New dinuclear macrocyclic copper(II) complexes as potentially fluorescent and magnetic materials

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Table S3. Fluorescence data of the thin materials **K1**/Si and **K2**/Si obtained by thermal vapour deposition.

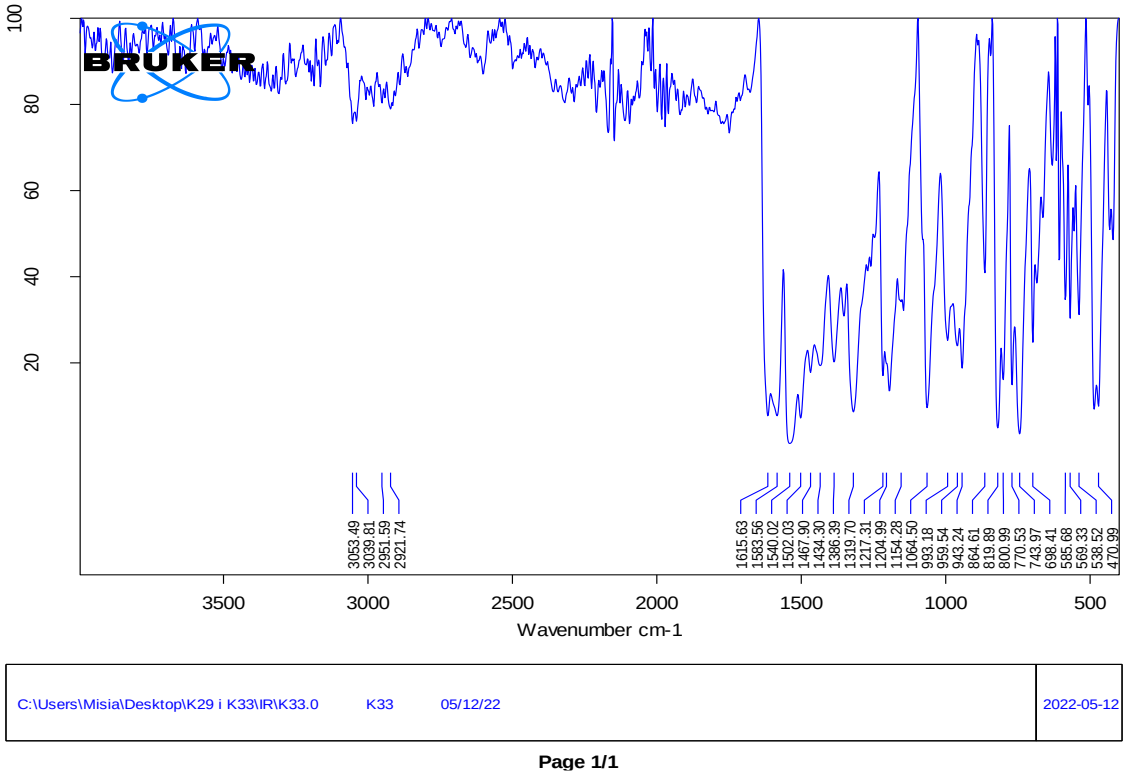


Figure S1. IR spectrum of **K1**.

