10]

b) State and describe the characteristics desired for adsorbents

[5]

d) Calculate the activity coefficients for methanol(1)-benzene(2) solution at 60°C if $x_1 = 0.6$ by using the NRTL equation.

$$\ln \gamma_1 = x_2^2 \left[\tau_{21} \left(\frac{G_{21}}{x_1 + x_2 G_{21}} \right)^2 + \frac{\tau_{12} G_{12}}{(x_2 + x_1 G_{12})^2} \right]$$

$$\ln \gamma_2 = x_1^2 \left[\tau_{12} \left(\frac{G_{12}}{x_2 + x_1 G_{12}} \right)^2 + \frac{\tau_{21} G_{21}}{(x_1 + x_2 G_{21})^2} \right]$$

[10]

QUESTION B3

- a) Why is mass transfer a major factor in separation processes? [5]
- b) Explain how polarization occurs in electrodialysis and reverse osmosis. [8]
- c) In a cooling crystallizer used to crystallise sodium acetate from a salt liquid solution, water is also removed by evaporation after cooling at 0°C. The feed is initially saturated at 80°C and cooled to 0°C. If we initially dissolve the anhydrous salt in 100kg/hr of H₂O, how many crystals are collected. [12]

Table 2: Solubilities of 1 selected compound adapted from Mullin(1972), grams anhydrous compound per 100g of water

Compound	Formula	Solubility °C								Stable hydrate 0-25°C
		0	10	20	30	40	60	80	100	
Sodium Acetate	NaC ₂ H ₃ O ₂	36.3	40.8	47	54.5	65.5	139	153	170	3

QUESTION B4

- a) What are the disadvantages of using mass separating agents? [5]
- b) Estimate the activity coefficients for the ethanol (1)-benzene (2) system at 340K and $x_i = 0.8$ using the UNIQUAC method.

$$\ln \gamma_i^c = \ln \frac{\Phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\Phi_i} + l_i - \frac{\Phi_i}{x_i} \sum_j x_j l_j$$

$$\ln \gamma_i^R = q_i \left[1 - \ln \left(\sum_j \theta_j \tau_{ji} \right) - \frac{\theta_j \tau_{ij}}{(\sum_k \theta_k \tau_{kj})} \right]$$

[20]

(END OF PAPER)

