

DFT investigation on nonlinear optical properties of some substitute amido alcohols

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In this paper, nonlinear optical (NLO) properties of twenty different substitute amido alcohols were studied as theoretically. Firstly, all amido alcohol molecules were optimized by DFT method with 6-31G(d,p) basis set. Then, the optical properties were calculated by DFT method with the 3-21G, 6-31G, 6-31G(d), 6-31G(d,p), 6-31G+(d,p), 6-31G++(d,p), 6-311G, 6-311G(d), 6-311G(d,p), 6-311G+(d,p) and 6-311G++(d,p) basis sets for the investigation of basis set effect on nonlinear optical properties. In general, it was determined that the relative changes from one basis set to another are nearly the same for studying amido alcohols. The NLO properties magnitude of molecules is dependent on the first-order hyperpolarizability which is clearly influenced more accurate after the addition of polarization and diffusion functions. For this reason, all discussion of NLO properties were made as 6-311G++(d,p) basis set. The calculated results show that the all amido alcohol molecules have more NLO properties than urea. These results indicate that the all molecules might have NLO behavior.

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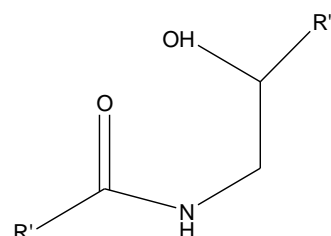
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1. Introduction

Since the invention of the laser in 1960, there have been significant developments in the field of nonlinear optical materials. Nonlinear optical (NLO) materials, defined as materials in which light waves can interact with each other, are key materials for the fast processing of information and optical storage applications. The important development in nonlinear optical materials occurred in 1970, when Davydov et al. reported a strong second harmonic generation (SHG) in organic materials [1]. In addition, nonlinear optical materials play a major role in the integration of optical devices into the current technology. This integration has led to the development of a large number of schemes for controlling and manipulating the phase, direction, polarization and amplitude of optical beams. The ability to control light intensity is of prime relevance in optical-related applications, such as optical communications, optical computing and light-driven chemical reactions. In these controls, it is used in nonlinear optical materials [2]. Therefore, the large number of works that have been studied the past two decades to synthesize the NLO materials [3-6], which are especially organic molecules. Generally, the strategies of these synthesis used mainly focused on utilizing molecules that contain extended π -electron systems [7]. The NLO properties magnitude of molecules is dependent on the first-order hyperpolarizability. The NLO property of molecules and their hyperpolarizabilities have become an important field of extensive research, especially in the theoretical research [8, 9].

On the other hand, the amido alcohol is an amide compound containing the amide and the hydroxyl groups. The general structure of amido alcohol is shown in Fig. 1,

which it can be intramolecular hydrogen bonding. Such molecules exhibit nonlinear optical properties as seen in the literature [10, 11]. In addition, it is thought that if the substitute phenyl groups are added in R' and R'', the molecule will exhibit even more nonlinear optical properties.



R' = -C₁₀H₇, -C₆H₄NO₂, -C₆H₄Cl, -C₆H₄Br

R'' = -H, -C₆H₅, -C₆H₄NO₂, -C₆H₄Cl, -C₆H₄Br

Fig. 1. General molecular structure of amido alcohol

In this context, the aim of this work is to study the NLO properties of twenty different substitute amido alcohols, of which containing amide group and π -electron systems. For this purpose, all molecules were optimized at density functional theory (DFT) using B3LYP method with 6-31G(d,p) basis set, then the basis set effect was investigated with 3-21G, 6-31G, 6-31G(d), 6-31G(d,p), 6-31G+(d,p), 6-31G++(d,p), 6-311G, 6-311G(d), 6-311G(d,p), 6-311G+(d,p) and 6-311G++(d,p) basis sets. The dipole moment (μ), the linear polarizability (α) and the first hyperpolarizability (β) were calculated with B3LYP/6-311G++(d,p) level. Urea is one of the reference

materials and frequently used for comparative purpose in the study of the NLO properties.

