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Research Article

A DFT-Based Investigation of Tosyl-D-Proline: Structure and Vibrational Spectroscopy

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Abstract

Tosyl-D-Proline, a chiral derivative of proline functionalized with a tosyl group, plays a significant role in asymmetric synthesis and organocatalysis. In this study, the molecular geometry of Tosyl-D-Proline was optimized using Density Functional Theory (DFT) at the B3LYP/6-311++G(d) level of theory. The optimized structure revealed stable conformations with no imaginary frequencies, confirming a true energy minimum on the potential energy surface. Vibrational frequency analysis was performed to obtain the theoretical infrared (IR) spectrum, and the characteristic vibrational modes were assigned. Key functional groups such as the sulfonyl, carboxyl, and amine groups were identified through their distinct IR absorption peaks. This computational investigation provides fundamental insights into the structural and vibrational properties of Tosyl-D-Proline, serving as a reference for future experimental and theoretical studies involving related chiral sulfonyl amino acids. The optimized structure and IR spectrum analysis of Tosyl-D-Proline molecule was performed using the Gaussian 09W software package.

Keywords: DFT, proline, optimization, vibrational frequency analysis

1. Introduction

Understanding the structural and vibrational properties of organic molecules at the atomic level is essential for advancing modern chemistry, especially in fields such as asymmetric catalysis, medicinal chemistry, and materials design. In this context, quantum chemical calculations, particularly those grounded in Density Functional Theory (DFT), have become powerful tools for predicting molecular geometry, electronic distribution, and spectroscopic behavior with remarkable accuracy. These computational approaches provide insights that are often inaccessible through experimental methods alone, thus enabling a deeper understanding of molecular interactions, stability, and reactivity (Aamir et al., 2022; Cui and Chen, 2021; Eschrig, 1996). Molecular modeling not only allows for the visualization of stable conformations and intramolecular forces but also facilitates the interpretation of spectroscopic data, especially in vibrational analyses such as infrared (IR) spectroscopy. By simulating theoretical IR spectra and comparing them with experimental findings, it is possible to assign characteristic vibrational modes to functional groups and evaluate how structural modifications influence molecular behavior. Among the wide array of biologically and synthetically important molecules, chiral proline derivatives have gained significant attention due to their utility in organocatalysis and enantioselective transformations. One such compound is Tosyl-D-Proline, a hybrid molecule that incorporates a D-proline backbone functionalized with a p-toluenesulfonyl (tosyl) group. This functional group significantly alters the molecule's electronic environment, introducing both steric hindrance and electron-withdrawing effects. As a result, Tosyl-D-Proline exhibits enhanced reactivity and selectivity, rendering it a valuable building block in the synthesis of pharmacologically and catalytically relevant compounds. Despite its synthetic potential, there is a notable lack of theoretical studies that address the molecular geometry and vibrational fingerprint of Tosyl-D-Proline in detail. To date, no comprehensive computational investigation has been reported that simultaneously examines the optimized geometry and infrared vibrational characteristics of this molecule. This gap in the literature represents a significant opportunity to explore its fundamental properties using modern quantum chemical techniques. In the present study, we employed DFT calculations at the B3LYP/6-311++G(d) level of theory to perform the first full geometry optimization and vibrational frequency analysis of Tosyl-D-Proline. The optimized geometry was evaluated to ensure the absence of imaginary frequencies, confirming its correspondence to a true energy minimum. The simulated IR spectrum was then used to identify the diagnostic vibrational modes associated with key functional groups such as carboxylic acid (–COOH), amine (–NH), and sulfonyl (–SO_2) functional groups. This work presents the first quantum chemical characterization of Tosyl-D-Proline, offering novel insights into its conformational stability and vibrational behavior. Beyond its intrinsic academic value, the findings may serve as a computational reference for future experimental and theoretical studies involving chiral sulfonylated amino acids, thereby contributing to the broader understanding of structure–function relationships in asymmetric synthesis and molecular design.

