



# 电子碰撞谱学的新机遇与新进展

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1. 背景
2. 电子与原子分子碰撞电离的实验和理论
  - (1) 实验技术
  - (2) 理论方法
3.  $(e, 2e)$ 电子动量谱学的新进展
  - (1) 谱仪技术新进展;
  - (2)  $(e, 2e)$ 的分子多中心干涉效应。
4. 扫描探针电子能谱学
  - (1) 谱仪技术的发展;
  - (2) 非线性非弹性电子散射现象。





# 1. 背景

## 2. 电子与原子分子碰撞电离的实验和理论

(1) 实验技术

(2) 理论方法

## 3. (e, 2e)电子动量谱学的新进展

(1) 谱仪技术新进展;

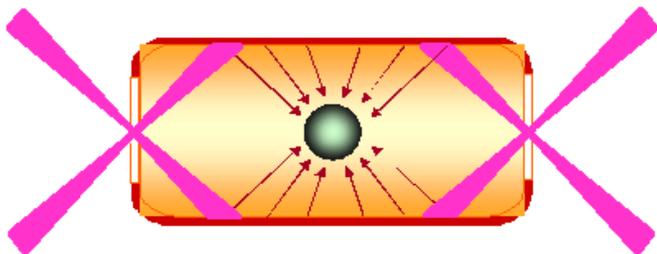
(2) (e, 2e)的分子多中心干涉效应。

## 4. 扫描探针电子能谱学

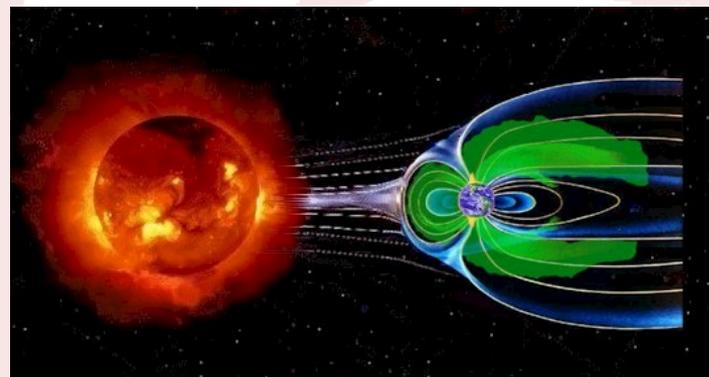
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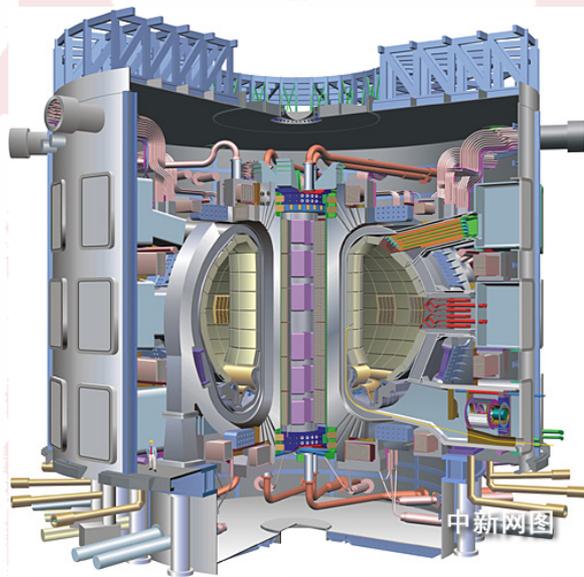




惯性约束聚变



空间物理



磁约束聚变

**Planetary Nebulae**

- > Gaseous envelopes ejected by low- and intermediate- mass stars in their advanced evolutionary stages
- > Major sources of C, N and s- process elements in the Universe
- > Idea laboratories to study astrophysical plasmas

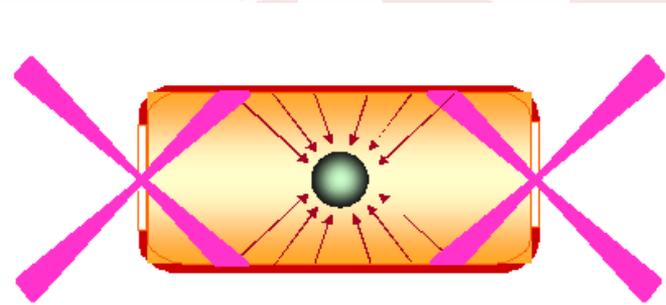
B. Balick

X - W. Liu, Atomic and molecular processes in ionized nebulae, Lan Zhou, 12 August 2002

