Analisis Molekular dan Karakteristik Hidrogen Sianida (HCN)

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- 1. Abstrak.** Hidrogen sianida dalam air membentuk asam lemah bersifat toksik. Tujuan review ini untuk menganalisis molekular dan transpor elektron hidrogen sianida. Metode yang digunakan adalah penggambaran molekul dengan aplikasi *Chem Office* versi 15.0, untuk mengetahui transpor ion asam sianida yaitu dengan parameter konduktivitas, viskositas, mobilitas ion, dan gerakan hanyut. Hasil yang didapat yaitu struktur molekul asam sianida pada analisis molekular 2D, dan bentuk molekul asam sianida dalam 3D. Berdasarkan metode ini diperoleh energi kinetik rotasi senyawa 2,0466 kcal/mol. Untuk konduktivitas, kecepatan hanyut, gerakan ion, dilakukan dengan menggunakan metode perhitungan dengan rumusan hasilnya dan beberapa soal yang dibuatkan grafiknya Analisis jari-jari atom hidrogen dengan carbon pada Chemdraw 3D didapatkan sebesar 1,1 Å, dan jari-jari atom carbon dengan nitrogen masing-masingnya sebesar 1,1 Å. Data yang didapat pada Analisa MM2 dynamics HCN adalah interaction time 0.024, 0.026, 0.028, 0.030, total energy 0.048, 0.082, potensial energy 0.38, 0.045, 0.016, 0.091. sifat dari asam sianida diantaranya massa molar 27,03 g/mol, densitas 0,687g/mL, viskositas : 201 µPa s. Sifat termodinamika hidrogen sianida adalah ΔG (energi Gibbs) 143,1 kJ/mol entropi (ΔS) 113,01 J/kmol, entalpi pembentukan standar ($\Delta_f H$) -141,2 kJ/mol, entalpi pembakaran standar ($\Delta_c H$) -426,5 kJ/mol dan kecepatan hanyut yang didapat berdasarkan perhitungan sebesar 2,33 V/cm.

Kata kunci : Asam sianida, transfer elektron

I. Pendahuluan

Asam sianida⁽¹⁻⁴⁰⁾ adalah senyawa kimia yang mengandung gugus siano $C \equiv N$ yang terikat dengan atom hidrogen^(7; 10; 26; 27; 32; 41-45), atom karbon terikat tiga ke atom nitrogen. Pada gugus CN sebagai ion sianida poliatomik yang bermuatan negatif (CN^-). Hidrogen Sianida salah satu senyawa yang sangat beracun. Anion CN^- bersifat isoelektronik jika berikatan dengan molekul nitrogen dan karbon monoksida.

Umumnya Sianida organik juga disebut nitril, dimana terdapat ikatan kovalen pada gugus CN dengan gugus, seperti metil ($-CH_3$) pada metil sianida (asetonitril). Pada umumnya nitril tidak melepas ion sianida maka bersifat tidak beracun, kecuali jika dibakar. Senyawa Asam^[203] Sianida merupakan cairan yang mudah menguap^[207].

Metode oksidasi Andrussow yang diciptakan oleh Leonid Andrussow menjelaskan proses pembuatan asam sianida (HCN) yang paling sering dilakukan menggunakan metode, yang diciptakan oleh Leonid Andrussow, dimana metana⁽¹⁵⁵⁻¹⁷⁴⁾, dan amonia bereaksi pada suhu^[206] sekitar 1200°C menggunakan katalis platina⁽¹⁷⁵⁻¹⁹⁴⁾, dengan reaksi sebagai berikut :

Energi yang dibutuhkan untuk reaksi ini berasal dari panas yang timbul akibat reaksi oksidasi parsial metana dan amonia.

Proses pembuatan HCN lainnya adalah proses Degussa (BMA proses) dimana tidak ada oksigen ditambahkan dan energi harus ditransfer secara tidak langsung melalui dinding reaktor, dengan reaksi sebagai berikut :

Asam hidrosianat (HCN) juga bisa diekstrak dari daun, bunga, atau umbi-umbian dari tanaman beracun yang memiliki *cyanohydrins*, dengan cara hidrolisis yang diikuti proses pengasaman dan penyulingan.

