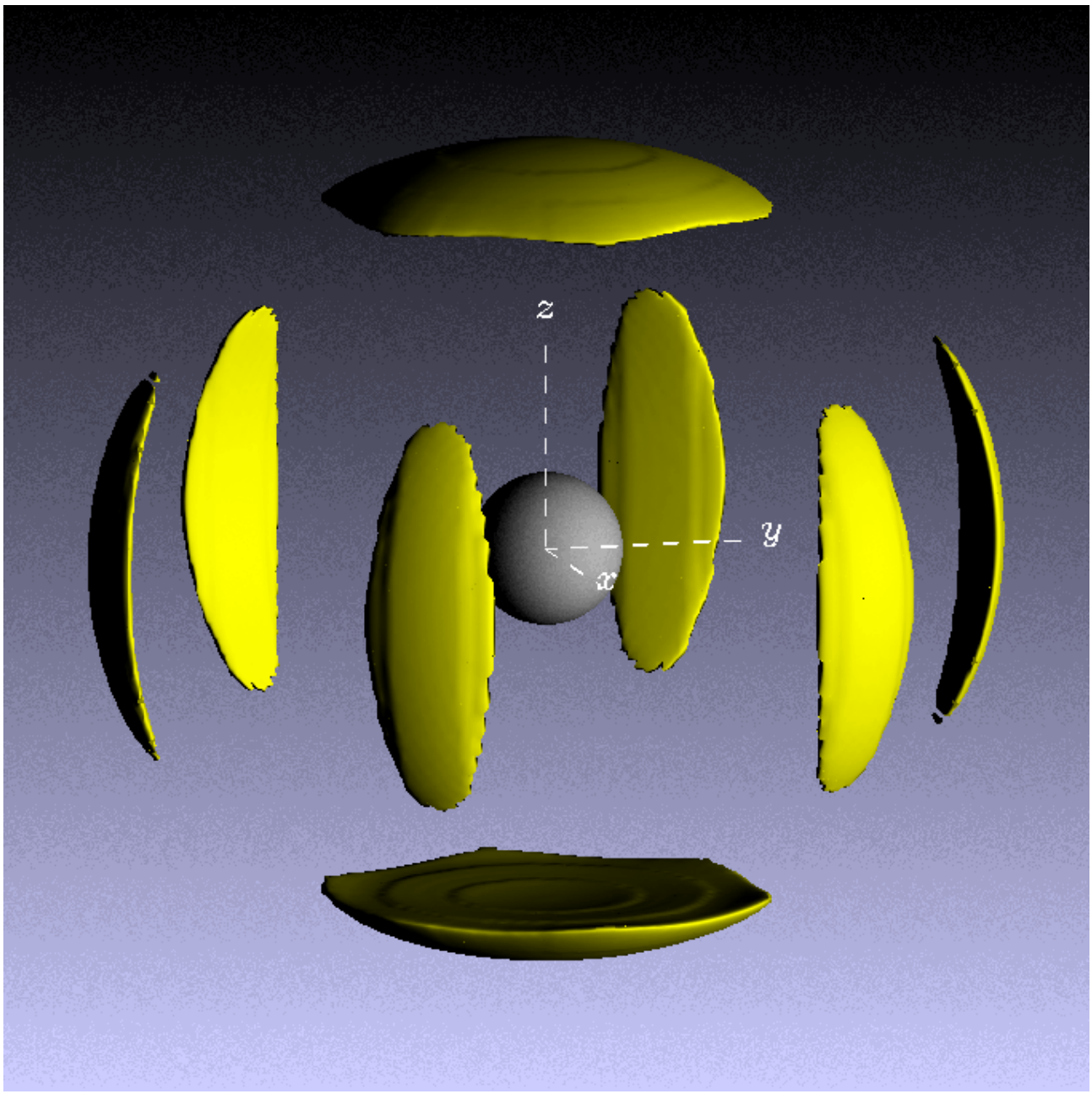

Fig 1 Benzene SDF – z-axis normal to molecule plane. Contour level set to 2.5 (-2.5 in input file to get absolute contours).

