

ESI

Table ESI 1. Potential parameters applied in simulations

Molecule/structure	centre	σ [nm]	ϵ [kJ/mole]	q/e
H ₂ O				
	H			-1.04
	O	0.3154	0.6480	0.00
	charge point			+0.52
Carbon nanotube	C	0.3400	0.2329	0.00; +0.25; +0.50; +0.75
	O	0.2960	0.8801	0.00; -0.25; -0.50; -0.75

Table 1. Values of the (12,6) Lennard-Jones parameters and the point charges used in the current study of H₂O (TIP4P) adsorption in carbon membranes composed of single-walled nanotubes. [M. W. Mahoney and W. L. Jorgensen, *J. Chem. Phys.* **112** (2000) 8910-8922; W. L. Jorgensen, J. Chandrasekhar, J. D. Madura, R. W. Impey, and M. L. Klein, *J. Chem. Phys.* **79** (1983) 926-935, W. L. Jorgensen and J. D. Madura, *Mol. Phys.* **56** (1985) 1381-1392, respectively; M. Jorge, C. Schumacher and N. A. Seaton **18** (2002) *Langmuir* 9296-9306]

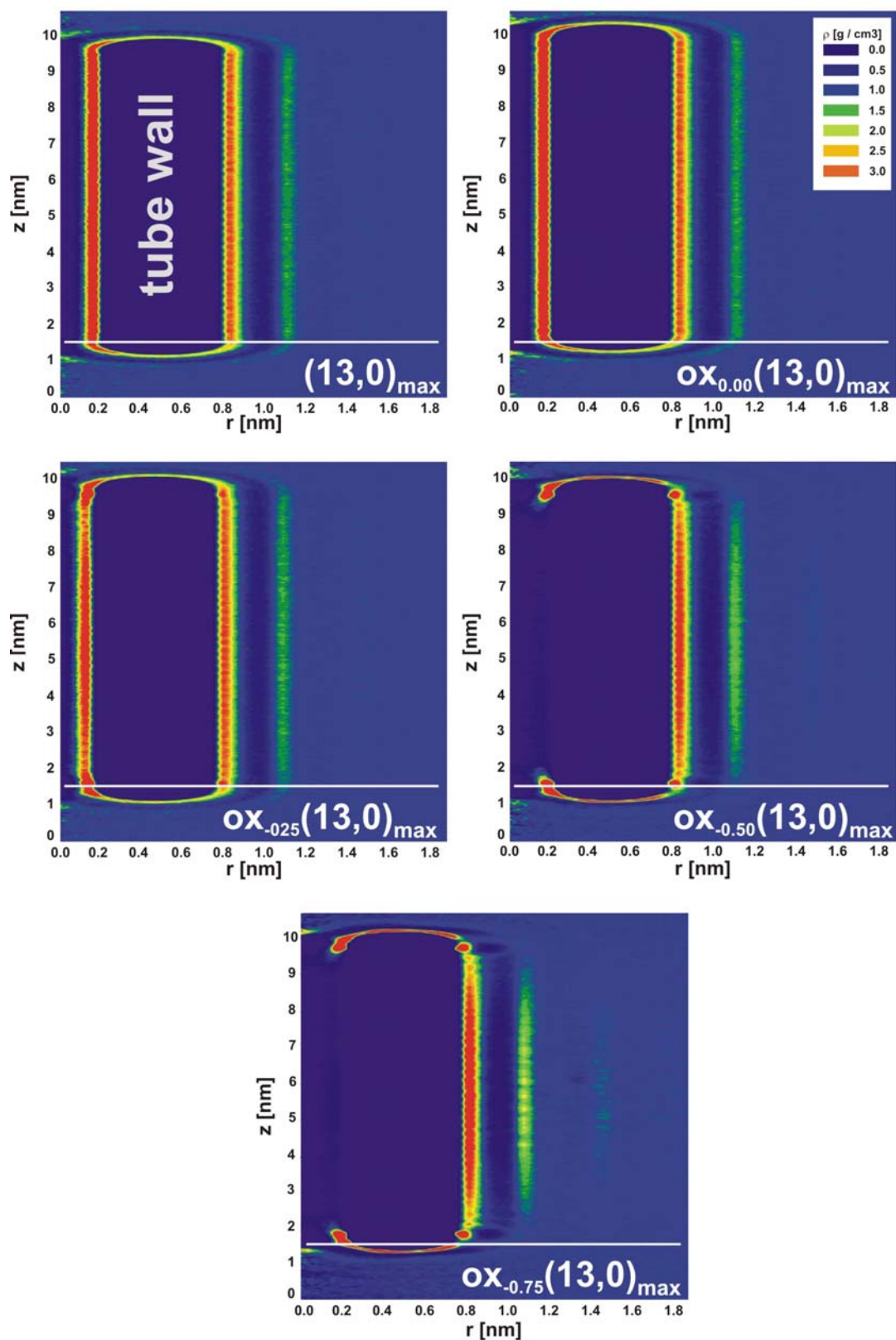


Fig. ESI 1. Density profiles (g/cm³) determined for selected tubes and assuming that the centre of the molecules is located on oxygen atom, r is the distance from the tube axis and z is the direction of the tube axis. The effect of charge distributions. White horizontal line shows the slice discussed in Fig. 5.