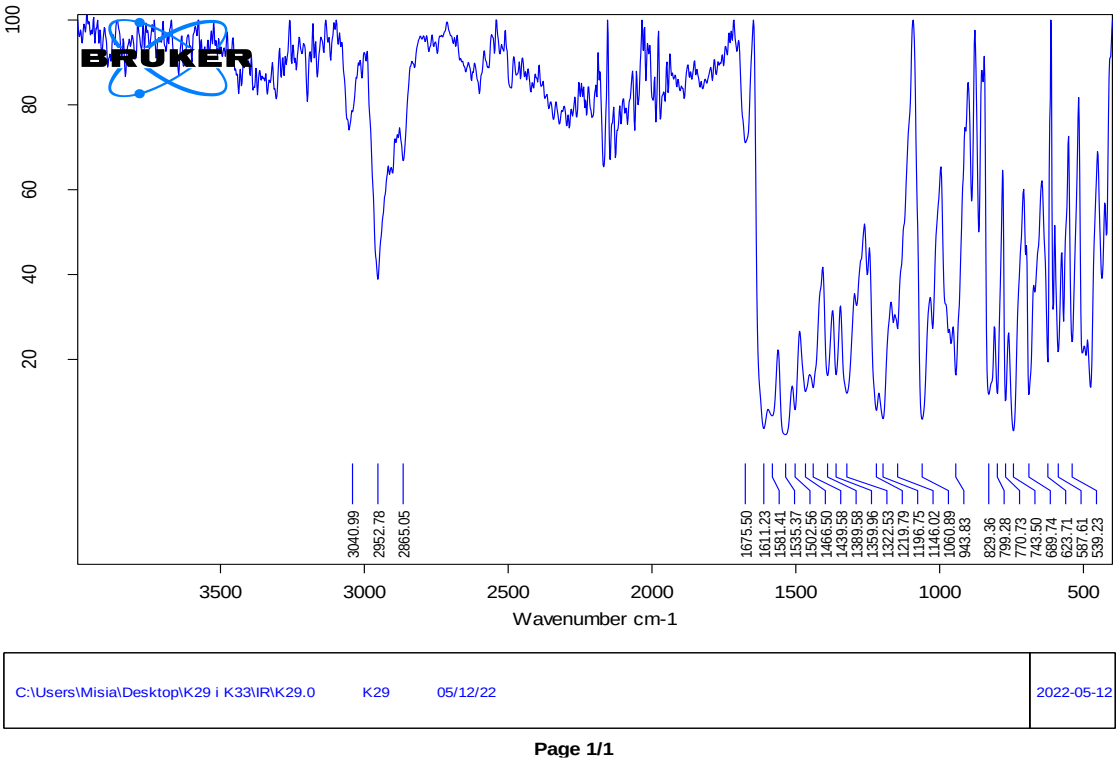
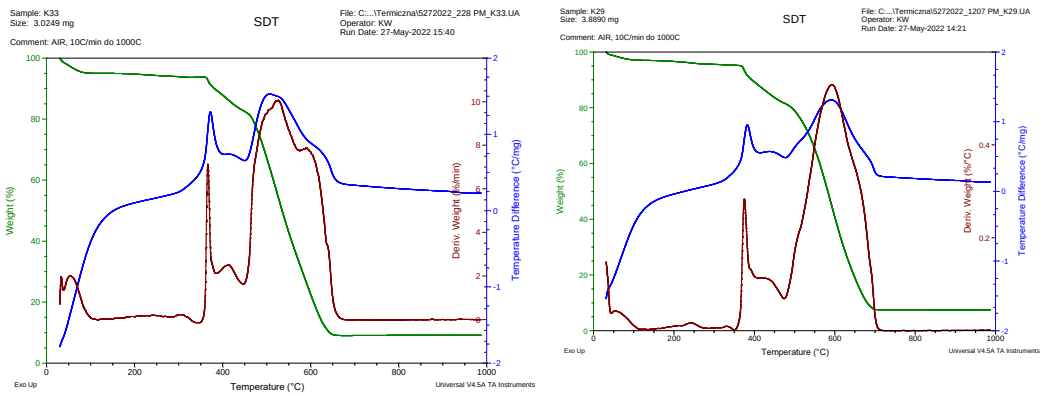


