

Corrosion Inhibition of Copper in Aqueous Chloride Solution by 1H-1,2,3-Triazole and 1,2,4-Triazole and their Combinations: Electrochemical, Raman and Theoretical Studies.

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SUPPLEMENTARY MATERIALS

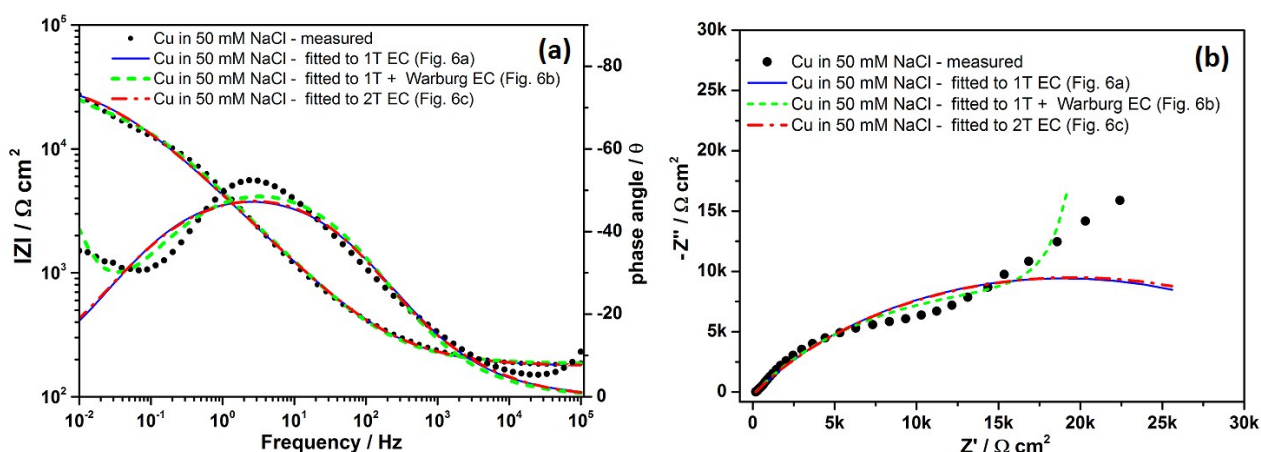
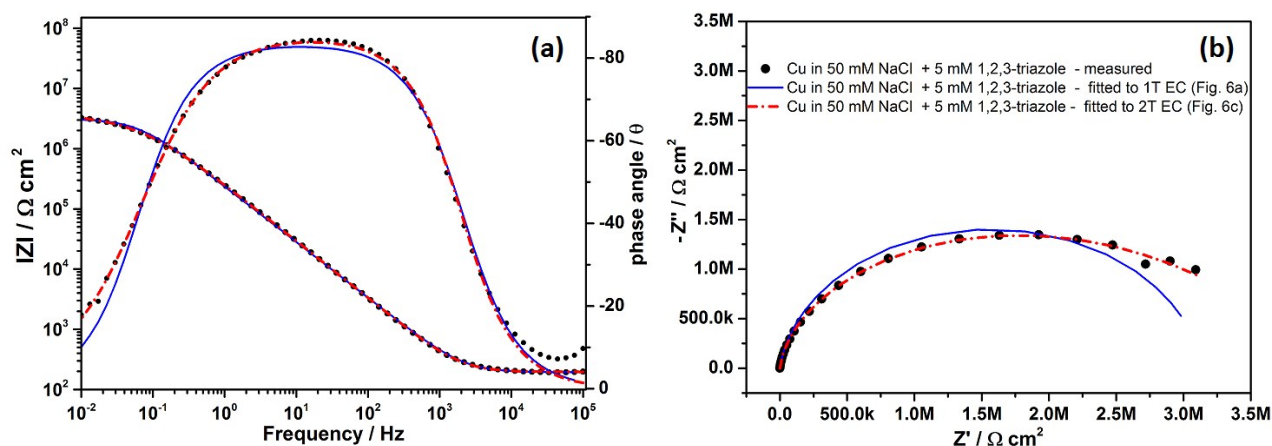


Figure S1: Measured and fitted spectra for copper to all the 3 equivalent circuits presented in Fig. 6. after 12 hours immersion in 50 mM NaCl.



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Figure S2: Measured and fitted spectra for copper after 12 hours immersion in 50 mM NaCl + 5 mM 1,2,3-triazole to the 1-time constant and 2-time constant equivalent circuits presented in Fig. 6a and Fig. 6c, respectively.

