Synthesis, characterization, and quantum chemical studies of new chiral acyclic (O,N,Te) type Schiff base, (*R*)-1-(((1-((4-methoxyphenyl)tellanyl)propan-2-yl)imino)methyl)naphthalen-2-ol

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Abstract. The reaction of the chiral telluro-amine, (*R*)-**2** with 2-hydroxy-1-naphthaldehyde has produced a new chiral telluro Schiff's base of (O,N,Te) type, (*R*)-1-(((1-((4-methoxyphenyl)tellanyl)propan-2-yl)imino)methyl)naphthalen-2-ol (*R*)-**3**. The SOR, CHN and spectroscopic analysis were used to characterize the structure of (*R*)-**3**. The different intermolecular interactions were shown by the fingerprint plots and Hirshfeld surface analysis. To describe the optimal structure, FMO, and reactive characteristics, DFT studies were carried out. Additionally, the RDG-based isosurface analysis conducted to investigate the type and nature of interactions.

Keywords: Schiff's base, chiral, tellurium, DFT, QTAIM

1 Introduction

As chiral ligands in transition metal-mediated asymmetric organic transformations [12–14], and in biochemistry [6–11], schiff bases of the organochalcogen (organosulphur, organoselenium, and organotellurium) compounds [1–5] have attracted a lot of attention because of their potential uses. A variety of hybrid organosulfur/selenium/tellurium ligands, as well nitrogen/oxygen ligand chemistry has been thoroughly researched over the past three decades [15–18]. Additionally, organotellurium compounds shown superior antioxidant activity in comparison to their comparable selenium and sulphur compounds [19,20]. In contrast to chiral organo-seleno- and -thioether Schiff bases compounds [21–25], the known

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chiral tellurated Schiff bases compounds are extremely rare and have been studied sparsely in biology [6–11, 15-20] and asymmetric organic synthesis. By the reaction of tellurated aldehydes with various chiral amines, the corresponding chiral telluro Schiff baseligands were reported [26–28] but this method is limited due to non commercial availability of the tellurated aldehydes and their synthesis is as not easy as like other.

Chemical and biological research has benefited immensely from the development of computational tools in current years, which have made to facilitate in investigation of basic physical and chemical characteristics and comprehend the nature of noncovalent interactions. Theoretical and experimental studies further improve the structures and characteristics of substances [29]. There are some known chiral tellurium-ether ligands, and their computational behavior has been insufficiently explored.

As a result, we have described the new chiral tellurium based Schiff base (*R*)-**3**, which was synthesized by utilizing chiral telluratedamine. (*R*)-**3** was characterized by FT-IR spectroscopy, elemental analysis, polarimetry, ^{1}H-NMR, and ^{13}C{^{1}H}-NMR. Furthermore, the QTAIM analysis and DFT computations were carried out.

2 Experimental

2.1 Materials and Methods

Merck Ind. Ltd. provided the tellurium, anisole, (*R*)-2-Amino-1-propanol, 2-Hydroxy-1-naphthaldehyde, and sodium borohydride ($NaBH_4$), which were utilized exactly as supplied. Standard procedures were used to purify and dry the solvents as needed [30]. Merck 60 F_{254} silica gel pre-coated aluminum TLC plates were used to monitor the reaction and the results were observed using UV light, $KMnO_4$ solution, or ninhydrine stain.

As described in the literature, the precursor compounds bis (4-methoxyphenyl) ditelluride (Ar_2Te_2) [31,32] and chiral telluro-amine, (*R*)-**2** [28] were made. Melting points of the compounds measured , and the results were reported uncorrected. A cell with a path length of 100 mm was used to measure the specific optical rotation (SOR) using a Rudolph Autopol-I automatic polarimeter. ^{1}H-NMR and ^{13}C{^{1}H}-NMR spectras were recorded by using tetramethylsilane (TMS) as an internal standard (0 ppm) and the values are expressed in δppm.

