Advance Sustainable Science, Engineering and Technology (ASSET)
Vol. 8, No.4, October 2026, pp. 02604030-01 ~ 02604030-011
ISSN: 2715-4211 DOI: https://doi.org/10.26877/asset.v8i4.2990

Electronic Structure–Property Relationships in Ketohexoses: Implications for Crystal Engineering and Functional Rare Sugar Materials

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Abstract. Rare sugars have garnered significant attention owing to their beneficial biological activities and their potential applications in sustainable materials, agriculture, and medicine. However, despite extensive crystallographic and hydrogen-bonding studies, the electronic factors governing their molecular stability and crystal packing are still not fully understood. In this study, the DV-Xα molecular orbital method was employed to systematically analyze intramolecular charge distribution in ketohexoses, comparing D-chiral and D,L-racemic forms. The results reveal a clear distinction between two types of electronic behavior: (i) electronically stable sites (C2 and C5), where charge variation remains minimal (typically < 1 %), and (ii) adaptive sites (C3, C4, and C6), where charge distribution exhibits significant responsiveness to molecular environment. This finding provides a new electronic-structure-based framework that explains how localized charge stability and flexibility cooperatively govern crystal packing and intermolecular interactions, particularly hydrogen bonding. Even subtle variations in charge (< 1 %) were found to be chemically meaningful, as they systematically influence interaction patterns across different ketohexoses. These insights go beyond conventional structural analyses by establishing a direct link between intramolecular electronic structure and macroscopic material behavior. The present approach offers a foundation for rational design and functionalization of rare sugars in applications such as crystal engineering, pharmaceuticals, and sustainable agrochemical materials.

Keywords: Crystal engineering, Electronic polarization, Ketohexose, Rare sugar, Structure–property relationship

(Received 2025-11-15, Revised 2026-08-15, Accepted 2026-08-17, Available Online by 2026-10-31)

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1. Introduction

Monosaccharides constitute the most fundamental class of carbohydrates consisting of a single sugar unit that cannot be further hydrolyzed. They are classified into naturally abundant monosaccharides and rare sugars, with the latter defined by the International Society of Rare Sugars as “monosaccharides and their derivatives that occur only in limited quantities in nature.[1]” Monosaccharides can be broadly divided into two categories: aldoses, which possess an aldehyde group, and ketoses, which contain a ketone group. Among the ketoses, the six-carbon sugars, known as ketohexoses, comprise four types: fructose, psicose, tagatose, and sorbose. Their Fischer projection formulas are illustrated in Figure 1. Hexoses follow an internationally established numbering convention, in which the six carbon atoms are sequentially designated from C1 to C6, as also shown in Figure 1.

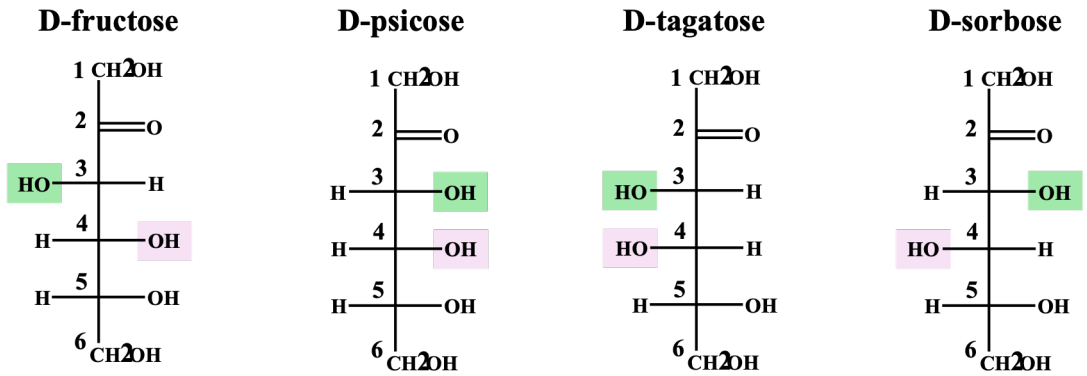


Figure 1. Fischer projections of ketohexoses.