2. Theoretical details

In this study, firstly the optimized geometries of the all amido alcohol molecules were determined by using DFT/B3LYP method [12] with 6-31G(d,p) basis set. The optimized structures were then used to calculate the electrostatic potential, nonlinear optical properties and frontier molecular orbitals of all amido alcohol molecules. The effects of basis sets on calculations are studied at the B3LYP levels with 3-21G, 6-31G, 6-31G(d), 6-31G(d,p), 6-31G+(d,p), 6-31G++(d,p), 6-311G, 6-311G(d), 6-311G(d,p), 6-311G+(d,p) and 6-311G++(d,p) basis sets. All theoretical calculations in this work were carried out using Gaussian 03 program [13] and GaussView molecular visualization program [14]. The optimized geometries of all amido alcohols are shown in Fig. 1. The obtained structures were used to calculate the different physical properties of the all amido alcohol molecules.

3. Result and discussion

The most stable molecular structures of the 20 different substitute amido alcohols were optimized by the DFT/B3LYP method with 6-31G(d,p) basis set. The optimized structures obtained GaussView program are shown in Fig. 2. Generally, the most important bonds of amido alcohols are amide carbonyl, amide N-H and hydroxyl O-H bond. These bond lengths were calculated between 1.239 and 1.256 Å for carbonyl, between 0.997 and 1.001 Å for N-H and between 1.007 and 1.108 Å for hydroxyl O-H bond lengths. In addition, all the amido alcohols have intramolecular hydrogen bonding. The amido alcohol molecules linked by the O-H...O intramolecular hydrogen bond involving the hydroxyl H atom and the carbonyl O atom. This hydrogen bond distance is calculated between 2.182 and 2.212 Å for all amido alcohols. This intramolecular hydrogen bond adds structural stability for all amido alcohols.

