

Degradation mechanisms of selected aminopolycarboxylic acid molecules by DFT method

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In this study, pentetic acid or diethylenetriamine pentaacetic acid (DTPA), ethylenediamine tetraacetic acid (EDTA) and hydroxyethylenediamine tetraacetic acid (HEDTA) were investigated, selected from the group of aminopolycarboxylic acids (APCA), which are chemical compounds in which one or more nitrogen atoms are bonded to two or more carboxyl groups *via* carbon atoms and used in various chemical, medical, and environmental applications. The toxicological properties of these compounds are important for both human health and environment. Aminopolycarboxylic acids, such as EDTA and DTPA, are compounds that can persist in the environment and are difficult to biodegrade. Therefore, the risk of EDTA becoming a "persistent organic pollutant," is being discussed. Environmental degradation generally occurs through sunlight, and this process is slow which increases the risk of accumulation in wastewater and natural environment. The ability of these acids to bind metal ions can reduce the bioavailability of some metals in aquatic environments and lead to imbalances in ecosystems. This and similar factors have led to the investigation of the degradation pathways of these molecules in nature.

The aim of this study is to theoretically elucidate the fate of both the main molecule and its hydroxylated fragments in nature as they enter the natural cycle as a result of mixing with wastewater. Geometric optimizations of the fragments were performed using the DFT/B3LYP/6-31G(d) basis set of quantum mechanical density functional theory (DFT) to theoretically determine all possible reaction pathways of the selected molecules with the OH radical.

Keywords: DFT, aminopolycarboxylic acids (APCA), DTPA, EDTA, HEPTA

INTRODUCTION

An aminopolycarboxylic acid (APCA) is a chemical compound containing one or more nitrogen atoms bonded to two or more carboxyl groups *via* carbon atoms. Aminopolycarboxylates, that have lost their acidic protons, form strong complexes with metal ions. This property makes APCAs useful complexing agents in a wide variety of chemical, medical and environmental applications [1]. APCAs are synthetic chelators because they contain multiple carboxylate and amine groups and can form strong, stable complexes with metal ions. The most used of these compounds are: pentetic acid or diethylenetriamine pentaacetic acid (DTPA), ethylenediamine tetraacetic acid (EDTA) and hydroxyethylenediamine tetraacetic acid (HEDTA) [2, 3].

DTPA consists of a diethylenetriamine structure with five carboxymethyl groups. The DTPA molecule can be seen as an extended version of EDTA and is used similarly.

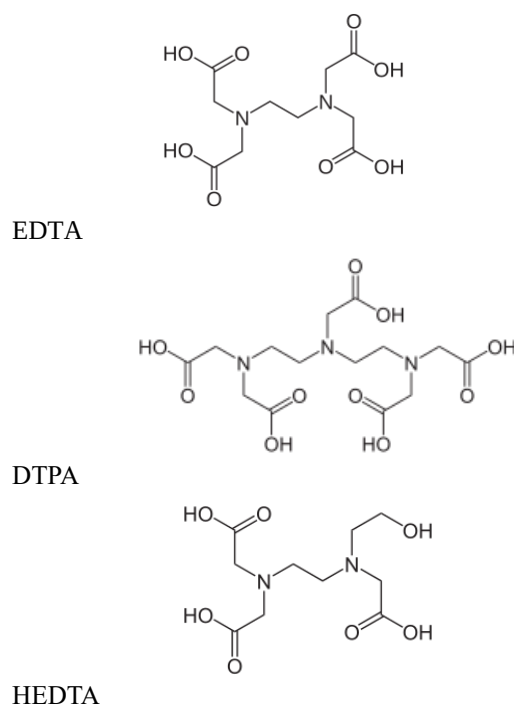


Figure 1. Two-dimensional representations of DTPA, EDTA, and HEDTA molecules

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It is a white solid with limited solubility in water. In the textile industry, EDTA is used to bind metal ions in aqueous solution, preventing dyed products from changing color. In the pulp and paper industry, EDTA inhibits the ability of metal ions, particularly Mn^{2+} , to catalyze the disproportionation of hydrogen peroxide used in chlorine-free bleaching. While it is used as a preservative or stabilizer in some foods to prevent catalytic oxidative discoloration catalyzed by metal ions, in the cosmetics industry, EDTA salts are used in shampoos, cleaners, and other personal care products to improve their stability in air [4-6]. Sodium calcium edetate, an EDTA derivative, is used to bind metal ions in chelation therapy for conditions such as mercury and lead poisoning. It is also used to remove excess iron from the body. This therapy is used to treat complications of repeated blood transfusions, as well as in the treatment of thalassemia [7].

