Ion Clustering

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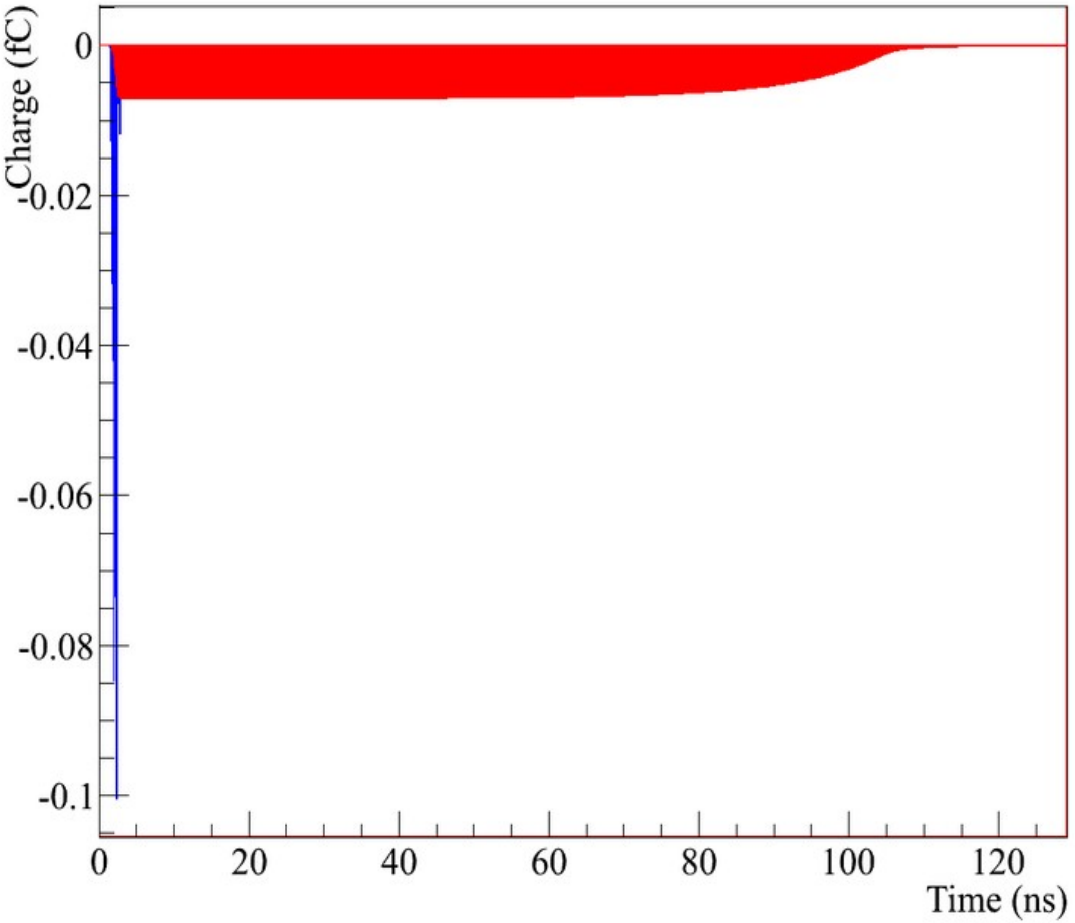
Introduction

- Ions effect in gas detectors
- Mobility of ions
- Clusters
- Structure of $(CO_2)_n$ clusters

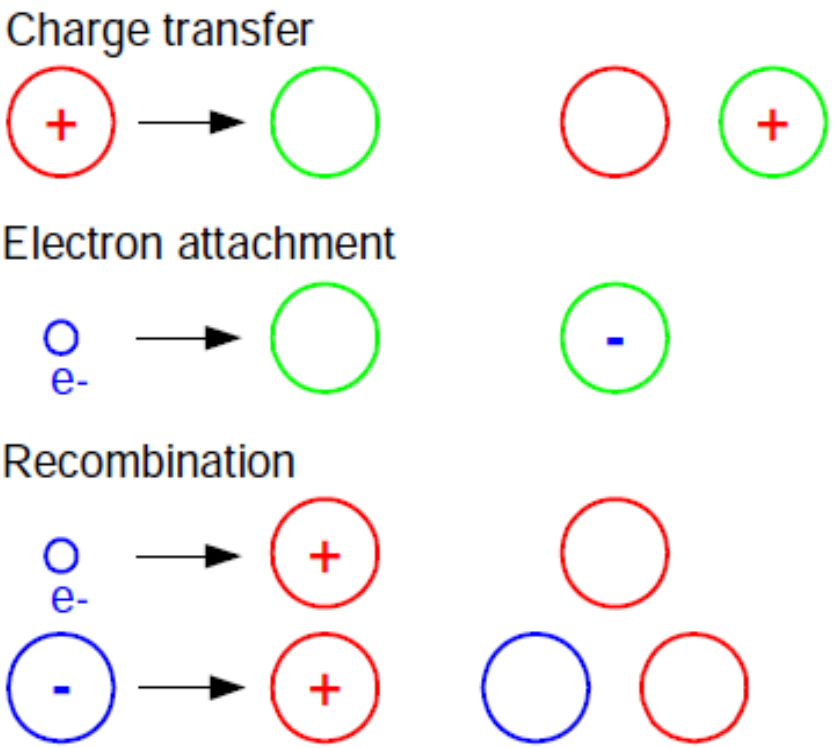
Ion Effect in Gas Detectors



- Ions can effect directly to signal.

