

LABORATORIUM KIMIA FISIKA
Jurusan Kimia - FMIPA
Universitas Gadjah Mada (UGM)

MATEMATIKA KIMIA

Informasi Kuliah

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INFORMASI KULIAH

Judul kuliah : Matematika Kimia
Kode : MKK-2701
SKS : 2 SKS
Sifat : Wajib
Jadwal : Jumat, jam 09.30-11.10 di ruang K6
Dosen : 1. Dr. Ria Armunanto, M.Si / Dr Ahmad Syoufian (kelas A)
2. Prof. Dr. Karna Wijaya (kelas B)
3. Drs. Iqmal Tahir, M.Si. (kelas C)

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MANAJEMEN WAKTU KULIAH

KALENDER AKADEMIK SEMESTER I TA. 2014/2015

No	Tanggal	Kegiatan
1	18 Agustus 2014 - 20 Agustus 2014	Registrasi dan KRS Mahasiswa Lama
2	21 Agustus 2014	Pengumuman Matakuliah yang tidak terakreditasi
3	21 Agustus 2014 - 22 Agustus 2014	Perubahan KRS & Key in Perubahan Matakuliah yang tidak terakreditasi
4	25 Agustus 2014 - 19 Desember 2014	Kuliah/Praktikum/Ujian Skripsi
5	29 September 2014 - 10 Oktober 2014	Pengambilan Kartu Ujian Tengah Semester
6	13 Oktober 2014 - 25 Oktober 2014	Ujian Tengah Semester
7	15 Desember 2014 - 26 Desember 2014	Pengambilan Kartu Ujian Akhir Semester
8	22 Desember 2014 - 26 Desember 2014	Minggu Tenang
9	29 Desember 2014 - 10 Januari 2015	Ujian Akhir Semester
10	12 Januari 2015 - 6 Februari 2015	Sibar Semester/Pengumuman Hasil Ujian (PHU)

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MATEMATIKA KIMIA

Kuliah Matematika Kimia bukan untuk menggantikan matakuliah kalkulus, tetapi memberikan bekal konsep dan terapan matematika guna penyelesaian masalah dalam bidang kimia khususnya kimia fisika.

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CONTOH PERSAMAAN MATEMATIKA DALAM KIMIA

Straight Line Equation $y = mx + c$

Wave Nature of Light $c = \lambda \nu$

Concentration of Molecules $c = \frac{n}{V}$

Chemical Equilibrium $K = \frac{[C]^c [D]^d}{[A]^a [B]^b}$

Enthalpy of Reaction and Temperature $H_2 - H_1 = C_p(T_2 - T_1)$

Kinetics of a Complex Chemical Reaction $v = \frac{k[H_2][Br_2]^{1/2}}{[Br_2] + k'[HBr]}$

The van der Waals Equation $\left(p + \frac{a}{V^2}\right)(V - nb) = nRT$

Vapour Pressure of a Liquid $\ln\left(\frac{p_2}{p_1}\right) = \frac{\Delta H_{vap}}{R} \left(\frac{1}{T_1} - \frac{1}{T_2}\right)$

Kinetics of a Second-Order Chemical Reaction $\frac{1}{a_0 - x} \ln \frac{b_0 - x}{b_0 - a_0}$

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CONTOH PERSAMAAN MATEMATIKA DALAM KIMIA

Binomial Formula $\binom{n}{k} = \frac{n!}{k!(n-k)!}$

Photons of Light $E = h\nu$

Rates of Chemical Reactions and Concentrations $v_{total} = \frac{k[A]^a [B]^b}{[C]}$

Lattice Enthalpy of an Ionic Crystal

$$\Delta H_{lattice}^{\circ} = -\Delta H_{ionization}^{\circ} + \Delta H_{electron affinity}^{\circ} + \frac{1}{2} \Delta H_{dissociation}^{\circ} + \Delta H_{ionization}^{\circ} + \Delta H_{electron affinity}^{\circ}$$

Lindemann's Treatment of Unimolecular Reaction $k_1[A] - k_2[A^*][A] - k_3[A^*] = 0$

Enthalpy of Combustion of Benzene

$$\Delta H_{comb}^{\circ} = 6 \Delta H_f^{\circ}(CO_2) + 3 \Delta H_f^{\circ}(H_2O) - \left(\Delta H_f^{\circ}(C_6H_6) + \frac{15}{2} \Delta H_f^{\circ}(O_2) \right)$$

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Rydberg Equation $\nu = R_{\infty} \left(\frac{1}{n_1} - \frac{1}{n_2} \right)$