Sianida memiliki peran yang sangat penting dalam ekstraksi emas berukuran mikro dan nano batuan asalnya. Umumnya jenis sianida yang digunakan dalam proses ekstraksi emas⁽¹²⁸⁻¹⁵³⁾ adalah alkali sianida, yang bisa berupa senyawa NaCN atau KCN

Berdasarkan reaksi diatas, logam emas larut dalam ion sianida, membentuk anion kompleks $4\text{Na}[\text{Au}(\text{CN})_2]_{(l)}$. Larutan emas ini selanjutnya diadsorpsi menggunakan adsorbent karbon aktif atau granular resin (195-200) anion yang bisa dipisahkan dari lumpur melalui proses penyarigan partikel kasar. Disamping NaCN dan KCN, ion kompleks heksasianoferat III juga bisa digunakan sebagai oksidator dan pelarut emas dalam proses sianidasi. Senyawa ferri sianida dan ferrosianida memiliki tingkat toksik yang relatif rendah dibanding senyawa alkali sianida yang lain, disebabkan ikatan antara ion besi II dan besi III dan ion sianida yang jauh lebih kuat. Namun perubahan pH yang terjadi akibat naiknya konsentrasi ion hidrogen dalam larutan ferri atau ferro sianida dapat melepaskan senyawa hidrogen sianida yang beracun dari larutannya.

Prussian Blue atau zat kimia biru prussia merupakan pigmen biru tua dengan rumus kimia yang ideal $\text{Fe}_7(\text{CN})_{18}$. Prussian Blue dibuat dari reaksi kimia antara larutan alkali ferro-sianida dan larutan jenuh besi III klorida. Kombinasi dari ion ferri berasal dari larutan jenuh besi III klorida dan ion ferro sianida membentuk pigmen warna yang memiliki warna biru tua. Prussian Blue bersifat non-toksik (tidak beracun) dan justru digunakan sebagai obat.

Prussian Blue juga digunakan secara luas dalam berbagai bidang. Penggunaan terbesar dari pigmen ini adalah industri cat dan tinta cair, pembiru pakaian putih saat dibilas (blau). Prussian Blue juga digunakan sebagai obat bagi beberapa jenis keracunan logam berat, misalnya keracunan yang disebabkan oleh logam thallium dan isotop radioaktif cesium, untuk pengobatan keracunan.

II. Metode

Asam sianida secara makroskopik⁽⁷¹⁻⁷³⁾ berwujud cair. Untuk itu, pengkajian secara mikroskopik seperti bentuk molekul, karakteristik serta interaksi yang terjadi sangat dibutuhkan guna mengenalinya lebih dalam. Pada perolehan yang menggunakan literasi jurnal disitasi melalui aplikasi *EndNote* dan menghasilkan fishbone state of art. Pada analisa molekular, maka dilakukan metode komputasi⁽⁷⁴⁾ atau permodelan menggunakan aplikasi ChemOffice 15.0 dimana sub aplikasi yang digunakan yaitu ChemDraw professional 15.0 untuk molekul 2D dan Chem3D 15.0.

Pengolahan data dapat dilakukan melalui beberapa tahapan diantaranya:

- (1) Analisis molekul HCN secara dua dimensi menggunakan ChemDraw professional 15.0 2D;
- (2) Analisis molekul⁽⁷⁵⁾ secara tiga dimensi dengan ChemDraw professional 15.0 2D yang diproyeksikan pada Chem 3D. Permodelan ini dengan mengasumsikan pada satu molekul HCN dengan beberapa kemungkinan pergerakan dan vibrasional yang terjadi^(76; 77).

Molekul HCN mulanya digambarkan pada software dari ChemDraw professional 15.0 2D dengan cara klik *Structure*, pilih bagian bawah "*Convert Name to Structure*". Setelah itu muncul pada layar kerja, tulis boric acid, lalu pilih OK. Setelah rumus molekul terbentuk, lakukan analisis senyawa. Proses analisis dilakukan pada bagian *View*, dengan optional show analysis window dan show chemical properties windows.

Pada analisis molekul secara 3D dilakukan dengan merubah molekul 2D ke Chem 3D. Pada bagian Chem 3D, struktur HCN menjadi tiga dimensi dan dapat dianalisis keadaan sebelum optimasi dengan pilihan select, sesuai pengukuran dan observasi yang diinginkan.