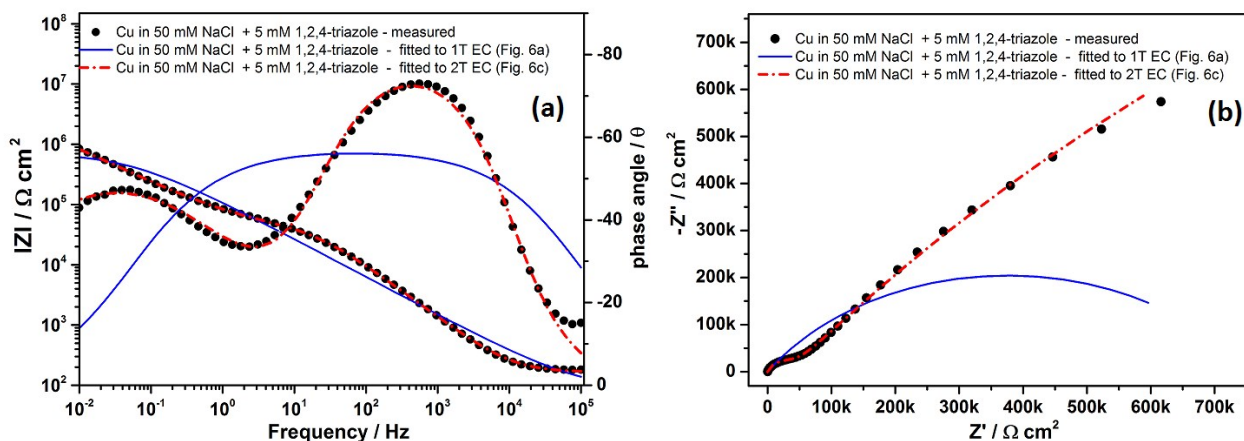


Figure S3: Measured and fitted spectra for copper after 12 hours immersion in 50 mM NaCl + 5 mM 1,2,4-triazole to the 1-time constant and 2-time constant equivalent circuits presented in Fig. 6a and Fig. 6c, respectively.

