Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Alkali Metal Complexes of Non-Steroidal Anti-inflammatory Drugs Inhibit Lung and Oral Cancers In Vitro

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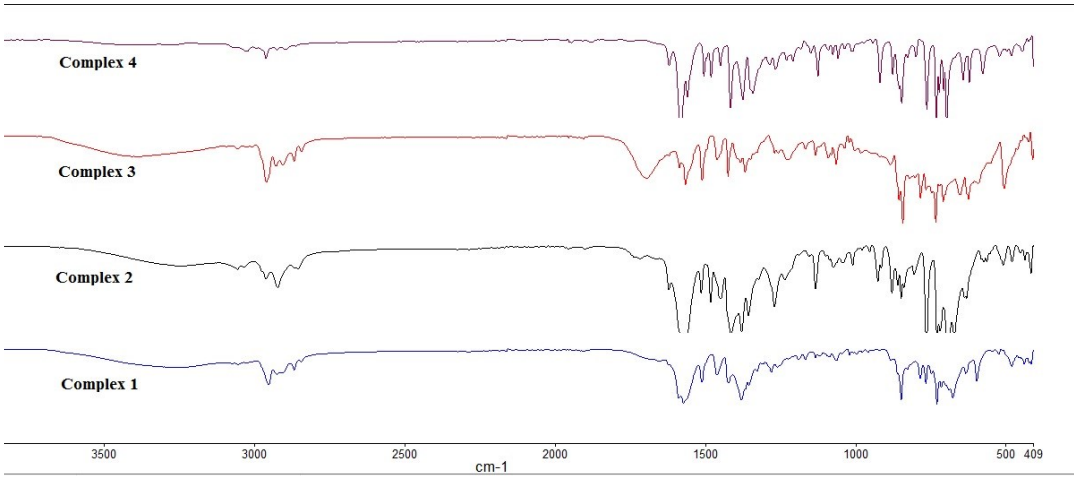

Figure S1: FT-IR spectra of complexes **1 – 4**.

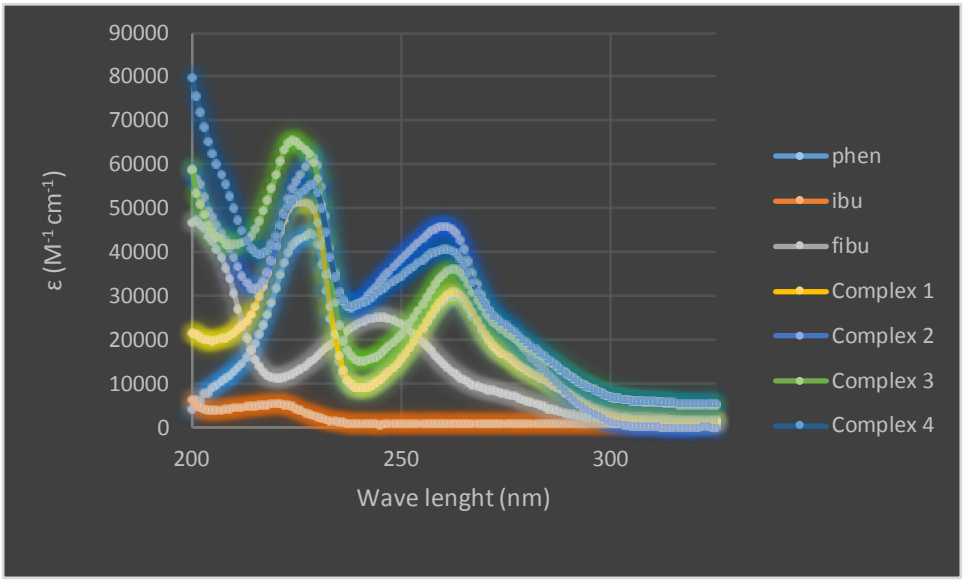

Figure S2: UV–Vis solution spectra of complex **1 – 4** and free ligands **phen**, **ibu**, **fibu** (MeOH, rt, concentration 10^{-5} – 10^{-6} M).

