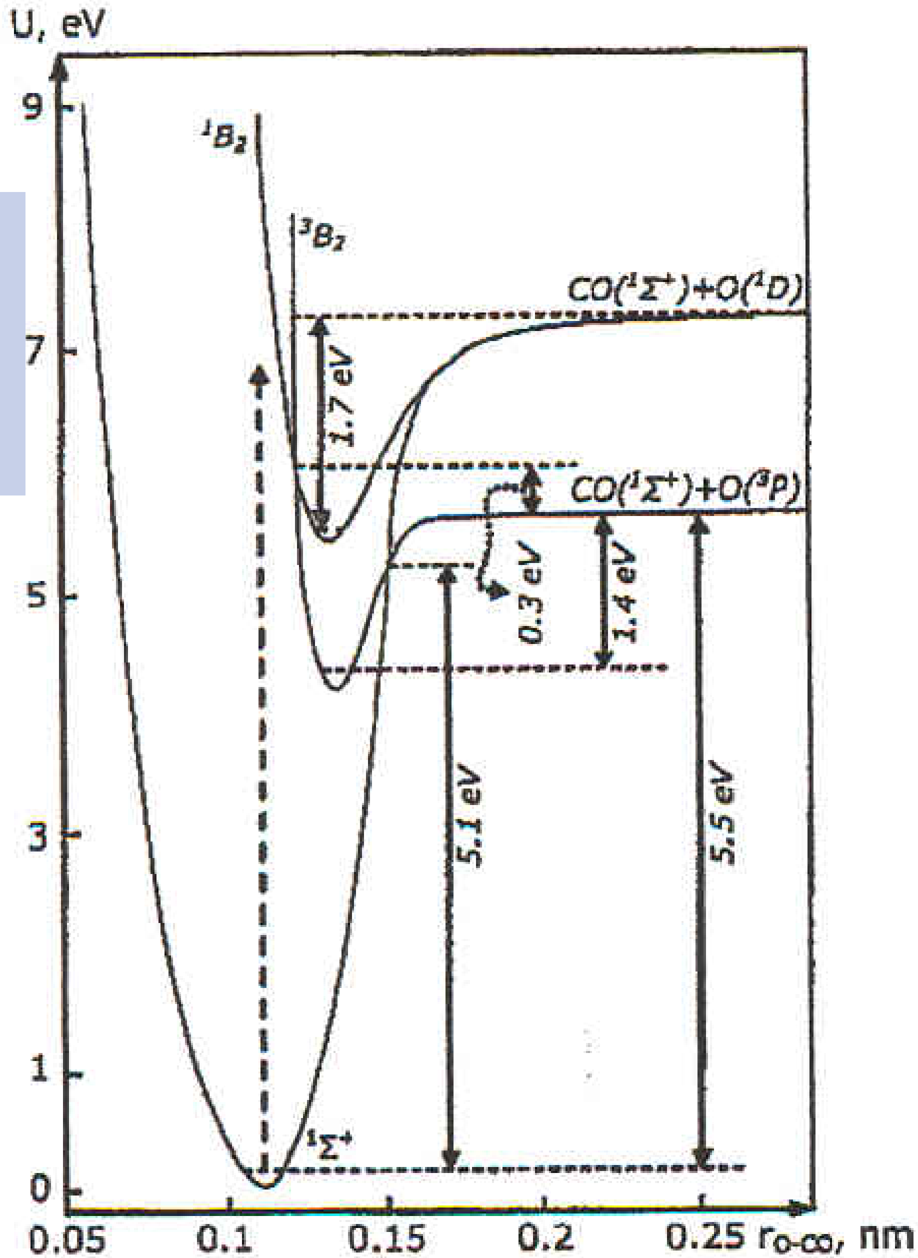
6°) carbon dioxide properties

$CO2 \rightarrow CO + O$

