**Supplementary data**

# A silicon-containing polyazomethine and derived metal complexes: synthesis, characterization and evaluation of the properties

Mirela-Fernanda Zaltariov, Maria Cazacu, Sergiu Shova, Cristian Varganici, Loredana Vacareanu, Valentina Musteata, Anton Airinei

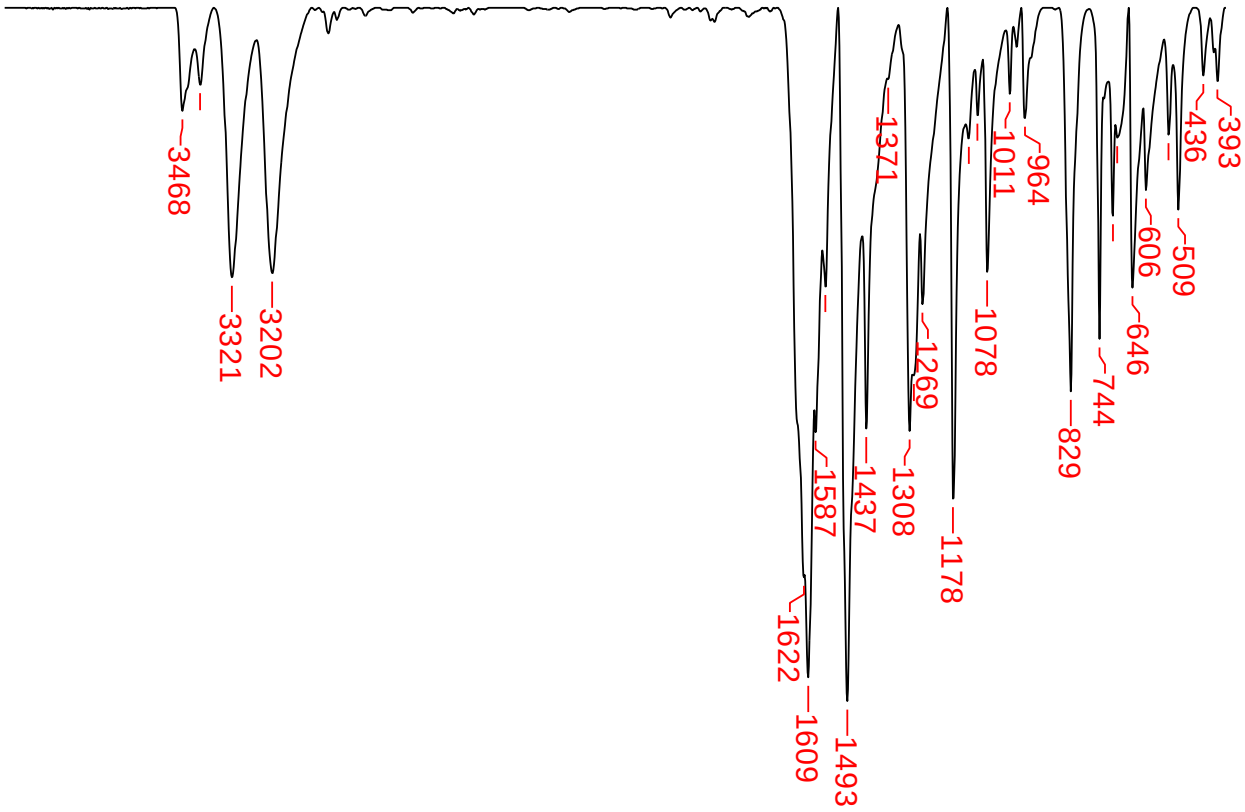