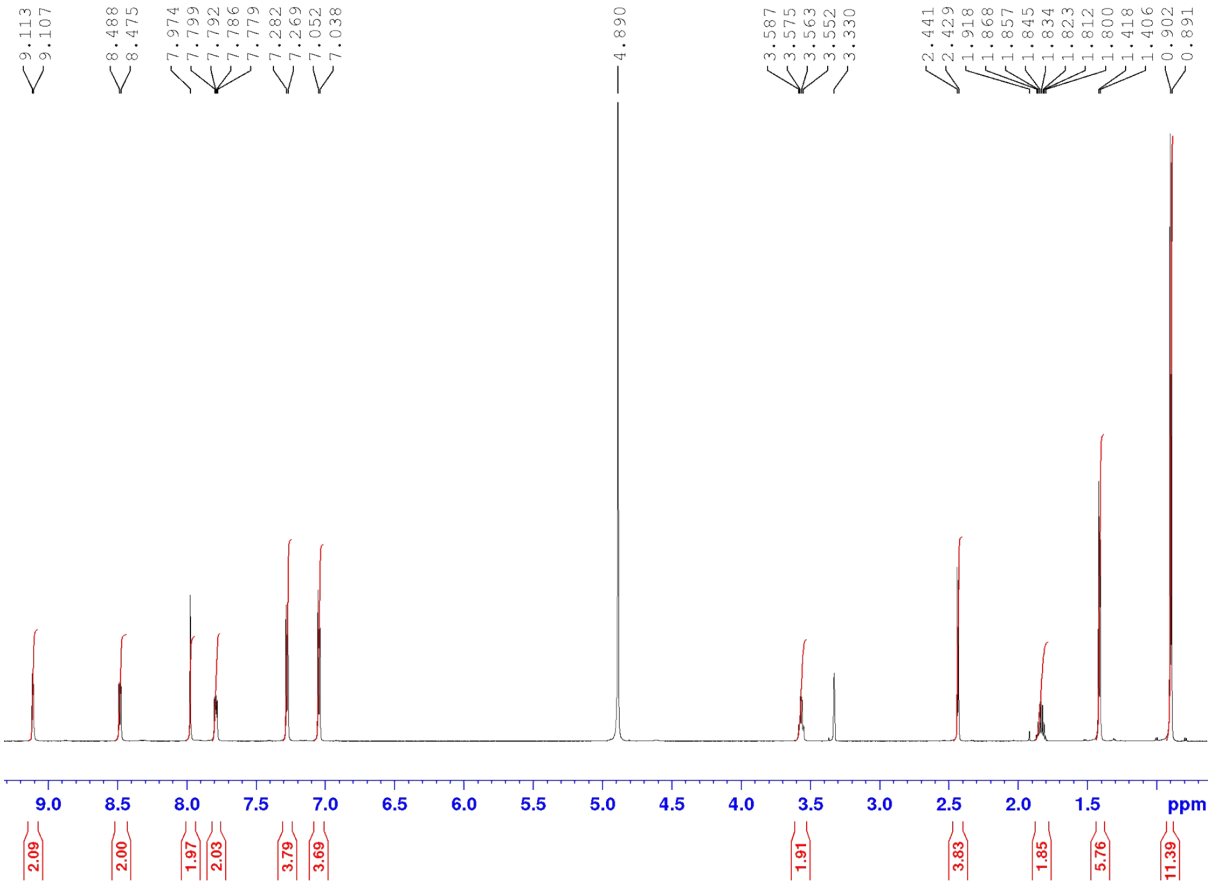

Figure S3: ^{1}H NMR spectrum of **1** in MeOD.

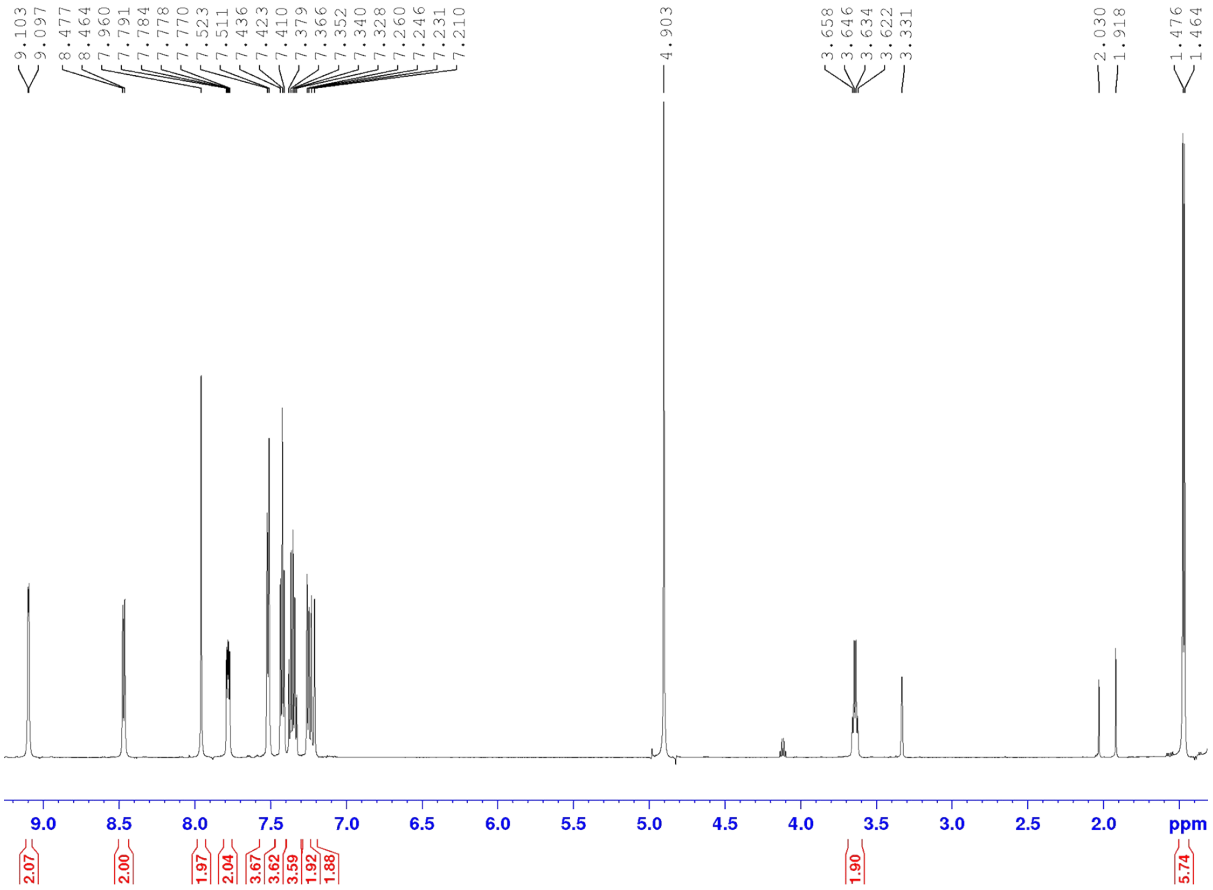

Figure S4: 1H NMR spectrum of **2** in MeOD.