IUPAC Periodic Table of the Elements

1 H hydrogen 1.0080 ± 0.0002																	18 He helium 4.0026 ± 0.0001						
3 Li lithium 6.94 ± 0.06	4 Be beryllium 9.0122 ± 0.0001																	13 B boron 10.81 ± 0.02	14 C carbon 12.011 ± 0.002	15 N nitrogen 14.007 ± 0.001	16 O oxygen 15.999 ± 0.001	17 F fluorine 18.998 ± 0.001	10 Ne neon 20.180 ± 0.001
11 Na sodium 22.990 ± 0.001	12 Mg magnesium 24.305 ± 0.002																	13 Al aluminium 26.982 ± 0.001	14 Si silicon 28.085 ± 0.001	15 P phosphorus 30.974 ± 0.001	16 S sulfur 32.06 ± 0.02	17 Cl chlorine 35.45 ± 0.01	18 Ar argon 39.95 ± 0.16
19 K potassium 39.098 ± 0.001	20 Ca calcium 40.078 ± 0.004	21 Sc scandium 44.956 ± 0.001	22 Ti titanium 47.867 ± 0.001	23 V vanadium 50.942 ± 0.001	24 Cr chromium 51.996 ± 0.001	25 Mn manganese 54.938 ± 0.001	26 Fe iron 55.845 ± 0.002	27 Co cobalt 58.933 ± 0.001	28 Ni nickel 58.693 ± 0.001	29 Cu copper 63.546 ± 0.003	30 Zn zinc 65.38 ± 0.02	31 Ga gallium 69.723 ± 0.001	32 Ge germanium 72.630 ± 0.008	33 As arsenic 74.922 ± 0.001	34 Se selenium 78.971 ± 0.008	35 Br bromine 79.904 ± 0.003	36 Kr krypton 83.798 ± 0.002						
37 Rb rubidium 85.468 ± 0.001	38 Sr strontium 87.62 ± 0.01	39 Y yttrium 88.906 ± 0.001	40 Zr zirconium 91.224 ± 0.002	41 Nb niobium 92.906 ± 0.001	42 Mo molybdenum 95.95 ± 0.01	43 Tc technetium [97]	44 Ru ruthenium 101.07 ± 0.02	45 Rh rhodium 102.91 ± 0.01	46 Pd palladium 106.42 ± 0.01	47 Ag silver 107.87 ± 0.01	48 Cd cadmium 112.41 ± 0.01	49 In indium 114.82 ± 0.01	50 Sn tin 118.71 ± 0.01	51 Sb antimony 121.76 ± 0.01	52 Te tellurium 127.60 ± 0.03	53 I iodine 126.90 ± 0.01	54 Xe xenon 131.29 ± 0.01						
55 Cs caesium 132.91 ± 0.01	56 Ba barium 137.33 ± 0.01	57-71 lanthanoids	72 Hf hafnium 178.49 ± 0.01	73 Ta tantalum 180.95 ± 0.01	74 W tungsten 183.84 ± 0.01	75 Re rhenium 186.21 ± 0.01	76 Os osmium 190.23 ± 0.03	77 Ir iridium 192.22 ± 0.01	78 Pt platinum 195.08 ± 0.02	79 Au gold 196.97 ± 0.01	80 Hg mercury 200.59 ± 0.01	81 Tl thallium 204.38 ± 0.01	82 Pb lead 207.2 ± 1.1	83 Bi bismuth 208.98 ± 0.01	84 Po polonium [209]	85 At astatine [210]	86 Rn radon [222]						
87 Fr francium [223]	88 Ra radium [226]	89-103 actinoids	104 Rf rutherfordium [267]	105 Db dubnium [268]	106 Sg seaborgium [269]	107 Bh bohrium [270]	108 Hs hassium [269]	109 Mt meitnerium [277]	110 Ds darmstadtium [281]	111 Rg roentgenium [282]	112 Cn copernicium [285]	113 Nh nihonium [286]	114 Fl flerovium [290]	115 Mc moscovium [290]	116 Lv livermorium [293]	117 Ts tennessine [294]	118 Og oganesson [294]						

Key:
atomic number
Symbol
name
abridged standard
atomic weight



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57 La lanthanum 138.91 ± 0.01	58 Ce cerium 140.12 ± 0.01	59 Pr praseodymium 140.91 ± 0.01	60 Nd neodymium 144.24 ± 0.01	61 Pm promethium [145]	62 Sm samarium 150.36 ± 0.02	63 Eu europium 151.96 ± 0.01	64 Gd gadolinium 157.25 ± 0.03	65 Tb terbium 158.93 ± 0.01	66 Dy dysprosium 162.50 ± 0.01	67 Ho holmium 164.93 ± 0.01	68 Er erbium 167.26 ± 0.01	69 Tm thulium 168.93 ± 0.01	70 Yb ytterbium 173.05 ± 0.02	71 Lu lutetium 174.97 ± 0.01
89 Ac actinium [227]	90 Th thorium 232.04 ± 0.01	91 Pa protactinium 231.04 ± 0.01	92 U uranium 238.03 ± 0.01	93 Np neptunium [237]	94 Pu plutonium [244]	95 Am americium [243]	96 Cm curium [247]	97 Bk berkelium [247]	98 Cf californium [251]	99 Es einsteinium [252]	100 Fm fermium [257]	101 Md mendelevium [258]	102 No nobelium [259]	103 Lr lawrencium [262]

For notes and updates to this table, see www.iupac.org. This version is dated 4 May 2022.
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Table A.18 Margules, van Laar, Wilson, NRTL and UNIQUAC parameters for some selected binary systems*