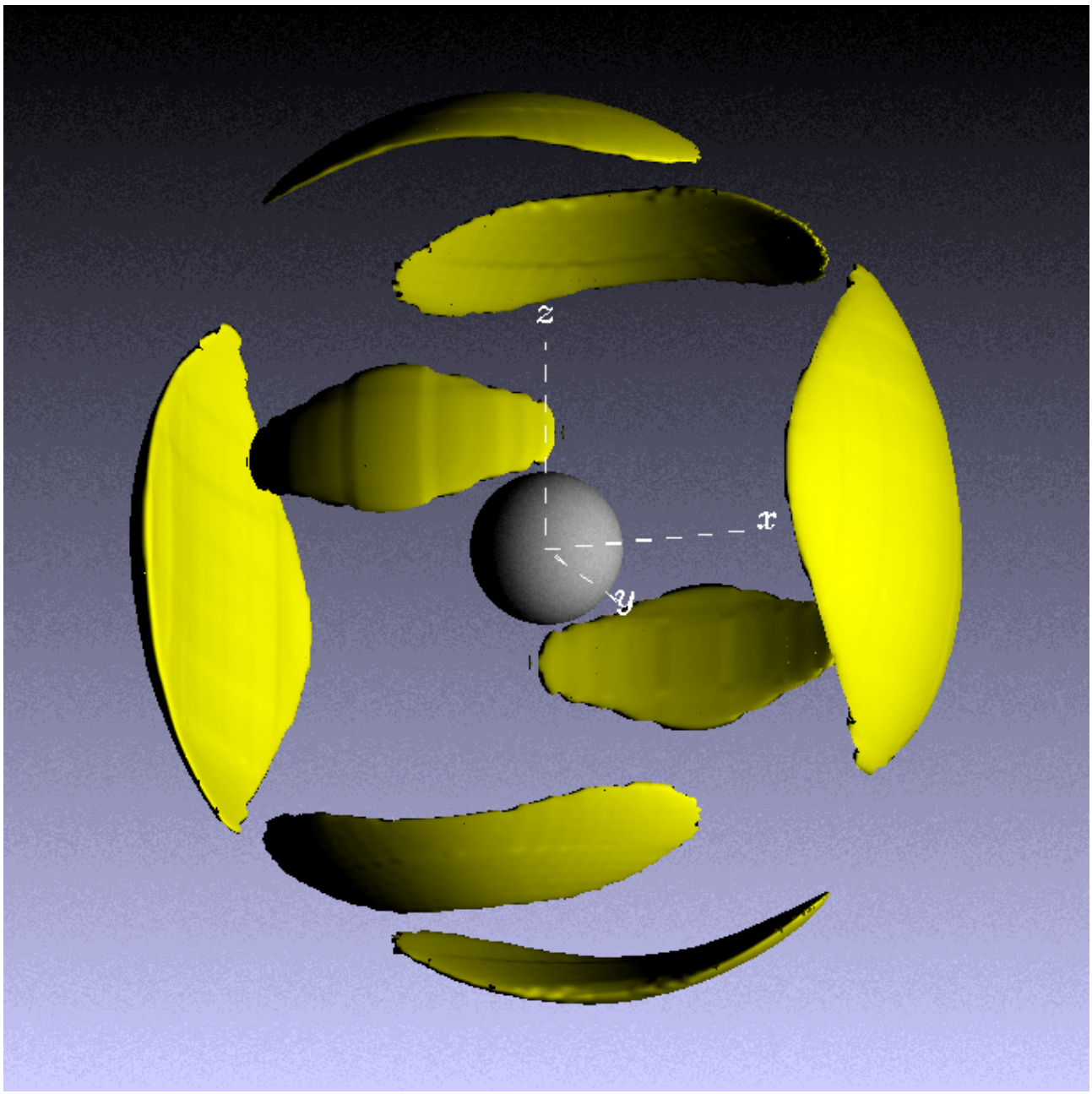

Fig 2. Benzene SDF – z-axis in plane of molecule, contour level set to 2.5 (-2.5 in input file).