EDTA is used so widely that questions are being raised about whether it is a persistent organic pollutant. While EDTA has many positive functions in industrial, pharmaceutical, and other fields, its longevity can cause serious problems for the environment. EDTA degrades slowly, mostly abiotically in the presence of sunlight [8]. EDTA and its derivatives are widely used in wastewater treatment, particularly for binding and removal of heavy metal ions, and as stabilizers in the food and cosmetics industries [9, 10]. DTPA stands out as a radionuclide carrier in nuclear medicine and as an industrial cleaning agent, while HEDTA is preferred in agricultural micronutrient fertilizers and detergent formulations [11]. The widespread use of these compounds leads to their accumulation as persistent organic pollutants in environmental settings and the emergence of potential ecotoxicological risks [12]. Owing to their high chemical stability and difficult biological degradation, APCAs such as EDTA and DTPA are detected in wastewater, surface, and groundwater [13, 14]. EDTA is among the substances recommended for monitoring under the European Union Water Framework Directive and attracts attention due to its environmental persistence [15]. The fate of these compounds in the environment is closely related to the toxicological profiles not only of the parent molecules but also of their degradation products. For example, nitrilotriacetic acid (NTA), formed during the environmental degradation of EDTA, is classified as a probable human carcinogen (group 2B) by the International Agency for Cancer Research (IARC) [16].

To understand the environmental fate and toxicological effects of APCAs, it is necessary to

examine the degradation mechanisms of these molecules in detail. Degradation processes occurring under environmental conditions (light, pH, microbial activity) are generally slow and lead to the formation of intermediate products rather than complete mineralization [17]. Therefore, the persistence and potential risks of APCAs in the environment are investigated not only by experimental studies but also by computational chemistry methods. Density functional theory (DFT) stands out as a powerful tool in understanding chemical reactions and degradation mechanisms at the molecular level. DFT-based studies play an important role in elucidating the structural properties of APCA metal complexes, bond breaking energies, and possible intermediate formation pathways [18]. Recent DFT studies have shown that the key step in the biodegradation of chelators such as EDTA and S, S-EDDS is the breaking of the C–N bond, and the energy barrier required for this step determines the environmental persistence of the compound [19]. Similarly, the environmental degradation mechanisms of derivatives such as DTPA and HEDTA, and the toxicological profiles of their intermediates are better understood thanks to calculations made with DFT.

The molecules to be examined are organic compounds. Recent studies show that organic pollutants are present in water at very low concentrations. Therefore, purifying drinking water from organic pollutants is very important. Sunlight on Earth helps to naturally purify lakes, rivers, and other water systems. Large organic molecules are broken down into smaller molecules by sunlight [20, 21]. Organic compounds undergo photolysis by reacting with OH radicals, and this is the most dominant decomposition reaction in the atmosphere. Biomolecules, which are hydroxyl scavengers at various rates, are specific detectors for hydroxyl radicals due to their hydroxylation capabilities. Any hydroxyl radical attack on an aromatic compound result in the formation of a hydroxylated product, and these newly formed products can be far more harmful than the original products at the beginning of the process. Therefore, monitoring these products is very important. The OH radical acts as an electrophile in its reaction with any organic molecule and therefore readily binds to unsaturated bonds, while the O radical is a nucleophile and therefore does not interact with these bonds. When an aliphatic side chain is attached to an aromatic molecule, the OH radical prefers the aromatic ring to bind to [21-29].

