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Research Article

An Original FORTRAN Code Combined with an XMGRACE© Graphical Routine Aimed at the Parameter Calculations and Drawing of Newton Diagrams for Crossed Molecular Beams (CMB) Experiments Planning

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Abstract

This work presents a detailed computational method for analyzing and visually representing molecular collision dynamics in crossed molecular beam (CMB) experiments. An original UNIX-based FORTRAN code was created to calculate important kinematic parameters and build Newton diagrams for reactive systems where two monoenergetic beams intersect at any angle between 0° and 180°. The program finds center-of-mass velocities, collisional energies, product scattering velocities, angular ranges, and coordinate changes between laboratory and center-of-mass reference frames, using the principles of classical mechanics. A related XMGRACE-compatible routine creates high-resolution Newton diagrams that are ready for publication. This allows users to visualize reaction kinematics, scattering circles, and time-of-flight (TOF) detection angles accurately. An extra DOS/GW-Basic executable is included for quick on-screen visualization. The method has been thoroughly tested with different reactive channels and various chemical systems. By combining analytical derivations with automated graphical output, the tool provides a flexible platform for planning CMB experiments, interpreting dynamic results, and comparing theoretical predictions with observed scattering behavior. The codes are free for scientific use with proper credit.

I. Introduction

Newton Diagrams are vector representations of the collisional events between two particles treated based on classical physics. Such types of diagrams are extensively used for the planning and the cinematic analysis of collisional events that typically occur in Crossed Molecular Beams (CMB) experiments performed in a high vacuum environment, which are at the basis of the Reaction Dynamics investigations [1-7].

The present work describes in detail a UNIX-based code aimed at the collisional parameter calculation and at the drawing of Newton Diagrams for two reacting molecular beams intersected at any angle g between 0 and 180 degrees. The global code, written in FORTRAN, was implemented by the author during his Ph.D. course in Chemistry and has been used and tested for a great variety of reactions.

It consists of two main parts: The first one calculates the reaction parameters of two monoenergetic beams of particle interacting at a given angle **g**, for a given elementary reaction; the second one generates and save an XMGRACE©-readable file which after the launch/opening of an UNIX© executable, draws an high-resolution graphical scheme of the reactions knematics, which in turn can be modified, printed or exported in the desired format for its final inclusion in a publication.

Moreover, it is also alleged to be a simple GW-Basic©/DOS© executable which can generate a Newton Diagram for a quick on-screen visualization for a given reaction.

The codes cited in this article can be freely used or copied by the reader(s), provided that due credit is given by the user(s) to the author.

II. Theoretical treatment of the collision of two particles, according to the classical physics

II.a. Vector derivation of the expressions for Center-Mass velocity ($V_{c.m.}$) and angle ($Q_{c.m.}$): Considering the generic reaction:

A + BC → AB + C (I)

Between two particle reagent beams **A** and **BC** crossed at whatever angle **g** (with $0^0 < g < 180^0$) e with velocities $\mathbf{V}_A$ e $\mathbf{V}_{BC}$, for the conservation of the linear momentum in the C.M. reference system:

$$m_A\mathbf{U}_A + m_{BC}\mathbf{U}_{BC} = 0 \quad \text{(A.I.1)}$$

And the vectorial differences:

$$\mathbf{U}_A = \mathbf{V}_A - \mathbf{V}_{c.m.} \quad \text{(A.I.2a)}$$

$$\mathbf{U}_{BC} = \mathbf{V}_{BC} - \mathbf{V}_{c.m.} \quad \text{(A.I.2b)}$$

(**Figure** II.1.) We obtain from (A.I.1):

$$m_A\mathbf{V}_A - m_A\mathbf{V}_{c.m.} + m_{BC}\mathbf{V}_{BC} - m_{BC}\mathbf{V}_{c.m.} = 0$$

Namely:

$$\mathbf{V}_{c.m.} = (m_A\mathbf{V}_A + m_{BC}\mathbf{V}_{BC}) / (m_A + m_{BC}) \quad \text{(A.I.3)}$$

Using the unit vectors **i**, **j** for representing $\mathbf{V}_A$ and $\mathbf{V}_{BC}$ (Figure A.I.1), for g = 90^0:

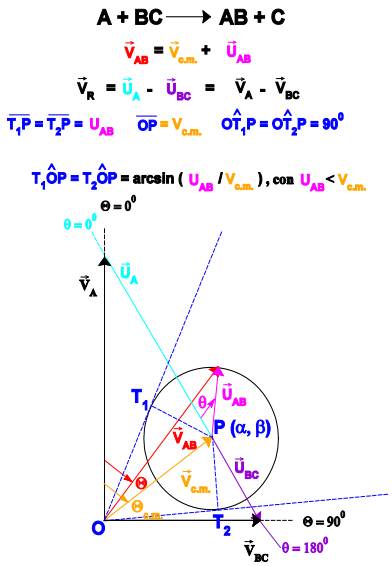

Figure A.II.1: Vectorial relations for the generic reaction: A + BC → AB + C.

$$\mathbf{V}_{BC} = V_{BC}\mathbf{i} \quad \text{(A.I.4a)}$$

$$\mathbf{V}_A = V_A\mathbf{j} \quad \text{(A.I.4b)}$$

By substituting the (A.I.4a, b) into (A.I.3):

$$\mathbf{V}_{c.m.} = [(m_{BC}V_{BC})/(m_A+m_{BC})](\mathbf{i}) + [(m_AV_A)/(m_A+m_{BC})](\mathbf{j}) \quad \text{(A.I.5)}$$

By expressing the vector $\mathbf{V}_{c.m.}$ as a function of its components parallel to the X and Y axes of the Laboratory reference system:

$$\mathbf{V}_{c.m.} = [a](\mathbf{i}) + [b](\mathbf{j}) \quad \text{(A.I.6)}$$

The modules of these component vectors a e b correspond to the Cartesian coordinates of the point **P** (the tip of the $\mathbf{V}_{c.m.}$ vector) in the reference system XOY.

By confronting (A.I.5) with (A.I.6) we get:

$$a = (m_{BC}\mathbf{V}_{BC}) / (m_A+m_{BC}) \text{ e } b = (m_A\mathbf{V}_A) / (m_A+m_{BC}) \quad \text{(A.I.7)}$$

Moreover, by letting $p_{BC} = m_{BC}V_{BC}$ and $p_A = m_AV_A$,:

$$V_{c.m.} = (p_A^2 + p_{BC}^2)^{1/2} / (m_A + m_{BC}) \quad \text{(A.I.8a)}$$

and

$$\tan(Q_{c.m.}) = (a / b) = (p_{BC} / p_A) \quad \text{(A.I.8b)}$$

For $0^0 < g < 90^0$, we have:

$$\mathbf{V}_{BC} = (V_{BC})_X\mathbf{i} + (V_{BC})_Y\mathbf{j} \quad \text{(A.I.9a)}$$

$$\mathbf{V}_A = V_A\mathbf{j} \quad \text{(A.I.9b)}$$

The modules of the component vectors of $\mathbf{V}_{BC}$ are given by:

$$(V_{BC})_X = v_{BC}\sin g;\ (V_{BC})_Y = V_{BC}\cos g \quad \text{(A.I.10a,b)}$$

By substituting the (A.I.10a, b) into (A.I.9a) and then the (A.I.9a, b) into (A.I.3), we obtain:

$$\mathbf{V}_{c.m.} = [(m_{BC}V_{BC}\sin g)(\mathbf{i}) + (m_AV_A + m_{BC}V_{BC}\cos g)(\mathbf{j})]/(m_A+m_{BC}), \quad \text{(A.I.11)}$$

from which:

$$a = (m_{BC}V_{BC}\sin g) / (m_A+m_{BC}), \quad \text{(A.I.12a)}$$

$$b = (m_AV_A + m_{BC}V_{BC}\cos g) / (m_A+m_{BC}) \quad \text{(A.I.12b)}$$

And:

$$V_{c.m.} = (p_A^2 + p_{BC}^2 + 2p_Ap_{BC}\cos g)^{1/2}/(m_A+m_{BC}) \quad \text{(A.I.13)}$$