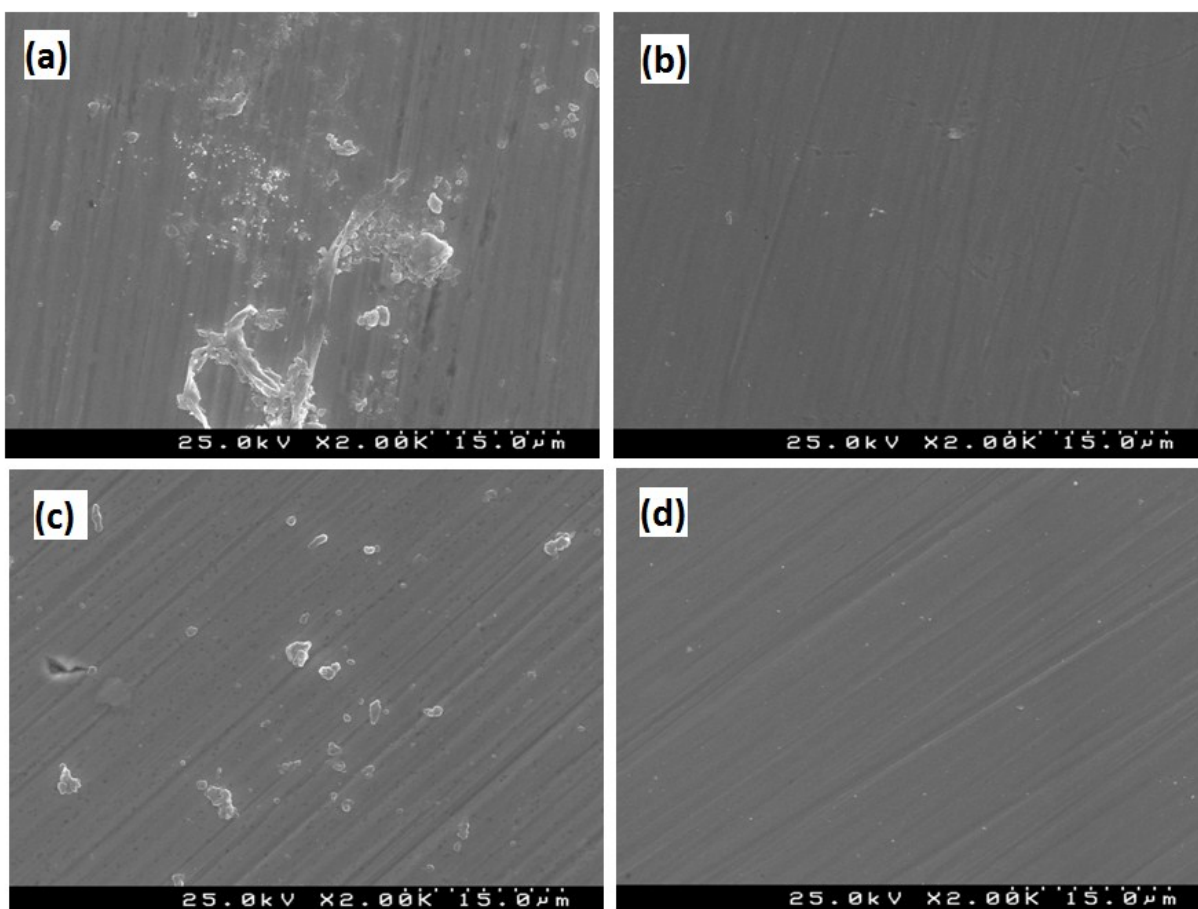


Figure S4: SEM images of copper surface after 12 hours immersion in (a) 50 mM NaCl only, (b) 50 mM NaCl + 5 mM 1,2,3-triazole, (c) 50 mM NaCl + 5 mM 1,2,4-triazole, and (d) 50 mM NaCl + 5 mM 1,2,4-triazole.

with 5 mM 1,2,3-triazole, (c) with 5 mM 1,2,4-triazole, and (d) with 5 mM of both 1,2,3-triazole and 1,2,4-triazole.

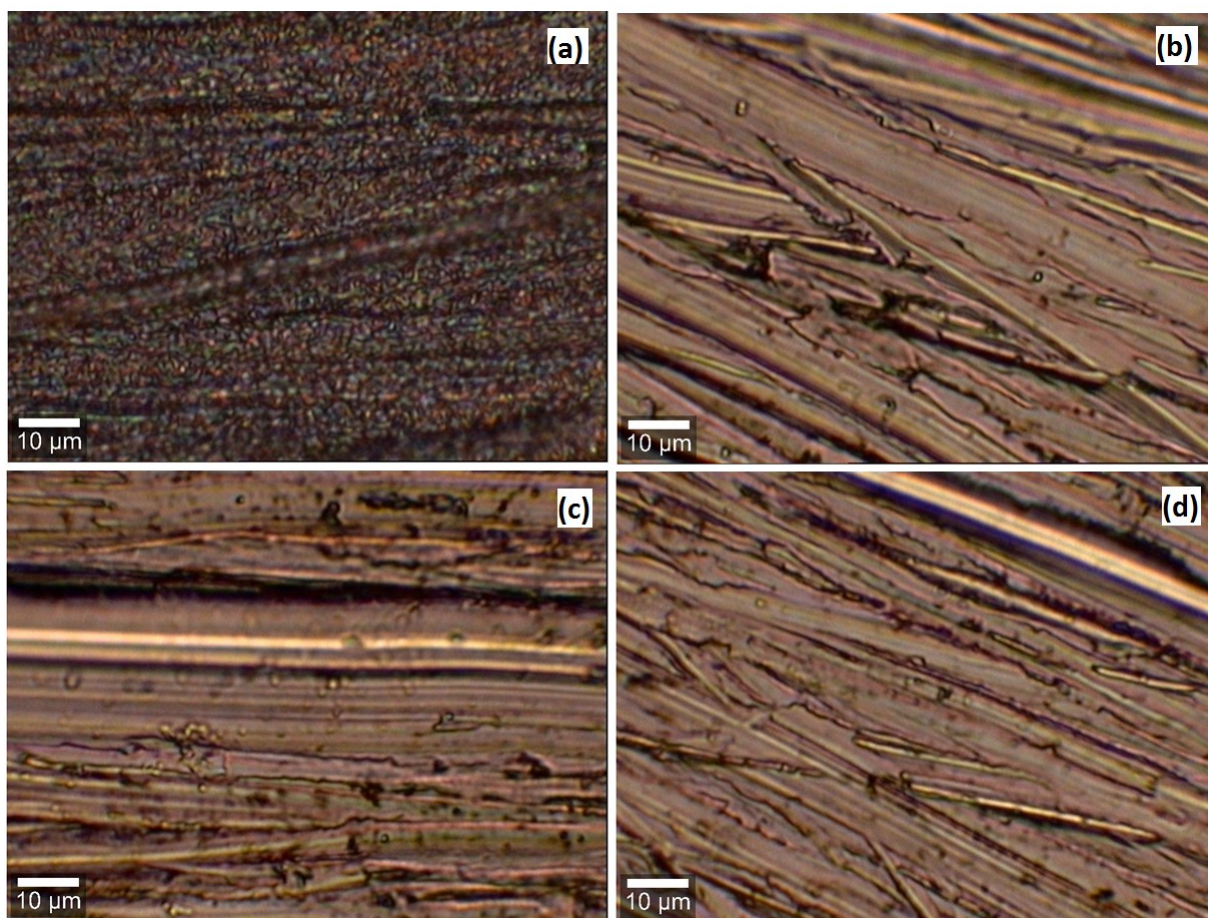


Figure S5: Images of copper surfaces obtained with the confocal microscope after 12 hours immersion in (a) 50 mM NaCl only, (b) with 5 mM 1,2,3-triazole, (c) with 5 mM 1,2,4-triazole, and (d) with 5 mM of both 1,2,3-triazole and 1,2,4-triazole.