The main objective of this study is to track the initial products released into the environment, as

well as the new products that may be more dangerous as a result of a degradation reaction, and to explain the degradation reaction. Because the decomposition reactions of organic pollutants can produce products that are even more harmful than the main pollutants themselves, knowledge of intermediate products is crucial for air and water treatment. The reactions that cause organic pollutants to disappear in the atmosphere are those involving OH, NO₃ radicals, O₃, and Cl atoms. Among these radicals, the most active are those involving OH radicals. Knowing the half-lives of these substances in the troposphere is the most important factor in providing information about whether they will be transported to the stratosphere [30-32].

MATERIALS AND METHODS

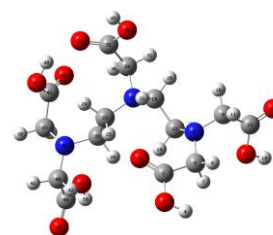
In order to theoretically determine all possible reaction pathways for the molecules under study, geometric optimizations were performed using the DFT/B3LYP/6-31G(d) basis set of the quantum mechanical density functional theory (DFT), an electronic structure method. Energy values for all fragments were calculated using the Gauss View 6 molecular representation program and the Gaussian16 program for trajectory calculations, and geometric optimizations [33]. The fragmentation reaction energy is affected by the water molecules in the aqueous medium. In addition, the geometric stress in the solutions is triggered by H₂O. In other words, the presence of a dielectric medium such as H₂O causes the geometry associated with the solute to relax and has a stabilizing effect by reducing the energy of this mechanism [21]. Therefore, in this study, the CPCM in the COSMO (conductor-like shielding solvation model) solvent model in the Gaussian 16 package was used to explain the solvent effect of the H₂O molecule +. OH reaction [33].

Gaussian 16 is a comprehensive program that includes molecular mechanics, quasi-empirical and ab initio methods. It offers a wide range of theory and fundamental set options for all three methods. The program enables the calculation of atomic and molecular energies, geometric optimizations, and the calculation of vibration frequencies, force constants, and dipole moments. Gauss View 6 is a graphical interface designed for creating input files and visualizing outputs for Gaussian package programs. Gauss View 6 allows us to rotate, move, and arrange molecules as desired by visualizing them. It also easily prepares input files even for complex calculations. It allows us to graphically examine the results calculated by the Gaussian 16 program. These results may include optimized

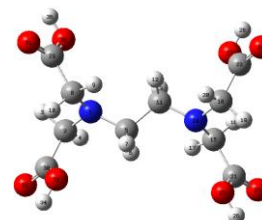
molecular structures, molecular orbitals, electrostatic potential surfaces, atomic charges, IR, Raman, and NMR spectra, and normal mode animations based on vibration frequencies [33].

Since the reactions of molecules with the OH radical are important for both water treatment and atmospheric chemistry, calculations were performed in both gas phase and water phase using the COSMO (conductor-like screening solvation model) model, using CPCM. The Mulliken charges of molecules, the electronegative atoms in the molecule and the arrangement of the atoms surrounding them, stable double bonds, weak bonds at the ends of the molecule, calculated energies, bond lengths, and bond angles between atoms were examined, and these data helped select all the fragments that would determine the degradation mechanism. By examining the molecules for their reactions with OH radicals in air or water, the degradation reaction of each molecule was documented, starting with the lower-energy fragments, and their fate in nature was determined.

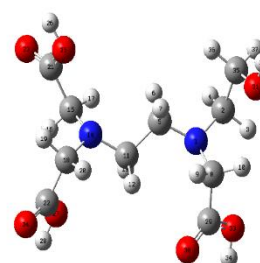
RESULTS AND DISCUSSION



DTPA



EDTA



HEDTA

Figure 2. Geometric structure of DTPA, EDTA, and HEDTA molecules optimized by the DFT method (C atom is shown in gray, O atom in red, N atom in blue, and H atom in white)

Figures 1 and 2 show the two-dimensional and the optimized geometric structures of the three molecules studied. Double bonds in molecules are stable structures. If they are to be separated from the molecule, they initially do not want to separate. Single bonds at the ends of the molecule indicate atoms that can be removed from the compound. When writing the fragmentation path, the first thing to consider is whether there is a closed loop or double bond in the molecule, and what kind of arrangement exists around electronegative atoms. Table 1 shows the bond lengths, bond angles, and Mulliken charges of electronegative atoms in the DTPA molecule.