For $90^0 < g < 180^0$:

$$\mathbf{V}_{BC} = (V_{BC})_X\mathbf{i} + (V_{BC})_Y(-\mathbf{j}) \quad \text{(A.I.14a)}$$

$$\mathbf{V}_A = V_A\mathbf{j} \quad \text{(A.I.14b)}$$

The modules of the component vectors of $\mathbf{v}_{BC}$ are given by:

$$(V_{BC})_X = V_{BC}\sin g \quad \text{(A.I.15a)}$$

$$(V_{BC})_Y = - V_{BC}\cos g \qquad \text{(A.I.15b)}$$

By substituting the (A.I.15 a,b) into (A.I.14a) and then the (A.I.14a,b) into (A.I.3), we get the (A.I.11) again:

$$\mathbf{V}_{c.m.}=[(m_{BC}\cdot V_{BC}\sin g)(\mathbf{i})+(m_A\cdot v_A+m_{BC}\cdot V_{BC}\cdot\cos g)(\mathbf{j})]/(m_A+m_{BC}), \qquad \text{(A.I.11)}$$

the (A.I.12a,b):

$$a = (m_{BC}\cdot V_{BC}\sin g) / (m_A+m_{BC}),$$

$$b = (m_A\cdot V_A+m_{BC}\cdot V_{BC}\cos g) / (m_A+m_{BC})$$

And the:

$$V_{c.m.}= (p_A^2 + p_{BC}^2 + 2p_A\cdot p_{BC}\cos g)^{1/2} /(m_A+m_{BC}) \qquad \text{(A.I.13)}$$

Generally, it is more convenient to express the $Q_{c.m.}$ angle as a function of V_A, $V_{c.m.}$, and u_A rather than directly as the arctangent of the ratio a / b, because in this fashion it can be obtained a single general formula effective for each value of g between 0^0 and 180^0.

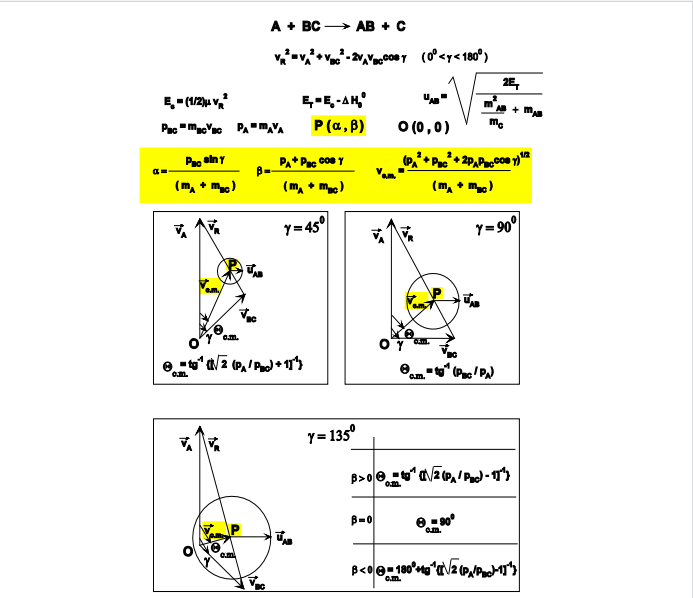

Figure. A.II.2. $\Theta_{c.m.}$ values for γ = 45°, 90° and 135°.

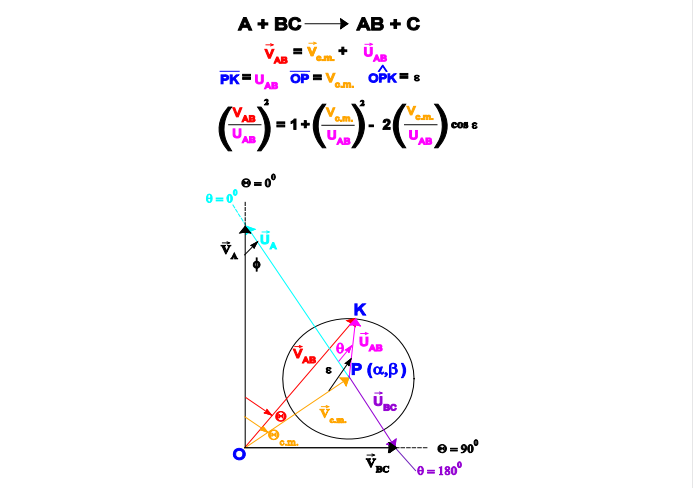

Figure. A.II.3. "Jacobian" operator.