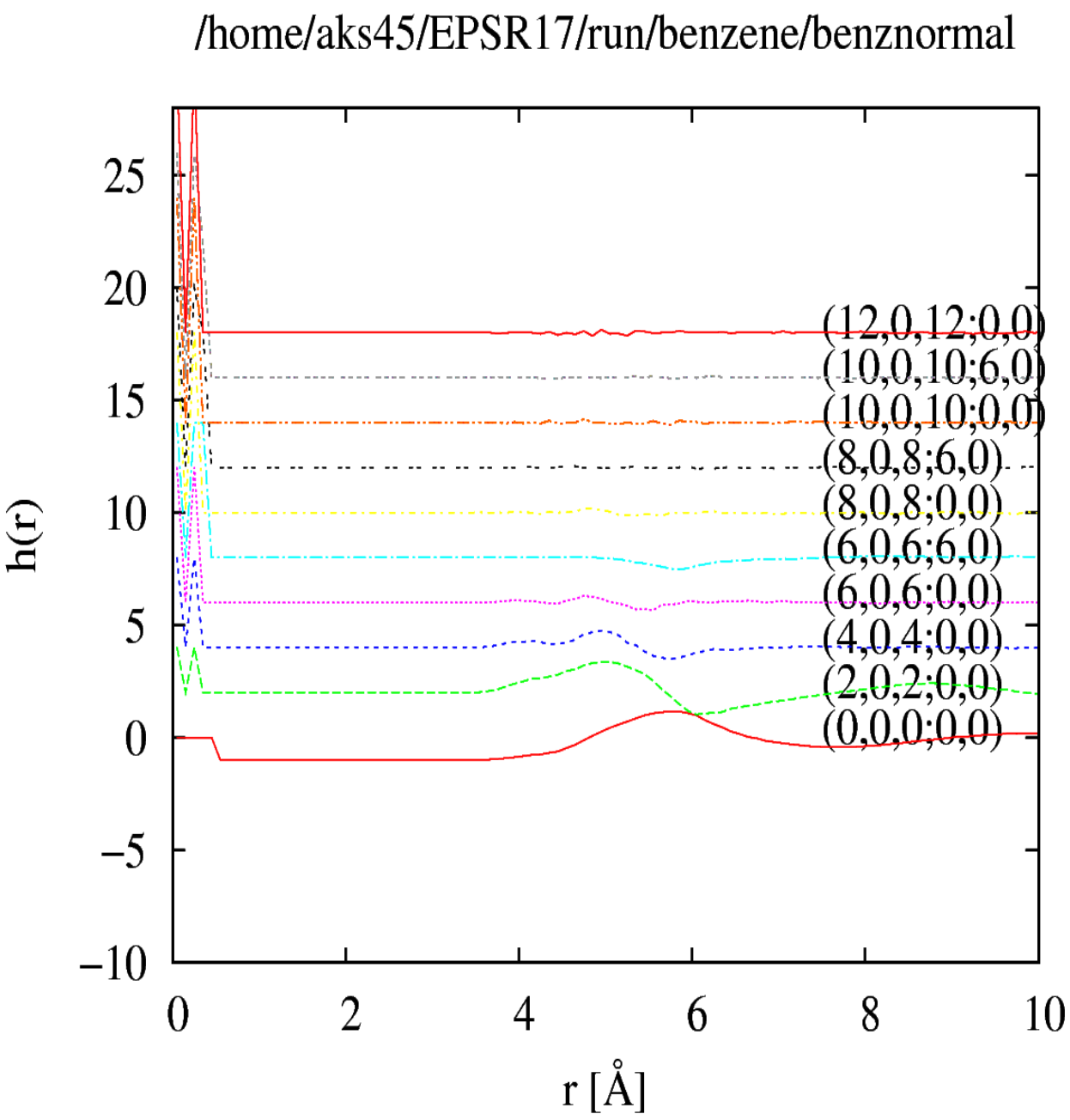

Fig 3. Spherical harmonic expansion coefficients as a function of radius for liquid benzene, with the z-axis normal to the plane of the benzene ring.