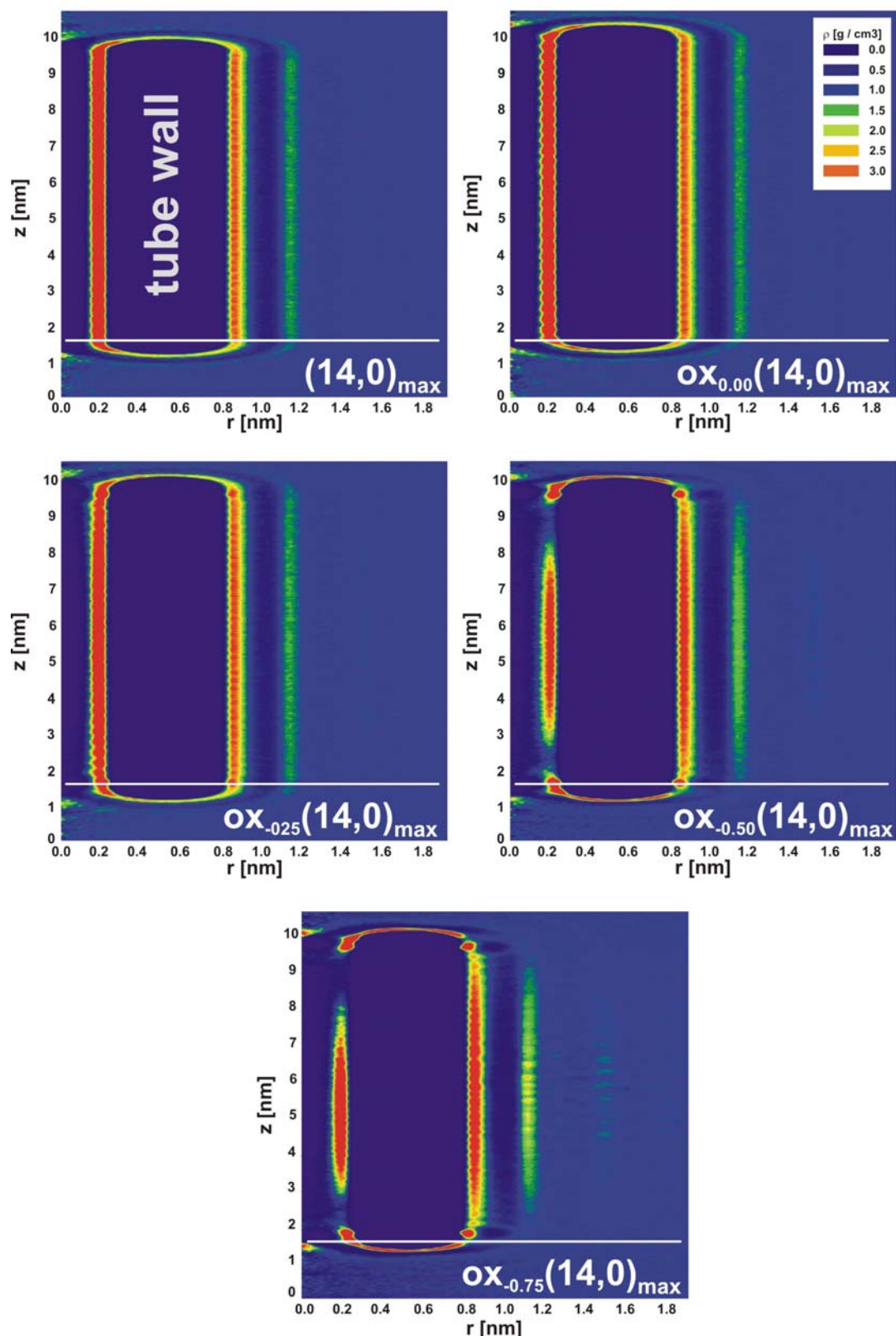


Fig. ESI 2. Density profiles (g/cm^3) determined for selected tubes and assuming that the centre of the molecules is located on oxygen atom, r is the distance from the tube axis and z is the direction of the tube axis. The effect of charge distributions. White horizontal line shows the slice discussed in Fig. 5.