Analisa molekular melalui aplikasi bertujuan untuk mengetahui bentuk molekul,⁽²²³⁻²²⁵⁾ jenis ikatan pada molekul, pergerakan molekul,⁽⁷⁸⁻⁸⁰⁾ energi yang dihasilkan molekul tersebut serta bagian-bagian lainnya yang tidak dapat diamati secara langsung oleh mata tanpa bantuan alat. Data yang diperoleh berupa gambar molekular 2D dan 3D. Selain itu, melalui ChemOffice 15.0 diperoleh optimasi MM2 pada HCN. Data yang diperoleh juga dimaksudkan untuk dibandingkan kesesuaiannya dengan literatur yang didapat.

Untuk pengolahan data secara fisika dilakukan metode perhitungan dengan rumusan hasilnya angka-angka dan simulasi beberapa soal yang dibuatkan grafiknya.

Berdasarkan sumber wikipedia sifat dari asam sianida diantaranya massa molar : 27,03 g/mol, penampilan : cairan transparan atau gas tak berwarna, densitas : 0,687g/mL, kelarutan dalam air : bercampur, viskositas : 201 μ Pa s.

III. Hasil dan Pembahasan

1. Result

Hidrogen sianida^(7; 10; 26; 27; 32; 46-60) atau biasa disebut formic anammonide, asam hidrosianat, atau asam sianida yang merupakan suatu monobasa dari asam Lewisboron lemah yang dapat digunakan sebagai penyepuhan emas, dan pembuatan pewarna prussian blue (blau),⁽¹⁰⁸⁾. Asam sianida akan larut dalam air^(109; 110), senyawa ini didalam air akan membentuk ion CN^- dan ion H^+ . Senyawa dengan rumus kimia HCN cairan tak berwarna dan sangat beracun. Asam sianida memiliki bentuk molekul⁽¹¹⁵⁾ linear⁽¹¹⁶⁻¹²⁰⁾ dengan momen dipol⁽¹²¹⁾ 2.98 D.

Tabel 1. Sifat Fisika dan Sifat Kimia Asam Borat

https://en.wikipedia.org/wiki/Hydrogen_cyanide

Sifat	
Massa molar	27.0253 g/mol
Titik lebur	-13.29 °C (8.08 °F; 259.86 K)
Titik didih	26 °C (79 °F; 299 K)
Densitas	0.6876 g cm ⁻³
Keasaman	9.21
Kebasaan	4,79

Densitas^(94; 125; 126) disebut juga dengan kerapatan merupakan massa per satuan volume suatu zat⁽²¹¹⁻²¹³⁾ pada suhu^(127; 128) tertentu dan tidak hanya ditentukan gaya interaksi antar molekul⁽²³¹⁻²³⁵⁾. Senyawa asam sianida memiliki sifat melarut sempurna pada air, dan sedikit larut dalam etanol. Ada beberapa faktor yang memengaruhi kelarutan suatu senyawa diantaranya sifat dari zat terlarut (solute)⁽¹³⁹⁻¹⁴³⁾ dan pelarut⁽¹⁴⁴⁾ (solvent)^(94; 129; 132; 145; 146) dimana zat terlarut yang bersifat polar⁽²¹⁴⁻²¹⁶⁾ akan mudah larut dalam solvent⁽²⁴³⁻²⁴⁶⁾ atau yang disebut pelarut yang bersifat polar, begitupun sebaliknya, disini berlaku asas *like dissolve like*. Suhu, konsentrasi,^(95; 139; 147-149) pengaruh penambahan ion senama⁽²³⁶⁻²³⁷⁾ juga sangat mempengaruhi kelarutan⁽²⁴⁷⁻²⁴⁹⁾ suatu senyawa.

2. Data Molekul HCN

Gambar 2. B(OH)_3 3D

https://id.wikipedia.org/wiki/Hidrogen_sianida

Stretch : 2.0466
Bend : 0.0000
Stretch-Bend : 0.0000
Torsion : 0.0000
Non-1,4 VDW : 0.0000
1,4 VDW : 0.0000
Total Energy : 2.0466 kcal/mol

Total energy for this frame: 2.047 kcal/mol

3. Analisa Molekul HCN

Analisa molekular bertujuan untuk mendapatkan data optimasi, energi dan gambar pada molekul HCN. Untuk memperoleh data pada analisa molekular ini digunakan metode komputasi menggunakan ChemOffice 15.0.

a. Analisa molekul 2D HCN

Pada tahap analisa molekul asam sianida secara 2D digunakan ChemDrawProfessional 15.0.