天体物理



- 在高能量密度环境中原子结构的变化?
- 原子动力学行为的变化?
  - a. 光过程
  - b. 电子碰撞过程
  - c. 重粒子碰撞过程

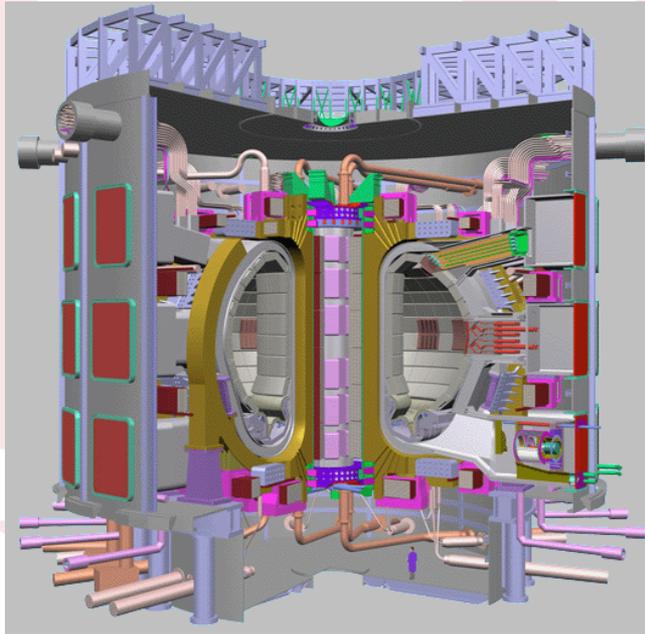


惯性约束聚变

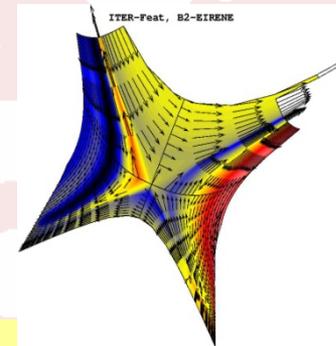
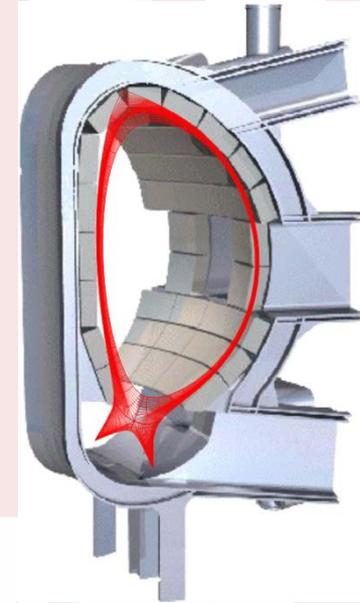




# Plasma edge/divertor region



磁约束聚变



**ITER: Furnace chamber:**

**Ø 15 m   6.8 m high   5.3 T   15 MA   500 MW   8 min**



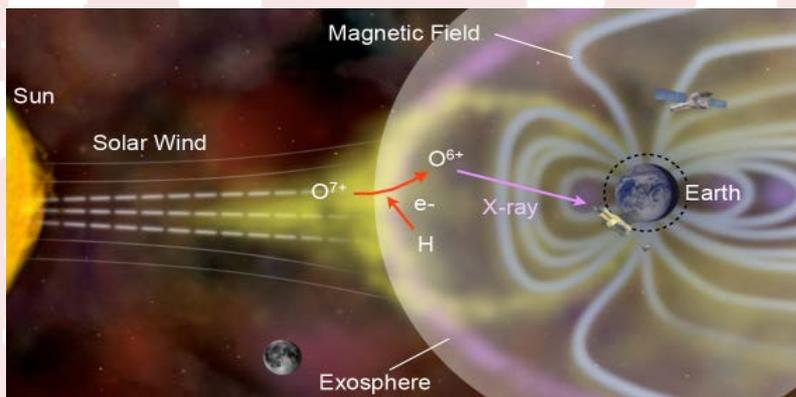


## Atomic and molecular processes in edge/divertor plasma regions

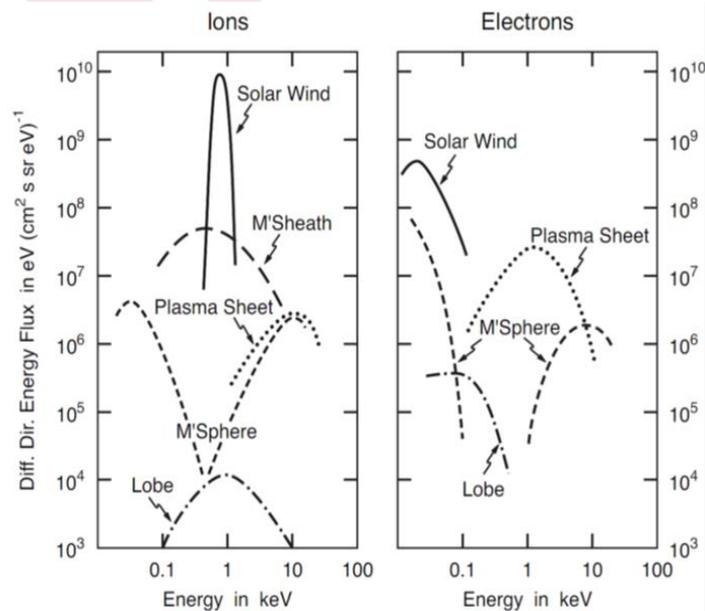
- Plasma compositions: ( $T \sim 0.5 - 100$  eV)
    - e, p, H,  $H_2$ ,  $H_2^+$ ,  $H_3^+$ ,  $H^-$ ;
    - neutral and low-q atomic impurities (Be, C, B, N, W);
    - molecular impurities and their singly charged ions (BeH,  $BeH_2$ , BH,  $BH_2$ , CH .....  $C_3H_8$ ,  $N_2$ )
- \*\*\* Molecular species are vibrationally excited!!