Excited states of

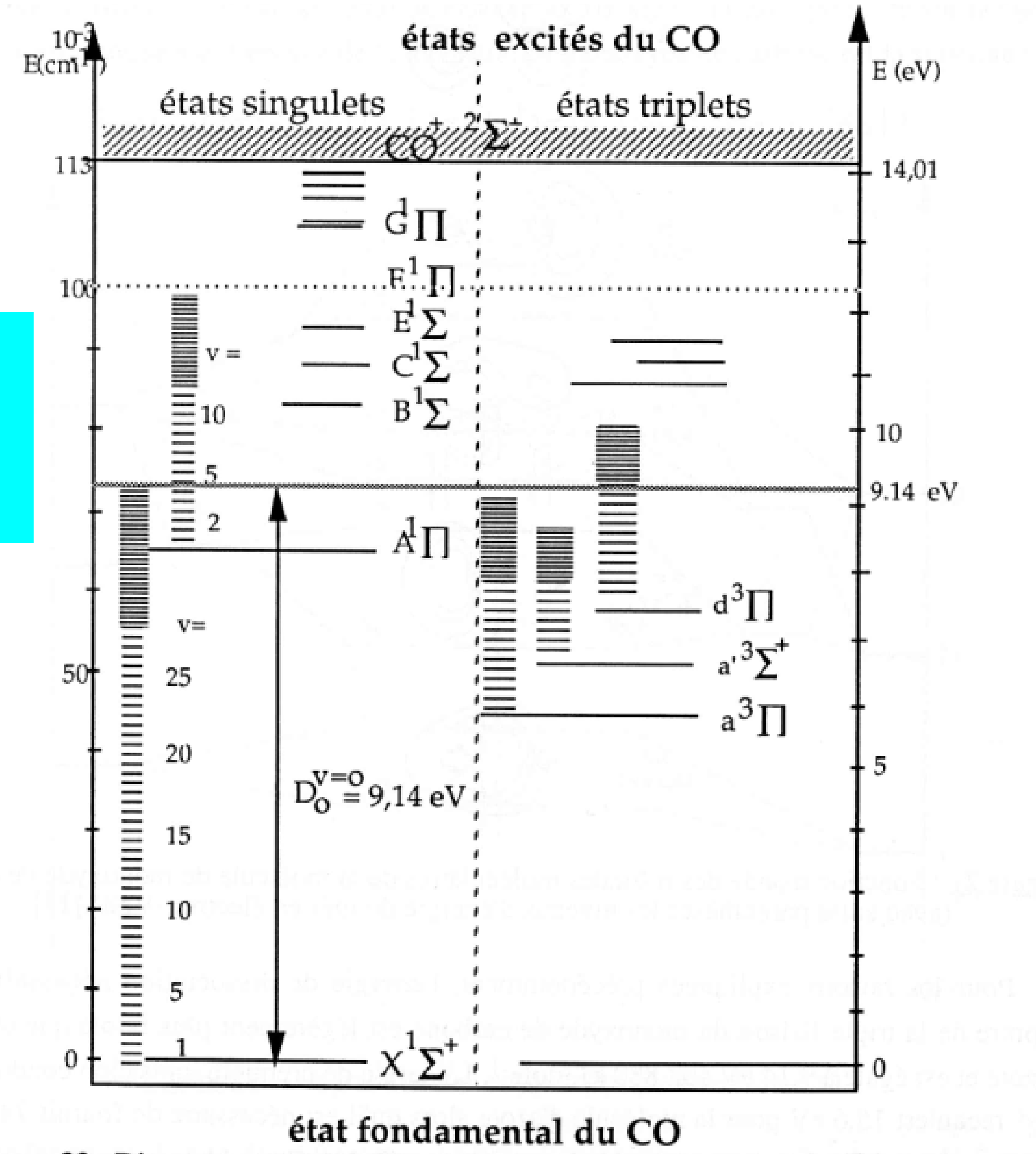
carbone dioxide

(energy states versus distance)