Dari analisa ini didapatkan gambar dan bentuk molekul seperti berikut:

Chemical Formula : CHN
Exact Mass : 27,01
Molecular Weight : 27,03
m/z : 27,01(100,0%)
Elemental Analysis : C,44,44 H, 3,73 N,51,83

b. Analisa molekul 3D HCN

Analisa molekul HCN menggunakan metode komputasi dibuat dengan *software* ChemDraw Professional 15.0 kemudian diproyeksikan pada ChemDraw 3D untuk dianalisis struktur tiga dimensinya. Proses ini memperlihatkan kepada kita bagaimana pola pergerakan molekul secara optimal dan bagaimana dinamika interaksi antara HCN dengan H₂O.

Gambar 3. Analisis 3D pada molekul HCN model Ball and Stick. (a) atom C(1) dan H(3)
(b) atom C(1) dan N(2) (Rahmadani,A. *ChemOffis* 2015)

Gambar 4. Analisis 3D pada molekul HCN model Ball and Stick. (a) molekul HCN terdiri dari atom H (bola putih), atom C (bola abu-abu), atom N (bola biru) (b) penampang girasi molekul HCN pada permukaan molekul pada sisi positif (merah) dan pada sisi bermuatan negative (biru) (Rahmadani,A. *ChemOffis* 2015).

Gambar 5. Analisis 3D Surface HCN. (a) Surface Solvent Accessible molekul HCN, (b) Surface Solvent Accessible molekul HCN Display Mode Wire Mesh (c) Surface Solvent Accessible molekul HCN Display Mode Translucent, (d) Surface Connolly Molecular molekul HCN, (e) Surface Connolly Molecular molekul HCN Display Mode Wire Mesh, (f) Surface Connolly Molecular molekul HCN Display Mode Translucent.

Gambar 6. Jarak antara atom pada molekul HCN dengan menggunakan Measurements Window

Optimasi MM2 pada HCN

Optimasi molekul HCN dilakukan dengan Molekular^[212] Mekanik (MM2) dan menghasilkan output data dalam bentuk data geometri atom atom dalam molekul dan Energi optimumnya. Hasil output yang diperoleh dapat dilihat sebagai berikut :

1. Optimasi MM2 Minimization
2. Optimasi MM2 Dynamics
3. Optimasi MM2 Properties

Minimize Energy

Stretch : 2.0466
Bend : 0.0000
Stretch-Bend : 0.0000
Torsion : 0.0000
Non-1,4 VDW : 0.0000
1,4 VDW : 0.0000
Total Energy : 2.0466 kcal/mol

Total energy for this frame: 2.047 kcal/mol

1) Analisa MM2 dynamics pada HCN

Translational Kinetic Energy: 0.0000 Rotational Kinetic Energy: 0.3165

2) Analisa MM2 Properties HCN

Stretch	:	2.0466
Bend	:	0.0000
Stretch-Bend	:	0.0000
Torsion	:	0.0000
Non-1,4 VDW	:	0.0000
1,4 VDW	:	0.0000
Total Energy	:	2.0466 kcal/mol

The total energy for this frame : 2.047 kcal/mol

Dari hasil optimasi MM2 terhadap molekul menggunakan metode komputasi diperoleh energi stretch molekul HCN sebesar 2,0466 energy bend, torsion, dan 1,4 VDW masing-masing 0,0000 sehingga total energi keseluruhan adalah 2,047 kcal/mol.

4. Jari-Jari Atom Penyusun HCN

Asam sianida⁽¹⁻⁴⁰⁾ adalah senyawa kimia yang mengandung gugus siano $C \equiv N$ yang terikat dengan atom hidrogen^(7; 10; 26; 27; 32; 41-45), atom karbon terikat tiga ke atom nitrogen. Pada gugus CN sebagai ion sianida poliatomik yang bermuatan negatif (CN⁻). Hidrogen Sianida salah satu senyawa yang sangat beracun. Anion CN⁻ bersifat isoelektronik jika berikatan dengan molekul nitrogen dan karbon monoksida.

