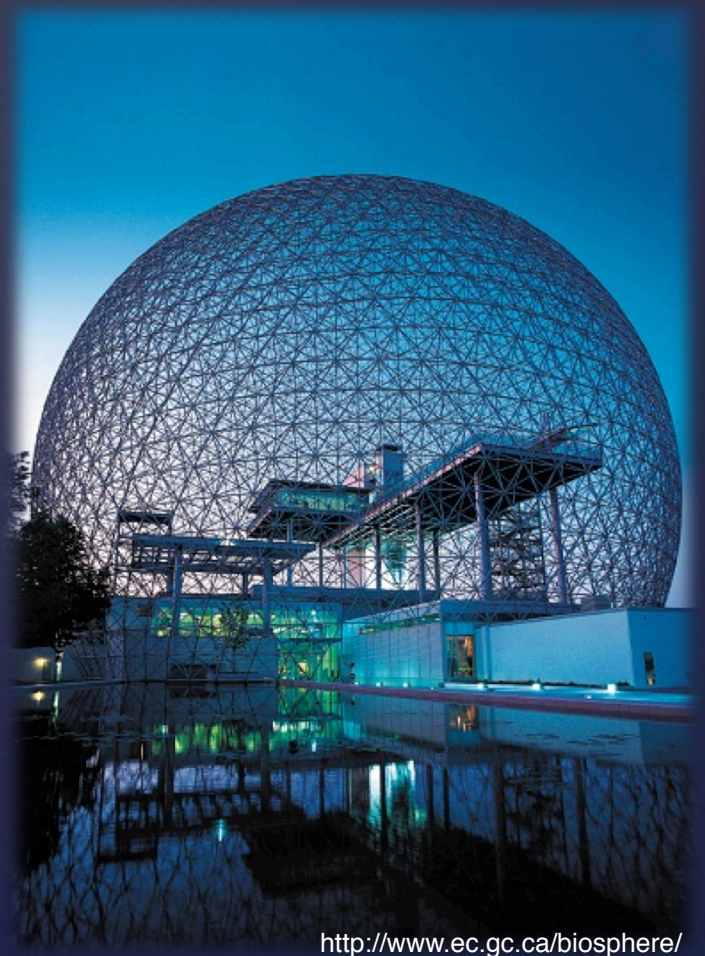
Buckminsterfullerene -Aromaticity and Molecule@C_{60}-

May 27, 2013

Kumiko Yamamoto

Contents



http://www.ec.gc.ca/biosphere/

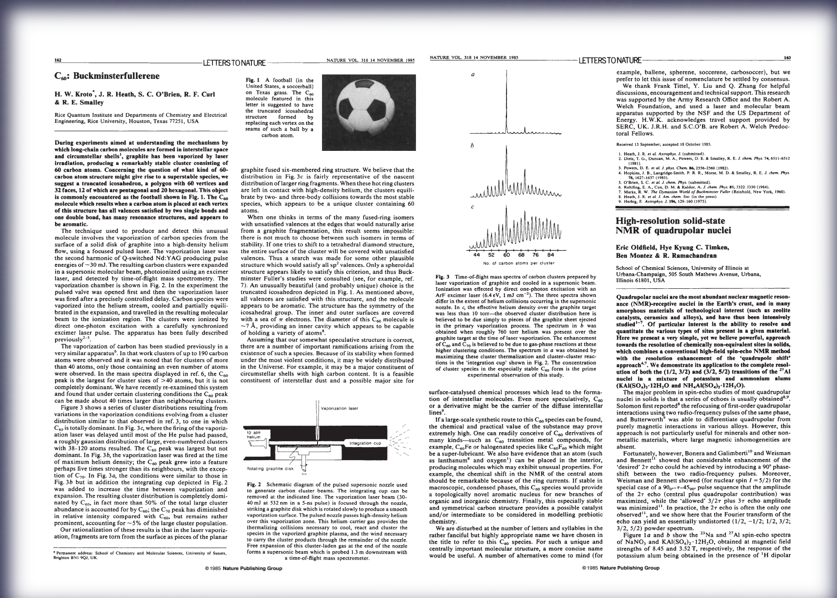
History of Buckminsterfullerene

1970 first prediction by E. Osawa

E. Osawa, *Kagaku* **1970**, *25*, 854.

1985 discovery of Buckminsterfullerene by H. W. Kroto, R. E. Smalley

H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R. E. Smalley, *Nature* **1985**, *318*, 162.



LETTERS TO NATURE

C_{60}: Buckminsterfullerene

H. W. Kroto*, J. R. Heath, S. C. O'Brien, R. F. Curl & R. E. Smalley

Rice Quantum Institute and Departments of Chemistry and Electrical Engineering, Rice University, Houston, Texas 77251, USA

High-resolution solid-state NMR of quadrupolar nuclei

Eric Oldfield, Hye Kyung C. Timken, Ben Montez & R. Ramachandran

© 1985 Nature Publishing Group

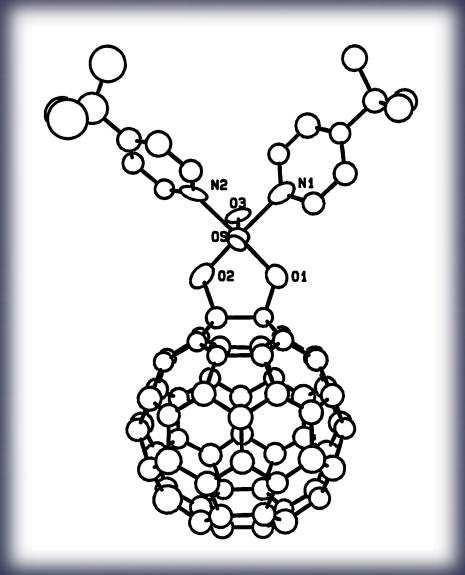
Buckminsterfullerene was named after Richard Buckminster Fuller.
←Biosphere, Environment Museum

1990 preparation of substantial amounts of Buckminster fullerene by W. Krätschmer, D. R. Huffman

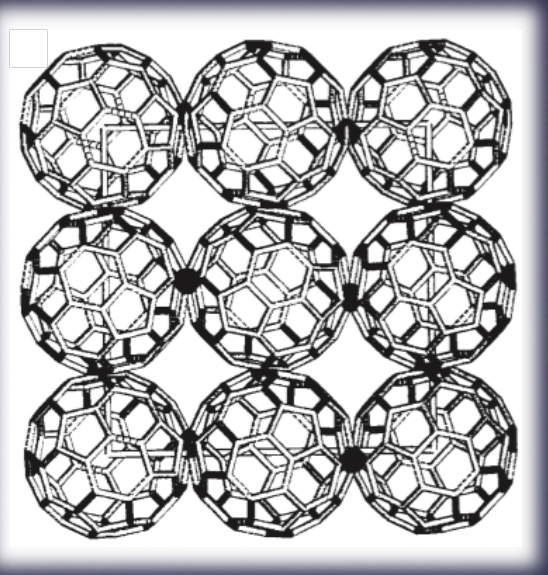
W. Krätschmer, L. D. Lamb, K. Fostiropoulos, D. R. Huffman, *Nature* **1990**, *347*, 354.

History of Buckminsterfullerene

1991 crystal structure of Buckminsterfullerene

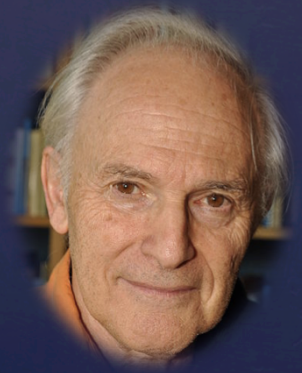


J. M. Hawkins, A. Meyer, T. A. Lewis, S. Loren, F. J. Hollander, *Science* **1991**, *252*, 312.

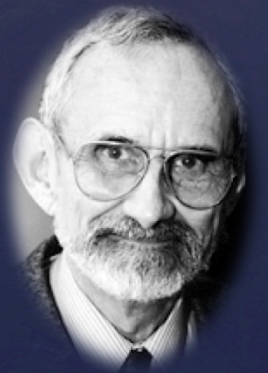


W. I. F. David, R. M. Ibberson, J. C. Matthewman, K. Prassides, T. J. S. Dennis, J. P. Hare, H. W. Kroto, R. Talor, D. R. M. Walton, *Nature* **1991**, *353*, 147.

1996 Nobel Prize in Chemistry; discovery of new carbon compounds called fullerenes



H. W. Kroto

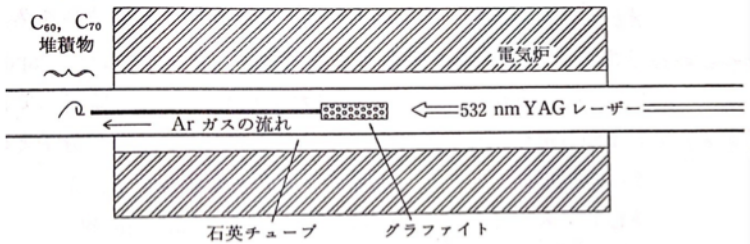


R. F. Curl

R. E. Smalley

How to Produce Fullerenes?

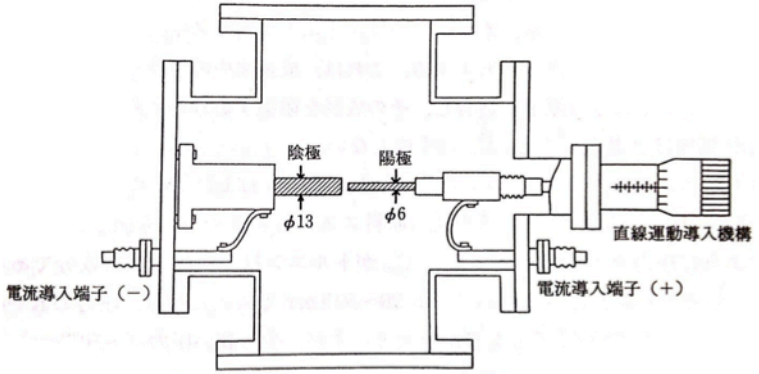
laser-vaporization



- good generation efficiency of C_{60}
- small scale synthesis

篠原久典, 齋藤弥八, 『フラーレンとナノチューブの科学』, 名古屋大学出版会, 2011.

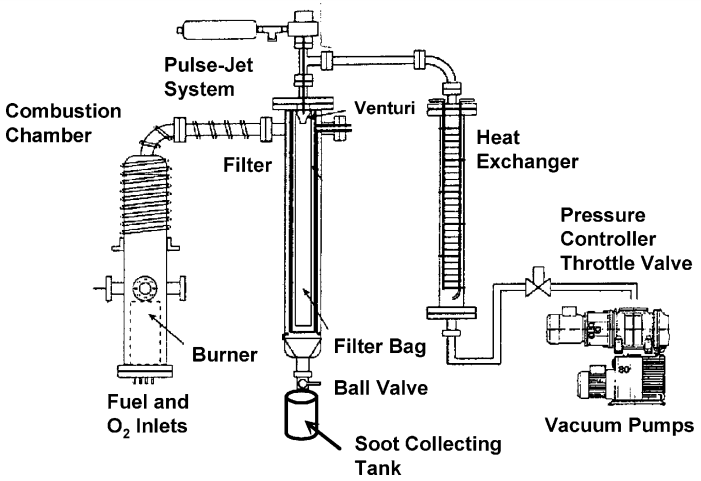
arc discharge



- low generation efficiency of C_{60}
- can obtain soot in gram scale

篠原久典, 齋藤弥八, 『フラーレンとナノチューブの科学』, 名古屋大学出版会, 2011.

combustion synthesis



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Wako

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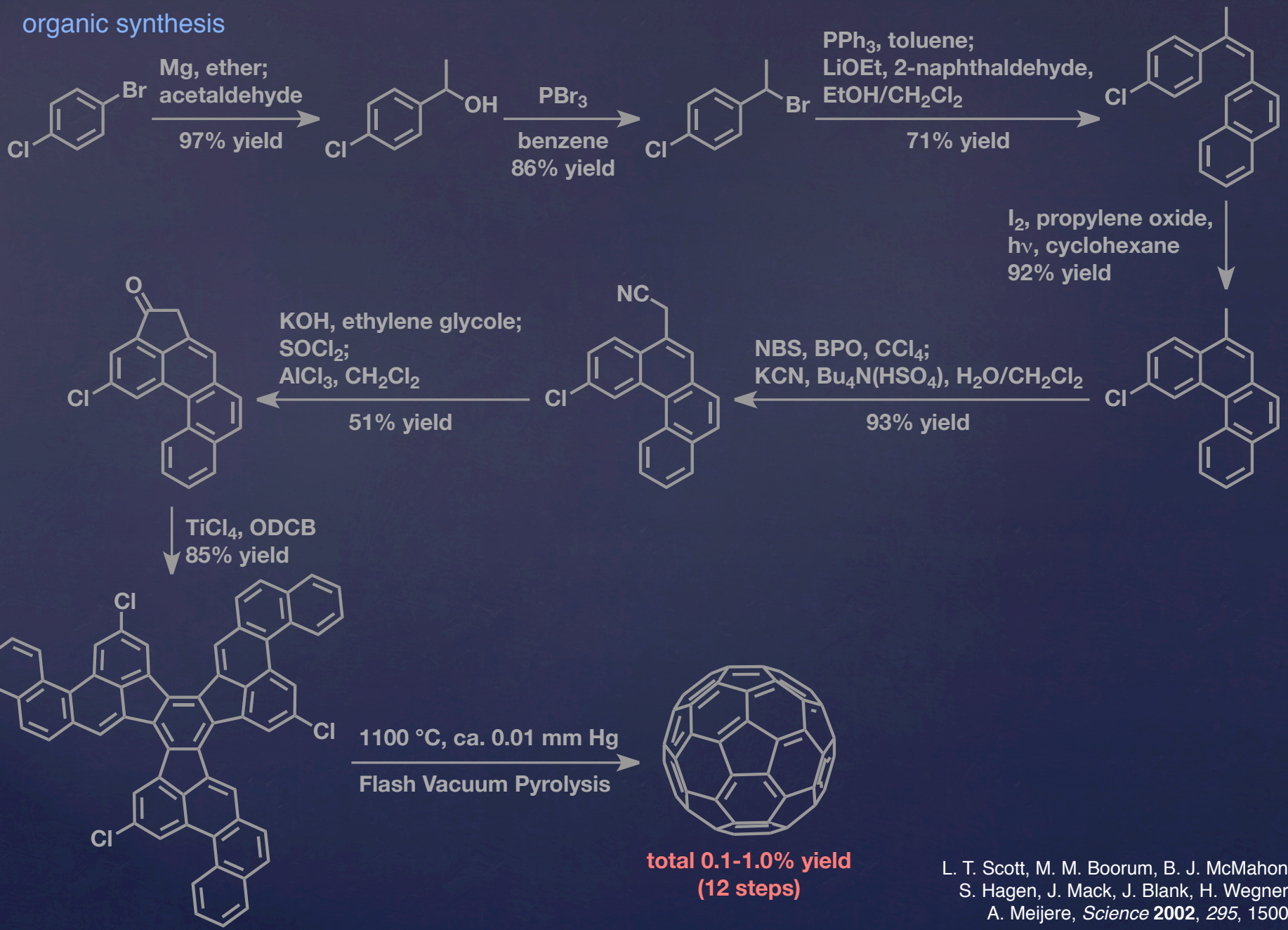
H. Takehara, M. Fujiwara, M. Arikawa, M. D. Diener, J. M. Alford, *Carbon* **2005**, *43*, 311.

How to Produce Fullerenes?