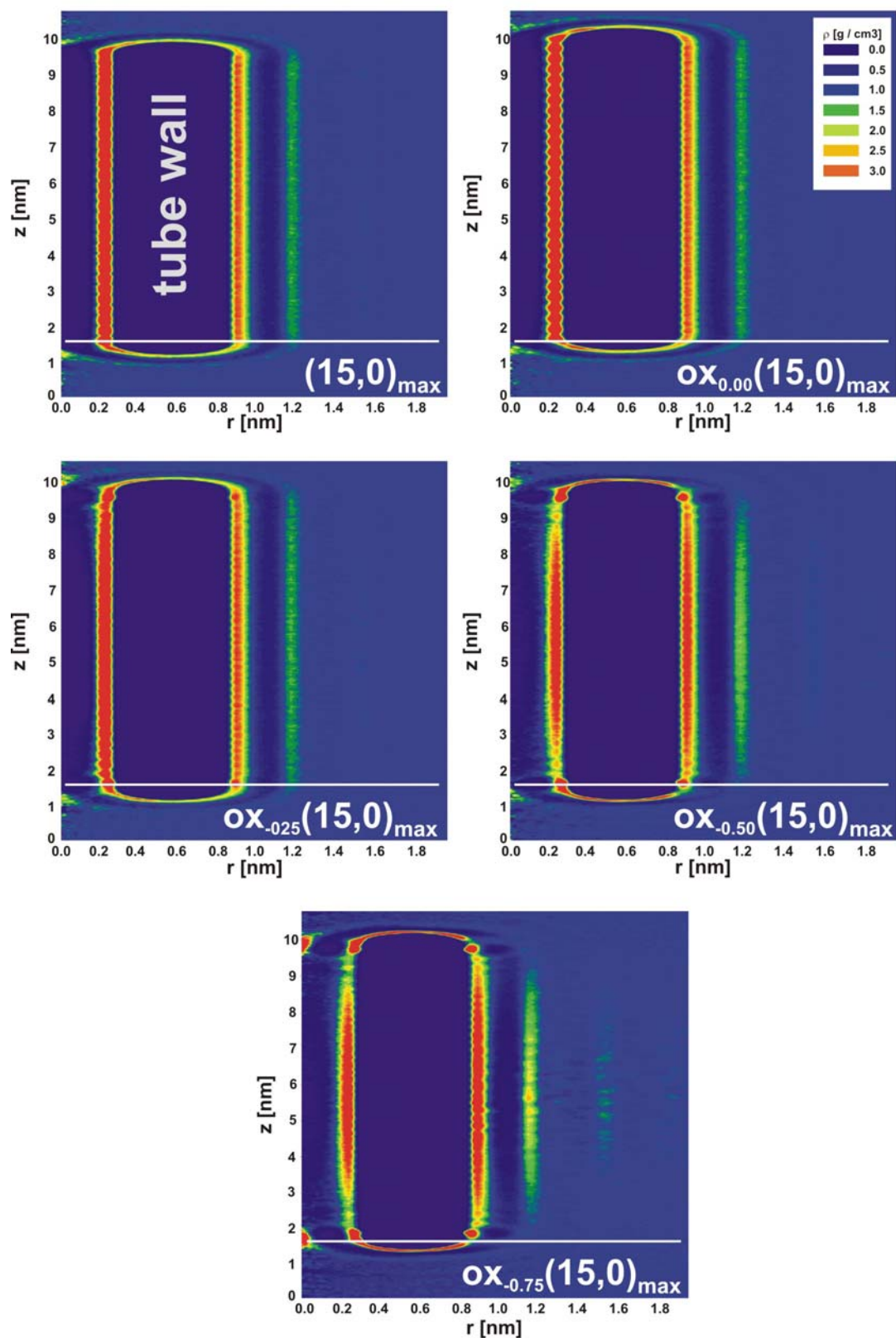


Fig. ESI 3. Density profiles (g/cm^3) determined for selected tubes and assuming that the centre of the molecules is located on oxygen atom, r is the distance from the tube axis and z is the direction of the tube axis. The effect of charge distributions. White horizontal line shows the slice discussed in Fig. 5.