http://en.wikipedia.org/wiki/MicroMegas_detector#mediaviewer/File:MMsigsimu.png
Simulation of induce signal on a Micromegas
MMsigsimu

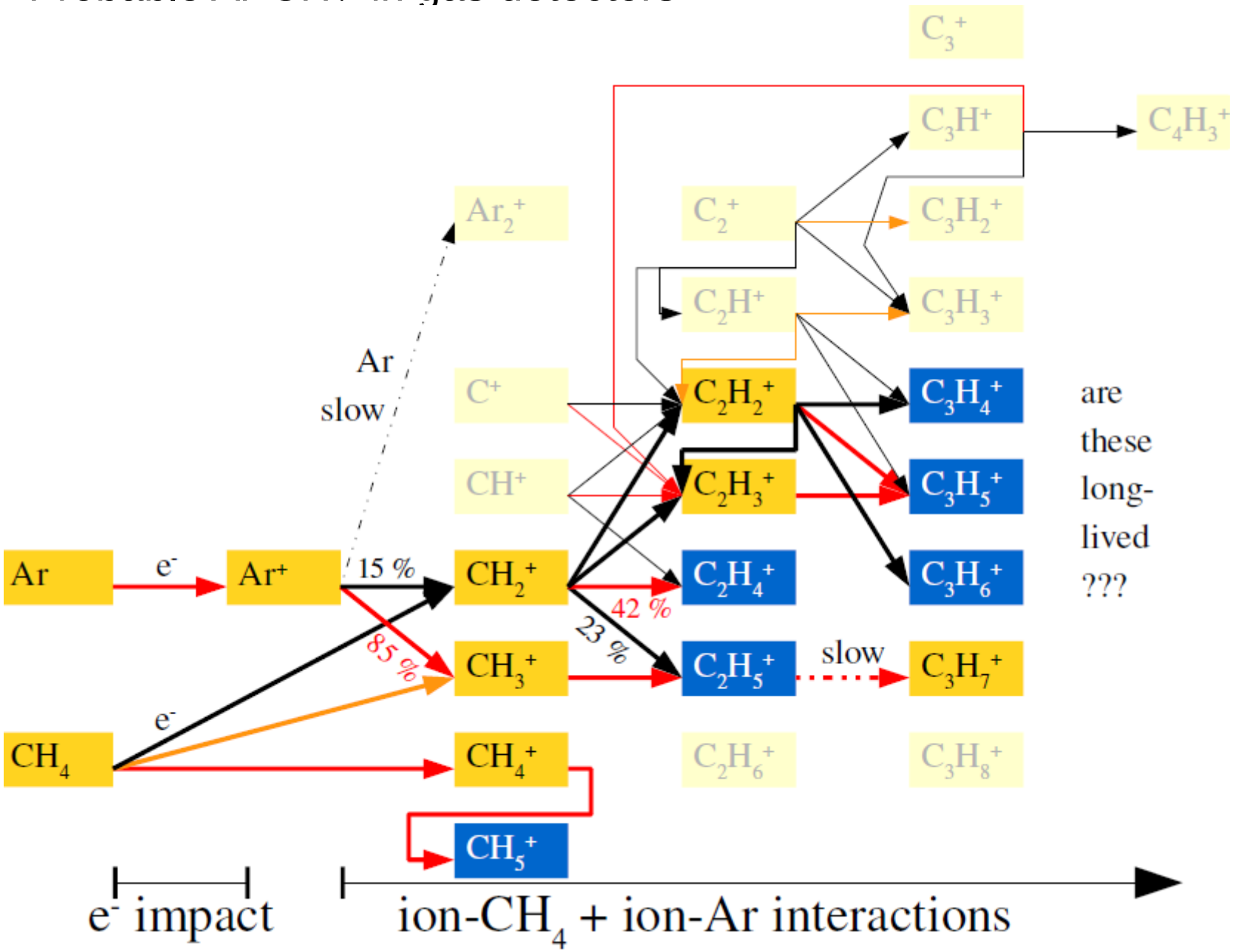
- Electron-ion pairs are in the random thermal motion and diffuse away..
- Charge transfer occurs when a positive ion encounters a neutral molecule.



Collisions between free electrons, ions and neutral gas molecules.

https://www.science.mcmaster.ca/medphys/images/files/courses/4R06/4R6Notes3_GasFilled_Detectors.pdf