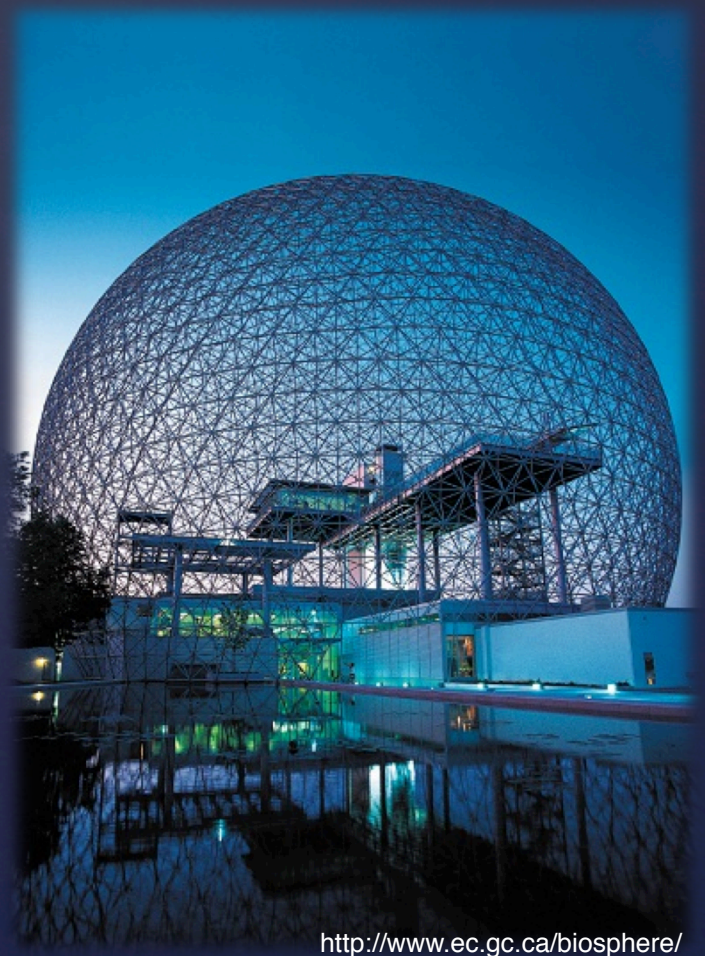
organic synthesis



total 0.1-1.0% yield
(12 steps)

L. T. Scott, M. M. Boorum, B. J. McMahon, S. Hagen, J. Mack, J. Blank, H. Wegner, A. Meijere, *Science* **2002**, *295*, 1500.

Contents

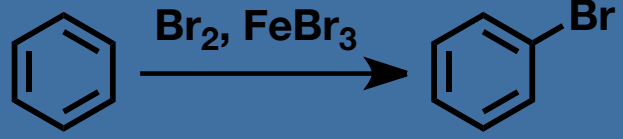


http://www.ec.gc.ca/biosphere/

What is Aromaticity?

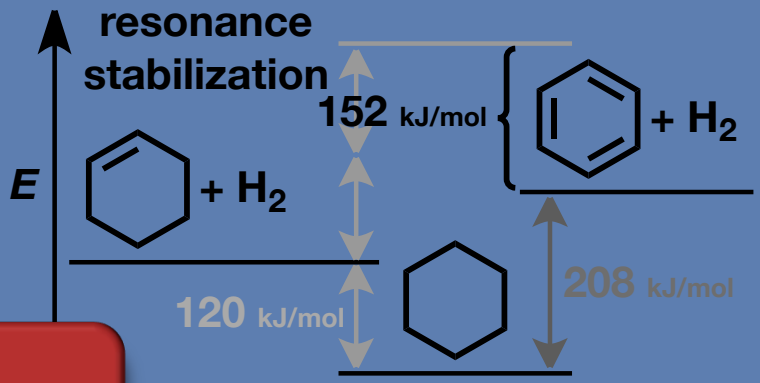
Reactivity Criteria

electrophilic aromatic substitution



Energetic Criteria

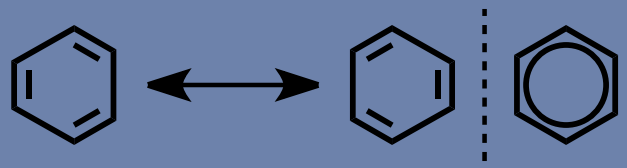
enhanced stability (large resonance energy)



Aromaticity

Structural Criteria

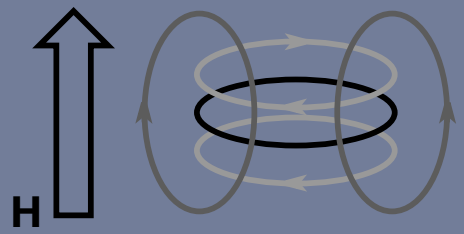
bond length equalization due to cyclic delocalization



HOMA etc.

Magnetic Criteria

ring current effects



NMR chemical shift
diamagnetic susceptibility exaltation (Λ)
NICS value
etc.

Structural Criteria

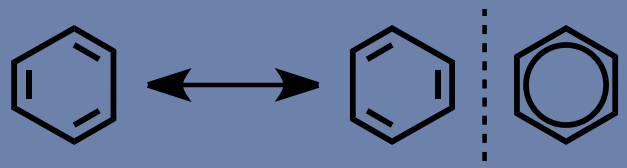
the valence bond (VB) structure

method	[5,6]-bonds	[6,6]-bonds
HF(STO-3G)	1.465 (Å)	1.376
HF(7s3p/4s2p)	1.453	1.369
LDF(11s6p)	1.43	1.39
HF	1.448	1.370
MP2	1.446	1.406
NMR	1.45	1.40
neutron diffraction	1.444	1.391
electron diffraction	1.458	1.401
X-ray	1.467	1.355

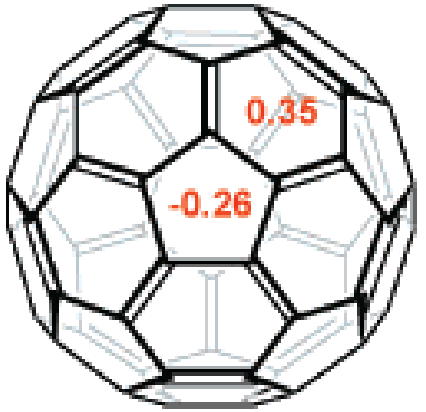
Aromaticity

Structural Criteria

bond length equalization due to cyclic delocalization



HOMA etc.



whole molecule; 0.14

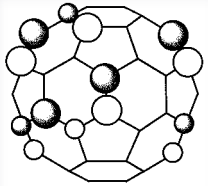
HOMA values

T. M. Krygowski, A. Ciesielski, *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 1001.
M. Bühl, A. Hirsch, *Chem. Rev.* **2001**, *101*, 1153.

Structural Criteria

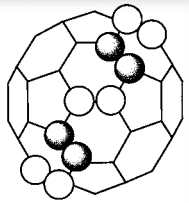
the valence bond (VB) structure

[6,6]-bonds: double bond character
[5,6]-bonds: single bond character
(from calculations & experimental results)



LUMO

C_{60}^{6-}
[6,6]-bonds: 1.42 Å
[5,6]-bonds: 1.45 Å



HOMO

C_{60}
[6,6]-bonds: 1.45 Å
[5,6]-bonds: 1.37 Å

C_{60}^{10+}
no significant bond-length alternation is expected
[6,6]-bonds: 1.48 Å
[5,6]-bonds: 1.44 Å

C_{60} has ambiguous aromatic character;
aromatic hexagons and antiaromatic pentagons within neutral C_{60}.

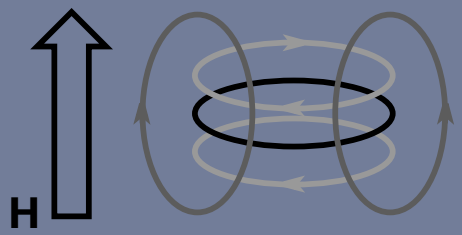
M. Bühl, A. Hirsch, *Chem. Rev.* **2001**, *101*, 1153.

Magnetic Criteria

Aromaticity

Magnetic Criteria

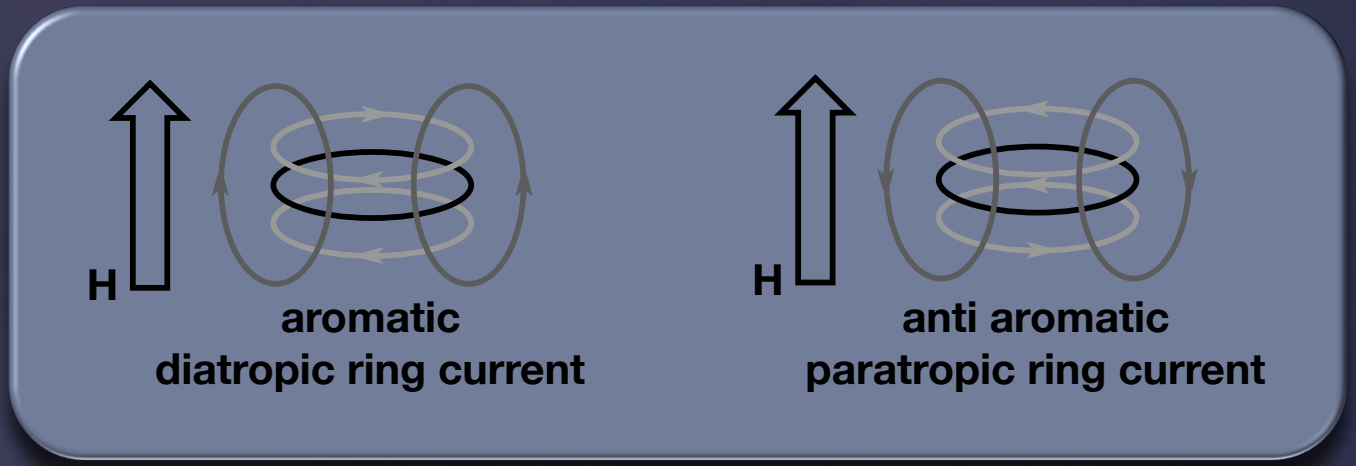
ring current effects

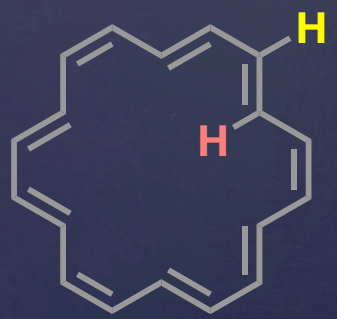


NMR chemical shift
diamagnetic susceptibility exaltation (Λ)
NICS value
etc.

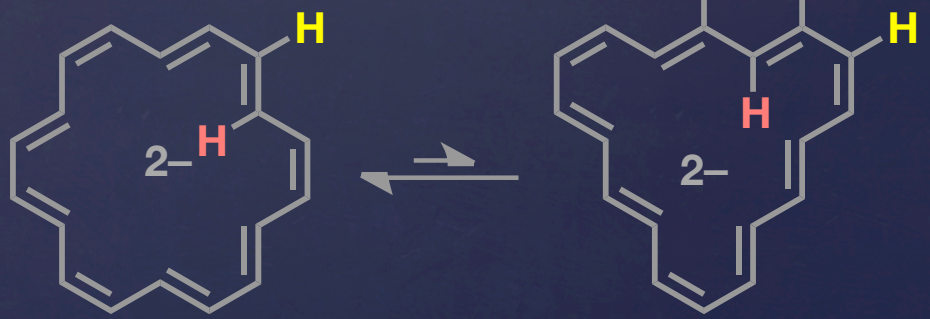
Magnetic Criteria

^{1}H NMR chemical shift





9.28 ppm (outer protons)
–2.99 ppm (inner protons)
[18]annulene



–1.13 ppm (outer protons)
29.5, 28.1 ppm (inner protons)
dianion of [18]annulene

J. F. M. Oth, E. P. Woo, F. Sondheimer, *J. Am. Chem. Soc.* **1973**, *95*, 7337.

Magnetic Criteria

diamagnetic susceptibility exaltation (Λ)

$$\Lambda = \chi_M - \chi_{M'}$$

Λ < 0: aromatic compounds
Λ ~ 0: non aromatic compounds

χ_M: the experimentally determined molar susceptibility of a compound
$\chi_{M'}$: the susceptibility estimated for a cyclopolyene of that structure

compound	χ_M	$\chi_{M'}$	
	−68.1	−68.1	0.0
	−57.5	−58.3	0.8
	−48.6	−49.3	0.7
	−54.8	−41.1	−13.7

compound		$\chi_{M'}$	
	-	-	−17.2**
	−44.5	−38.0	−6.5 (−2.4**)
	-	-	32.6**

*All values of χ_M, $\chi_{M'}$ and Λ are given in units of 10^{-6} cm^3 mol^{-1} (ppm cgs).
**The calculated magnetic susceptibility exaltations.

H. J. Dauben, Jr., J. D. Wilson, J. L. Laity, *J. Am. Chem. Soc.* **1968**, *90*, 811.
H. J. Dauben, Jr., J. D. Wilson, J. L. Laity, *J. Am. Chem. Soc.* **1969**, *91*, 1991.

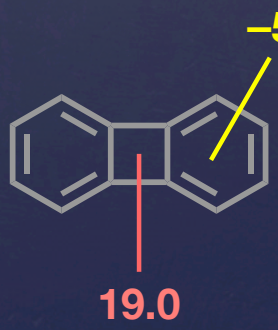
Magnetic Criteria

NICS (nucleus-independent chemical shift)

absolute magnetic shieldings, computed at ring centers

NICS < 0: aromaticity
NICS > 0: antiaromaticity

compound		NICS	compound		NICS
	0.0	−2.2		−17.2**	−14.3
	−13.7	−9.7		−6.5 (−2.4**)	−3.2
				32.6**	54.2



*All values of Λ are given in units of 10^{-6} cm^3 mol^{-1} (ppm cgs) and NICS are given in units of ppm.
**The calculated magnetic susceptibility exaltations.

P. v. R. Schleyer, C. Maerker, A. Dransfeld, H. Jiao, N. J. R. van E. Hommes, *J. Am. Chem. Soc.* **1996**, *118*, 6317.

Magnetic Criteria

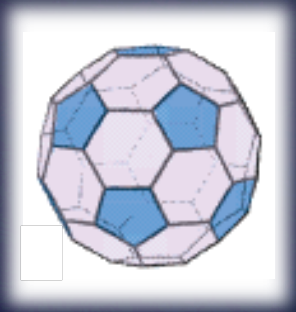
diamagnetic susceptibility exaltation (Λ)

compound	χ_M	$\chi_{M'}$	Λ
	−54.8	−41.1	−13.7
C_{60}	−260±20	−262±40	2±60

*All values of χ_M, $\chi_{M'}$ and Λ are given in units of 10^{-6} cm^3 mol^{-1} (ppm cgs).

R. C. Haddon, L. F. Schneemeyer, J. V. Waszczak, S. H. Glarum, R. Tycko, G. Dabbagh, A. R. Kortan, A. J. Muller, A. M. Mujsce, M. J. Rosseinsky, S. M. Zahurak, A. V. Makhija, F. A. Thiel, K. Raghavachari, E. Cockayne, V. Elser, *Nature* **1991**, *350*, 46.