# 太阳风与星际介质或行星大气相互作用； 行星外层大尺度鞘层结构。



空间物理



近地空间中离子和电子的能量分布



## 天体物理中的重大问题

### ● 黑洞的性质

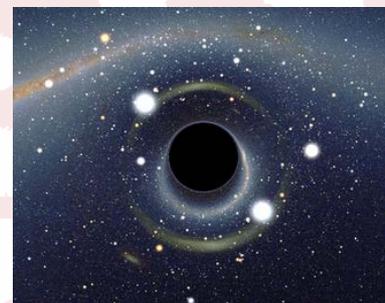
质量



黑洞近邻区域  
物质的化学构成  
和物理条件



天文观测光谱



黑洞模拟图

自旋



黑洞视界附近  
超大引力条件  
下物质化学构成  
和物理条件



天文观测光谱

### ● 天体起源中关键问题：恒星系统的形成与演化

恒星形成



分子云团的  
化学构成和  
物理条件



天文观测光谱



大麦哲伦星云中的  
LH95恒星孕育

恒星是由星际介质中最致密的分子云团形成的



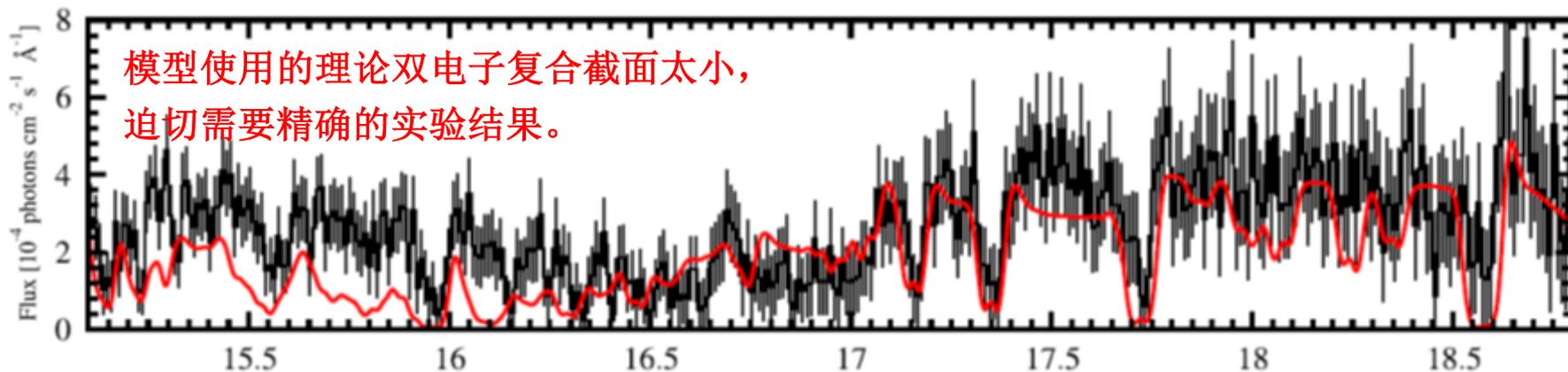
## 原子分子参数与高精度谱学数据

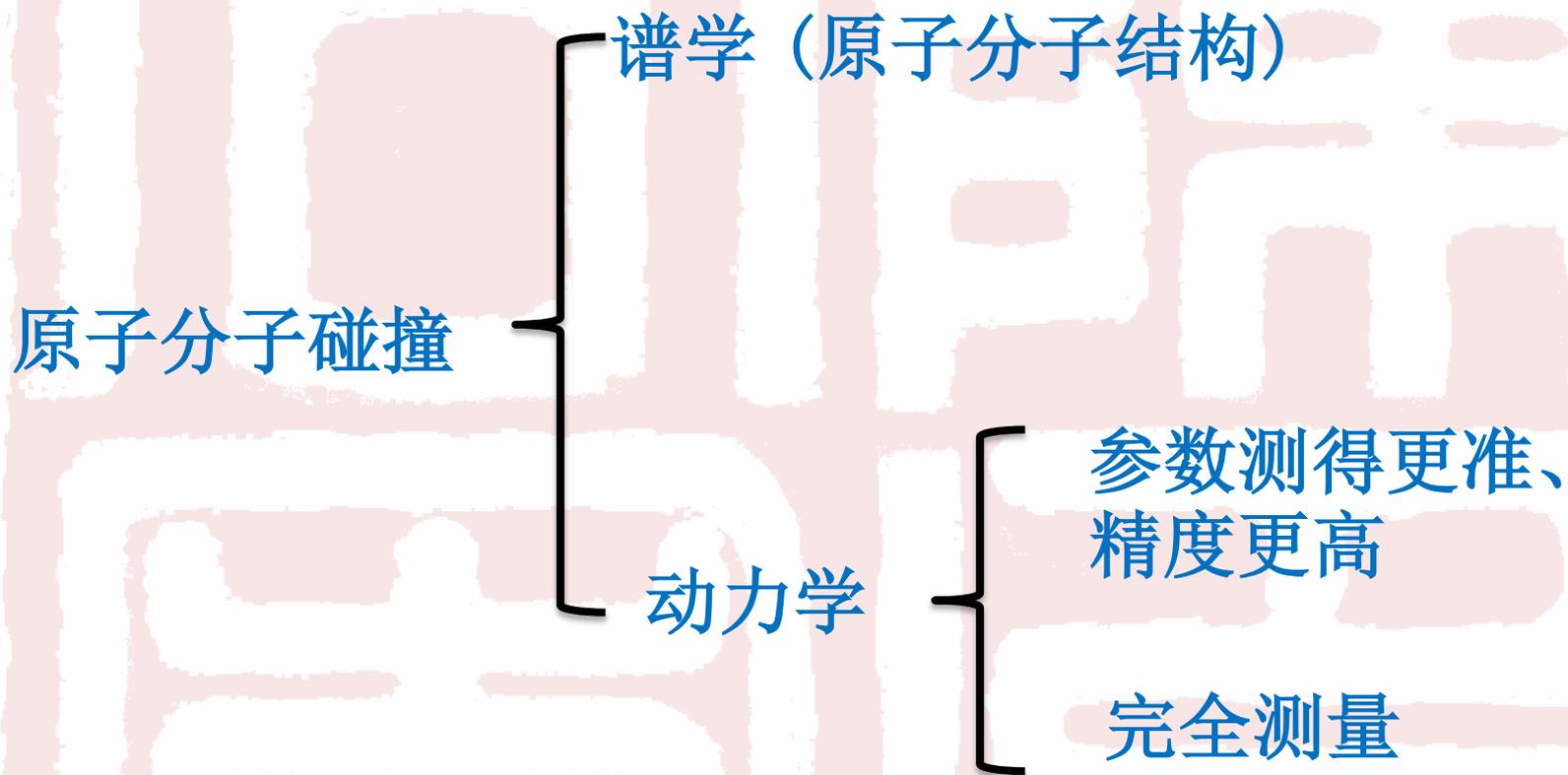
天文模型：依赖于精确的原子分子物理参数，包括：光激发、电离、解离，以及电子、离子、原子和分子的碰撞激发、电离、解离等原子分子物理参数。

高精度的实验室谱学数据：对天文观测光谱的准确解释极大地依赖于天文模型和高精度的谱学数据和准确标识。

**Chandra天文卫星观测结果：**

**AGN (Active Galactic Nuclei) NGC 3783**







## 原子分子碰撞最显著的发展方向

简单体系  复杂体系

- (1) 从单电子原子、双电子原子向重原子的开壳层体系发展；
- (2) 从双原子分子向多中心体系发展；
- (3) 从弹性散射、激发向单电离、多电离和电离解离发展；
- (4) 从随机取向分子的碰撞向取向分子的碰撞发展；
- (5) 从基态原子分子的碰撞向激发态的碰撞发展；
- (6) 从孤立环境下的原子分子过程向极端环境下的原子分子过程发展。