- Probable Ar-CH_4 in gas detectors



Experimental Results: CO_2

Appearance Energies

CO_2^+	13.8 eV
CO^+	19.5 eV
O^+	19.1 eV

IONIZATION

$CO_2 + e \rightarrow CO_2^+ + e$ — above threshold 13.8 eV

$CO_2 + e \rightarrow CO_2^+ + e$ 84.7 %

$\rightarrow CO^+ + 1/2O_2 + e$ 3.7 %

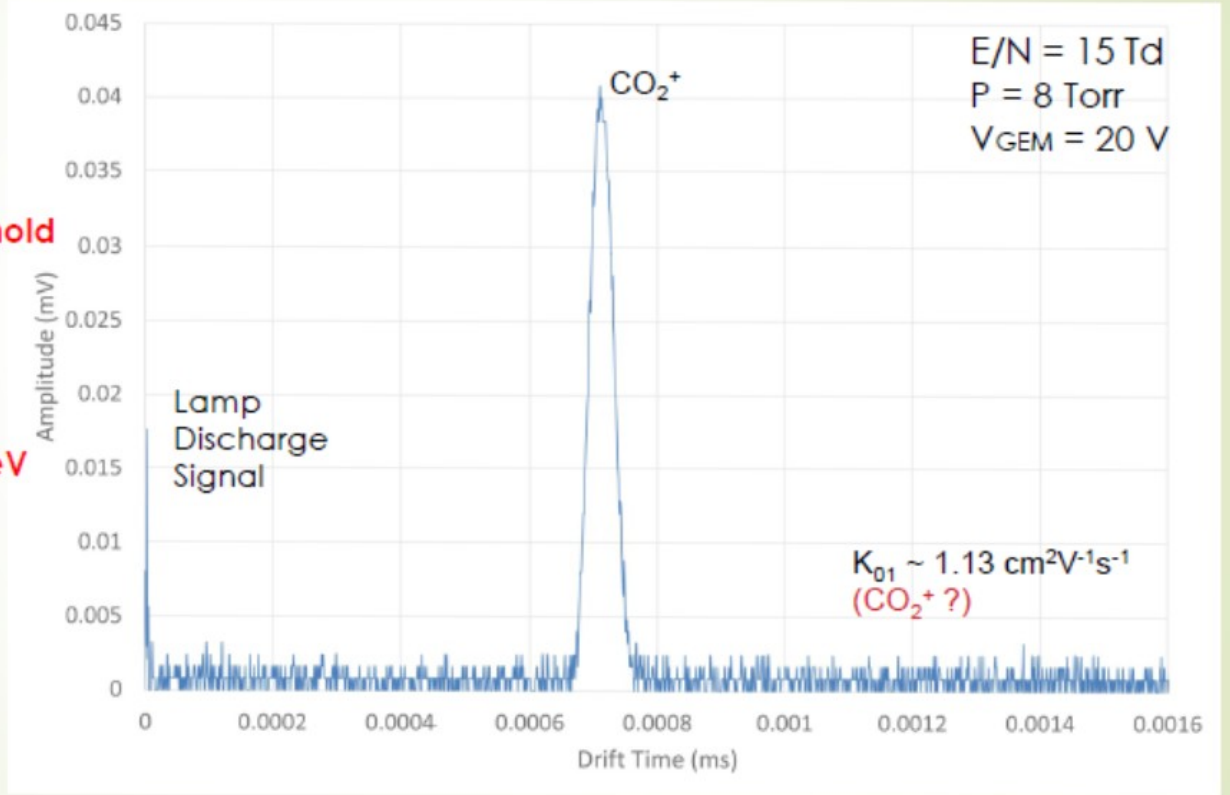
$\rightarrow O^+ + CO + e$ 5.4 % * — above 19.5 eV