2.2 Synthesis of telluro Schiff base, (*R*)-3

At room temperature, telluroamine, (*R*)-**2** (1 mmol) dissolved in absolute ethanol, which is added to 2-hydroxy naphthaldehyde solution (1 mmol) dissolved in absolute ethanol with stirring, continued for 3 hrs. After employing a rotary evaporator pale yellow solid resulted of (*R*)-**3**. (Yield: 0.38 g, 85%); M.P.: 77-79 °C; $[\alpha]_D^{26} = -178°$; Anal. Calcd. (found) for $C_{17}H_{18}N_2OS$: C 42.91 (42.78), H 3.43 (3.34), N 2.38 (2.25); FTIR (ATR) *ν*, cm^{-1}: 3436 (O-H), 2919 (C-H), 1629 (C=N), 690 (ArC-Te), 606 (alkylC-Te); ^{1}H-NMR (Solvent:DMSO-d_6, 400 MHz) *δ* ppm: 1.343-1.359 (doblet, *J*=6.4Hz, 3H, methyl), 2.691-2.742 (doublet of doublet, *J*=7.2Hz, 1H, -CH_2-), 2.795-2.841 (doublet of doublet, *J*=7.6Hz, 1H, -CH_2-), 3.811 (singlet, 3H, OCH_3), 3.846-3.893 (sextet, 1H, CH-N), 6.753-6.776 (doublet, *J*=9.2Hz, 2H, ArH, *meta* to Te), 7.130-7.263 (multiplet, 3H, ArH), 7.419-7.456 (doublet, 1H, ArH), 7.623-7.642 (doublet, 1H, ArH), 7.712-7.736 (doublet, 1H, ArH), 8.062-8.083 (doublet, *J*=8.4Hz, 2H, ArH, *ortho* to Te), 9.080-9.103 (doublet, *J*=9.2Hz, 1H, -CH=N), 13.154 (singlet, 1H, OH); $^{13}C\{^1H\}$-NMR (Solvent:DMSO-d_6, 100.64 MHz) δ: 21.895 (CH_3), 27.343 (C-2), 31.605 (OCH_3), 58.428 (C-1), 119.137 (C-8), 122.795 (C-16), 125.179 (C-10), 125.947 (C-5), 127.027 (C-14), 128.321 (C-15), 128.808 (C-13), 129.314 (C-12), 134.509 (C-11), 137.233 (C-17), 139.782 (C-4), 157.442 (C-9), 159.282 (C-6), 175.916 (C-7).