Based on a generic reactive system geometry (Figure I.2.; Figure II.2.), we have:

$$U_A^2 = V_A^2 + V_{c.m.}^2 - 2\,V_A\cdot V_{c.m.}\cos(Q_{c.m.}) \qquad \text{(A.I.14)}$$

hence:

$$Q_{c.m.}= \arccos[(V_A^2 + V_{c.m.}^2 - U_A^2) / (2\,V_A\cdot V_{c.m.})]. \qquad \text{(A.I.15)}$$

But:

$$V_{c.m.}^2 = a^2 + b^2 \text{ and } U_A^2 = a^2 + (V_A - b)^2$$

Then:

$$Q_{c.m.}= \arccos[(b) / (a^2 + b^2)]. \qquad \text{(A.I.16)}$$

By substituting into (A.I.16) the (A.I.12a, b) we obtain finally:

$$Q_{c.m.}= \arccos[(p_A + p_{BC}\cos g) /(p_A^2 + p_{BC}^2 + 2p_A\cdot p_{BC}\cdot\cos g)^{1/2}], \qquad \text{(A.I.17)}$$

Valid for each g between 0^0 and 180^0.

II.b. Relations between the Cartesian coordinate system of the Center of Mass and the Laboratory system for a generic point P in the velocity plane.

The Center of Mass reference system can be seen as the result of a translation of the origin O(0,0) of the Laboratory reference system axes $\mathbf{V}_{xLAB}$, $\mathbf{V}_{yLAB}$ into the point **P(a, b)**, which is the Center of Mass followed by an anti-clockwise rotation of **f** degrees (Figure A.II.1), where **f** is given by :

$$f = \arctan(V_{BC}\sin g / [V_A - V_{BC}\cos g]) \qquad \text{(A.II.1)}$$

and $0^0 < \mathbf{g} < 180^0$.

It follows that the relations which allow the passage from Center of Mass coordinates to the Laboratory ones for a generic point **P** are given by:

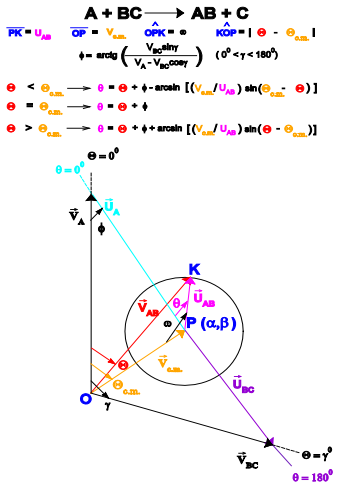

Figure. A.II.4. Laboratory and C.M. system vector relationships.

$$V_{xLAB} = V_{xc.m.} \cos f - Vy_{c.m.} \sin f + a \qquad \text{(A.II.2 a,b)}$$

$$V_{yLAB} = V_{xc.m.} \sin f + Vy_{c.m.} \cos f + b$$

II.b.1. Relations between Cartesian and Polar Coordinates in the two reference systems

Based on Figure A.II.1, we can also write:

$$Vx_{LAB} = V_P \sin Q \qquad \text{(A.II.3)}$$

$$Vy_{LAB} = V_P \cos Q$$

And:

$$Vx_{c.m.} = U_P \sin q \qquad \text{(A.II.4)}$$

$$Vy_{c.m.} = U_P \cos q$$

Where $\mathbf{V_P}$, $\mathbf{U_P}$ are respectively the **P** product velocity in the Laboratory reference system and in the Center of Mass one and **Q** e **q** the corresponding angles.

By substituting the (A.II.3) and (A.II.4) into (A.II.2), we have:

$$V_P \sin Q = U_P \sin q \cos f - U_P \cos q \sin f + a \qquad \text{(A.II.5)}$$

$$V_P \cos Q = U_P \sin q \sin f + U_P \cos q \cos f + b$$

Namely:

$$V_P \sin Q = U_P \sin(q - f) + a \qquad \text{(A.II.6 a, b)}$$

$$V_P \cos Q = U_P \cos(q - f) + b$$

Dividing member by member the (A.II.6)*:*

$$\tan Q = (U_P \sin(q - f) + a) / (U_P \cos(q - f) + b) \qquad \text{(A.II.7)}$$

By combining the (A.II.6 a, b) as a function of the angle **Q**:

$$\tan (q - f) = (V_P \sin(Q) - a) / (V_P \cos(Q) - b) \qquad \text{(A.II.8)}$$

A.II.3. Jacobian operator and relations for the conversion of the Laboratory reference frame angles Q into the Center of Mass reference system ones.