NICS (nucleus-independent chemical shift)



hexagons: -5.31 ppm
pentagons: 8.89 ppm
(benzene: -9.7 ppm)

M. Bühl, *Chem. Eur. J.* **1998**, *4*, 734.

NMR chemical shift

$\delta_{RC} = 2\chi_M / r^3$
r: radius of the sphere ⇒ 0.57 ppm

V. Elser, R. C. Haddon, *Nature* **1987**, *325*, 792.

^{3}He NMR: δ(He@C_{60}) = −6.3 ppm

= [ring current] + [σ-bond anisotropy]

M. Saunders, H. A. J.-Vázquez, R. J. Cross, S. Mroczkowski, D. I. Freedberg, F. A. L. Anet, *Nature* **1994**, *367*, 256.

sophisticated theoretical calculation
δ(He@$C_{60}H_{60}$) = −5.2 ppm

M. Bühl, W. Thiel, H. Jiao, P. R. Schleyer, M. Saunders, F. A. L. Anetl, *J. Am. Chem. Soc.* **1994**, *116*, 6005.

ring-current chemical shift $\delta_{RC}(C_{60})$ = ca. −1 ppm

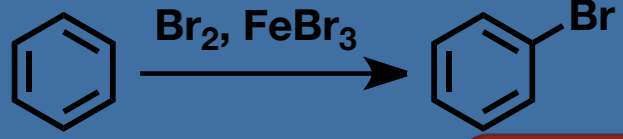
C_{60} has ambiguous aromatic character.

R. C. Haddon, *Nature* 1995, *378*, 249.
M. Bühl, A. Hirsch, *Chem. Rev.* **2001**, *101*, 1153.

Summary

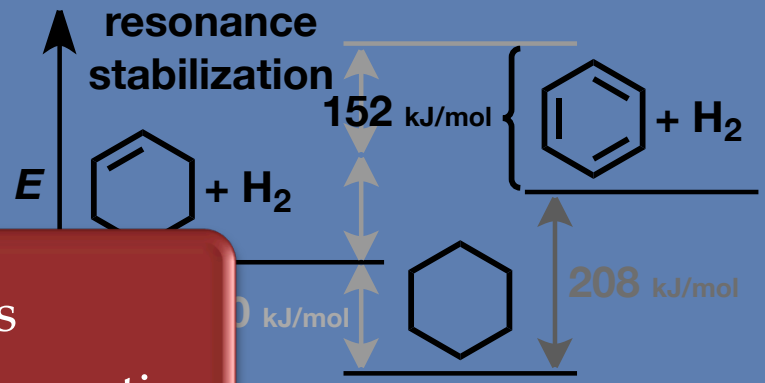
Reactivity Criteria

electrophilic aromatic substitution



Energetic Criteria

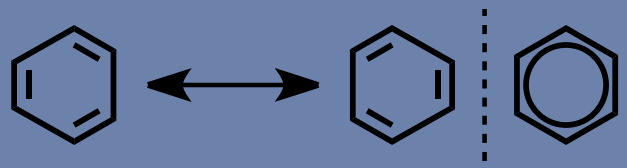
enhanced stability (large resonance energy)



C_{60} has ambiguous aromatic character.

Structural Criteria

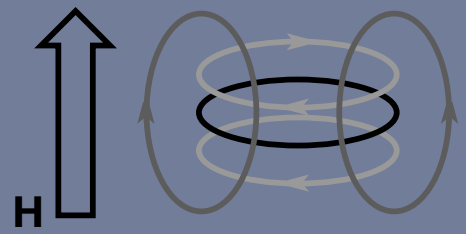
bond length equalization due to cyclic delocalization



HOMA etc.

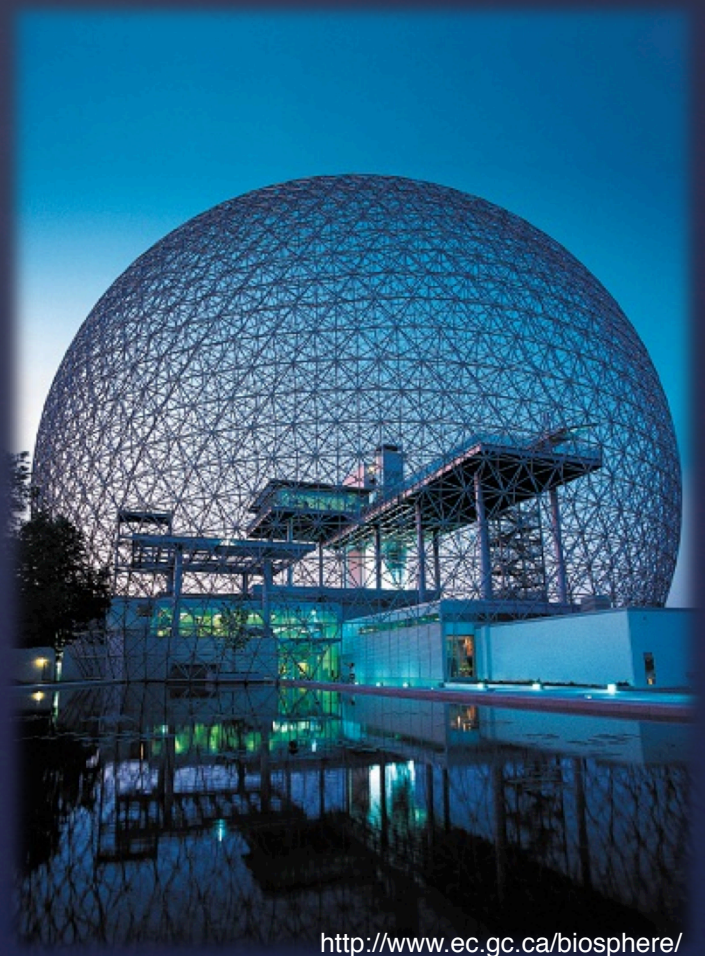
Magnetic Criteria

ring current effects



NMR chemical shift
diamagnetic susceptibility exaltation (Λ)
NICS value
etc.

Contents



http://www.ec.gc.ca/biosphere/

Endohedral Fullerenes Encapsulating a Molecule

endohedral fullerenes: fullerenes with atom(s) or molecule(s) encapsulated

Endhedral fullerenes which have been synthesized and isolated till May 2011

篠原久典, 齋藤弥八, 『フラーレンとナノチューブの科学』, 名古屋大学出版会, 2011, pp. 207.

Why Endohedral Fullerenes?

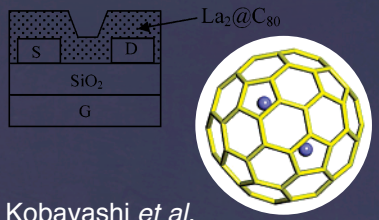
Scientific interest!!

+

expected to be important for their potential use in various fields such as…

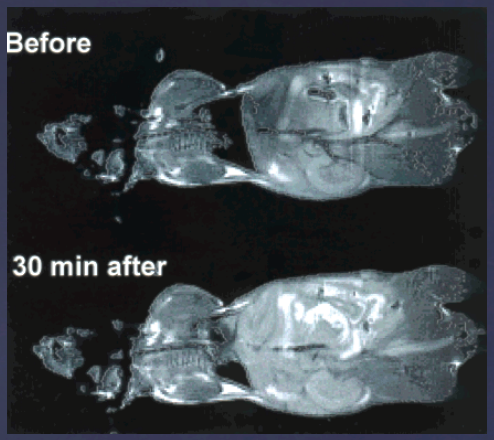
molecular electronics

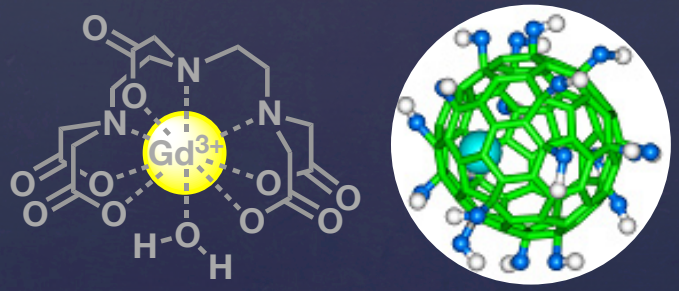
field effect transistor



S. Kobayashi *et al.*
J. Am. Chem. Soc. **2003**, *125*, 8166.

MRI contrast agent





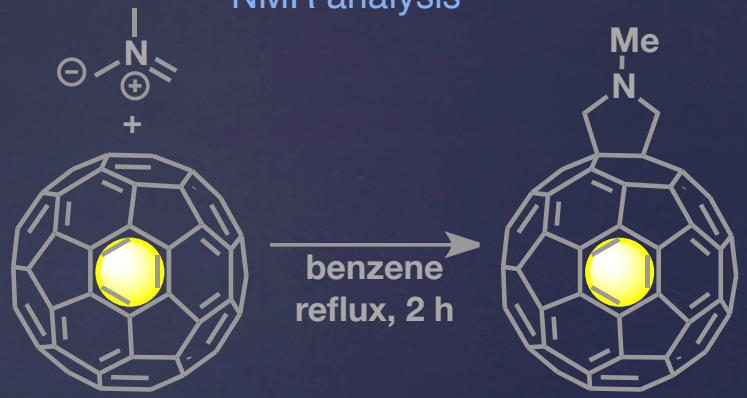
Gd-DTPA
100 μmol Gd/kg

$Gd@C_{82}(OH)_n$
5 μmol Gd/kg

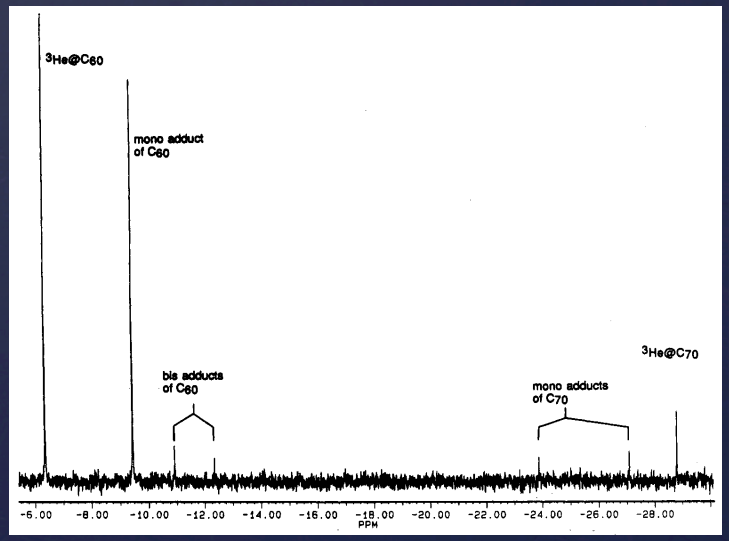
1/20

H. Shinohara *et al.*
Bioconjugate Chem. **2001**, *12*, 510.
J. Am. Chem. Soc. **2003**, *125*, 4391.

NMR analysis



$He@C_{60}$:$He@C_{70}$ = 7:3



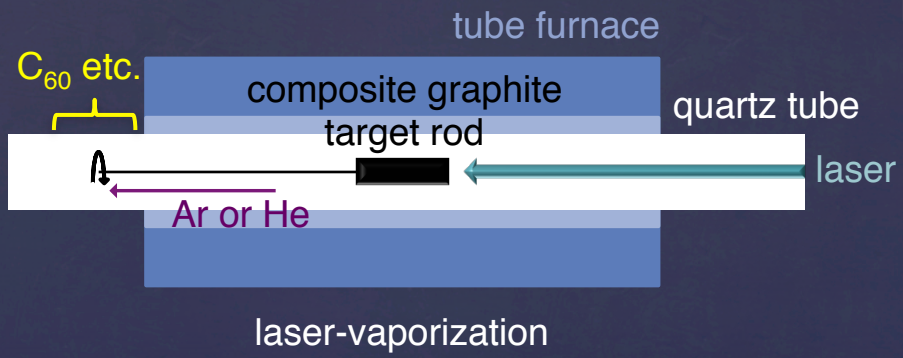
M. Saunders *et al.*
J. Am. Chem. Soc. **1994**, *116*, 3621.

Conventional Synthesis of Endohedral Fullerenes

physical methods under harsh conditions such as…

co-vaporization of carbon and metal atoms
→ metallofullerenes

laser-vaporization, arc discharge, etc.
with composite graphite target rods; made by mixing metal powder with graphite powder, pressing, and carbonized by baking.



first example: R. E. Smalley *et al. J. Am. Chem. Soc.* **1985**, *107*, 7779.
篠原久典, 齋藤弥八, 『フラーレンとナノチューブの科学』, 名古屋大学出版会, 2011.

high-pressure/temperature treatment with gases
→ non-metal doped fullerenes (noble gas atom@fullerene)

650 °C, 3000 atm, under noble gas atmosphere
ca. 0.1% yield

first example: M. Saunders *et al. J. Am. Chem. Soc.* **1994**, *116*, 2193.
日本化学会編, 『π電子系の化学』, 化学同人, 2013.

problems

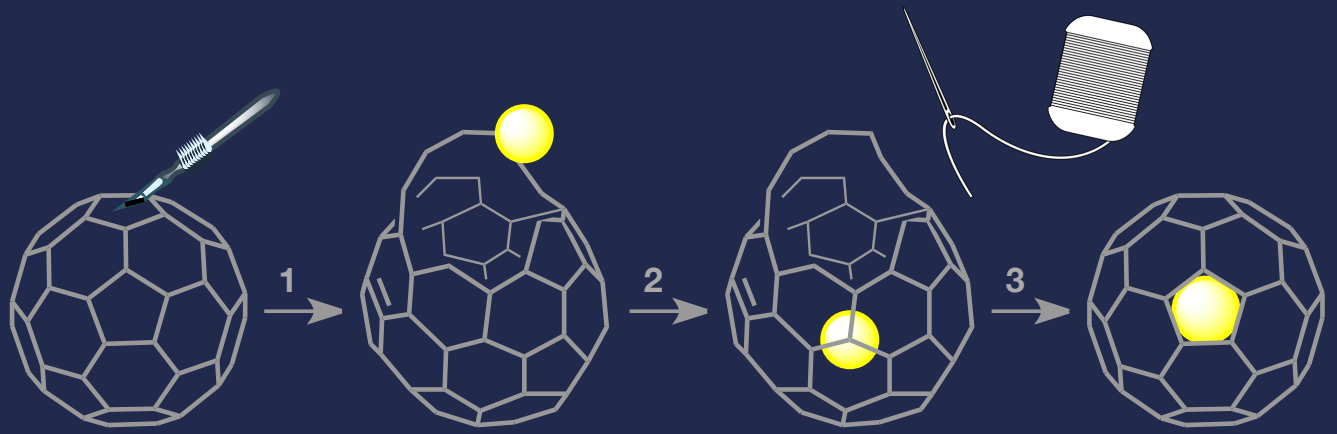
difficult to control the reaction; no selectivity in controlling both the cage-size and product distribution.
low yield & laborious purification; yield only mg quantities of pure product after tedious isolation procedures.

