

Fractional coordinates of the geometry optimised UMP structure (starting point for MD simulation). Lattice parameters (Å): a = 22.880000, b = 8.877000, c = 19.592000; Cell Angles (degrees) alpha = 90.000000, beta = 90.000000, gamma = 90.000000

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H	0.797988707725507	0.371724617211405	0.185047271988791
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