第７回　（１）BX_3のルイス酸性度

テキストp.117 (e)-118

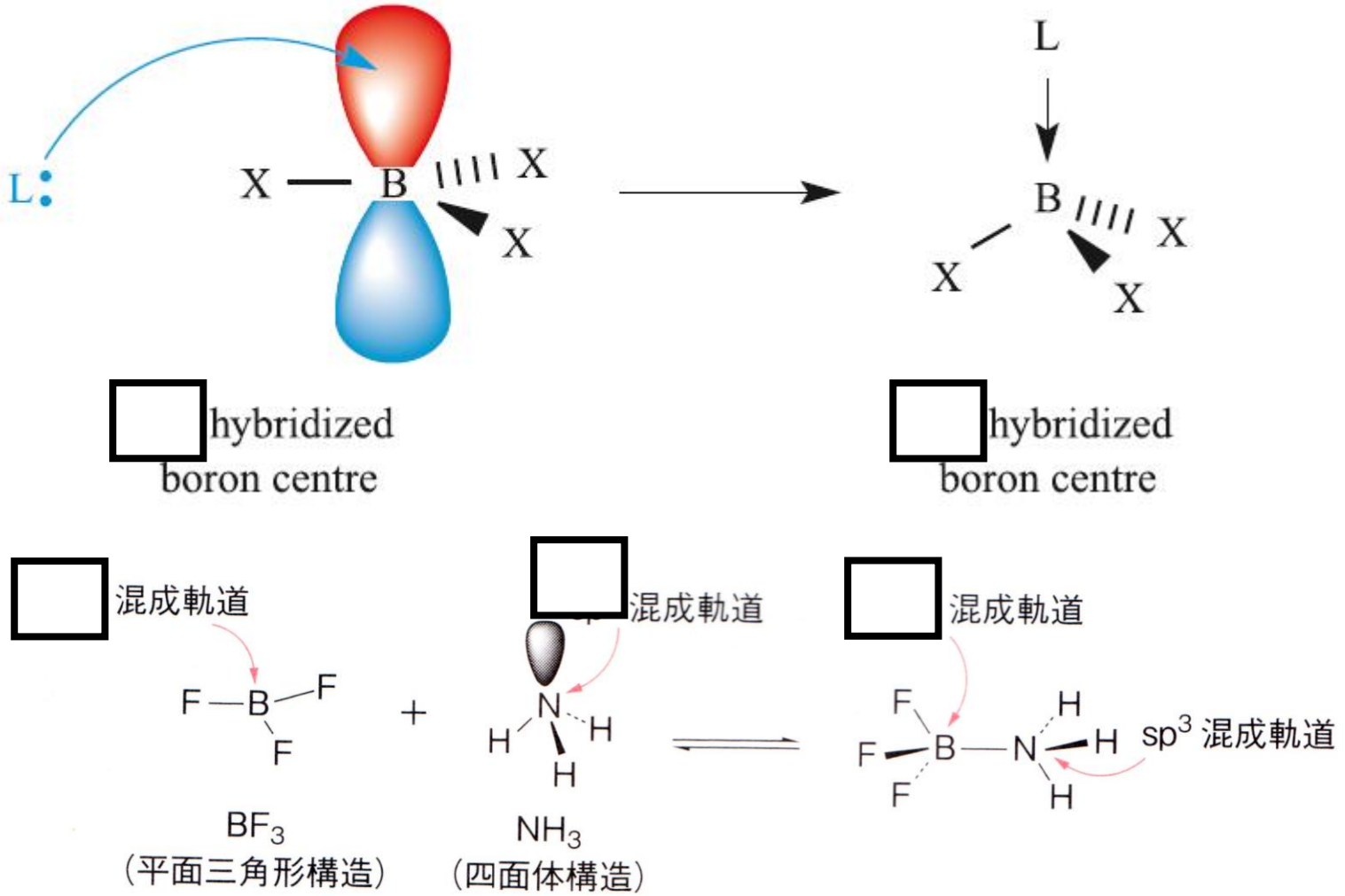
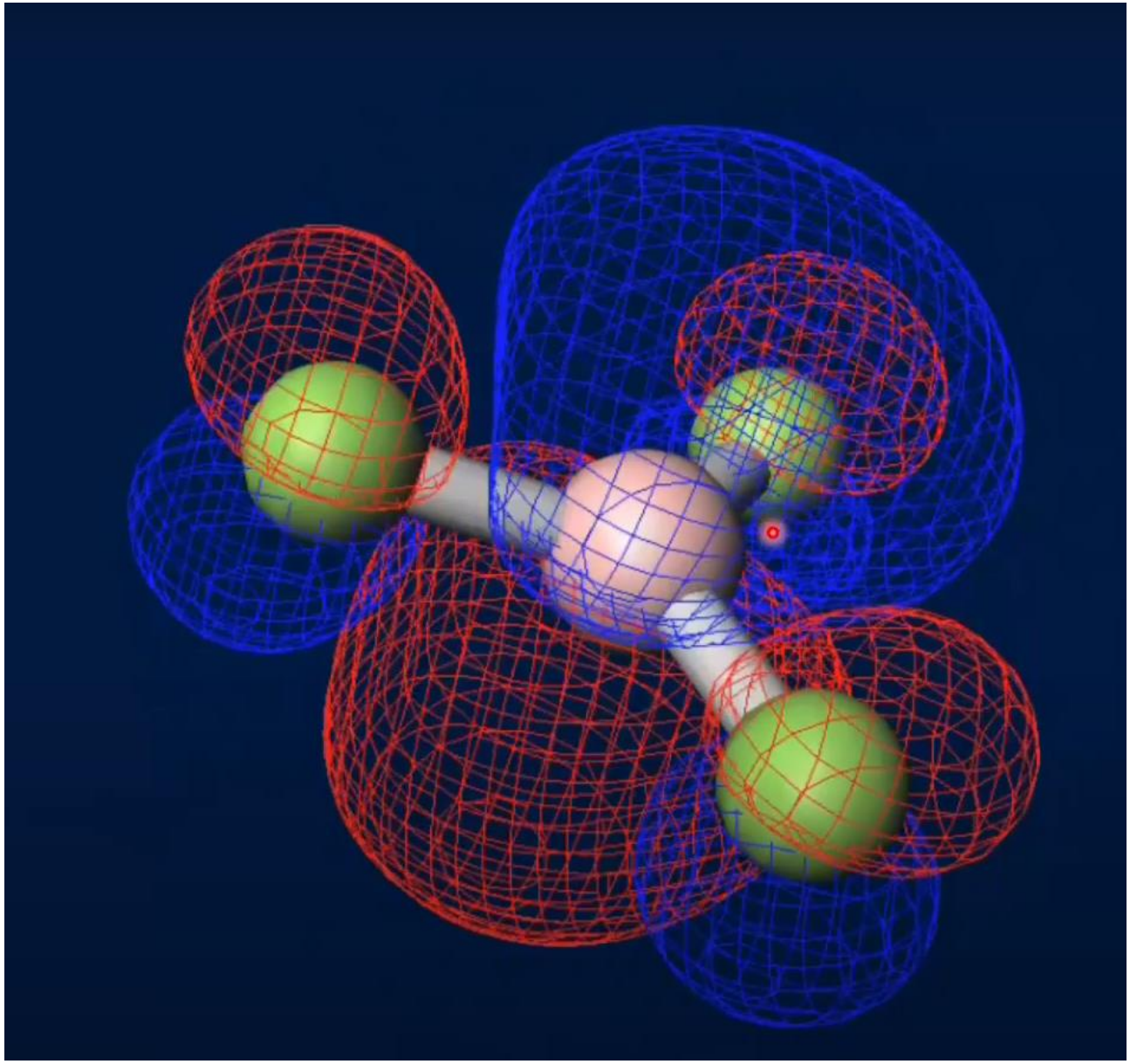