"Molecular Surgery"

by Yves Rubin

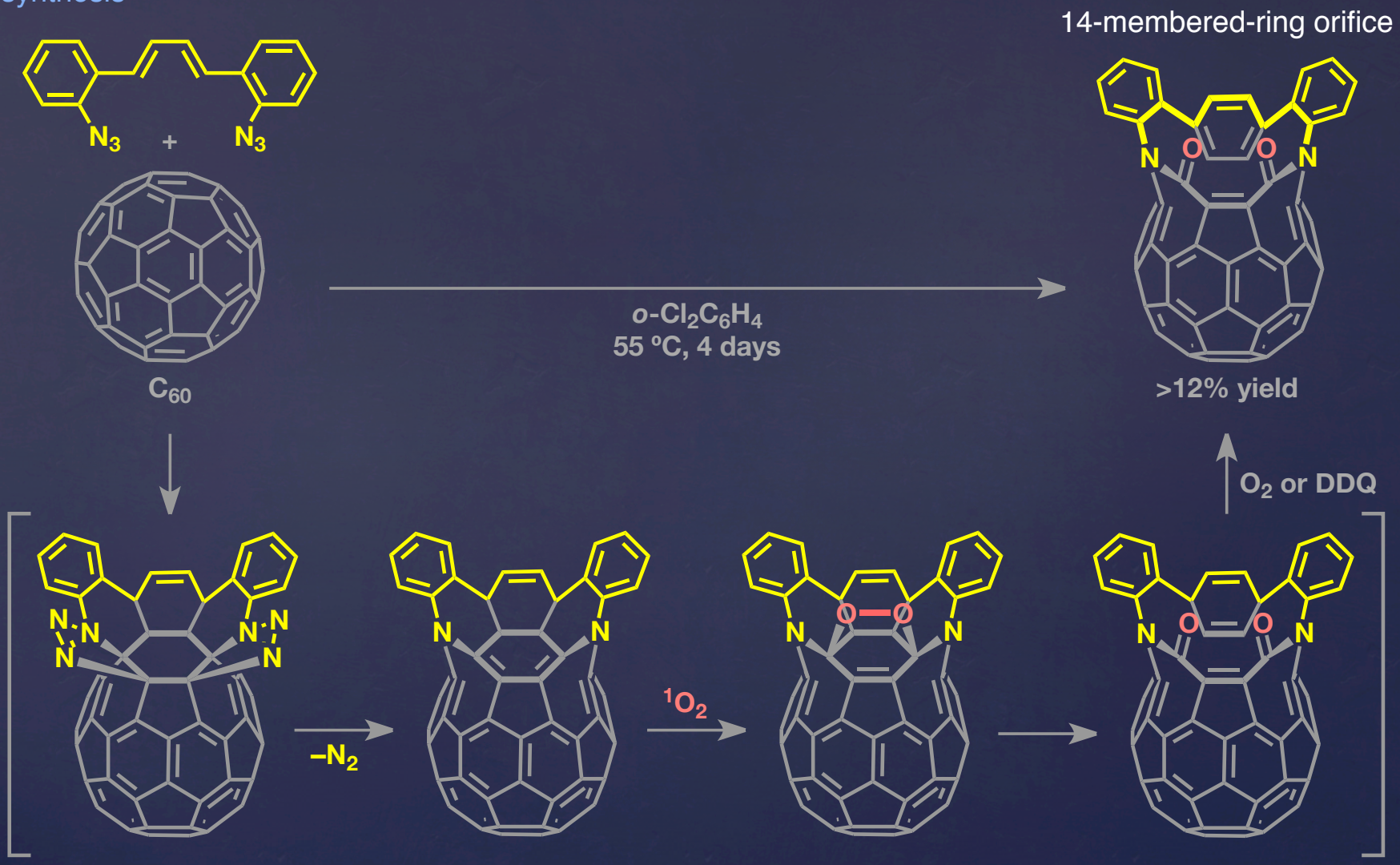
1) "incision" of the fullerene cage to form an opening on the surface.
2) insertion of some small atom(s) or molecule(s) through the opening.
3) "suture" of the opening to reproduce the fullerene cage while retaining the guest species.

Y. Rubin, K. N. Houk, M. Saunders, R. J. Cross *et al. Angew. Chem. Int. Ed.* **2001**, *40*, 1543.
M. Murata, Y. Murata, K. Komatsu, *Chem. Commun.* **2008**, 6083.



Insertion of He & H_2 Through the Orifice of an Open Fullerene

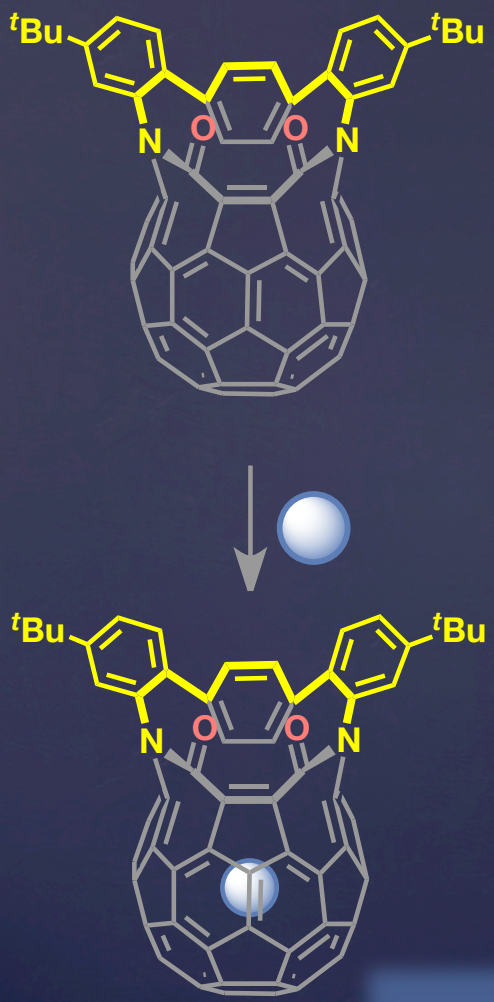
synthesis



G. Schick, T. Jarrosson, Y. Rubin, *Angew. Chem. Int. Ed.* **1999**, *38*, 2360.

Insertion of He & H_2 Through the Orifice of an Open Fullerene

insertion of He & H_2



calculated activation barrier

Guest	Volume[22] [Å^3]	Est. insertion temperature [°C]	Barrier to insertion	Energy of encapsulation	Barrier to escape
He	11.0	124	+24.5	+0.2	+24.3
H_2	19.0	397	+41.4	+1.4	+40.0
Ne	14.6	384	+40.6	−1.1	+41.7
N_2	35.3	1550	+112.4	+5.6	+106.8
Ar	28.9	1930	+136.3	+6.1	+130.2

experimental results

He

100 °C, 3-4 atm, 24 h → 0.04% yield
300 °C, 475 atm, 7.5 h → 1.5% yield

^{3}He NMR: δ = -10.10 ppm

H-H

400 °C, 100 atm, 48 h → 5% yield

^{1}H NMR: δ = -5.43 ppm

He and H_2 are strongly shielded by the fullerene π-electron shell of the open fullerene.

"The important step of closing back the fullerene framework also needs to be studied."

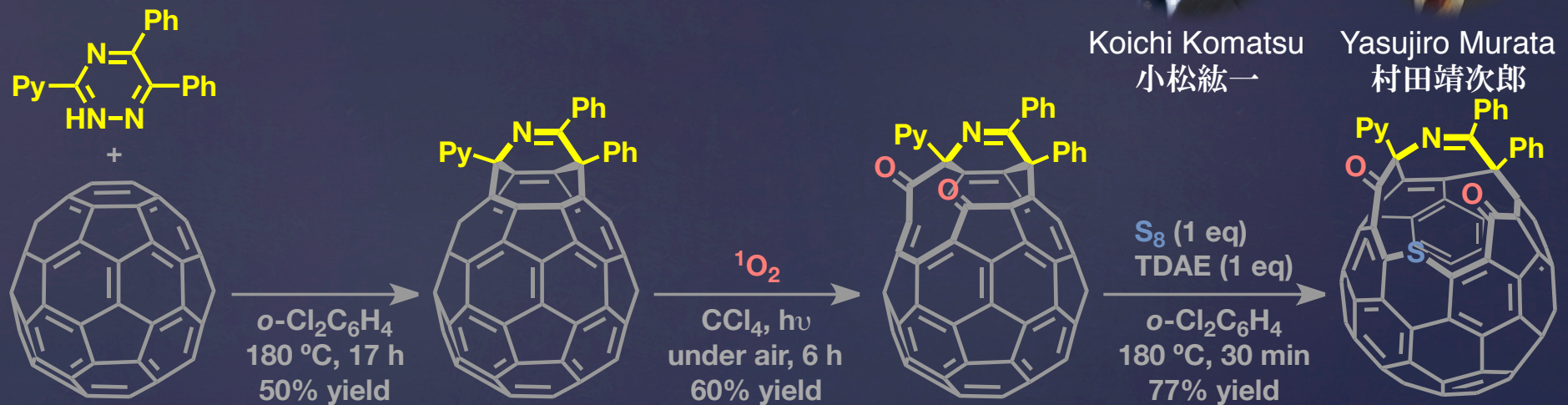
Y. Rubin, T. Jarrosson, G.-W. Wang, M. D. Bartberger, K. N. Houk, G. Schick, M. Saunders, R. J. Cross, *Angew. Chem. Int. Ed.* **2001**, *40*, 1543.

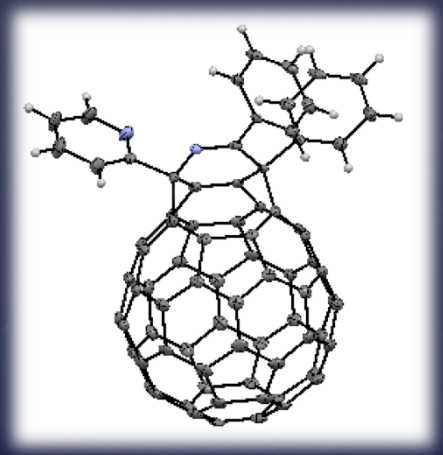
Encapsulation of H_2 in C_{60} by Organic Synthesis

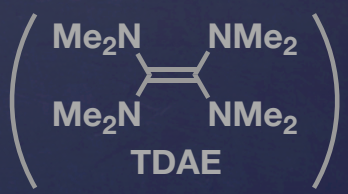
"incision" of the fullerene cage

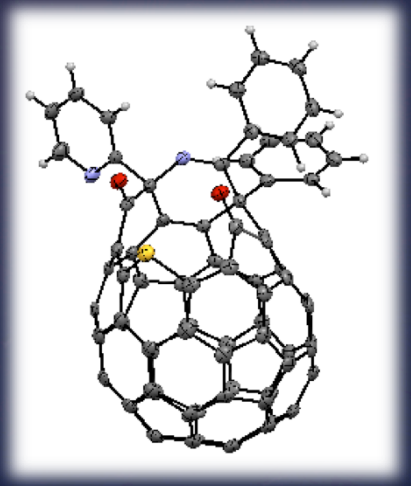
Koichi Komatsu
小松紘一

Yasujiro Murata
村田靖次郎





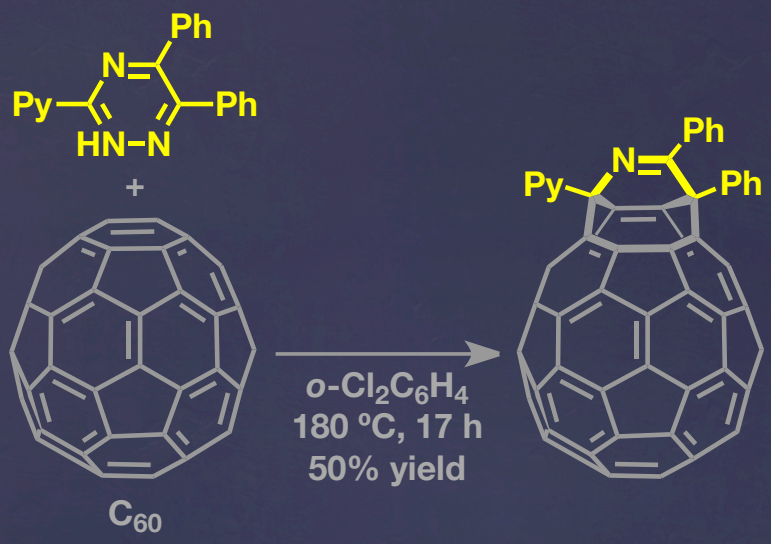


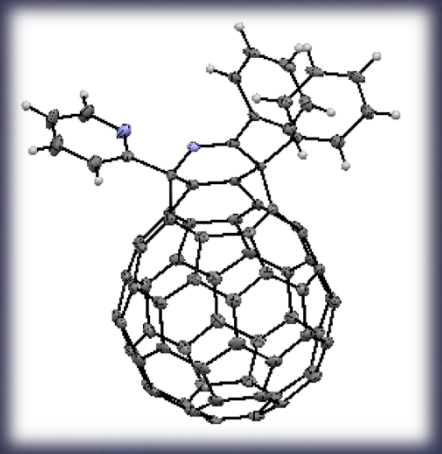


Y. Murata, M. Murata, K. Komatsu, *Chem. Eur. J.* **2003**, *9*, 1600.

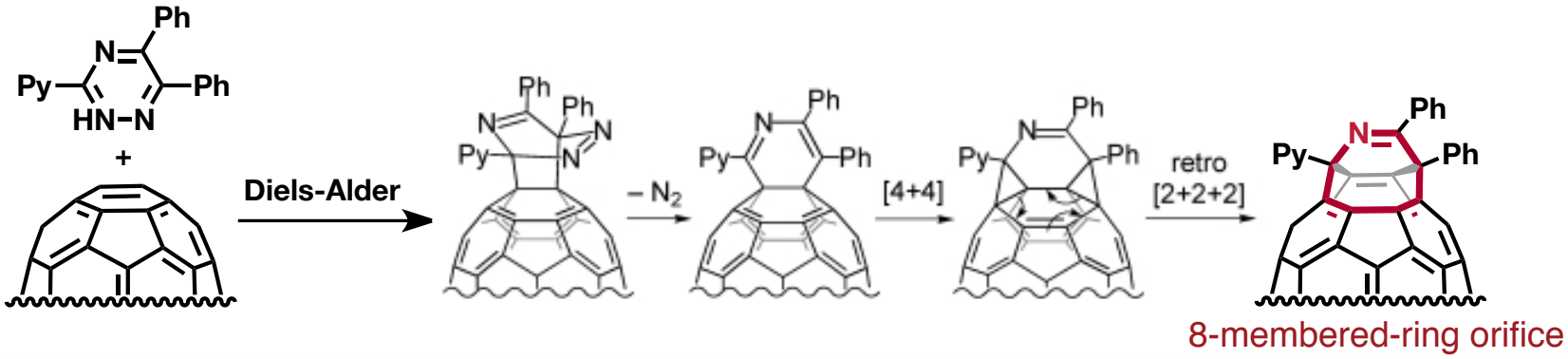
Encapsulation of H_2 in C_{60} by Organic Synthesis

8-membered-ring orifice





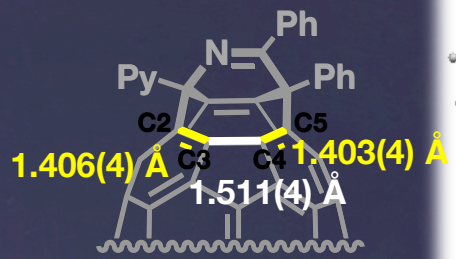
X-ray structure

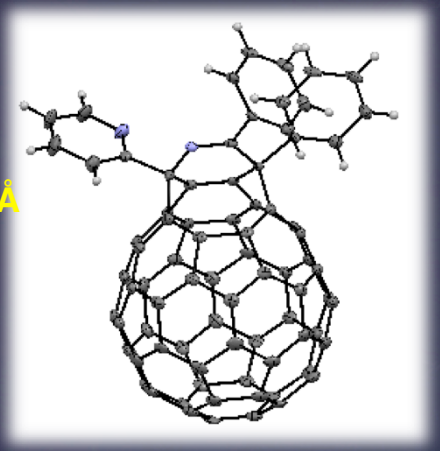


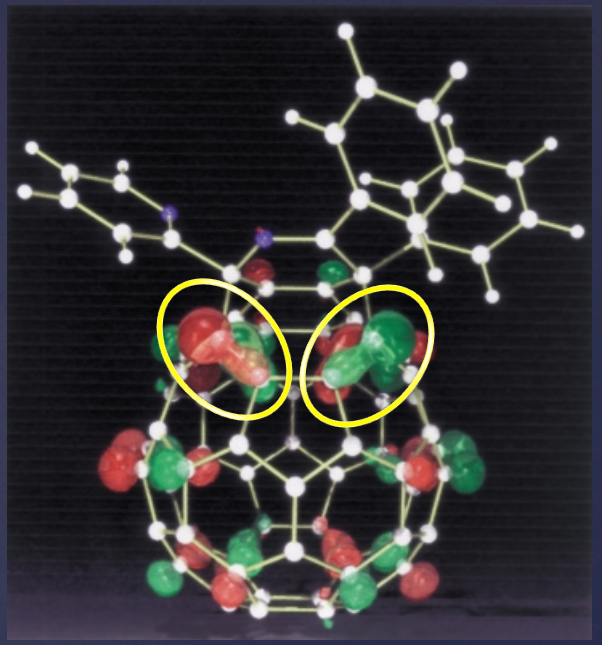
Y. Murata, M. Murata, K. Komatsu, *Chem. Eur. J.* **2003**, *9*, 1600.