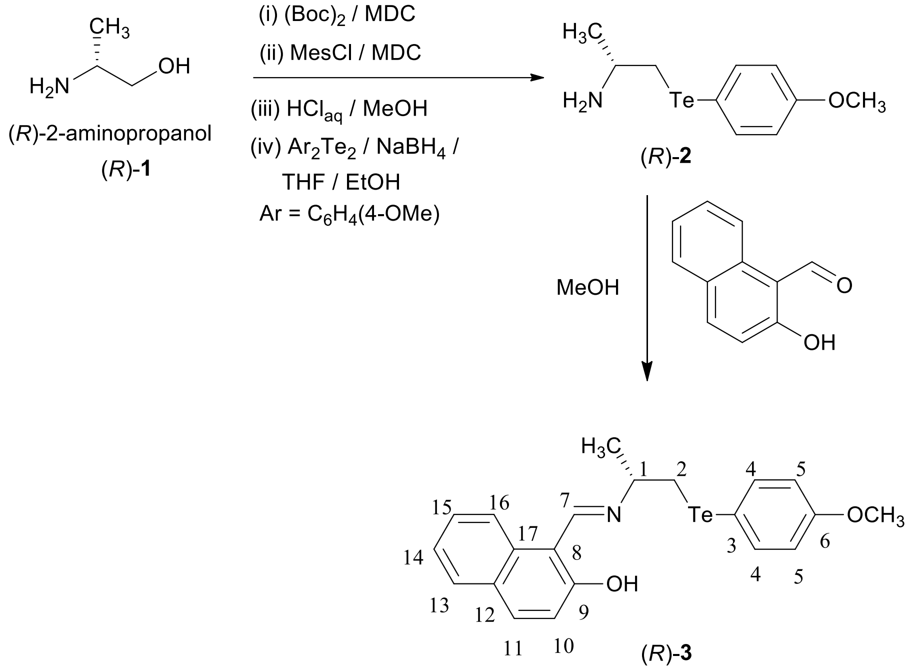
2.3 Quantum computational studies

The LANL2DZ and B3LYP functional basis set are used in DFT to optimize the geometry of (*R*)-**3**. The absence of imaginary frequencies showed that the optimized structure corresponded to the true energy minima configuration. To investigate the electronic-properties, global-reactivity parameters, and electrostatic-potential-surface, the FMO and MEP map were plotted respectively and examined at the same theoretical level. All calculations were done by using the Gaussian 16, and the Gaussview 5.0 tool was utilized to show the DFT findings [33]. Furthermore, the reduced density gradient (RDG) based isosurface was developed. The Bader's QTAIM analysis were conducted in order to understand the various types of interactions displayed by (*R*)-**3**. The Multiwfn software [34] was utilized to perform the QTAIM analysis, and Visual Molecular Dynamics (VMD) tool [35] was used to construct the isosurface plot.

3 Results and discussion

3.1 Synthesis

Chiral telluro Schiff base, (*R*)-**3** has been synthesised through the condensation reaction of telluro amine, (*R*)-**2** with 2-hydroxynaphthaldehyde as mentioned in **Scheme 1**. Schiff base, (*R*)-**3** was found insoluble in n-hexane, heptane, THF, benzene, toluene, and diethyl ether but freely soluble in CH_3CN, DMF, $CHCl_3$, CH_2Cl_2, CH_3OH and DMSO.



Scheme 1 Synthesis of (*R*)-**3**

3.2 Spectroscopy

The compound (*R*)-**3** was characterized by, SOR, CHN analysis, IR, proton and carbon-13 NMR spectroscopy.

As per the FT-IR data of (*R*)-**3**, the O-H and >C=N- stretching vibrational frequencies were appeared at 3436 and 1629 cm^{-1}. The ArC-Te and RC-Te stretching frequencies were appeared at 690 cm^{-1} and 606 cm^{-1}. The appeared frequencies are found characteristic with the respective functional groups as reported in the literature. [36]