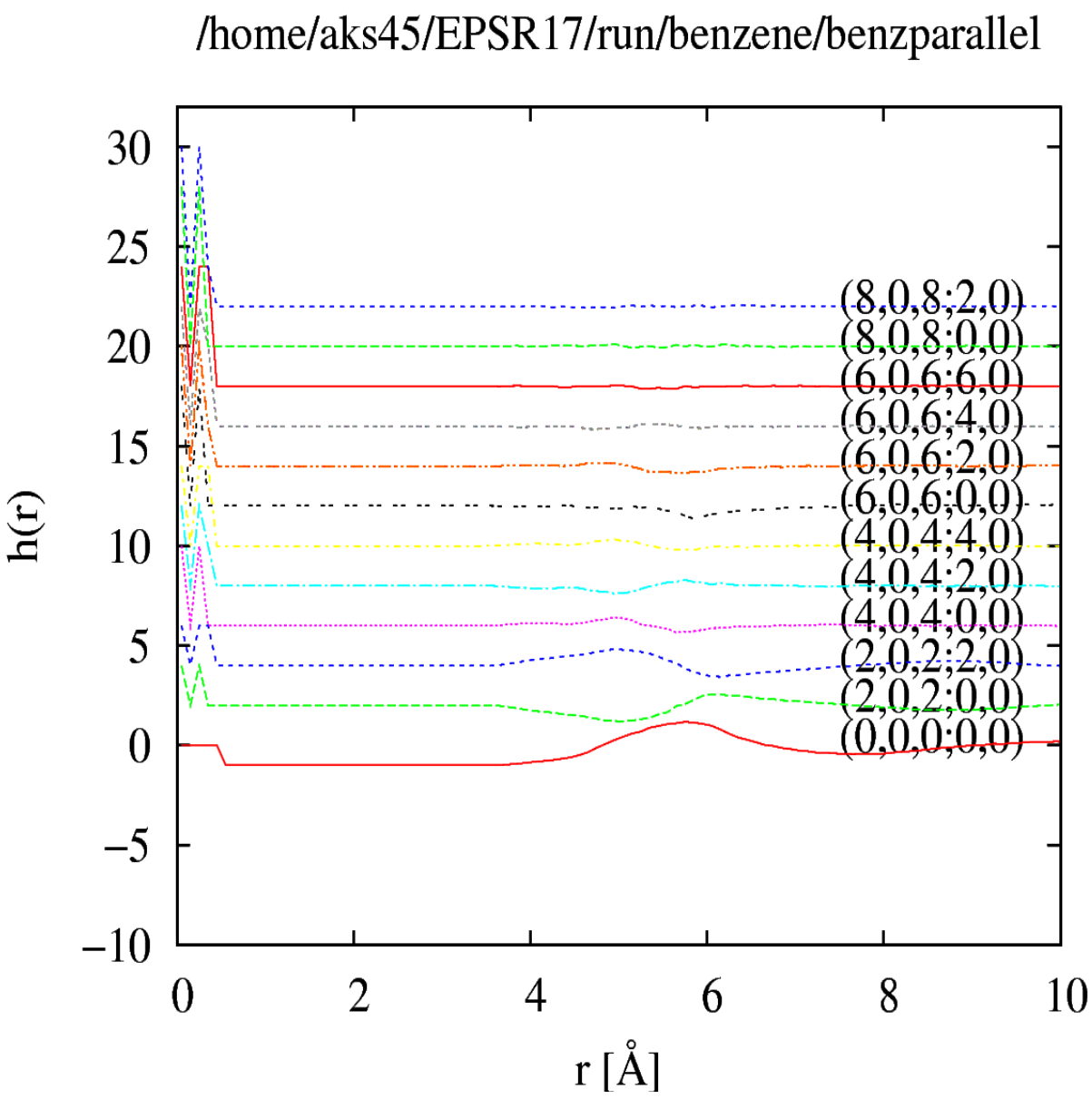

Fig 4 Spherical harmonic expansion coefficients as a function of radius for liquid benzene, with the z-axis parallel to the plane of the benzene ring.