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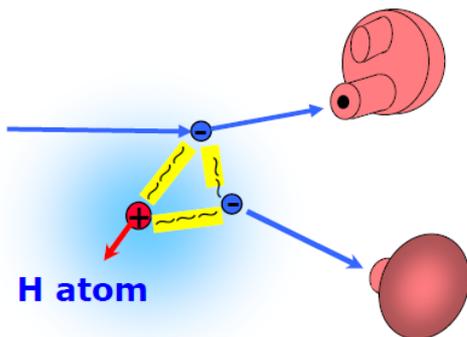


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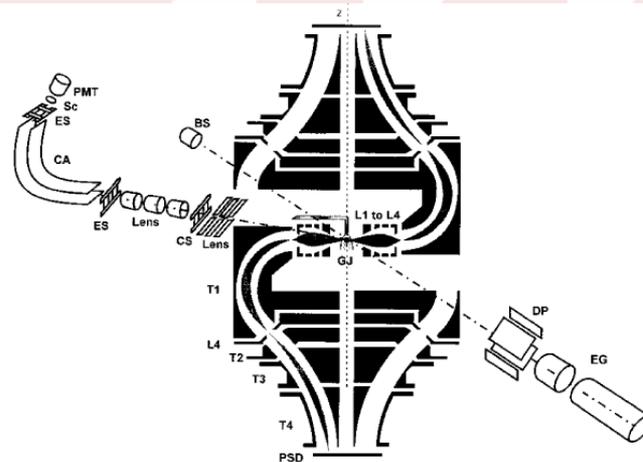
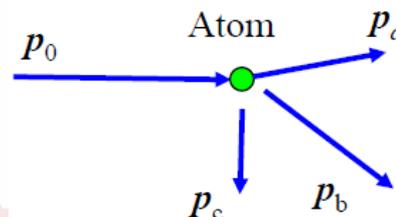


# 实验 (多重符合技术的发展)

Coincident (e,2e) measurement  
 $e + H \rightarrow H^+ + e + e$



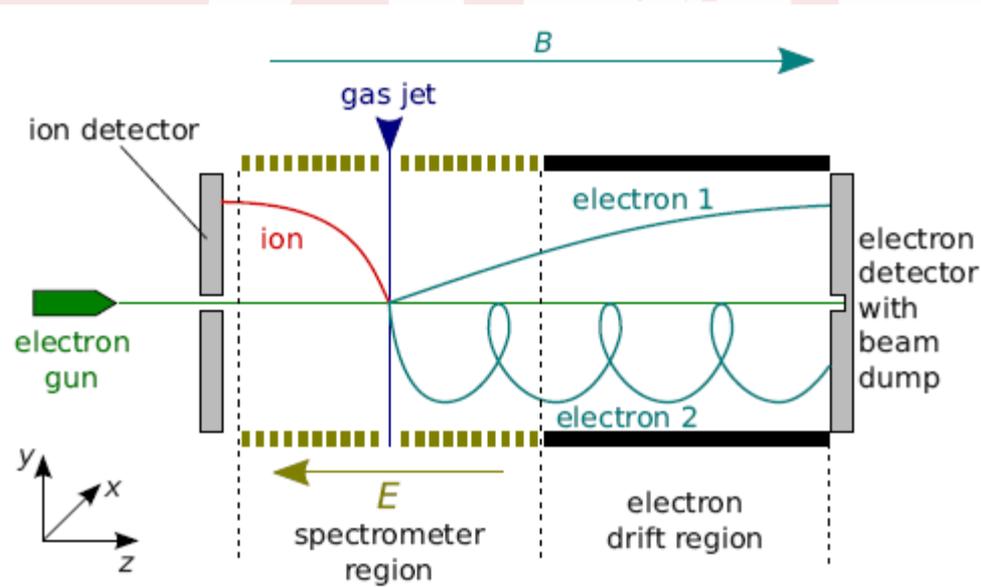
H. Ehrhardt, Freiburg 1969



A. Duguet et al  
Rev. Sci. Instrum. 69 (1998) 3524.

reaction microscopes

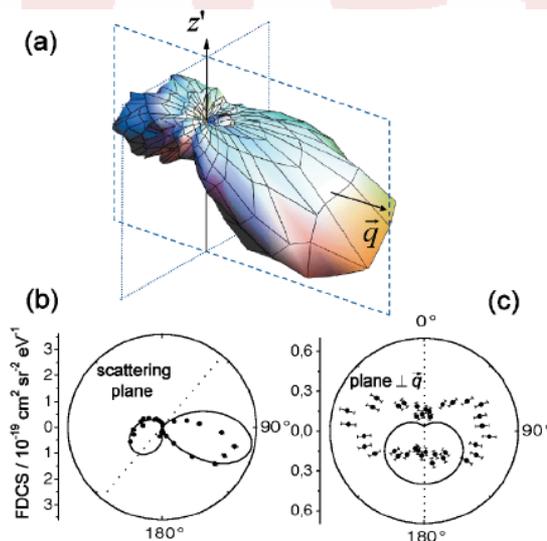
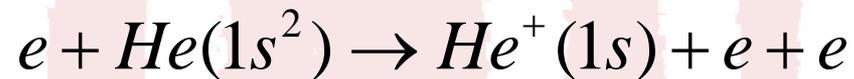
COLTRIMS