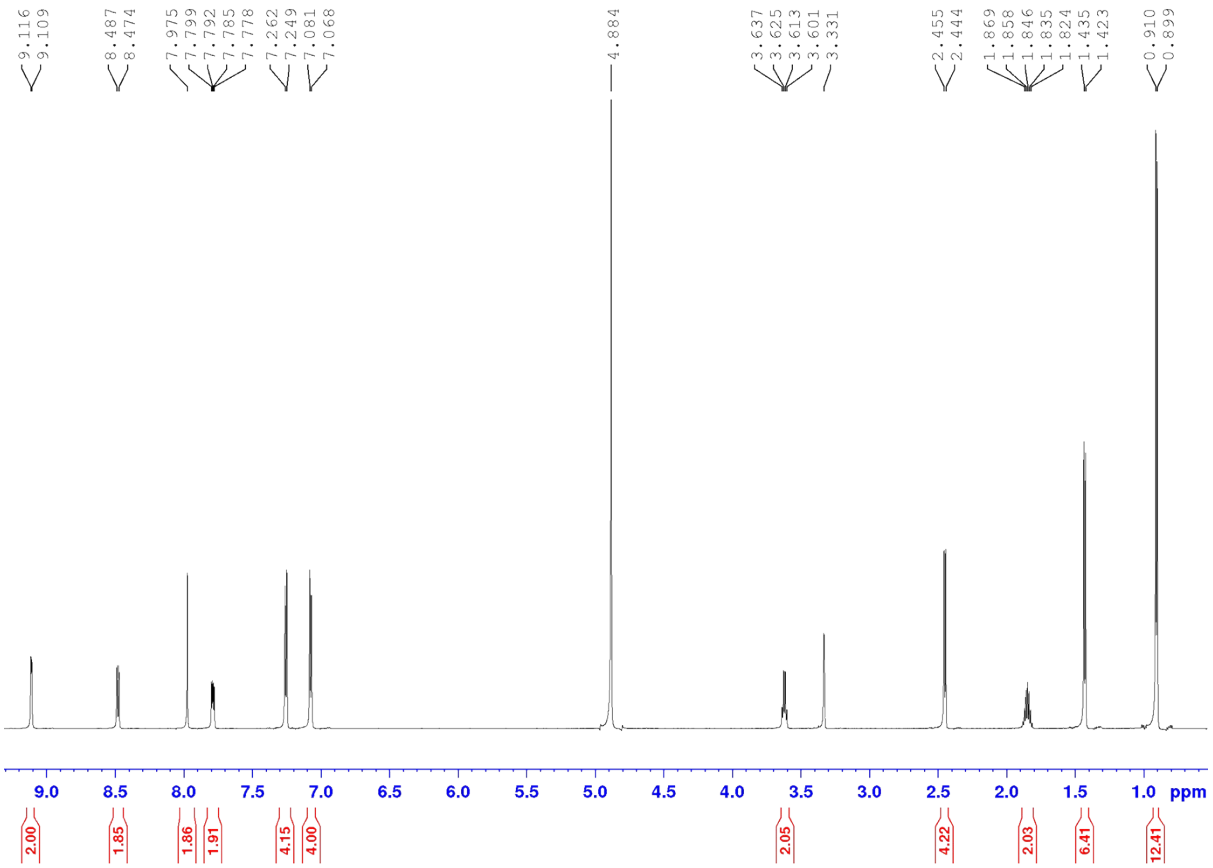

Figure S5: ^{1}H NMR spectrum of **3** in MeOD.

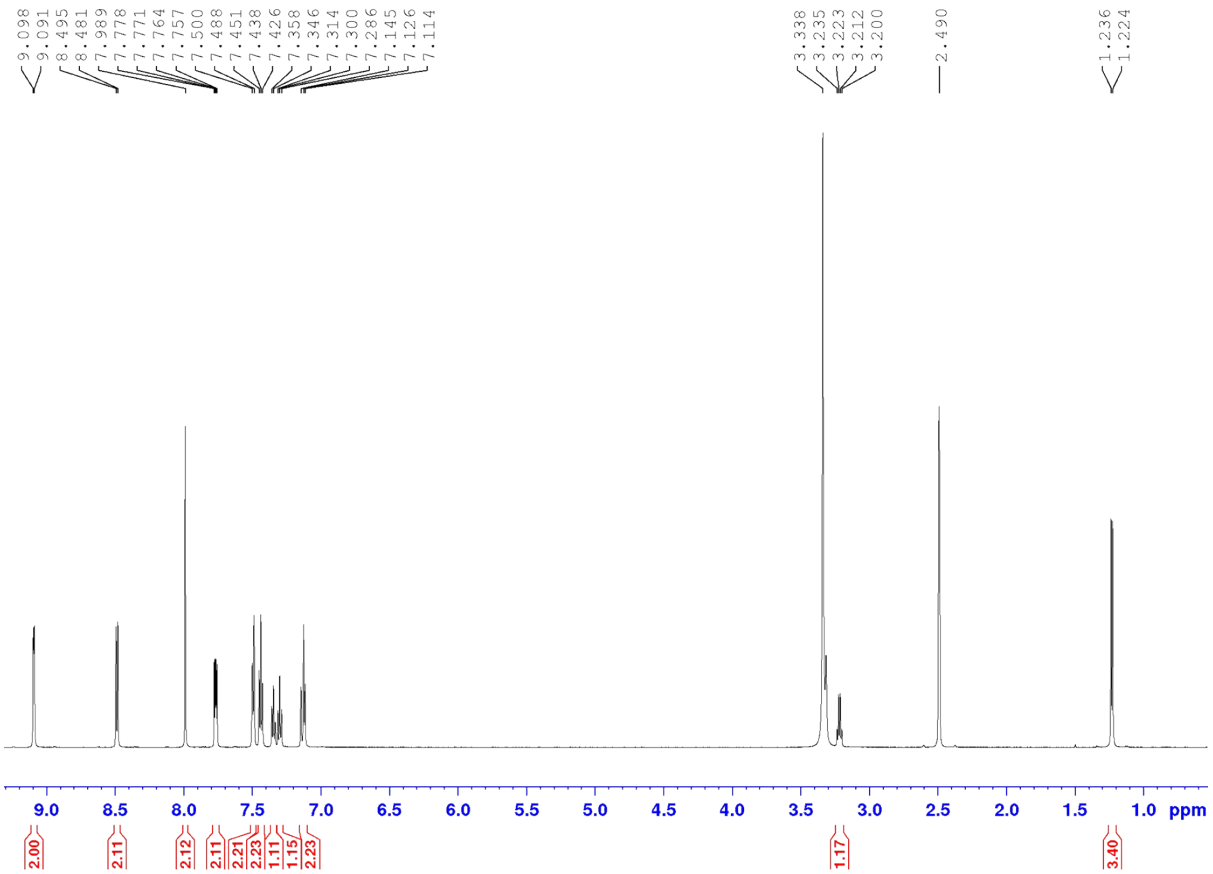

Figure S6: ^{1}H NMR spectrum of **4** in DMSO-d_6.