S.No.	System	Temperature range (°C)	Margules		van Laar	
			A_{12}	A_{21}	A	B
1.	Acetaldehyde(1)/Benzene(2)	20.80 – 80.10	0.5028	-0.4772	0.5022	0.0889
2.	Acetaldehyde(1)/Ethanol(2)	5.80 – 62.80	-2.1035	-0.0792	-21.4912	-0.6377
3.	Acetone(1)/Benzene(2)	56.18 – 80.10	0.5176	0.3283	0.5337	0.3379
4.	Acetone(1)/Chloroform(2)	57.00 – 64.50	-1.0482	-0.6055	-1.1050	-0.6579
5.	Acetone(1)/Methanol(2)	55.70 – 62.80	0.2980	0.7142	0.3624	0.7900
6.	Acetone(1)/2-propanol(2)	56.78 – 79.78	0.5136	0.6323	0.5207	0.6319
7.	Acetone(1)/Toluene(2)	58.71 – 88.28	0.3913	0.5890	0.4184	0.5954
8.	1-Butanol(1)/Benzene(2)	81.00 – 109.20	0.7334	1.3305	0.7925	1.4530
9.	Carbon disulfide(1)/Methanol(2)	37.70 – 58.80	2.5978	1.8151	2.6062	1.8569
10.	Carbon tetrachloride(1)/Ethanol(2)	63.88 – 74.82	1.6358	1.9486	1.6211	2.0534
11.	Carbon tetrachloride(1)/1-propanol(2)	73.10 – 97.16	1.1535	1.9768	1.2189	2.0547
12.	Chloroform(1)/Methanol(2)	53.50 – 63.00	0.8320	1.7365	0.9356	1.8860
13.	Ethanol(1)/Acetic acid(2)	76.80 – 115.80	-0.2389	0.0091	-0.2586	-0.0866
14.	Ethanol(1)/Benzene(2)	67.90 – 76.90	1.8362	1.4717	1.8570	1.4785
15.	Ethanol(1)/Ethyl acetate(2)	72.20 – 76.50	0.9417	0.6640	0.9482	0.6925
16.	Ethanol(1)/2-propanol(2)	78.80 – 81.90	0.0382	-0.0510	-0.0080	1066.0345
17.	Ethanol(1)/Toluene(2)	77.00 – 110.60	1.6485	1.5707	1.6506	1.5702
18.	Methanol(1)/Benzene(2)	58.02 – 70.67	2.1411	1.7950	2.1623	1.7925
19.	Methanol(1)/Carbon tetrachloride(2)	55.65 – 76.10	2.3187	1.9027	2.3265	1.9118
20.	Methanol(1)/Ethanol(2)	65.80 – 77.00	0.0342	0.0130	0.0415	0.0155
21.	Methanol(1)/Ethyl acetate(2)	62.10 – 74.80	1.0178	1.0194	1.0172	1.0200
22.	Methanol(1)/Hexane(2)	49.90 – 63.50	2.9377	2.6151	3.0091	2.5961
23.	Methanol(1)/2-propanol(2)	67.45 – 79.38	0.0122	-0.1767	0.0446	0.0006
24.	Methanol(1)/Toluene(2)	63.58 – 70.25	1.9535	2.0385	1.9492	2.0425
25.	1-propanol(1)/Chlorobenzene(2)	95.90 – 117.00	1.1172	1.2587	1.1239	1.2586
26.	2-propanol(1)/Benzene(2)	71.70 – 82.26	1.7688	1.1250	1.8432	1.1722
27.	Toluene(1)/1-Butanol(2)	105.50 – 117.70	0.8533	1.2440	0.8813	1.2749

Contd.

Table A.18 Contd.