Equilibrium Constant and Concentrations $K = \frac{[H]^{21}}{[H_2][I_2]} = 55.64$

Bragg Equation $n\lambda = 2d \sin(\theta)$

Polymer Random Coil $r^2 = N l^2 \frac{1 - \cos\theta}{1 + \cos\theta}$

Wavefunction for n -Electrons in a Linear Polyene Molecule $\psi = A \cos(kx) + B \sin(kx)$

Acidity Constant $K_a = \frac{[H_3O^+][CH_3COO^-]}{[CH_3COOH]}$

Synthesis of Ammonia $K = \frac{(P_{NH_3})^2}{P_{N_2}(P_{H_2})^3} = 977$

Quadratic Formula $x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$

Logarithms $\log_e(xy) = \log_e(x) + \log_e(y)$ $\log_e\left(\frac{x}{y}\right) = \log_e(x) - \log_e(y)$ $\log_e(x^n) = n \log_e(x)$

Natural Number and Power Series $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots$

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Acidity and Alkalinity $pH = -\log_{10}[H^+]$ $pOH = -\log_{10}[OH^-]$

Henderson-Hasselbalch Equation $pH = pK_a + \log\left(\frac{[base]}{[acid]}\right)$

First Order Kinetics $[A] = [A]_0 e^{-kt}$

Arrhenius Equation $k = A e^{-\left(\frac{E_a}{RT}\right)}$

Nernst Equation $E = E^\circ - \frac{RT}{nF} \ln\left(\frac{[redox]}{[oxidant]}\right)$


Gibbs Free Energy $\Delta G^\circ = -RT \ln(K)$

Experimental Determining of the Order of a Chemical Reaction $v = k [H_2]^m$ $\log(v) = \log(k) + m \log[H_2]$

Temperature Variation of Vapour Pressure $\ln(p) = -\frac{\Delta H_{vap}}{RT} + K$

Maxwell-Boltzmann Distribution of Speeds of Gas Molecules $f(v) = 4\pi \left(\frac{M}{2\pi RT}\right)^{3/2} v^2 e^{-\left(\frac{Mv^2}{2RT}\right)}$

Differential of the Maxwell-Boltzmann Equation and the Most Probable Speed $v_{mp} = \left(\frac{2RT}{M}\right)^{1/2}$

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Lennard Jones Equation $V = -4\epsilon \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right)$

Consecutive Chemical Reactions $[B] = [A]_0 \frac{k_1}{k_2 - k_1} (e^{-k_1 t} - e^{-k_2 t})$

First-Order Reaction $\frac{d[A]}{dt} = -k[A]$


Second-Order Reaction $\frac{d[A]}{dt} = -k[A]^2$

Expanding Gas and Thermodynamic Work $w = -\int p \, dV$

Enthalpy of a Molecule and Temperature Changes $dH = (a + bT + cT^2) dT$

Quantum Mechanics of a Conjugated Polyene Molecule $\int_0^l B^2 \sin^2\left(\frac{n\pi x}{l}\right) dx = 1$

Hydrogen Atom Is Electron Radial Distribution Function $P = \frac{4}{a_0^3} r^2 e^{-\frac{2r}{a_0}}$


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MATERI KULIAH

Mata kuliah ini menyajikan materi matematika yang umum digunakan dalam ilmu kimia seperti :


- Fungsi
- Operator
- Integral
- fungsi variabel banyak
- Vektor
- Deret
- Matrik
- Determinan
- persamaan differensial
- analisis Fourier

Masing-masing sebagai alat untuk menjembatani mahasiswa dalam menganalisa dan menyelesaikan persoalan-persoalan dalam perkuliahan, terutama ketika menyelesaikan tugas akhir.

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SUPLEMEN KULIAH

- Aplikasi MS Excell untuk penyelesaian kasus perhitungan dan pemodelan numerik dalam bidang kimia
- Pemrograman komputer

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BUKU PEGANGAN

1. D. Hirst, 1976, Mathematics for Chemists, Dept. of Molecular Science, University of Warwick, Coventry
2. Robert G. Mortimer, 1999, Mathematic for Physical Chemistry, Edisi ke-2, Academic Press, California 92101-4495, USA
3. Boas, M. I., 1983, Mathematic Methods in the Physical Science, Edisi ke-2, John Wiley & Sons
4. J.R. Barrante, 1996, Applied Mathematics for Physical Chemistry, Prentice Hall.
5. R. G. Mortimer, 1999, Mathematics for Physical Chemistry, Academic Press

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