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## RESEARCH ARTICLE

# A NEW APPROACH FOR THE MOLECULAR WEIGHT DETERMINATION

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**ABSTRACT**

Molecular weight determination of both micro and macro, molecules without a molecular peak and fragment peaks in spectrum is the characteristic feature of this method. In this method molecular crystal ions are generated separated, and plotting a graph between their abundance and weight, m/z molecular weight of sample is determined.



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## INTRODUCTION

There are many methods for the molecular weight determination, with common feature of molecular ion formation, and its analytical studies. The present method is with its characteristic feature, of molecular crystal ions (MCI) generation, and their analytical studies. Molecular crystal ions are the precursor ions for the molecular ions generation. It is MCI generated, in almost all the molecular ions generation techniques and particularly in the desorption ionization technique, prior to the generation of molecular ions. When in almost all molecular ions generation techniques, molecular ions are generated from MCIS, trough an expenditure of an extera energy, which causes fragmentation and denaturing of molecule, I thought why MCIS are not used, with almost no fragmentation and no denaturing effects. In this method MCI, are generated, and are analytically studied. A graph is plotted between the abundances of different MCI, and their masses m/z. Form the graph differences between the peaks of different MCI peaks is determined by subtraction. The smallest difference between any two adjacent peaks in spectrum is the molecular weight, if it is a whole number multiple for all other differences in between the peaks in spectrum.

If smallest differences is not whole number multiple, for all other differences in between the peaks, then the simple fraction of it, as 1/2, 1/3, 1/4 …. is a whole number multiple for all other differences in between peaks. If the smallest difference or a simple fraction of this, determined by subtraction is not a whole number multiple, for all the difference in between the peaks in spectrum, it is not the molecular mass of the compound. The spectrum should be rejected a new spectrum may be taken by making changes in ionization process and electric and magnetic sector. In the new spectrum, taken by making changes of ionization processes and electric and magnetic sector, repeat the whole exercise described above, and find out the minimum, difference, whole number multiple for all other differences in between the peaks in spectrum.

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## MATERIALS AND METHODS

There are many methods for M.wt determinations, with different degree of accuracy as EI, CI, gives the nominal mass until it's not attached with H.R devices in all their methods. One thing is common and is the molecular ion formation and its analytical studies. In all methods molecular ion informed and its mass is determined to quiet exactness through H.R techniques and from its molecular formula and atomic composition is confirmed (2). The idea for molecular weight determination, which I have evolved does not involved molecular ion formation and its analysis but in my method for molecular weight determination.

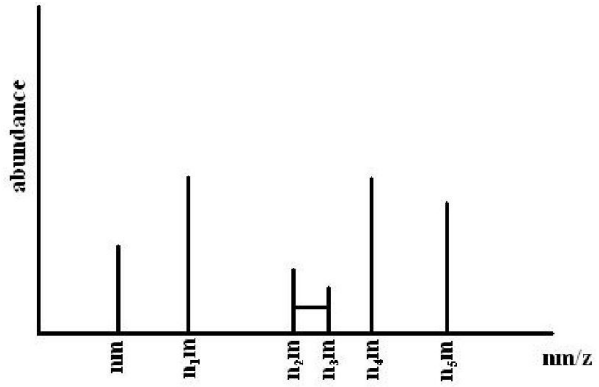
I have the concept of molecular crystal ion generation (MCI). It is the MCI from which the molecular ion is being generated in

ESI, D.I, APDI, thermal D.I (1) in all the ionization first the MCI a chunk of molecules a lump a group of molecule is formed and on simplify excesses energy from it a molecular ion is obtained. One Sample in the solid or liquid state is taken on a crucible in an ionization chamber with the normal pressure in the chamber. Sample is fired with Argon gas trough a nozzle at pressure 5 atms. This pressure splashes the sample from its, source as sample crusts, these sample crusts are counter attacked with Ar+HCl gas in ration 10:1, through a nozzle with positive charge and pressure 5 atm. Counter attack smashes the crusts of sample into small molecular chunks, with different number of molecules, with different number of charges, are the molecular crystal ions (MCI).

The MCI produced in ionization chamber are $nm^z$, $n_1m^z{}_1$, $n_2m^z{}_2$, $n_3m^z{}_3$, $nm^z{}_1$, $n_4m^z{}_2$, $nm^z{}_3$, $n_1m^z$, $n_1m^z{}_2$, $n_7m^z{}_3$. The MCI are with different number of molecules (n), and with different number of charges (z). Pass these molecular crystal ions from filters to obtain the molecular ions with same charge, unit charge. Electric filters are the sieves to filter out the MCI, with charges more than unity. Now we have MCI with unit charge, but of different weight as in these MCI different number of molecules are present. There are MCI with same charge, but with different number of molecules and in different abundance, these molecular crystal ions are $nm^+$, $n_1m^+$, $n_2m^+$, $n_3m$ . . . . . in numbers $x$, $x_1$, $x_2$, $x_3$ . . . . . .

