Low Temperature Heat Capacities of NO Encapsulated in Open-Cage Fullerenes

Low temperature heat capacity measurements were performed for a NO encapsulated fullerene derivative (NO@**1**) and empty one (**1**). Magnetic field dependence of the Schottky anomaly originating from the unpaired electrons on NO unit was observed in NO@**1**, which was simulated by S = 1/2 spin with anisotropic g-factor. According to the theoretical calculations, NO molecule should not show magnetic moment because the orbital angular momentum (***L***) and the spin angular momentum (***S***) compensate with each other. In case of NO@**1**, orbital angular momentum of the NO unit was partially quenched by the encapsulation, resulting in the emergence of the net magnetic moment. In addition, Schottky anomaly was observed at zero dc magnetic field in NO@**1**, possibly due to a low energy vibration.

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Table 1. Principal values of g-tensor.

	NO(calc)	NO@**1**(exp)	NO@**1**(calc)
g_{xx}	0.0669	1.42	1.515
g_{yy}	0.0669	1.42	1.515
g_{zz}	0.00344	0.59	0.723

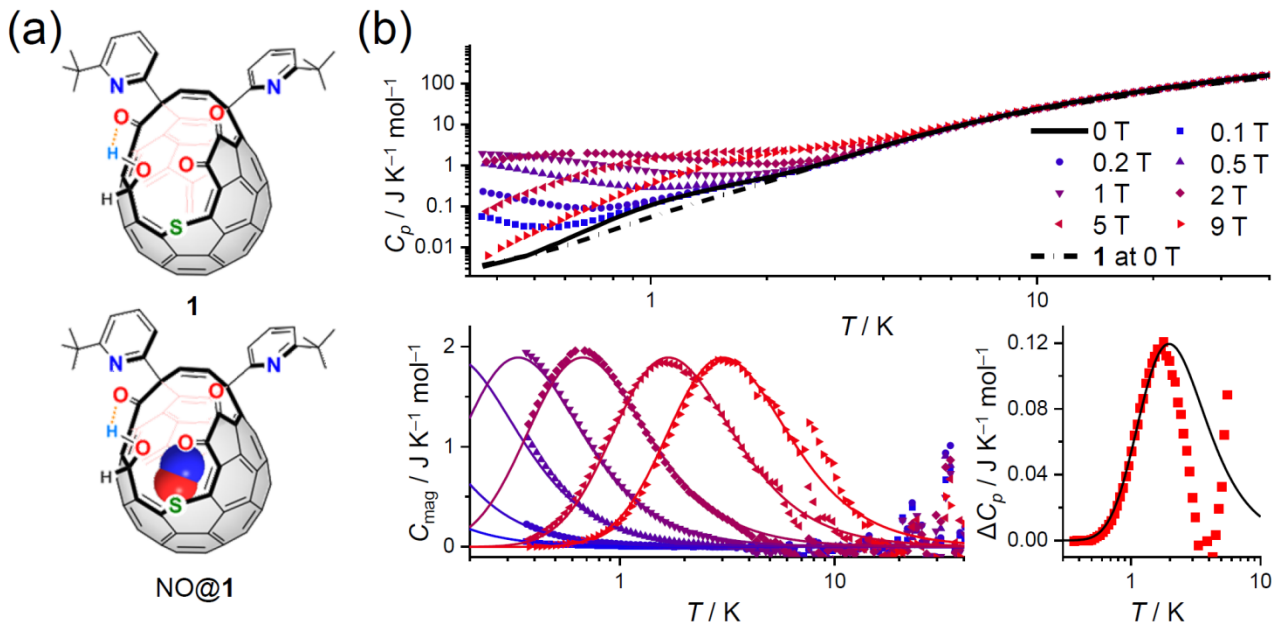

Fig. 1. (a) Molecular structures and (b) heat capacities of **1** and NO@**1**.

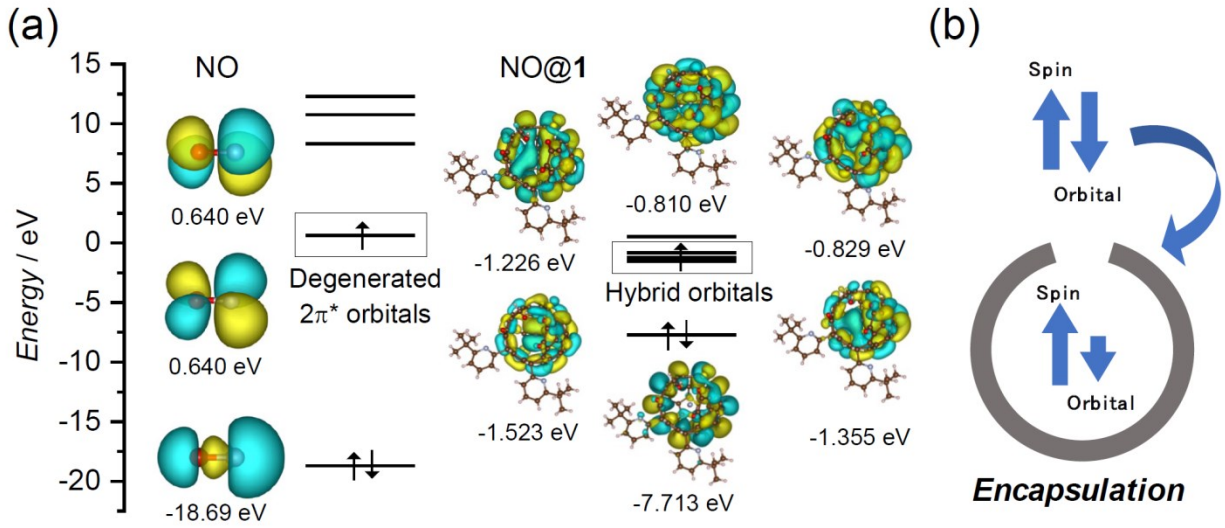

Fig. 2. (a) Active orbitals and their energy levels of NO and NO@**1**. (b) Quenching of the orbital angular momentum by the encapsulation.