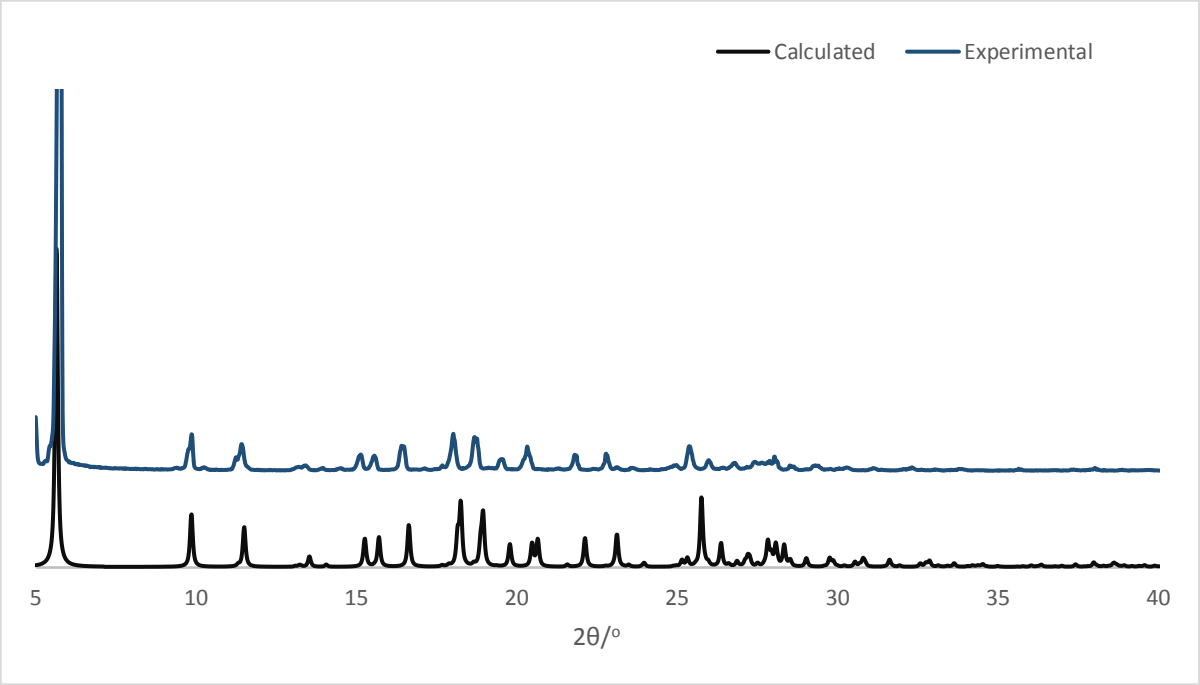

Figure S 7:The calculated (bottom) and observed (top) powder X-ray diffraction patterns of 1.

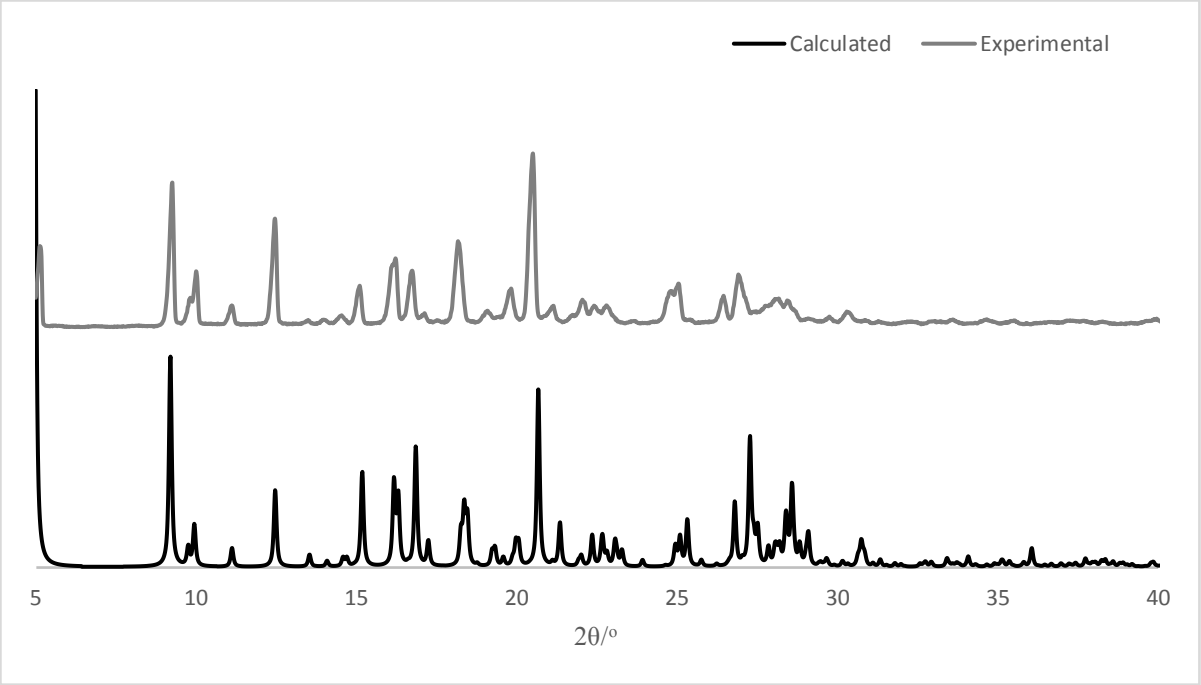

Figure S 8:The calculated (bottom) and observed (top) powder X-ray diffraction patterns of **2**.