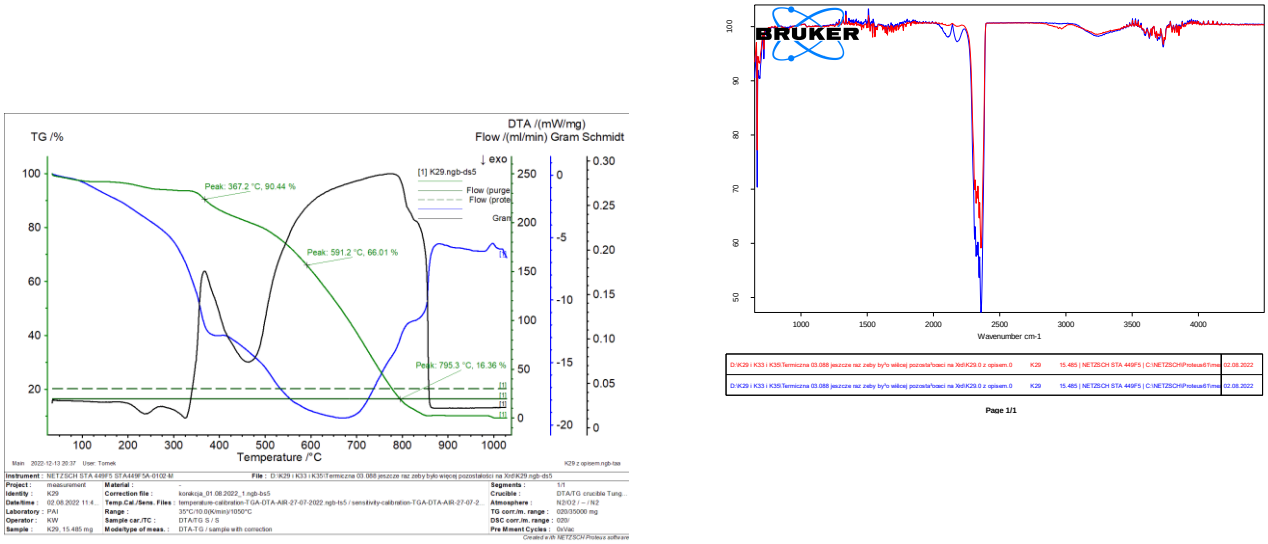
Figure S2. IR spectrum of **K2**.

Thermal analysis



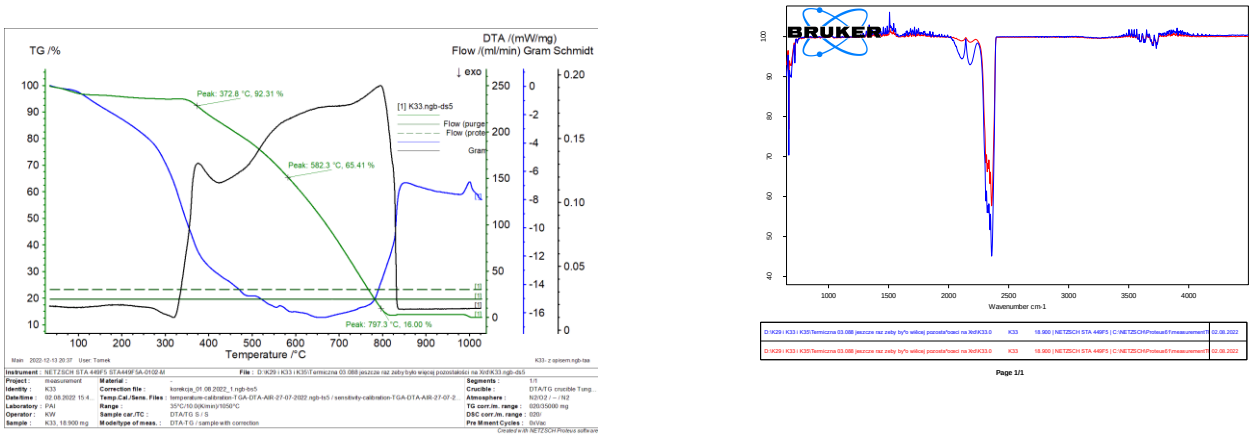
a) **b)**

Figure S3. **a)** TG-DTA traces of **K1** and **b) K2.**



a) **b)**

Figure 4. a) TG-DTA traces of **K1** and **b)** IR spectra decomposition product



a) **b)**

Figure S5. **a)** TG-DTA traces of **K2** and **b)** IR spectra decomposition products.