Previous studies have demonstrated that rare sugars possess a variety of beneficial physiological activities[2-7]. For example, D-allulose (D-psicose) exhibits approximately 70 % of the sweetness of sucrose while being virtually calorie-free, and has been shown to suppress weight gain. In 2014, it was granted Generally Recognized As Safe (GRAS) status by the U.S. Food and Drug Administration (FDA), enabling its use in food applications. Furthermore, in 2020, D-tagatose was reported by Mochizuki and co-workers at Kagawa University to suppress plant diseases, leading to its development as an “edible pesticide.[8]” Owing to such unique properties not observed in naturally abundant monosaccharides, rare sugars are now being applied across diverse fields, including medicine, agriculture, and food science.

Our laboratory has long been engaged in single-crystal structural analyses of a wide range of rare sugars [9-12]. For example, in the case of ketohexoses, we have successfully determined the crystal structures of D-psicose in its chiral form, as well as all four species in their racemic forms, thereby elucidating both their molecular and crystal structures. In addition, by performing molecular orbital calculations, we have pursued a deeper understanding of their electronic states [9-12]. Recent findings demonstrated that sorbose and its derivatives consistently exhibit the strongest hydrogen bonding between the O3 and O4 groups, which plays a pivotal role in crystal formation. In contrast, such a strong hydrogen-bonding was not observed in tagatose derivatives, suggesting that despite their strikingly similar molecular frameworks, each ketohexose possesses a distinct electronic structure.

Despite significant progress in crystallographic analysis and hydrogen-bond characterization of rare sugars, the fundamental electronic factors governing these structural features remain insufficiently understood. In particular, previous studies have primarily focused on geometric and intermolecular aspects, while the role of intramolecular electronic structure—especially site-specific charge distribution—has not been systematically clarified. This lack of electronic-level understanding limits our ability to rationally interpret crystal packing behavior and to design functional sugar-based materials for sustainable applications. Therefore, a detailed analysis of intramolecular charge distribution is

essential for bridging the gap between electronic structure and macroscopic material properties. This perspective is also consistent with recent studies in sustainable materials science, which emphasize the importance of understanding electronic structure–property relationships in molecular systems. In this context, the DV-Xα method provides a suitable framework for analyzing localized electronic properties and site-specific charge characteristics in complex molecular systems [13].

Nevertheless, many questions remain unresolved, including the fundamental factors that give rise to these unique electronic states and how they influence crystal packing. To address this issue, the present study systematically investigates the intramolecular electronic structures of ketohexoses using DV-Xα molecular orbital calculations, with a particular focus on identifying site-specific charge stability and adaptability. By comparing D-chiral and D,L-racemic forms, this work aims to establish a fundamental electronic framework that explains both molecular stability and crystal packing behavior.

2. **Methods**

The DV-Xα method was employed in this study because it provides a robust and reliable description of localized electronic states and atomic charge distribution in molecular systems with relatively low computational cost. In particular, DV-Xα is well suited for analyzing site-specific electronic characteristics, such as the relative stability of atomic positions and charge redistribution, which are central to the present study. Compared to density functional theory (DFT), DV-Xα allows a direct and transparent evaluation of atomic contributions to electronic structure, making it advantageous for systematic comparison across multiple ketohexose molecules. Furthermore, DV-Xα has been successfully applied in previous studies on rare sugars and related molecular systems, demonstrating its validity for interpreting electronic features relevant to crystal structure formation. All calculations were performed using the DV-Xα program package. The basis set consisted of numerical atomic orbitals. The cluster size, exchange-correlation potential, and convergence criteria were set according to standard parameters used in previous DV-Xα studies. Net charges were evaluated using Mulliken population analysis.