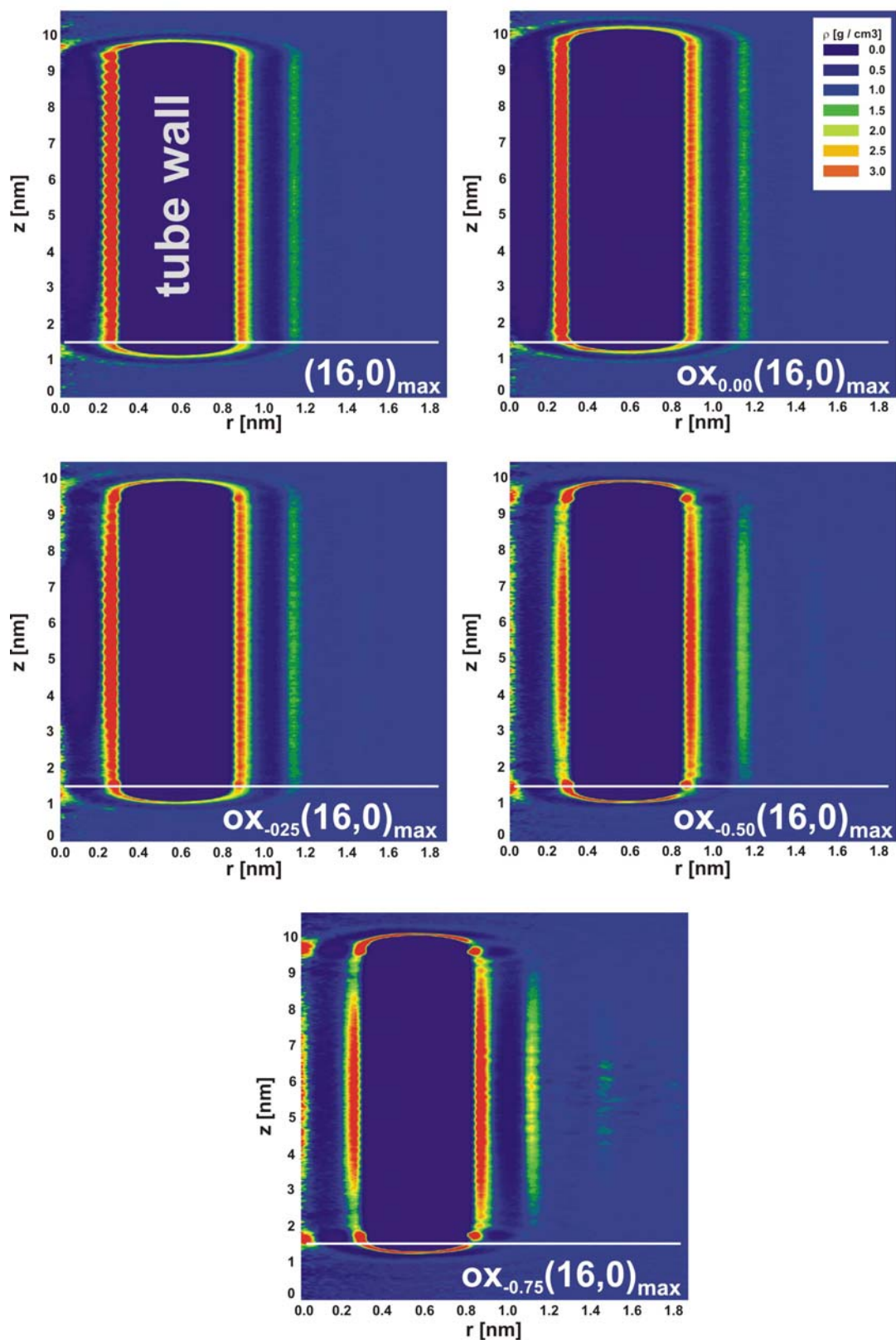


Fig. ESI 4. Density profiles (g/cm³) determined for selected tubes and assuming that the centre of the molecules is located on oxygen atom, r is the distance from the tube axis and z is the direction of the tube axis. The effect of charge distributions. White horizontal line shows the slice discussed in Fig. 5.