Table 1. Bond lengths, bond angles, and Mulliken charges of electronegative atoms in the DTPA molecule

Bond Lengths	(Å)	Bond Angles	(°)	Mulliken Charges
C ₁₅ O ₁₇	1.35797	C ₉ C ₁₅ O ₁₇	113.42037	O ₂ -0.429521
C₉C₁₅	1.53616	N₈C₉C₁₅	119.28590	O₃ -0.563245
N ₈ C ₉	1.44302	N ₈ C ₅ C ₁	112.81975	C ₅ -0.257605
C ₅ N ₈	1.44279	C ₅ C ₁ O ₃	113.98490	N ₈ -0.356586
C₅C₁	1.53410	C₅N₈C₁₂	116.33977	C ₉ -0.250553
O ₃ C ₁	1.36111	N ₈ C ₁₂ C ₁₉	111.70246	C ₁₂ -0.133821
C ₁₂ N ₈	1.46684	C ₁₂ C ₁₉ N ₂₂	110.38509	O ₁₆ -0.450194
C₁₂C₁₉	1.53677	C ₁₉ N ₂₂ C ₂₃	114.81808	O₁₇ -0.562539
N ₂₂ C ₁₉	1.46522	N ₂₂ C ₂₃ C ₂₆	112.17940	C ₁₉ -0.138476
C ₂₉ N ₂₂	1.46245	C ₂₃ C ₂₆ N ₃₅	111.32709	N ₂₂ -0.393991
N ₂₂ C ₂₃	1.47242	C₂₆N₃₆C₄₀	117.01964	C ₂₃ -0.170861
C₂₃C₂₆	1.54726	N₃₆C₄₀C₄₄	119.41875	C ₂₆ -0.153528
C ₂₆ N ₃₆	1.47102	N ₃₆ C ₃₇ C ₄₃	110.06062	C ₂₉ -0.228362
N ₃₆ C ₃₇	1.46362	N ₂₂ C ₂₉ C ₃₂	114.12929	O ₃₃ -0.485948
N ₃₆ C ₄₀	1.44105	C ₂₉ C ₃₂ O ₃₄	112.38119	O₃₄ -0.547331
C₄₀C₄₄	1.53665	C ₄₀ C ₄₄ O ₄₉	113.45427	N ₃₆ -0.374885
C ₄₄ O ₄₉	1.35604	C ₃₇ C ₄₃ O ₄₇	112.69966	C ₃₇ -0.169482
C ₃₇ C ₄₃	1.52521	C ₃₇ N ₃₆ C ₄₀	114.77181	C ₄₀ -0.244046
C ₄₃ O ₄₇	1.34136	C₁₉N₂₂C₂₉	115.70621	C ₄₀ -0.244046
		C₅N₈C₉	116.20264	O ₄₅ -0.466818
		C₉N₈C₁₂	115.42464	O ₄₆ -0.457541
				O₄₇ -0.566968
				O₄₉ -0.555565

When examining the Mulliken charges in Table 1, the most electronegative atoms are dark colored

These are shown with the following values: O₄₇ - 0.566968, O₃ -0.563245, O₁₇ -0.562539, O₄₉ - 0.555565. Following these are O₃₃, O₄₅, O₄₆, O₁₆, O₂, N₂₂, and N₈. If we were to try to predict the decay path by only looking at these electronegative atoms, decay would be expected to occur at this stage.

Looking at the bond lengths in Table 1, the longest bond lengths are highlighted in dark color. These are, in order, the C-C bond lengths of C₂₃C₂₆, C₁₂C₁₉, C₄₀C₄₄, C₉C₁₅, C₅C₁. Following these are the C-N bond lengths of N₂₂C₂₃, C₂₆N₃₆, C₁₂N₈, N₂₂C₁₉, C₂₉N₂₂, ... If we try to predict the decay path by only looking at the bond lengths between these pairs of atoms, decay would be expected to occur in that order.