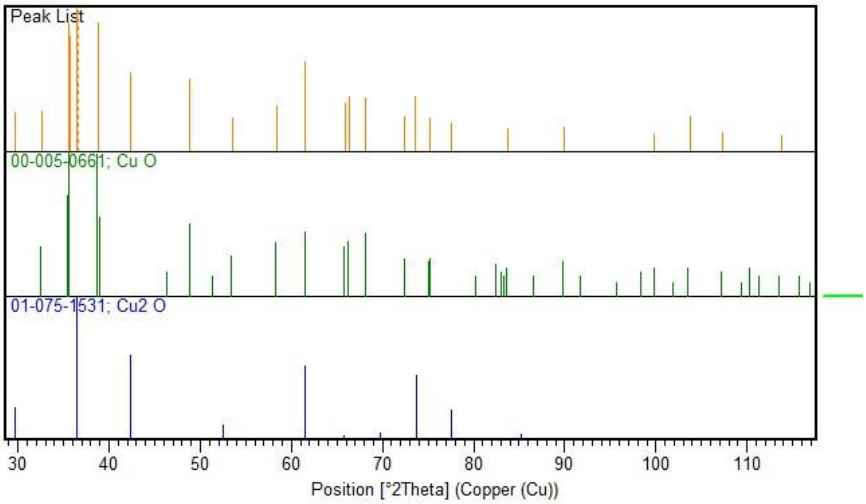


Figure S6. XRD of the thermal analysis residue of **K1**.

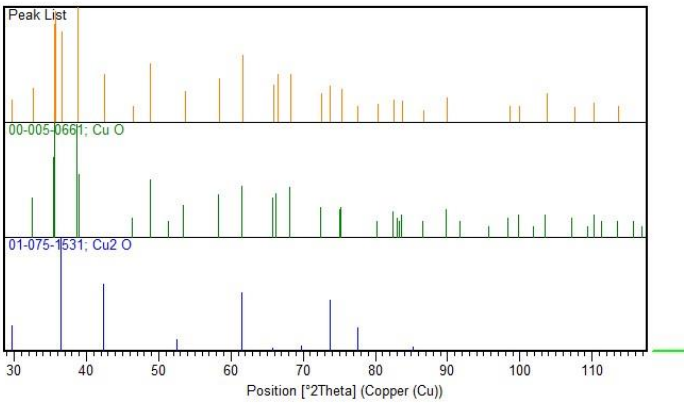


Figure S7. XRD of the thermal analysis residue of **K2**.

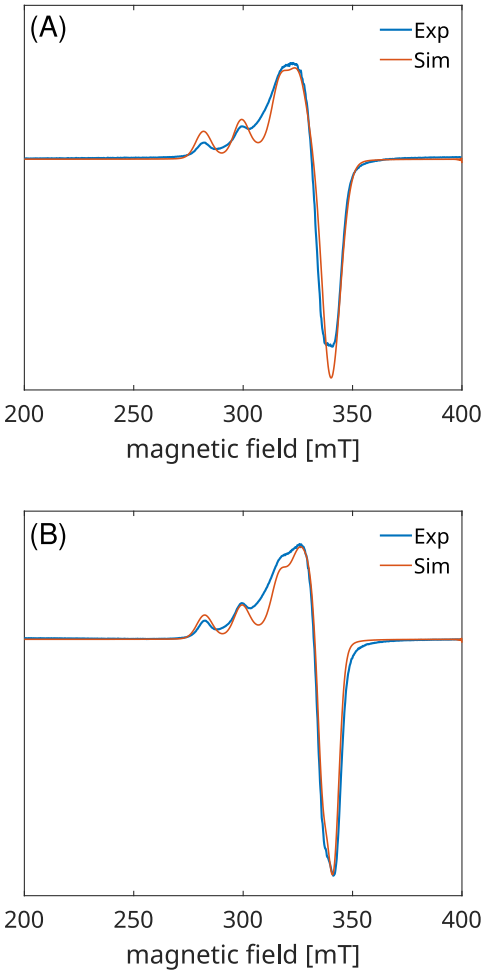


Figure S8. Powder EPR spectra recorded for **K1** (A) and **K2** (B) at 77 K.