Plot g(r)'s in different directions for normal and parallel coordinate systems. Values of theta and phi used were:

Direction (z-axis normal to molecular plane, x-axis through ring carbon)	Thetal	Phil	Equivalent direction (z-axis through ring carbon, x-axis normal to molecular plane)	Thetal	Phil
001	0	0	100	90	0
010	90	90	010	90	90
100	90	0	001	0	0
110	90	45	011	45	90
101	45	0	101	45	0
011	45	90	110	90	45
111	54.7	45	111	54.7	45

The g(r)'s corresponding to these directions are shown below

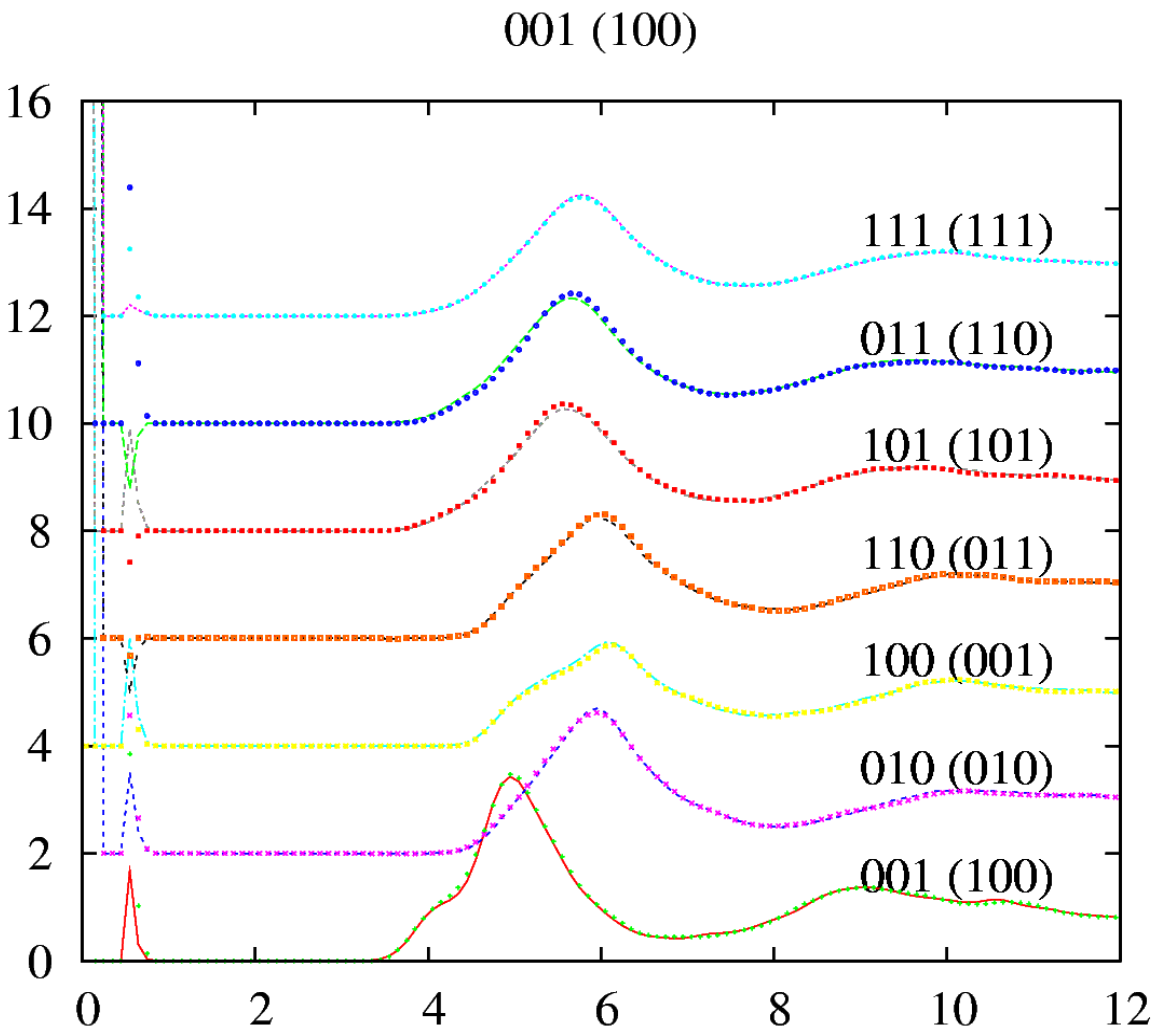

Figure 5. g(r)'s in particular directions (Miller indices hkl) for the z-axis normal to the benzene ring (lines). The dots correspond to the equivalent directions when the z-axis is parallel to the plane of the ring. The brackets show the Miller indices corresponding to the latter axes in each case.

