POSTER

DIPOLAR LATTICE ENERGY FOR $KC_{24}(THF)_x$

A. Charlier†,M.F. Charlier†,A. Laurent†,F. Foureson† and R. Setton‡

† Laboratoire de Physique du Solide, 1 Bld Arago, 57068 Metz France

‡CRSOC/CNRS, 1B rue de la Férollerie, 45071 Orléans France

INTRODUCTION

Evaluation of ionic, ion-dipolar and dipolar interaction energies for $KC_{24}(THF)_x$ first stage intercalation compounds (with x=1 or 2) enables determination of tetrahydrofuran's dipole orientation in the lattice cell.

STRUCTURE OF $KC_{24}(THF)_x$

In tetrahydrofuran $(CH_2)_40$ or THF we cannot say that the oxygen atom is negatively charged and the carbon atoms positively but rather that the binding is charged with δ^- on O and δ^+ on the C atoms. Oxygen has two pairs of noncoupled electrons: gaseous THF exhibits a permanent dipolar momentum.
The THF molecule is planar as the sum of angles equal 540° (see table 1 and figure 1) .

Table 1 Tetrahydrofuran

$\widehat{COC}$= 111°	
$\widehat{CCC}$= 105.5°	$d_{C-C} = 1.54\AA$
$\widehat{CCH}$= 127.3°	$d_{C-H} = 1.10\AA$
$\widehat{HCH}$= 109.5°	$d_{C-O} = 1.43\AA$
$\widehat{CCO}$= 109°	

The studied graphite intercalation compounds $KC_{24}(THF)_x$ are all first stage compounds. They present monoclinic or orthorhombic structures [1],[2],[3].

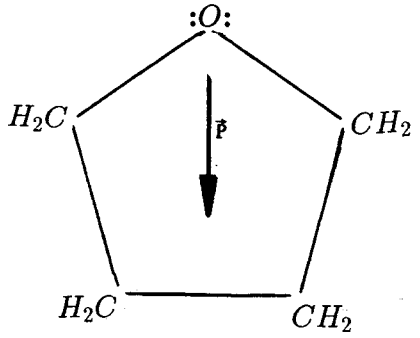

Figure 1 Tetrahydrofuran

In table 2 we present the first stage monoclinic $KC_{24}(THF)_2$ unit cell

Table 2 First stage monoclinic $KC_{24}(THF)_2$ unit cell

	x	y	z
a	$7.41d-10$	0.0	0.0
b	$-2.456d-10$	$8.564d-10$	0.0
c	0.0	0.0	$8.84d-10$

Table 3 Atoms in monoclinic $KC_{24}(THF)_2$ first stage

		q	a	b	c
1	C	$-1/24$	0.055	1/6	0.0
2	C	$-1/24$	0.194	1/12	0.0
3	C	$-1/24$	0.389	1/6	0.0
4	C	$-1/24$	0.528	1/12	0.0
5	C	$-1/24$	0.722	1/6	0.0
6	C	$-1/24$	0.861	1/12	0.0
7	C	$-1/24$	0.110	1/3	0.0
8	C	$-1/24$	0.304	5/12	0.0
9	C	$-1/24$	0.444	1/3	0.0
10	C	$-1/24$	0.638	5/12	0.0
11	C	$-1/24$	0.777	1/3	0.0
12	C	$-1/24$	0.972	5/12	0.0
13	C	$-1/24$	0.028	7/12	0.0
14	C	$-1/24$	0.223	2/3	0.0
15	C	$-1/24$	0.362	7/12	0.0
16	C	$-1/24$	0.556	2/3	0.0
17	C	$-1/24$	0.696	7/12	0.0
18	C	$-1/24$	0.890	2/3	0.0
19	C	$-1/24$	0.139	11/12	0.0
20	C	$-1/24$	0.278	5/6	0.0
21	C	$-1/24$	0.472	11/12	0.0
22	C	$-1/24$	0.611	5/6	0.0
23	C	$-1/24$	0.806	11/12	0.0
24	C	$-1/24$	0.945	5/6	0.0
25	K	$+1.0$	0.0	0.0	0.5

Table 3 shows the atomic and electric distribution in a unit cell of monoclinic $KC_{24}(THF)_2$ first stage. Figure 2 is the representation of atoms in a unit cell.

LATTICE ENERGY

We give in table 4 Madelung energy [4] values or ion-ion interaction energies for the three studied compounds. The interaction energies produced by ionic and dipolar lattices are computed by formulas derived from *Ewald's* [5] and *Kornfeld's* [6] methods. The value of the permanent dipolar momentum for tetrahydrofuran is taken equal to 1.63 Debye (to be compared to 1.85 for H_2O or 1.5 for NH_3. They permit to show that in terms of energy the anti-parallel structure is more stable than the parallel.

Table 4 Madelung energies

Compound	*Struct.*	$10^{-19}J$	eV
$KC_{24}(THF)_2$	*Monocl.*	-1.69	-1.05
$KC_{24}(THF)_2$	*Orthor.*	-1.65	-1.03
$KC_{24}(THF)_1$	*Monocl.*	-0.45	-0.28

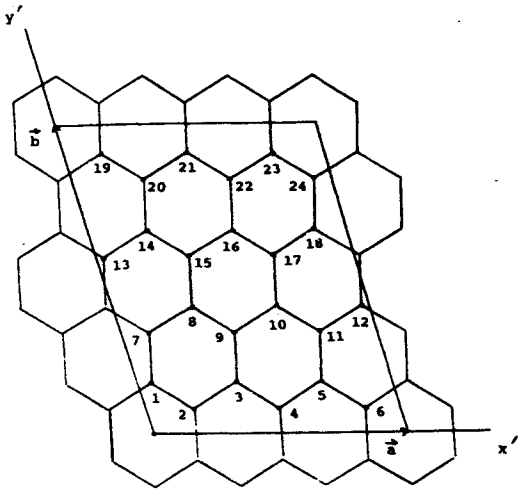

Figure 2 Atoms in monoclinic $KC_{24}(THF)_2$ first stage

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