J. Ullrich *et al.*, *Rep. Prog. Phys.* **66**, 1463 (2003).



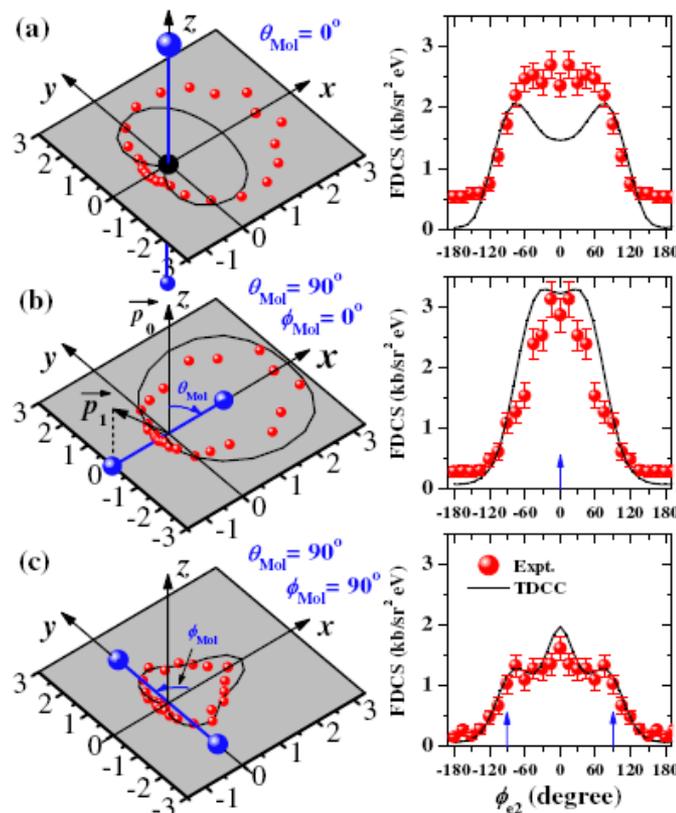
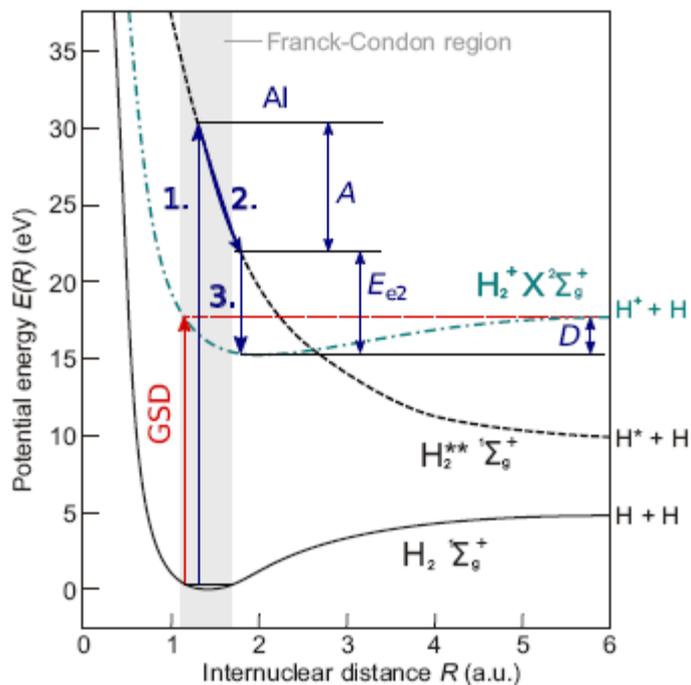
# 碰撞单电离、激发电离和双电离等三体、四体库仑连续态问题



*Phys. Rev. Lett.* **96**, 243202 (2006)

*Nature* **422**, 48 (2003)

# 分子体系的电离解离



X. Ren, T. Pflüger, S. Xu, et al., *Phys. Rev. Lett.* **109**, 123202 (2012).





## 理论

$e + H \rightarrow e + H$       两体，弹性散射

$e + H(1s) \rightarrow e + H(nl)$       两体，非弹性散射

$e + H(1s) \rightarrow H^+ + e + e$       三体，碰撞电离





库仑三体问题

Bray and Stelbovics

*Phys. Rev. Lett.* **70**, **746** (1993)

*Phys. Rev. Lett.* **70**, **746** (1993)

Convergent Close-Coupling

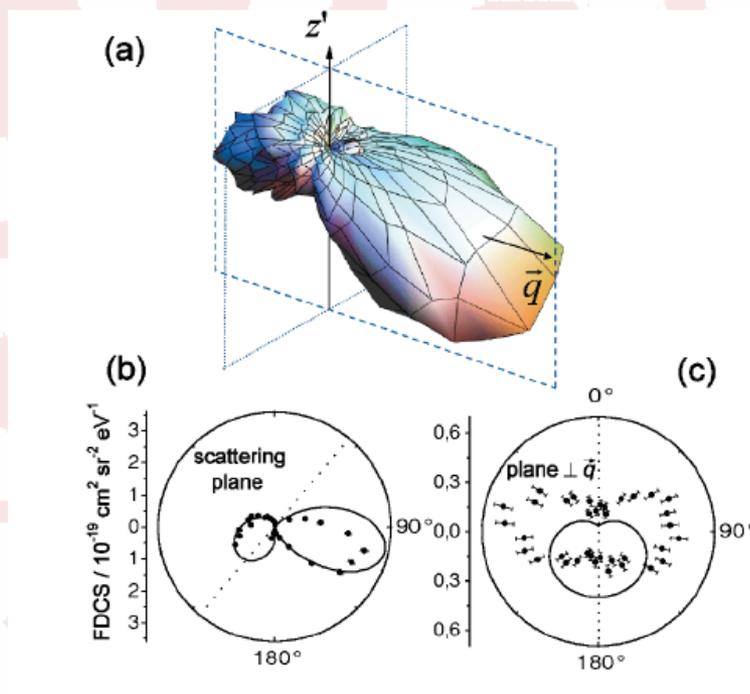
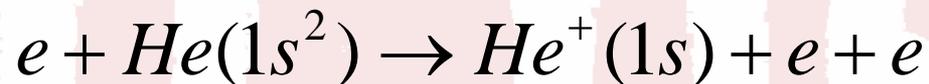
Rescigno and McCurdy

*Science* **286**, **2474** (1999)

Exterior complex scaling (ECS)