In this study, molecular orbital calculations were performed using the DV-Xα method within a single-molecule model. For D,L-tagatose, experimentally determined structural data obtained from single-crystal X-ray diffraction were employed. For the other ketohexoses, we utilized either experimental data previously obtained in our laboratory or crystallographic information deposited in the Cambridge Structural Database (CSD), with the following identifiers: TAGTOS01 (D-tagatose)[14], SORBOL01 (L-sorbose)[15], HELYOP (D,L-sorbose)[16], FRUCTO12 (D-fructose)[17], NUPSUO (D,L-fructose)[18], OGETAW01 (D-psicose)[19], and XULKIA (D,L-psicose)[20]. The geometric parameters of the ketohexoses used in the present analysis are summarized in Table 1. Notably, all of the ketohexoses adopt chair-type six-membered ring conformations in their crystalline state, and the numbering of atoms was defined in accordance with international conventions, as illustrated in Figure 2.

Table 1. Geometrical parameters of ketohexoses.

	D-fructose	D-psicose	D-tagatose	L-sorbose
Formula	$C_6H_{12}O_6$	$C_6H_{12}O_6$	$C_6H_{12}O_6$	$C_6H_{12}O_6$
Crystal System	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space Group	$P2_12_12_1$ (#19)	$P2_12_12_1$ (#19)	$P2_12_12_1$ (#19)	$P2_12_12_1$ (#19)
a [Å]	8.0818 (4)	8.693 (2)	6.22010 (10)	6.545 (2)
b [Å]	9.1394 (4)	11.185 (4)	6.50220 (10)	18.062 (7)
c [Å]	9.9546 (5)	7.745 (2)	17.6629 (4)	6.310 (2)
α [º]	90	90	90	90
β [º]	90	90	90	90
γ [º]	90	90	90	90
Cell Volume [Å³]	735.275	753.056	714.364	745.942
Z	4	4	4	4
Z′	1	1	1	1
R-Factor [%]	2.03	4.3	2.47	3.7

	D,L-fructose	D,L-psicose	D,L-tagatose	D,L-sorbose
Formula	$C_6H_{12}O_6$	$C_6H_{12}O_6$	$C_6H_{12}O_6$	$C_6H_{12}O_6$
Crystal System	Triclinic	Orthorhombic	Monoclinic	Monoclinic
Space Group	$P\bar{1}$ (#2)	$Pna2_1$ (#33)	$P2_1/c$ (#14)	$P2_1/a$ (#14)
a [Å]	5.43124 (19)	11.2629(5)	8.11340 (10)	12.8152 (3)
b [Å]	7.2727 (3)	5.3552(3)	9.4936 (2)	6.29489 (13)
c [Å]	10.1342 (4)	12.6538(6)	10.4731 (2)	18.9482 (4)
α [º]	69.120 (2)	90	90	90
β [º]	83.907 (2)	90	103.067 (7)	108.3472 (12)
γ [º]	78.381 (2)	90	90	90
Cell Volume [Å³]	366.088	763.215	785.806	1450.85
Z	2	4	4	8
Z′	1	1	2	2
R-Factor [%]	3.68	4.75	3.77	4.42