**Figure 1S.** FTIR spectrum of 2,5-bis(*p*-aminophenyl)-1,3,4-oxadiazole.

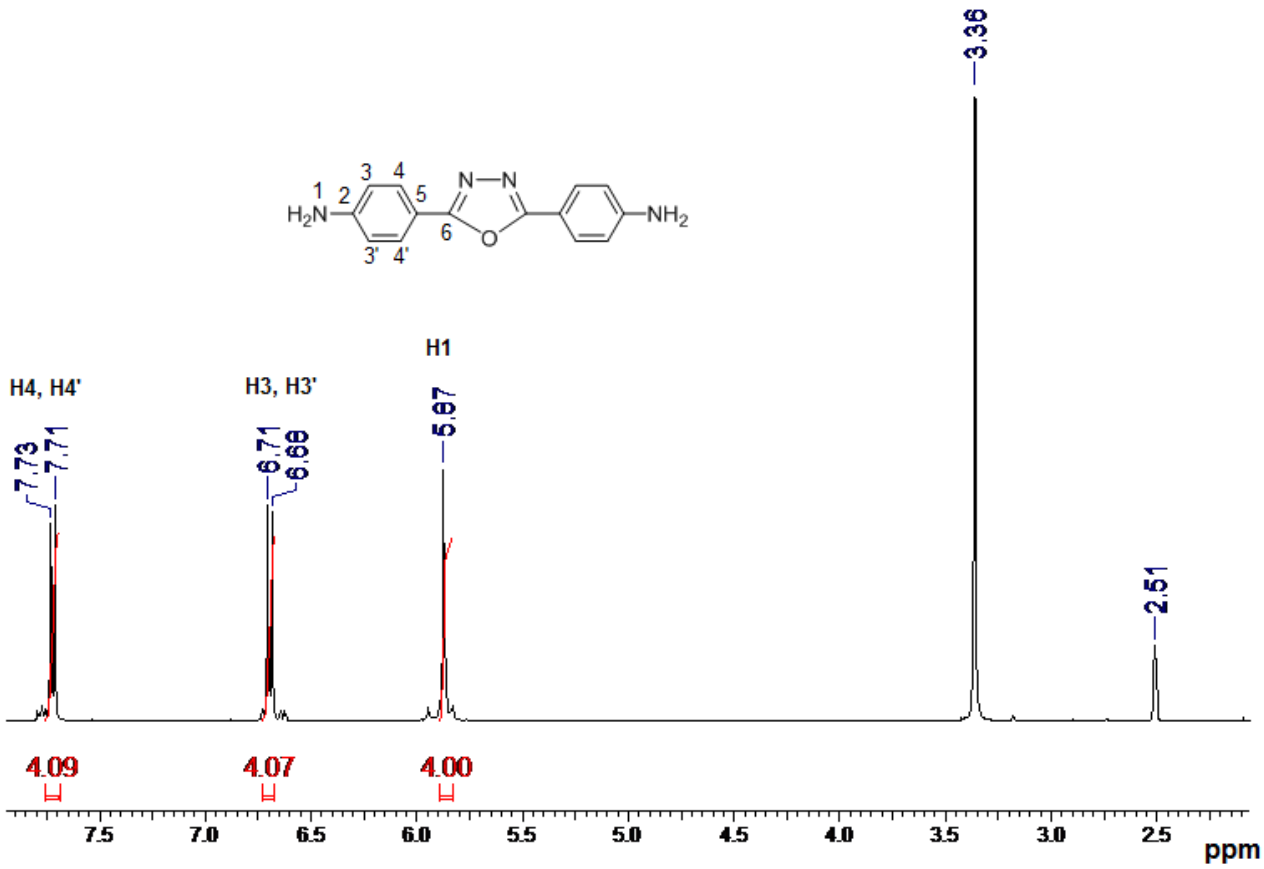


**Figure 2S.** $^{1}$H NMR Spectrum for 2,5-bis(*p*-aminophenyl)-1,3,4-oxadiazole.

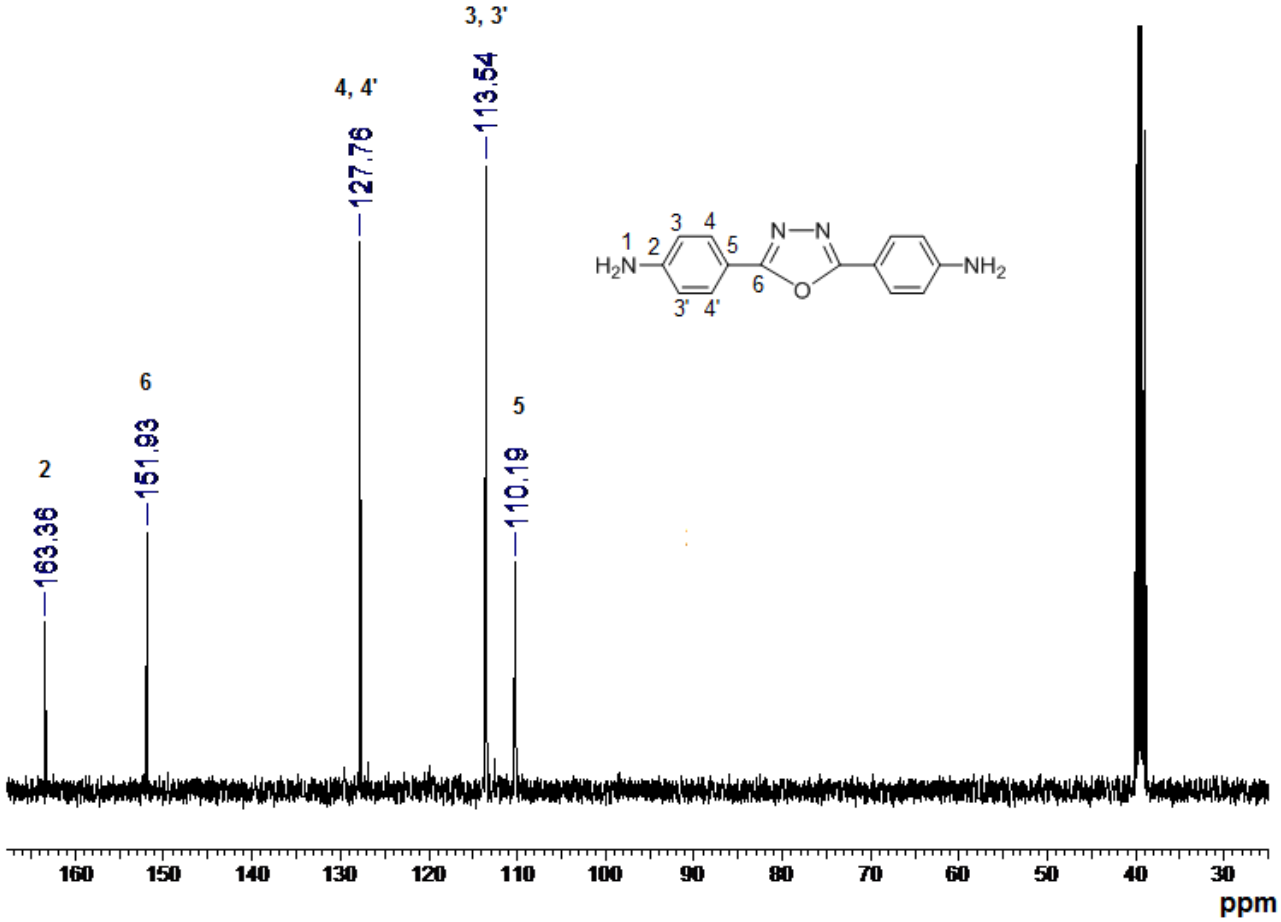


**Figure 3S.** $^{13}$C NMR Spectrum for 2,5-bis(*p*-aminophenyl)-1,3,4-oxadiazole.

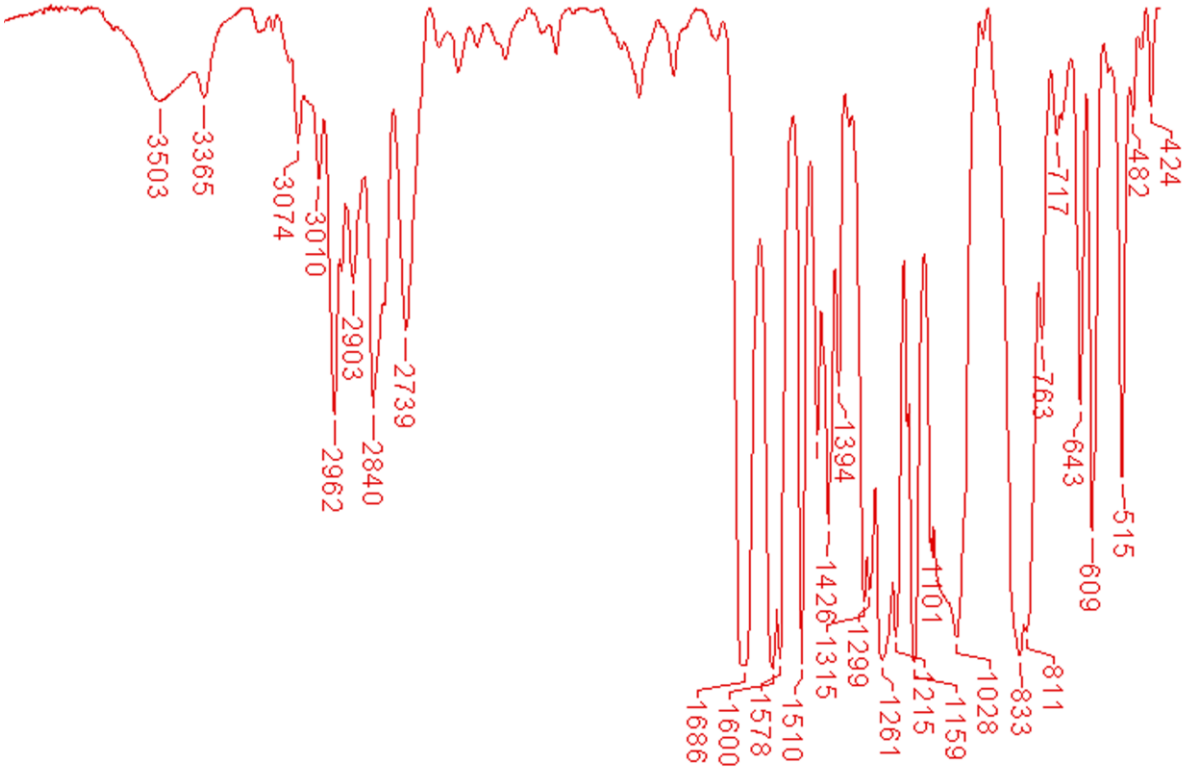