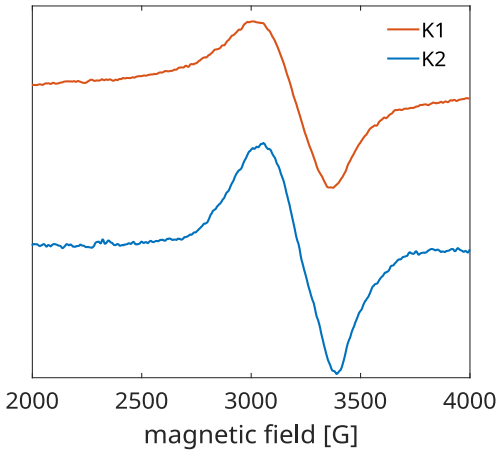


Figure S9. Powder EPR spectra recorded for **K1** and **K2** at 350 K.

Table S1. The theoretical values of the J(Cu_1-Cu_2) magnetic coupling constants [cm^{-1}], estimated within the broken-symmetry and spin-flip approach with B3LYP functional and def2-SVP/def2-QZVPP(Cu) basis set according to the three schemes: spin-projected (SP), spin-unprojected (SUP) and approximate spin-projected (AP).

	K1	**K2**
	Broken Symmetry/B3LYP/def2-SVP+def2-QZVPP for Cu	
E(High-Spin)-E(BrokenSym)	673.941 (antiferromagnetic)	693.172 (antiferromagnetic)
J(SP)	-673.94	-693.17
J(SUP)	-336.97	-346.59
J(AP)	-632.18	-649.28
	Spin-Flip/B3LYP/def2-SVP+def2-QZVPP for Cu	
E(High-Spin)-E(BrokenSym)	674.353 (antiferromagnetic)	693.295 (antiferromagnetic)
J(SP)	-674.35	-693.29
J(SUP)	-337.18	-346.65
J(AP)	-632.58	-649.42

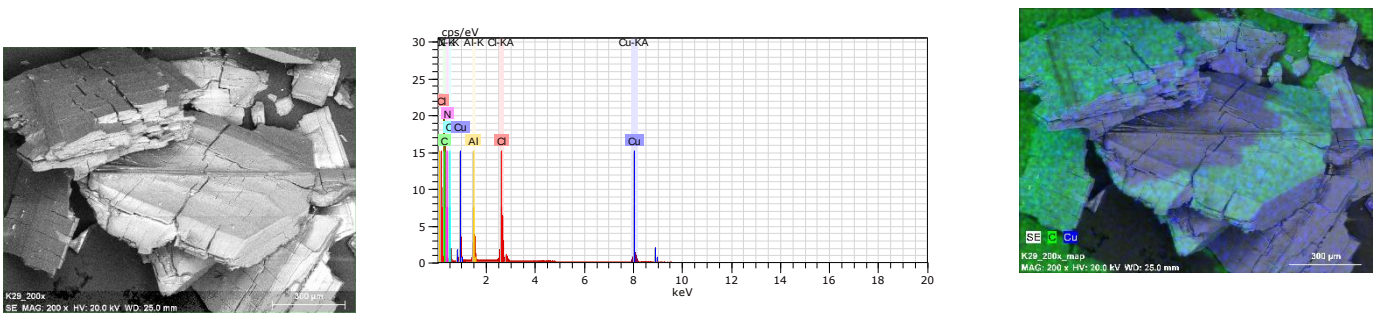


Figure S10. SEM/EDX images of **K1** maping scanning size 300 µm.