2. Material and Methods

All quantum chemical calculations were carried out using the Gaussian 09W software (Frisch et al., 2009) package, and molecular visualizations were performed via the GaussView 5.0 (Dennington et al., 2009) graphical interface. The molecular geometry of Tosyl-D-Proline was optimized at the B3LYP/6-311++G(d) level of theory. To confirm the nature of the stationary point, frequency calculations were performed, ensuring the absence of imaginary frequencies. Furthermore, detailed vibrational mode analyses were conducted using the VEDA 4 program (Jamroz, 2004; Jamróz, 2013) to assist in the assignment of IR spectral bands.

3. Optimization analysis

The molecular geometry of Tosyl-D-Proline was thoroughly optimized using Density Functional Theory (DFT) at the B3LYP functional level in combination with the 6-311++G(d,p) basis set within the gas phase. These calculations were conducted using the Gaussian 09W software package (Frisch et al., 2009) to identify the global minimum structure on the potential energy surface. The absence of imaginary frequencies in the subsequent vibrational analysis confirmed that the optimized geometry corresponds to a true local minimum. The resulting geometric parameters-namely bond lengths, bond angles, and dihedral angles-were presented comprehensively in Table 1. The optimization revealed a structurally rigid framework stabilized by intramolecular interactions, particularly between the sulfonyl and carboxylic acid groups. Notable geometric features include the shortened S=O bond lengths (~1.58 Å), which are indicative of strong double-bond character within the sulfonyl moiety, and the slightly elongated C–N bond between the proline ring and the sulfonyl group, which reflects the electronic influence of the electron-withdrawing tosyl substituent. Furthermore, the dihedral angles reveal a well-defined spatial arrangement, underscoring the conformational stability of the chiral center in D-proline. This defined geometry is expected to play a pivotal role in the molecule's stereoselectivity and reactivity in asymmetric transformations. The optimized structure, depicted in Fig. 1, demonstrates a non-planar conformation that aligns with the steric bulk and electronic distribution of the tosyl group. These geometric insights provide a solid foundation for correlating molecular conformation with vibrational properties and reactivity patterns, especially in contexts where stereochemistry and non-covalent interactions govern chemical behavior.

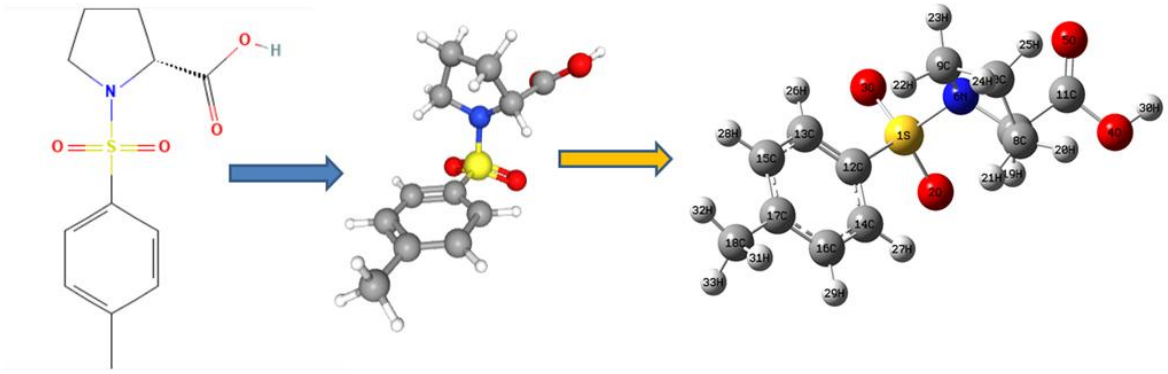

Figure 1. The 2D, 3D (Kim et al., 2025) and optimized structures, respectively of Tosyl-D-Proline molecule.