HCN terdiri atas tiga atom penyusun yaitu atom H,C,dan N , jari-jari ketiga atom ini memiliki perbedaan jari-jari. Jari-jari atom merupakan jarak antara inti ke elektron terluar atom di suatu atom. Perbedaan jari-jari ini dapat dilihat dari tabel dibawah ini :

Tabel 2. Jari-jari atom H, B, dan O

https://id.wikipedia.org/wiki/Jari-jari_atom

Simbol	Nama	Jari-jari (pm)			
		Empiris	Hasil Perhitungan	Van der Waals	Kovalen
H	Hidrogen	25	53	120	37
C	Carbon	70	67	170	77
N	Nitrogen	60	56	155	75

Jari -jari molekul merupakan jarak antara satu atom ke atom lainnya dalam susunan tertentu yang terikat secara bersama melalui sebuah ikatan kimia.

Gambar 6. Jarak antara atom pada molekul HCN dengan menggunakan Measurements Window

Pada fasa⁽¹⁵¹⁾ liquid asam sianida terdiri atas lapisan⁽¹⁵²⁾ molekul HCN yang terikat bersama dengan ikatan hidrogen⁽¹⁵³⁾ (seperti gambar) Dimana panjang ikatan H-C 1,1 amstrong dan C dengan N 1,1 amstrong .

5. Sifat Termodinamika

Keadaan termodinamika⁽¹⁵⁵⁾ merupakan keadaan secara makroskopik^(72; 73; 156) dari suatu sistem dimana sifat-sifatnya hanya sebatas percobaan menggunakan peralatan laboratorium yang menjaga sifat-sifat tersebut pada nilai tertentu yang dipilih dan keadaannya tidak bergantung pada waktu.

Berdasarkan percobaan didapatkan sifat termodinamika asam borat sebagai berikut:

Termodinamika	
<u>Kapasitas kalor</u> (C)	71,00/(mol·K)
<u>Entropi molar standar</u> (S°)	113,01 J/(mol·K)
<u>Entalpi pembentukan standar</u> (Δ _f H°)	109,9 kJ/mol
<u>Energi bebas Gibbs</u> (Δ _f G)	143,1 kJ/mol

Tabel 3. Sifat Termodinamika Hidrogen Sianida

pembuatan asam sianida (HCN) yang paling sering dilakukan menggunakan metode, yang diciptakan oleh Leonid Andrussow, dimana metana⁽¹⁵⁵⁻¹⁷⁴⁾, dan amonia bereaksi pada suhu⁽²⁰⁶⁾ sekitar 1200° C menggunakan katalis platina⁽¹⁷⁵⁻¹⁹⁴⁾, dengan reaksi sebagai berikut :

Energi yang dibutuhkan untuk reaksi ini berasal dari panas yang timbul akibat reaksi oksidasi parsial metana dan amonia.

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Asam hidrosianat (HCN) juga bisa diekstrak dari daun, bunga, atau umbi-umbian dari tanaman beracun yang memiliki *cyanohydrins*, dengan cara hidrolisis yang diikuti proses pengasaman dan penyulingan.

Harga ΔH_f° komponennya pada suhu 298 K dapat dilihat pada tabel 5. dibawah ini:

Tabel 4. Harga ΔH_f° Masing-masing Komponen⁽¹⁵⁷⁾

Komponen	ΔH_f° (kJ / mol)
CH₄	-74,9
NH₃	-46,3
HCN	-20
H₂	0

$$\begin{aligned} \Delta H_R^\circ &= \Delta H_f^\circ \text{ produk} - \Delta H_f^\circ \text{ reaktan} \\ &= (\Delta H_f^\circ \text{ HCN} + 3 \times \Delta H_f^\circ \text{ H}_2) - (\Delta H_f^\circ \text{ CH}_4 + \Delta H_f^\circ \text{ NH}_3) \\ &= ((-20) + (3 \times 0)) - ((-74,9) + (-46,3)) \text{ kJ / mol} \\ &= -141,2 \text{ kJ / mol} \end{aligned}$$

6. Gerakan ion

Sebelum menentukan pengukuran konduktivitas, terlebih dahulu mengetahui penyebab dari pergerakan ion dengan laju yang berbeda-beda, dan penyebab ion tersebut memiliki konduktivitas molar yang berlainan, serta sebab konduktivitas molar⁽¹⁶⁶⁾ elektrolit kuat berkurang dengan akar konsentrasi.⁽¹⁶⁷⁾

Konsep nya adalah makin besar mobilitas ion^(168; 169) dalam larutan,⁽¹³⁴⁾ maka semakin besar pula kontribusinya pada konduktivitas (untuk muatan tertentu).