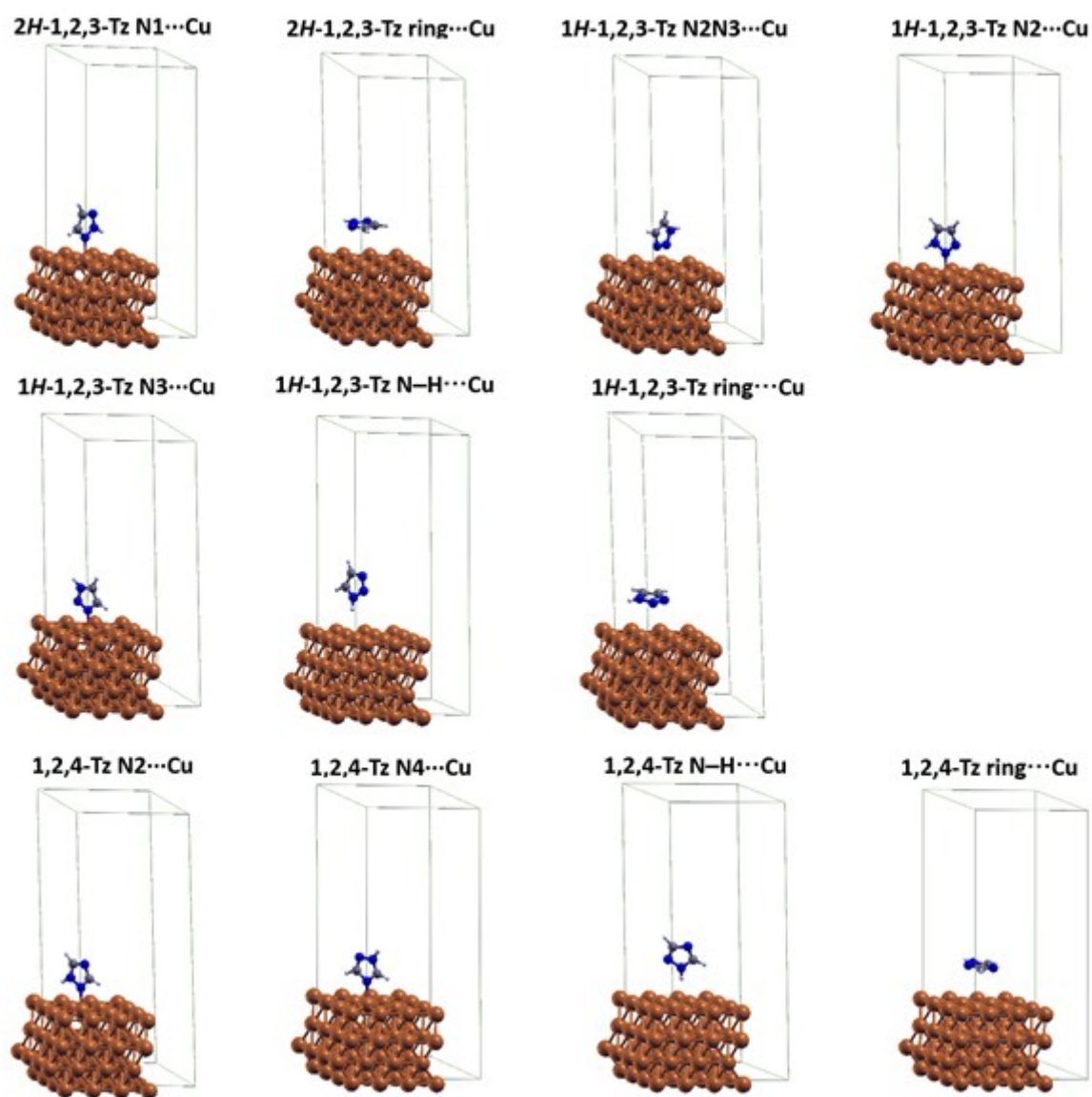


Figure S6: Representation of the periodic supercells and boundary conditions for the interaction between 1*H*-1,2,3-triazole (1*H*-1,2,3-Tz), 2*H*-1,2,3-triazole (2*H*-1,2,3-Tz) and 1,2,4-triazole (1,2,4-Tz) with a Cu(111) surface (spheres color code: C, grey; N, blue; H, white; Cu, brown).