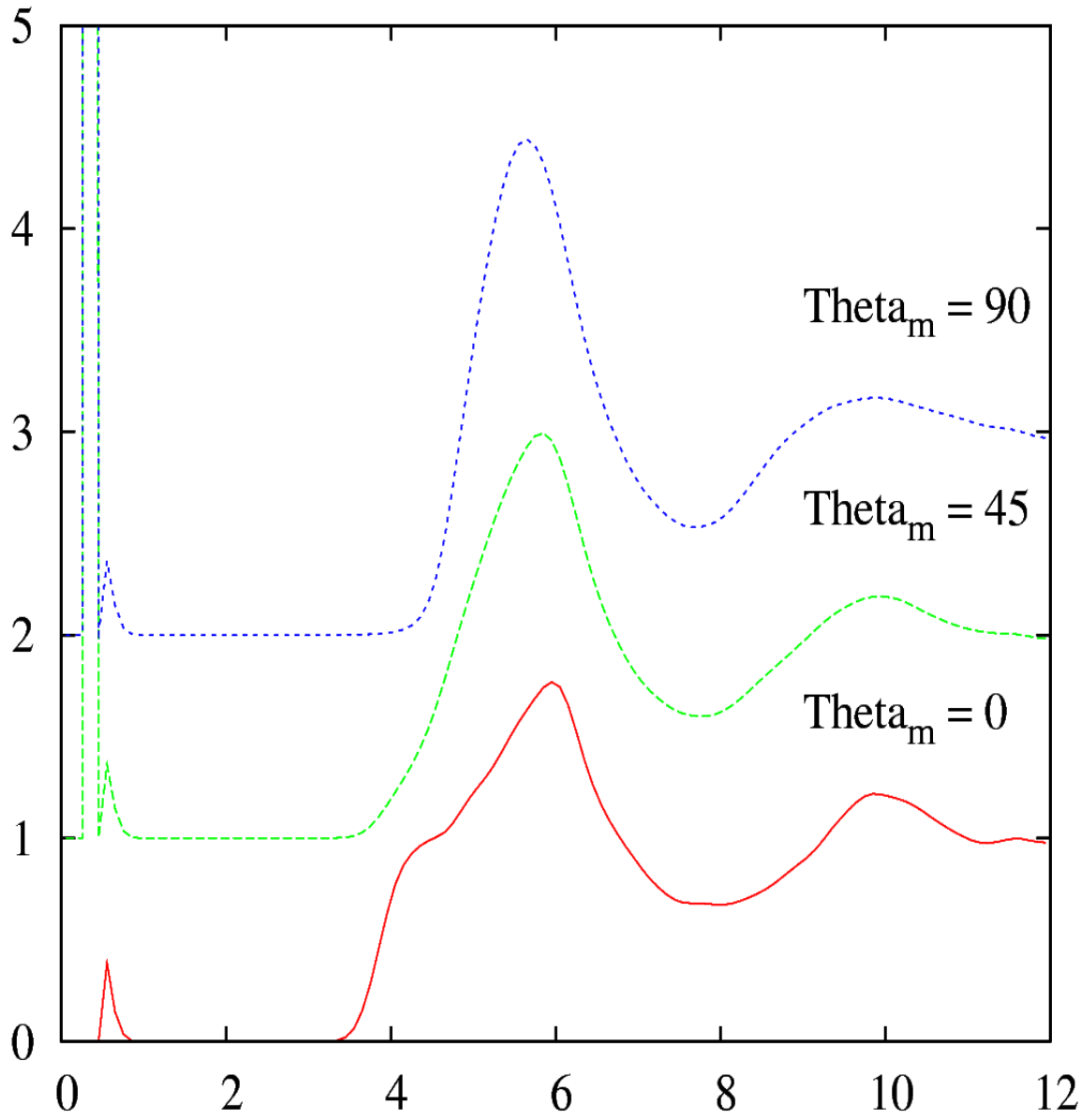

Fig. 6 Plot of the orientational correlation function for benzene, averaged over spatial directions theta_l and phi_l, internal rotations chi_m, for three values of the relative angle, theta_m. For this plot l = m = 0.