REACTIONS

$CO_2^+ + CO_2 \rightarrow CO_2 + CO_2^+$

$CO^+ + CO_2 \rightarrow CO_2^+ + CO$

$O^+ + CO_2 \rightarrow O_2^+ + CO$



* values obtained from ionization cross sections for electron impact of 25 eV

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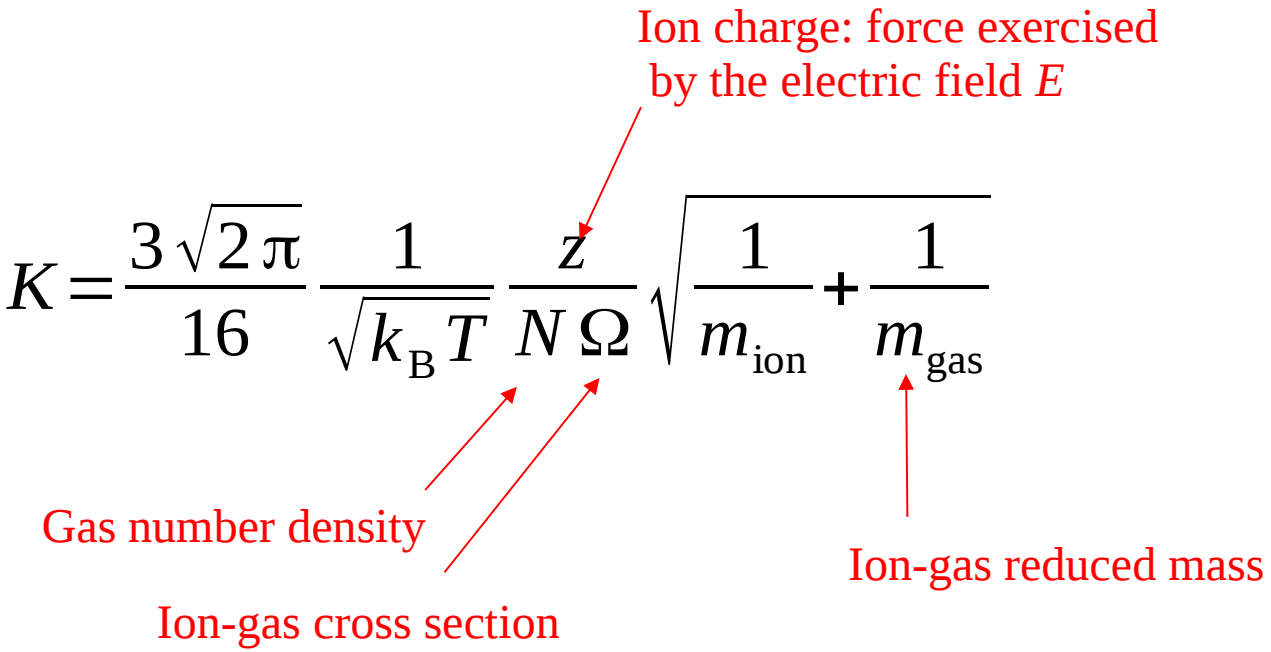
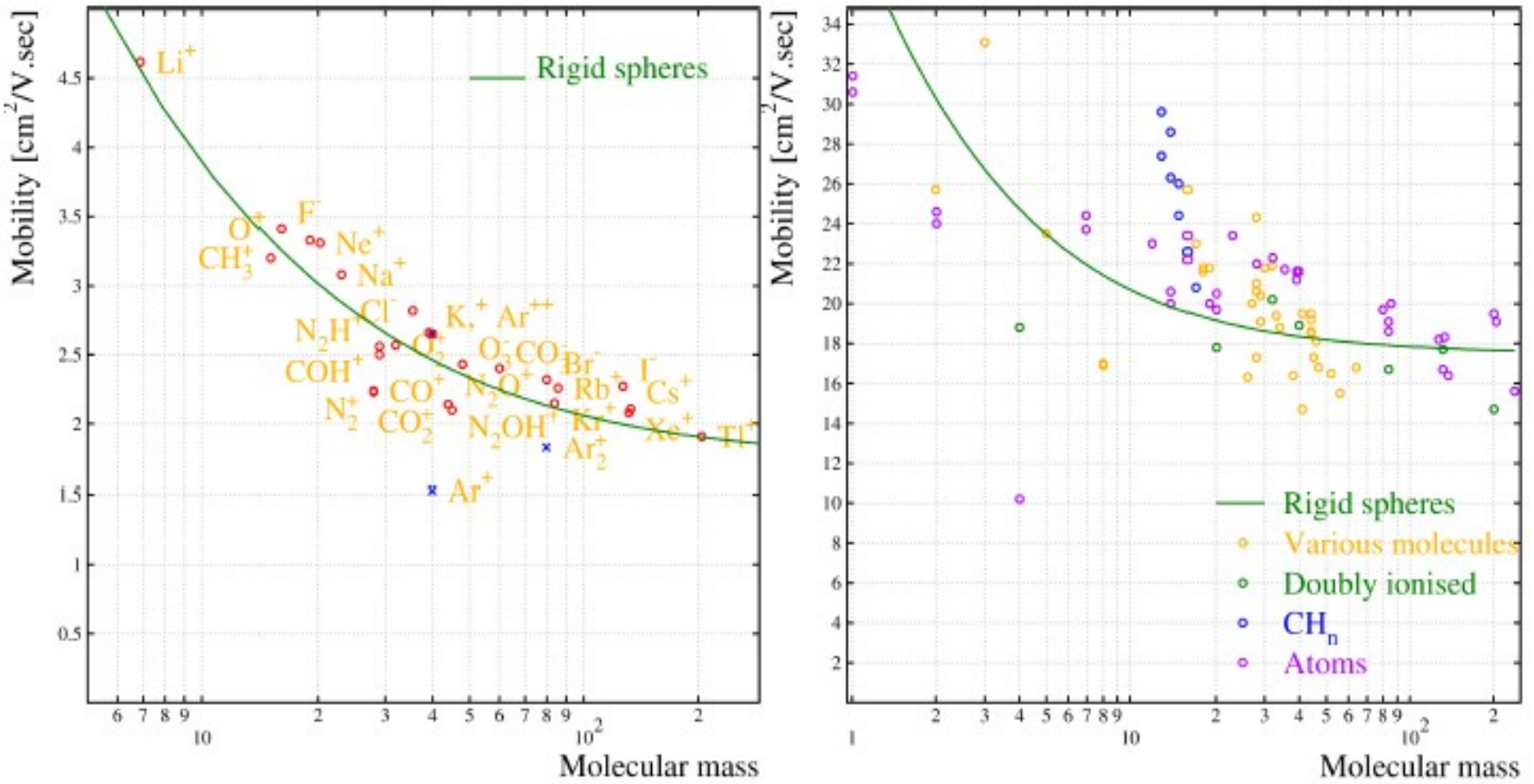
Mobility of ions

- Mason-Schamp (1958) relation:



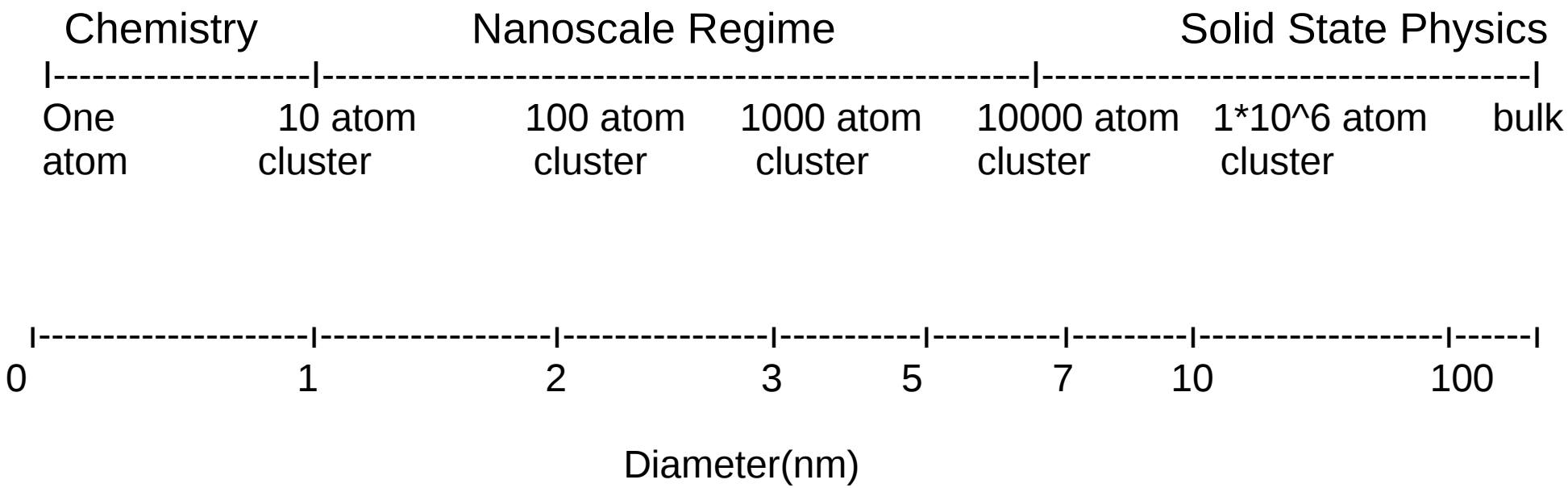
- *K* = velocity / *E*



- Some ions,atoms and molecules mobility have prepared to use to Garfield++ simulation program.

- In figures ; while some ions mass increases, their mobilities decreases in Argon gas .

Clusters



- Figure 1-1Size relationships of chemistry, nanoparticles, and solid state physics.

What are Clusters ????

Carbon dioxide clusters:
$(CO_2)_6$ to $(CO_2)_{13}$

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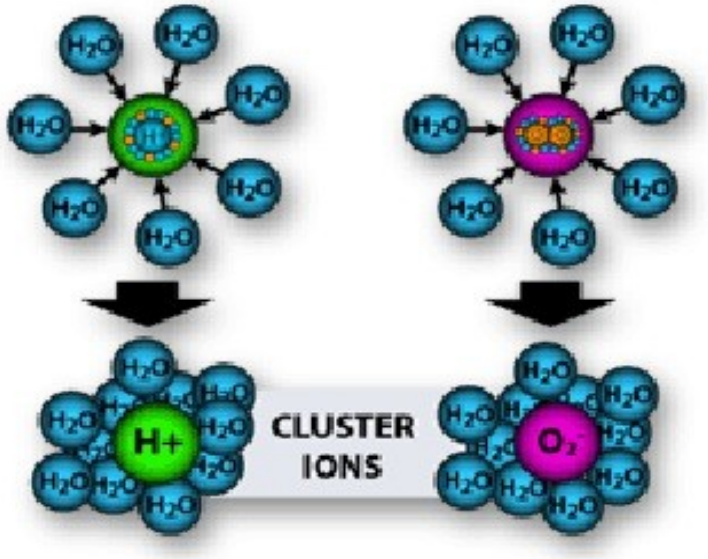
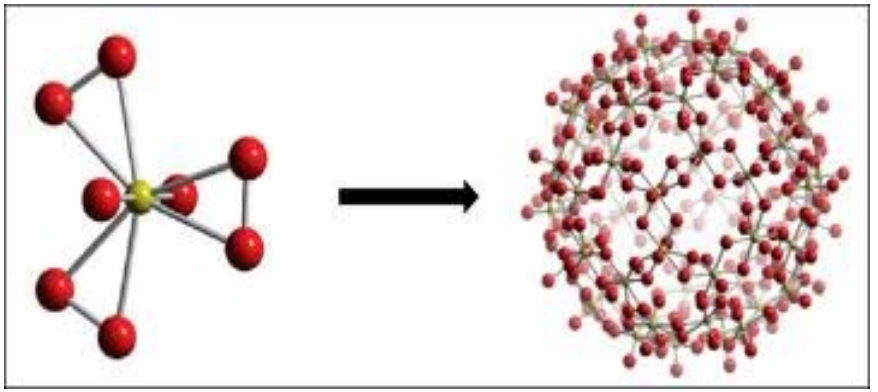
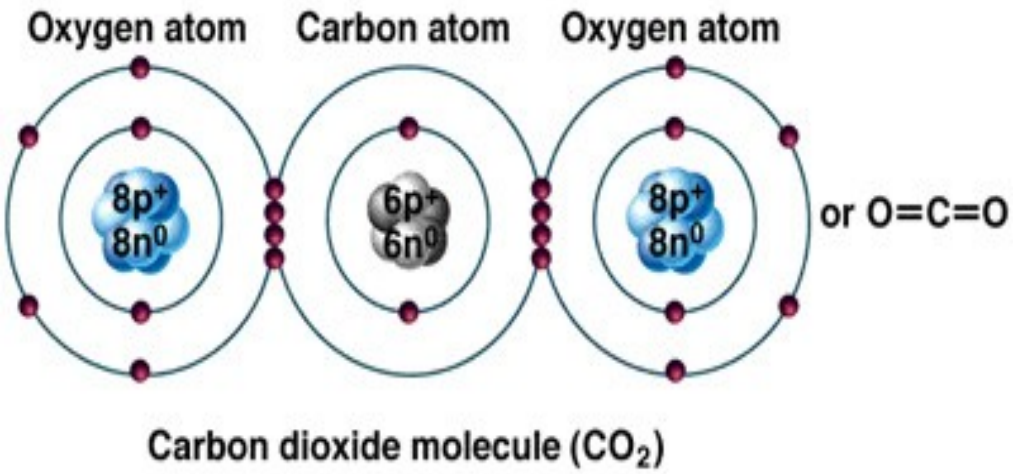