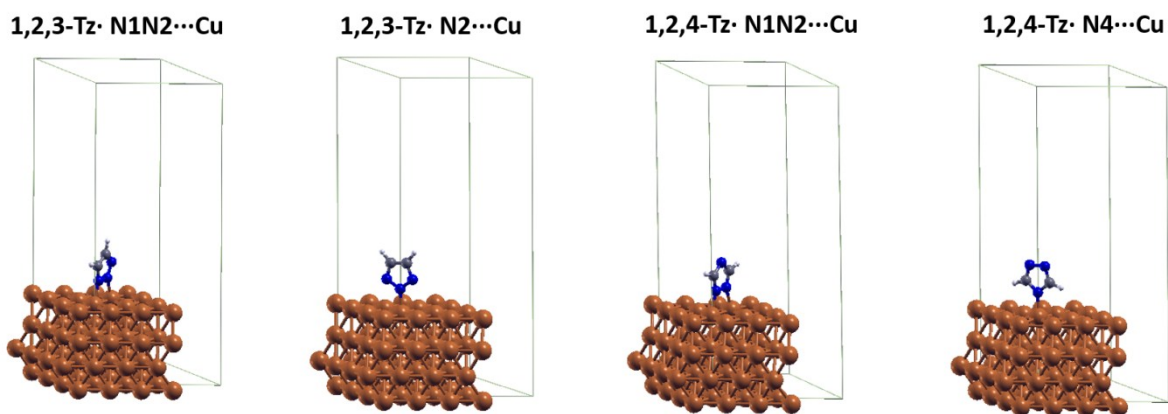


Figure S7: Representation of the periodic supercells and boundary conditions for the interaction between dehydrogenated 1,2,3-triazole (1,2,3-Tz) and 1,2,4-triazole (1,2,4-Tz) with a Cu(111) surface (spheres color code: C, grey; N, blue; H, white; Cu, brown).

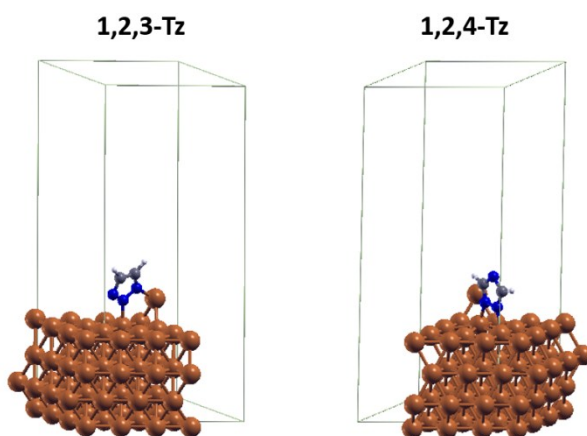


Figure S8: Representation of the periodic supercells and boundary conditions for the interaction between dehydrogenated 1,2,3-triazole (1,2,3-Tz) and 1,2,4-triazole (1,2,4-Tz) with a Cu(111) surface with a Cu adatom (spheres color code: C, grey; N, blue; H, white; Cu, brown).