S.No.	Wilson		$(g_{12} - g_{22})$ J/mol K	NRTL $(g_{21} - g_{11})$ J/mol K	α_{12}	UNIQUAC	
	$(\lambda_{12} - \lambda_{11})$ J/mol K	$(\lambda_{12} - \lambda_{22})$ J/mol K				$(u_{12} - u_{22})$ J/mol K	$(u_{21} - u_{11})$ J/mol K
1.	5387.4244	-3233.5215	-10900.744	15354.5500	0.0653	815.9046	-793.2959
2.	5594.2535	-4857.4296	-1530.2122	-828.5762	9.1690	-3443.8432	3886.3133
3.	2722.4615	-1108.2453	-1180.6603	2871.7430	0.3015	-1293.6830	2087.8892
4.	839.0968	-2612.2876	-4262.4660	3520.1499	0.2870	-2179.0099	1922.1887
5.	-2562.1897	4926.7649	4095.4955	-1665.6244	0.3029	3510.2054	-1420.9118
6.	599.2075	1177.8223	1479.4023	251.5163	0.3007	500.6674	196.0792
7.	1024.1957	618.1428	2157.3676	-501.3756	0.2994	273.9785	132.8507
8.	383.6764	3997.7945	4759.9604	-565.8629	0.2901	1635.1110	-420.8755
9.	4800.0029	3639.4597	-2564.4625	9761.7017	0.0737	1445.3084	3015.5251
10.	605.9523	9981.7797	9356.9494	3346.3882	0.5143	3676.1828	-397.4319
11.	738.3838	5759.4453	4951.1033	1263.8452	0.4109	3133.4394	-671.3736
12.	-1513.4945	7086.6110	5708.7525	-562.0585	0.2932	5294.1251	-1147.0709
13.	824.6991	-1109.7856	-1228.5620	875.4718	0.2992	-680.7241	511.8770
14.	5289.4975	1115.3171	1625.1619	4016.9799	0.2910	-241.2287	2799.5827
15.	3879.3724	-1082.5887	-149.8650	2891.0351	0.2979	-1014.9430	2742.0398
16.	334.9217	-335.6257	503.5196	-512.9642	0.3040	-1467.0038	2011.3449
17.	5316.4284	972.5993	2269.0755	3231.3457	0.2937	-408.1366	2922.5299
18.	6971.2226	950.4985	3291.9421	4619.3371	0.4790	-226.3266	4651.0615
19.	7365.2623	871.1722	2101.3461	4944.3289	0.2400	-195.8914	5346.9635
20.	2122.5512	-1892.9692	-1292.6631	1579.9663	0.3053	-758.3737	1034.8543
21.	4241.7110	-883.5284	1428.2635	1695.9190	0.2977	-617.4522	3236.1603
22.	12630.4310	1912.1220	5387.1709	8011.3450	0.4240	-132.8089	7653.0336
23.	586.3614	555.1457	918.4895	-1049.9924	0.3047	-1558.3433	2332.5131
24.	7677.1579	1097.1060	4149.5839	5155.2885	0.5073	-202.7943	4684.1004
25.	2994.3016	1498.8530	2387.4984	1737.5424	0.2946	315.0247	924.2880
26.	5143.2615	820.0536	396.9232	4955.1419	0.2893	-447.0592	2424.2567
27.	300.4613	3933.1705	3946.7729	75.4897	0.2954	1896.3543	-665.0041

* Compiled from Gmehling, J. and Onken, U., "Vapor-Liquid Equilibrium Data Collection", DECHEMA Chemistry Data Series, Vol. I (1977).

Shankar

Table A.19 *UNIQUAC/UNIFAC group volume (R_k) and surface area (Q_k) parameters**