図 5.1　ハロゲン化物とルイス塩基との反応



BF_3の分子軌道(LUMO, 下図の13の軌道)

HOMO: 12

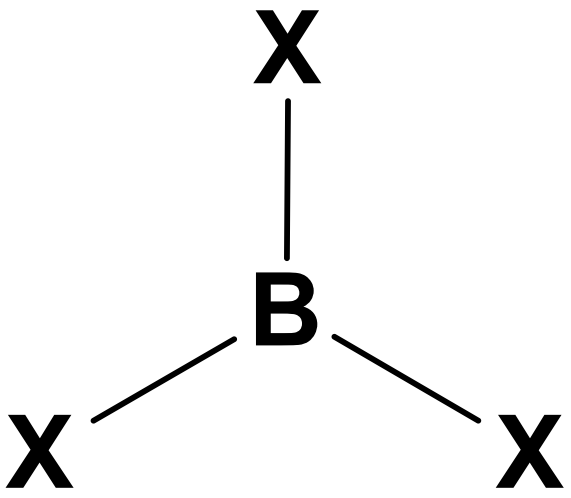
HOMO-LUMO Gap : 16.7039 eV

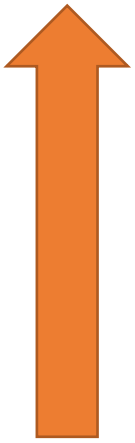
Unit: ○ a.u. ◉ eV

16	6.5434
15	6.5431
14	1.8723
13	1.7643
12	-14.9396
11	-14.9397
10	-15.1505
9	-15.1928
8	-15.1929
7	-18.4593
6	-18.8345
5	-18.8347
4	-22.8042
3	-50.6128
2	-50.6131
1	-51.6471