Encapsulation of H_2 in C_{60} by Organic Synthesis

12-membered-ring orifice



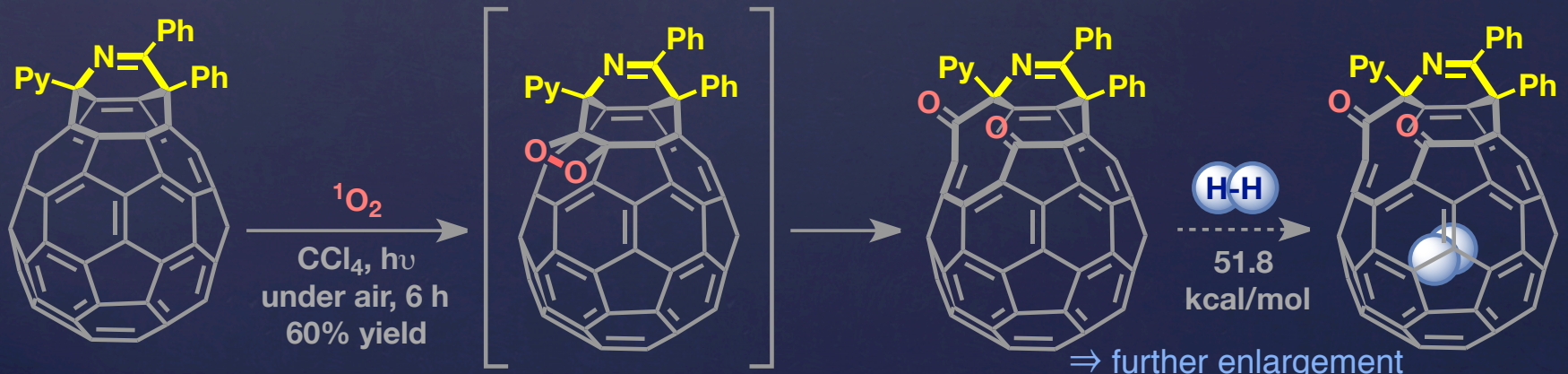




C2-C3 and C4-C5 have double bond character.

HOMO is localized primarily at C2-C3 and C4-C5.

⇒ O_2 addition is expected to take place on these bonds.

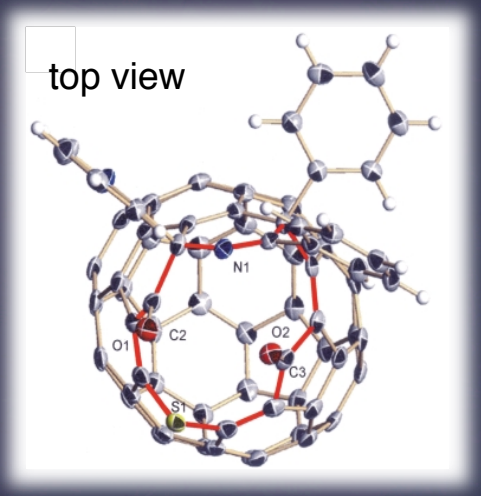


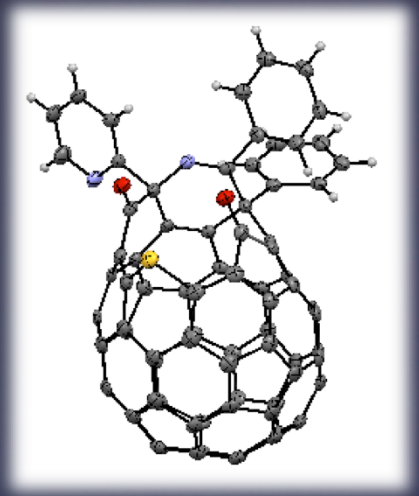
⇒ further enlargement of the opening is necessary

Y. Murata, M. Murata, K. Komatsu, *Chem. Eur. J.* **2003**, *9*, 1600.
M. Murata, Y. Murata, K. Komatsu, *Chem. Commun.* **2008**, 6083.

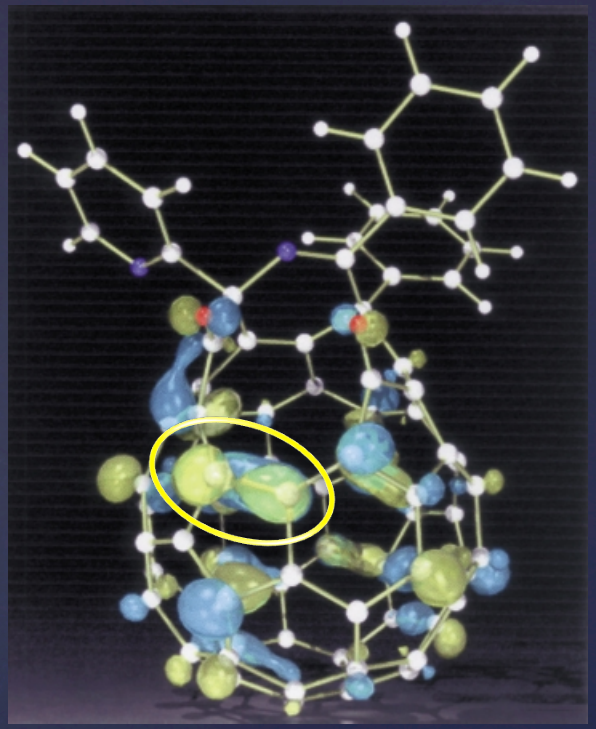
Encapsulation of H_2 in C_{60} by Organic Synthesis

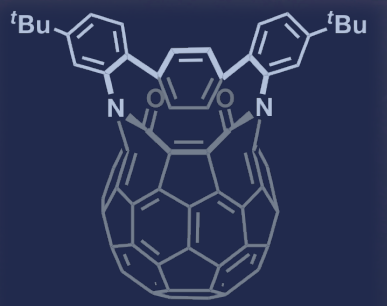
13-membered-ring orifice





X-ray structure





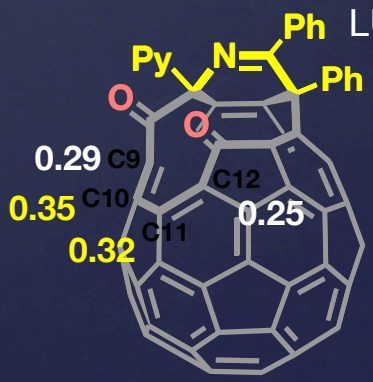
elliptic shape
(14-membered ring)

the largest hole
(at that time)

relatively circular shape
(13-membered ring)

S_8 (1 eq)
TDAE (1 eq)

o-$Cl_2C_6H_4$
180 °C, 30 min
77% yield



absolute values
of the coefficients

LUMO is relatively localized at C9-C10-C11-C12.

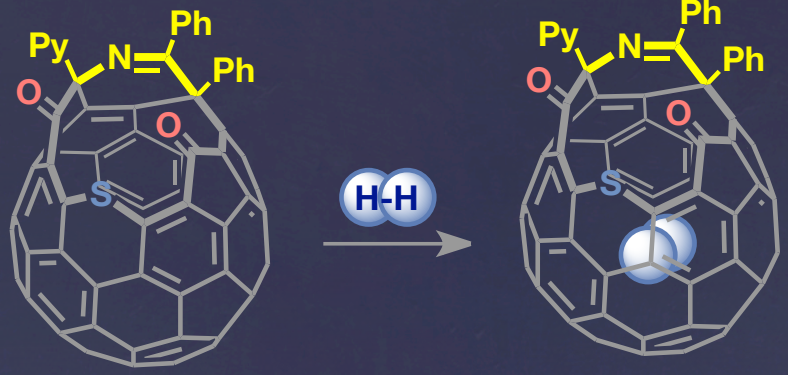
Absolute values of the coefficients of C10 and C11 are 0.35 and 0.32.

⇒ S_8 inserted into the C10-C11 bond.

Y. Murata, M. Murata, K. Komatsu, *Chem. Eur. J.* **2003**, *9*, 1600.

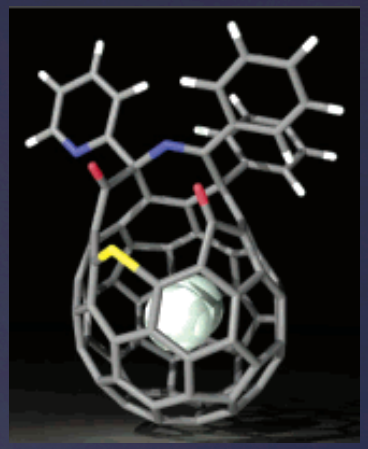
Encapsulation of H_2 in C_{60} by Organic Synthesis

insertion of H_2



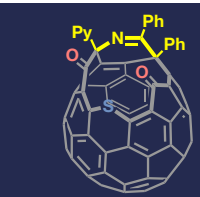
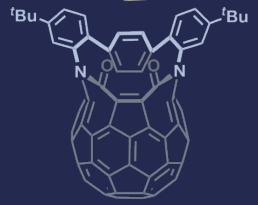
the largest hole
(at that time)

relatively circular shape
(13-membered ring)



calculated structre

calculated activation barrier for the insertion of H_2 (kcal/mol)

	barrier to insertion	energy of encapsulation	barrier to escape
	30.1	1.4	28.7
	41.4	1.4	40.4

by Rubin *et al.*

experimental results

200 °C, 800 atm, 8 h → 100% yield

stable at room temp. for more than 3 months.

^{1}H NMR: δ = -7.25 ppm

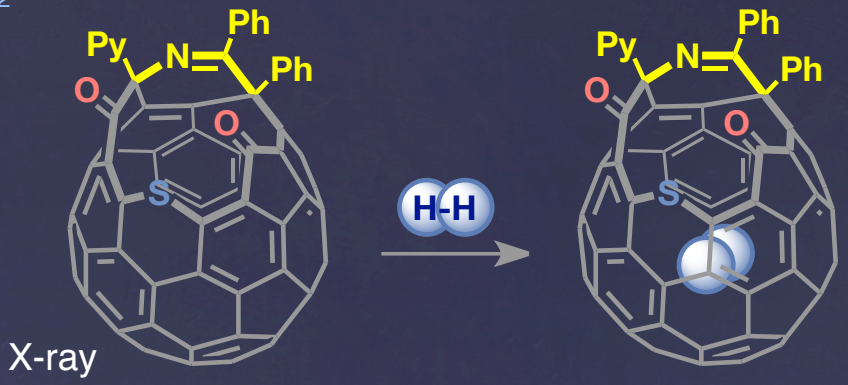
MALDI-TOF mass: H_2@open-cage fullerene
open-cage fullerene
C_{60}
$H_2@C_{60}$

