

## Bismuth Hybrid Halide with Dual Inhibition against Alzheimer's and Type 2 Diabetes Probed by Structural, Vibrational, and Theoretical Analysis

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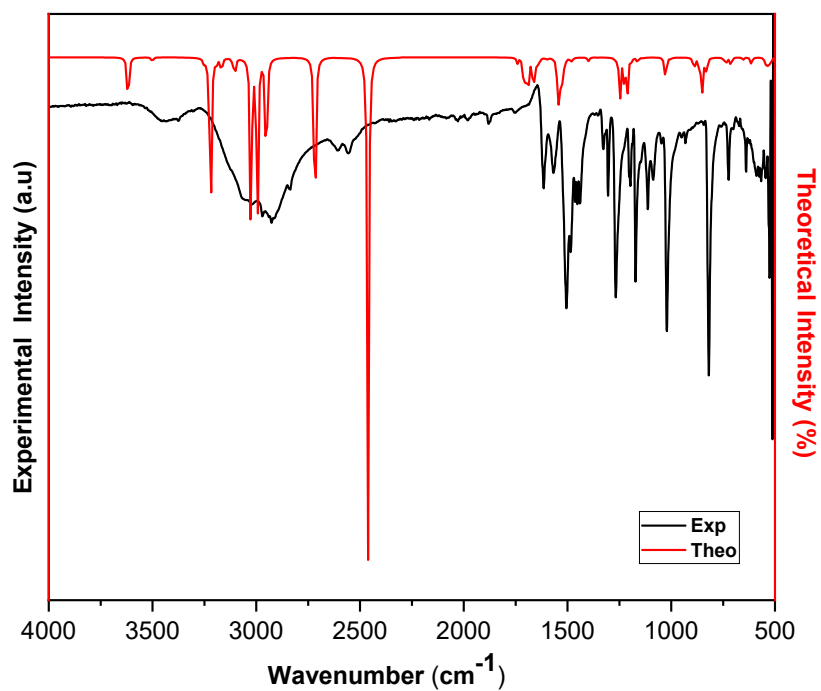
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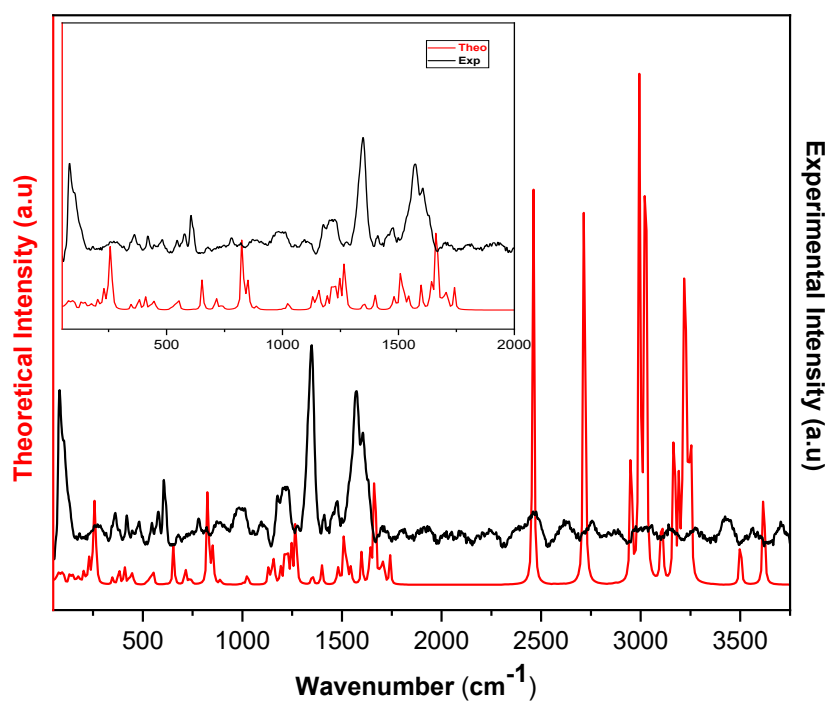
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**Table 1.S.** The character table for C<sub>2h</sub>.

