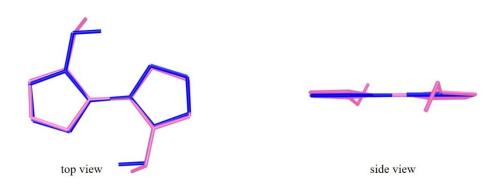
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2023



S2: optimized structure of isolate HOC_2N_8OH in blue and mauve fragment $C_2N_8O_2H_2$ in molecule II . Total root mean square displacement/deviation (RMSD): 0.3488