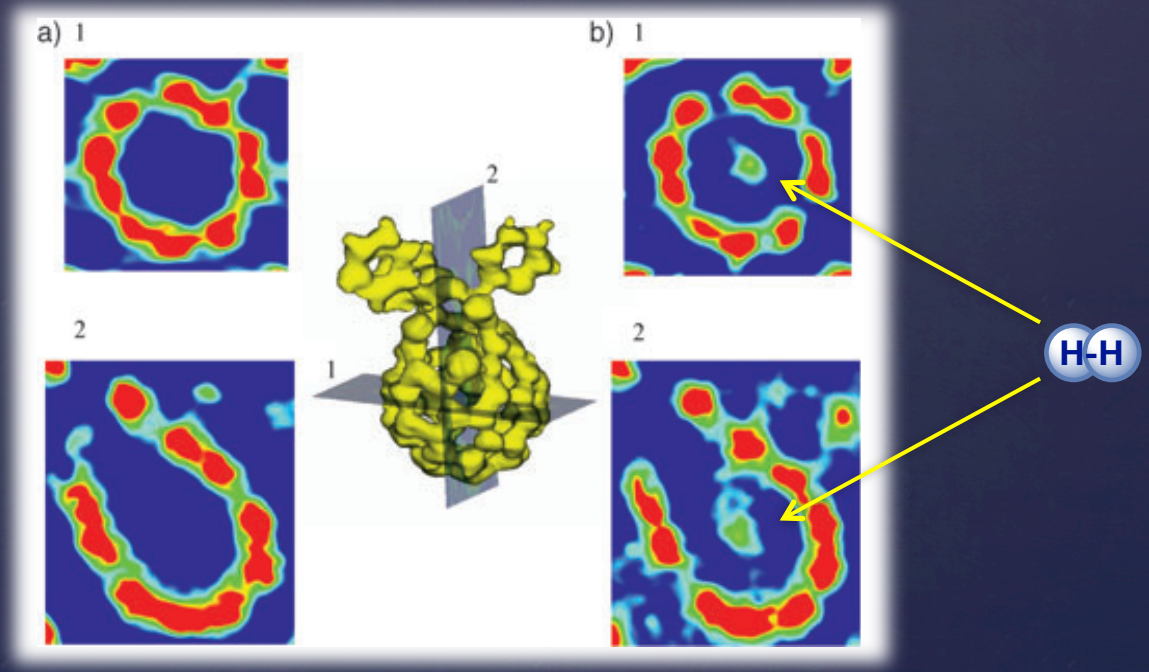
X-ray diffraction study

Y. Murata, M. Murata, K. Komatsu, *J. Am. Chem. Soc.* **2003**, *125*, 7152.

Encapsulation of H_2 in C_{60} by Organic Synthesis

characterization of H_2@ATOCF



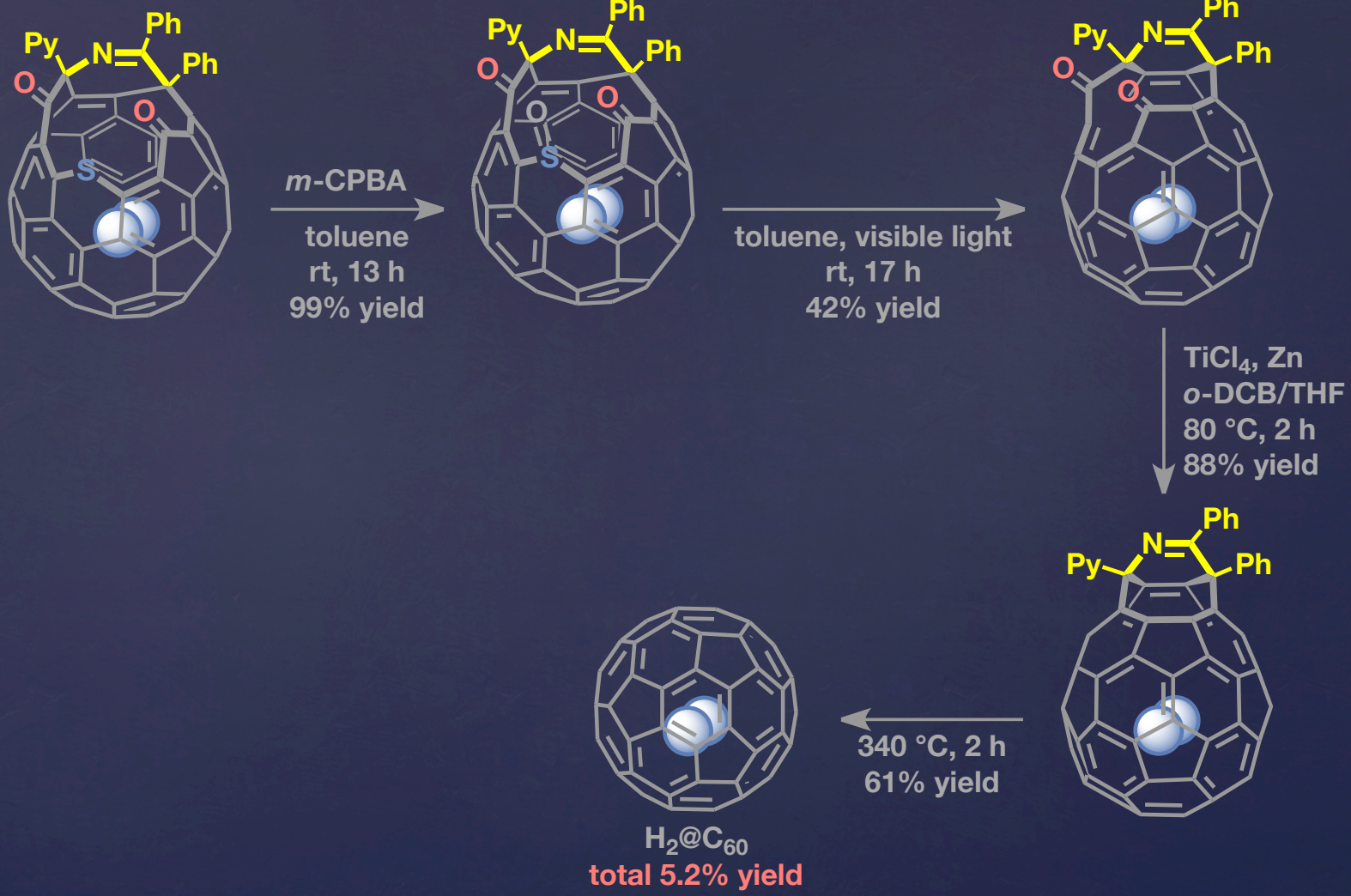


electron density was observed at the center of the fullerene cage.
the number of electrons was calculated to be 2.0 ± 0.1 (= H_2).

H. Sawa, Y. Wakabayashi, Y. Murata, M. Murata, K. Komatsu, *Angew. Chem. Int. Ed.* **2005**, *44*, 1981.

Encapsulation of H_2 in C_{60} by Organic Synthesis

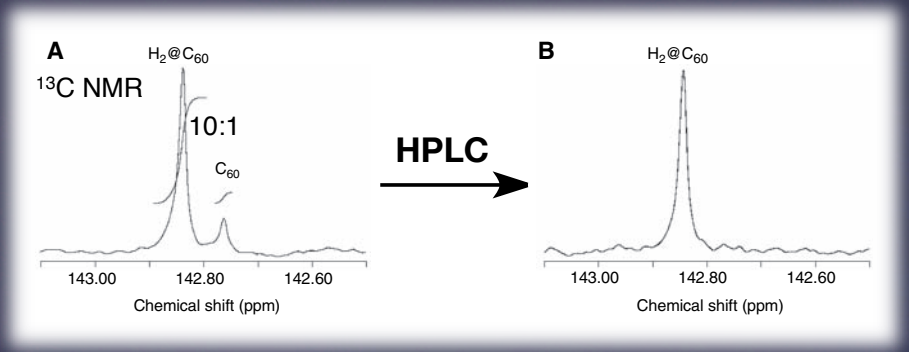
"suture" of the opening



K. Komatsu, M. Murata, Y. Murata, *Science* **2005**, *307*, 238.

Encapsulation of H_2 in C_{60} by Organic Synthesis

purification of $H_2@C_{60}$



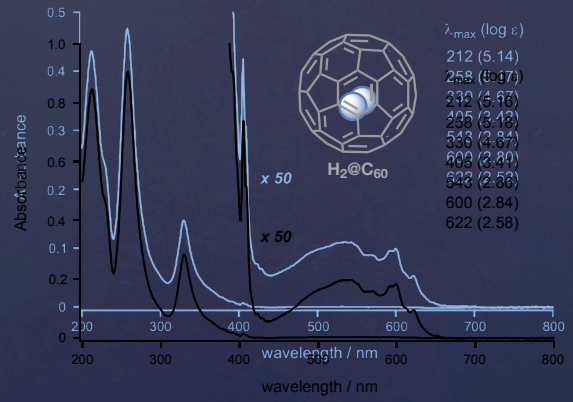
by recycling HPLC (20 cycles)

⇒ "very weak but appreciable van der Waals interaction must be operating between the inner hydrogen molecule and the π-electron cloud of outer C_{60}".

characterization of $H_2@C_{60}$

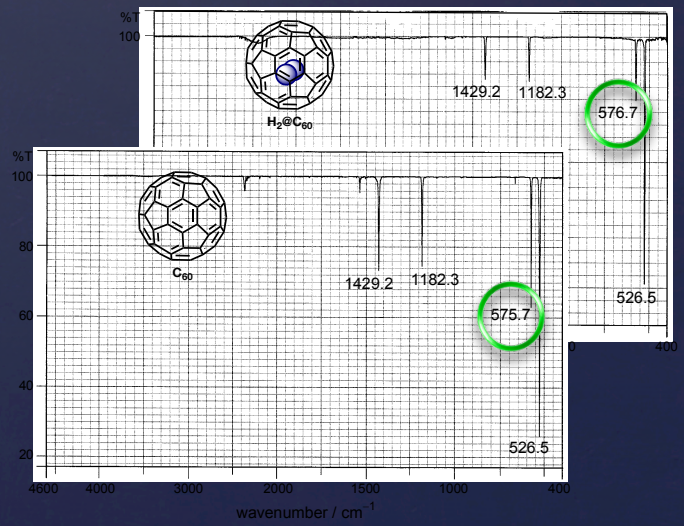
FAB mass
MALDI-TOF mass
elemental analysis
^{1}H NMR
^{13}C NMR

UV-vis spectrum



⇒ UV-vis spectrum is also the same as that of C_{60}.

IR spectrum

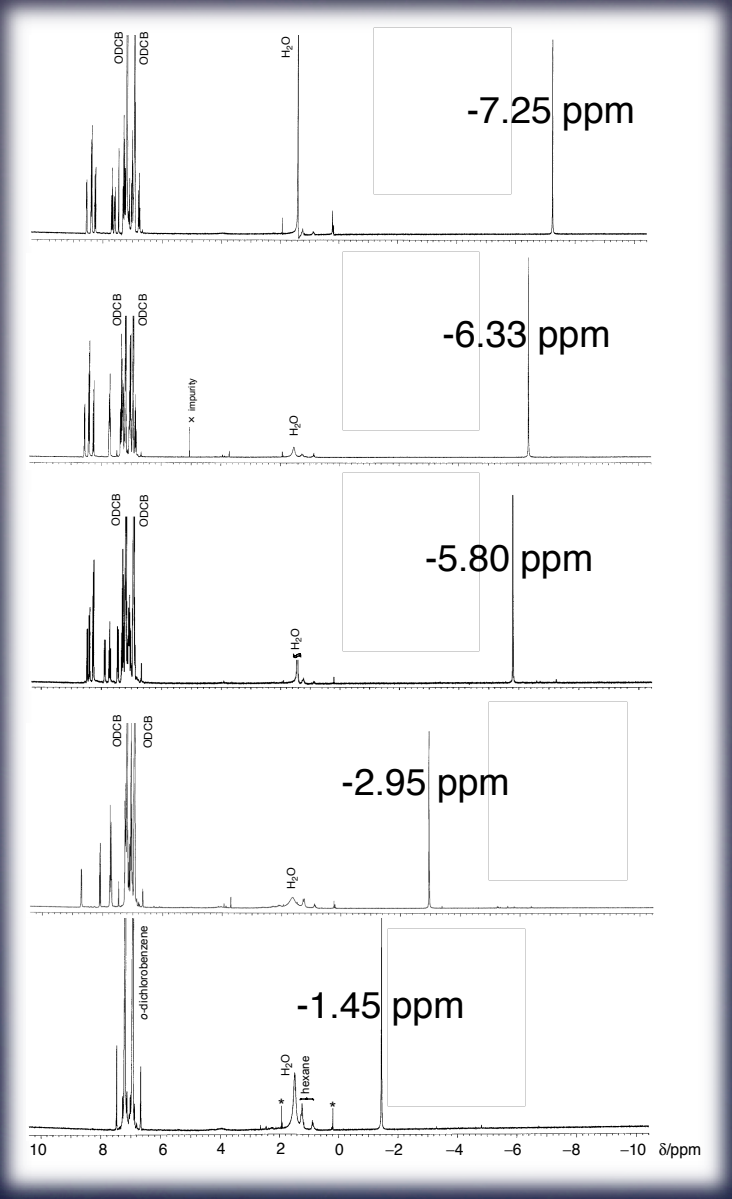


⇒ "slight repulsive interaction with the inner H_2 molecule caused a very slight deformation of the spherical cage of $H_2@C_{60}$".

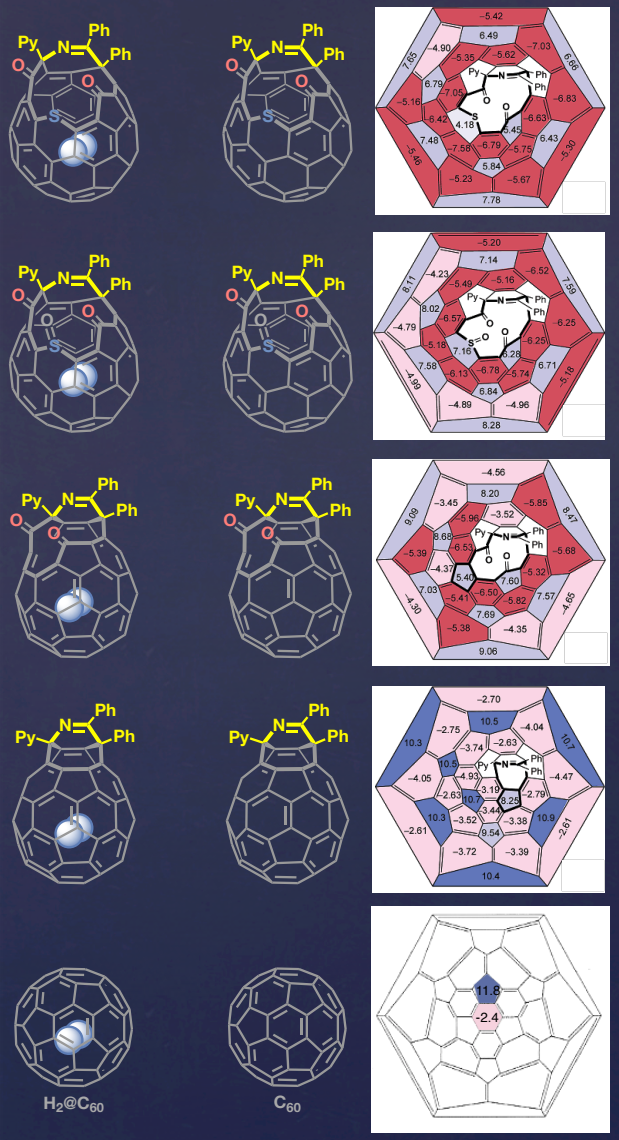
M. Murata, Y. Murata, K. Komatsu,
J. Am. Chem. Soc. **2006**, *128*, 8024.

Encapsulation of H_2 in C_{60} by Organic Synthesis

about ^{1}H NMR chemical shift



NICS values

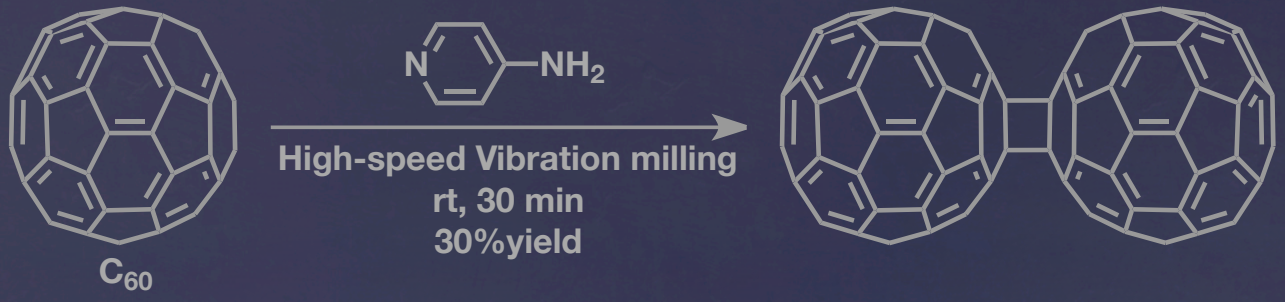


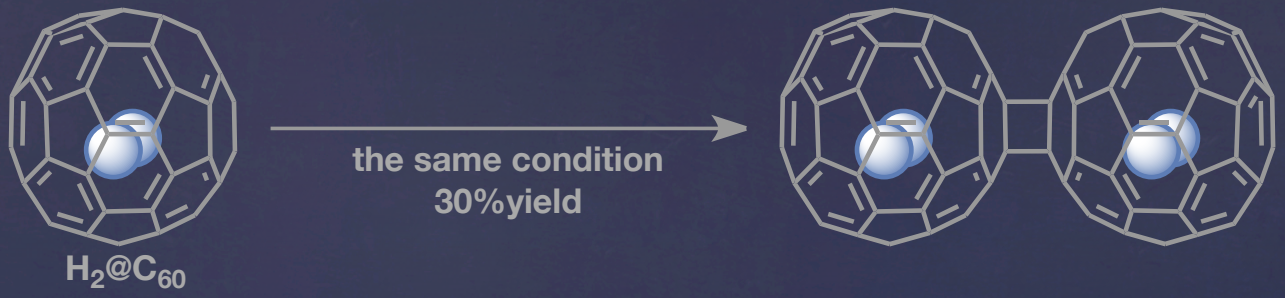
"the size reduction of the orifice in each step is shown to lower the aromatic character of the fullerene cage as a whole".