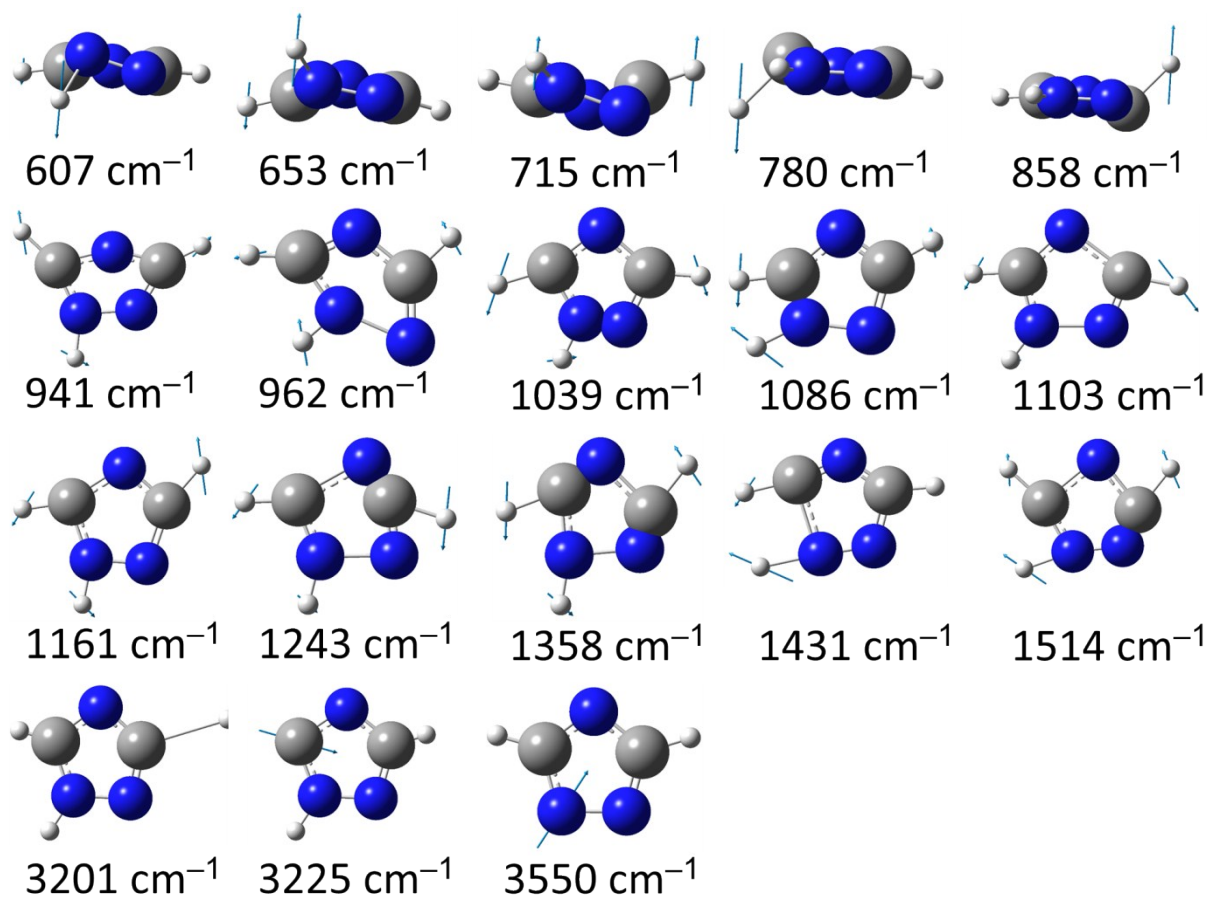


Figure S9: Raman vibrational frequencies of 1*H*-1,2,3-triazole.

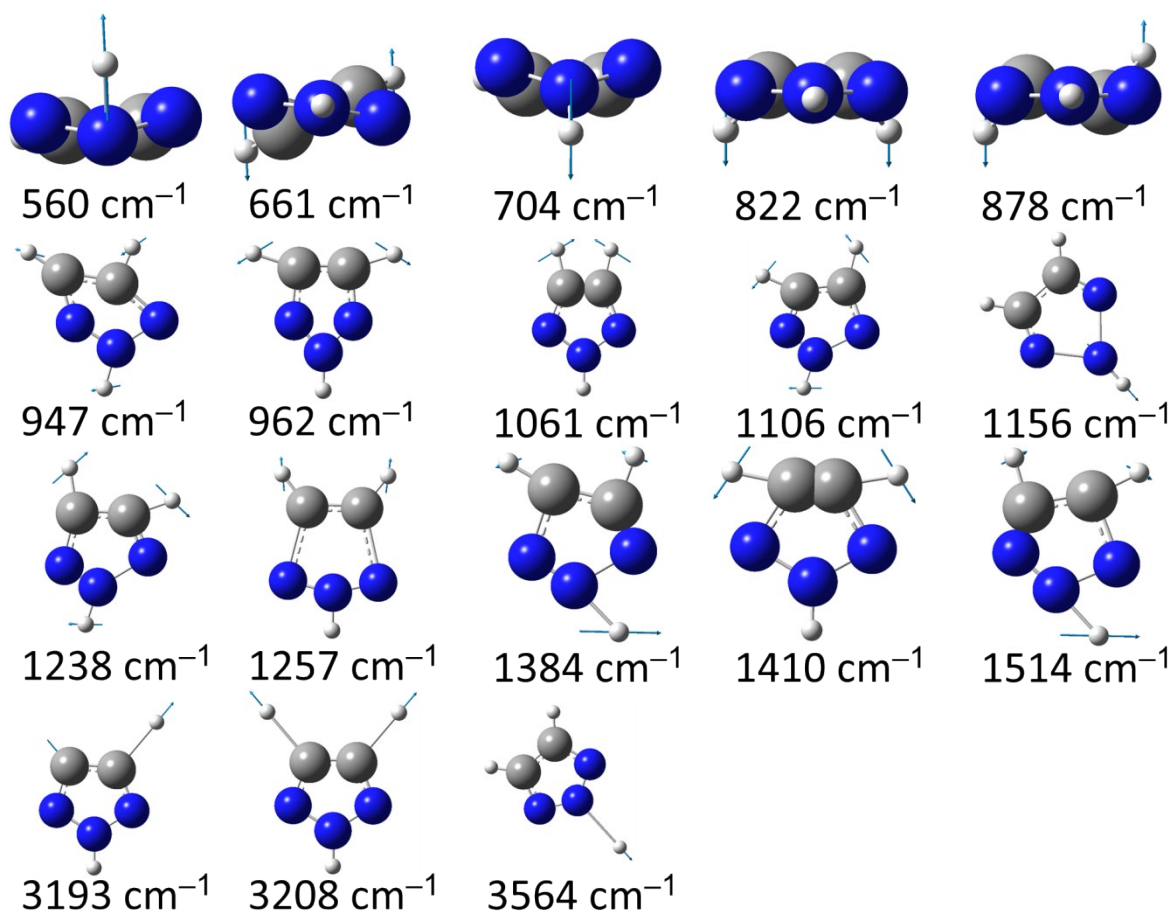


Figure S10: Raman vibrational frequencies of 2H-1,2,3-triazole.