C <sub>2h</sub>	E	C <sub>2</sub>	i	σ <sub>h</sub>	Linear/Quadratic Functions	Activity
<b>Ag</b>	1	1	1	1	X <sup>2</sup> , y <sup>2</sup> , z <sup>2</sup> , xy	Raman-active
<b>Bg</b>	1	-1	1	-1	xz, yz	Raman-active
<b>Au</b>	1	1	-1	-1	z, translations (Tz)	IR-active
<b>Bu</b>	1	-1	-1	1	x, y, translations (Tx, Ty)	IR-active



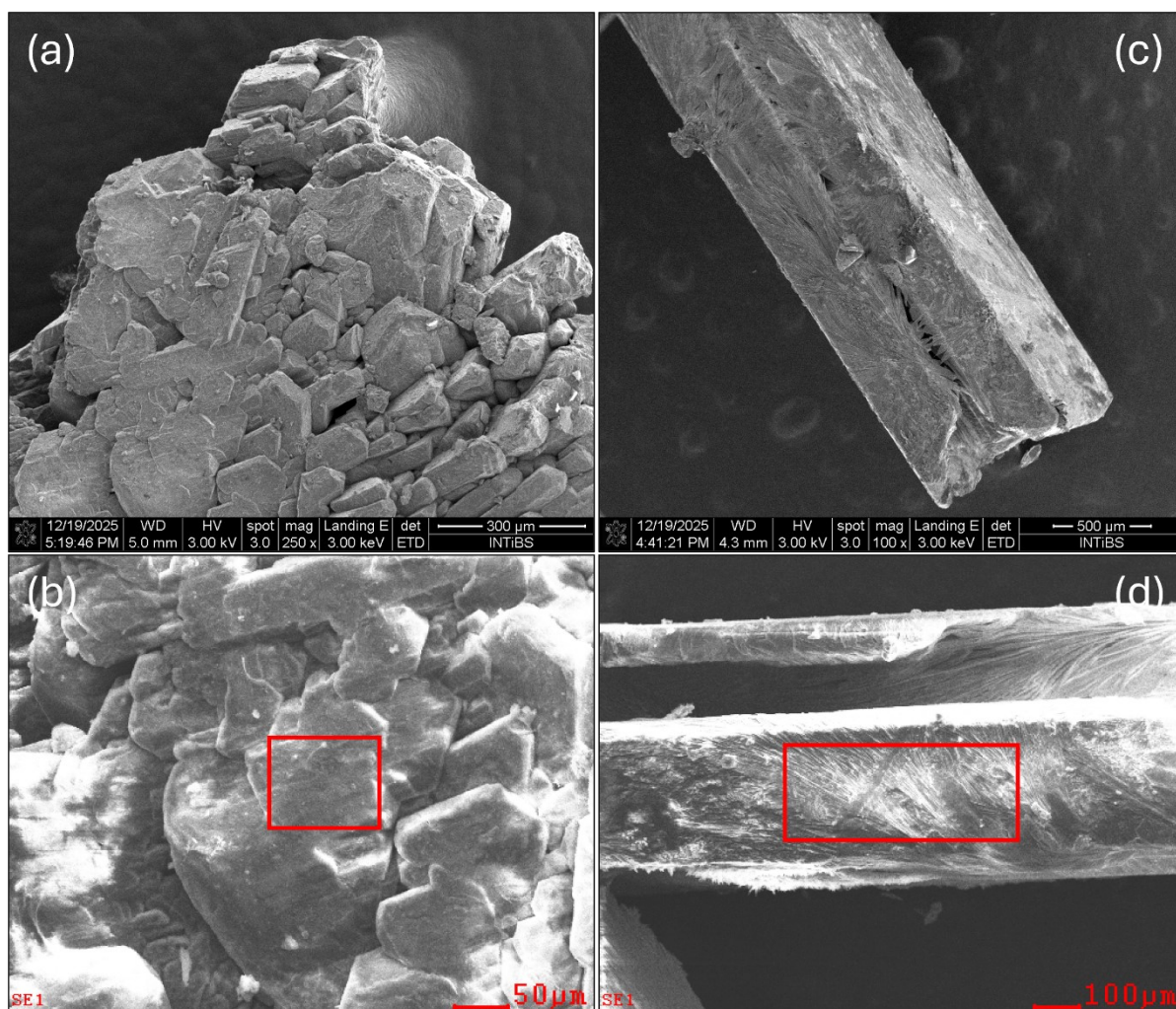
**Fig. 1.S.** Raman FT-IR spectrum of the hybrid compound  $(C_7H_{10}NO)_4[BiCl_6] \cdot Cl \cdot H_2O$ .



