## Supplementary Information (SI) for CrystEngComm. This journal is © The Royal Society of Chemistry 2025



Figure S1. Optical microscope and SEM photographs of crystals of complexes 1(a), 2(b), 3(c), 4(d) and 5(e)



*Figure S2a.* Comparison of the experimental powder XRD pattern (red line) of complex 1 with the calculated one (black line). X-ray source; Copper  $K\alpha$  radiation.



*Figure S2b.* Comparison of the experimental powder XRD pattern (red line) of complex 2 with the calculated one (black line). X-ray source; Copper  $K\alpha$  radiation. The (\*) represent unidentified crystalline impurities within the sample.



*Figure S2c.* Comparison of the experimental powder XRD pattern (red line) of complex **3** with the calculated one (black line). X-ray source; Copper  $K\alpha$  radiation.



*Figure S2d.* Comparison of the experimental powder XRD pattern (red line) of complex 4 with the calculated one (black line). X-ray source; Copper  $K\alpha$  radiation.



*Figure S2e.* Comparison of the experimental powder XRD pattern (red line) of complex **5** with the calculated one (black line). X-ray source; Copper  $K\alpha$  radiation.



*Figure S3a.* Infrared spectroscopy analysis in the  $4000 - 400 \text{ cm}^{-1}$  range for the tantalum complexes 1 (a), 2 (b), 3 (c), 4 (d), 5 (e) (blue lines). The free ligands anthracene-9-carboxylic acid (a), 4'-methylbiphenyl-4-carboxylic acid (b), benzoic acid (c), 1-naphtoic acid (d) and 2-naphtoic acid (e) (red lines) and the tantalum precursor Ta(OEt)<sub>5</sub> (black lines).



*Figure S3b.* Infrared spectroscopy analysis in the  $2000 - 400 \text{ cm}^{-1}$  range for the tantalum complexes 1 (a), 2 (b), 3 (c), 4 (d), 5 (e) (blue lines). The free ligands anthracene-9-carboxylic acid (a), 4'-methylbiphenyl-4-carboxylic acid (b), benzoic acid (c), 1-naphtoic acid (d) and 2-naphtoic acid (e) (red lines) and the tantalum precursor Ta(OEt)<sub>5</sub> (black lines).



Figure S4. TGA of the tantalum complexes 1 (a), 2 (b), 3 (c), 4 (d), 5 (e).



**Figure S5.** Catalytic reaction scheme of the conversion of dihydroxyacetone (DHA) into lactic acid (LA), pyruvaldehyde (PA) and sugars ( $C_6$ , such as glucose or fructose).