Supporting information for

Corrosion inhibition properties of triazine derivatives containing carboxylic acid and amine groups in 1.0 M HCl solution

Seung-Hyun Yoo[1], Young-Wun Kim[1,*], Keunwoo Chung[1], Nam-Kyun Kim[1], and Joon-Seop Kim[2,*]

[1]*Green Chemistry Research Division, Surfactant & Lubricant Research Team, KRICT, Daejeon 305-600, South Korea*

[2]*Department of Polymer Science & Engineering, Chosun University, Gwangju 501-759, South Korea*

It is seen in Table S1 taht the ^{1}H-NMR peak at δ = 3.15 ppm for the hydrogen at the alpha position of primary amine (s, 2H, H_2N–C$\underline{H}_2$-) of Gly shifts to δ = 3.64 ppm (s, 2H, Ar–HN–C$\underline{H}_2$-) upon the S_NAr reaction of Gly with cyanuric chloride. In addition, the ^{13}C-NMR peak at δ = 174.7 ppm for the carbonyl carbon of Gly shifts to δ = 178.4 ppm upon the reaction, and a new peak at δ = 165.1 ppm for the three carbons of 1,3,5-triazine appears. In the case of FT-IR spectra, the IR band at 1633 cm^{-1} for the carbonyl group of Gly, involving hydrogen-bonding,[1,2] appears at 1705 cm^{-1} for Tris-Gly. It is also seen that the IR band for the alkyl group of Tris-Gly appears at 2964 cm^{-1}, and the IR bands for the deformation vibration of –NH– and in-plane ring stretching vibration of –C=N– are observed in the range of 1500–1630 cm^{-1}, and multiple bands are seen for the secondary amine in the range of 3000–3300 cm^{-1}. The EA and MS results are in good agreement with the calculated values based on the chemical formula of Tris-Gly. The spectroscopic data and the EA and MS data of Tris-IDA also indicate the reaction completed successfully.

References

(1) Iuliano, A.; Lecci, C.; Salvadori, P. The *s*-triazine moiety as a scaffold for connecting different chiral auxiliaries: synthesis of new biselector CSPs for enantioselective chromatography. *Tetrahedron: Asymmetry* **2003**, *14*, 1345.

(2) Afonso, C. A. M.; Lourenço, N. M. T.; Rosatella, A. A. Synthesis of 2,4,6-tri-substituted-1,3,5-triazines. *Molecules* **2006**, *11*, 81.

Table S1. Notation, name, ^{1}H- and ^{13}C-NMR, FT-IR, EA, and MS data of the corrosion inhibitors

notation	name	^{1}H-NMR (ppm)	^{13}C-NMR (ppm)	FT-IR (KBr, cm^{-1})	EA	MS
Gly	2-aminoacetic acid (glycine)	--	--	--	--	--
IDA	2,2'-azanediyldiacetic acid	--	--	--	--	--
5-APA	5-aminopentanoic acid	--	--	--	--	--
Tris-Gly	2,2',2''-((1,3,5-triazine-2,4,6-triyl)tris(azanediyl))triacetic acid	(D_2O•NaOH /TMS) 3.64 (s, 2H)	(D_2O•NaOH /TMS) 178.4, 165.1, 43.3	3261, 3114, 2964, 1705, 1628, 1578, 1397, 1354, 1219, 787	(calcd: C, 36.00; H, 4.03; N, 27.99) found: C, 35.46; H, 3.99; N, 27.90	MS-EI m/z $[M]^{+}$ 300
Tris-IDA	2,2',2'',2''',2'''',2'''''-((1,3,5-triazine-2,4,6-triyl)tris(azanetriyl))hexaacetic acid	(D_2O /TMS) 4.22 (s, 2H)	(D_2O /TMS) 175.8, 165.1, 51.1	3000, 2551, 1735, 1651, 1621, 1481, 1392, 1337, 1091, 811, 716	(calcd: C, 37.98; H, 3.82; N, 17.72) found: C, 37.05; H, 3.65; N, 17.62	MS-FAB m/z $[M+H]^{+}$ 475

The ^{1}H-NMR peak at δ = 3.15 ppm for the hydrogen at the alpha position of primary amine (s, 2H, $H_2N–C\underline{H_2}$-) of Gly shifts to δ = 3.64 ppm (s, 2H, Ar–HN–C$\underline{H_2}$-) upon the S_NAr reaction of Gly with cyanuric chloride. In addition, the ^{13}C-NMR peak at δ = 174.7 ppm for the carbonyl carbon of Gly shifts to δ = 178.4 ppm upon the reaction, and a new peak at δ = 165.1 ppm for the three carbons of 1,3,5-triazine appears. In the case of FT-IR spectra, the IR band at 1633 cm^{-1} for the carbonyl group of Gly, involving hydrogen-bonding,[18,19] appears at 1705 cm^{-1} for Tris-Gly. It is also seen that the IR band for the alkyl group of Tris-Gly appears at 2964 cm^{-1}, and the IR bands for the deformation vibration of –NH– and in-plane ring stretching vibration of –C=N– are observed in the range of 1500–1630 cm^{-1}, and multiple bands are seen for the secondary amine in the range of 3000–3300 cm^{-1}. The EA and MS results are in good agreement with the calculated values based on the chemical formula of Tris-Gly. The spectroscopic data and the EA and MS data of Tris-IDA also indicate the reaction completed successfully.