Between the product flux in the two reference systems, the following relation holds:

$$I_{LAB}(Q,V_P) = (V_P^2/U_P^2) \cdot I_{c.m.}(q,U_P) \qquad \text{(A.II.9)}$$

The product's density measured in the Laboratory reference system is:

$$N(Q,V_P) = (V_P/U_P^2) \cdot I_{c.m.}(q,U_P) \qquad \text{(A.II.10)}$$

Where $\mathbf{(V^2/U^2)}$ is the **Jacobian** operator, which converts the effective Center of Mass flux into the one observed in the Laboratory reference frame.

By expressing the velocity of a generic product's particle **P** as $\mathbf{V_P}$ in the Laboratory frame as a function of the corresponding velocity in the Center of Mass reference system $\mathbf{U_P}$ and of the Center of Mass velocity $\mathbf{V_{c.m.}}$:

$$V_P^2 = U_P^2 + V_{c.m.}^2 - 2U_P \cdot V_{c.m.} \cos w \qquad \text{(A.II.11)}$$

Where **w** is the **{OPK}** triangle angle defined by the half-lines where are the vectors $\mathbf{U_P}$ and $\mathbf{V_{c.m.}}$ (Figure A.II.3.). The expressions for **w** as a function of the angle **Q** formed by the vectors $\mathbf{V_P}$ and $\mathbf{V_A}$ are given by:

$$w = p - f - Q_{c.m.} + q \qquad \text{for } Q < Q_{c.m.}$$

$$w = p \qquad \text{for } Q = Q_{c.m.}$$

$$w = p + f + Q_{c.m.} - q \qquad \text{for } Q > Q_{c.m.} \qquad \text{(A.II.12 a, b, c)}$$

Dividing each part of (A.II.11) by U_P^2, it can be obtained the expression for the *"Jacobian"* as a function of w:

$$(V_P^2/U_P^2) = 1 + (V_{c.m.} / U_P)^2 - 2(V_{c.m.} / U_P) \cos w \qquad \text{(A.II.13)}$$

or:

$$(V_P/U_P^2) = \{[1 + (V_{c.m.} / U_P)^2 - 2(V_{c.m.} / U_P) \cos w\,]^{1/2}\}/U_P \qquad \text{(A.II.14)}$$

Applying the sine's theorem to the same triangle **{OPK}** above, by varying the angle, Q it is possible to obtain expressions for the conversion of the Q angles of the Laboratory system to the angles q of the center of Mass reference system (Figure A.II.4):

$$\text{for } Q < Q_{c.m.}. \quad q = Q + f - \arcsin \{(V_{c.m.} / U_{AB})\sin(Q_{c.m.} - Q)\}$$

$$\text{for } Q = Q_{c.m.} \quad q = Q_{c.m.} + f$$

$$\text{for } Q > Q_{c.m.}. \quad q = Q + f + \arcsin \{(V_{c.m.} / U_{AB})\sin(Q - Q_{c.m.})\}. \qquad \text{(A.II.14 a, b, c)}$$

A.II.4. Collisional energy (E_c), angular range amplitude (DA), velocity (vCM), and angle (Q_{CM}) of the center of mass dependence on g (intersection angle of the reagents beams).

Considering two reagent beams **A** and **BC** crossed at an angle **g** between 0^0 and 180^0, the collisional energy is given by:

$$E_c = (½)\, m\, V_r^2 \qquad \text{(A.II.15)}$$

Where **m** is the reduced mass of the reagents and their relative velocity:

$$V_r = (V_A^2 + V_{BC}^2 - 2V_A \cdot V_{BC} \cos g)^{1/2} \qquad \text{(A.II.16)}$$

E_c as a function of g in the range (0, p) is in general always growing when the angle g increases, with a flection at the point (p/2, ½ $m(V_A^2 + V_{BC}^2)$ of the plane {E_c, g}, corresponding to a beam configuration of 90^0. The velocity vector of a generic product AB in the Center of mass reference system is given by:

$$U_{AB} = (2E_T / [\{m_{AB}^2 / m_C\} + m_{AB}])^{1/2} \qquad \text{(A.II.17)}$$

Where the total energy E_T is given by the sum of the collisional energy and the exothermicity of the considered reaction:

$$E_T = (½)m V_r^2 - DH^0_0 \quad \text{(A.II.18)}$$

It is always growing in the interval (0,p) of the angle g (Figure A.II.3b). If the quantity:

$$(2V_A \cdot V_{BC}) / (V_A^2 + V_{BC}^2 - 2DH^0) \quad \text{(A.II.19)}$$

Is less then 1, the $U_{AB} = f(g)$ a flex point at $g = (2V_A V_{BC}) / (V_A^2 + V_{BC}^2 - 2DH^0_0)$.