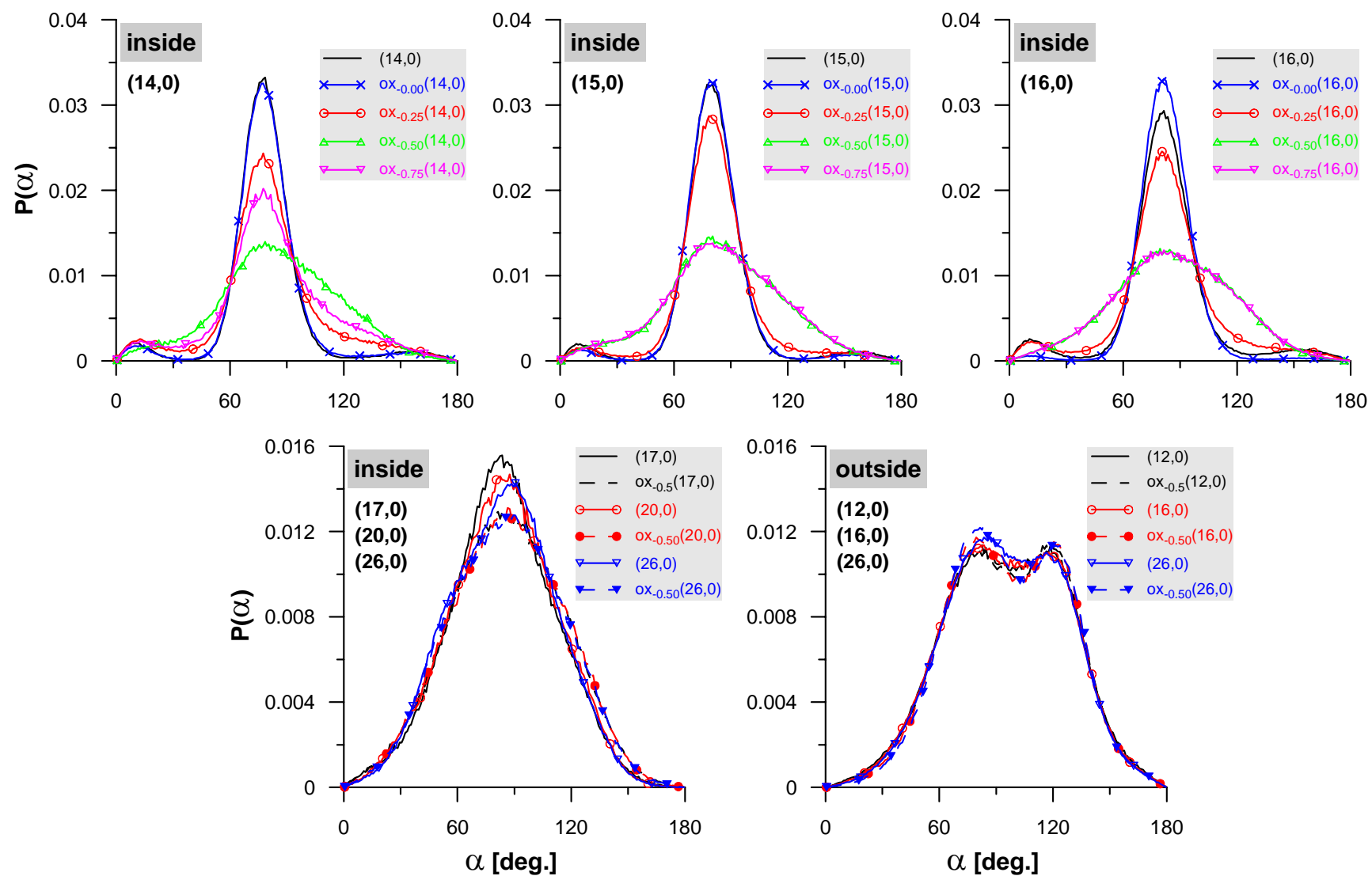


Fig. ESI 5. Histograms of the orientation of water dipole moment vector with respect to the surface of selected tubes.