**Figure 4S.** FT-IR Spectrum for bis(formyl-*p*-phenoxymethyl)-dimethylsilane, DA.

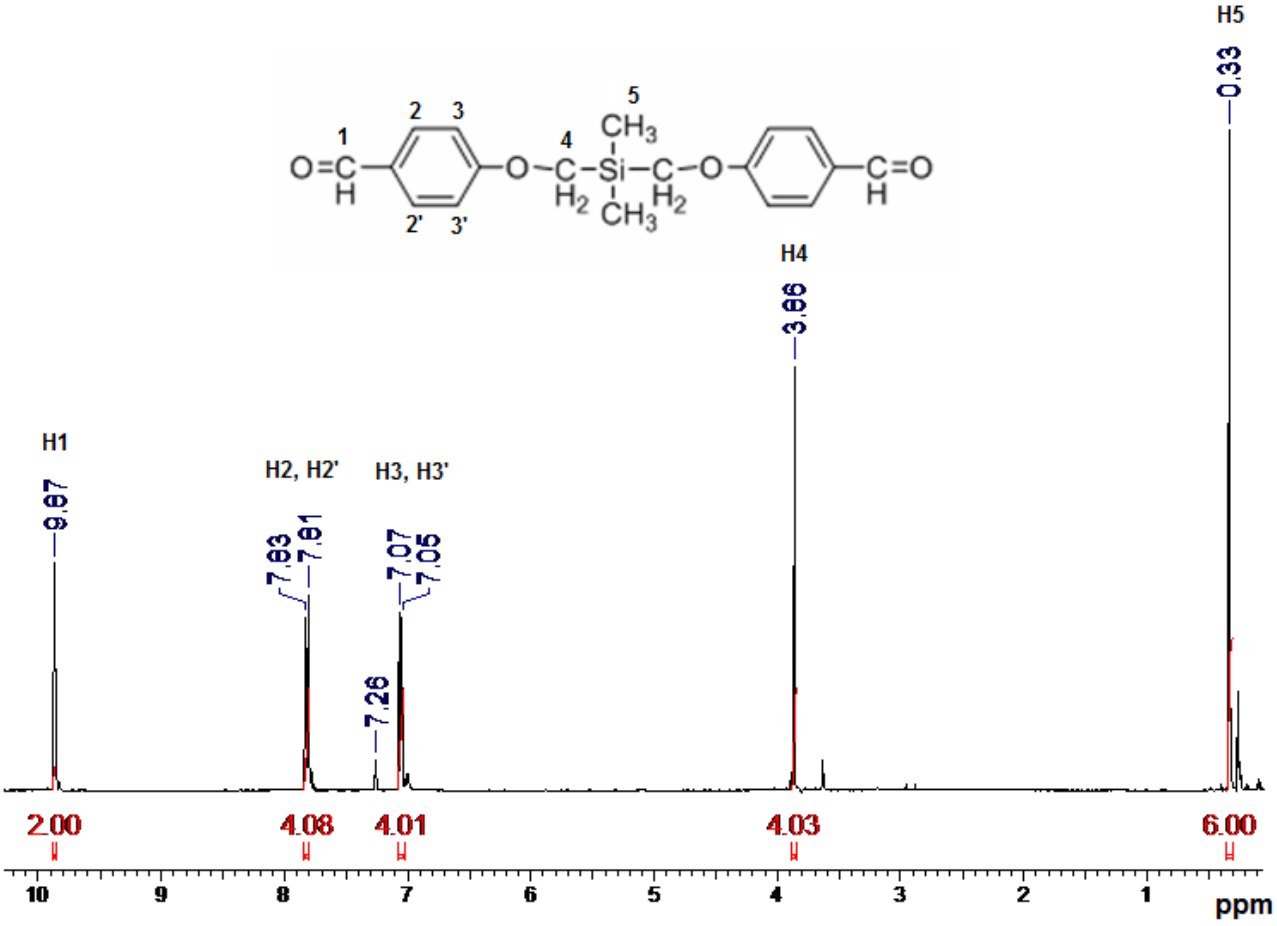


**Figure 5S.** $^{1}$H NMR Spectrum for bis(formyl-*p*-phenoxymethyl)-dimethylsilane, DA.

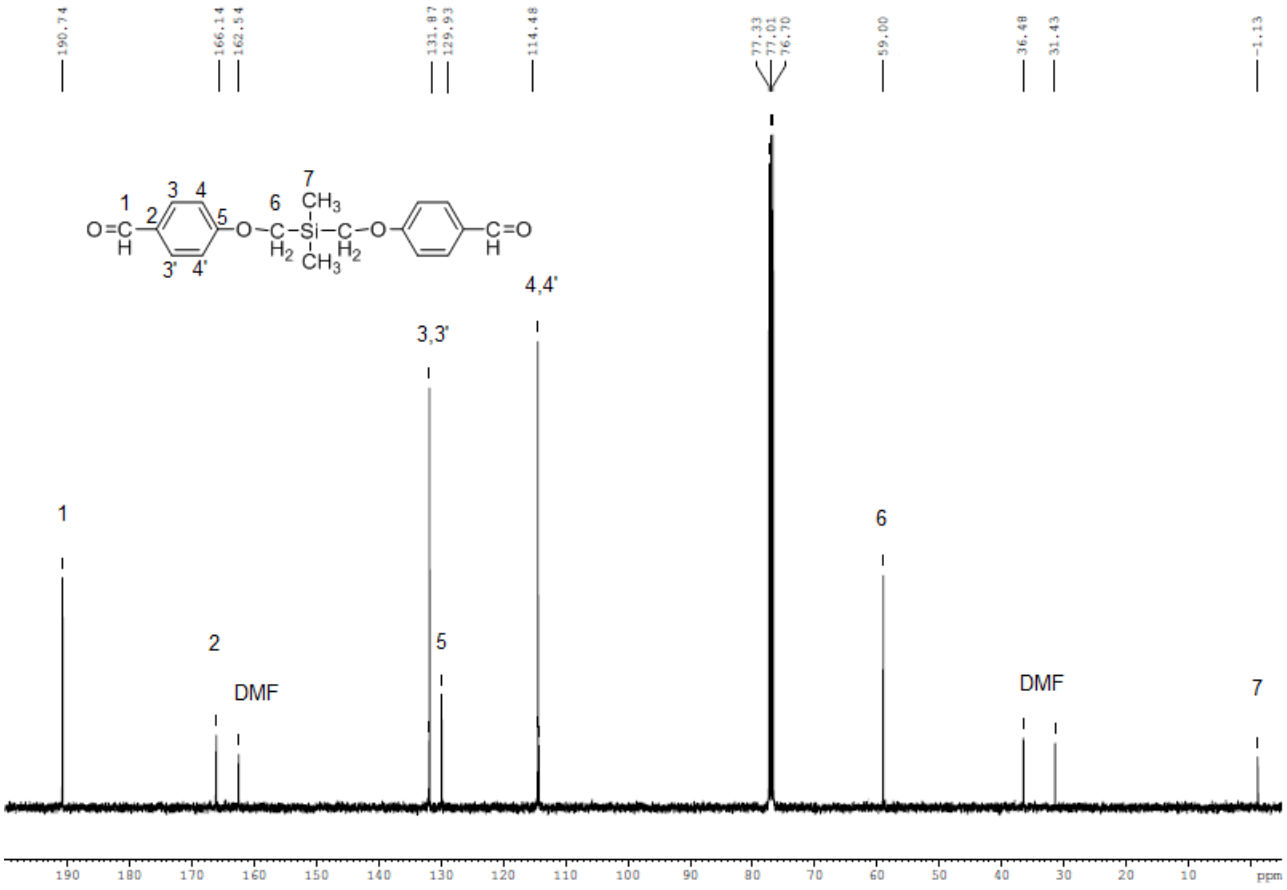