MCI secured after passing from electronic sieves, are $nm^+$, $n_1m^+$, $n_2m^+$, $n_3m^+$ . . . . in numbers $x$, $x_1$, $x_2$, $x_3$ . . . . . With unit charge. The MCI, are of different energy being of different masses and of different velocity, $v$, $v_1$, $v_2$, $v_3$ . . . . . Now the heterogeneous energy beam of MCI, is passed from Electric sector to obtain the homogeneous energy MCI beam. In homogeneous energy beam of MCI, energy of MCI, irrespective of their masses (nm) and velocities ($v$) will be the same. In the homogeneous energy beam, there are present MCI with masses nm, $n_1m$, $n_2m$, $n_3m$ with velocity $v$, $v_1$, $v_2$, $v_3$ . . . . and energy $\frac{nmv^2}{r}$, where r is the path subtended by MCI, with same energy in electric sector. In the beam with homogeneous energy of MCI, there are present MCI, nm, $n_1m$, $n_2m$, $n_3m$ . . . . with velocity $v$, $v_1$, $v_2$, $v_3$ . . . . and same charge. This energy beam is secured from heterogeneous energy beam of MCI by electric sector interaction with electrical part of MCI's moving through the electric sector. Function of electric sector is to squash the MCI, with same energy through interaction with the electrical part of MCI, under its influence. Now the homogeneous energy beam of MCI, coming from electric sector is exposed to the magnetic sector with strength 3 torr. MCIS with same masses will get coalesced and give the beam of MCI's with same masses as nm, $n_1m$, or $n_2m$,. . . . from magnetic sector, MCI beams with masses nm, $n_1m$, $n_2m$, $n_3m$ and in abundance $x$, $x_1$, $x_2$, $x_3$ . . . . ... are obtained from homogeneous energy beam from magnetic sector. Graph is plotted between the MCI, masses nm, $n_1m$, $n_2m$, $n_3m$ and their abundance $x$, $x_1$, $x_2$, $x_3$ . . . . is as follows

Now the smallest difference between adjacent peaks is calculated by subtraction method. Let this smallest difference between any two adjacent peaks is $dx$, and other adjacent differences are $dx_1$, $dx_2$, $dx_3$ . . . . .




The smallest difference $dx$, will be the molecular weight, if it is a whole number multiple, for the differences $dx_1$, $dx_2$, $dx_3$ . . . . or a simple fraction as $dx/2$, $dx/3$, or $dx/4$ … is a whole number multiple for all the differences in between the peaks. If the smallest difference '$dx$' is not the whole number multiple for the differences $dx_1$, $dx_2$, $dx_3$ . . . . . or its fraction $dx/2$, $dx/3$, or $dx/4$ …is also not the whole number multiple for differences, reject the whole exercise, and take a new spectrum, making changes in ionization process, in electric and magnetic sector,and again determination the smallest difference, and see if it is or a fraction of it is, a whole number multiple for the differences in between the peaks. For the determination of molecular weight of macro molecule, the method as stated above is employed, with simple change that the multiply charged MCI are generated. Multiply charged MCI are passed from electric sieve to secure the MCI of macro molecules with same multiple charges, may be of the order of 100 and rest of the method is the same as it is for micro molecules MCI, stated above.

## RESULTS

Simple mathematic is used for the molecular weight determination. If this mathematics, consisting of subtraction, division and multiplication is incorporated with computer program there is no need for the graph and molecular weight can be determined directly, as a reading in spectrometer. The molecular weight determined is a nominal molecular weight.

### Conclusion

It is a very simple technique for nominal molecular weight determination. Although the weight is not as exact as it is in case of high resolution molecular weight determination, still it will provide a guideline for sample nature and classification, and exact molecular weight can be determined, connecting H R, devices. In this method, no sophisticated technology involves and, no vacuum conditions are required, and with single electrical and magnetic, maneuvering, results are obtained. No molecular or isotopic peaks, isolation and identification, and nothing of the type of fragment and background peaks confusion. Simple MCI peaks, determination of differences between them, and finding the smallest difference, the whole number multiple, for all the differences, it is the molecular weight. I feel instrumentation for this will be quite handy of small size and low cost.

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