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Supporting information for article:

**Psilocybin: crystal structure solutions enable phase analysis of
prior art and recently patented examples**

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A Crystallographic Information Format (CIF) file is provided, containing the results of the Rietveld refinements (including the raw data) and the DFT optimizations.

Form_A	The refined structure of Form A
Form_A_VASP	The VASP-optimized structure of Form A
Form_B	The refined structure of Form B
Form_B_VASP	The VASP-optimized structure of Form B
OKOKAD_VASPIoT	The VASP-optimized structure of psilocybin trihydrate, using the fixed 152K lattice parameters.



Figure S1 Sample 1 container. Printed date on bottle is “12/13/63.”



Figure S1 Sample 3 container. First record of use printed “1/10/76.” Label also states, “This material contains about 0.8% moisture.”