**Fig. 6S** $^{13}$C NMR Spectrum for bis(formyl-*p*-phenoxymethyl)-dimethylsilane, DA

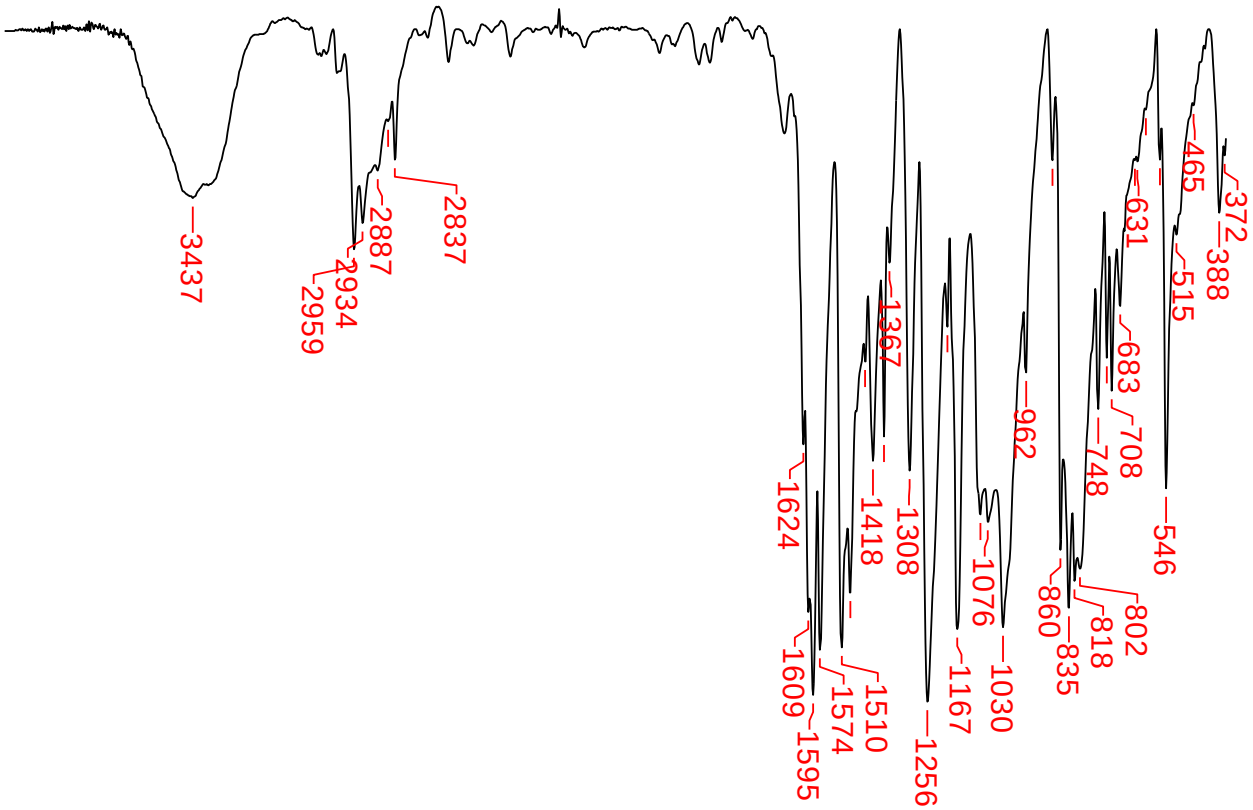


**Figure 7S.** FTIR spectrum of polyazomethine PAZ.

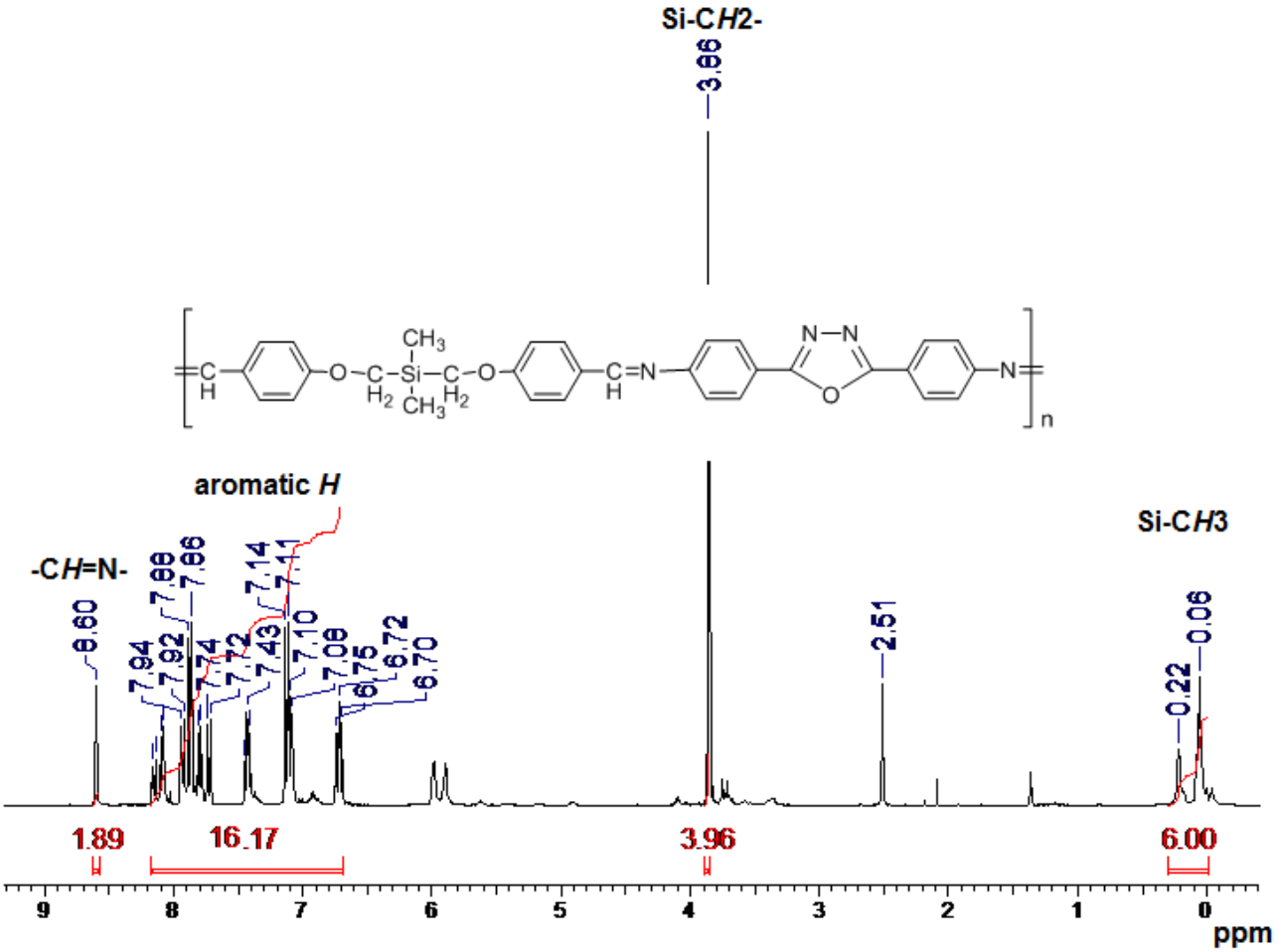


**Figure 8S.** [1]HNMR spectrum for polyazomethine PAZ.

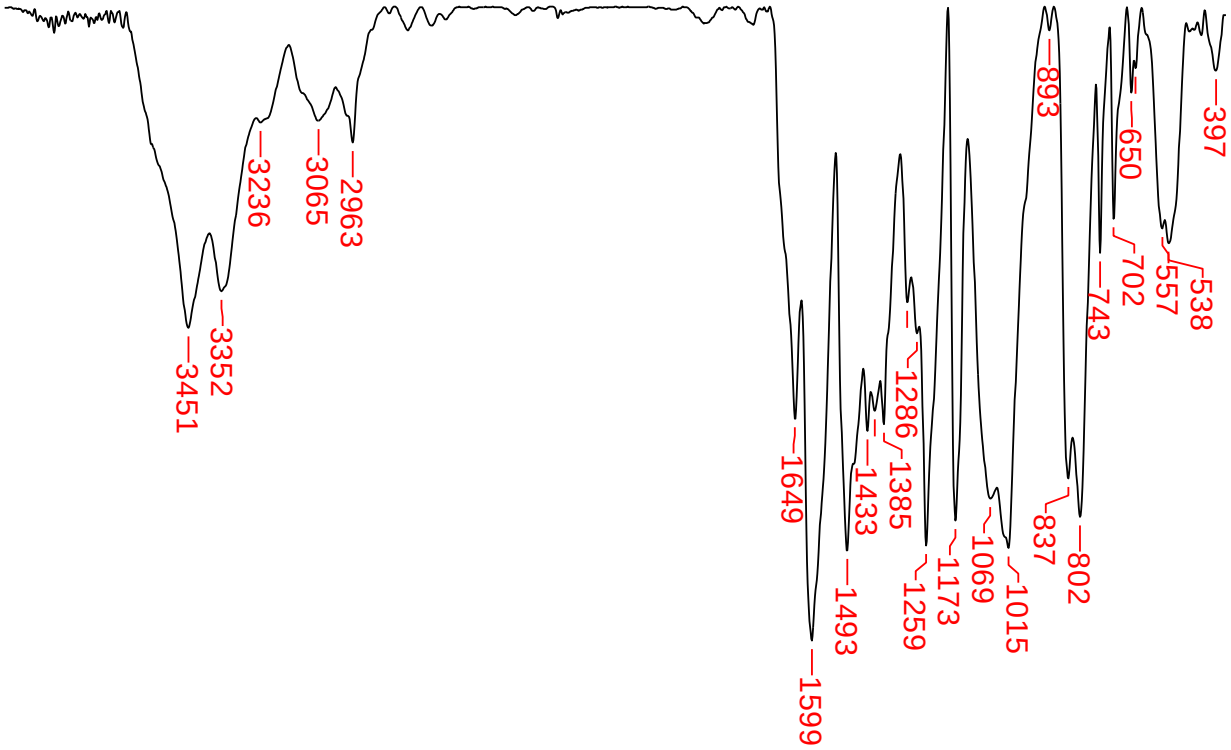