Table 1. The optimized structure parameters of Tosyl-D-Proline molecule

Bond Lengths (Å)	Values	Bond Angles (°)	Values	Dihedral Angles (°)	Values
S1-O2	1.60	O2-S1-O3	122.0	O2-S1-N6-C7	-14.2
S1-O3	1.58	O2-S1-N6	105.5	O2-S1-N6-C9	-146.4
S1-N6	1.80	O2-S1-C12	106.1	O3-S1-N6-C7	-146.5
S1-C12	1.85	O3-S1-N6	108.6	O3-S1-N6-C9	81.3
O4-C11	1.39	O3-S1-C12	107.1	C12-S1-N6-C7	98.3
O4-H30	1.00	N6-S1-C12	106.8	C12-S1-N6-C9	-33.8
O5-C11	1.22	C11-O4-H30	108.4	O2-S1-C12-C13	-154.5
N6-C7	1.48	S1-N6-C7	114.0	O2-S1-C12-C14	23.2
N6-C9	1.50	S1-N6-C9	117.6	O3-S1-C12-C13	-22.8
C7-C8	1.55	C7-N6-C9	110.8	O3-S1-C12-C14	154.9
C7-C11	1.52	N6-C7-C8	104.1	N6-S1-C12-C13	93.3
C7-H19	1.09	N6-C7-C11	109.1	N6-S1-C12-C14	-88.9
C8-C10	1.55	N6-C7-H19	110.2	H30-O4-C11-O5	-1.6

C8-H20	1.09	C8-C7-C11	108.1	H30-O4-C11-C7	-177.2
C8-H21	1.10	C8-C7-H19	114.8	S1-N6-C7-C8	-116.4
C9-C10	1.56	C11-C7-H19	110.2	S1-N6-C7-C11	128.4
C9-H22	1.10	C7-C8-C10	101.5	S1-N6-C7-H19	7.3
C9-H23	1.09	C7-C8-H20	111.7	C9-N6-C7-C8	19.0
C10-H24	1.09	C7-C8-H21	109.5	C9-N6-C7-C11	-96.2
C10-H25	1.09	C10-C8-H20	113.6	C9-N6-C7-H19	142.7
C12-C13	1.38	C10-C8-H21	110.6	S1-N6-C9-C10	139.6
C12-C14	1.39	H20-C8-H21	109.7	S1-N6-C9-H22	21.2
C13-C15	1.40	N6-C9-C10	103.7	S1-N6-C9-H23	-100.4
C13-H26	1.08	N6-C9-H22	110.9	C7-N6-C9-C10	6.0
C14-C16	1.39	N6-C9-H23	109.8	C7-N6-C9-H22	-112.5
C14-H27	1.08	C10-C9-H22	110.4	C7-N6-C9-H23	126.0
C15-C17	1.40	C10-C9-H23	112.2	N6-C7-C8-C10	-35.9
C15-H28	1.08	H22-C9-H23	109.8	N6-C7-C8-H20	-157.3
C16-C17	1.41	C8-C10-C9	103.7	N6-C7-C8-H21	81.0
C16-H29	1.08	C8-C10-H24	113.1	C11-C7-C8-C10	80.0
C17-C18	1.52	C8-C10-H25	109.4	C11-C7-C8-H20	-41.4
C18-H31	1.10	C9-C10-H24	111.8	C11-C7-C8-H21	-163.1
C18-H32	1.09	C9-C10-H25	109.0	H19-C7-C8-C10	-156.5
C18-H33	1.10	H24-C10-H25	109.6	H19-C7-C8-H20	82.1
		O4-C11-O5	123.3	H19-C7-C8-H21	-39.6
		O4-C11-C7	107.9	N6-C7-C11-O4	-167.8
		O5-C11-C7	128.7	N6-C7-C11-O5	16.9
		S1-C12-C13	119.1	C8-C7-C11-O4	79.6
		S1-C12-C14	118.1	C8-C7-C11-O5	-95.7
		C13-C12-C14	122.8	H19-C7-C11-O4	-46.6
		C12-C13-C15	118.4	H19-C7-C11-O5	138.1
		C12-C13-H26	119.4	C7-C8-C10-C9	39.7
		C15-C13-H26	122.2	C7-C8-C10-H24	161.0
		C12-C14-C16	118.4	C7-C8-C10-H25	-76.5
		C12-C14-H27	119.2	H20-C8-C10-C9	159.8
		C16-C14-H27	122.4	H20-C8-C10-H24	-79.0
		C13-C15-C17	120.7	H20-C8-C10-H25	43.5
		C13-C15-H28	119.7	H21-C8-C10-C9	-76.4
		C17-C15-H28	119.6	H21-C8-C10-H24	44.9
		C14-C16-C17	120.7	H21-C8-C10-H25	167.4
		C14-C16-H29	119.8	N6-C9-C10-C8	-28.6
		C17-C16-H29	119.5	N6-C9-C10-H24	-150.7
		C15-C17-C16	119.1	N6-C9-C10-H25	87.9
		C15-C17-C18	120.9	H22-C9-C10-C8	90.2
		C16-C17-C18	120.1	H22-C9-C10-H24	-32.0
		C17-C18-H31	110.8	H22-C9-C10-H25	-153.3
		C17-C18-H32	111.0	H23-C9-C10-C8	-147.0
		C17-C18-H33	110.5	H23-C9-C10-H24	90.8
		H31-C18-H32	108.4	H23-C9-C10-H25	-30.5
		H31-C18-H33	107.9	S1-C12-C13-C15	179.7
		H32-C18-H33	108.2	S1-C12-C13-H26	1.5
				C14-C12-C13-C15	2.1
				C14-C12-C13-H26	-176.1
				S1-C12-C14-C16	-179.6
				S1-C12-C14-H27	-2.0
				C13-C12-C14-C16	-1.9
				C13-C12-C14-H27	175.7
				C12-C13-C15-C17	-0.8
				C12-C13-C15-H28	180.0
				H26-C13-C15-C17	177.4
				H26-C13-C15-H28	-1.9