Main Group	Sub group	No.	R_k	Q_k	Sample Group Assignment	
*CH ₂ *	CH ₃	1	0.9011	0.348	Hexane:	2 CH ₃ , 4 CH ₂
	CH ₂	2	0.6744	0.540		
	CH	3	0.4469	0.228	2-Methylpropane:	3 CH ₃ , 1 CH
	C	4	0.2195	0.000	Neopentane:	4 CH ₃ , 1 C
C=C	CH ₃ =CH	5	1.3454	1.176	Hexene-1:	1 CH ₃ , 3 CH ₂ , 1 CH ₂ =CH
	CH=CH	6	1.1167	0.867	Hexene-2:	2 CH ₃ , 2 CH ₂ , 1 CH=CH
	CH ₂ =C	7	1.1173	0.988	2-Methyl-1-butene:	2 CH ₃ , 1 CH ₂ , 1 CH ₂ =C
	CH=C	8	0.8886	0.676	2-Methyl-2-butene:	2 CH ₃ , 1 CH=C
	C=C	70	0.6605	0.485	2,3-Dimethylbutene:	4 CH ₃ , 1 C=C
ACH	ACH	9	0.5313	0.400	Naphthalene:	8 ACH, 2 AC
	AC	10	0.3652	0.120	Styrene:	1 CH ₂ =CH, 5 ACH, 1 AC
*ACCH ₂ *	ACCH ₃	11	1.2663	0.968	Toluene:	5 ACH, 1 ACCH ₃
	ACCH ₂	12	1.0396	0.660	Ethylbenzene:	1 CH ₃ , 5 ACH, 1 ACCH ₂
	ACCH	13	0.8121	0.348	Cumene:	2 CH ₃ , 5 ACH, 1 ACCH
OH	OH	14	1.0000	1.200	Propanol-2:	2 CH ₃ , 1 CH, 1 OH
CH ₂ OH	CH ₂ OH	15	1.4311	1.432	Methanol:	1 CH ₂ OH
H ₂ O	H ₂ O	16	0.9200	1.400	Water:	1 H ₂ O
ACOH	ACOH	17	0.8952	0.680	Phenol:	5 ACH, 1 ACOH
CH ₂ CO	CH ₃ CO	18	1.6724	1.488	Butanone:	1 CH ₃ , 1 CH ₂ , 1 CH ₃ CO
	CH ₂ CO	19	1.4457	1.180	Pentanone-3:	2 CH ₃ , 1 CH ₂ , 1 CH ₂ CO
CHO	CHO	20	0.9980	0.948	Propionic aldehyde:	1 CH ₃ , 1 CH ₂ , 1 CHO
CCOO	CH ₃ COO	21	1.9031	1.728	Butyl acetate:	1 CH ₃ , 3 CH ₂ , 1 CH ₃ COO
	CH ₂ COO	22	1.6764	1.420	Methyl propionate:	2 CH ₃ , 1 CH ₂ COO
HCOO	HCOO	23	1.2420	1.188	Ethyl formate:	1 CH ₃ , 1 CH ₂ , 1 HCOO
CH ₂ O	CH ₃ O	24	1.1450	1.088	Dimethyl ether:	1 CH ₃ , 1 CH ₃ O
	CH ₂ O	25	0.9183	0.780	Diethyl ether:	2 CH ₃ , 1 CH ₂ , 1 CH ₂ O
	CHO	26	0.6908	0.468	Diisopropyl ether:	4 CH ₃ , 1 CH, 1 CHO
	THF	27	0.9183	1.100	Tetrahydrofuran:	3 CH ₂ , 1 THF
*CNH ₂ *	CH ₂ NH ₂	28	1.5959	1.544	Methylamine:	1 CH ₂ NH ₂
	CH ₂ NH ₂	29	1.3692	1.236	Ethylamine:	1 CH ₃ , 1 CH ₂ NH ₂
	CHNH ₂	30	1.1417	0.924	Isopropylamine:	2 CH ₃ , 1 CHNH ₂
CNH	CH ₃ NH	31	1.4337	1.244	Dimethylamine:	1 CH ₃ , 1 CH ₃ NH
	CH ₂ NH	32	1.2070	0.936	Diethylamine:	2 CH ₃ , 1 CH ₂ , 1 CH ₂ NH
	CHNH	33	0.9795	0.624	Diisopropylamine:	4 CH ₂ , 1 CH, 1 CHNH
(C)3N	CH ₃ N	34	1.1865	0.940	Trimethylamine:	2 CH ₃ , 1 CH ₃ N
	CH ₂ N	35	0.9597	0.632	Triethylamine:	3 CH ₃ , 2 CH ₂ , 1 CH ₂ N
*ACNH ₂ *	ACNH ₂	36	1.0600	0.816	Aniline:	5 ACH, 1 ACNH ₂
Pyridine	C ₅ H ₅ N	37	2.9993	2.113	Pyridine:	1 C ₅ H ₅ N
	C ₅ H ₄ N	38	2.8332	1.833	2-Methylpyridine:	1 CH ₃ , 1 C ₅ H ₄ N
	C ₅ H ₃ N	39	2.6670	1.553	2,3-Dimethylpyridine:	2 CH ₃ , 1 C ₅ H ₃ N
CCN	CH ₃ CN	40	1.8701	1.724	Acetonitrile:	1 CH ₃ CN
	CH ₂ CN	41	1.6434	1.416	Propionitrile:	1 CH ₃ , 1 CH ₂ CN
COOH	COOH	42	1.3013	1.224	Acetic acid:	1 CH ₃ , 1 COOH
	HCOOH	43	1.5280	1.532	Formic acid:	1 HCOOH

Contd.