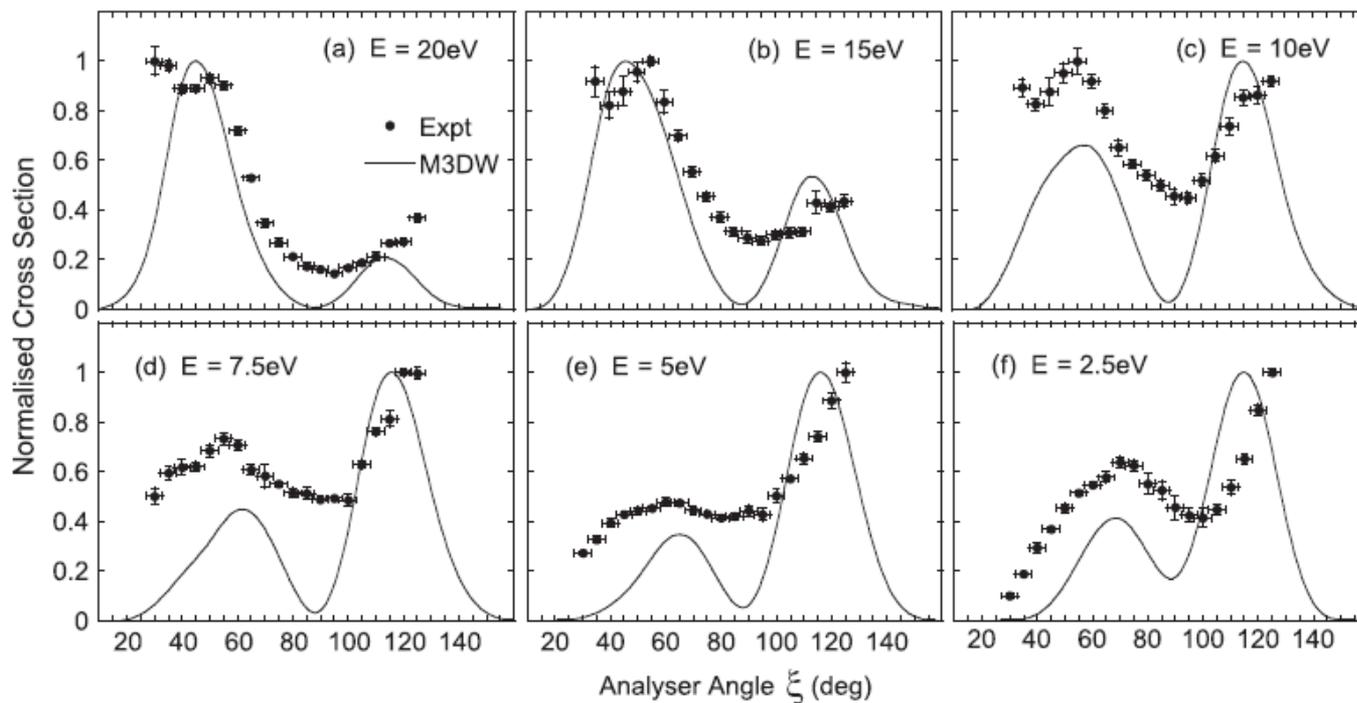


复杂原子分子和多体动力学，理论描述仍然面临重大挑战。



理论是CCC

*Phys. Rev. Lett.* **96**, 243202 (2006)



*J. Chem. Phys.* **134**, 174304 (2011)

理论 M3DW, MBBK, MDW





## Non-perturbative methods

converge close-coupling (CCC) method

time-dependent close-coupling (TDCC) method

exterior complex scaling (ECS) method

B-spline R-matrix approach

## Perturbative methods

molecular three-body distorted-wave (M3DW) method

+ orientation averaged molecular orbital (OAMO) approximation

+ **a proper average over all molecular orientations**

Brauner, Briggs, and Klar (BBK) model

complex Kohn treatment

Generalized Sturmian functions approach





## Multicenter distorted-wave (MCDW)

## Multicenter distorted-wave Born Approximation (MC-DWBA)



Dr. SongBin Zhang

Song Bin Zhang *et al.* , Phys. Rev. A 89,052711(2014).

Xingyu Li *et al.* , Phys. Rev. A 95, 012703 (2017).

Maomao Gong *et al.*, Phys. Rev. A 96, 042703 (2017).

Maomao Gong *et al.*, J. Phys. B (2018) online.

Xiaojie Xu *et al.*, J. Chem. Phys. (2018) in press.

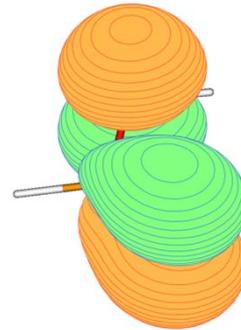
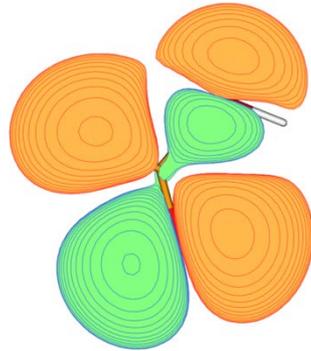




# formic acid (HCOOH)

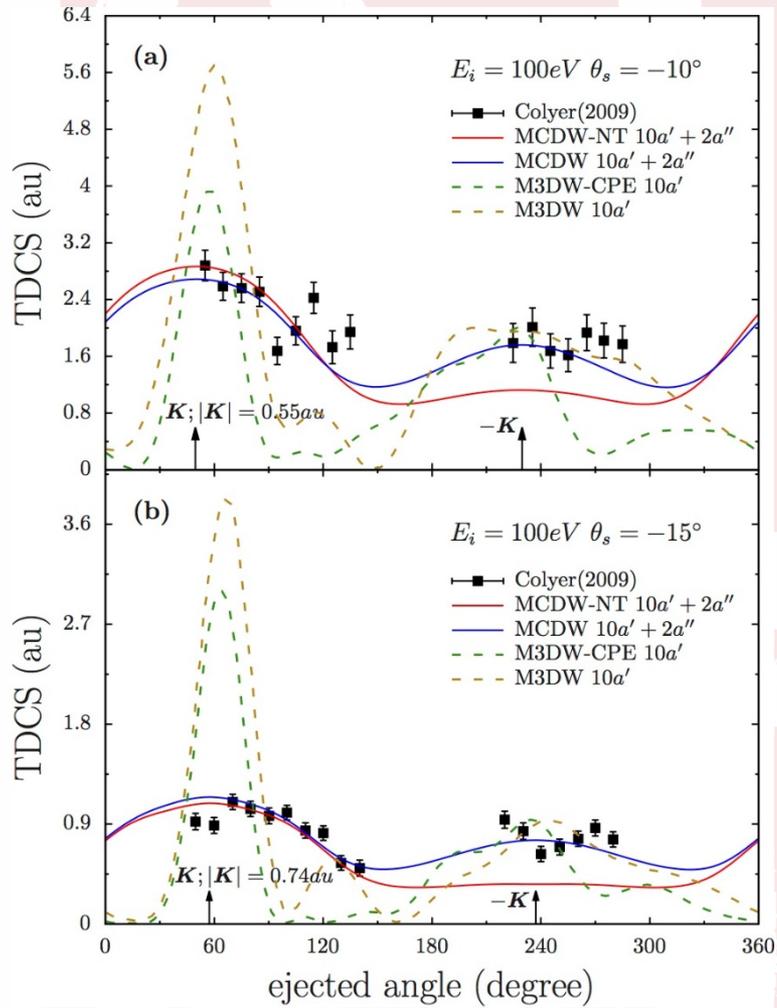
Xingyu Li *et al.* , Phys. Rev. A 95, 012703 (2017).