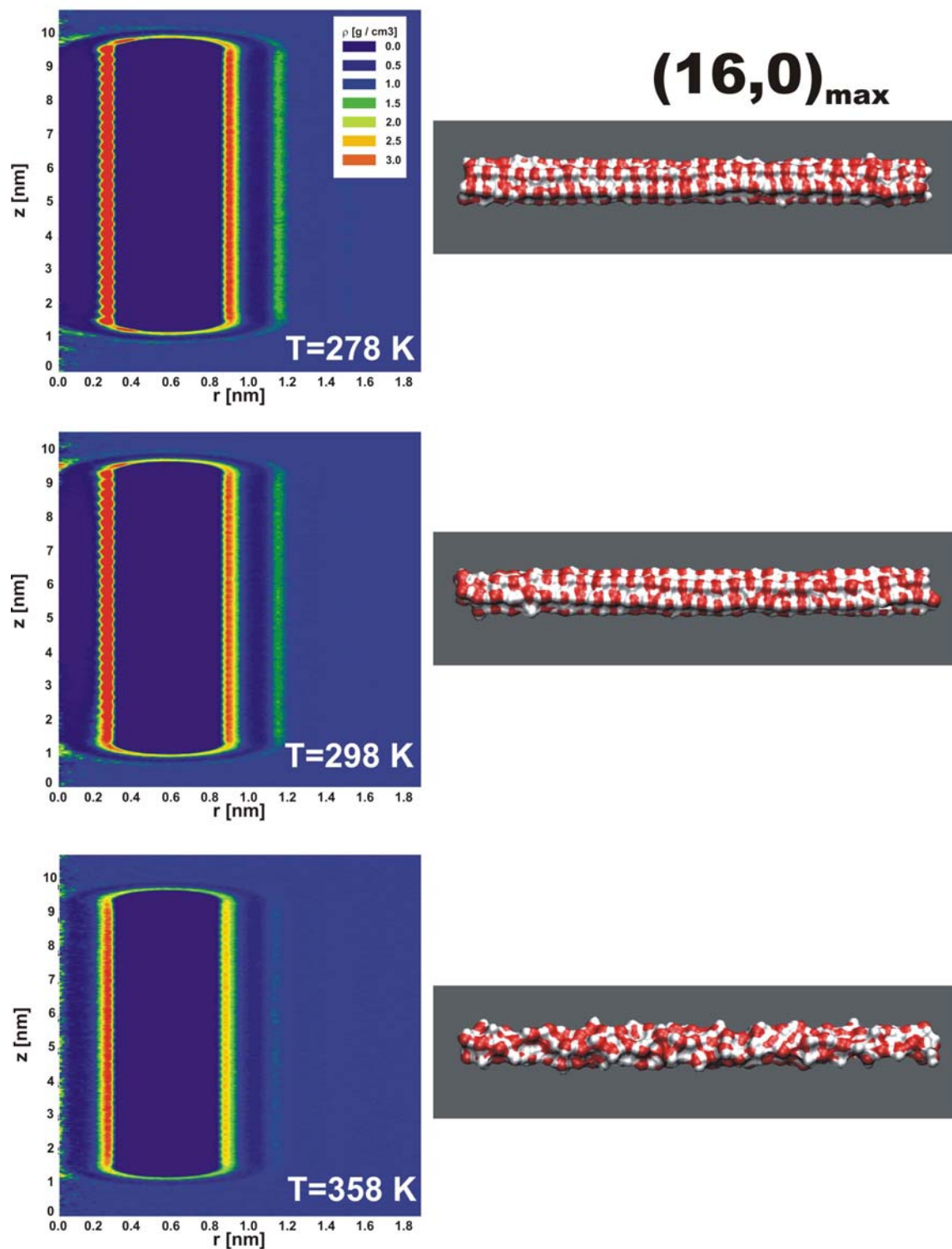


Fig. ESI 6. Density profiles (g/cm^3) determined for selected tubes and assuming that the centre of the molecules is located on oxygen atom, r is the distance from the tube axis and z is the direction of the tube axis. The effect of temperature.