M. Murata, Y. Murata, K. Komatsu, *J. Am. Chem. Soc.* **2006**, *128*, 8024.

Encapsulation of H_2 in C_{60} by Organic Synthesis

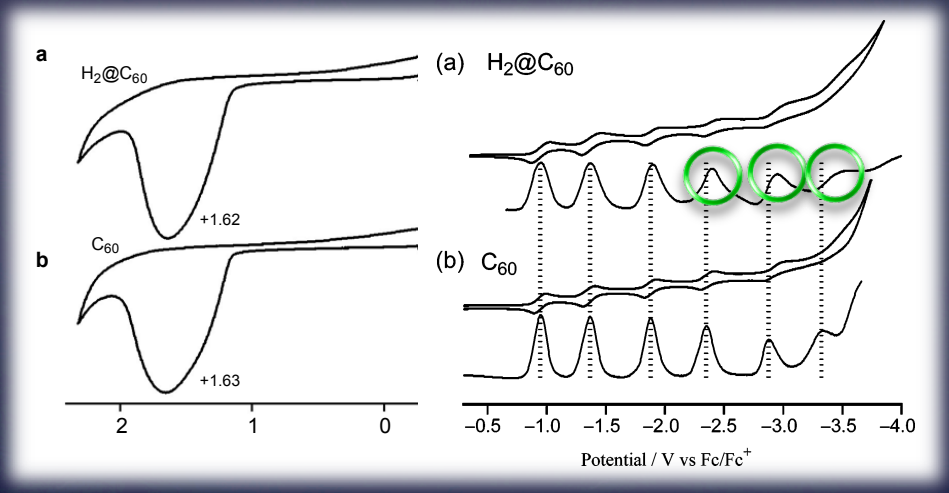
properties of $H_2@C_{60}$





⇒ "the inside hydrogen does not affect the reactivity of the outer C_{60} cage".

electronic property of $H_2@C_{60}$



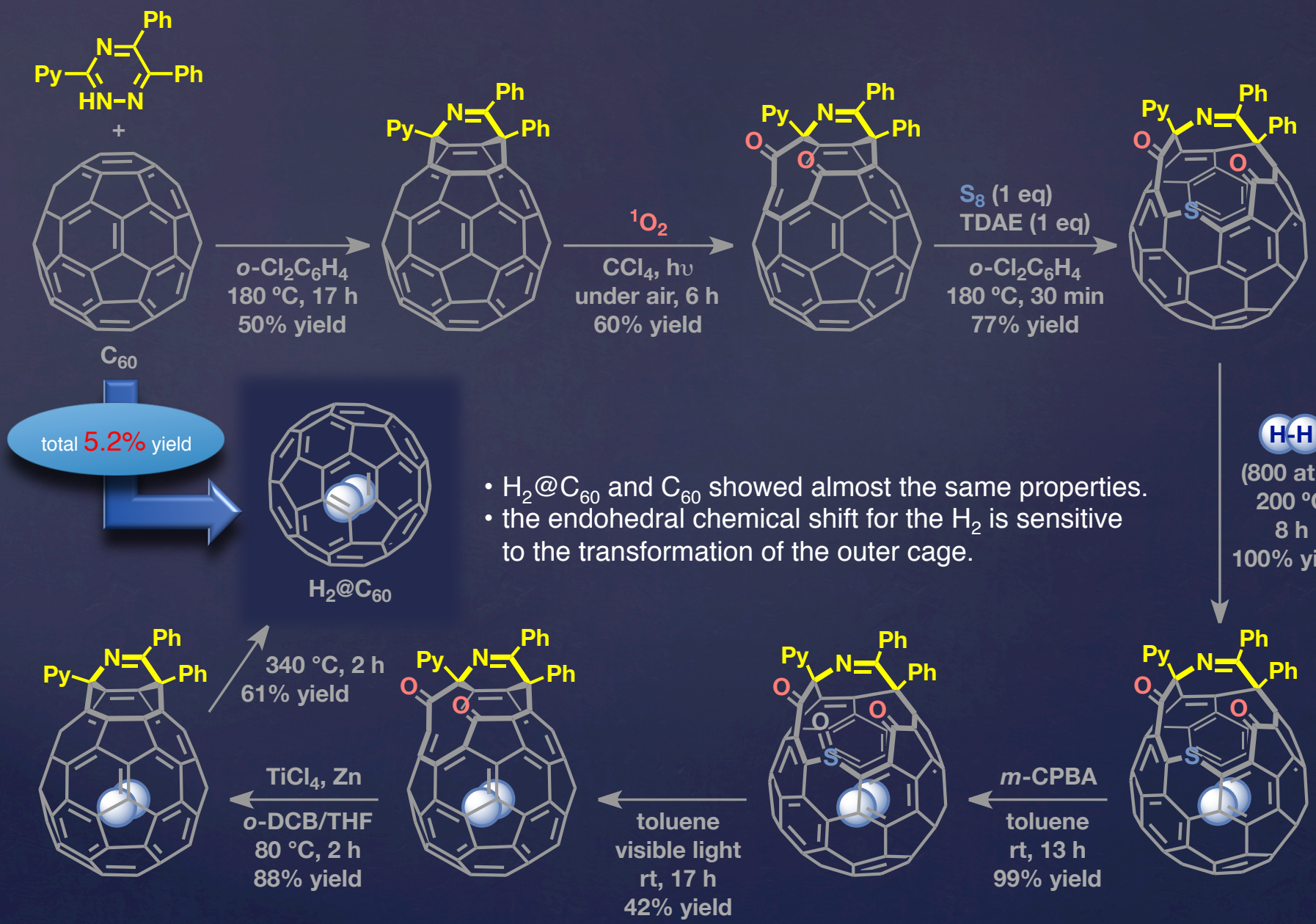
CV and DPV of $H_2@C_{60}$ and C_{60}

⇒ $H_2@C_{60}$ becomes more difficult to be reduced as it acquires more than three electrons.

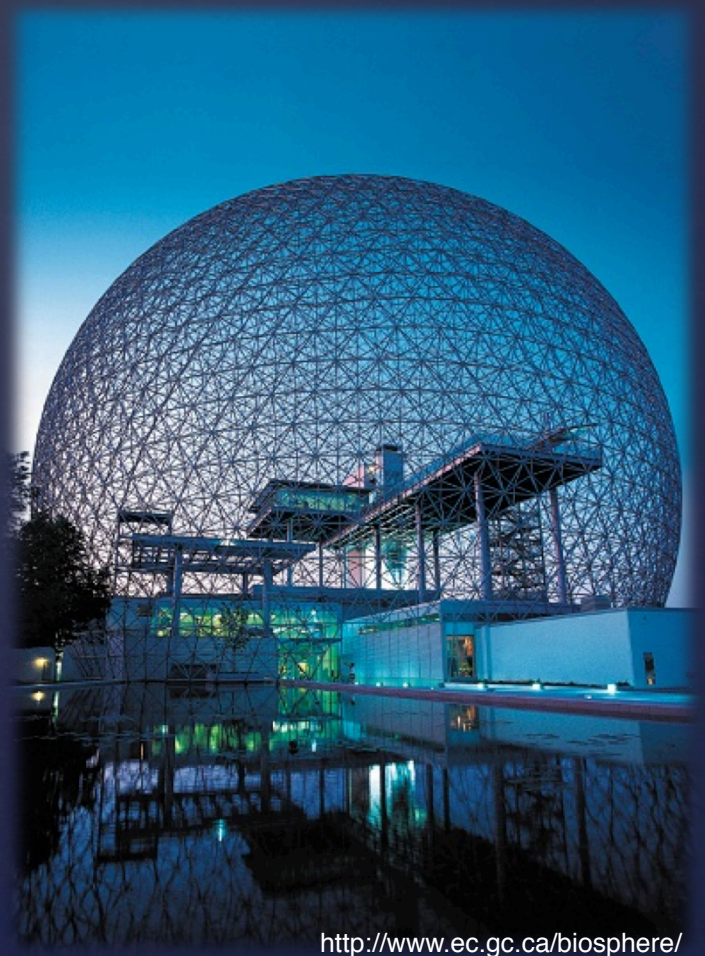
K. Komatsu, M. Murata, Y. Murata, *Science* **2005**, *307*, 238.
M. Murata, Y. Murata, K. Komatsu, *J. Am. Chem. Soc.* **2006**, *128*, 8024.