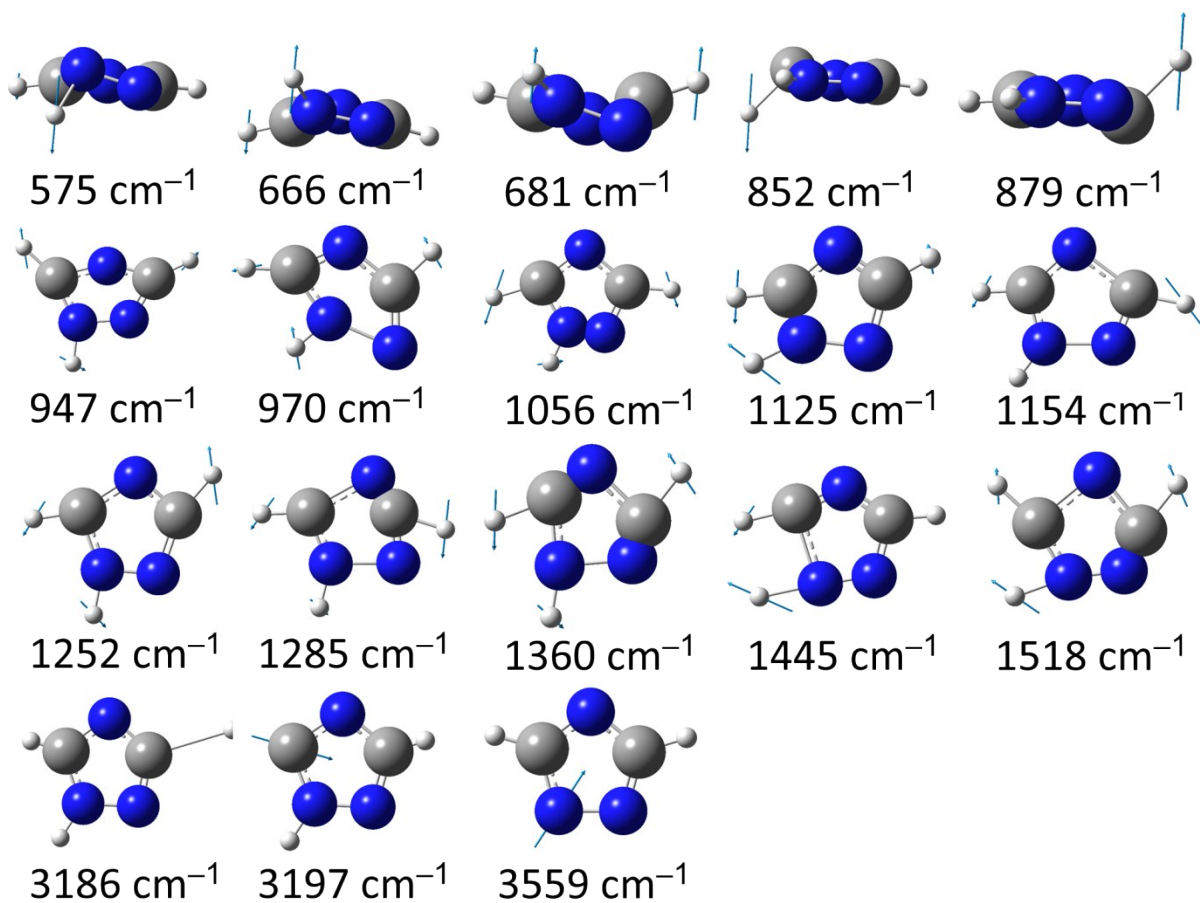


Figure S11: Raman vibrational frequencies of 1,2,4-triazole.