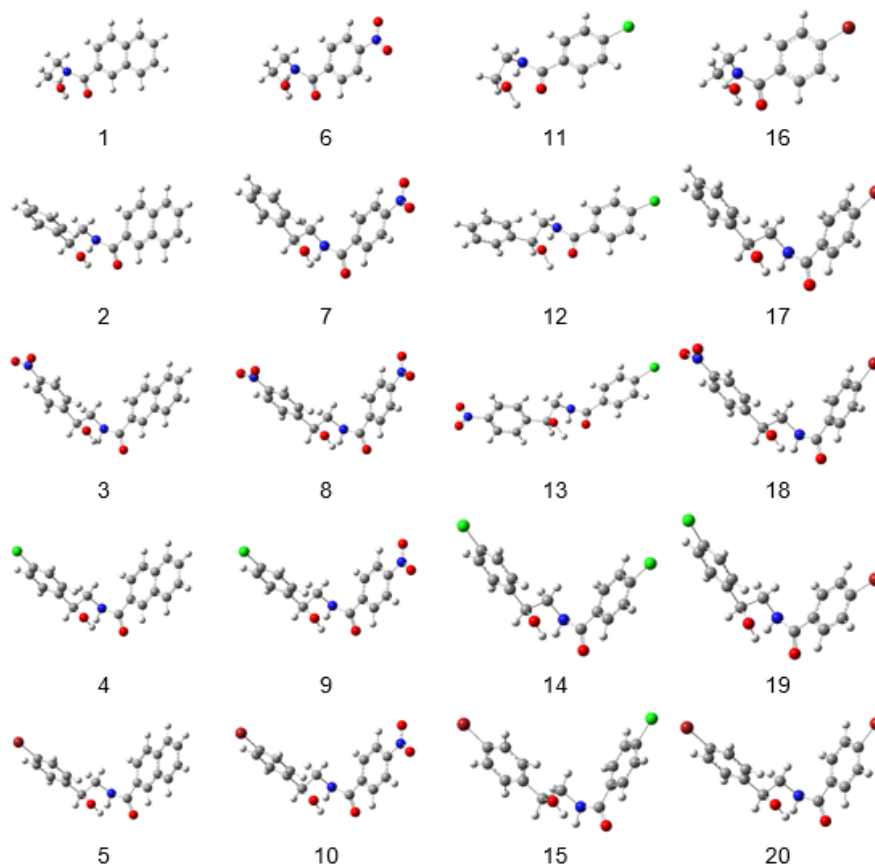


Fig. 2. Optimized geometries of substitute amido alcohols. Abbreviations of amido alcohols: 1-Naphthalene-2-carboxylic acid (2-hydroxy-ethyl)-amide, 2-Naphthalene-2-carboxylic acid (2-hydroxy-2-phenyl-ethyl)-amide, 3-Naphthalene-2-carboxylic acid [2-hydroxy-2-(4-nitro-phenyl)-ethyl]-amide, 4-Naphthalene-2-carboxylic acid [2-(4-chloro-phenyl)-2-hydroxy-ethyl]-amide, 5-Naphthalene-2-carboxylic acid [2-(4-bromo-phenyl)-2-hydroxy-ethyl]-amide, 6- N-(2-Hydroxy-ethyl)-4-nitro-benzamide, 7-N-(2-Hydroxy-2-phenyl-ethyl)-4-nitro-benzamide, 8-N-[2-Hydroxy-2-(4-nitro-phenyl)-ethyl]-4-nitro-benzamide, 9-N-[2-(4-Chloro-phenyl)-2-hydroxy-ethyl]-4-nitro-benzamide, 10-N-[2-(4-Bromo-phenyl)-2-hydroxy-ethyl]-4-nitro-benzamide, 11-4-Chloro-N-(2-hydroxy-ethyl)-benzamide, 12-4-Chloro-N-(2-hydroxy-2-phenyl-ethyl)-benzamide, 13-4-Chloro-N-[2-hydroxy-2-(4-nitro-phenyl)-ethyl]-benzamide, 14-4-Chloro-N-[2-(4-chloro-phenyl)-2-hydroxy-ethyl]-benzamide, 15-4-Chloro-N-[2-(4-bromo-phenyl)-2-hydroxy-ethyl]-benzamide, 16-4-Bromo-N-(2-hydroxy-ethyl)-benzamide, 17-4-Bromo-N-(2-hydroxy-2-phenyl-ethyl)-benzamide, 18-4-Bromo-N-[2-hydroxy-2-(4-nitro-phenyl)-ethyl]-benzamide, 19-4-Bromo-N-[2-(4-chloro-phenyl)-2-hydroxy-ethyl]-benzamide, 20-4-Bromo-N-[2-(4-bromo-phenyl)-2-hydroxy-ethyl]-benzamide

A good non-linear optical material has been frequently used in communication technology, signal processing, optical switches and optical memory devices. Theoretical studies on electronic properties have been done in order to understand the microscopic origin of nonlinear behavior of the different substitute amido alcohol molecules. The presence of electron donor group and an electron acceptor group also enhance the non-linear optical properties. The study includes the calculation of the total static dipole moment (μ), the linear polarizability (α) and the first hyperpolarizability (β) tensor for the all amido alcohol molecules. The first hyperpolarizability is a third rank tensor which can be described by a $3 \times 3 \times 3$ matrix. Due to the fact that Kleinman symmetry was used in calculations, the 20 substitute amido alcohol molecules of the 3D matrix can be reduced to 10 components [15]. The Gaussian 03 outputs give 10 components of this matrix as $\beta_{xxx}, \beta_{xyx}, \beta_{xyy}, \beta_{yyy}, \beta_{xxz}, \beta_{xyz}, \beta_{yyz}, \beta_{xzz}, \beta_{yzz}, \beta_{zzz}$ respectively. The first hyperpolarizability were reported as different type in the literature. It was generally named as β_{vec} (β vector), $\beta_{||}$ (β parallel), β_{tot} (β total) [16]. β_{vec} is the component along the dipole moment direction. On the other hand, $\beta_{||}$ which theoretical chemists are more concerned with this, is the component parallel to the ground state charge transfer direction, and the other is the total hyperpolarizability β_{tot} . Using the x, y, z components, the total static dipole moment (μ), the linear polarizability (α) and the first hyperpolarizability (β) for the all amido alcohol molecules can be calculated by the following equations [17]:

$$\mu = \sqrt{\mu_x^2 + \mu_y^2 + \mu_z^2} \quad (1)$$

$$\alpha = \frac{\alpha_{xx} + \alpha_{yy} + \alpha_{zz}}{3} \quad (2)$$

$$\beta = \sqrt{(\beta_{xxx} + \beta_{yyy} + \beta_{zzz})^2 + (\beta_{xyx} + \beta_{xyy} + \beta_{yzz})^2 + (\beta_{xzz} + \beta_{xxz} + \beta_{yyz})^2} \quad (3)$$

In the calculation of the first hyperpolarizability, the origin of the Cartesian coordinate system was chosen as the centre of mass of the all molecules [18]. Since the values the first hyperpolarizability tensors were calculated as atomic units (a.u.), these values were converted in to electrostatic units (e.s.u.) with following equation:
 $1 \text{ a.u.} = 8.6393 \times 10^{-33} \text{ cm}^5 \text{ e.s.u.}^{-1}$.