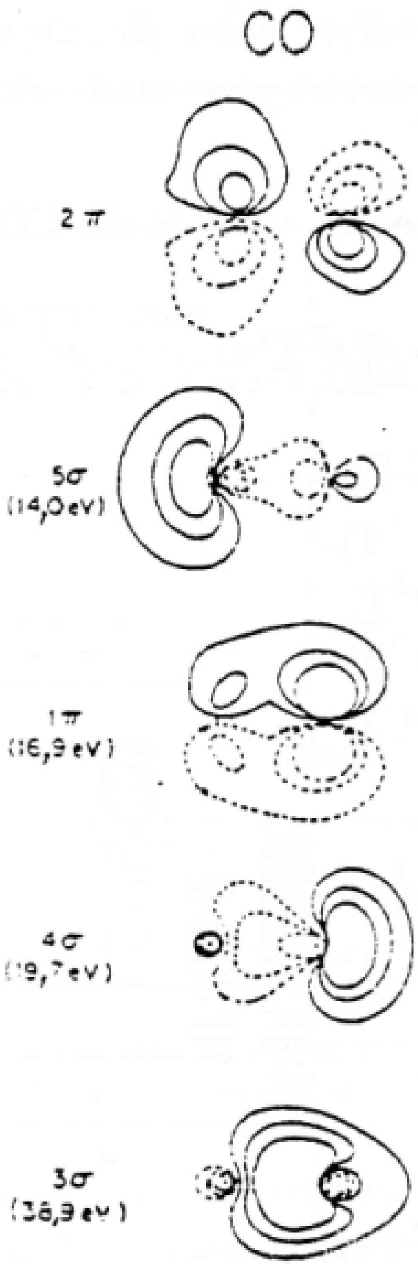
EMRS FALL MEETING
Varsaw 13-15 sept 2010

Excited states of Carbone monoxide molecule



gure 22 : Diagramme simplifié des différents états électroniques et vibrationnels du monoxyde de carbone en fonction de l'énergie potentielle de la molécule [14][15]

Molecular shapes of carbone monoxide molecule



Excited state 2
Lumo orbital

Very strong polar
Homo orbital

Figure 21 : Fonction d'onde des orbitales moléculaires de la molécule de monoxyde de carbone (avec entre parenthèses les niveaux d'énergie donnés en électron-Volt).[13]

Main mechanisms during plasma excitation of CO_2 molecules

1 – Electron impact

- $e + CO_2 \rightarrow CO_2^-$
- $e + CO_2 \rightarrow CO_2^+ + 2e$
- $e + CO_2 \rightarrow CO_2^* + e$

2 – Dissociatif attachment

- $CO_2 + e \rightarrow CO^+ + O + 2e$
- $\rightarrow CO + O+ + 2e$
- $e + CO_2 \rightarrow CO_2^+ + 2e$
- $e + CO_2 \rightarrow CO_2^* + e$

3 – Molecular reaction

- $CO_2^+ + CO_2 + CO_2 \rightarrow C_2O_4^+ + CO_2$
- $C_2O_2^- + CO_2 + CO_2 \rightarrow C_3O_4^- + CO_2$
  cluster formation
- $C_2O_4^+ + e \rightarrow CO + CO + O_2$
- $CO_2^- + CO_2 \rightarrow C_2O_4^-$
- $C_2O_4^- \rightarrow CO + CO_2 + O^-$
- $C_2O_4^- + CO \rightarrow C_2O_3^- + CO_2$

4 – Carbon monoxide reaction

- $CO \rightarrow CO^+ + e-$
- $CO + CO \rightarrow C_2O_2 \rightarrow C_4^+O_4 + e$
- $CO \rightarrow C_2O + O + e$