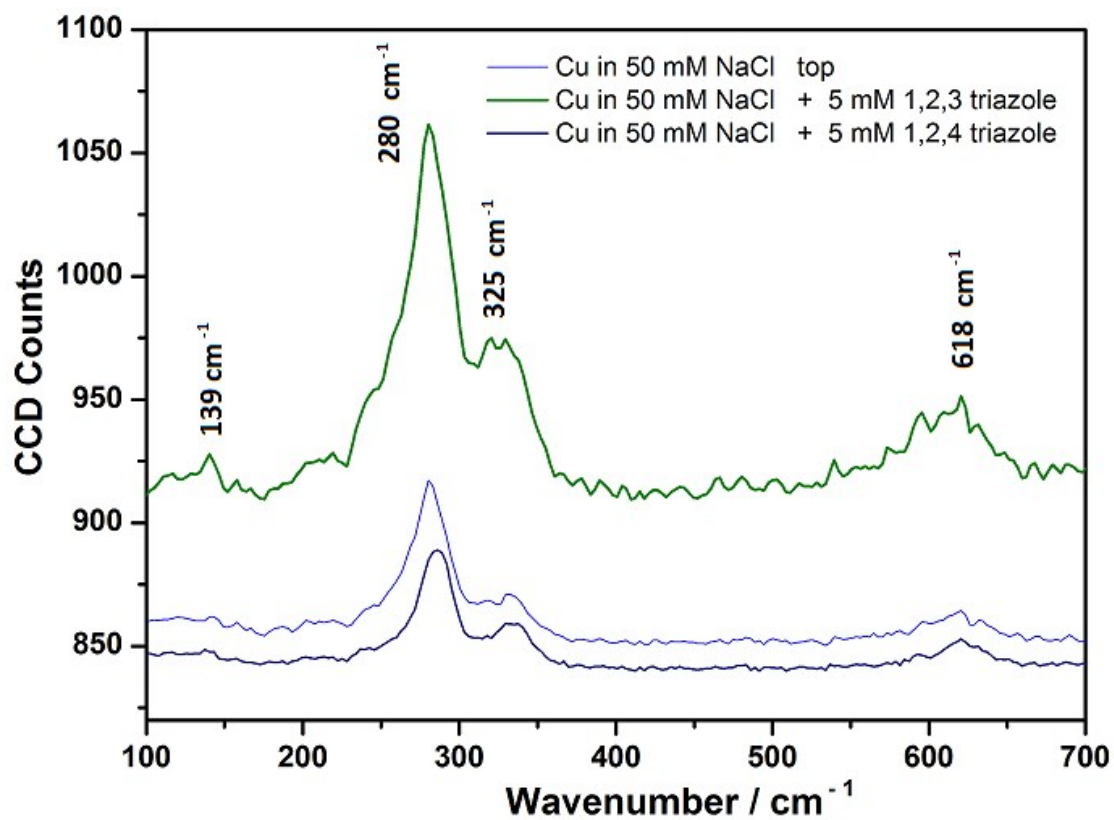


Figure S12: Segment of Raman spectra of Cu in 50 mM NaCl only, with 5 mM 1,2,3-triazole, and with 5 mM 1,2,4-triazole respectively.

Table S1 : Total electronic energy calculated at the vdw-DF level of theory.

Molecular system	E_{el} / Ry
Cu(111)	-13782.298427
2 <i>H</i> -1,2,3-Triazole	-127.2498346
1 <i>H</i> -1,2,3-Triazole	-127.2404923
1,2,4-Triazole	-127.2872886
2 <i>H</i> -1,2,3-Triazole N1...Cu(111)	-13909.595310
2 <i>H</i> -1,2,3-Triazole ring...Cu(111)	-13909.588838
1 <i>H</i> -1,2,3-Triazole N2N3...Cu(111)	-13909.580937
1 <i>H</i> -1,2,3-Triazole N2...Cu(111)	-13909.588220
1 <i>H</i> -1,2,3-Triazole N3...Cu(111)	-13909.590108
1 <i>H</i> -1,2,3-Triazole N-H... Cu(111).	-13909.562842
1 <i>H</i> -1,2,3-Triazole ring...Cu(111)	-13909.582592
1,2,4-Triazole N2...Cu(111)	-13909.637159
1,2,4-Triazole N4...Cu(111)	-13909.641242
1,2,4-Triazole N-H...Cu(111)	-13909.609958
1,2,4-Triazole ring...Cu(111)	-13909.627214
1,2,3-Triazole dehydrogenated	-125.8384322
1,2,4-Triazole dehydrogenated	-125.8872295
1,2,3-Triazole dehydrogenated N1N2...Cu(111)	-13908.365127
1,2,3-Triazole dehydrogenated N2...Cu(111)	-13908.336125
1,2,4-Triazole dehydrogenated N1N2...Cu(111)	-13908.408767
1,2,4-Triazole dehydrogenated N4...Cu(111)	-13908.331215
H...Cu(111)	-13783.532748
Cu(111)·Cu(adatom)	-13997.511080
1,2,3-Triazole dehydrogenated...Cu(111)·Cu(adatom)	-14123.721862
1,2,4-Triazole dehydrogenated...Cu(111)·Cu(adatom)	-14123.732762

1 Ry = 1312.7496997450642 kJ·mol⁻¹