As the experimental values for the first hyperpolarizability (β) of amido alcohols in the literature are not reported, it is difficult to conclude which basis set computes reliable values of β . The 6-31G(d,p) basis set has been a common strategy for study in many previous theoretical investigations of the NLO properties of organic molecules [19, 20]. Though it is well established that diffuse and polarization functions are required for a quantitative description of both the electronic and hyperpolarizability of medium size organic molecules [21]. It has previously been noted that the 6-311G++(d,p) basis set has been found to be more adequate for obtaining reliable hyperpolarizability (β) values [22, 23]. In this study, firstly, the effects of basis sets on calculations are investigated at the B3LYP levels with 3-21G, 6-31G, 6-31G(d), 6-31G(d,p), 6-31G+(d,p), 6-31G++(d,p), 6-311G, 6-311G(d), 6-311G(d,p), 6-311G+(d,p) and 6-311G++(d,p) basis sets and are given in Table 1.

Fig. 3 shows that the variation of the first hyperpolarizability for studying amido alcohols. It can be seen from Fig. 3 that the relative changes from one basis set to another are nearly the same for studying amido alcohols. In general, the first polarizability values obtained using 3-21G basis set for all molecules are lower than the other basis sets. However, as seen Fig. 3 and Table 1, when diffuse functions are added to these basis sets on heavy atoms and hydrogen atoms, the magnitude of hyperpolarizability increases significantly.

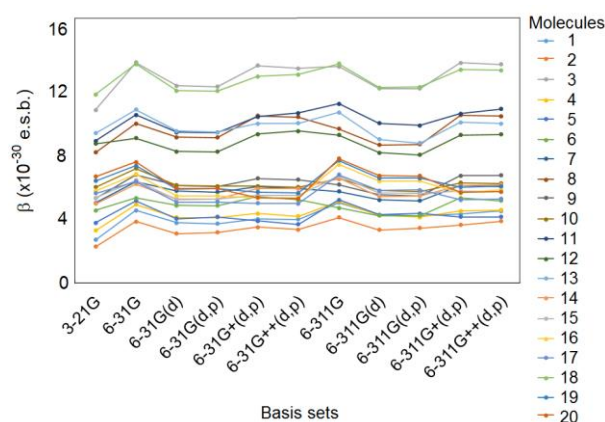


Fig. 3. Variation of the first hyperpolarizability (β) of different substitute amido alcohols at different basis sets

Table 1. Calculated components of the first hyperpolarizability (β) of 20 different substitute amido alcohol molecules at different basis sets from DFT/B3LYP calculations ($\times 10^{-30} \text{ e.s.u.}$)

