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APPENDIX A
PROPERTY DATA BANK

The following tables is listing of the component currently available in database system. The data of component receive from reference data(Ried R.C and et al., 1987) and Sinnott R.K., 1983). Tables consist of five groups of compounds as follows:

1. HYDROCARBON

1.1. PARAFINS

Number	Formula	Compound name
1	CH ₄	Methane
2	C ₂ H ₆	Ethane
3	C ₃ H ₈	Propane
4	C ₄ H ₁₀	Isobutane
5	C ₄ H ₁₀	N-butane
6	C ₅ H ₁₂	N-pentane
7	C ₆ H ₁₄	N-hexane
8	C ₇ H ₁₆	N-heptane
9	C ₈ H ₁₈	N-octane
10	C ₉ H ₂₀	N-nonane
11	C ₉ H ₂₂	N-decane

1.2. AKYL PARAFINS

Number	Formula	Compound name
1	C ₅ H ₁₂	2,2-dimethylpropane
2	C ₆ H ₁₄	2-methylpentane
3	C ₆ H ₁₄	3-methylpentane
4	C ₆ H ₁₄	2,2-dimethylbutane
5	C ₆ H ₁₄	2,3-dimethylbutane
6	C ₇ H ₁₆	2-methylhexane
7	C ₇ H ₁₆	3-methylhexane
8	C ₇ H ₁₆	3-ethylpentane
9	C ₇ H ₁₆	2,2-dimethylpentane
10	C ₇ H ₁₆	2,4-dimethylpentane
11	C ₇ H ₁₆	3,3-dimethylpentane
12	C ₇ H ₁₆	2,2,3-trimethylbutane
13	C ₈ H ₁₈	2-methylheptane
14	C ₈ H ₁₈	3-methylheptane
15	C ₈ H ₁₈	4-methylheptane
16	C ₈ H ₁₈	2,2-dimethylhexane
17	C ₈ H ₁₈	2-methyl-3-ethylpentane
18	C ₈ H ₁₈	3-methyl-3-ethylpentane
19	C ₈ H ₁₈	2,2,3-trimethylpentane
20	C ₈ H ₁₈	2,2,4-trimethylpentane

1.3 CYCLOPARAFINS

Number	Formula	Compound name
1	C ₂ H ₆	Cyclopropane
2	C ₄ H ₈	Cyclobutane
3	C ₅ H ₁₀	Cyclopentane
4	C ₆ H ₁₂	Cyclohexane
5	C ₆ H ₁₂	Methylcyclopentane
6	C ₇ H ₁₄	Methylcyclohexane
7	C ₇ H ₁₄	Ethylcyclopentane
8	C ₇ H ₁₄	1,1-dimethylcyclopentane
9	C ₇ H ₁₄	Cycloheptane
10	C ₈ H ₁₆	Ethylcyclohexane

1.4 AROMATICS

Number	Formula	Compound name
1	C ₆ H ₆	Benzene
2	C ₇ H ₈	Toluene
3	C ₈ H ₁₀	Ethylbenzene
4	C ₈ H ₁₀	o-Xylene
5	C ₈ H ₁₀	m-Xylene
6	C ₈ H ₁₀	p-Xylene
7	C ₈ H ₈	Styrene
8	C ₉ H ₁₂	N-propylbenzene
9	C ₉ H ₁₂	1-methyl-2-ethylbenzene
10	C ₉ H ₁₂	1-methyl-3-ethylbenzene
11	C ₉ H ₁₂	1-methyl-4-ethylbenzene
12	C ₁₀ H ₈	Napthalene

1.5 OLEFINS

Number	Formula	Compound name
1	C ₂ H ₄	Ethylene
2	C ₃ H ₆	Propene
3	C ₃ H ₄	Propadiene
4	C ₄ H ₆	1,2-Butadiene
5	C ₄ H ₆	1,3-Butadiene
6	C ₄ H ₈	1-Butene
7	C ₄ H ₈	Isobutylene
8	C ₅ H ₈	1,2-Pentadiene
9	C ₅ H ₈	3-methyl-1,2-butadiene
10	C ₅ H ₁₀	1-Pentene
11	C ₆ H ₁₂	1-Hexene
12	C ₆ H ₁₂	cis-2-Hexene
13	C ₆ H ₁₂	trans-2-Hexene
14	C ₇ H ₁₄	1-Heptene
15	C ₈ H ₁₆	1-Octene
16	C ₁₀ H ₂₀	1-Decene