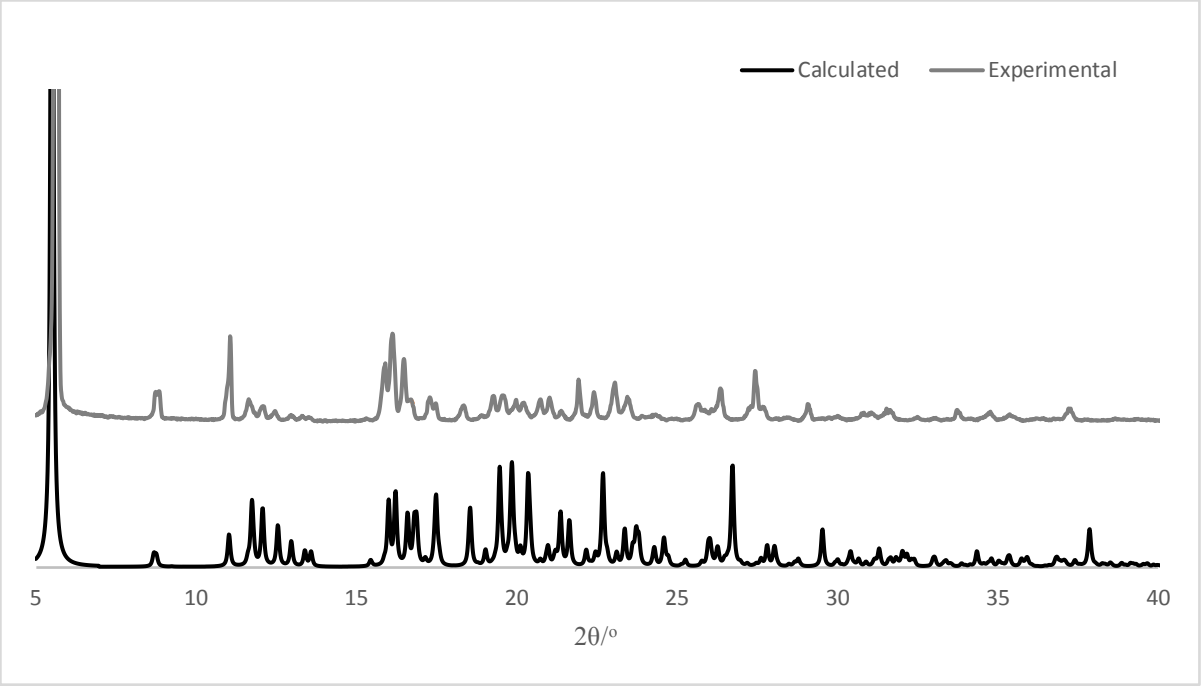

Figure S 9:The calculated (bottom) and observed (top) powder X-ray diffraction patterns of 3.

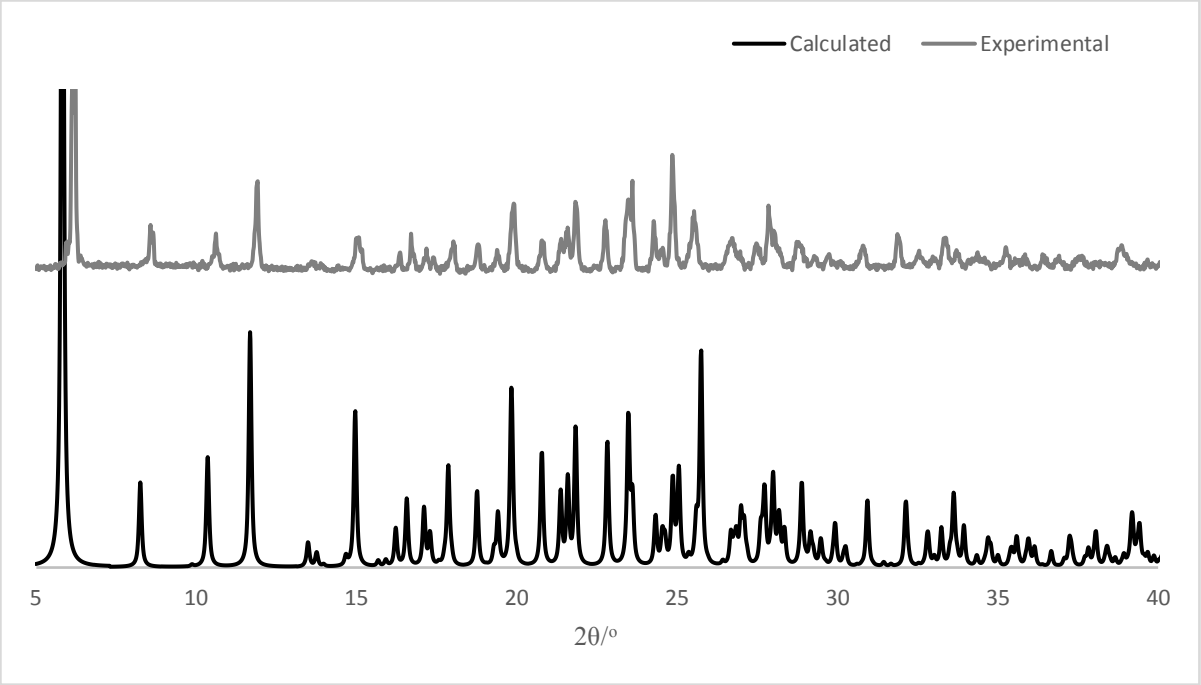

Figure S 10:Figure S 9:The calculated (bottom) and observed (top) powder X-ray diffraction patterns of **4**.

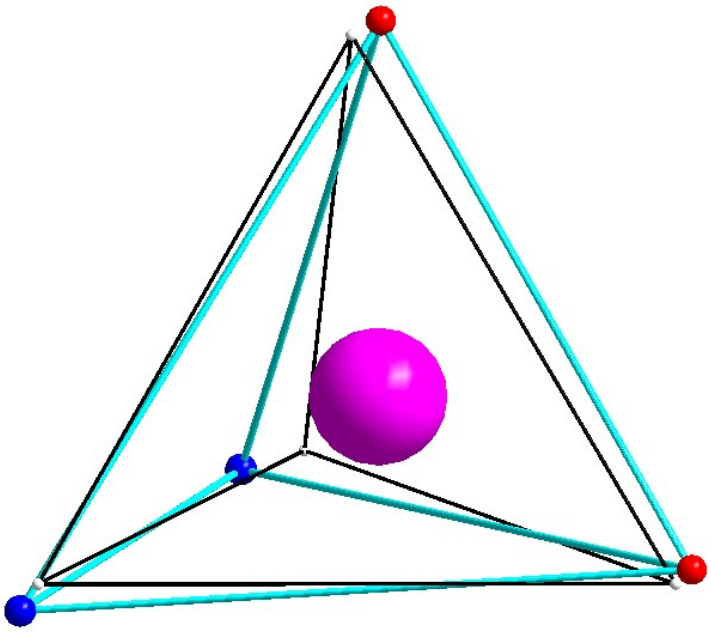

Figure S 11:Observed distorted polyhedron (black lines) and ideal calculated prism polyhedron (blue lines) in **1**, calculated by the continuous shape measure (CshM) theory utilizing SHAPE software.[1] Colour Codes of atoms: Nitrogen (blue), Oxygen (Red), Lithium (pink) CshM = 2.38 (Table S1).

1. Llunell, M.; Casanova, D.; Cirera, J.; Alemany, P.; Alvarez, S. SHAPE, Version 2.1.; Univ. Barcelona: Barcelona, Spain, 2013; p2103.

Table S1:Continuous Shape Measures calculation in **1** (geometries which give the smallest deviation from the experimental structure are highlighted).