Molecules	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
3-21G	2.70	2.27	10.90	3.28	3.77	4.56	5.04	8.22	5.33	6.02	8.95	8.77	9.43	4.97	5.35	5.80	5.63	11.88	6.43	6.69
6-31G	4.56	3.86	13.89	4.94	5.16	5.34	6.39	10.04	6.81	7.21	10.60	9.13	10.93	6.22	6.47	6.85	6.39	13.80	7.38	7.61
6-31G(d)	3.78	3.09	12.44	4.12	4.04	4.87	5.79	9.18	6.12	6.14	9.49	8.29	9.57	5.28	5.25	5.48	5.08	12.12	5.91	5.96
6-31G(d,p)	3.72	3.18	12.38	4.12	4.15	4.85	5.72	9.17	6.06	6.09	9.48	8.27	9.49	5.27	5.27	5.48	5.09	12.10	5.95	5.95
6-31G+(d,p)	4.02	3.50	13.70	4.37	3.89	5.42	6.07	10.54	6.57	6.08	10.48	9.38	10.05	5.93	5.53	5.35	5.01	13.02	5.72	5.37
6-31G++(d,p)	3.99	3.34	13.53	4.19	3.69	5.22	5.95	10.45	6.50	6.02	10.70	9.57	10.06	5.93	5.53	5.37	4.99	13.13	5.65	5.30
6-311G	5.05	4.11	13.65	5.12	5.22	4.72	5.75	9.71	6.19	6.56	11.30	9.32	10.75	6.59	6.71	7.46	6.82	13.82	7.71	7.84
6-311G(d)	4.28	3.32	12.25	4.27	4.28	4.23	5.22	8.70	5.56	5.81	10.07	8.21	9.05	5.44	5.66	6.41	5.81	12.32	6.59	6.75
6-311G(d,p)	4.23	3.44	12.25	4.13	4.37	4.22	5.17	8.73	5.48	5.76	9.92	8.07	8.81	5.48	5.64	6.43	5.85	12.36	6.60	6.74
6-311G+(d,p)	4.32	3.65	13.88	4.53	4.15	5.35	6.14	10.58	6.76	6.30	10.67	9.32	10.12	6.13	5.80	5.65	5.23	13.45	6.02	5.70
6-311G++(d,p)	4.53	3.66	13.79	4.58	4.16	5.16	6.07	10.51	6.78	6.26	10.97	9.35	10.04	6.19	5.75	5.85	5.28	13.41	6.08	5.74

Table 2. Calculated dipole moment (μ), the linear polarizability (α) and the first hyperpolarizability (β) for 20 different substitute amido alcohols at B3LYP/6-311G++(d,p) level