B3LYP/TZVP



orbital maps of  $10a'$  (left) and  $2a''$  (right)

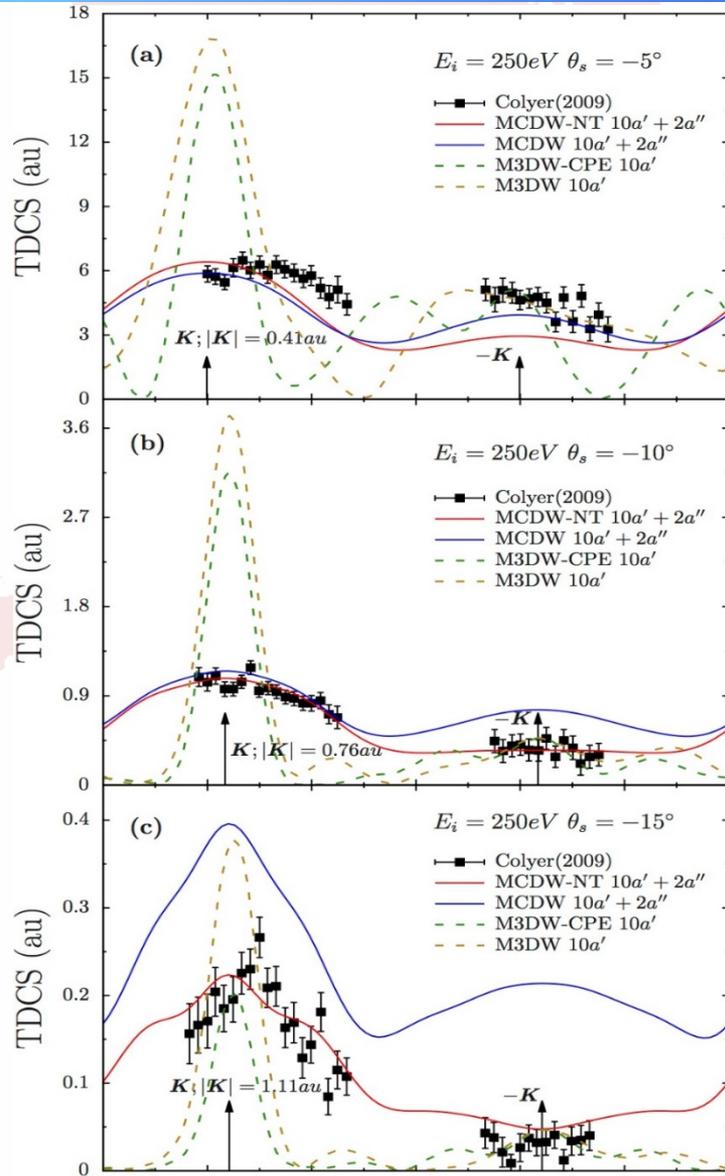




$E_i = 100\text{ eV}, E_e = 10\text{ eV}$

Exp & M3DW:  
C. J. Colyer et al, J. Phys. B At. Mol. Opt. Phys.  
42, 235207 (2009).





$E_i = 250\text{ eV}, E_e = 10\text{ eV}$

Exp & M3DW:

C. J. Colyer et al, J. Phys. B At. Mol. Opt. Phys. 42, 235207 (2009).

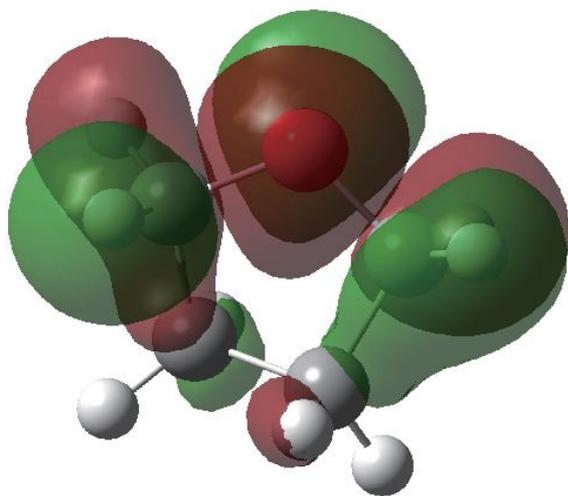




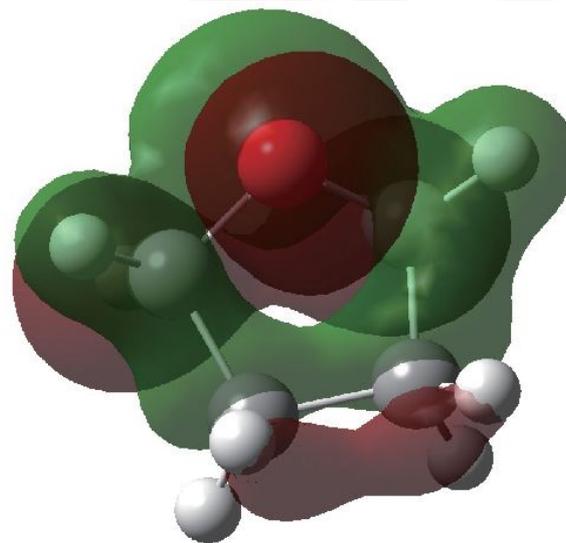
# Tetrahydrofuran (THF)