**Figure 9S.** FTIR spectrum of Cu complex, PAZ-Cu.

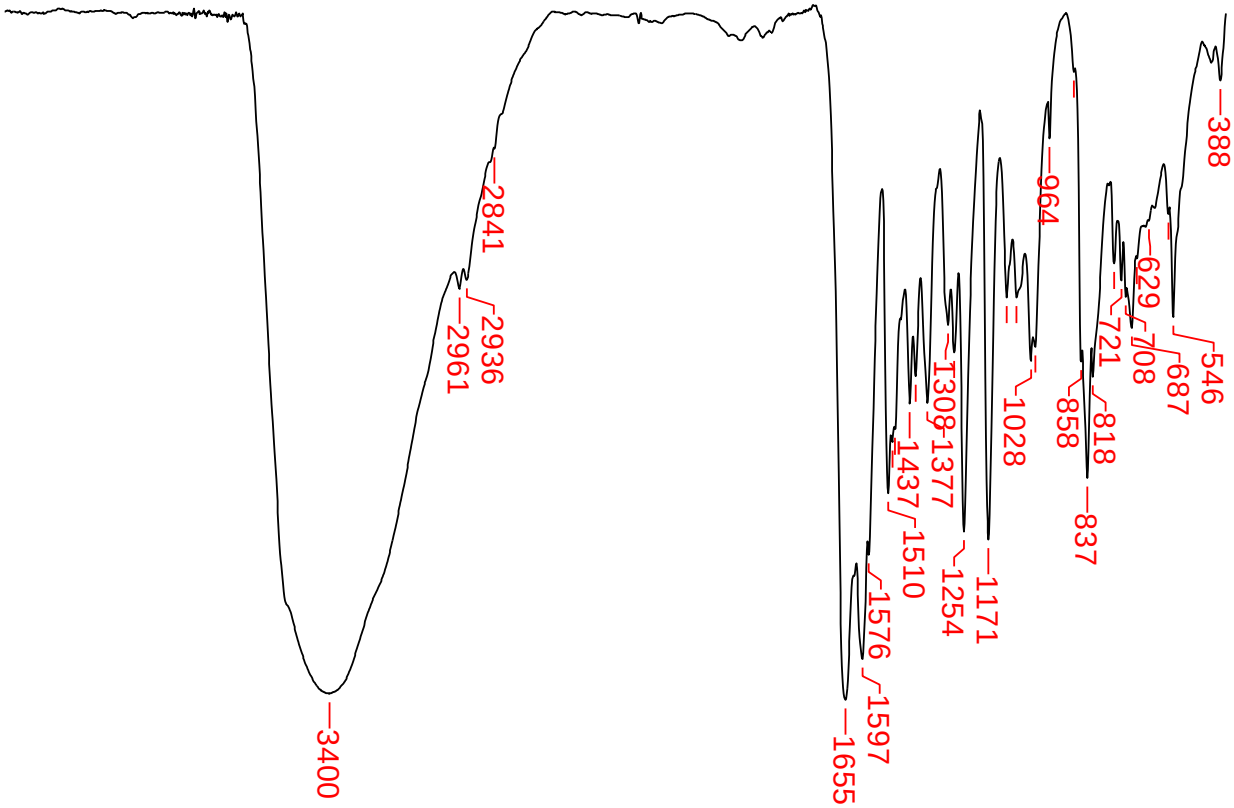


**Figure 10S.** FTIR spectrum of Co complex, PAZ-Co.

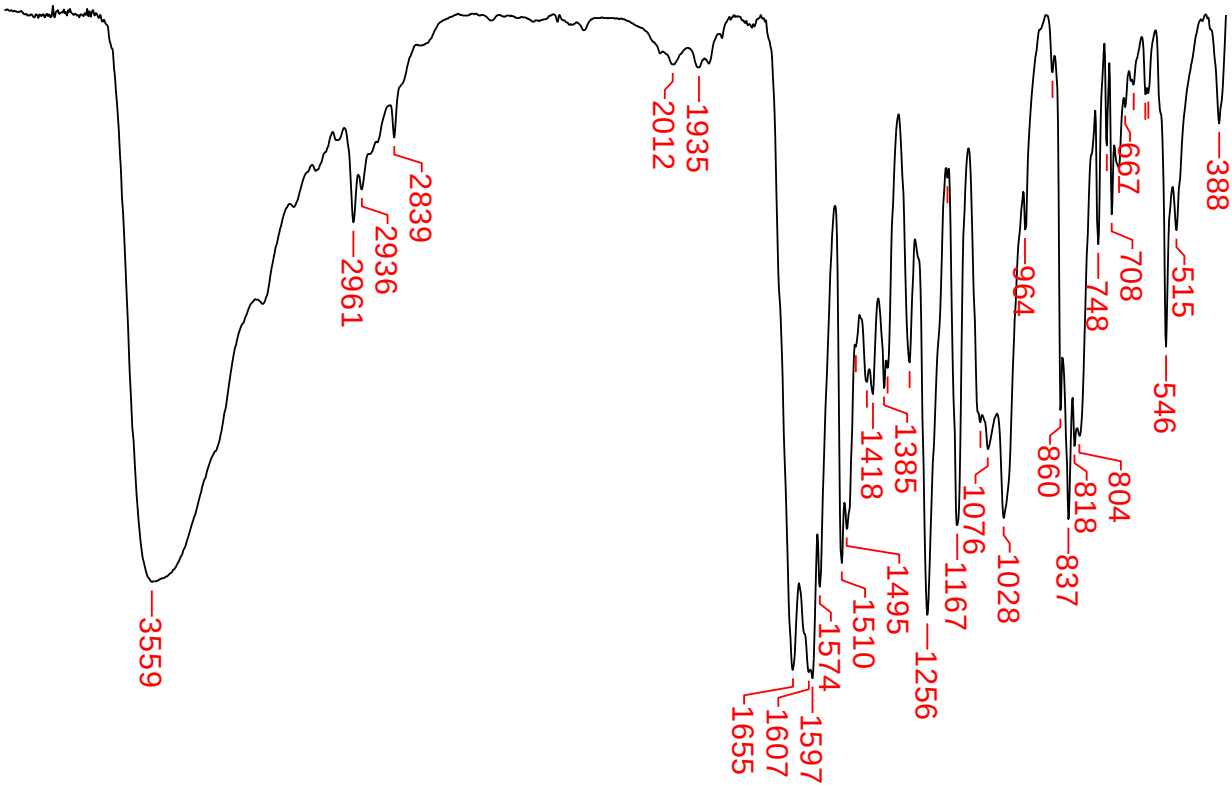


**Figure 11S.** FTIR spectrum of Zn complex, PAZ-Zn.

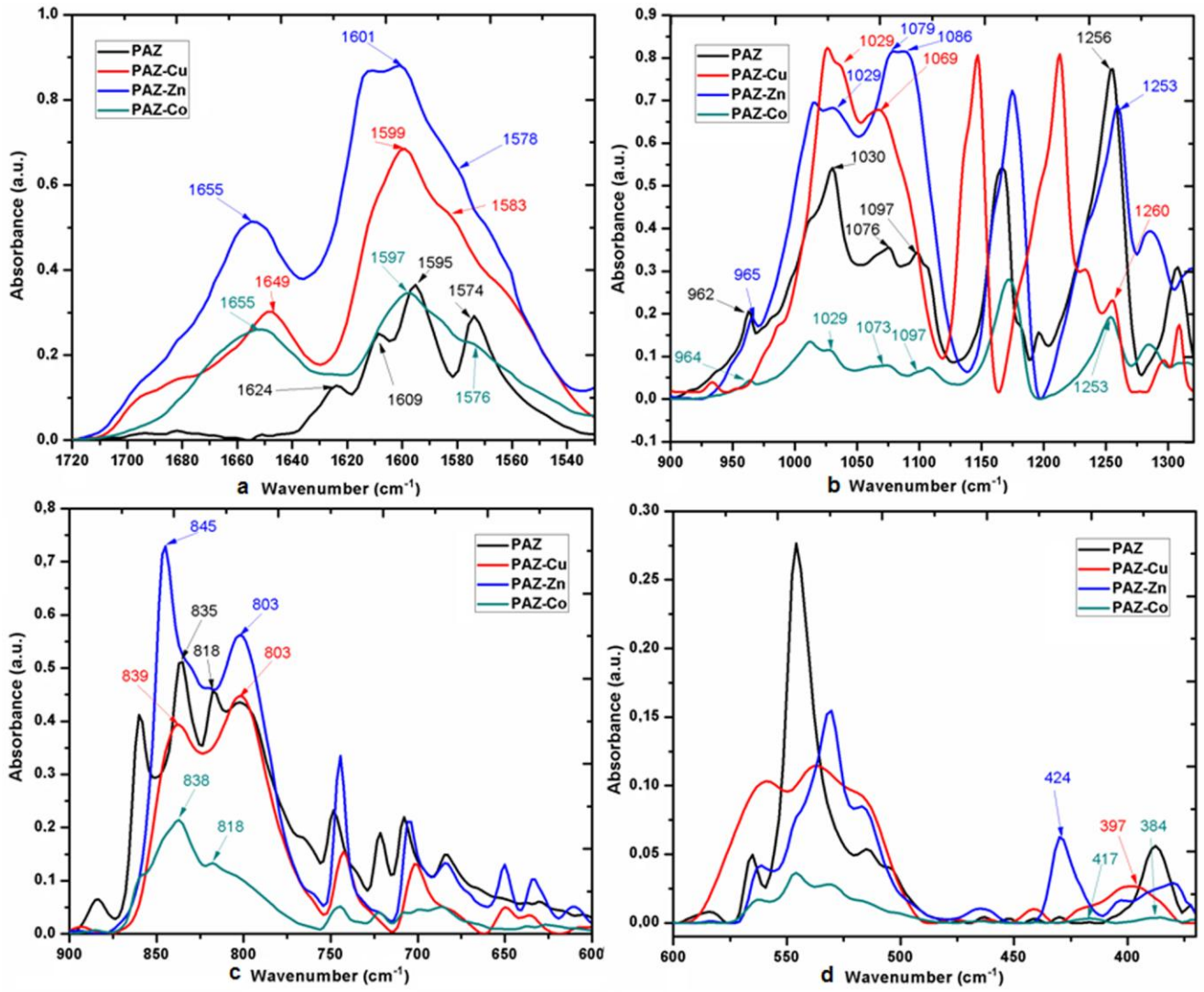


Figure 12S. Comparative IR spectra details for polyazomethine and metal complexes