	SP-4 Square D_{4h}	T-4 Tetrahedron T_d	SS-4 Seesaw C2v
CShM	26.14	2.38	7.950

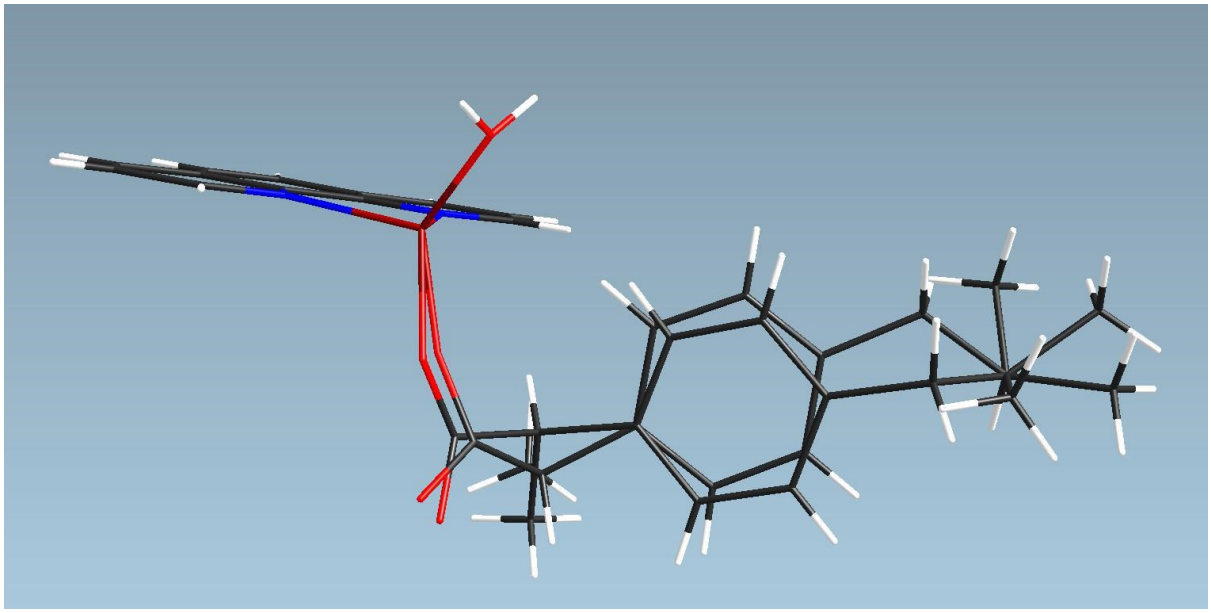

Figure S 12:The crystal structure of 1 highlighting the disorder in **ibu** moiety.

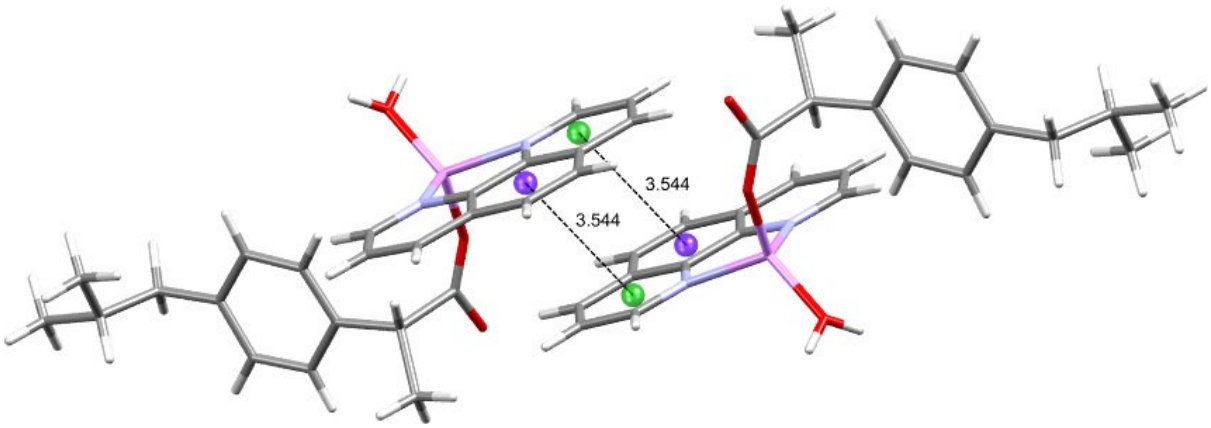

Figure S 13:The crystal packing of **1**, highlighting the centroid–centroid (Cg···Cg) distances (black dotted lines). The disorder part of ibu is removed for clarity.

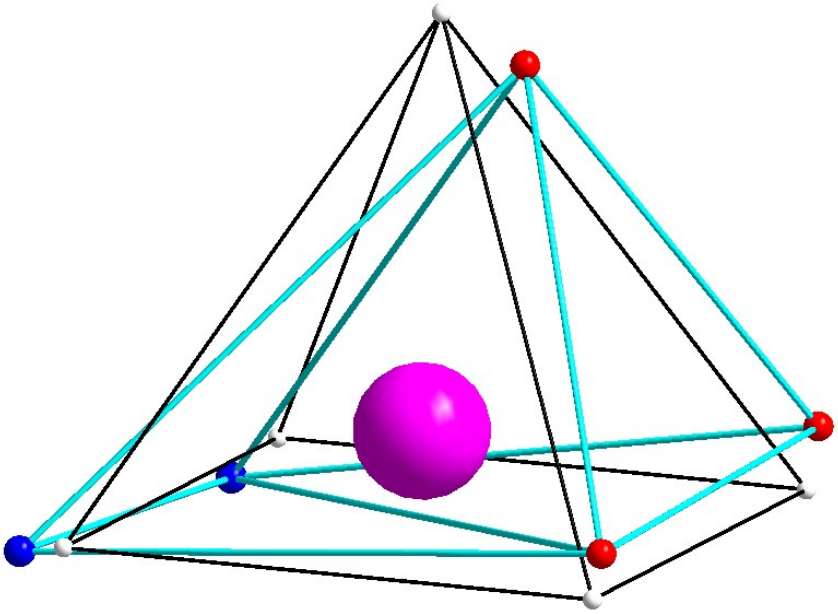

Figure S 14: Observed distorted polyhedron (black lines) and ideal calculated prism polyhedron (blue lines) in **2** , calculated by the continuous shape measure (CshM) theory utilizing SHAPE software.[1] Colour Codes of atoms: Nitrogen (blue), Oxygen (Red), Lithium (pink) CshM = 2.78 (Table S2).

Table S 2:Continuous Shape Measures calculation in **2** (geometries which give the smallest deviation from the experimental structure are highlighted).