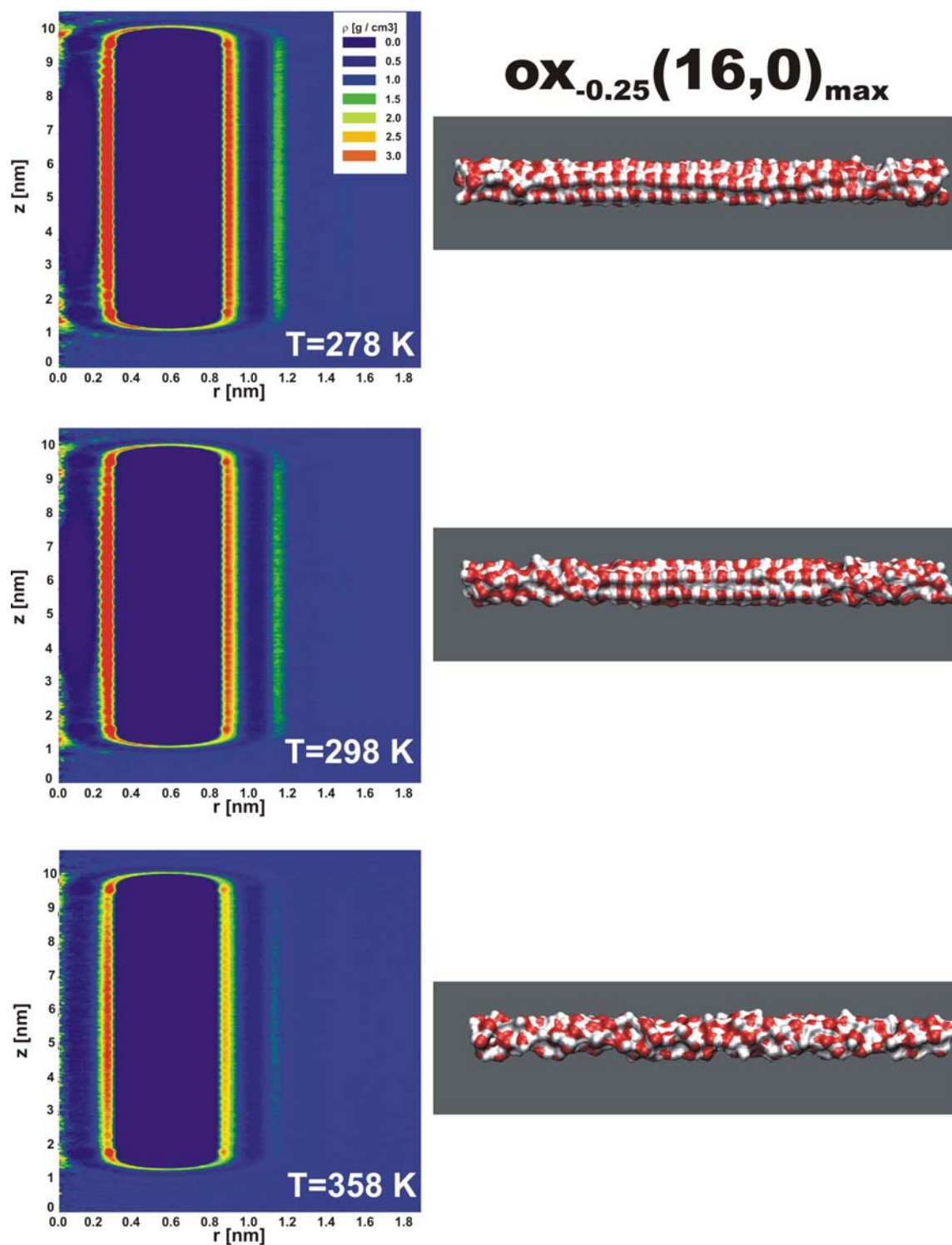


Fig. ESI 7. Density profiles (g/cm^3) determined for selected tubes and assuming that the centre of the molecules is located on oxygen atom, r is the distance from the tube axis and z is the direction of the tube axis. The effect of temperature.

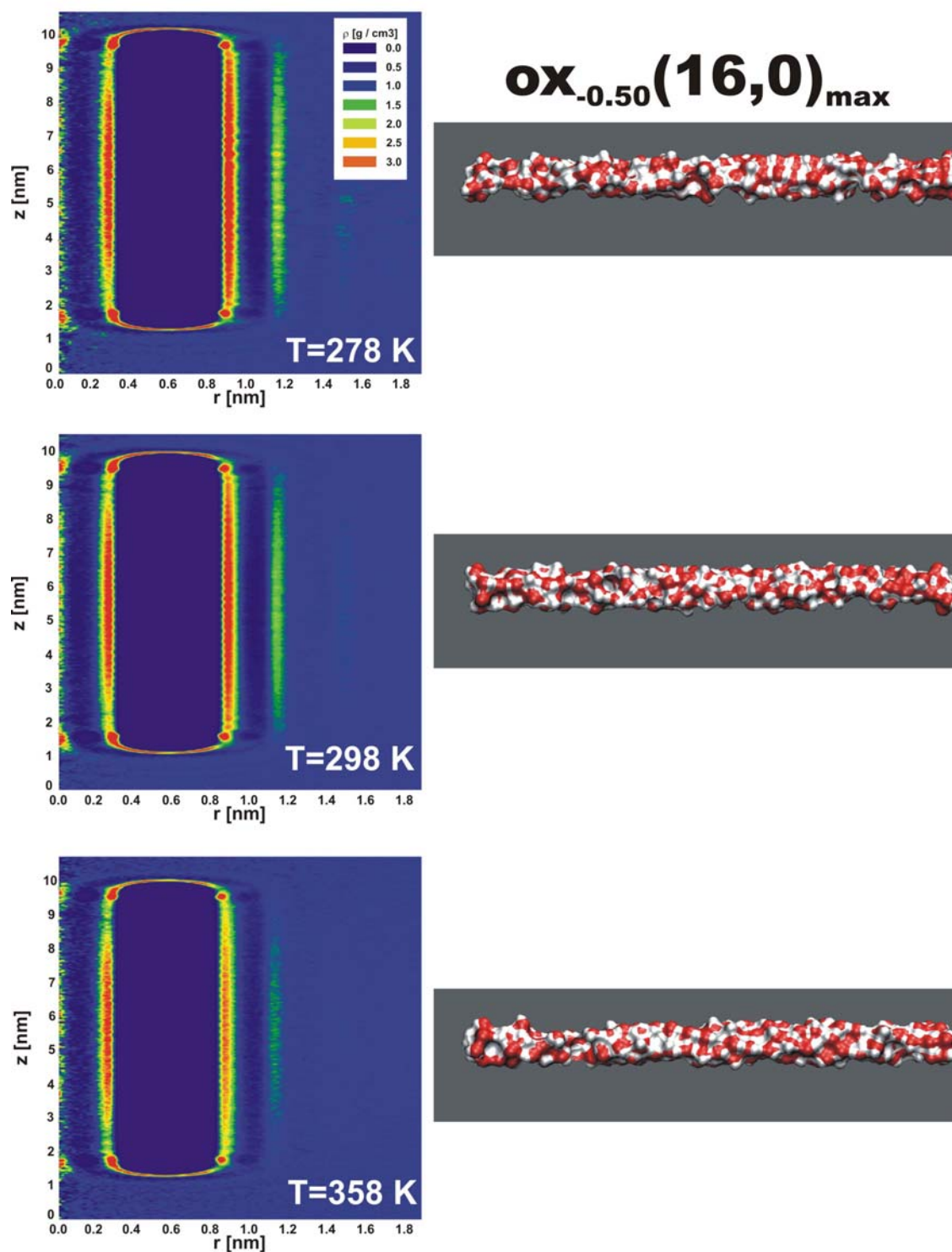


Fig. ESI 8. Density profiles (g/cm³) determined for selected tubes and assuming that the centre of the molecules is located on oxygen atom, r is the distance from the tube axis and z is the direction of the tube axis. The effect of temperature.

