

Hydration Structure of Osmolyte TMAO: Concentration- / Pressure-induced Response

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Electronic Supplementary Information

The optimized structure of TMAO

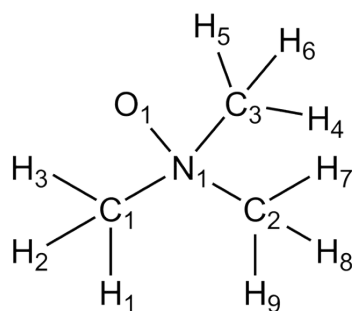


Figure S-1. Schematic representation with atom labeling for TMAO

Table S-1. Atom coordinates of TMAO with atom labeling according to Fig. S-1.

Atom	$x, \text{Å}$	$y, \text{Å}$	$z, \text{Å}$
N1	-0.401	0.207	0.566
O1	-0.254	1.509	0.948
C1	-1.243	-0.504	1.568
C2	0.942	-0.433	0.489
C3	-1.059	0.162	-0.770
H1	-0.732	-0.402	2.519
H2	-2.185	0.031	1.605
H3	-1.387	-1.551	1.301
H4	-1.197	-0.862	-1.115
H5	-2.008	0.675	-0.657
H6	-0.421	0.726	-1.441
H7	1.382	-0.334	1.474
H8	0.871	-1.478	0.185
H9	1.515	0.150	-0.224