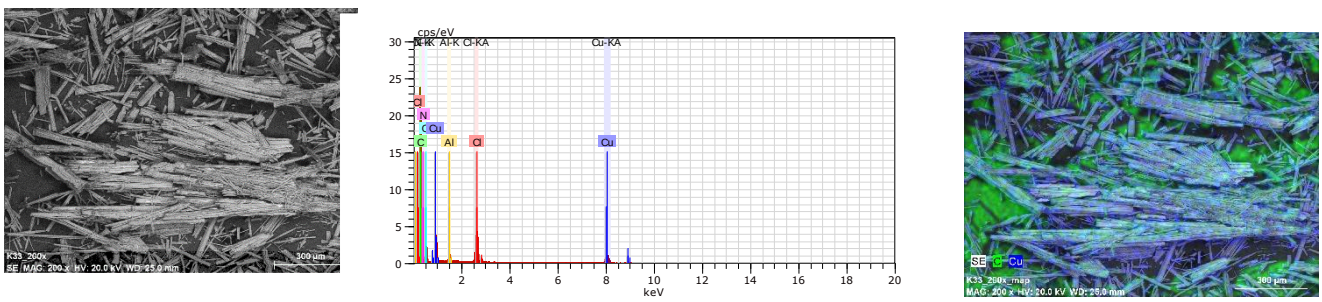
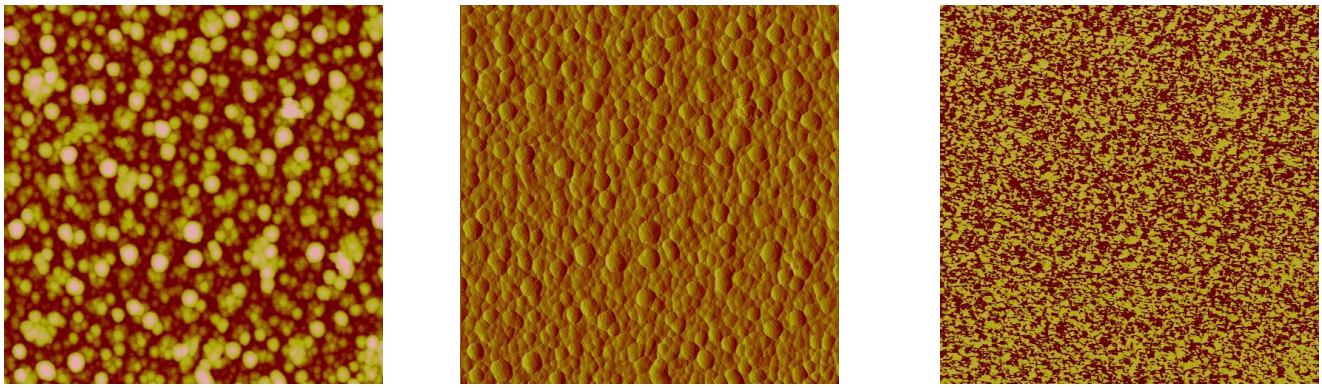


Figure S11. SEM/EDX images of **K2** maping scanning size 300 µm.



Height **Amplitude** **Phase**

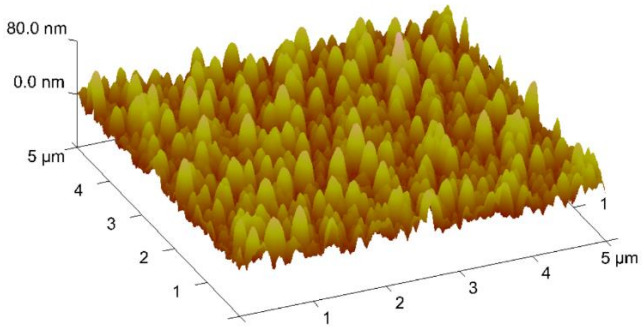


Figure S12. AFM of **K1**/Si, thermal deposition, scan size 5 µm, R_a=4.02 nm, R_q=5.36 nm.