Encapsulation of H_2 in C_{60} by Organic Synthesis

summary



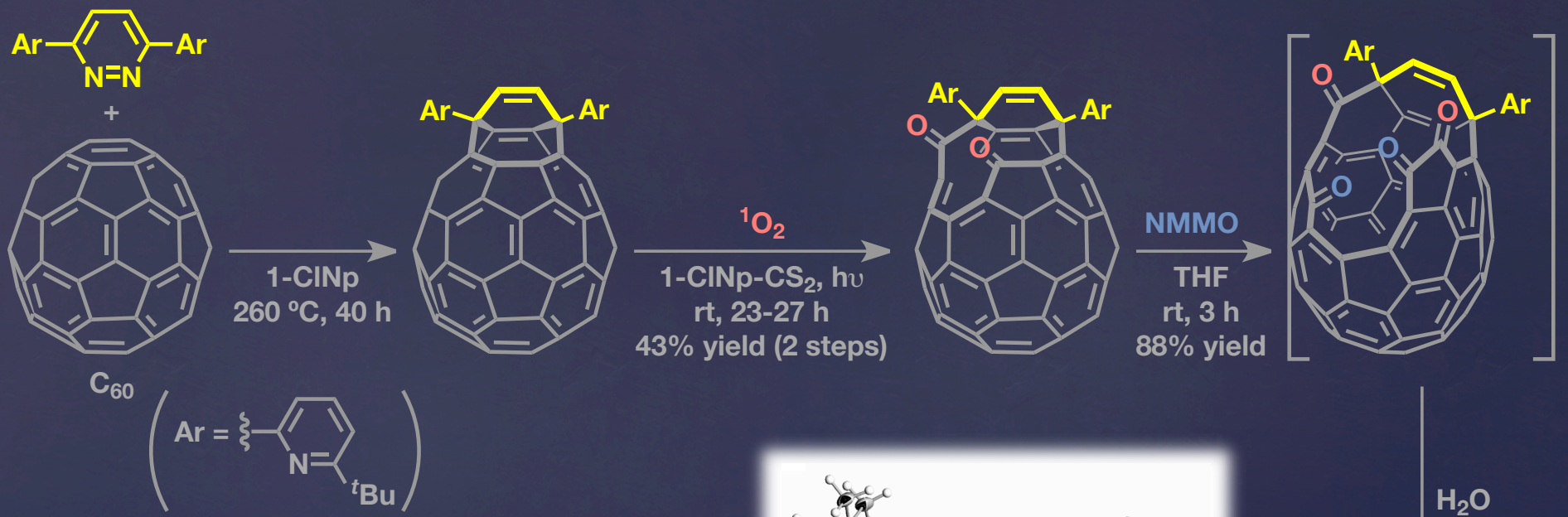
Contents

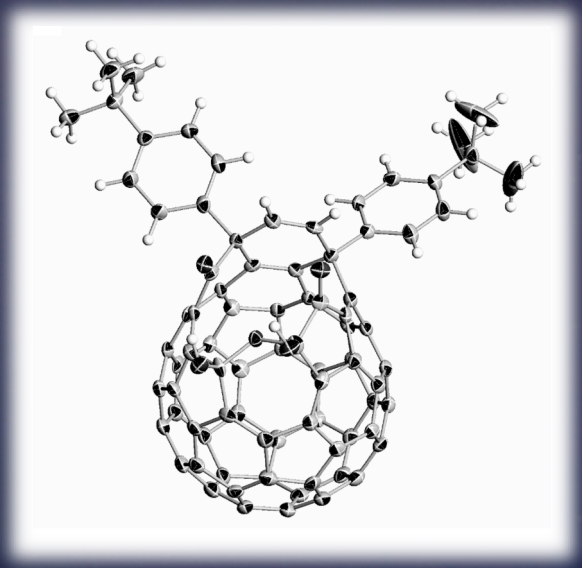


http://www.ec.gc.ca/biosphere/

Encapsulation of H_2O in C_{60} by Organic Synthesis

synthesis



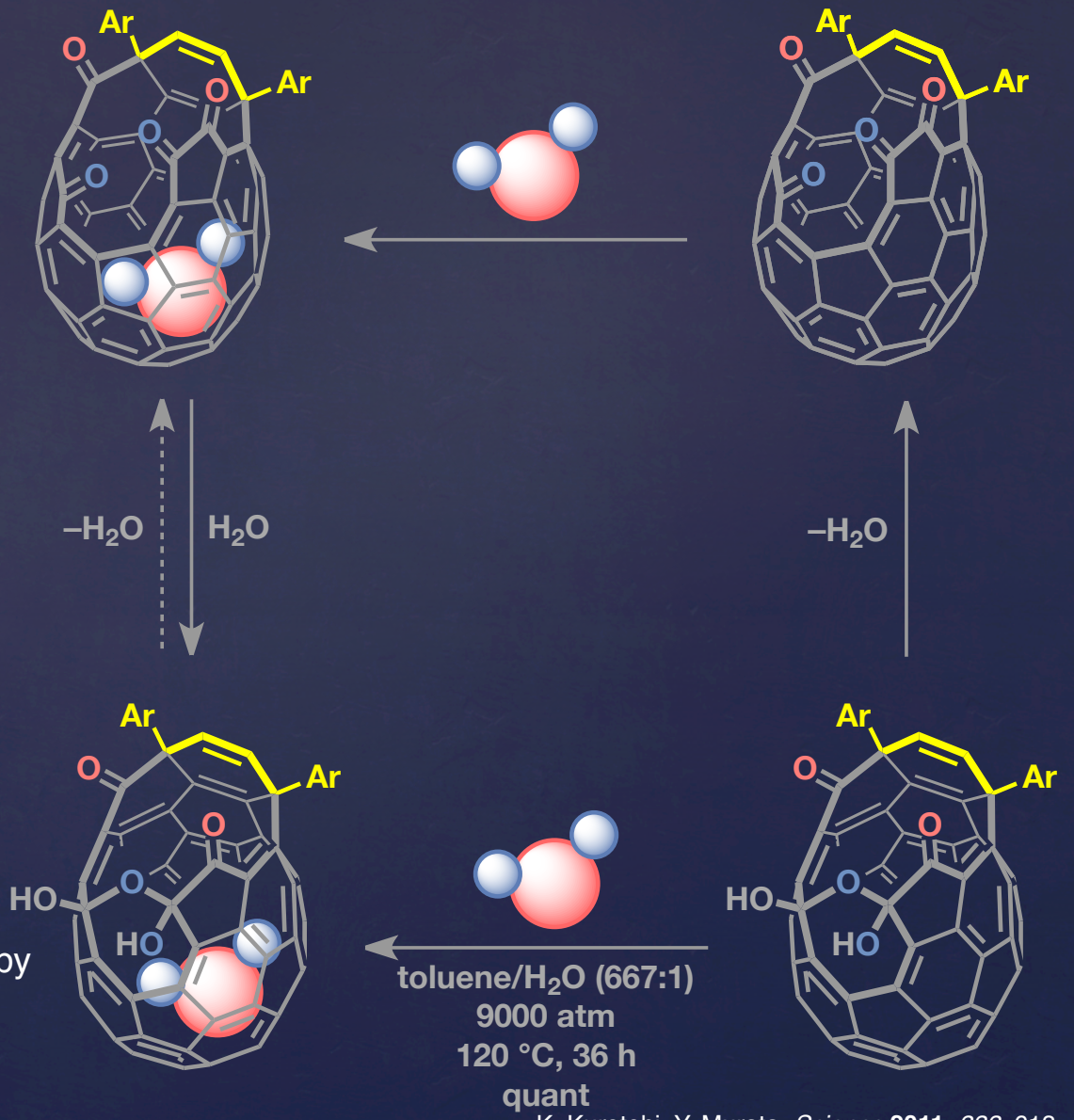


X-ray $\left(\text{Ar} = \text{}^{t}\text{Bu}\right)$

K. Kurotobi, Y. Murata, *Science* **2011**, *333*, 613.

Encapsulation of H_2O in C_{60} by Organic Synthesis

synthesis

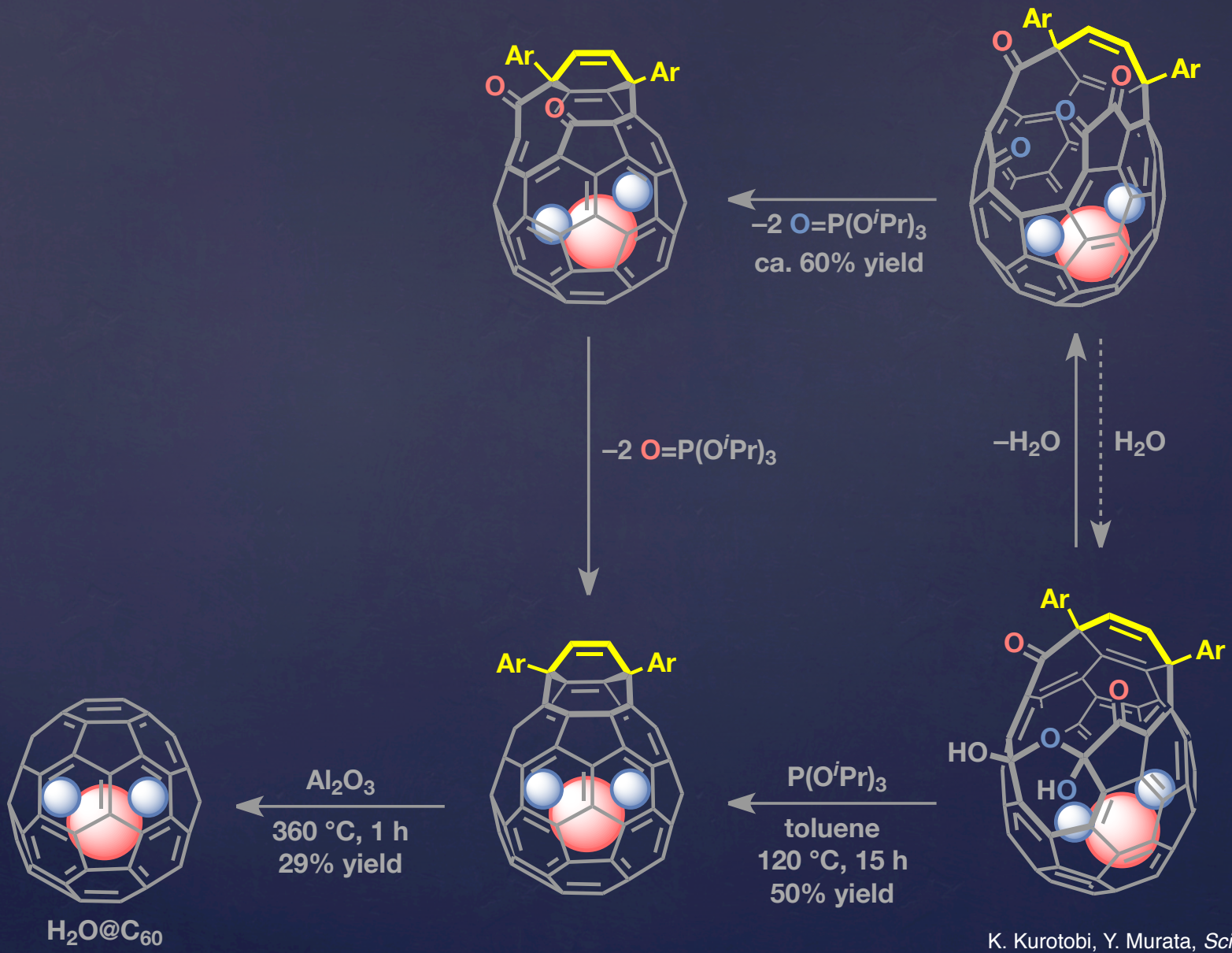


encapsulation of H_2O was supported by
^1H NMR: δ = -9.87 ppm
FAB mass

K. Kurotobi, Y. Murata, *Science* **2011**, *333*, 613.

Encapsulation of H_2O in C_{60} by Organic Synthesis

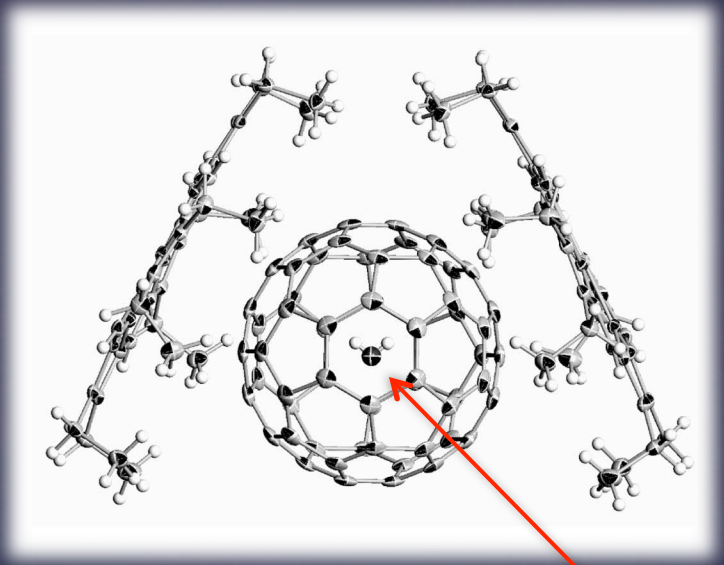
synthesis



K. Kurotobi, Y. Murata, *Science* **2011**, *333*, 613.

Encapsulation of H_2O in C_{60} by Organic Synthesis

evidence for the existence of the encapsulated H_2O



X-ray of $H_2O@C_{60}\cdot(NiOEP)_2$

just at the center of the C_{60} cage

^1H NMR: δ = -4.81 ppm

^{13}C NMR: δ = 142.89 ppm (C_{60}: 143.78 ppm)

⇒ "rapid rotation of the encapsulated H_2O".

APCI mass

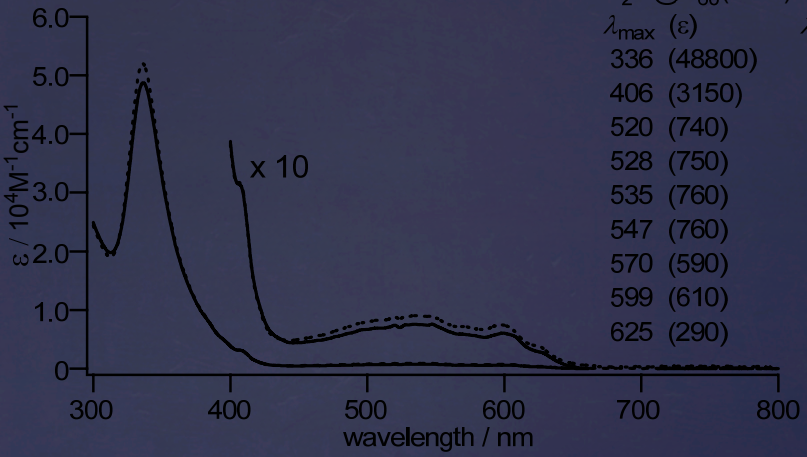
no escape of H_2O was observed (420 °C, 30 min)

"wet fullerene"
"polar C_{60}"

$H_2O@C_{60}$

properties

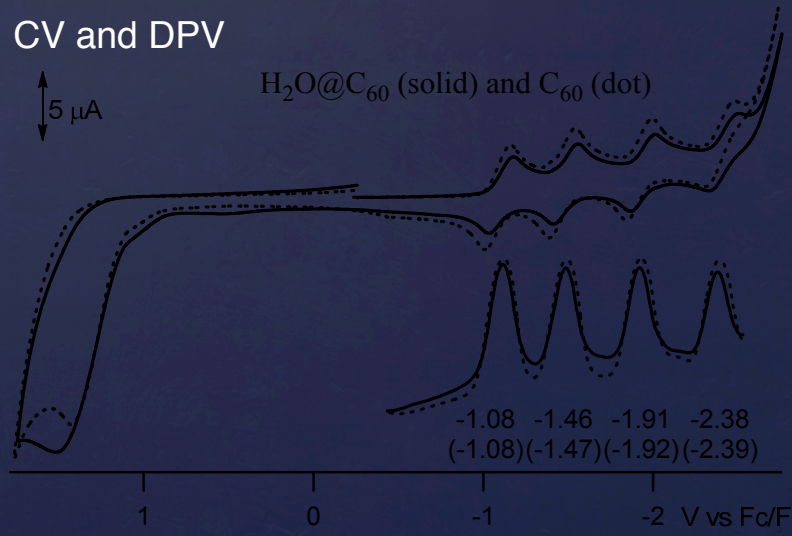
UV-Vis spectra



$H_2O@C_{60}$(solid)		C_{60}(dot)	
λ_{max}	(ε)	λ_{max}	(ε)
336	(48800)	336	(52000)
406	(3150)	406	(3170)
520	(740)	520	(880)
528	(750)	528	(890)
535	(760)	535	(900)
547	(760)	545	(890)
570	(590)	570	(720)
599	(610)	598	(750)
625	(290)	624	(380)

⇒ "no detectable electronic interaction present between the encapsulated H_2O and C_{60} cage".

CV and DPV

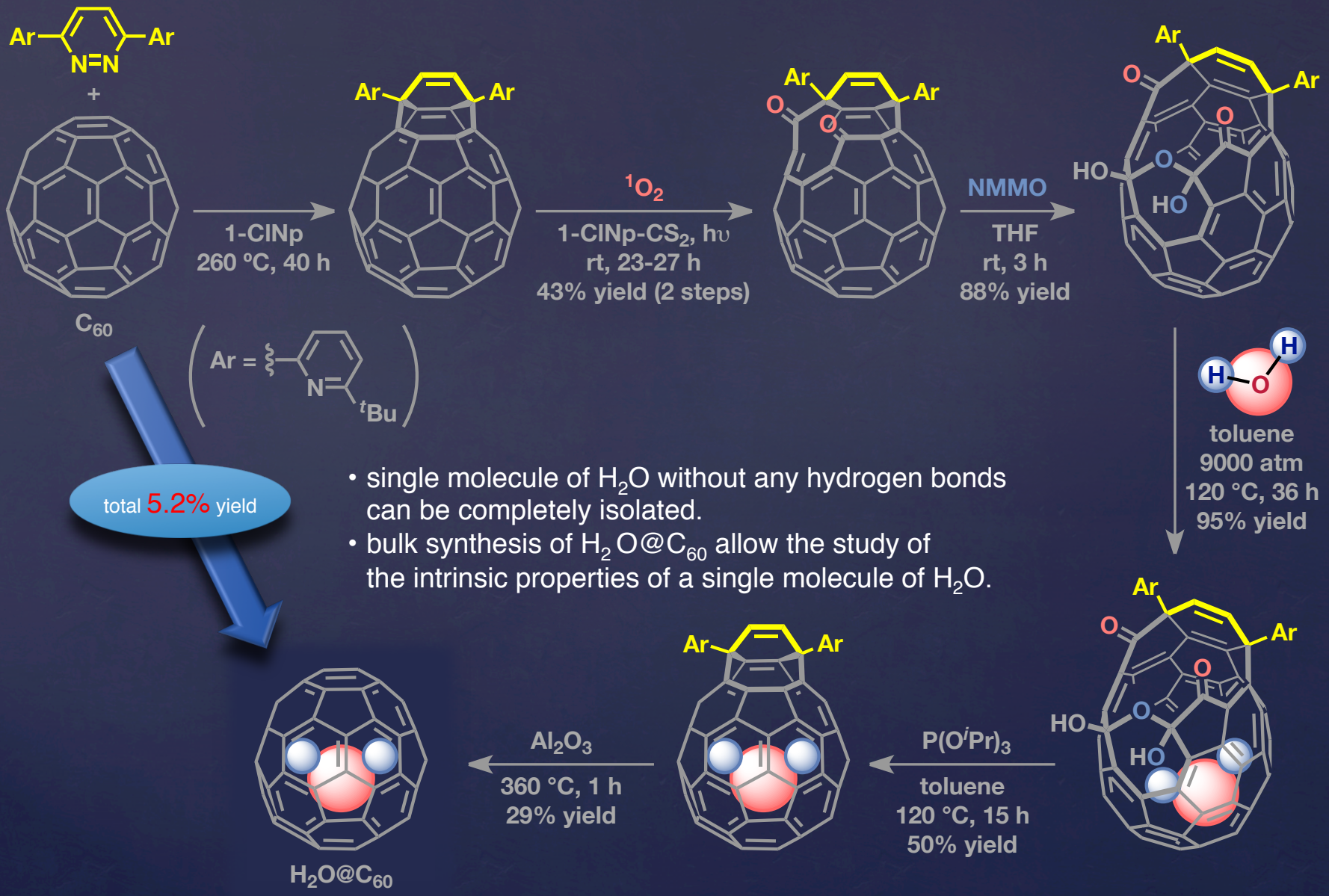


⇒ encapsulated H_2O is electrochemically stable.

K. Kurotobi, Y. Murata, *Science* **2011**, *333*, 613.

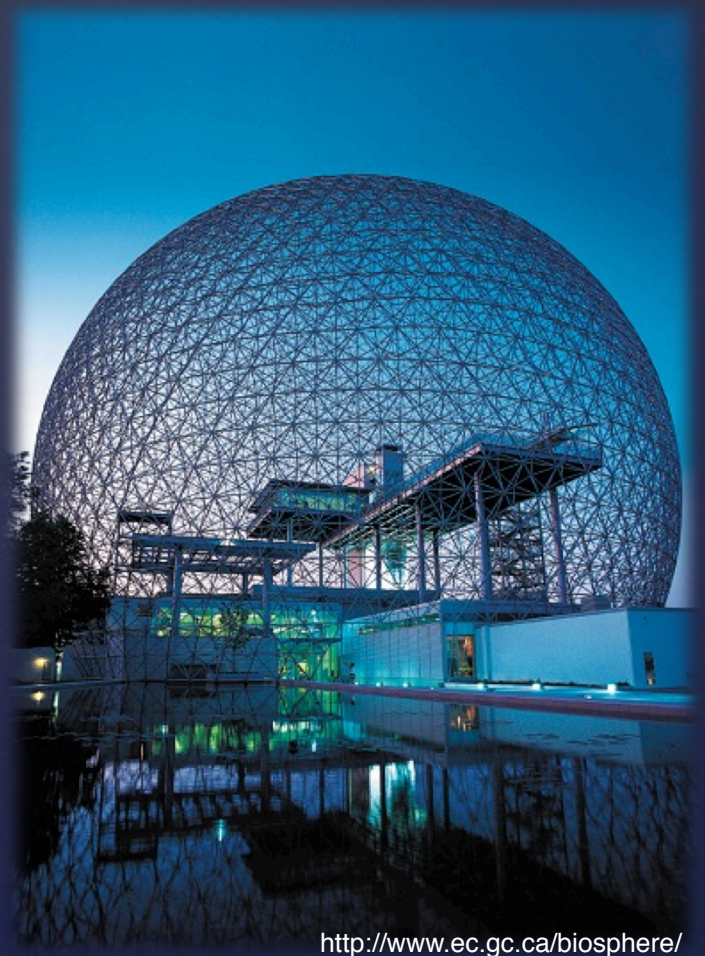
Encapsulation of H_2O in C_{60} by Organic Synthesis

summary



- single molecule of H_2O without any hydrogen bonds can be completely isolated.
- bulk synthesis of $H_2O@C_{60}$ allow the study of the intrinsic properties of a single molecule of H_2O.

Contents



http://www.ec.gc.ca/biosphere/

Summary & Outlook

Introduction

-History of Buckminsterfullerene
-How to Produce Fullerenes?

Aromaticity of Fullerenes

-What is Aromaticity?
-Aromaticity of Buckminsterfullerene

C_{60} has ambiguous aromatic character.

Endohedral Fullerenes Encapsulating a Molecule

-Why Endohedral Fullerenes?
-Conventional Synthesis of Endohedral Fullerenes
-"Molecular Surgery"
$H_2@C_{60}$, $H_2O@C_{60}$

total 5.2% yield

total 5.2% yield

Summary & Outlook

Endohedral Fullerenes Encapsulating a Molecule

Scientific interest!!

+

expected to have high potential such as…

-synthesis of new endohedral fullerenes which can't be obtained by conventional methodologies
-highly efficient (gram scale) synthesis of endohedral fullerenes → material sciences
-control π-electron system from the inside of fullerenes
-completely "isolated" molecule
-encapsulation of highly active species

etc.