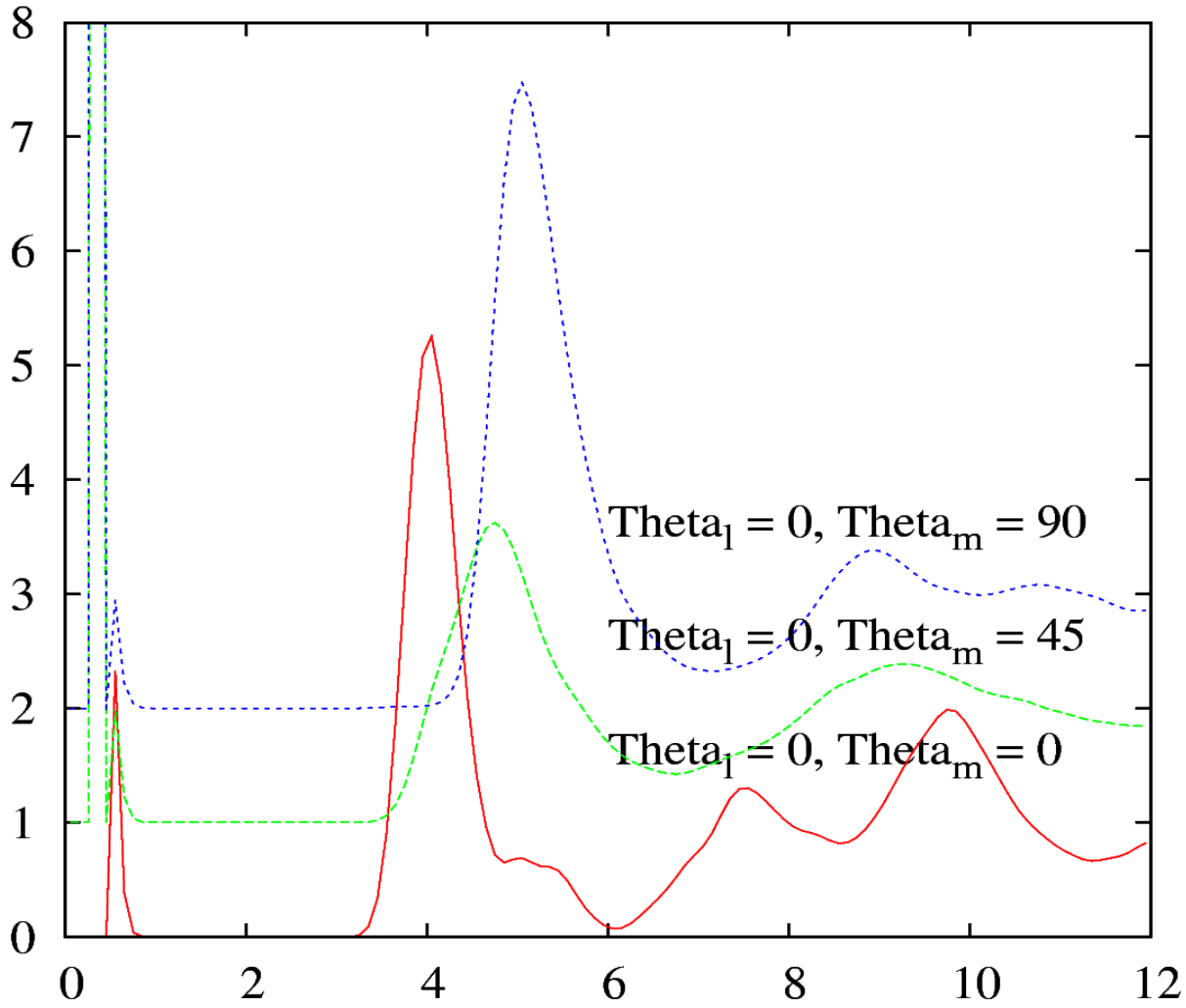

Fig. 7 Plot of the orientational correlation function for benzene, averaged over directions phi_l, and chi_m for three values of the relative angle, theta_m, and with theta_l = 0, corresponding to along the polar z-axis (normal to the molecular plane). For this plot m = 0.