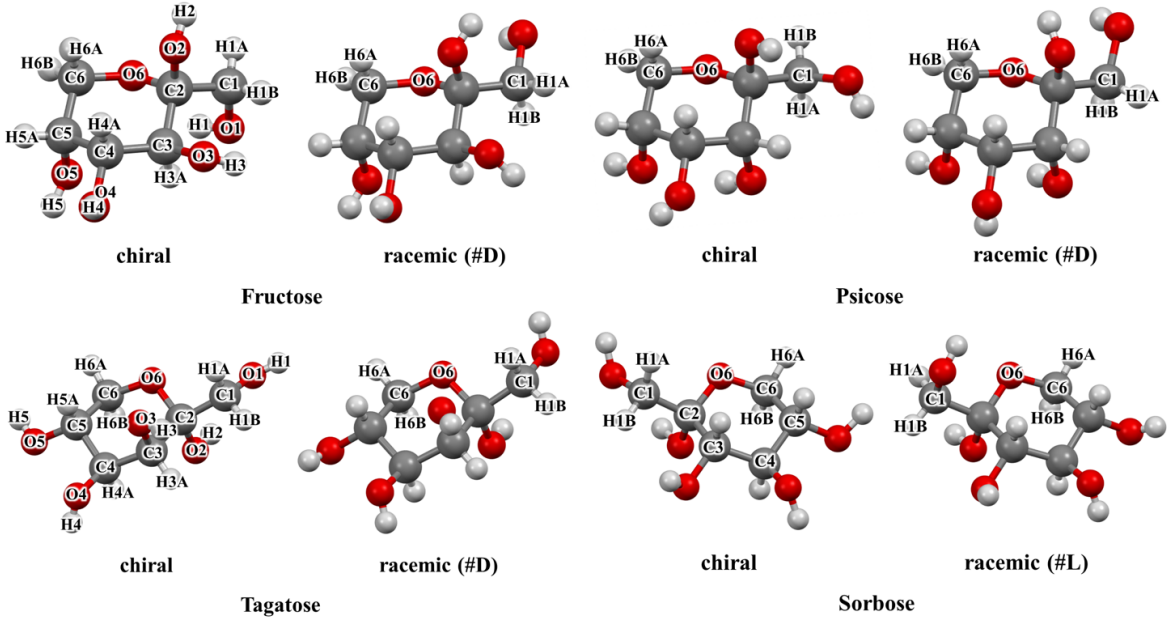


Figure 2. Numbering of ketohexoses.

2.1. Polarity analysis by atom numbering

In this study, the carbons, oxygens, and hydrogens constituting the six-membered ring were grouped according to their atom numbering, such that atoms bearing the same number were considered as one group. The net charges (Net Charge) for each group were then calculated. Since oxygen atoms act as electron acceptors, their Net Charge values were obtained as negative, whereas carbon and hydrogen atoms, functioning as electron donors, yielded positive values. However, in order to evaluate the degree of charge polarization within each group, the absolute values of the oxygen contributions were employed. The overall polarity of each numbering group was then calculated as the sum of these values.

2.2. Variation in intramolecular charge values

To conduct a more detailed analysis, we calculated the variations in the Net Charge of each atom. Specifically, we examined how the intramolecular charges in the racemic forms changed relative to their corresponding chiral counterparts. First, the Net Charge of each atom in the molecules was determined, and the degree of concordance between the D-form and the D,L-form was calculated. By subtracting this value from 100, the percentage increase or decrease in charge was obtained. The calculation formula used for this analysis is presented in Equation (1),

$$\Delta_{\text{Charge}}\,(\%) = (\text{NetCharge_D,L} / \text{NetCharge_D}) \times 100 - 100 \quad . \qquad (1)$$

2.3. Variation in intramolecular charge distribution

We further investigated how the relative distribution of intramolecular charges changed between the chiral and racemic forms of each sugar. To this end, the total Net Charge for each sugar was first calculated, followed by determination of the proportion contributed by each atom. The difference in these proportions between the racemic and chiral forms was then evaluated, allowing us to discuss the extent to which atom polarity was altered.

It should be noted that the present calculations were performed within a single-molecule framework and therefore do not explicitly include intermolecular interactions in the crystal environment. However,

since the primary objective of this study is to identify intrinsic electronic characteristics of individual atomic positions, the single-molecule approximation provides a reasonable first-order description. The influence of intermolecular interactions, such as hydrogen bonding and crystal packing, is discussed qualitatively based on the electronic trends obtained from the calculations.

3. Results and Discussion

3.1. Polarity analysis of numbering group

The obtained charge distribution trends are consistent with previously reported experimental observations [9-12], particularly the strong hydrogen-bonding tendency involving O3–O4 groups in sorbose derivatives. This agreement supports the validity of the present DV-Xα-based analysis. The total Net Charge values calculated for each numbering group are summarized in Table 2. Here, the groups were defined as follows: the C1 group = C1 + O1 + H1 + H1A + H1B; the C2 group = C2 + O2 + H2; the C3 group = C3 + O3 + H3 + H3A; and the C6 group = C6 + O6 + H6 + H6B. The C4 and C5 groups were defined analogously to the C3 group.

Table 2. Total polarity of each numbering group.