Molecules	1	2	3	4	5	6	7	8	9	10
Parameters										
μ_x	-0.066	-0.831	3.180	0.364	0.241	5.481	-5.317	0.372	-3.413	-2.913
μ_y	2.852	-2.141	1.470	-0.700	-0.747	-2.460	1.395	-6.113	3.809	4.185
μ_z	1.303	2.160	1.662	1.960	1.955	-0.953	2.062	1.696	1.938	1.956
μ (D)	3.137	3.153	3.878	2.113	2.107	6.083	5.871	6.355	5.469	5.461
α_{xx}	175.507	230.288	249.405	242.531	248.637	137.553	189.798	207.330	198.627	205.642
α_{xy}	10.418	34.403	46.412	44.581	47.877	9.131	29.509	40.033	39.679	41.627
α_{yy}	111.099	204.877	243.355	233.416	248.306	96.718	191.743	230.061	221.027	236.429
α_{xz}	-29.095	-44.597	-48.429	-43.401	-41.754	-3.242	-17.648	-21.982	-15.907	-15.115
α_{yz}	-13.266	-11.483	-4.547	-7.542	-5.368	-11.062	-6.715	-0.229	-2.883	-0.726
α_{zz}	243.327	296.970	303.985	300.683	304.744	189.029	242.051	248.786	247.960	250.926
α (a.u)	176.644	244.045	265.582	258.877	267.229	141.100	207.864	228.726	222.538	230.999
α (Å³)	26.18	36.17	39.36	38.37	39.60	20.91	30.81	33.90	32.98	34.23
β_{xxx}	63.894	59.822	36.950	17.453	39.388	78.896	86.053	46.372	47.038	73.701
β_{xxy}	-13.116	-27.431	121.093	-75.064	-53.761	0.185	-1.522	75.036	-49.616	-25.840
β_{xyy}	19.543	-22.398	505.164	-92.005	-74.890	26.627	-27.278	380.563	-102.474	-91.672
β_{yyy}	3.338	49.883	1242.299	-169.425	-79.136	-14.372	-31.139	1043.667	-290.152	-212.781
β_{xxz}	40.346	72.294	77.782	51.633	60.122	-41.401	-13.958	-0.830	-32.917	-20.910
β_{xyz}	31.055	64.149	92.749	39.702	45.655	33.171	70.637	114.658	48.769	56.626
β_{yyz}	89.896	117.581	142.806	99.607	92.833	31.913	100.176	161.547	82.224	78.649
β_{xzz}	99.552	94.494	100.208	92.353	103.282	7.073	-12.304	-31.287	-29.608	-18.538
β_{yzz}	14.979	14.380	12.381	9.382	29.148	-68.029	-137.022	-158.728	-154.565	-140.635
β_{zzz}	-621.620	-590.475	-713.371	-625.719	-618.155	589.828	593.848	472.595	554.873	559.184
β (a.u)	524.370	423.367	1596.297	529.832	481.424	596.851	702.455	1216.213	785.258	725.095
β (10^{-30} e.s.u.)	4.53	3.66	13.79	4.58	4.16	5.16	6.07	10.51	6.78	6.26
xtimes urea	12.1	9.8	37.0	12.3	11.2	13.8	16.3	28.2	18.2	16.8
Molecules	11	12	13	14	15	16	17	18	19	20
Parameters										
μ_x	-0.035	-0.084	5.236	-0.915	-0.839	1.660	2.215	-1.705	1.017	0.907
μ_y	-1.556	-0.825	0.697	-0.841	-0.917	-2.766	-1.248	3.100	0.638	0.726
μ_z	-1.756	-1.837	2.202	-2.050	-2.057	-1.332	-2.139	-1.905	-2.071	-2.051
μ (D)	2.346	2.015	5.723	2.398	2.403	3.490	3.322	4.019	2.394	2.358
α_{xx}	132.924	179.111	200.649	192.837	199.349	131.621	186.428	205.051	196.094	204.221
α_{xy}	2.348	9.750	13.560	40.138	44.226	9.090	30.374	40.897	40.232	44.125
α_{yy}	85.158	158.072	165.691	219.500	233.706	101.527	195.627	234.829	224.817	239.006
α_{xz}	-0.826	-30.362	-34.801	-17.187	-15.942	-3.689	-19.068	-22.632	-16.896	-16.634
α_{yz}	-7.288	-19.570	-29.599	-3.813	-1.613	-11.347	-8.316	-1.686	-3.586	-3.435
α_{zz}	205.823	305.653	333.798	56.997	246.840	201.522	254.007	260.254	258.765	262.696
α (a.u)	141.302	214.279	233.379	156.445	226.632	144.890	212.021	233.378	226.559	235.308
α (Å³)	20.94	31.76	34.59	23.19	33.59	21.47	31.42	34.59	33.58	34.87
β_{xxx}	63.847	31.399	-74.124	42.071	69.181	85.467	82.976	49.868	45.989	68.268
β_{xxy}	-29.832	-48.378	-77.181	-60.610	-39.538	-6.264	-13.181	96.942	-59.223	-41.198
β_{xyy}	28.440	14.188	-12.065	-78.921	-66.632	31.524	-7.765	458.491	-78.436	-66.571
β_{yyy}	-33.604	-35.925	-82.181	-166.814	-91.388	2.897	42.817	1180.833	-189.144	-100.098
β_{xxz}	26.678	76.569	134.065	56.997	69.058	60.370	88.519	98.272	64.069	79.693
β_{xyz}	-12.324	38.173	37.029	35.842	46.193	32.051	63.034	97.589	37.583	49.013
β_{yyz}	-1.020	22.630	54.095	35.999	33.347	67.083	88.284	120.601	69.376	66.910
β_{xzz}	44.926	-58.704	-40.819	2.501	16.647	9.809	13.384	0.132	5.180	15.914
β_{yzz}	24.396	-53.543	-21.212	27.657	44.840	18.793	36.995	27.730	31.555	50.455
β_{zzz}	-1287.350	-1172.866	-1328.557	-780.472	-762.414	-792.347	-777.796	-885.789	-802.000	-804.008
β (a.u)	1269.731	1082.559	1161.569	716.736	665.877	677.053	611.132	1551.671	703.362	663.885
β (10^{-30} e.s.u.)	10.97	9.35	10.04	6.19	5.75	5.85	5.28	13.41	6.08	5.74
xtimes urea	29.4	25.1	26.9	16.6	15.4	15.7	14.2	35.9	16.3	15.4