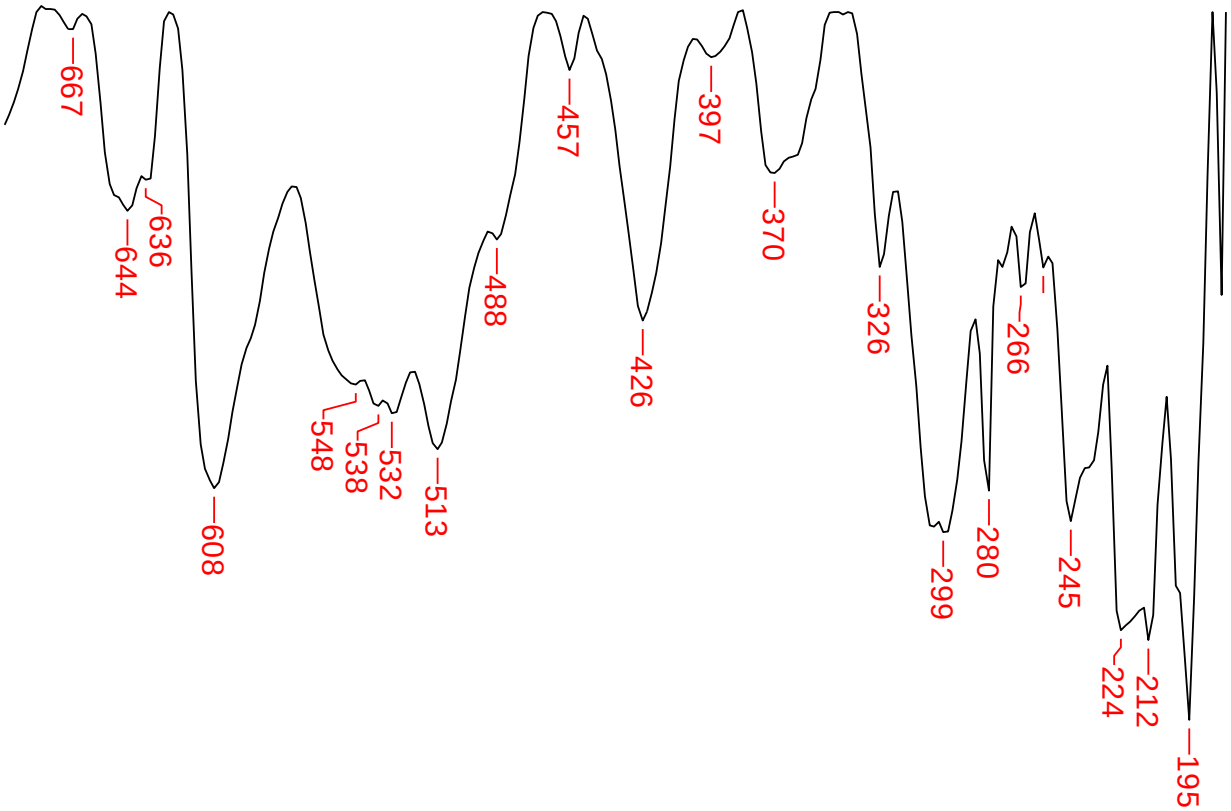


**Figure 13S.** Far-IR spectrum of Cu complex, PAZ-Cu.

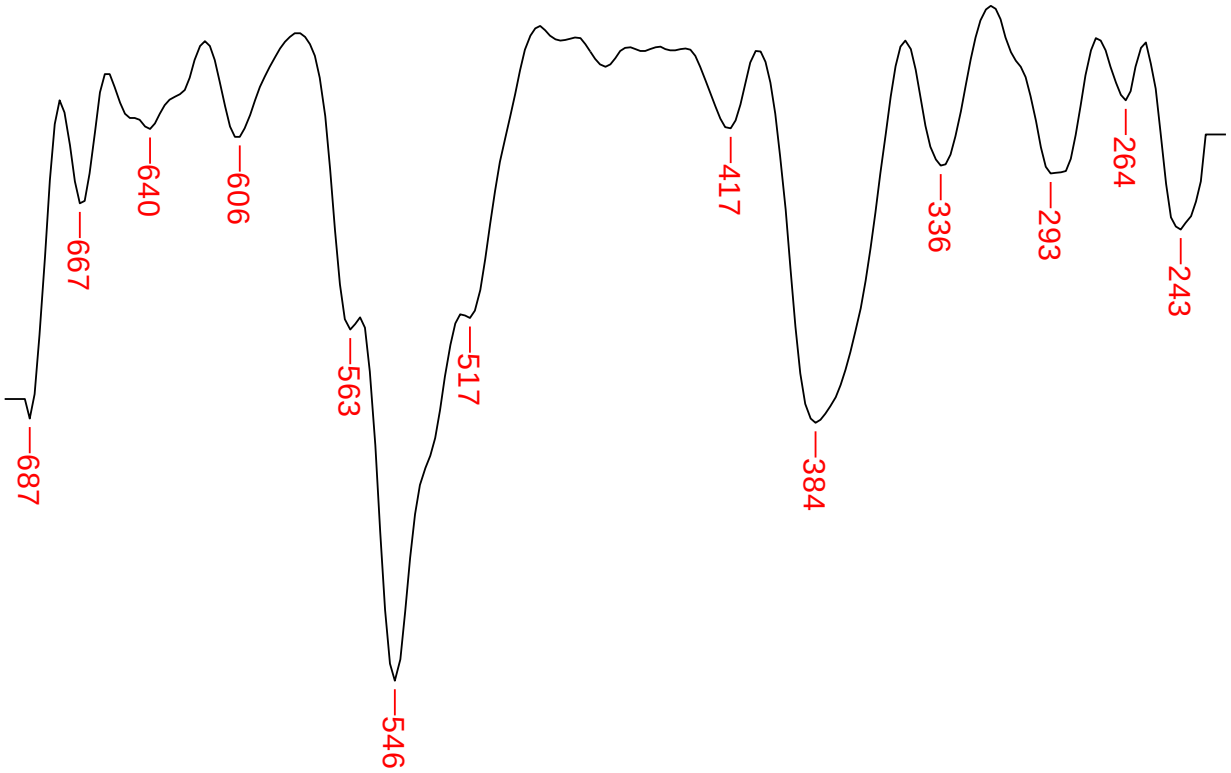


**Figure 14S.** Far-IR spectrum of Co complex, PAZ-Co.

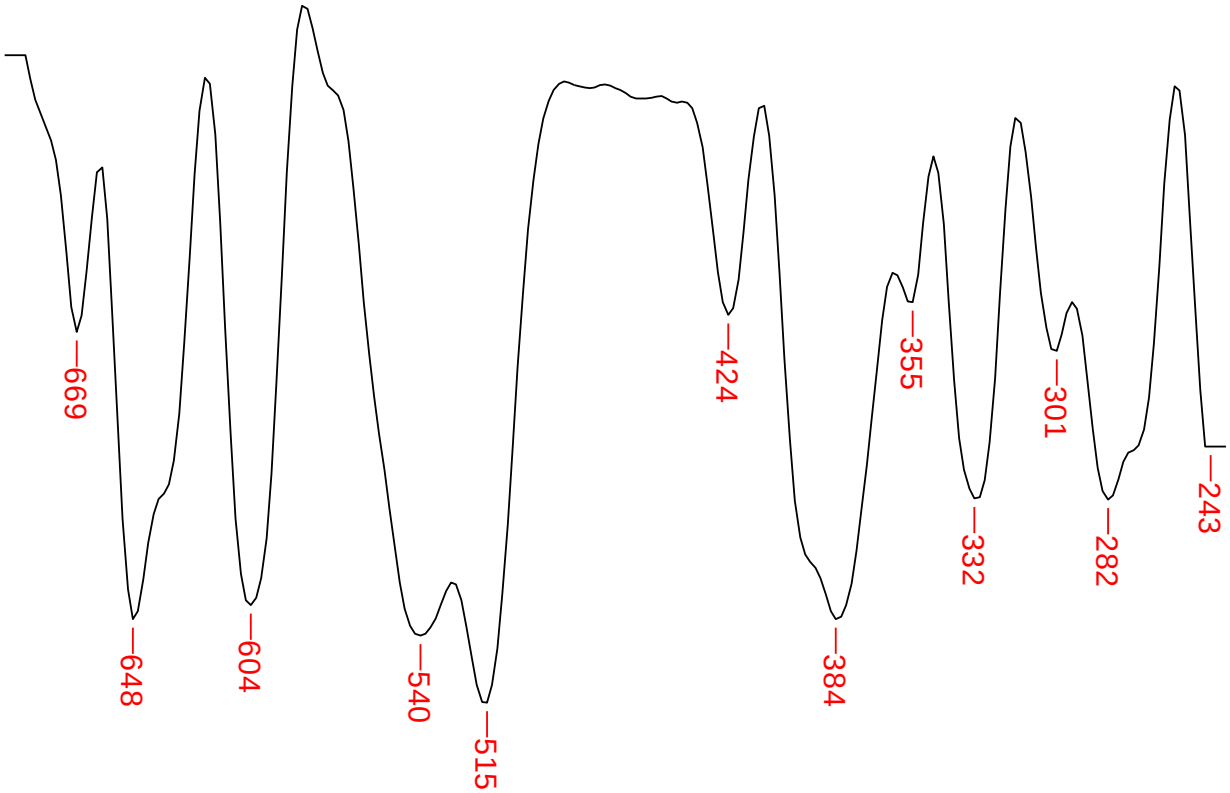


**Figure 15S.** Far-IR spectrum of Zn complex, PAZ-Zn.

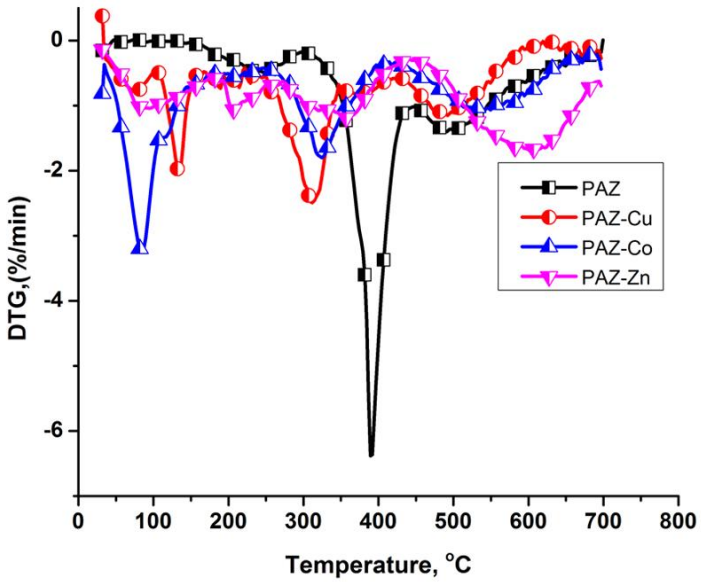


**Figure 16S.** DTG curves of the polyazomethine-based structures

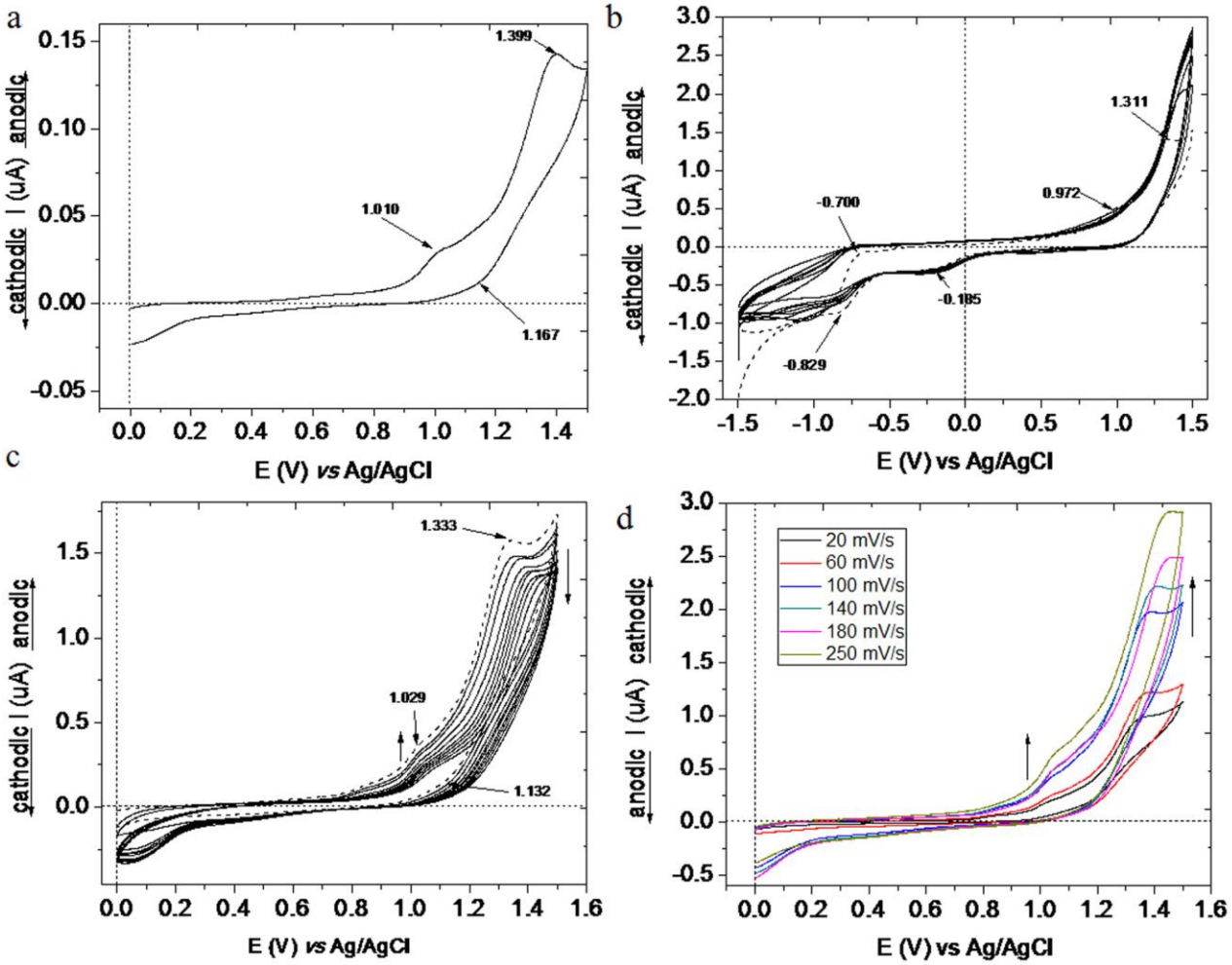


**Figure 17S.** PAZ-Co: (a) cyclic voltammogram recorded during the potential electrode scanning from 0.0 V to 1.5 V range with 50 mV/s; (b) cyclic voltammogram recorded during the electrode potential scanning from +1.5 V to -1.5 V range with 