LUMO: lowest unoccupied molecular orbital （最低空軌道）＝電子を受け取るときに重要になる軌道. （テキストp.93）プリントの最後に若干の説明あり.

BX_3のルイス酸性度





電気陰性度

B－X distance

X = F	131 pm
X = Cl	174 pm
X = Br	189 pm
X = I	210 pm

BF_3, BCl_3, BBr_3, BI_3 ← ルイス酸性度の大きさは？

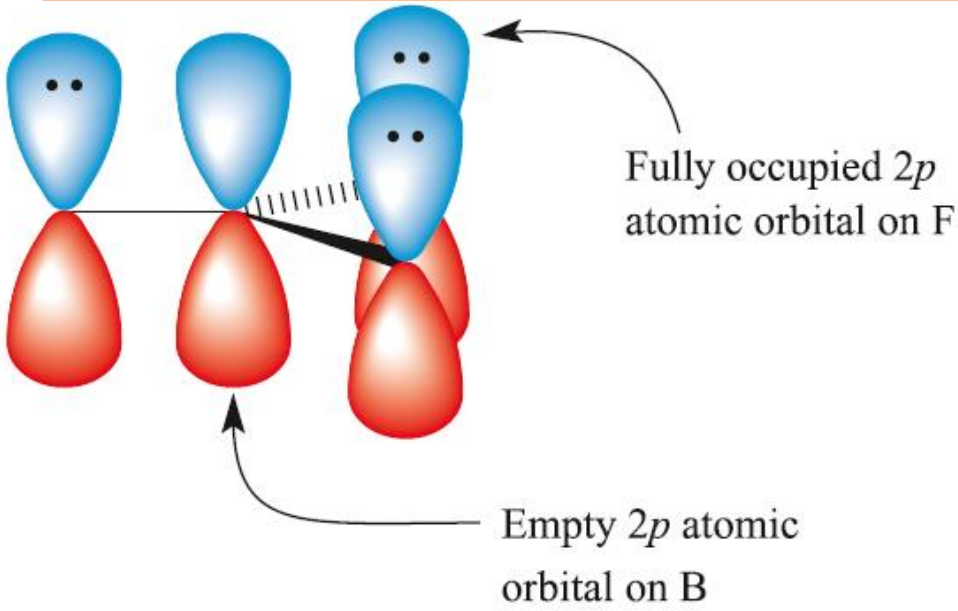
BX_3のルイス酸性度

B-X結合には,□結合性が一部含まれている.

(BI_3を除く）

π結合性の割合：B□$_3$ > B□$_3$ >B□$_3$

Lewis acidity: □ < □ < □



	B-X distance (pm)	*)共有結合半径
X = F	131 pm	71 pm
X = Cl	171 pm	99 pm
X = Br	189 pm	114 pm
X = I	210 pm	133 pm