CO_2 dissociation

1 – Vitrational state
- $CO_2*(^1\Sigma^+) \rightarrow CO(^1\Sigma^+) + O(^1D)$ E # 7 eV/mol
- $CO_2*(^1\Sigma^+) \rightarrow CO2*(^3B_2) \rightarrow CO(^1\Sigma^+) + O(^3P)$ E = 5.5 eV/mol
- $O + CO_2* \rightarrow CO + O_2$ E # 0.5 – 1 eV/mol

2 – Direct electronic impact
- $e + CO_2(^1\Sigma^+) \rightarrow CO(a^3\Pi) + O(^3P)$
- $e + CO_2 \rightarrow CO + O^-$

3 – Intermolecular collision
- $CO_2(^1\Sigma^+) + CO(a^3\Pi) \rightarrow CO(^1\Sigma^+) + CO\ (^1\Sigma^+) + O(^3P)$

4 – Vibrational excitation of CO
- $CO(X'\Sigma^+,V) + e \rightarrow CO(X^1\Sigma^+,W) + e$

5 – Electronic excitation
- $CO(X^1\Sigma^+,V) + e \rightarrow CO(Y,W) + e$

6 – Ionisation
- $CO(X^1\Sigma^+,V) + e \rightarrow CO+(X^2\Sigma^+,W) + 2\ e$

7 – Dissociation
- $CO(X^1\Sigma^+,V) + e \rightarrow C(^3P) + O(Y) + e$
- $\rightarrow C(Y) + O(^3P) + O(Y) + e$

8 – Vibrational relaxation
- $CO(X^1\Sigma^+,V) + CO(X^1\Sigma^+,W) \rightarrow CO(X^1\Sigma^+,V-1) + CO(X^1\Sigma^+, W + 1)$

9 – Electronic energy emission
- $CO(B'Z^+\ v) \rightarrow CO(A'\Pi,W) + hu$

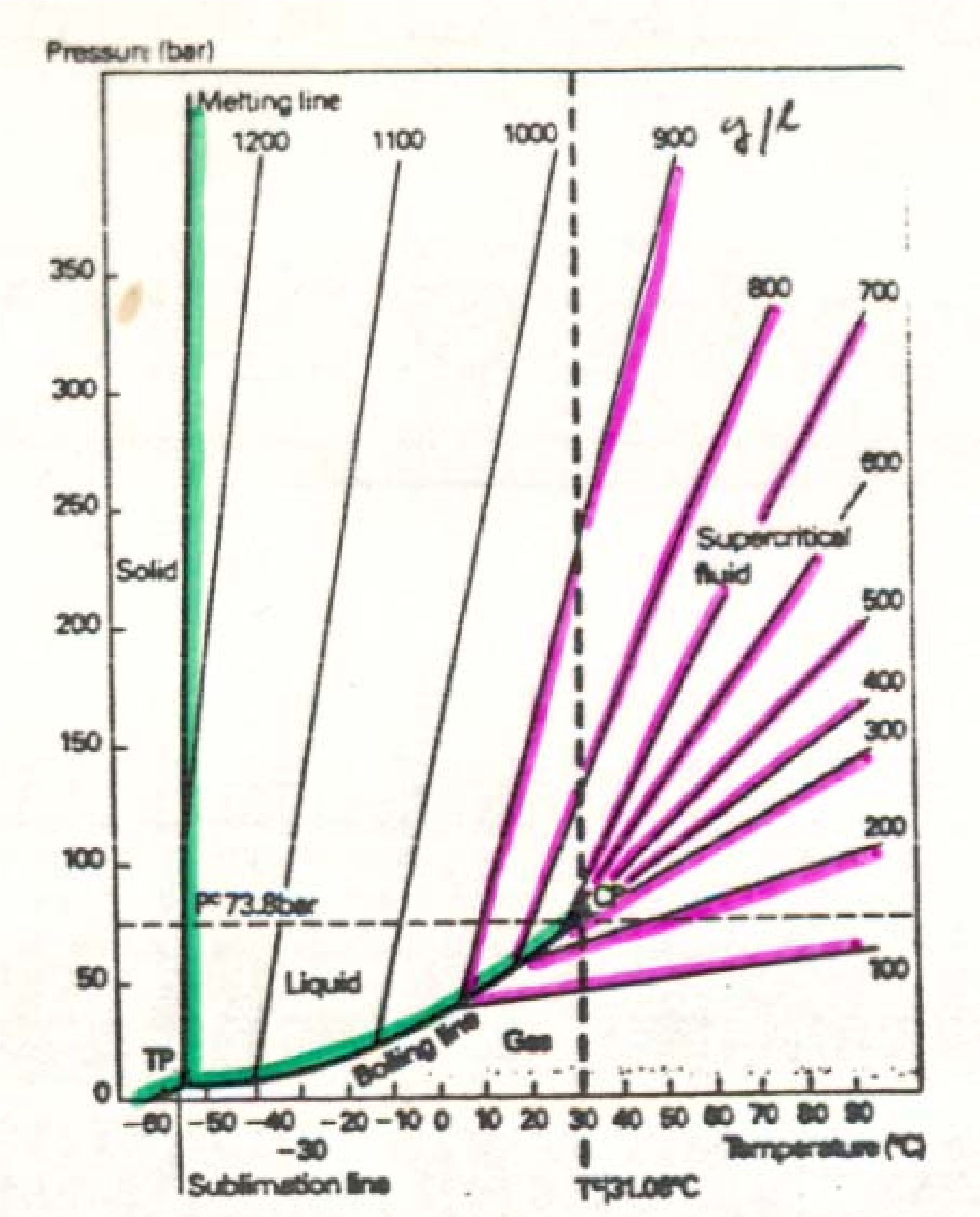
10 – Recombinaison
- 10.1. $C(^3P) + O(^3P)$ + wall $\rightarrow CO(Y,V)$ + paroi
- 10.2. $C(^3P)$ + wall $\rightarrow$ deposit C_s
- 10.3. $O(^3P)$ + wall $\rightarrow$ Oads $\rightarrow O_{2g}$ + wall