The Vc dependence g is given by:

$$V_{c.m.} = (p_A^2 + p_{BC}^2 + 2p_A \cdot p_{BC} \cos g)^{1/2} / (m_A + m_{BC}) \quad \text{(A.II.20)}$$

It is always decreasing when the value of g increases, with an inflexion point at $g_F = \arccos(-p_y / p_x)$, if $py/px < 1$, and $g_F = \arccos(-px/py)$ if $py/px > 1$, with $90^0 < g_F \pounds 180^0$.

The angular range amplitude of a scattering circle with respect to the Laboratory frame is:

$$DA(g) = Q_{max} - Q_{min} = 2 \arcsin (U_P / V_{c.m.}) \quad \text{(A.II.23)}$$

Where:

$$Q_{Max} = Q_{c.m.} + \arcsin (U_P / V_{c.m.}) \quad \text{(A.II.21)}$$

$$Q_{Min} = Q_{c.m.} - \arcsin (U_P / V_{c.m.}). \quad \text{(A.II.22)}$$

And $Q_{c.m.}$ is the center of mass vector angle, U_P is the scattering velocity of the product P(= AB, C) with respect to the center of mass frame, and $V_{c.m.}$ is the center of mass vector module.

The function $DA(g) = 2 \arcsin (U_P / V_{c.m.})$ (with $U_P \pounds V_{c.m.}$) is always growing in the interval $(0, g_l)$, in cui g_l is the limit angle (lesser than 180^0) between the beams when $u_P = v_{c.m.}$ (isotachic point: iso - tachis =same velocity).

The general expression for the center of mass angle is given by:

$$Q_{c.m.} = \arccos[(p_A + p_{BC} \cdot \cos g) / (p_A^2 + p_{BC}^2 + 2p_A p_{BC} \cos g)^{1/2}] \quad \text{(A.II.24)}$$

By the substitution: $R = (p_A / p_{BC})$, it can be written as:

$$Q_{c.m.} = \arccos[(R + \cos g) / (R^2 + 1 + 2R \cos g)^{1/2}] \quad \text{(A.II.25)}$$

It can be demonstrated that for reactions with $0<R<1$ (namely with $p_A < p_{BC}$), the corresponding curves $Q_{c.m.} = f(g)$ are always growing when g increasing and are comprised in the cartesian plane $\{Q_{c.m.}, g\}$ region between the straight lines :

$Q_{c.m.} = g$ and $Q_{c.m.} = ½(g)$ (Figure A.II.5).

$Q_{c.m.} = ½(g)$ is the (A.II.25) for R =1, namely for those reactions with $p_A = p_{BC}$. If R > 1 (namely for ractions with $p_A > p_{BC}$), the corresponding curves $Q_{c.m.} = f(g)$ show a relative maximum for $g_{MAX} = \arccos(-1 / R) = \arccos(- p_{BC} / p_A)$, and are comprised between the two straight lines:

$Q_{c.m.} = ½(g)$, $Q_{c.m.} = 0$.

For R tending to +¥, the curves $Q_{c.m.} = f(g)$ approximate to the line $Q_{c.m.} = 0$, while for R tending to 0, they approach asymptotically the $Q_{c.m.} = g$.

(Figure A.II.5)

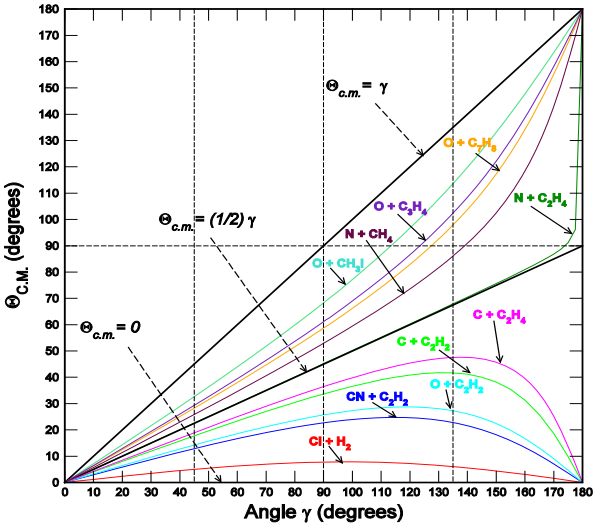

Figure. A.II.5. Θ_{cm} dependence from the crossing angle γ for some reactive systems.