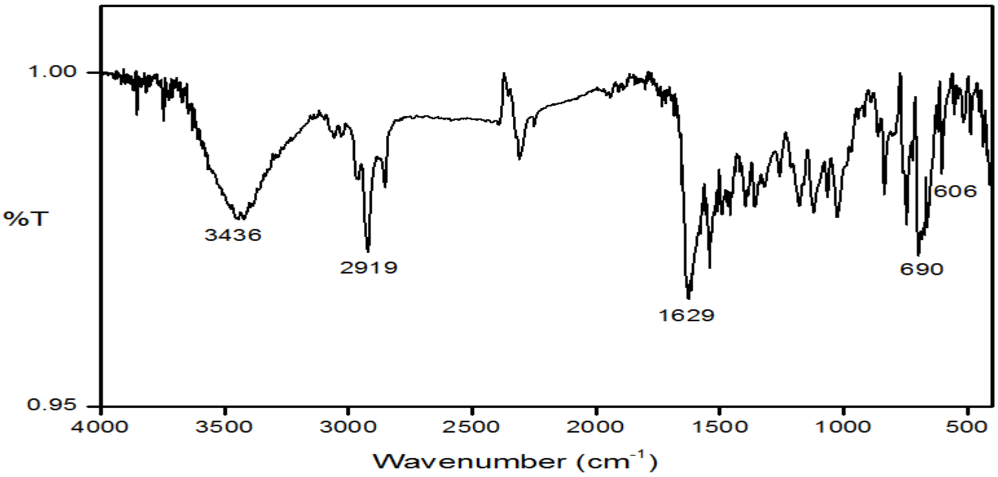


Fig. 1 FT-IR spectrum of (*R*)-**3**

In the proton Nuclear Magnetic Resonanace spectrum of (*R*)-**3** (as shown in **Fig. 2**), At the low field region, the aromatic OH proton was appeared,at 14.3 δ ppm it was found as broad singlet and highly deshielded due to hydrogen bonding with imine nitrogen. The proton of the imine (CH=N) was acquired. at δ, 9.1 ppm. The asymmetric CH proton shown a broad quartet at δ, 3.85-3.89 ppm due to coupling with three protons of CH_3 and CH_3 protons formed a doublet at δ, 1.30-1.35 ppm due to coupling with one proton of CH. At δ, 2.69-2.74 and 2.79-2.84 ppm, a series of doublets was produced by diasteroid CH2Te protons that are chemically non-equivalent. At their distinctive locations (δ ppm), the additional aromatic proton signals were visible [36,37].

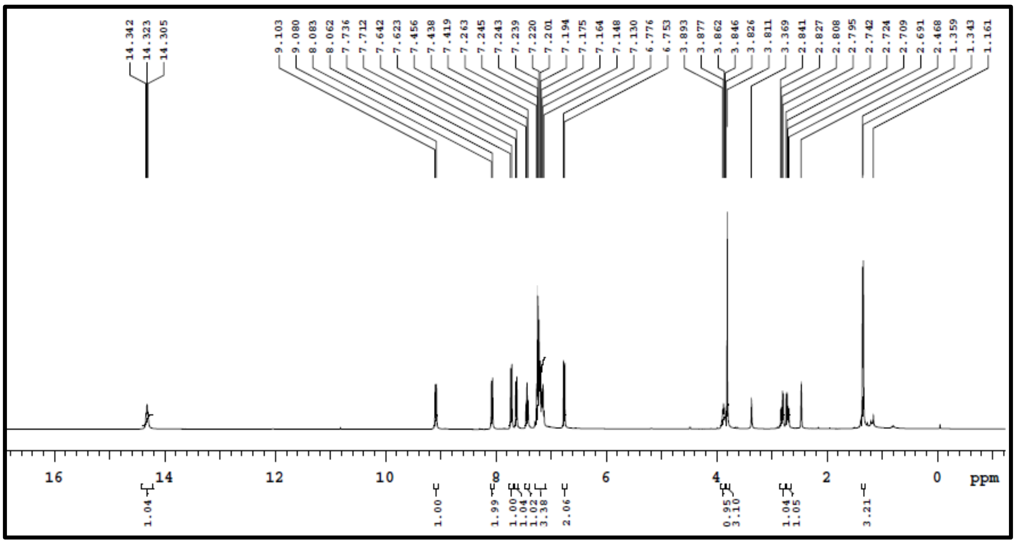


Fig. 2 ^{1}H NMR spectrum of (*R*)-3

In the carbon-13 Nuclear Magnetic Resonance spectrum of (*R*)-**3** (as shown in **Fig. 3**) the CH_2Te-C signal was obtained at 21.89 δ ppm. The CH -C gave peak at 58.43 δ ppm and imine carbon (C=N) was obtained at δ, 175.92 ppm and was found more deshielded. The Aromatic Carbon-OH peak was obtained at 159.28 δ ppm. The ArC-Te carbon signal was appeared at δ, 106.31 ppm. At their distinctive locations (δ ppm), the other carbon signals were visible [36,37].