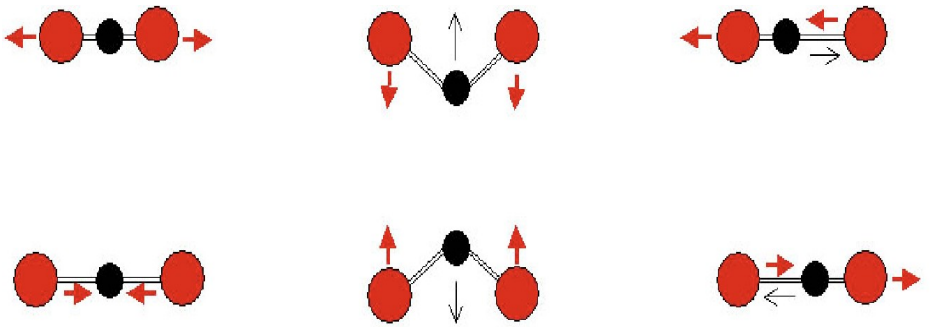
Formation of Covalent Bonds



Carbon dioxide molecule (CO_2)

O=C=O

116.3 pm



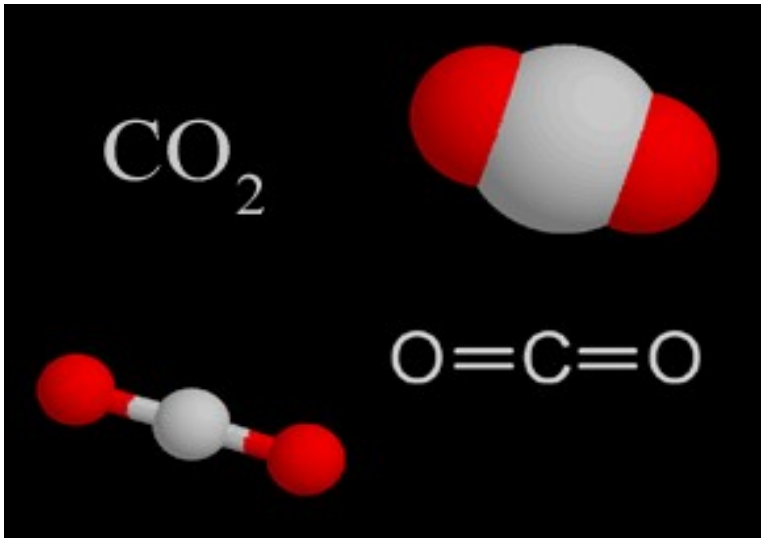
Symmetric Stretch
1366 cm^{-1}

Bending Mode
667 cm^{-1}

Asymmetric Stretch
2349 cm^{-1}

Oxygen

Carbon



Clusters are separated two groups;

1.Small Clusters between (1-100 atoms):

2.Large Clusters almost (5000 atoms):

.

- For a large cluster this size is small compared to the cluster radius r_0, and this leads to the hard sphere model for interactions between an atomic particle and a cluster with the following model potential:

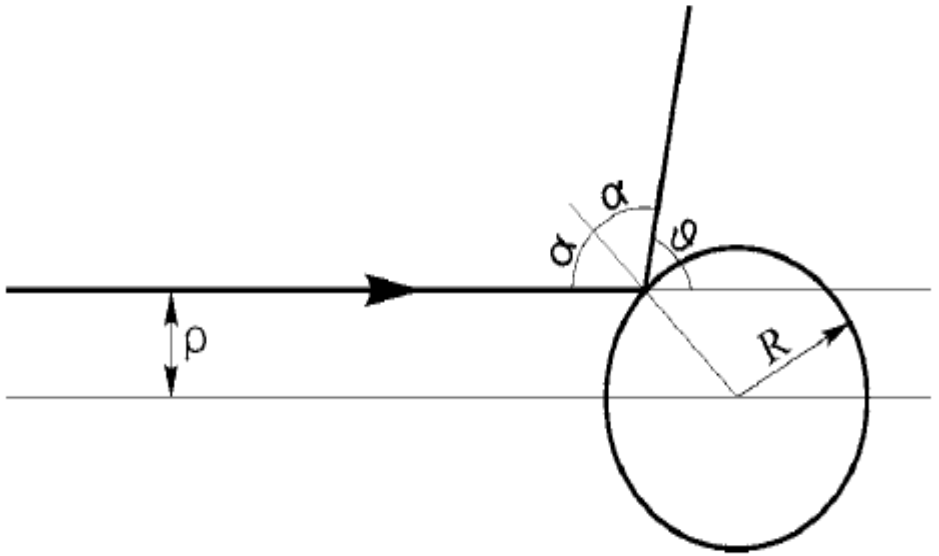
$$U(r) = \begin{pmatrix} 0, & r > r_0 \\ \infty, & r \le r_0 \end{pmatrix}$$