On the other hand, the first hyperpolarizability of all molecules were generally calculated smallest at 3-21G, biggest at 6-31G and 6-311G basis sets as seen in Fig. 3 and Table 1. However, when the diffuse functions were added, the calculated values were more stable. Therefore, the results obtained with the addition of diffuse functions in calculations are more meaningful as in the literature [22, 23]. The calculated dipole moment (μ), the linear polarizability (α) and the first hyperpolarizability (β) have

been performed at the B3LYP method with 6-311G++(d,p) level for the all substitute amido alcohols to provide its nonlinear properties, and are listed in Table 2. On the other hand, urea is one of the reference materials and frequently used for comparative purpose in the study of the NLO properties. The dipole moment (μ), the linear polarizability (α) and the first hyperpolarizability (β) were calculated using DFT/B3LYP method and 6-311G++(d,p) basis set at 1.3732 D, 3.8312 Å³ and 0.3729×10^{-30}

$\text{cm}^5\text{e.s.u.}^{-1}$ respectively for urea molecule. Urea crystals attract the attention of both theoreticians and experimentalist due to the NLO piezoelectric properties. On the other hand, urea is representative of one class of materials, which are applicable to photonics and reference material in the DMOS (diffusive mixing of organic solution) experiment in microgravity carried out by NASA.

They are potentially useful materials for frequency doubling of near IR laser radiation single crystals of the materials which have very high laser damage threshold. NLOs are playing a major role in emerging photonic and optoelectronic technologies. Therefore, new NLO frequency conversion materials have a significant impact on laser technology and optical data storage. The dipole moment is an important property of a molecule, used to investigate intermolecular interactions. Higher the dipole moment, stronger is the intermolecular interaction. The small band gap and high dipole moment of amido alcohols may contribute to multiply its NLO activity. The dipole moments were calculated between 2.015 and 6.355 D in all different substitute amido alcohols. The smallest dipole moment was performed in molecule 5, while highest dipole moment was calculated in molecule 8. The linear polarizability (α) for the 20 different substitute amido alcohol molecules was calculated between 20.91 and 39.60 \AA^3 . The calculated value of α for urea molecule is 3.8312 \AA^3 . Thus, all of the amido alcohol molecules were performed greater than the α value of urea molecule. The first hyperpolarizability (β) of all amido alcohol molecules were calculated between 3.34×10^{-30} and $13.79 \times 10^{-30} \text{ cm}^5 \text{ e.s.u.}^{-1}$. The calculated values of the first hyperpolarizability (β) for the selected compounds are greater at least ten times than this of urea (the β of urea is $0.37289 \times 10^{-30} \text{ cm}^5 \text{ e.s.u.}^{-1}$ obtained by B3LYP/6-311G++(d,p) method). The highest β was performed to be $13.79 \times 10^{-30} \text{ cm}^5 \text{ e.s.u.}^{-1}$ in molecule 3. Theoretically, the first-order hyperpolarizability (β) of the molecule 3 is of 37.0 times higher than urea. In addition, it has been observed that this molecule has higher β value than similar molecules in the literature. For example, the β value of (E)-N²-(furan-2-ylmethylene) nicotinohydrazide (F2CNH) was calculated as $2.09 \times 10^{-30} \text{ cm}^5\text{e.s.u.}^{-1}$ with same basis set. The β value of molecule 3 is of 6.6 times higher than F2CNH [24]. These results indicate that the all amido alcohol molecules possess good nonlinear optical properties [25, 26].

4. Conclusion

In this present investigation, we have reported theoretical calculation of the nonlinear optical (NLO) properties of twenty different substitute amido alcohols. Firstly, the most appropriate basis set was determined as 6-311G++(d,p) with calculating different basis sets. Then, the molecular properties have been calculated by using DFT/B3LYP method with same basis set. The optimized molecules show that the amido alcohol molecules have an

intramolecular interaction. The calculated dipole moment (μ), the linear polarizability (α) and the first hyperpolarizability (β) have been performed for the all substitute amido alcohols between 2.015 and 6.355 D, between 20.91 and 39.60 \AA^3 , between 3.34×10^{-30} and $13.79 \times 10^{-30} \text{ cm}^5 \text{ e.s.u.}^{-1}$ respectively. The results indicated a good nonlinear optical property of all amido alcohol molecules. In addition, the molecule 3 shows the most nonlinear optical property and the molecule 10 has the highest electron accepting ability among all amido alcohol molecules.

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