	PP-5 Pentagon (D_{5h})	vOC-5 Vacant octahedron (C_{4v})	TBPY-5 Trigonal bipyramid (D_{3h})	SPY-5 Spherical square pyramid (C_{4v})	JTBPY-5 Johnson trigonal bipyramid J12 D3h (D_{3h})
CShM	23.38	2.90	7.05	2.78	8.78

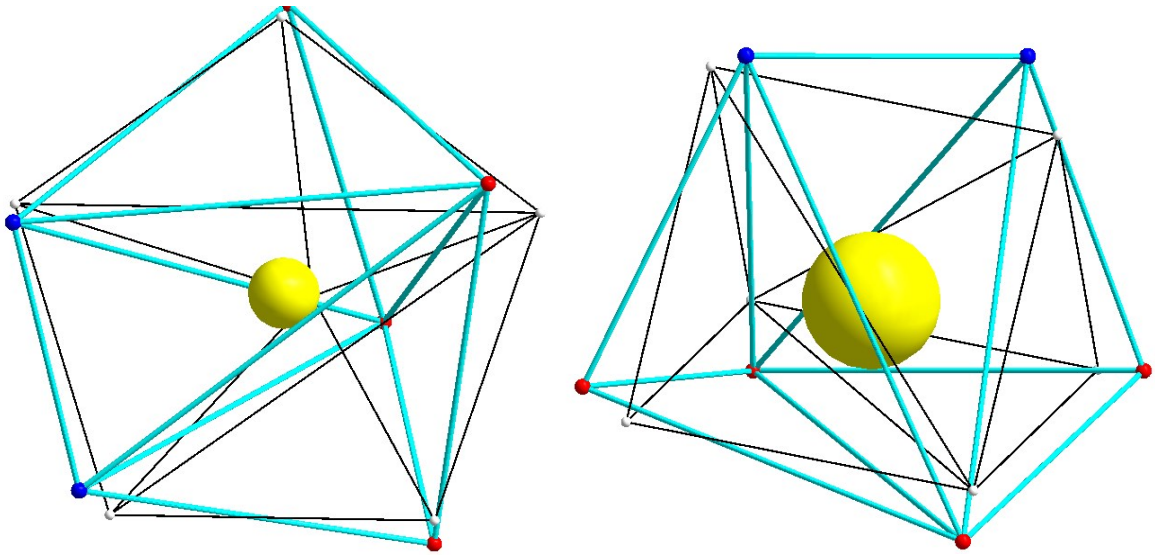

Figure S 15:Observed distorted polyhedron (black lines) and ideal calculated prism polyhedron (blue lines) in **3** , calculated by the continuous shape measure (CshM) theory utilizing SHAPE software.[1] Colour Codes of atoms: Nitrogen (blue), Oxygen (Red), Potassium (Yellow) CshM = 7.91 (Table S3).

Table S 3:Continuous Shape Measures calculation in **3** (geometries which give the smallest deviation from the experimental structure are highlighted).

	HP-6 Hexagon (D_{6h})	PPY-6 Pentagonal pyramid (C_{5v})	OC-6 Octahedron (O_h)	TPR-6 Trigonal prism (D_{3h})	JPPY-6 Johnson pentagonal pyramid J2 (C_{5v})
CShM	22.12	7.911	22.36	7.912	10.77

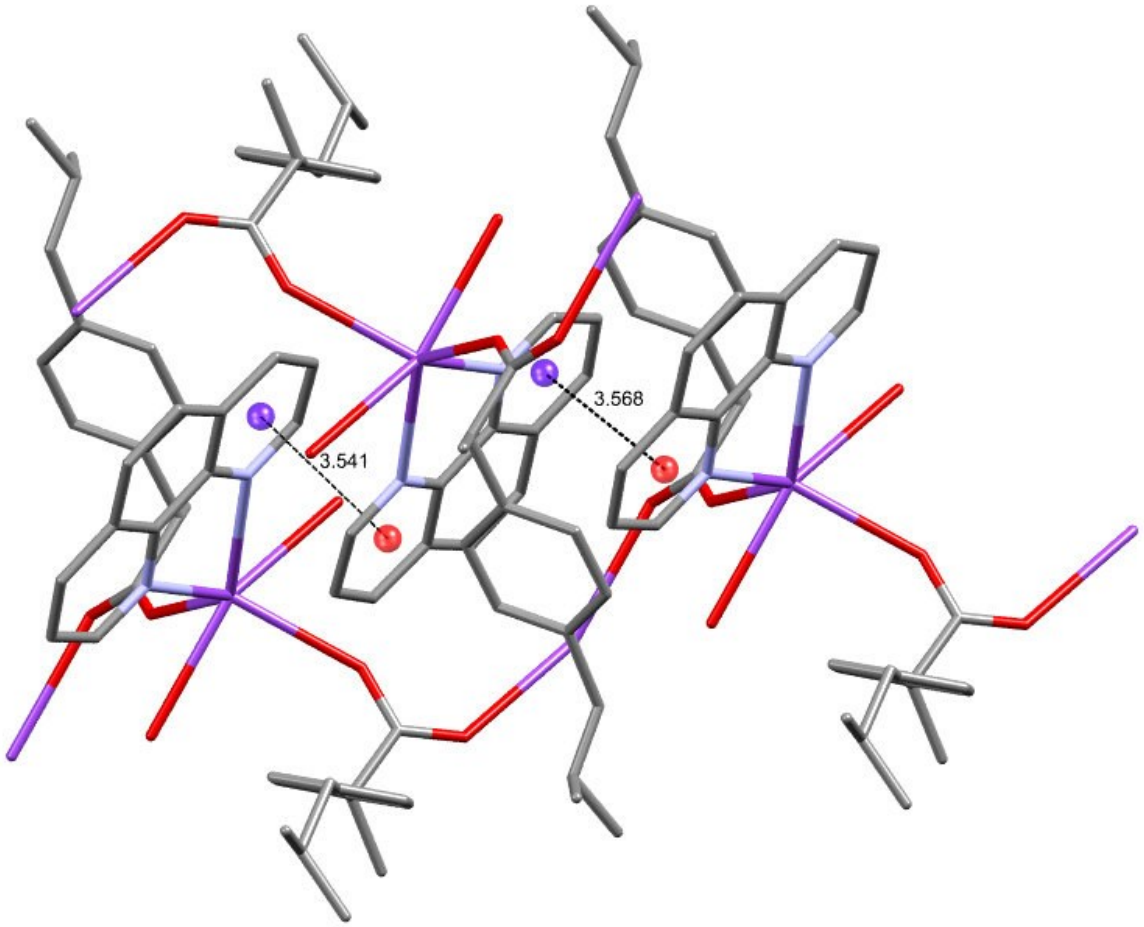

Figure S 16:The crystal packing of **3**, highlighting the Cg···Cg distances (black dotted lines). H-atoms are removed for clarity.