- In the case of an elastic scattering in the collision of an atomic particle with a cluster;

$$\frac{\rho}{r_0} = \sin\frac{\pi - \vartheta}{2} = \cos\frac{\vartheta}{2}$$

- For the differential cross section of scattering:

$$d\sigma = 2\pi\rho d\rho = \pi r_0^2 d\cos\vartheta$$

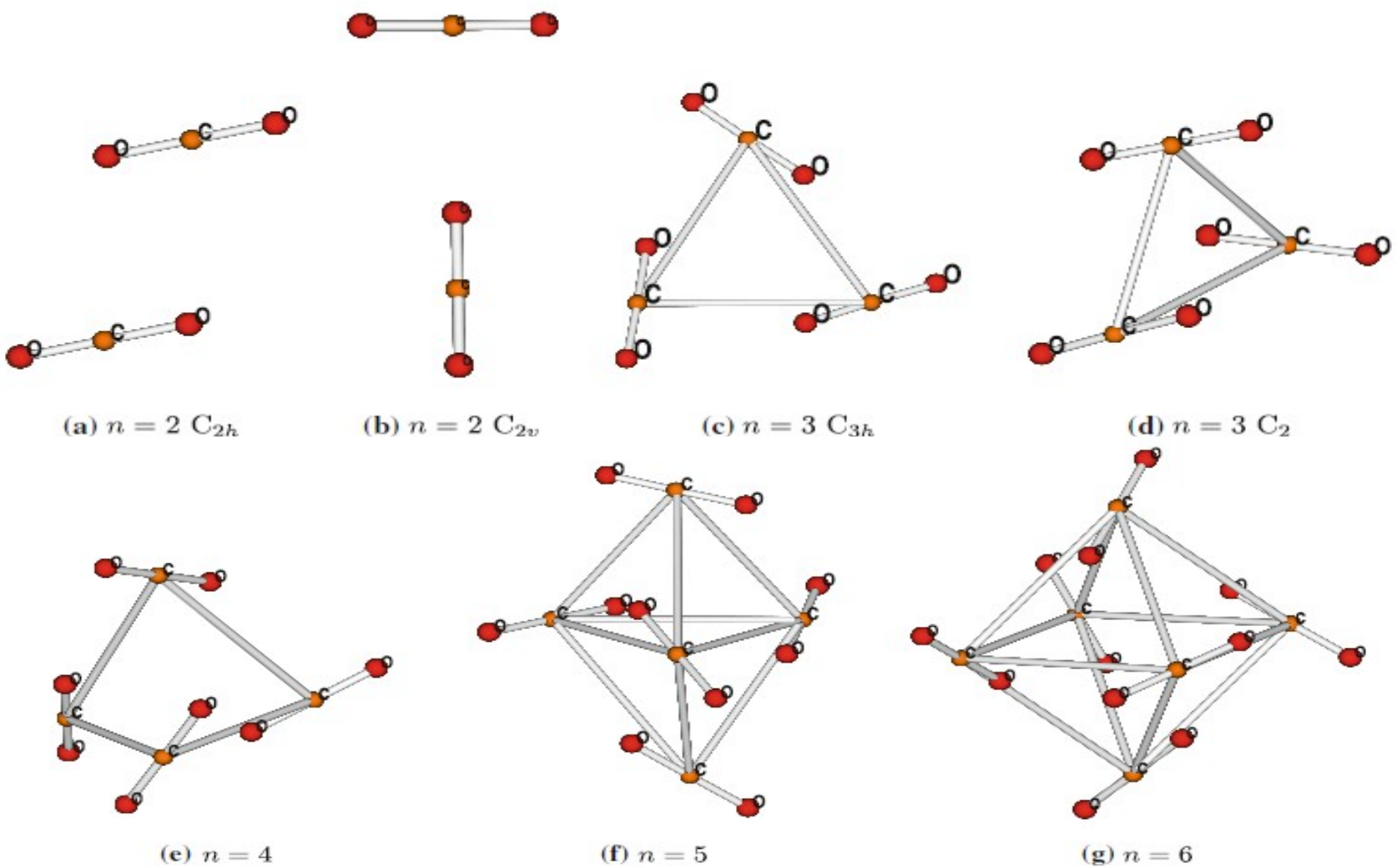


The following relations follow from this figure $\rho = R \sin \alpha$, $\vartheta = \pi - 2\alpha$, where ρ is the impact parameter of collision, R is the hard sphere radius, ϑ is the scattering angle.