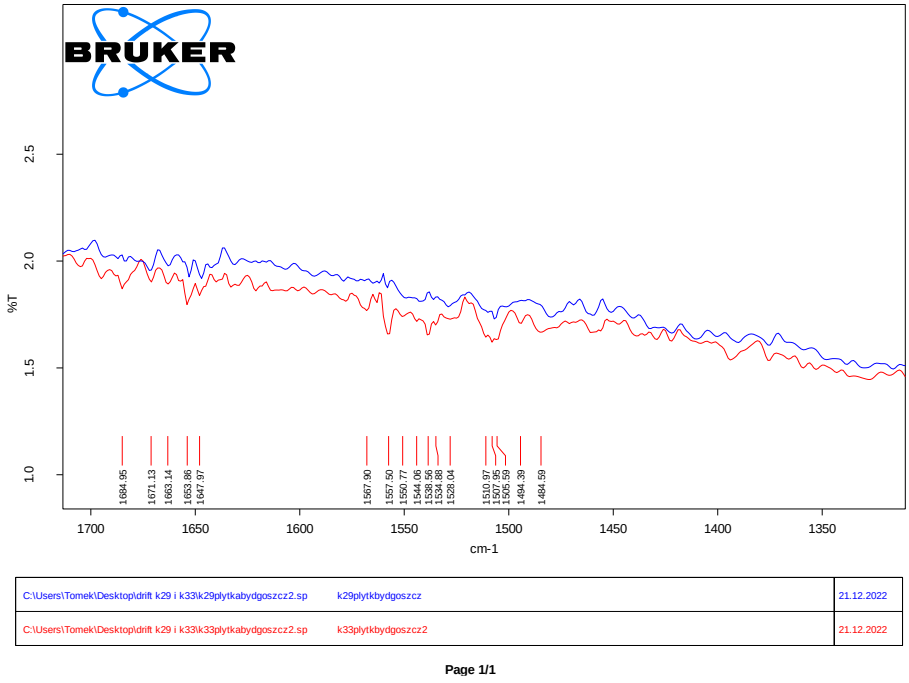


Figure 13. IR DRIFT of **K1**/Si and **K2**/Si materials- thermal vapour deposition.

Table S2. Relevant photophysical data of studied compounds: $ë_{em}$, $ë_{ex}$ [nm] Bp=8; λ[nm] (ε [dm^3 mol^{-1} cm^{-1}]); Stoke shift [nm], [cm^{-1}]; Q Bp=5.

Comp.	Solvent	λ_{ex} [nm]	λ_{em} [nm]	Fluoresc. Intensity a. u.	λ[nm] (ε [dm^3 mol^{-1} cm^{-1}])	A	Q	Stoke shift [nm]	Stoke shift [cm^{-1}]
K1	acetone	350	**409**	1688725	**402** (39628)	**0,128**	0,027	**7**	**1428571**
	methanol		**412**	1151660	**388** (43963); 324 (46440) sh; 274 (104025)	**0,142**; 0,150; 0,336	0,013	**24**	**416667**
	chloroform		**398**	201250	**408** (37461); 324 (40248) sh; 272 (114861) 660 (13313)	**0,121**; 0,130; 0,371 **0,043**	0,0019	**10**	**1000000**
	DMSO		**424**	3021975	**398** (44582); 290 (130960) sh	**0,144**; 0,423	0,017	**26**	**384615**
K2	acetone	350	**408**	1315030	**400** (40867)	**0,132**	0,035	**8**	**1250000**
	methanol		**420**	438415	**388** (49845); 326 (50774) sh; 274 (123220)	**0,161**; 0,164; 0,398	0,011	**32**	**312500**
	chloroform		**392**	260640	**404** (43344); 328 (42724) sh; 272 (124458) 664 (12384)	**0,140**; 0,138; 0,402 **0,040**	0,003	**12**	**833333**
	DMSO		**424**	1934125	**394** (45201)	**0,146**	0,021	**30**	**333333**
	acetonitrile		**409**	982115	**392** (46749)	**0,151**	0,038	**17**	**588235**

Table S3. Fluorescence data of the thin materials **K1**/Si and **K2**/Si – thermal vapour deposition.

Comp.	λ_{ex} [nm]	λ_{em} [nm]	Fluoresc. Intensity a. u.
K2	250	318	11715
		390	13580
		531	7320
	320	386	27980
		481	15870
		575	5050
		686	9145
K1	250	326	367045
		377	271315
		472	68955
	300	376	414115
		472	89570
	320	372	518885
		474	107320