

Supporting Information

Cis-to-trans photoconversion of azobenzene self-assembled monolayers on gold nanoparticle surfaces investigated by Raman spectroscopy

Sung Ik Yang,^a Ki-Hyun Kim,^b Daeseung Kang,^{c,*} and Sang-Woo Joo^{d,*}

^a *College of Environmental and Applied Chemistry, Kyunghee University, Suwon 151-742, Korea*

^b *Atmospheric Environmental Laboratory, Department of Earth and Environmental Sciences, Sejong University, Seoul 143-747, Korea*

^c *School of Electrical Engineering, Soongsil University, Seoul 156-743, Korea*

^d *Department of Chemistry, Soongsil University, Seoul 156-743, Korea*

Corresponding author. Fax: +1-82-2-820-0434

E-mail address: sjoo@ssu.ac.kr ; dkang@ssu.ac.kr

Table 1. Spectral Data and Vibrational Assignment of 4DAzC^a

4DAzC				Assignment ^b
Cal.		OR	Au SERS	
Trans	Cis			
1149	1145	1124	1128	9a _g (E), 20a (Z)
1162		1132	1138	10a _g (E)
	1178		1168	22a (Z)
1229		1200	1188	11a _g (E)
1274	1273		1221	11b _u (E), 22a (Z)
1325	1325	1299	1268	22b (Z), 23(a) (Z)
1341	1340	1312	1308	12a _g (E)
1369	1369	1362	1357	14a _g (E), 20a (Z)
1396	1395	1392	1392	13b _u (E), 23b (Z), COO ⁻
1442	1451	1420	1417	15a _g (E), 26a (Z)
1475		1445	1442	16a _g (E),
	1673		1502	27a (Z)
1652	1644	1596	1598	18a _g (E), 29a (Z)
1658	1660	1605	1618	17b _u (E), 27b(Z)

^aUnit in cm⁻¹. ^bBased on ref. 15. Scale factor: 0.97

Table 2. Density Functional Calculations of 4DAzC ^a

Dihedral Angles of <i>cis</i> form	
C-N-N-C	11.2°
N-N-C-C	50.0°
Energy Difference	
$\Delta(\text{cis-trans})$	16.0 Kcal/mol

^a B3LYP/6-31G++ (d,p)