III. Algorithm for the drawing of Newton Diagrams

Considering a generic reactive channel relative to a given multichannel reaction:

A + BC ® AB(i) + C(i)

Between two beams of reagents **A** and **BC** crossed at a whatever angle **g** (between 0^0 and 180^0) with velocities $\mathbf{V}_A$ and $\mathbf{V}_{BC,}$ respectively. If N is the number of the global reaction, it is possible to define the following algorithm for the Newton Diagrams drawing:

2. Results

Input data subroutine

Read:

masses velocities of the reagents: $\mathbf{m}_{A,} \mathbf{V}_{A,} \mathbf{m}_{BC,} \mathbf{V}_{BC}$

Angle between the two beams: **g**

number of reactive channels: **N**

TOF spectra angles number: **NTOF**

TOF spectra angles:

for i = 1 to NTOF { Q(i) } end

Produces masses and reactive channels' Enthalpies:

For i = 1 to N { $m_{AB}(i), m_C(i), DH_0^0(i)$ } end

Interval extremes for the drawing: $V_{Xmax}=V_{Ymax}$

SUBROUTINE for the cinematic parameters calculations

Calculate:

Reagents total mass: $m_T = m_A + m_{BC}$

Reagents reduced mass: $m = m_A \cdot m_{BC} / m_T$

Reagents linear momenta:

$p_{BC} = m_{BC}V_{BC}$;

$p_A = m_AV_A$

Scattering circles coordinates:

$a = (p_{BC} \sin g) / m_T$; $b = (p_A + p_{BC} \cos g) / m_T$

Center of Mass velocity modulus:

$V_{c.m.} = (a^2 + b^2)$

Center of Mass velocity vector angle:

$Q_{c.m.} = \arccos [(b) / (a^2 + b^2)]$.

Relative velocity modulus: $V_r^2 = V_A^2+V_{BC}^2-2V_AV_{BC}\cos g$

Collisional energy:

$Ec= (1/2)mV_r^2$

Total energies for the reactive channels:

For i = 1 to N

$\{E_T(i) = E_c - DH_0^0(i)\}$

end

Products scattering circles rays:

For = i = 1 a N

$U_{AB}(i) = \{2E_T/([m_{AB}^2(i) / m_C(i)] + m_{AB}(i))\}^{1/2}$;

$U_C(i) = (m_{AB}(i) / m_C(i)) \cdot U_{AB}(i)$

End

Reactive circles range EXTREMES angles SCATTERING calculation SUBROUTINE

Calculate:

For i = 1 to N

if $U_{AB}(i)$ £ Vc then

i-th Circle Angular range amplitude:

$DA(i) = 2 \cdot \arcsin (U_{AB}(i) / V_{c.m.})$

Minimum angle: $Amin(i) = Q_{c.m.} - DA(i) / 2$

Maximum angle: $Amax(i) = Q_{c.m.} + DA(i) / 2$

if $U_{AB}(i) > V_{c.m.}$ then i = i+1; continue

end

Coordinates of the scattering circles points calculations subroutine

Calculate:

For i = 1 to N

for q = 0 to 2p step $(5^0 / 180^0)\cdot p$

$x(i) = a + U_{AB}(i)\cdot \cos q$

$y(i) = b + U_{AB}(i)\cdot \sin q$

end

end

SUBROUTINE for the calculations of the limiting angles of the straight lines which define the RANGES of SCATTERING and of the TOF spectra angles

Calculate:

For i = 1 to N

for e= Amin(i), Amax(i), Q(i)

$y_R = Xmax\cdot\cos |e|$

$x_R = y_R / \{\tan([p/2]-e)\}$

end

SUBROUTINE for the T.O.F. spectra angles calculation in the Center of Mass reference system

Calcolate:

$f = \arctan (V_{BC} \sin g / [V_A - V_{BC} \cos g])$

for i = 1 to NTOF

if $Q(i) < Q_{c.m.}$ then

$q(i) = Q(i) + f - \arcsin \{(V_{c.m.}/U_{AB}(j))\sin(Q_{c.m.} - Q(i))\}$

if $Q(i) = Q_{c.m.}$ then

$q(i) = Q_{c.m.} + f$

if $Q(i) > Q_{c.m.}$ then

$q(i) = Q(i) + f + \arcsin \{(V_{c.m.}/U_{AB}(j))\sin(Q(i) - Q_{c.m.})\}$

end

Evaluated results OUTPUT SUBROUTINE

Print:

Center of Mass angle of the C.M. velocity vector: $\mathbf{Q_{c.m.}}$

C. M. velocity vector modulus: $\mathbf{V}_{c.m.}$

Collisional energy: **Ec**

Total energies of the **N** reactive channels $\mathbf{E}_T(\mathbf{i})$

Reagents' elastic scattering velocities:

$\mathbf{Ve}_A$, $\mathbf{Ve}_{BC}$

Products' maximum reactive scattering velocities:

$\mathbf{U}_{AB}(\mathbf{i})$, $\mathbf{U}_C(\mathbf{i})$

Angular Ranges extremes of the scattering circles:

Amin(i), Amax(i)

(Figure A.III.1)

Graphical Output:

Newton Diagram drawn in the velocity plane

between: (Vxmin, Vxmax) - (Vymin, Vymax)

(Figure A.III.2)

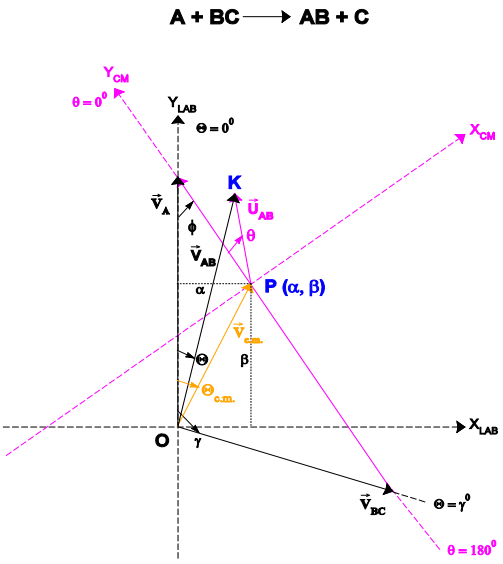

Figure. A.III.1. Relations between the Laboratory reference system coordinates and the Center of mass system ones.

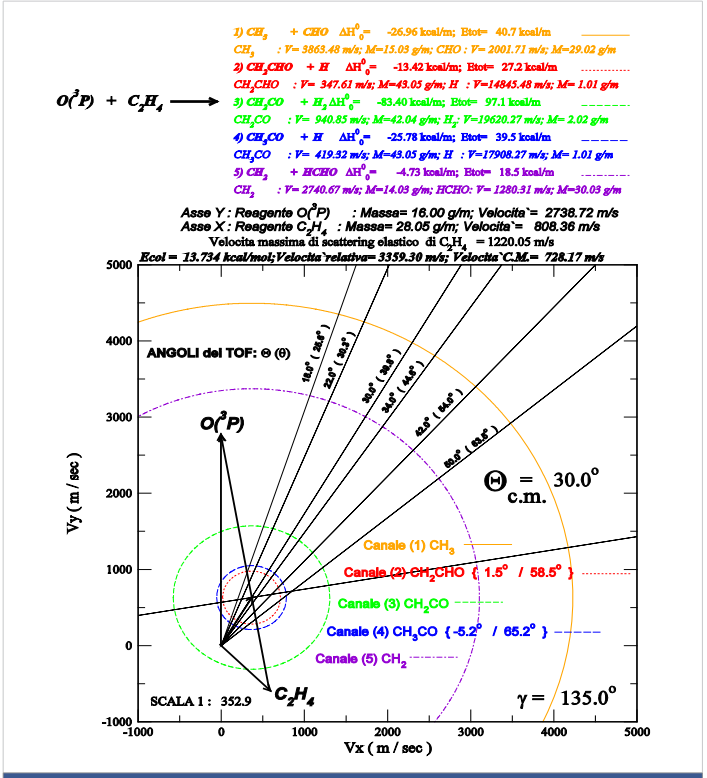

Figure. A.III.2. Example of graphical output obtained by the FORTRAN code and XMGRACE program.

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