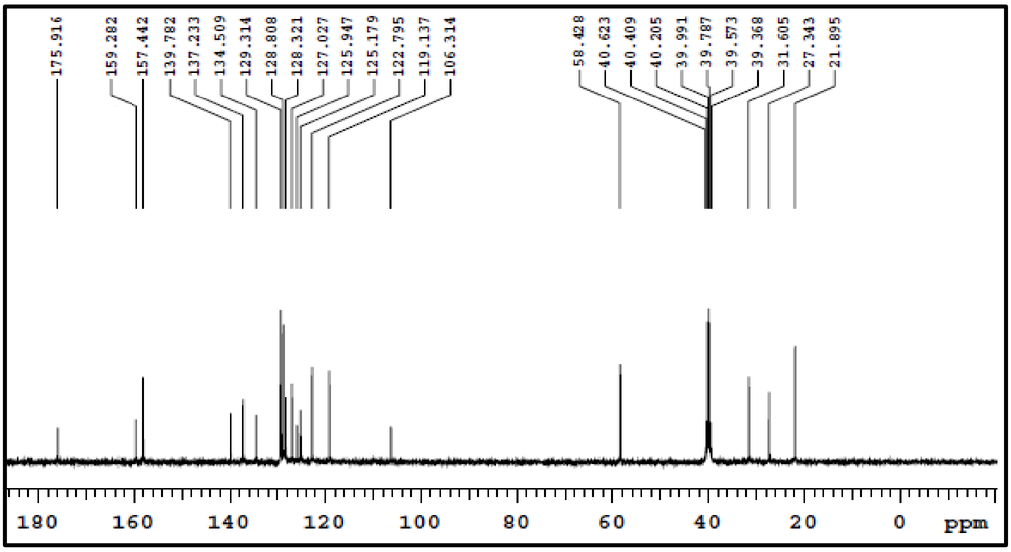


Fig. 3 $^{13}C\{^1H\}$ NMR spectrum of (*R*)-**3**

3.3 Quantum computational studies

The Schiff base, (*R*)-**3** optimized structure is shown in the **Fig. 4** and the HOMO and LUMO was calculated [38]. The HOMO-LUMO gap of (*R*)-**3** was obtained as 3.465 eV indicating the charge transfer occurring within the (*R*)-**3** molecule. The electrophilic behaviour of (*R*)-**3** was revealed by the higher electrophilicity index (3.665 eV) and lower chemical potential value (-3.564 eV). The HOMO and LUMO energies provide the valuable insights into several key parameters including the electronegativity (χ), energy gap (ΔEg), electron affinity (EA), ionization energy (IE), chemical potential (μ), global softness (s), electrophilicity (ω) and global hardness (η) of (*R*)-**3**, as tabulated in Table 1. An essential measure of a compound's stability and reactivity is its energy gap; a higher gap indicates more molecular stability and aromaticity as well as less chemical reactivity. The frontier molecular orbital distribution of (*R*)-**3** is as shown in **Fig. 5**. It is disclosed that the LUMO orbital is confined around the 2-hydroxy naphthalene moiety, while the HOMO is dispersed over the tellurium atom.

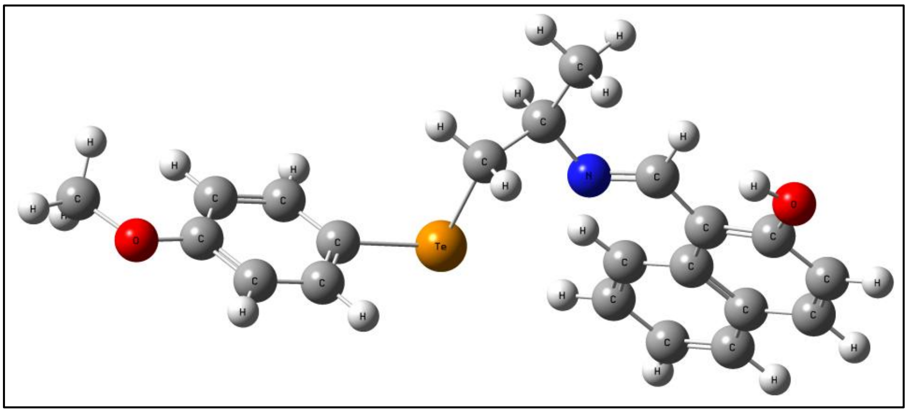


Fig. 4 Optimized structure of (*R*)-**3**

Table 1: The global quantum chemical parameters of (*R*)-**3**

Parameters	**Values**
E_{LUMO} (eV)	-1.831
E_{HOMO} (eV)	-5.296
ΔEg (eV)	3.465
IE (eV)	5.296
EA (eV)	1.831
χ (eV)	3.564
η (eV)	1.732
s $(eV)^{-1}$	0.577
ω (eV)	3.665
μ (eV)	-3.564

The optimal structure of (*R*)-**3** was obtained using the QTAIM analysis, and the VMD program was used to create the RDG-based isosurface plot. The isosurface plot of (*R*)-**3** is shown in the **Fig. 6** which reveals the existence and nature of various interactions. The varied color codes in the plot reflect the type of interaction. The existence of interactions of the van der Waals kind is shown by the green regions that are seen between the neighbouring atoms. Interestingly, the presence of the ring coloured region was observed between the carbon and the tellurium atom connected to it. All the rings of aromatic benzene are found to be associated with the red colored region in the center indicating the presence of steric repulsion.