Table A.19 Contd.

Main Group	Sub group	No.	R_k	Q_k	Sample Group Assignment
21 "CCl"	CH ₂ Cl	44	1.4654	1.264	Butane-1-chloro: 1 CH ₃ , 2 CH ₂ , 1 CH ₂ Cl
	CHCl	45	1.2380	0.952	
	CCl	46	1.0106	0.724	
22 "CCl ₂ "	CH ₂ Cl ₂	47	2.2564	1.998	2-Methylpropane-2-chloro: 3 CH ₃ , 1 CCl
	CHCl ₂	48	2.0606	1.684	
	CCl ₂	49	1.8016	1.448	
23 "CCl ₃ "	CHCl ₃	50	2.8700	2.410	Methane-dichloro: 1 CH ₂ Cl ₂
	CCl ₃	51	2.6401	2.184	
24 "CCl ₄ "	CCl ₄	52	3.3900	2.910	Ethane-1,1-Dichloro: 1 CH ₃ , 1 CHCl ₂
	CCl ₄	53	1.1562	0.844	
25 "ACCl"	ACCl	53	1.1562	0.844	Benzene-tetrachloro: 1 CCl ₄
	CH ₃ NO ₂	54	2.0086	1.868	
	CH ₂ NO ₂	55	1.7818	1.560	
26 "CNO ₂ "	CHNO ₂	56	1.5544	1.248	Propane-1-nitro: 1 CH ₃ , 1 CH ₂ , 1 CH ₂ NO ₂
	CHNO ₂	57	1.4199	1.104	
27 "ACNO ₂ "	ACNO ₂	57	1.4199	1.104	Benzene-nitro: 5 ACH, 1 ACNO ₂
28 "CS ₂ "	CS ₂	58	2.0570	1.650	Carbon disulfide: 1 CS ₂
29 "CH ₃ SH"	CH ₃ SH	59	1.8770	1.676	Methanethiol: 1 CH ₃ SH
	CH ₂ SH	60	1.6510	1.368	
30 "Furfural"	Furfural	61	3.1680	2.484	Ethanethiol: 1 CH ₃ , 1 CH ₂ SH
31 "DOH"	DOH	62	2.4088	2.248	Furfural: 1 Furfural
32 "I"	I	63	1.2640	0.992	1,2-Ethanediol: 1 DOH
33 "Br"	Br	64	0.9492	0.832	Iodoethane: 1 CH ₃ , 1 CH ₂ , 1 I
	CH ≡ C	65	1.2920	1.088	
34 "C ≡ C"	C ≡ C	66	1.0613	0.784	Bromoethane: 1 CH ₃ , 1 CH ₂ , 1 Br
	DMSO	67	2.8266	2.472	
35 "DMSO"	DMSO	67	2.8266	2.472	Hexyne-1: 1 CH ₃ , 3 CH ₂ , 1 CH ≡ C
36 "ACRY"	Acrylnitril	68	2.3144	2.052	Hexyne-2: 2 CH ₃ , 2 CH ₂ , 1 C ≡ C
	Cl - (C = C)	69	0.7910	0.724	
37 "ClCC"	Cl - (C = C)	69	0.7910	0.724	Dimethylsulfoxide: 1 DMSO
38 "ACF"	ACF	71	0.6948	0.524	Acrylnitrile: 1 Acrylnitril
	DMF	72	3.0856	2.736	
39 "DMF"	HCON(CH ₂) ₂	73	2.6322	2.120	Ethene-trichloro: 1 CH = C, 3 Cl - (C = C)
	CF	74	1.4060	1.380	
40 "CF ₂ "	CF ₂	75	1.0105	0.920	Hexafluorobenzene: 6 ACF
	CF	76	0.6150	0.460	
	CF	76	0.6150	0.460	
41 "COO"	COO	77	1.3800	1.200	N,N-Dimethylformamide: 1 DMF
	SiH ₃	78	1.6035	1.263	
	SiH ₂	79	1.4443	1.006	
	SiH	80	1.2853	0.749	
	Si	81	1.0470	0.410	
42 "SiH ₂ "	SiH ₂	80	1.2853	0.749	N,N-Diethylformamide: 2 CH ₃ , 1 HCON(CH ₂) ₂
	SiH	81	1.0470	0.410	
	Si	82	1.4838	1.062	
	SiH ₂ O	83	1.3030	0.764	
43 "SiO"	SiHO	83	1.3030	0.764	Perfluorohexane: 2 CF ₃ , 4 CF ₂
	SiO	84	1.1044	0.466	
	SiO	84	1.1044	0.466	
44 "NMP"	NMP	85	3.9810	3.200	Perfluoromethylcyclohexane: 1 CF ₃ , 5 CF ₂ , 1 CF
	NMP	85	3.9810	3.200	