	C12-C14-C16-C17	0.4
	C12-C14-C16-H29	179.5
	H27-C14-C16-C17	-177.1
	H27-C14-C16-H29	2.0
	C13-C15-C17-C16	-0.6
	C13-C15-C17-C18	-179.3
	H28-C15-C17-C16	178.6
	H28-C15-C17-C18	0.0
	C14-C16-C17-C15	0.8
	C14-C16-C17-C18	179.4
	H29-C16-C17-C15	-178.3
	H29-C16-C17-C18	0.3
	C15-C17-C18-H31	-128.1
	C15-C17-C18-H32	-7.7
	C15-C17-C18-H33	112.3
	C16-C17-C18-H31	53.3
	C16-C17-C18-H32	173.8
	C16-C17-C18-H33	-66.3

4. Vibrational analysis

The vibrational properties of the Tosyl-D-Proline molecule were systematically analyzed using Density Functional Theory (DFT) with the B3LYP functional and the 6-311++G(d,p) basis set in the gas phase. These calculations yielded no imaginary frequencies, confirming that the structure resides at a true local minimum on the potential energy surface. The computed sum of electronic and zero-point energies was determined to be -1213.237899 a.u., while the total dipole moment was calculated as 7.4578 Debye, indicating a pronounced polarity in the molecule due to the presence of the sulfonyl and carboxylic functional groups. Given that Tosyl-D-Proline consists of 33 atoms, it possesses 93 vibrational normal modes, as predicted by the 3N–6 rule for non-linear molecules (Kumar, 2006). The vibrational frequency analysis revealed detailed insights into the internal dynamics of the molecule, including stretching (ν), bending (β), torsional (τ), and out-of-plane (ω) deformations of key functional moieties. The theoretical infrared (IR) spectrum, presented in Fig. 2, reflects the molecular vibrational signature and exhibits well-resolved bands attributable to characteristic functional groups. The high-frequency region (~3000–3500 cm^{-1}) is dominated by O–H and C–H stretching vibrations, with the most intense peak observed at 3337 cm^{-1} corresponding to the ν(OH) mode. Likewise, symmetric and asymmetric C–H stretchings appear across 2947–3097 cm^{-1}, each varying slightly due to their distinct chemical environments. In the mid-infrared region, a prominent absorption band at 1732 cm^{-1} is attributed to C=O stretching (νOC) of the carboxylic acid group (Lin-Vien et al., 1991), a critical indicator of structural integrity and chemical reactivity. Additional bands in the 1200–1500 cm^{-1} region are assigned to bending vibrations (βHCH, βHCC) and provide diagnostic fingerprints for both aliphatic and aromatic environments. Notably, the sulfonyl (SO_2) group exhibits a strong and characteristic S=O stretching mode at 1050 cm^{-1}, aligned with literature expectations for such electron-withdrawing substituents. The full set of vibrational modes, including their calculated intensities, unscaled and scaled frequencies, and potential energy distribution (PED) assignments, were performed with VEDA4 and comprehensively tabulated in Table 2. The use of scaling factors correct the systematic overestimation of DFT-calculated harmonic frequencies and enhances agreement with experimental spectra. The vibrational assignments were supported by PED analysis using the VEDA 4.0 software (Jamroz, 2004; Jamróz, 2013), enabling a more precise decomposition of each mode into constituent atomic motions. Overall, the vibrational analysis provides a robust spectroscopic framework for identifying key functional groups and assessing intramolecular interactions. These findings are critical for future spectroscopic studies and can serve as a reliable computational reference for experimental characterization of Tosyl-D-Proline and structurally related molecules.

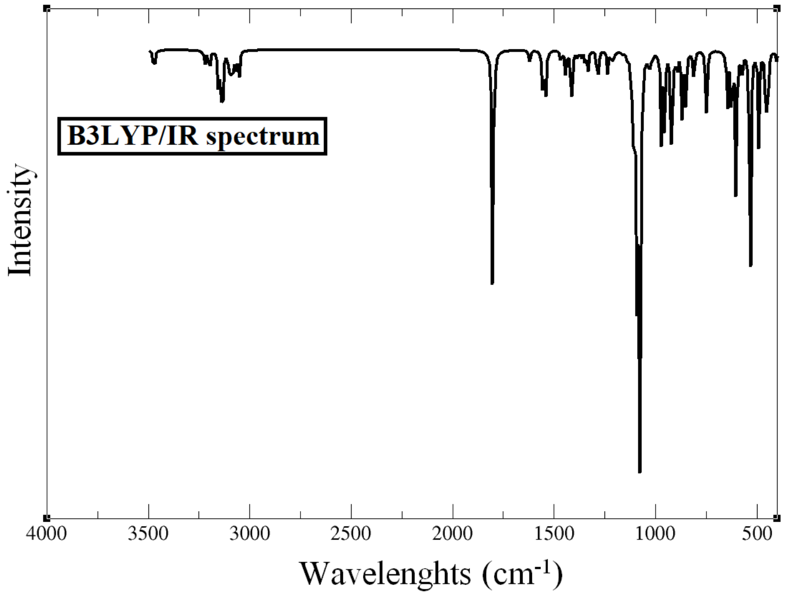

Figure 2. The theoretical IR spectra (B3LYP) of Tosyl-D-Proline molecule

Table 2. Calculated vibrational frequency with PED assignments of the title compound