Tabel 5. Mobilitas Ionik dalam Air pada suhu 298 K⁽¹⁵⁷⁾

Ion	Mobilitas ionik ($10^{-8} \text{ m}^2 \text{ s}^{-1} \text{ V}^{-1}$)
K⁺	7,62
Na⁺	5,19
Cl⁻	7,91
NO₃⁻	7,40
F⁻	5,70

Terdapat beberapa faktor yang mempengaruhi kecepatan ion diantaranya:

1. Muatan ion, dimana ion bergerak semakin cepat karena muatan ion semakin ringan.
2. Terdapat hidrasi, semakin sedikit molekul air yang melingkupi ion semakin cepat pergerakan ion.
3. Gaya tarik antar ion, dimana gaya tarik besar gerakan ion akan melambat.
4. Temperatur, dimana temperatur tinggi⁽¹⁷⁰⁾ maka kecepatan ion akan meningkat.

7. Viskositas

Viskositas merupakan suatu ukuran ketahanan dari fluida yang dipengaruhi oleh tekanan maupun tegangan. Viskositas larutan encer HCN dengan komposisi yang khas dari pendingin

reaktor daya air⁽¹⁷¹⁾ ringan telah diukur untuk tiga komposisi boron antara 1500 ppm(berat) dan 3500 ppm pada rentang suhu 30°C – 60°C menggunakan viskometer Cannon-Ubbelohde yang dikalibrasi. Viskositas larutan encer ini mengikuti persamaan Arrhenius dari bentuk (persamaan) dimana ν adalah viskositas kinematik (m^2/s) dari larutan HCN.

8. Kecepatan hanyut

Jika dua elektroda⁽¹⁷²⁻¹⁷⁶⁾ yang terpisah dengan jarak l berada pada selisih potensial $\Delta\phi$, maka ion dalam larutan diantara kedua elektroda⁽¹⁷⁷⁾ itu, mengalami medan listrik⁽¹⁷⁸⁻¹⁸²⁾ seragam, seperti:

$$E = \frac{\Delta\phi}{l} \quad (1)$$

Untuk ion (muatan ion) mengalami gaya sebesar :

$$F = zeE = \frac{ze\Delta\phi}{l} \quad (2)$$

Kation^(97; 173; 183-185) bereaksi dengan percepatan menuju elektroda⁽¹⁸⁶⁾ negatif dan anion^(97; 149; 183; 187; 188) bereaksi dengan percepatan menuju elektroda positif. Akan tetapi, saat ion bergerak melalui pelarut⁽¹⁸⁹⁻¹⁹¹⁾ maka ion akan mengalami gaya gesekan⁽¹⁹²⁻¹⁹⁶⁾ memperlambat muatan⁽¹⁹⁷⁾ yang setara dengan kecepatannya. dan jika dianalogikan hukum Stokes⁽¹⁹⁸⁻²⁰²⁾ untuk bola radius^(179; 203-206) a dan s berlaku pada skala mikroskopis, maka kita dapat menuliskan gaya perlambatan⁽²⁰⁷⁻²¹¹⁾ ini dibawah ini:

$$F' = fs \quad f = 6\pi\eta a \quad (3)$$

Kedua gaya itu bekerja dalam arah yang berlawanan, dan ion mencapai kecepatan akhir, yaitu kecepatan hanyut,⁽²¹²⁻²¹⁶⁾ jika gaya mempercepat I_e diimbangi oleh penahan kental I_e' . Gaya neto menjadi nol ($I_e = I_e'$), jika:

$$s = \frac{zeE}{f} \quad (4)$$

$$U = \frac{x}{t\left(\frac{dE}{dx}\right)} \quad (5)$$

Dimana:

x = jarak (m)

t = waktu (dt)

$\left(\frac{dE}{dx}\right)$ = kekuatan medan ($volt.m^{-1}$)

$$E = \frac{dE}{dx} \quad (6)$$

Maka,

$$U = \frac{\lambda_m}{zF} \quad (7)$$

z = valensi kation

F = Faraday

Karena adanya kecepatan hanyut⁽²¹⁷⁾ yang mengatur laju transportasi ion, sehingga diharapkan konduktivitas akan berkurang seiring bertambahnya viskositas pelarut akan ukuran ion.