- From this it follows for the diffusion (transport) cross section for elastic scattering of an atomic particle on a cluster within the framework of the hard sphere model

$$\sigma^* = \int (1 - \cos\vartheta) d\sigma = \pi r_0^2$$

STRUCTURE OF $(CO_2)_n$



(a) $n = 2$ C_{2h} (b) $n = 2$ C_{2v} (c) $n = 3$ C_{3h} (d) $n = 3$ C_2

(e) $n = 4$ (f) $n = 5$ (g) $n = 6$

http://link.springer.com/article/10.1007/s11224-013-0360-8/fulltext.html

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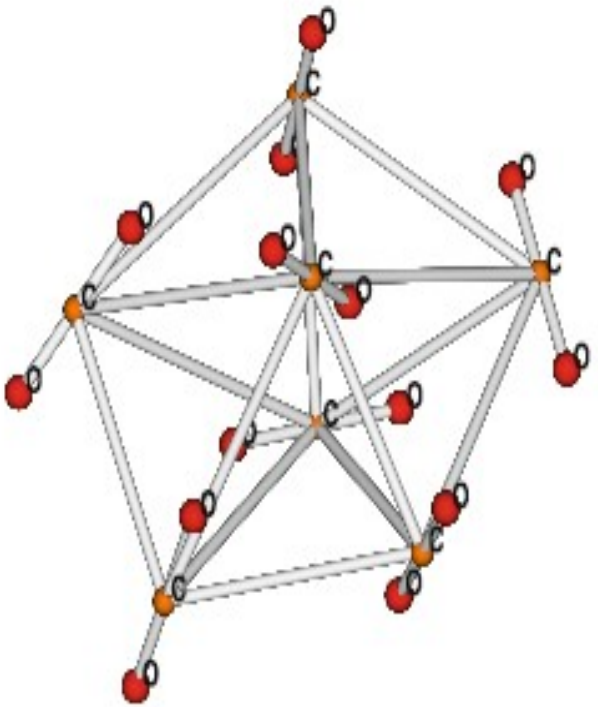
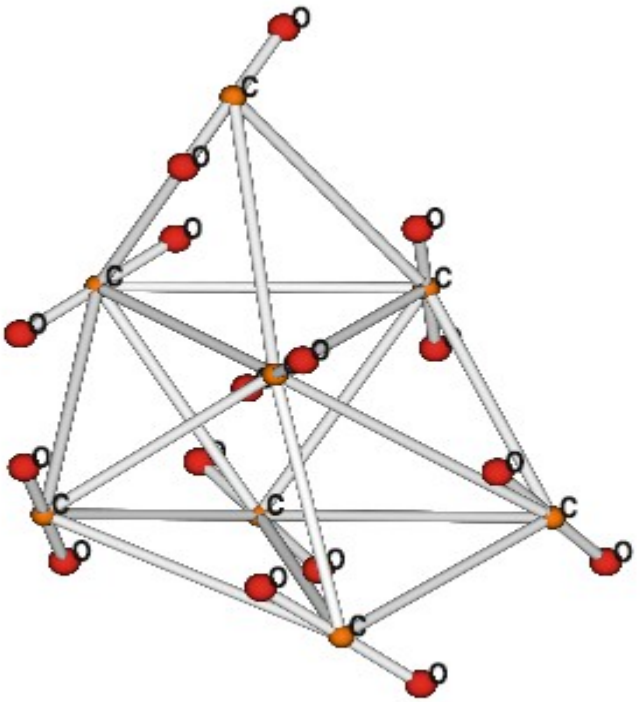


(h) $n = 7$



(i) $n = 8$

http://link.springer.com/article/10.1007/s11224-013-0360-8/fulltext.html

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- The C–O bond length is 1.16 A°
- The $(CO_2)n$ cluster potential energy function is given by;

$$U_{\text{total}} = \sum_i \sum_j \left(4\epsilon \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{r_{ij}} \right)$$

- where the index i denotes the carbon and the sum run overall atoms (j) of the cluster system.

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Table 1 Location of point charges in potential energy function for $(CO_2)_n$

Site	Z (Å)	Q (e)
1	−1.5232	0.1216
2	−1.0663	−0.6418
3/C	0.0000	1.0404
4	1.0663	−0.6418
5	1.5232	0.1216

Table 2 LJ parameters in potential energy function for $(CO_2)_n$

Atom pair	ϵ (K)	σ (Å)
C–C	26.3	2.824
C–O	75.2	3.026
O–O	44.5	2.925

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CO_2-cluster	Average C–C bondlength (Å)
$(CO_2)_2$	3.41
$(CO_2)_3$	3.44
$(CO_2)_4$	3.57
$(CO_2)_5$	3.60
$(CO_2)_6$	3.64
$(CO_2)_7$	3.53
$(CO_2)_8$	3.58
$(CO_2)_9$	3.61
$(CO_2)_{10}$	3.73
$(CO_2)_{11}$	3.69
$(CO_2)_{12}$	3.74
$(CO_2)_{13}$	3.64

Table 3 Variation of C–C bond length of $(CO_2)_n$ calculated at M062X/6-311++G(d,p)

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