

**Supplementary material to:**

P. Singh, K. Bisetty, P. Govender and G. Kruger, *S. Afr. J. Chem.*, 2011, **64**, 49–56.

Cluster No	Percentage of structures in MEOH	Phi angle (for TRIS residue) in RS	Psi angle (for TRIS residue) in RS	Tris conformation in RS
I	36.5	55.5	-70.5	C <sub>7ax</sub>
II	29.5	45.5	60.8	$\alpha_L$
III	21.0	-65.2	74.9	C <sub>7eq</sub>

**Table 3** Structural details of clusters I-III in case of MEOH.<sup>18</sup>

Cluster No	Percentage of structures in TIP3P	Phi angle (for TRIS residue) in RS	Psi angle (for TRIS residue) in RS	Tris conformation in RS
I	36.4	-55.9	76.2	C <sub>7eq</sub>
II	33.8	45.5	60.8	$\alpha_L$
III	18.8	70.2	55.4	$\alpha_L$

**Table 4** Structural details of clusters I-III in case of TIP3P.<sup>18</sup>