Mode No	Intensity	Unscaled	Scaled	Assignments
ν1	13.90	3471	3337	ϑ OH(100)
ν2	7.50	3222	3097	ϑ CH(88)
ν3	1.36	3219	3095	ϑ CH(99)
ν4	6.00	3201	3078	ϑ CH(87)
ν5	6.30	3196	3073	ϑ CH(91)
ν6	18.48	3155	3033	ϑ CH(87)
ν7	9.39	3145	3024	ϑ CH(96)
ν8	23.69	3138	3017	ϑ CH(99)
ν9	9.56	3133	3012	ϑ CH(86)
ν10	10.90	3131	3010	ϑ CH(89)
ν11	10.92	3103	2983	ϑ CH(94)
ν12	14.26	3094	2975	ϑ CH(98)
ν13	13.29	3081	2962	ϑ CH(85)
ν14	11.24	3065	2947	ϑ CH(97)
ν15	13.91	3052	2934	ϑ CH(90)
ν16	151.7	1802	1732	ϑ OC(85)
ν17	5.56	1622	1559	ϑ CC(56) + β HCC(14)
ν18	2.23	1618	1556	ϑ CC(45) + β CCC(25)
ν19	1.28	1569	1508	β HCH(82)
ν20	8.35	1557	1497	β HCH(65) + τ HCCC(21)
ν21	13.12	1554	1494	β HCH(59) + τ HCCC(19)
ν22	6.66	1545	1485	β HCH(75)
ν23	10.76	1542	1483	β HCH(85)
ν24	14.07	1540	1480	β CCC(10) + β HCC(65)
ν25	6.57	1465	1408	β HCH(88)
ν26	14.26	1442	1387	ϑ CC(14) + β HCC(47)
ν27	37.71	1414	1360	β HOC(11) + β HCC(29)
ν28	3.06	1386	1333	τ HCNS(28) + τ HCCN(41)
ν29	1.44	1382	1328	β HCC(34) + τ HCNS(10) + τ HCCN(22)