50 mV/s; (c) the multi cyclic voltammograms (10 cycles) recorded for PAZ-Co on the positive range of potential; (d) cyclic voltammograms of PAZ-Co recorded at different scan rates (from 20 to 250 mV/s).

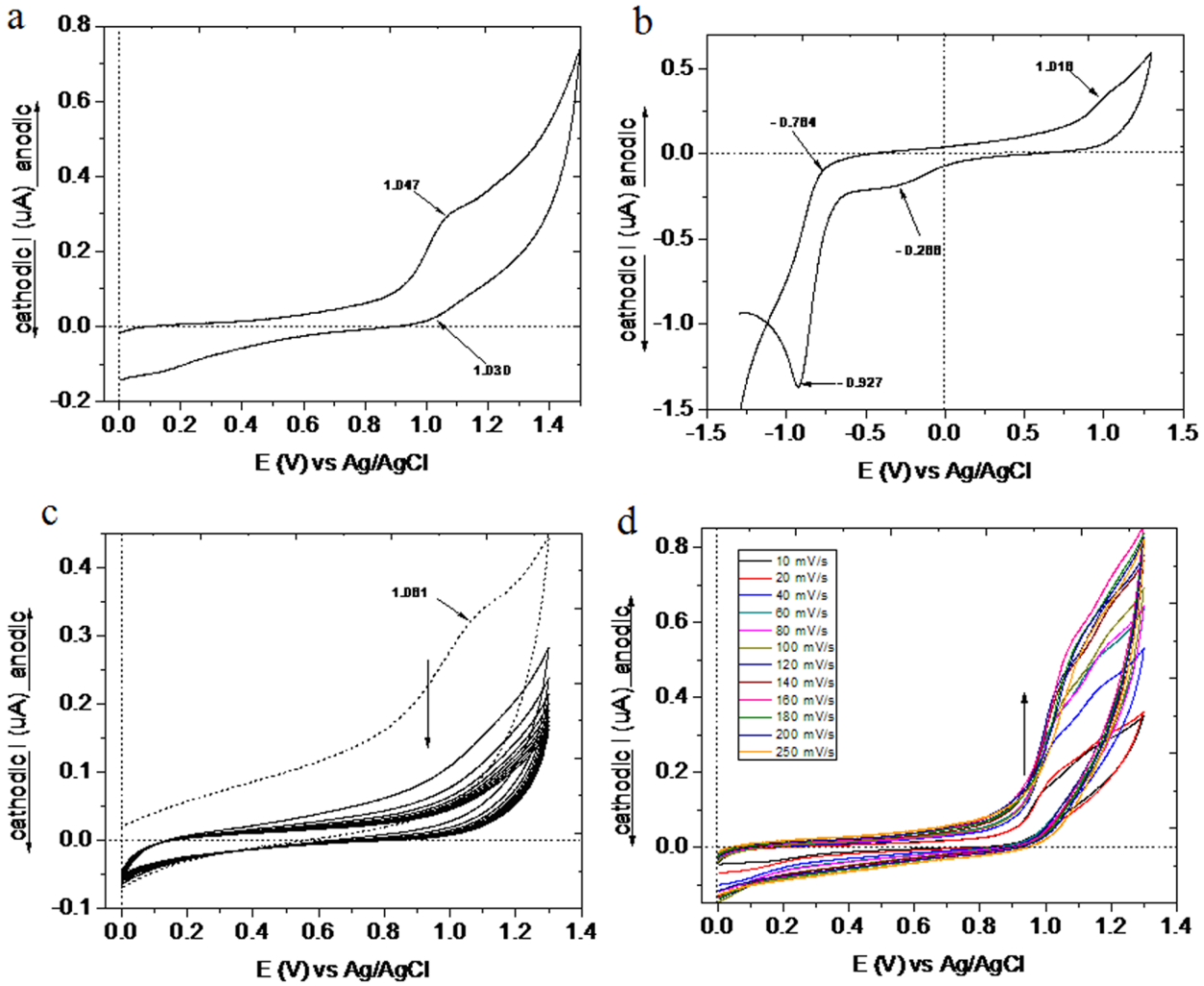


**Figure 18S.** PAZ-Zn: (a) cyclic voltammogram recorded during the potential electrode scanning from 0.0 V to 1.4 V range with 50 mV/s; (b) cyclic voltammogram recorded during the electrode potential scanning from +1.4 V to -1.4 V range with 50 mV/s; (c) the multi cyclic voltammograms (10 cycles) recorded for PAZ-Zn on the positive range of potential; (d) cyclic voltammograms of PAZ-Zn recorded at different scan rates (from 20 to 250 mV/s).