Contd.

Table A.19 <i>Contd.</i>		No.	R_k	Q_k	Sample Group Assignment	
Main Group	Sub group					
45 "CClF"	CCl ₃ F	86	3.0356	2.644	Trichlorofluoromethane: 1 CCl ₃ F	
	CCl ₂ F	87	2.2287	1.916	Tetrachloro-1,2-difluoroethane: 2 CCl ₂ F	
	HCCl ₂ F	88	2.4060	2.116	Dichlorofluoromethane: 1 HCCl ₂ F	
	HCClF	89	1.6493	1.416	1-Chloro-1,2,2,2-tetrafluoroethane: 1 CF ₃ , 1 HCClF	
	CClF ₂	90	1.8174	1.648	1,2-Dichlorotetrafluoroethane: 2 CClF ₂	
	HCClF ₂	91	1.9670	1.828	Chlorodifluoromethane: 1 HCClF ₂	
	CClF ₃	92	2.1721	2.100	Chlorotrifluoromethane: 1 CClF ₃	
	CCl ₂ F ₂	93	2.6243	2.376	Dichlorodifluoromethane: 1 CCl ₂ F ₂	
	46 "CON"	CONH ₂	94	1.4515	1.248	Acetamid: 1 CH ₃ , 1 CONH ₂
		CONHCH ₃	95	2.1905	1.796	N-Methylacetamid: 1 CH ₃ , 1 CONHCH ₃
CONHCH ₂		96	1.9637	1.488	N-Ethylacetamid: 2 CH ₃ , 1 CONHCH ₂	
CON(CH ₃) ₂		97	2.8589	2.428	N,N-Dimethylacetamid: 1 CH ₃ , 1 CON(CH ₃) ₂	
CONCH ₃ CH ₂		98	2.6322	2.120	N,N-Methylethylacetamid: 2 CH ₃ , 1 CONCH ₃ CH ₂	
CON(CH ₂) ₂		99	2.4054	1.812	N,N-Diethylacetamid: 3 CH ₃ , 1 CON(CH ₂) ₂	
47 "OCCOH"	C ₂ H ₅ O ₂	100	2.1226	1.904	2-Ethoxyethanol: 1 CH ₃ , 1 CH ₂ , 1 C ₂ H ₅ O ₂	
	C ₂ H ₄ O ₂	101	1.8952	1.592	2-Ethoxy-1-propanol: 2 CH ₃ , 1 CH ₂ , 1 C ₂ H ₄ O ₂	
48 "CH ₂ S"	CH ₃ S	102	1.6130	1.368	Dimethylsulfide: 1 CH ₃ , 1 CH ₃ S	
	CH ₂ S	103	1.3863	1.060	Diethylsulfide: 2 CH ₃ , 1 CH ₂ , 1 CH ₂ S	
	CHS	104	1.1589	0.748	Diisopropylsulfide: 4 CH ₃ , 1 CH, 1 CHS	
49 "morpholine"	MORPH	105	3.4740	2.796	Morpholine: 1 MORPH	
50 "thiophene"	C ₄ H ₄ S	106	2.8569	2.140	Thiophene: 1 C ₄ H ₄ S	
	C ₄ H ₃ S	107	2.6908	1.860	2-Methylthiophene: 1 CH ₃ , 1 C ₄ H ₃ S	
	C ₄ H ₂ S	108	2.5247	1.580	2,3-Dimethylthiophene: 2 CH ₃ , 1 C ₄ H ₂ S	

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