ν30	4.50	1366	1313	ϑ CC(12) + β HCC(81)
ν31	5.64	1347	1295	β HCC(12) + τ HCCO(62)
ν32	10.05	1334	1282	ϑ OC(10) + β HOC(43)
ν33	3.41	1331	1279	ϑ CC(82)
ν34	10.67	1288	1238	β HCC(50) + τ HCCO(11)
ν35	10.75	1281	1232	β HCC(18) + τ HCCO(19) + τ HCNS(18)
ν36	12.54	1236	1188	ϑ CC(14) + β HCC(62)
ν37	0.27	1223	1176	ϑ CC(62) + β HCC(10)
ν38	7.54	1215	1168	β HCC(25) + τ HCCO(22)
ν39	3.46	1201	1155	β HCC(35) + τ HCCO(11) + τ HCNS(16)
ν40	1.07	1163	1118	ϑ CC(37) + β HCC(43)
ν41	3.38	1136	1092	ϑ NC(17) + β HCC(15) + τ HCNS(11) + τ CCCN(13)
ν42	21.21	1119	1076	ϑ NC(24) + ϑ SO(10) + β CCC(10)
ν43	30.00	1108	1065	ϑ CC(45) + ϑ SC(10)
ν44	17.62	1103	1060	β HCH(11) + τ HCCC(45)
ν45	129.8	1092	1050	ϑ SO(57)
ν46	279.0	1077	1036	ϑ OC(39) + ϑ NC(13) + β HOC(22)
ν47	7.90	1060	1019	β CCC(58)
ν48	0.86	1039	999	β CCC(11) + τ HCCC(41)
ν49	11.31	1031	991	ϑ CC(39) + β CNC(18) + β CCN(13)
ν50	2.58	1020	981	τ HCCC(68) + τ CCCC(10)
ν51	1.78	1014	974	τ HCCC(57) + τ CCCC(24)
ν52	50.31	971	934	ϑ NC(12) + τ HCNS(16)
ν53	41.39	955	918	ϑ CC(32) + ϑ NC(19)
ν54	76.21	921	885	ϑ SO(34)
ν55	3.05	909	874	ϑ CC(37) + β CNC(10) + τ HCCO(10)
ν56	12.83	894	860	ϑ NC(17) + ϑ SO(30) + β CCN(18)
ν57	1.02	878	844	τ HCCC(96)
ν58	37.02	868	835	ϑ NC(22) + τ HCNS(12)
ν59	27.70	852	819	τ HCCC(73)
ν60	6.67	843	810	ϑ CC(19) + ω CCNC(12)
ν61	14.60	813	781	ϑ CC(14) + β CCC(10)
ν62	2.48	803	772	τ HCCC(13) + τ CCCC(43) + ω CCCC(13)
ν63	7.49	753	724	ω OCOC(48)
ν64	32.16	748	719	β CCC(79)
ν65	0.28	670	644	β OCO(17) + τ HOCC(32)
ν66	35.40	645	620	ϑ CC(21) + ϑ SC(26) + β CCC(18)
ν67	40.57	625	601	β OCO(35) + τ HOCC(33)
ν68	89.22	602	579	β OCO(10) + β CCC(20) + τ HOCC(19) + τ HCCO(15)
ν69	13.42	574	552	β OSO(10) + τ CCCC(12) + ω CCCC(22) + ω SCCC(15)
ν70	130.1	533	512	β CCC(10) + ω ONOS(27)
ν71	56.67	490	471	β OSO(29) + τ CCCC(14) + ω CCCC(15)
ν72	24.79	457	440	β OCC(17) + ω ONOS(18) + ω ONCS(17)
ν73	42.78	448	431	τ HCCC(19) + τ CCCC(73)