Perhitungan kecepatan hanyut :

Misalkan potensial HCN 3,50 V dan jarak antar elektroda adalah 1,5 cm, maka kecepatan hanyutnya dapat dihitung sebagai berikut :

$$E = \frac{\Delta\phi}{l}$$

$$E = \frac{3.50 \text{ V}}{1.5 \text{ cm}} = 2.33 \text{ V/cm}$$

Jadi kecepatan hanyut HCN adalah 2,33 V/cm

9. Konduktiviti

Konduktiviti merupakan suatu ukuran kemampuan suatu senyawa dalam menghantarkan listrik.⁽²¹⁸⁾ Berdasarkan penelitian, pengukuran konduktivitas listrik⁽²¹⁹⁾ dari larutan asam sianida

(15-110 g/kg-H₂O = 0,251-1,815 mol/kg-H₂O) dapat diukur dalam rentang suhu 25 sampai 75°C⁽¹⁶⁷⁾ pada tekanan uap jenuh dalam sel kaca menggunakan elektroda platinum konsentris. Konduktansi spesifik dari HCN_{3(aq)} dapat dihitung setelah koreksi untuk konduktansi pelarut (air) dan ditabulasikan. Konduktivitas suatu larutan dapat dipengaruhi oleh besarnya konsentrasi larutan tersebut. Semakin tinggi konsentrasi maka semakin tinggi pula konduktivitasnya. Untuk mengetahui pengaruh konsentrasi terhadap konduktivitas maka dapat dianalogikan sebagai berikut:

Suatu larutan X 0,1% ditimbang 0,1 gram, lalu dilarutkan dalam labu ukur 100 ml kemudian dilakukan penambahan air sampai tanda batas. Lalu larutan diencerkan menjadi 0,08%, 0,06%, 0,04% dan 0,02% dan diukur menggunakan konduktimeter sehingga diperoleh data sebagai berikut.

Tabel 6. Hasil pengukuran konduktivitas larutan X

Konsentrasi (%)	Konduktivitas (mS/cm)
0,1	2,45
0,08	1,75
0,06	1,25
0,04	0,82
0,02	0,50

Dari data diatas dapat diasumsikan bahwa konduktivitas larutan X meningkat seiring bertambahnya konsentrasi larutan. Konsentrasi berbanding lurus dengan konduktivitas. Sehingga dari data didapatkan grafik sebagai berikut:

Selain menggunakan konduktimeter, konduktivitas bisa ditentukan melalui rumus berikut:

$$K = 1P(\Omega - 1\text{cm} - 1) \quad (1)$$

Konduktivitas biasanya terdapat dalam mScm^{-1} dan konsentrasi M. Sehingga hubungannya diketahui dalam mho/cm seperti:

$$R = \rho \times lA \quad (2)$$

$$k = 1RA \quad (3)$$

$$Am = \frac{100 \times \frac{K}{(\text{Scm}^{-1})} \text{cm}^2 \text{mol}^{-1}}{C/M} \quad (4)$$

10. Besaran Kimia Fisika 3

a. Bilangan Transport

Fraksi dari arus total⁽²²⁰⁻²²⁴⁾ yang dibawa oleh ion jenis tertentu. Untuk larutan dengan dua jenis ion, bilangan transport kation :

$$t_+ = \frac{I^+}{I} \quad (1)$$

I= arus total

$$I = t_+ + t_- \quad (2)$$

Bilangan transport pembatas (t^0) untuk limit konsentrasi nol dari larutan elektrolit.^(147; 225-229)

Jika $I \propto \kappa$ sehingga :

$$t^0 = \frac{z v u}{\sum_i z v u_i} \quad (3)$$

Untuk elektrolit simetris (bilangan muatan untuk kedua ion sama) maka persamaan diatas disederhanakan :

$$t^0 = \frac{u}{\sum_i u_i} \quad (4)$$

Hubungan antara konduktivitas ion dengan mobilitas ion^(188; 230-234) :

$$t^0 = \frac{v \lambda}{\sum_i v_i \lambda_i} = \frac{v \lambda}{\Lambda_m^0} \quad (5)$$