Again, when examining the bond angles in Table 1, the widest bond angles are highlighted in dark color. These are the bond angles between the C-N-C atoms N₃₆C₄₀C₄₄, N₈C₉C₁₅, C₂₆N₃₆C₄₀, C₅N₈C₉, C₁₉N₂₂C₂₉, and C₉N₈C₁₂, respectively. If we try to predict the decay path by only looking at the bond angles between these three atoms, decay would be expected to occur at this stage.

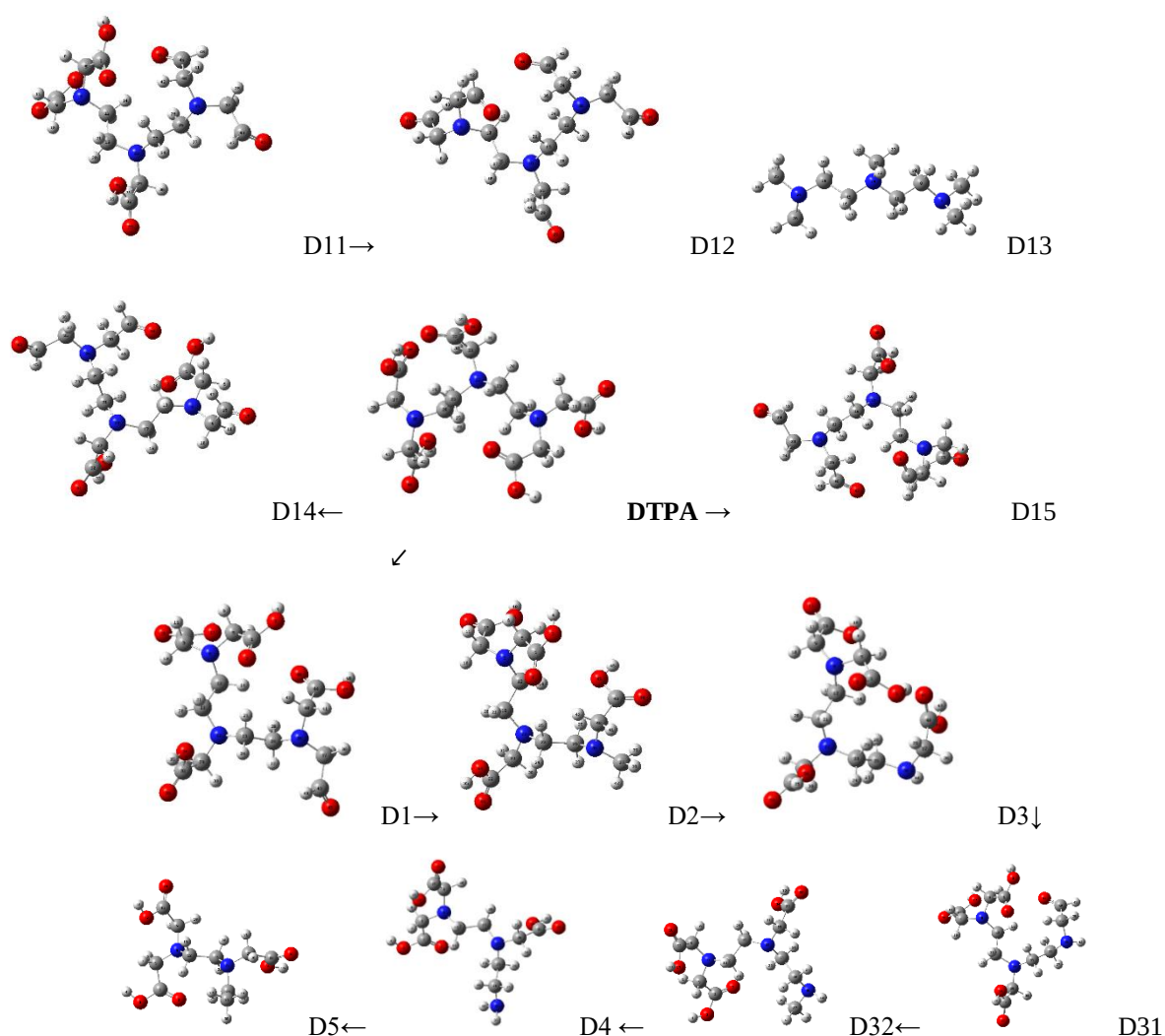
While one might expect the fission process to begin with atoms that have the longest bond lengths, atoms with the widest bond angles, or atoms surrounding the most electronegative atom, making the choice isn't that simple.