ν74	0.78	436	419	β CCC(24) + β SCC(15) + ω ONCS(16)
ν75	5.62	404	388	β CCC(26) + ω ONCS(11)
ν76	5.02	357	343	β CCC(11) + τ CCCN(11) + ω ONCS(19)
ν77	1.00	333	320	ϑ SN(14) + ω CCCC(13) + ω SCCC(12)
ν78	1.16	316	304	ϑ SN(14) + β CCC(12) + β OSO(21) + β OSC(11)
ν79	4.03	306	294	β OCC(22) + β CCC(11) + ω CSCN(13)
ν80	0.77	272	261	β OSO(16) + β OSC(34)
ν81	0.82	258	248	ϑ SC(29) + ω ONOS(26)
ν82	10.62	247	237	β CNS(26) + τ CCCN(16)
ν83	0.14	204	196	β CCC(19) + β NSC(15) + τ CCCC(12)
ν84	0.38	159	153	β CCC(11) + β SCC(23) + τ CCCC(12)
ν85	1.14	147	141	β SCC(20) + β NSC(11)
ν86	2.22	138	133	β CNS(22) + β SCC(14) + ω ONCS(11) + ω CCNC(20)
ν87	5.82	108	104	β NSC(25) + ω SCCC(34)

ν88	0.28	67	65	τ NSCC(87)
ν89	0.29	51	49	τ HCCC(81)
ν90	0.35	50	48	τ OCCC(70)
ν91	0.81	33	32	τ OCCC(13) + τ CCNS(53)
ν92	0.07	22	22	τ CNSC(87)
ν93	0.22	17	16	ϑ OH(100)

ϑ - streching, β - bending, τ - torsion, ω - out plane bending. Scale factor=0.9614.

5. Conclusion

In this study, the molecular structure and vibrational characteristics of Tosyl-D-Proline were thoroughly investigated using DFT calculations at the B3LYP/6-311++G(d) level. The optimized geometry revealed a stable, non-planar conformation stabilized by intramolecular interactions, particularly between sulfonyl and carboxylic acid groups. Vibrational frequency analysis provided a detailed assignment of characteristic modes, especially those corresponding to OH, C=O, and SO_2 groups, which were in agreement with theoretical expectations. The absence of imaginary frequencies confirmed the structural stability of the optimized conformation. Overall, this work offers the first comprehensive quantum chemical characterization of Tosyl-D-Proline and provides valuable spectral insights that can guide future experimental and theoretical studies involving sulfonylated chiral amino acids.

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