11 – Dismutation
- $CO(a^3\Pi) + CO \rightarrow CO_2 + C$ wall transfert or catalysis
- $CO(Y,V) + O(^3P) \rightarrow CO_2*$ + energy on wall

12 – Decomposition
- $CO_2 + C \rightarrow CO + CO$

Property/Molecule	CO_2	CH_4
Molecular weight	44	16
Boiling point (deg C)	-78.4 C	-161.5 C
Density (kg/m3)	775.3	424.0
Volume expansion factor	556.0	636.5
Moles/m3 (liquid)	17,620.5	26,500.8
Critical Point (T/P)	30.5 C ; 73.52 bar	-82.1 C ; 46.41 bar

CO2 a supercritic liquid



Isodensity diagram in g/l

Carbon dioxide

The solvating power can be tuned and controlled.

↓

Adjust the temperature and pressure

Above its critical point 31.7°C and 73.8 atmospheres), the distinction between a liquid and a gas disappears.

CARBON DIOXIDE FOR GREEN CHEMISTRY

Nidwaree Wanna G 5136122
Chemw.sc.mahidol.ac.th/html/scess/2008-scch503/CO2.ppt

Carbon dioxide

- Nontoxic
- Nonflamable
- Abundant
- Cheap

a substitute for harzadous organic solvents which are usually carcinogens.

CARBON DIOXIDE FOR GREEN CHEMISTRY

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Chemw.sc.mahidol.ac.th/html/scess/2008-scch503/CO2.ppt

carbon dioxide for oil recovery because of its solvant properties

- **one ton of CO2 gives 1.5 ton of oïl**

- **business plan**:
- 50euros CO2 ⇨ 900 euros of oil
- (average value)

- It needs for that an **european pipe for CO2 to the oil field of Scotland or Norway**

- ref Energy and environmental Science vol3,N°1,Jan 2010 p43-81, M.MikkelsenM.Jorgensen,F.C.Krebs