Table 2 presents the energy, enthalpy, and Gibbs free energy values for the three molecules studied, in both the gas and water phases, respectively, in atomic mass units. The values for the fragments are only for the gas phase. The reason for giving the energy values in atomic mass units (AU) is that the digits after the decimal point are very close to each other when converted to SI units.

Energy values are a determining factor for the decomposition pathway, as the pathway is written starting from the lowest energy value. The energy values in this table show that, without any external influence, molecules and their fragments spontaneously react with negative energy values and return to nature in the gaseous phase.

Table 2. ΔE , ΔH , ΔG (Au) values of DTPA, EDTA and HEDTA molecules and their fragments in the degradation pathways, respectively.

(AU)	DTPA	D1	D11	D2	D14
ΔE	-1463.395214	-1388.152850	-1312.906205	-1274.847813	-1237.659647
ΔH	-1463.394270	-1388.151906	-1312.905261	-1274.846869	-1237.658703
ΔG	-1463.489906	-1388.247331	-1312.999051	-1274.936787	-1237.750728
	D3	D15	D31	D32	EDTA
	-1235.576589	-1162.423835	-1160.326589	-1047.020875	-1095.762452
	-1235.575645	-1162.422891	-1160.325645	-1047.019931	-1095.761508
	-1235.660255	-1162.512971	-1160.409956	-1047.101265	-1095.841083
	D12	HEDTA	D4	H1	D5
	-1087.178138	-1021.991923	-1007.742701	-947.129545	-952.422596
	-1087.177193	-1021.990979	-1007.741756	-947.128601	-952.421652
	-1087.265588	-1022.067206	-1007.819769	-947.203927	-952.496679
	D6	D7	D8	D9	D10
	-913.137940	-873.860150	-798.614399	-685.312181	-646.033802
	-913.136996	-873.859206	-798.613455	-685.311237	-646.032858
	-913.208954	-873.926720	-798.679580	-685.371004	-646.089233
	D13	DTPA (water)	EDTA (water)	HEDTA (water)	
	-520.674327	-1463.429359	-1095.798667	-1022.023250	
	-520.673383	-1463.428415	-1095.797722	-1022.022306	
	-520.731514	-1463.528972	-1095.875473	-1022.098166	