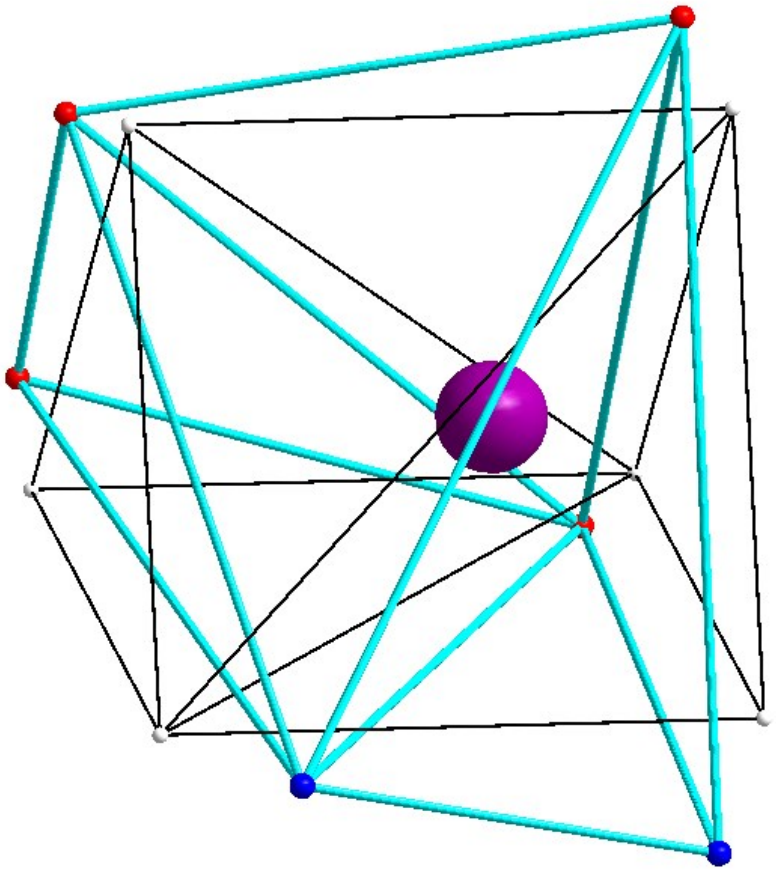

Figure S 17: Observed distorted polyhedron (black lines) and ideal calculated prism polyhedron (blue lines) in **4** , calculated by the continuous shape measure (CshM) theory utilizing SHAPE software.[1] Colour Codes of atoms: Nitrogen (blue), Oxygen (Red), Caesium (Purple) CshM = 9.30 (Table S3).

Table S4: Continuous Shape Measures calculation in **4** (geometries which give the smallest deviation from the experimental structure are highlighted).

	HP-6 Hexagon (D_{6h})	PPY-6 Pentagonal pyramid (C_{5v})	OC-6 Octahedron (O_h)	TPR-6 Trigonal prism (D_{3h})	JPPY-6 Johnson pentagonal pyramid J2 (C_{5v})
CShM	32.16	14.12	19.65	9.30	18.27

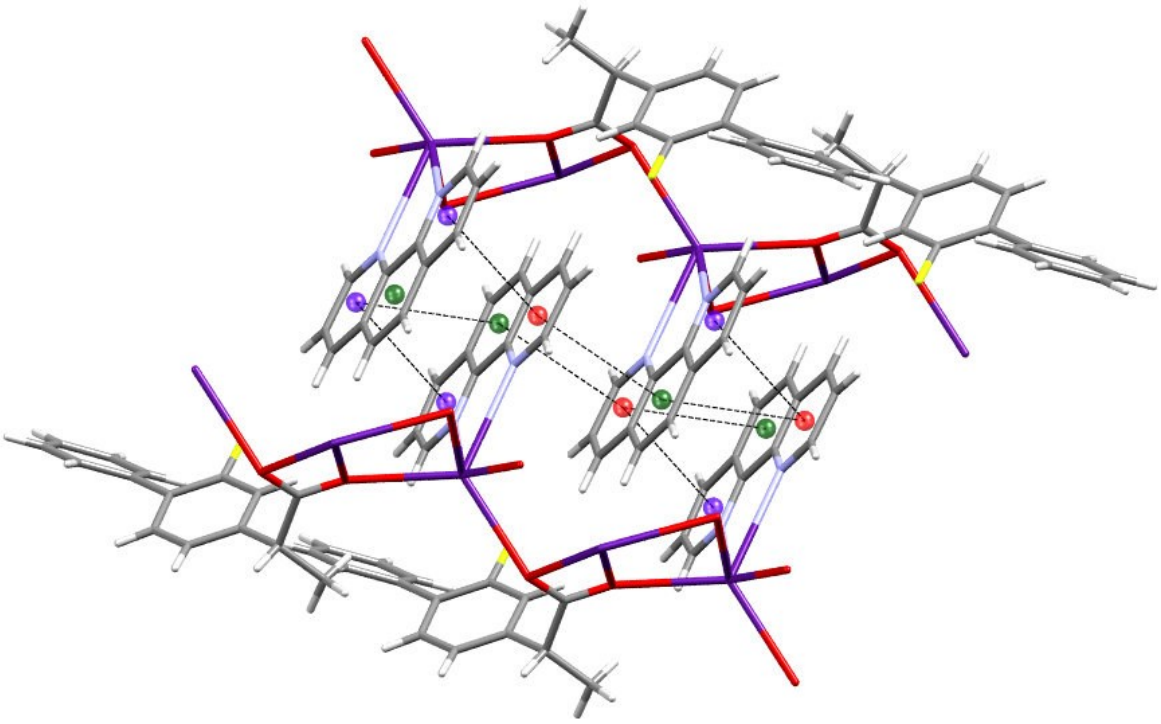

Figure S 18:The crystal packing of **4**, highlighting the Cg···Cg distances (black dotted lines).