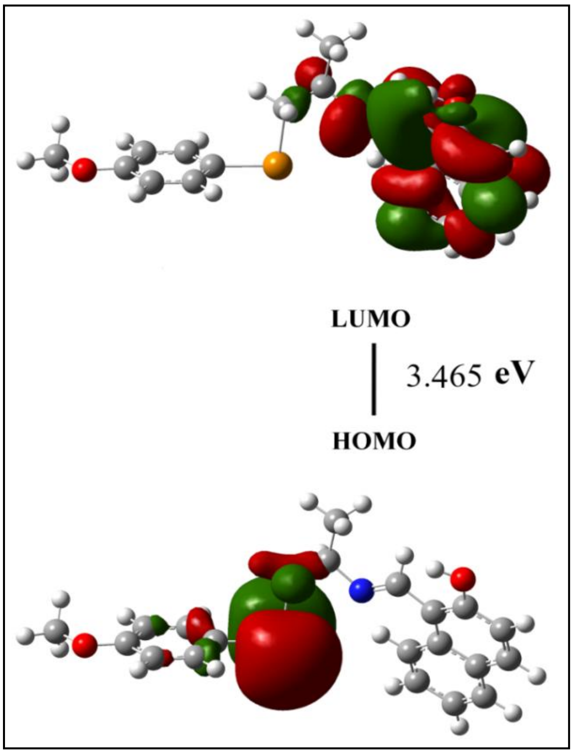


Fig. 5. Frontier molecular orbital distribution of (*R*)-**3**

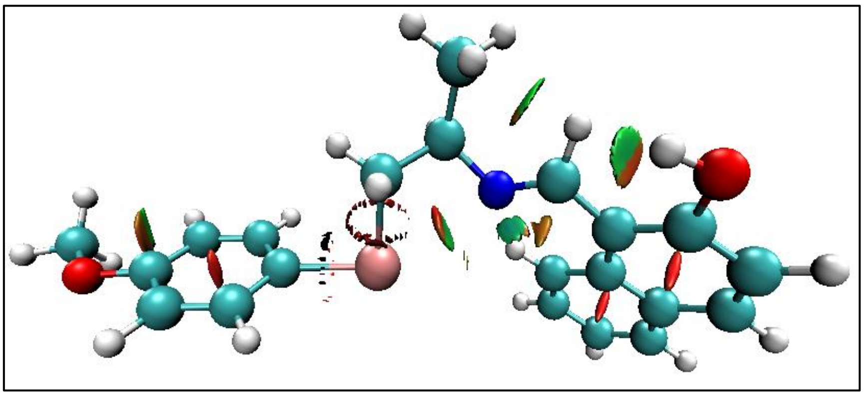


Fig. 6 RDG based isosurface of (*R*)-**3**

4 Conclusion

A new chiral tellurium based Schiff base, (*R*)-**3** was synthesized by the reaction of telluro-amine, and (*R*)-**2** and 2-hydroxy-1-naphthaldehyde. The synthesized Schiff's base is characterized by SOR, elemental and spectroscopic analysis. The geometrical coordinates of (*R*)-**3** was optimized using DFT and the orbital energy gap between HOMO-LUMO of (*R*)-**3** is found to be 3.465 eV. Further, the electrophilic behaviour of (*R*)-**3** was revealed by the higher electrophilicity index (3.665 eV) and lower chemical potential value (-3.564 eV). The HOMO orbital is found to be distributed over the telluriu atom, whereas the LUMO orbital is found to be localized over the 2-hydroxy napthalene moiety. The isosurface analysis revealed the nature and type of interactions exhibited by (*R*)-**3**.

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