1.6 ACETYLENE

Number	Formula	Compound name
1	C ₂ H ₂	Acetylene
2	C ₂ H ₄	Ethylene
3	C ₄ H ₄	Vinylacetylene
4	C ₄ H ₆	1-Butyne
5	C ₄ H ₆	2-Butyne
6	C ₅ H ₈	1-Pentyne

2. INORGANICS COMPOUND

Number	Formula	Compound name
1	N ₂	Nitrogen
2	CO ₂	Carbondioxide
3	H ₂ S	Hydrogen sulfide
4	H ₂ O	Water
5	H ₂	Hydrogen
6	CO	Carbonmonoxide
7	Ar	Argon
8	NH ₃	Ammonia
9	O ₂	Oxygen
10	COS	Carbonyl sulfide
11	He	Helium
12	CS ₂	Carbon disulfide
13	Cl ₂	Chlorine
14	F ₂	Fluorine
15	NO	Nitric oxide
16	NO ₂	Nitrogen dioxide
17	N ₂ O	Nitrous oxide
18	O ₃ S	Sulfur trioxide
19	Br ₂	Bromine
20	I ₂	Iodine
21	SO ₂	Sulfur dioxide
22	BCl ₃	Boron trichloride
23	D ₂	Deuterium
24	Ne	Neon
25	O ₃	Ozone
26	Xe	Xenon
27	HCN	Hydrogen cyanide

3. ALCOHOLS

Number	Formula	Compound name
1	CH ₄ O	Methanol
2	C ₂ H ₆ O	Ethanol
3	C ₃ H ₈ O	1-Propanol
4	C ₃ H ₈ O	Isopropyl alcohol
5	C ₄ H ₁₀ O	N-Butanol
6	C ₄ H ₁₀ O	2-Butanol
7	C ₄ H ₁₀ O	i-Butanol
8	C ₅ H ₁₂ O	1-Pentanol
9	C ₆ H ₁₄ O	1-Hexanol
10	C ₇ H ₁₆ O	1-Heptanol
11	C ₈ H ₁₈ O	1-Octanol

4. HALOGENATED HYDROCARBON

Number	Formula	Compound name
1	CCl ₄	Carbontetrachloride
2	CHCl ₃	Chloroform
3	C ₂ H ₅ Cl	Ethyl chloride
4	C ₃ H ₇ Cl	Propyl chloride
5	C ₄ H ₉ Cl	1-Chlorobutane
6	C ₄ H ₉ Cl	2-Chlorobutane
7	C ₆ H ₅ Cl	Chlorobenzene
8	CF ₄	Carbon tetrafluoride
9	C ₂ H ₃ Cl	Vinyl chloride
10	CH ₃ F	Methyl fluoride
11	CH ₂ F ₂	Difluoromethane
12	C ₂ F ₄	Perfluoroethane
13	C ₆ H ₅ F	Fluorobenzene

5. MISCELLANEOUS COMPOUNDS

Number	Formula	Compound name
1	CH ₅ N	Methyl amine
2	C ₂ H ₇ N	Ethyl amine
3	C ₃ H ₉ N	N-Propyl amine
4	C ₃ H ₉ N	Isopropyl amine
5	C ₄ H ₉ N	Pyrrolidine
6	C ₅ H ₅ N	Pyridine
7	C ₆ H ₇ N	Aniline
8	C ₃ H ₆ O	Acetone
9	C ₂ H ₂ O	Ketone
10	CH ₂ O	Formaldehyde
11	C ₂ H ₄ O	Acetaldehyde
12	C ₂ H ₄ O ₂	Methyl formate
13	C ₃ H ₆ O ₂	Ethyl formate
14	HCl	Hydrogen chloride
15	HF	Hydrogen fluoride
16	HBr	Hydrogen bromide
17	HI	Hydrogen iodide
18	C ₂ H ₄ O ₂	Acetic acid
19	C ₇ H ₆ O ₂	Benzoic acid
20	C ₂ H ₃ N	Acetonitrile
21	C ₃ H ₃ N	Acrylonitrile
22	C ₃ H ₅ N	Propionitrile
23	CH ₃ NO ₂	Nitromethane
24	C ₆ H ₆ O	Phenol

VITA

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