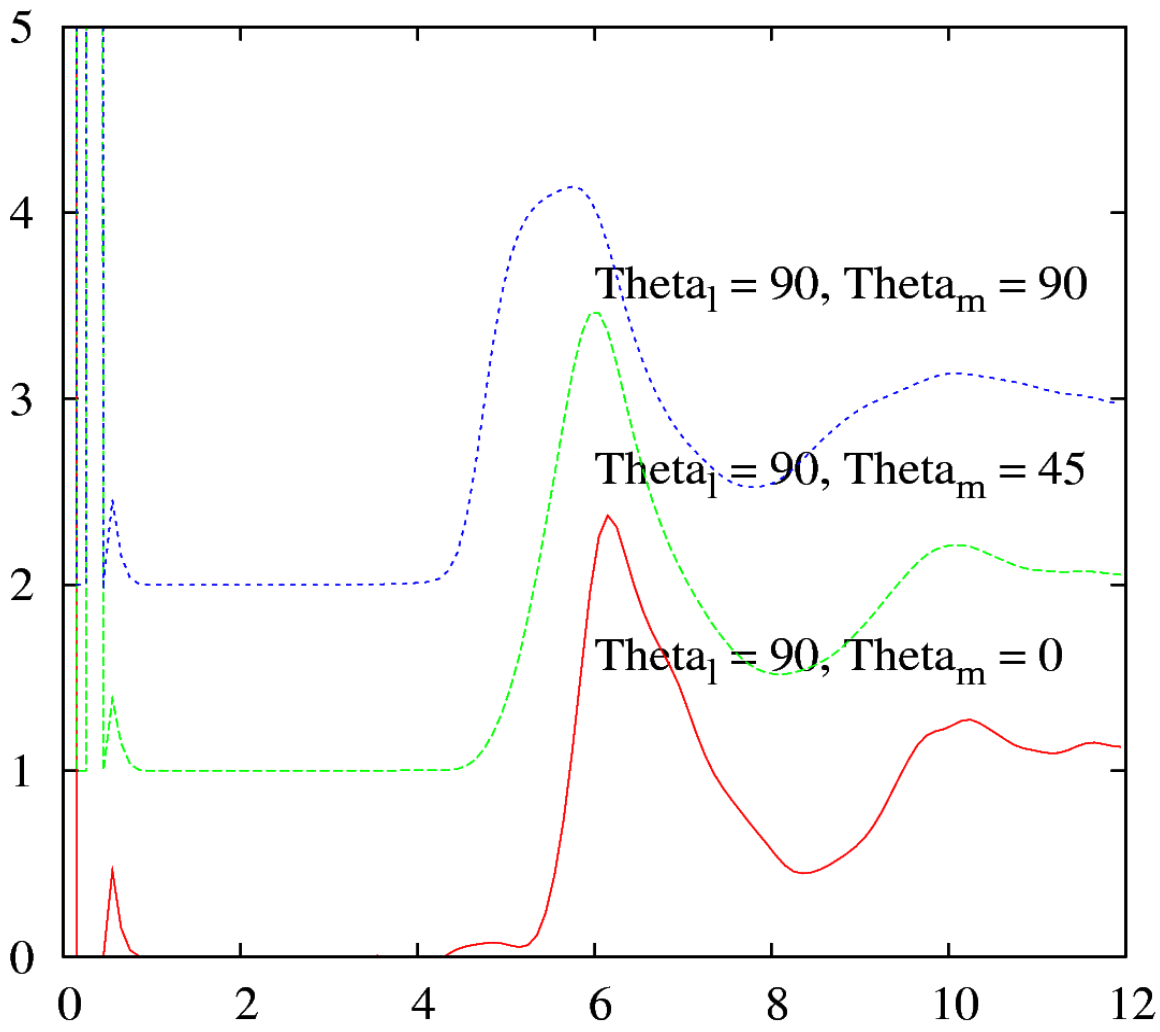

Fig 8. Same as Fig 7, but with Theta_l = 90, i.e. the equatorial plane