Xiaojie Xu *et al.*, J. Chem. Phys. (2018) in press

Tetrahydrofuran



C<sub>2v</sub>



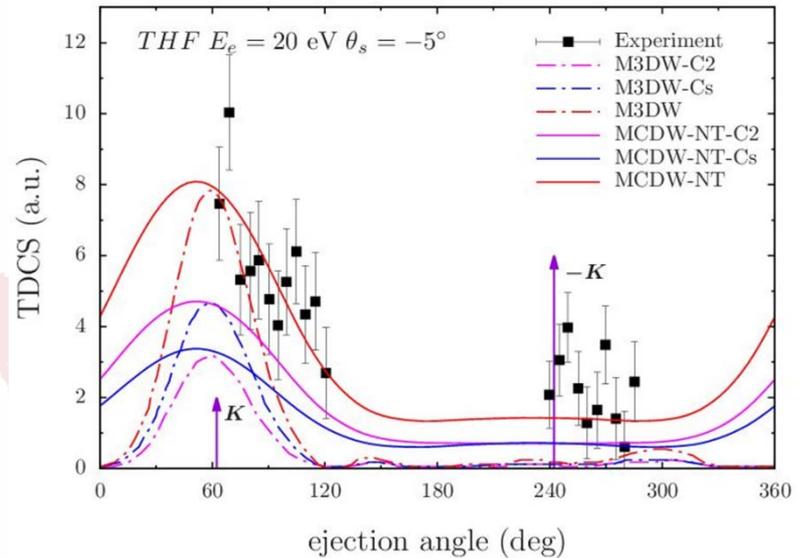
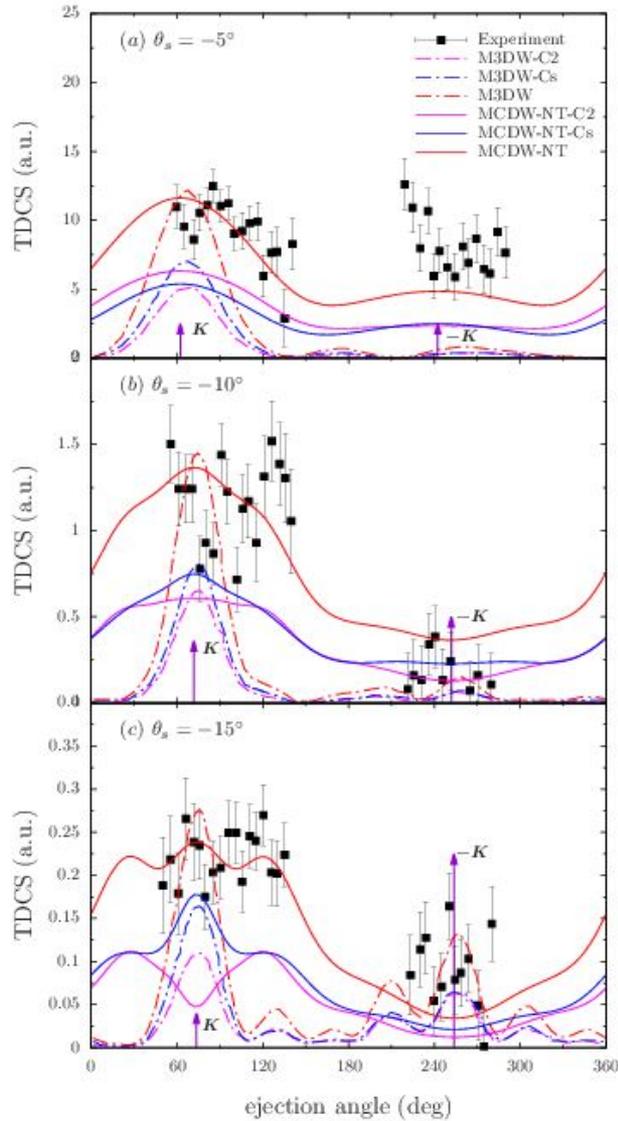
C<sub>s</sub>





$E_0=250\text{eV}$   $E_e=10\text{eV}$   $E_s=230.3\text{eV}$   $\theta_s = -5^\circ, -10^\circ, -15^\circ$

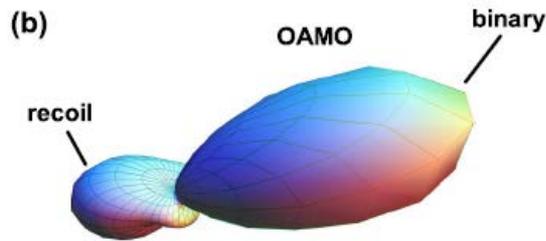
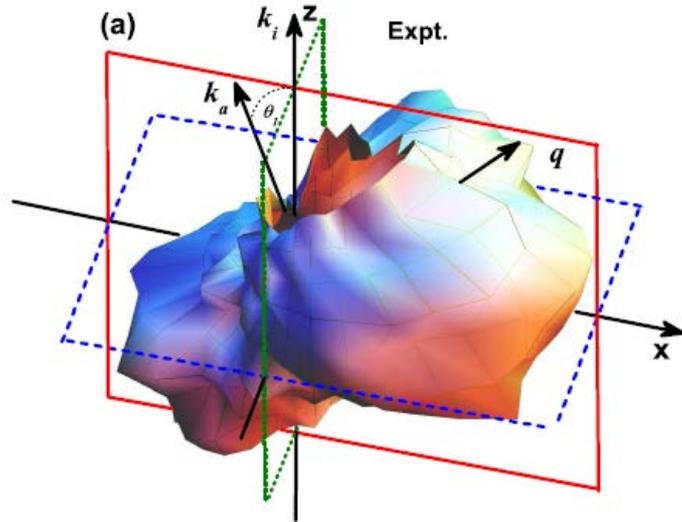
Exp: D. B. Jones et al, Chem. Phys. Lett. 572, 32 (2013)



Exp: J. D. Built-Williams et al, J. Chem. Phys. 139, 034306 (2013)

$E_0=250\text{eV}$   $E_e=20\text{eV}$   
 $E_s=220.3\text{eV}$   $\theta_s = -5^\circ$

(unpublished)



$1b_1 + 3a_1$  of  $H_2O$