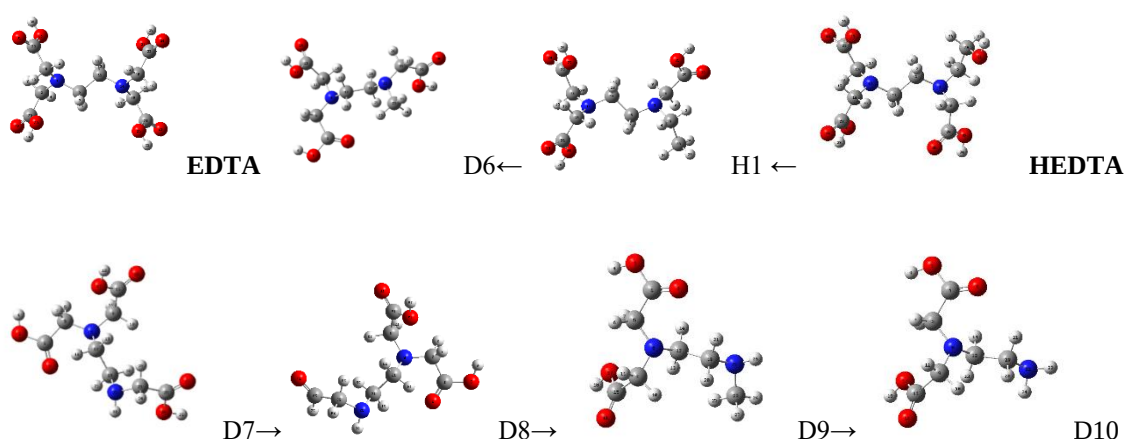


Figure 3. Designed degradation pathways for DTPA, EDTA, and HEDTA molecules

By examining all values in Figure 2 and Tables 1 and 2, that is, by looking at the bond lengths, bond angles, and Mulliken charges between electronegative atoms within the molecules and the atoms around them and supporting this with energy values, the degradation pathway shown in Figure 3 was determined.

Table 3. Half-life for the molecules studied [43-45]

Period	EDTA	DTPA	HEDTA
Photodegradation ($\lambda > 290$ nm, pH 7) half-life	20–30 days	10–15 days	18–25 days
Aerobic biological half-life (20 °C, activated sludge)	<10 %/60 days	<5 %/60 days	12 %/60 days
Soil	10–30 L/ kg (very mobile)	15–40	20–35
Wastewater treatment plant outlet average concentration.	35–120 $\mu\text{g/L}$	5–25 $\mu\text{g/L}$	2–10 $\mu\text{g/L}$

CONCLUSION

In the literature, EDTA and its derivatives are safely used in chelation therapies (e.g., in the treatment of lead and mercury poisoning) for human health. However, it is known that high doses or prolonged exposure can negatively affect kidney function and lead to the excretion of important minerals from the body. When used as a stabilizer in food and cosmetic products, according to international toxicology reports, it is considered safe only within the specified limits [34]. In terms of human and animal toxicity, $\text{CaNa}_2\text{-EDTA}$ and $\text{CaNa}_3\text{-DTPA}$ are FDA-approved chelators in lead/plutonium poisoning [35]. Parenteral administration of EDTA can cause significant decreases (15-40%) in serum calcium and zinc

levels, and cases of hypercalcaemic tetany have been reported [36]. In terms of renal and electrolyte imbalance, repeated EDTA infusions reduced glomerular filtration rate by 25% in rats [37]. Repeated administration of EDTA has been shown to reduce renal function, while urinary Ca^{2+} excretion increases fivefold after intravenous administration of DTPA [38]. In terms of in vitro genotoxicity, EDTA was found not to be genotoxic in the micronucleus test, but the Fe-EDTA complex increased reactive oxygen species (ROS) production by 180% [39].

In terms of regulation and limit values, the EU Water Framework Directive EQS-recommendation for EDTA is an average of 2.2 $\mu\text{g/L}$, the USEPA maximum secondary contaminant level (SMCL) for EDTA in drinking water is 0.25 mg/L, Cosmetics Europe's total release limit for EDTA is 2%, and the FAO/WHO JECFA acceptable daily intake (ADI) for EDTA in food is 2.5 mg/kg body weight [46-49]. When selected molecules are released onto the market, whether for therapeutic use or simply for disposal at the end of their shelf life, these organic compounds enter the natural cycle due to a lack of awareness in our country. Whether medical, commercial, or general waste, these organic compounds and their fragments enter the natural cycle. The half-lives of the molecules studied are presented in Table 3. They constitute a significant group of air and water pollutants. To remove these residues which persist in the environment for days from air and water, it is necessary to elucidate their degradation mechanisms.

Experimental kinetic data regarding the gas-phase and water-phase reactions of selected molecules with OH radicals are available in the literature. However, the reaction mechanisms of these substances have not been fully determined. In this study, the reactions of selected molecules with

OH radicals were investigated, and their degradation mechanisms were calculated using the DFT method. First, the gas-phase reactions were finalized, and their energy values in aqueous environments were also examined under the influence of water, due to their potential to cause pollution in wastewater. The mechanism of the reactions of the compounds with OH radicals in the atmosphere and in water was fully elucidated, and the reaction products were also fully identified. The findings were also evaluated from an environmental and toxicological perspective. Thus, the aim was to provide a more holistic view of the environmental fate and potential risks of these compounds.

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