



Figure 3. Overview of the three geometry-optimized structures of the cysteine thiyl radical, (a) 1st minimum, (b) 2nd minimum, and (c) 3rd minimum. The directions of the principal axes of the **g**-tensor: z (brown, parallel to the symmetry axis of the 3p orbital in the SOMO) and the y (light-blue) principal axis of the **g**-tensor are indicated. The x axis is parallel to the C β -S γ direction. Reproduced with permission from [128]. Copyright © 2004, American Chemical Society.