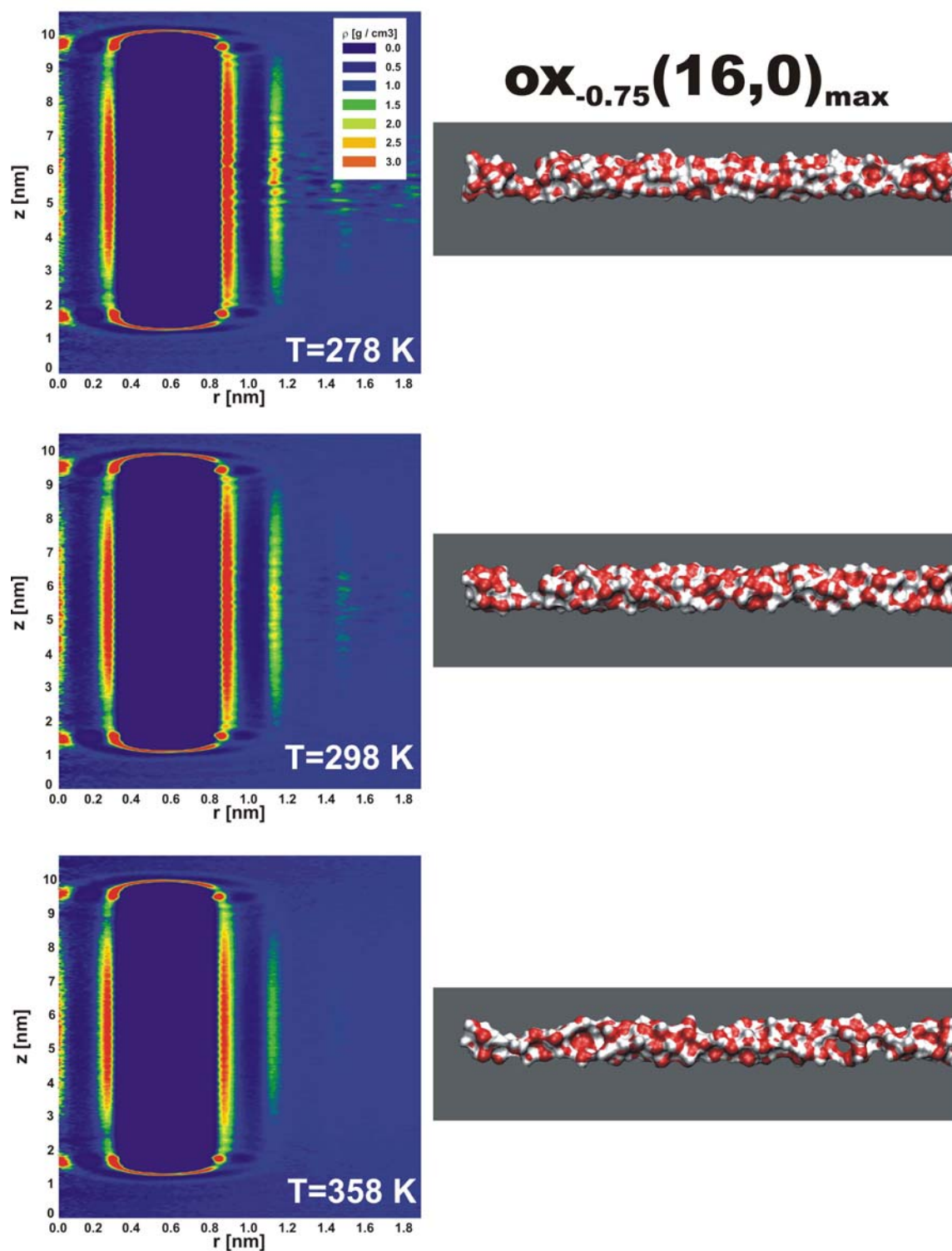


Fig. ESI 9. Density profiles (g/cm³) determined for selected tubes and assuming that the centre of the molecules is located on oxygen atom, r is the distance from the tube axis and z is the direction of the tube axis. The effect of temperature.