**Fig. 2.S.** Raman spectrum of the hybrid compound  $(C_7H_{10}NO)_4[BiCl_6] \cdot Cl \cdot H_2O$ .

**Table 2.S.** Correlation of  $O_h$  and  $C_{2h}$  Vibrational Modes and Their Spectroscopic Activity.

$O_h$ Mode	$C_{2h}$ Components	Activity
$A_{1g} (\nu_1)$	Ag (symmetric stretch)	Raman
$E_g (\nu_2)$	Ag + Bg (split)	Raman
$T_{1u} (\nu_3)$	Au + Bu (antisymmetric)	IR
$T_{2g} (\nu_4)$	Ag + Bg (split)	Raman
$T_{2u} (\nu_5)$	Au + Bu (split)	IR (if allowed)



**Fig. 3.S.** Scanning electron microscopy (SEM) images showing the surface morphology of  $(C_7H_{10}NO)_3[SbCl_5] \cdot Cl \cdot H_2O$  (a,b) and  $(C_7H_{10}NO)_4[BiCl_6] \cdot Cl \cdot H_2O$  (c,d) at different micrometer-scale magnifications.

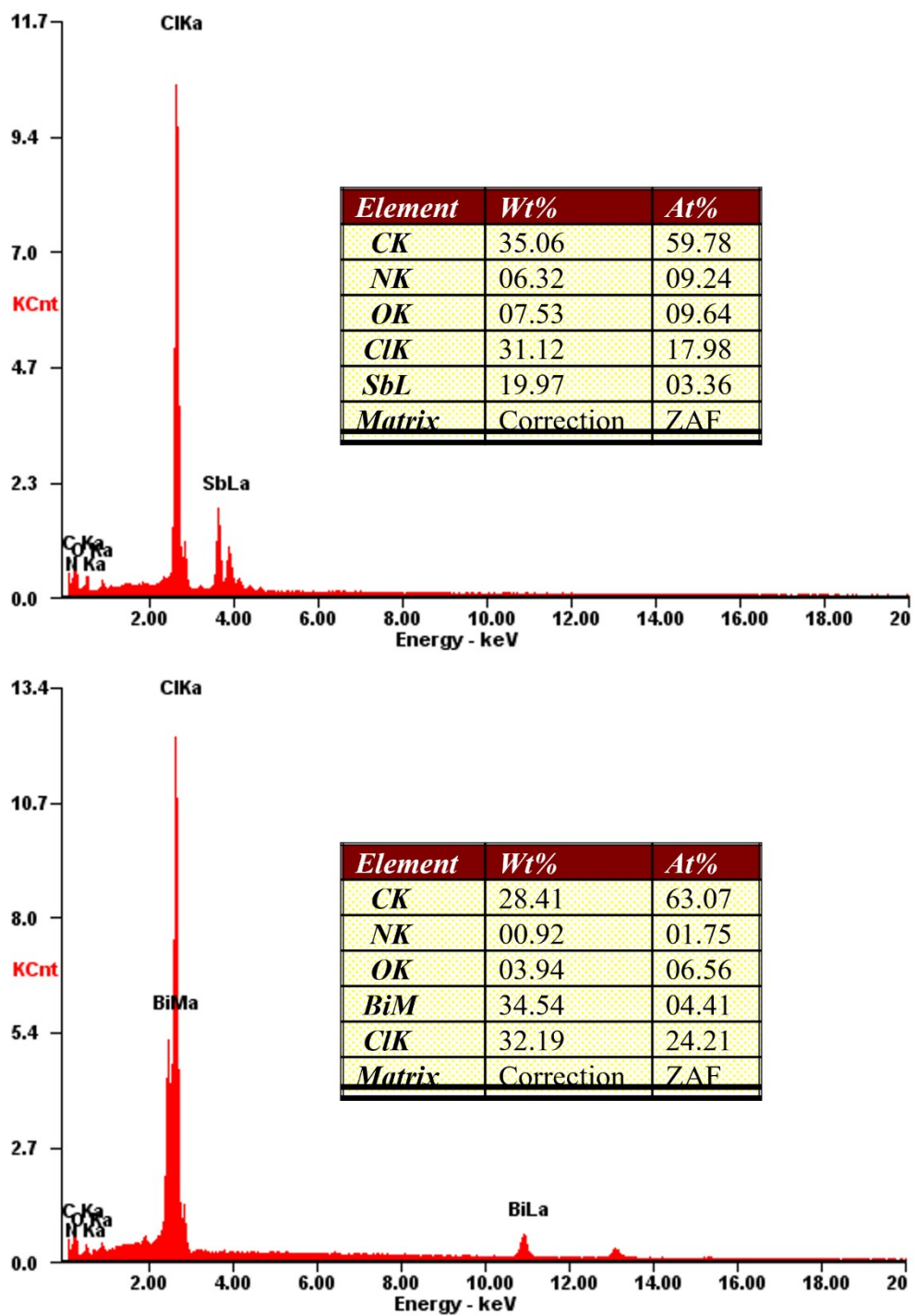
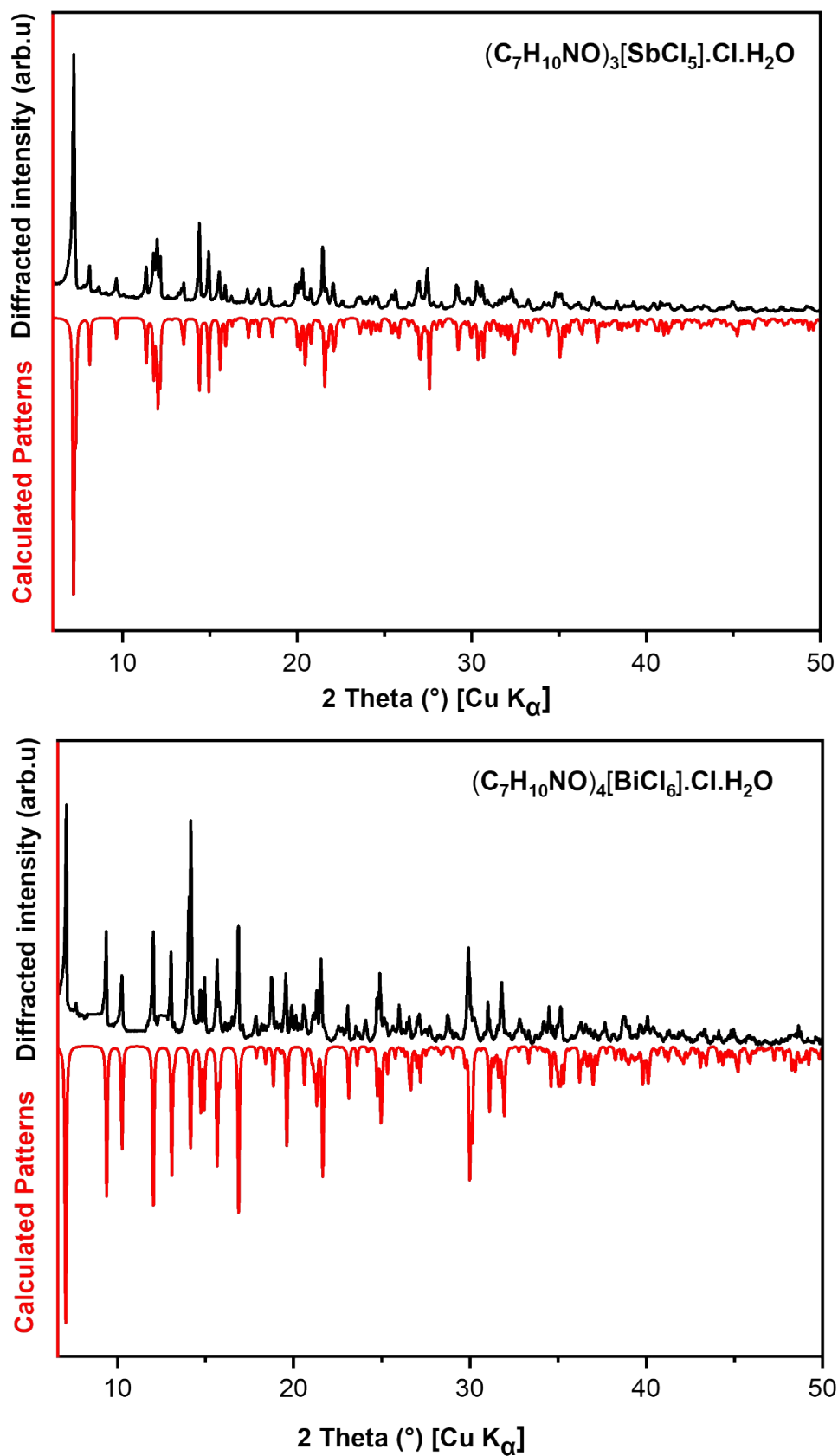


Fig. 4.S. EDS spectrum and elemental composition of  $(C_7H_{10}NO)_3[SbCl_5] \cdot Cl \cdot H_2O$  and  $(C_7H_{10}NO)_4[BiCl_6] \cdot Cl \cdot H_2O$ .



**Fig. 5.S.** Room-temperature experimental and simulated powder X-ray diffraction patterns of the Sb- and Bi-based hybrid compounds.