Bの共有結合半径：82 pm

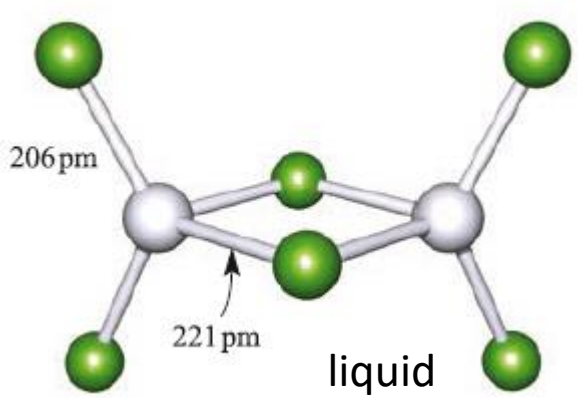
*)共有結合半径（テキストp.27 図2.2）

第13族元素のハロゲン化物

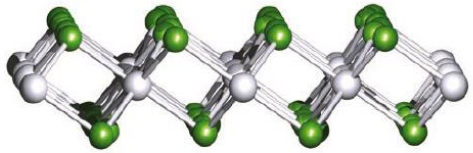
テキストp.115

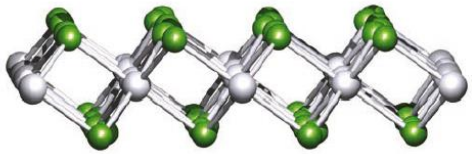
$AlCl_3$

強いLewis acid



liquid



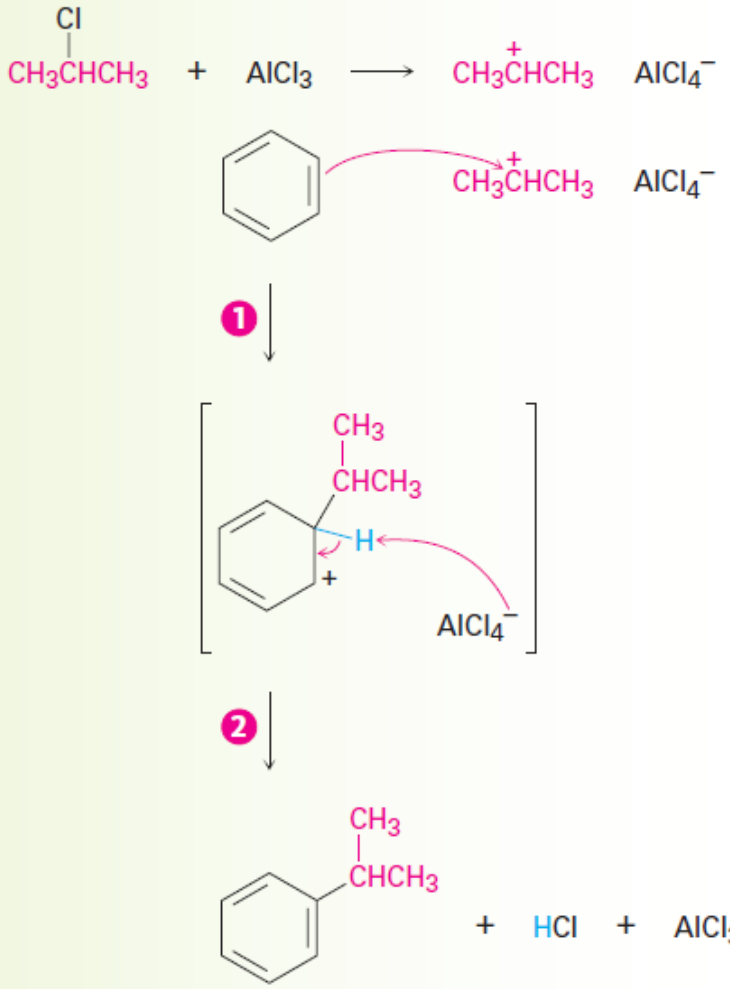


solid

Friedel-Craftsアルキル化

MECHANISM

Mechanism for the Friedel–Crafts alkylation reaction of benzene with 2-chloropropane to yield isopropylbenzene (cumene). The electrophile is a carbocation, generated by $AlCl_3$-assisted dissociation of an alkyl halide.

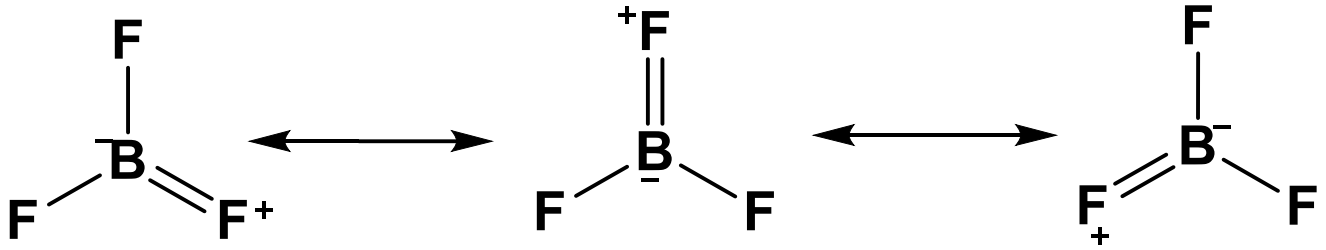


John McMurry, *Organic Chemistry* (9th Ed), 488

第７回　（１）BX_3のルイス酸性度

Lewis acidity: $BF_3 < BCl_3 < BBr_3$

B-X間のπ結合性の割合



$AlCl_3$ 強いLewis acid

Lewis酸触媒　Friedel-Craftsアルキル化

アシル化