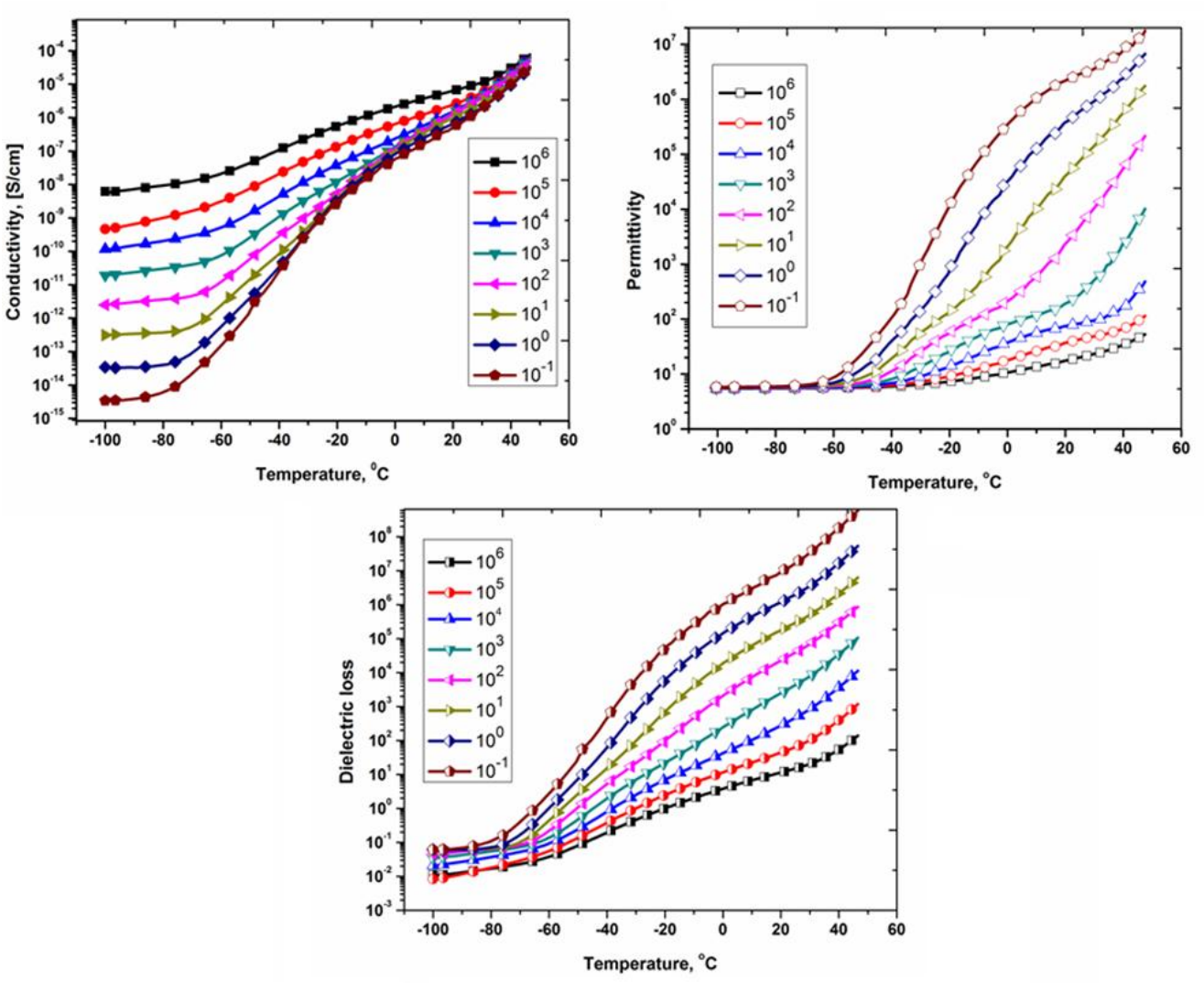


**Figure 19S.** Temperature dependence of the ac conductivity $\sigma_{ac}$, dielectric permittivity ε` and dielectric loss ε`` of **PAZ-Co** at different frequencies (in Hz).

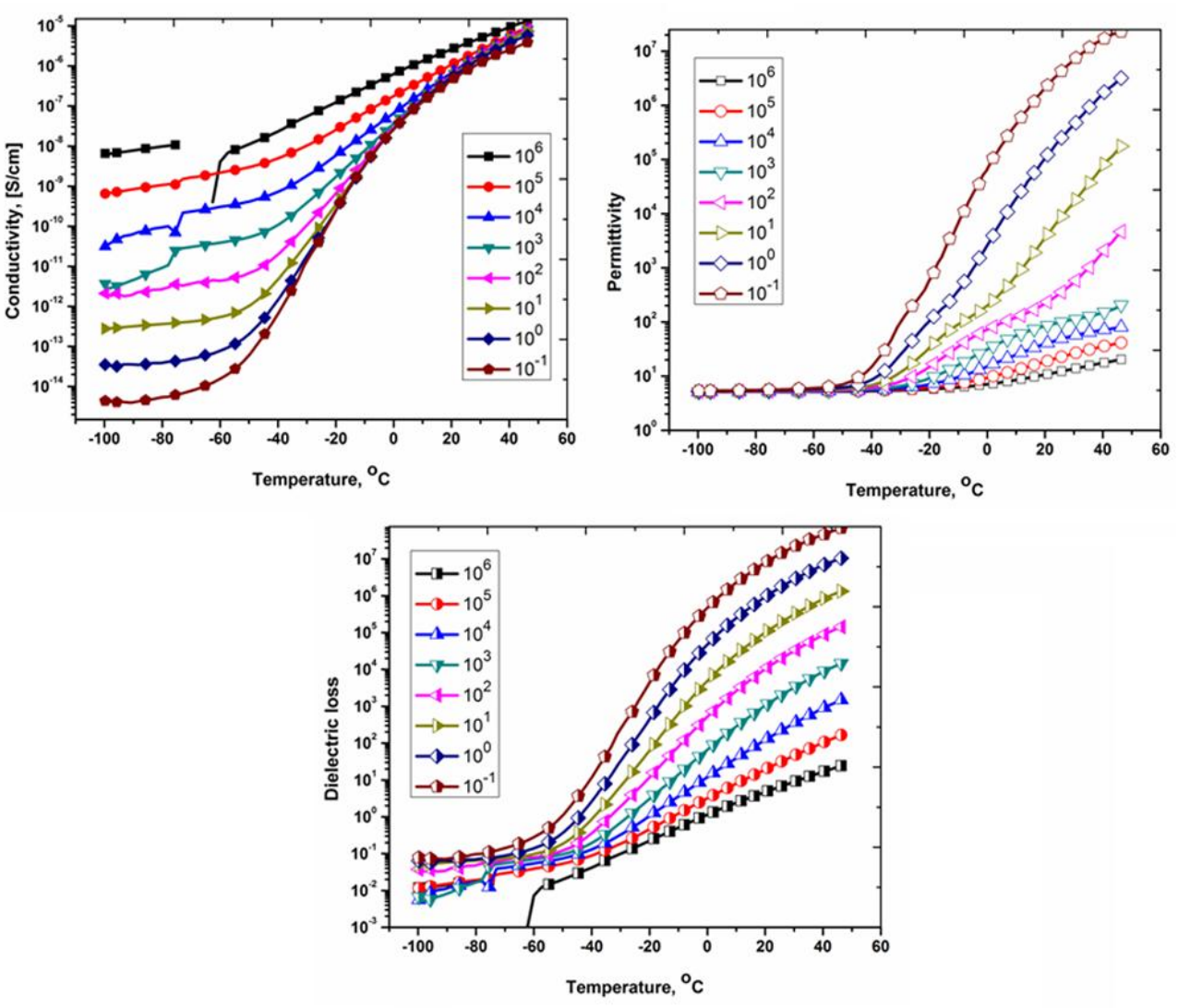


**Figure 20S.** Temperature dependence of the ac conductivity $\sigma_{ac}$, dielectric permittivity ε` and dielectric loss ε`` of **PAZ-Zn** at different frequencies (in Hz).

# checkCIF/PLATON report

**No syntax errors found.** **CIF dictionary** **Interpreting this report**

## Datablock: shi_1786_mz

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**Bond precision: C-C = 0.0044 A Wavelength=0.71070**

**Cell:** **a=10.2109(6)** **b=19.6215(8)** **c=9.5424(4)**
**alpha=90** **beta=110.916(6)** **gamma=90**
**Temperature:** **299 K**

| | Calculated | Reported |
|---|---|---|
| Volume | 1785.87(16) | 1785.87(15) |
| Space group | C c | C 1 c 1 |
| Hall group | C -2yc | C -2yc |
| Moiety formula | C18 H20 O4 Si | C18 H20 O4 Si |
| Sum formula | C18 H20 O4 Si | C18 H20 O4 Si |
| Mr | 328.43 | 328.43 |
| Dx,g cm-3 | 1.222 | 1.222 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.148 | 0.148 |
| F000 | 696.0 | 696.0 |
| F000' | 696.65 | |
| h,k,lmax | 12,24,11 | 12,24,11 |
| Nref | 1758[ 3504] | 3255 |
| Tmin,Tmax | 0.957,0.985 | 0.861,1.000 |
| Tmin' | 0.936 | |

**Correction method= MULTI-SCAN**

**Data completeness= 1.85/0.93** **Theta(max)= 26.000**

**R(reflections)= 0.0465( 2696)** **wR2(reflections)= 0.1177( 3255)**

**S = 1.031** **Npar= 210**

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The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

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**Alert level B**

Crystal system given = monoclinic
PLAT018_ALERT_1_B _diffrn_measured_fraction_theta_max .NE. _full !

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**Alert level C**

PLAT230_ALERT_2_C Hirshfeld Test Diff for Si1 -- C9 .. 6.0 su

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PLAT230_ALERT_2_C Hirshfeld Test Diff for    Si1    --  C10     ..        5.5 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    Si1    --  C11     ..        6.5 su
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Si1
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0044 Ang
```

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**Alert level G**

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed
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```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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**It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.**

**Publication of your CIF in IUCr journals**

**A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.**

**Publication of your CIF in other journals**

**Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.**

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**PLATON version of 05/11/2012; check.def file version of 05/11/2012**

**Datablock shi_1786_mz - ellipsoid plot**