

Pressure/GPa	0	0#	1.65	2.94	2.94#	3.70	3.70#
C8N3C9C10 (φ_1)	-85.3(5)	-89.3	-76.1(13)	116.7(7)	137.3	69.1(5)	64.7
C9C10O6H6 (ψ_1)	-178.2	174.3	173.6	30.5	-7.9	40.6	14.1
C6C7S1H1 (γ_2)	78.7	85.4	85.1	83.2	89.6	149.2	160.5
C3C2C1N1 (χ_3)	-71.0(4)	-69.2	-70.6(7)	-78.5(5)	-67.7	-72.5(4)	-64.1

Table of torsion angle parameters for GSH-I at 0 and 1.65 GPa, GSH-II at 2.94 GPa and GSH-III at 3.70 GPa. Angles in °. Values from the geometry optimised calculated structures are highlighted with a #.