Jadi untuk setiap jenis ion :

$$v \lambda = t^0 \Lambda_m^0 \quad (6)$$

a. **Hukum Pertama Fick Tentang Difusi**

Andaikan fluks partikel yang berdifusi, merupakan gerakan sebagai reaksi terhadap gaya termodinamika yang timbul dari gradient konsentrasi^[270-273]. Partikel^[266-269] akan mencapai kecepatan hanyut tetap s jika gaya termodinamika f sama dengan tahanan kental. kecepatan hanyut ini sebanding dengan gaya termodinamika, dan kita tuliskan $s \propto f$. Akan tetapi, fluks partikel J sebanding dengan kecepatan hanyut, dan gaya termodinamika sebanding dengan gradient konsentrasi dc/dx .

Rantai kesebandingan itu ($J \propto s$, $s \propto f$, dan $f \propto dc/dx$ menunjukkan bahwa:

$$J \propto \frac{dc}{dx} \quad (7)$$

b. **Hubungan Einstein**

Hukum Fick untuk fluks partikel dalam mol molekul⁽²²⁷⁾ per satuan luas per satuan waktu adalah:

$$J = -D \frac{dc}{dx} \quad (8)$$

Dengan D merupakan koefisien difusi dan dc/dx merupakan kemiringan dari konsentrasi molar.

Fluks partikel berhubungan dengan kecepatan hanyut, dengan:

$$J = s c \quad (9)$$

c. **Energy Stability**

Energi stabilitas yaitu stabilitas termodinamik dari sistem kimia,⁽²⁵¹⁾ dimana energi⁽⁷⁵⁾ yang terjadi ketika sebuah sistem berada dalam keadaan energi terendah atau kesetimbangan kimia dengan lingkungannya. Energi stabilitas dari molekul⁽²⁵²⁾ asam sianida yang diperoleh dari data aplikasi ChemDraw 3D dapat dilihat sebagai berikut:

Analisa MM2 dynamics pada HCN

MM2 Calculation completed successfully

-----MM2 Dynamics-----

Warning: Some parameters are guessed (Quality = 1).

Iteration	Time	Total Energy	Potential Energy	Temperature
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2.	0.024	0.048 ± 0.000	0.038 ± 0.000	1.05 ± 0.00
3.	0.026	0.082 ± 0.000	0.045 ± 0.000	4.18 ± 0.00
4.	0.028	0.089 ± 0.000	0.016 ± 0.000	8.08 ± 0.00
5.	0.030	0.093 ± 0.000	0.091 ± 0.000	0.18 ± 0.00

Translational Kinetic Energy: 0.0000 Rotational Kinetic Energy: 0.0000

Translational Kinetic Energy: 0.0000 Rotational Kinetic Energy: : 2.047 kcal/mol
Calculation ended

IV.Kesimpulan

Hidrogen Sianida larut dalam air. Hidrogen sianida bersifat toxic atau beracun. Analisis energi kinetik rotasi senyawa pada Chemdraw 2D 2,0466 kcal/mol Analisis jari-jari atom hidrogen dengan carbon pada Chemdraw 3D didapatkan sebesar 1,1 A, dan jari jari atom carbon dengan nitrogen masing-masingnya sebesar 1,1 A. Data yang didapat pada Analisa MM2 dynamics HCN adalah interaction time 0.024 , 0.026, 0.028, 0.030, total energy 0.048, 0.082, potensial energy 0.38, 0.045, 0.016, 0.091. Sifat termodinamika hidrogen sianida adalah entropi (ΔS) 113,01 J/kmol , entalpi pembentukan standar ($\Delta_f H$) -141,2 kJ/mol , entalpi pembakaran standar ($\Delta_c H$) -426,5 kJ/mol dan kecepatan hanyut yang didapat berdasarkan perhitungan sebesar 2,33 V/cmsifat dari asam sianida diantaranya massa molar : 27,03 g/mol, penampilan : cairan transparan atau gas tak berwarna, densitas : 0,687g/mL, kelarutan dalam air : bercampur, viskositas : 201 μ Pa s. Kegunaan hidrogen sianida dalam bidang industri pembuatan emas dan perak , kemudian pembuatan warna prussian blue (pewarna biru).

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