	C1 group	C2 group	C3 group	C4 group	C5 group	C6 group	total
D-tag	1.20974	1.66579	1.16340	1.30941	1.31398	0.62787	7.29019
D,L-tag (#D)	1.21990	1.65256	1.22754	1.28773	1.32384	0.65817	7.36974
L-sor	1.13299	1.43578	1.00510	1.18906	1.09625	0.69313	6.55231
D,L-sor (#L)	1.22798	1.60311	1.23935	1.29004	1.30259	0.69337	7.35644
D-fru	1.22695	1.53139	1.25240	1.29272	1.25771	0.66483	7.22600
D,L-fru (#D)	1.22541	1.61250	1.21275	1.30142	1.27841	0.64946	7.27995
D-psi	1.41365	1.61632	1.41685	1.59621	1.24707	0.65000	7.94010
D,L-psi (#D)	1.22087	1.61983	1.24287	1.31068	1.27622	0.63190	7.30237

[electrons]

As shown in Table 2, L-sorbose exhibits smaller Net Charge values across all groups except for the C6 group compared with the other ketohexoses (highlighted in blue). This result suggests that L-sorbose is the least polar sugar among the ketohexose family. In contrast, D-psicose displays notably larger Net Charge values in the C1, C3, and C4 groups, resulting in an overall higher molecular polarity than the other sugars (highlighted in red in Table 2). Moreover, a consistent trend was observed across all ketohexoses: the C2, C5, and C6 groups exhibited similar Net Charge values irrespective of stereochemistry or crystal packing. This indicates that these regions represent electronically stable sites within the ketohexose molecules.

Among all groups, the C2 group consistently exhibited the highest polarity. As the anomeric position, C2 plays a critical role in the stability of both molecular and crystalline states. The pronounced polarity at C2 likely arises not only from the necessity to maintain an electronically stable molecular structure through enhanced charge separation, but also from its pivotal role in facilitating intermolecular hydrogen-bond formation. Consequently, the C2 group substantially contributes to the stabilization of the overall crystal structure.

This electronic feature can be directly related to crystal structure formation. In particular, the high polarity at the C2 position enhances its ability to participate in intermolecular hydrogen bonding, thereby stabilizing the crystal packing. Similarly, variations in charge at the C3 and C4 positions may influence the formation and strength of O3–O4 hydrogen bonds, which have been reported to play a key role in

ketohexose crystal structures. Thus, the observed electronic distribution provides a mechanistic explanation for the experimentally observed hydrogen-bonding patterns and crystal packing behavior.

3.2. Variation in intramolecular charge values

As described in Section 3.1, the variation in Net Charge values between chiral and racemic forms was examined. For example, in D-tagatose, the O1 atom exhibited a Net Charge of -0.62108, whereas in D,L-tagatose, the corresponding value was −0.61542. The consistency ratio is calculated as $(-0.61542 / -0.62108) \times 100 = 99.09\,\%$. The percentage variation is therefore obtained as: Δ Charge (%) = 99.09 – 100 = –0.91 %, indicating that the polarity of the O1 atom in the D,L-racemic form decreased by 0.91 % relative to the D-chiral. In other words, a negative variation corresponds to a reduction in polarity, while a positive variation indicates an enhancement of polarity at that atomic site. The overall results are summarized in Table 3.

Table 3. Changes in intramolecular charge values (D → D,L (#D) or L → D,L (#L)).

	Tagatose	Sorbose	Fructose	Psicose
O1	-0.91	8.46	-0.77	-13.04
O2	-0.79	15.27	5.32	-1.18
O3	5.86	20.86	-1.79	-11.88
O4	0.92	13.68	1.09	-19.62
O5	0.28	16.67	2.12	2.24
O6	1.85	-3.96	-2.64	1.88
H1	-0.22	13.74	0.82	-10.82
H2	-1.58	10.98	9.86	0.07
H3	3.76	21.41	-1.80	-11.42
H4	-1.56	15.25	-0.15	-17.02
H5	1.63	19.35	2.02	0.87
C1	7.30	-41.95	-9.70	-49.25
C2	-0.20	3.20	2.00	2.24
C3	18.80	10.09	-7.20	-30.56
C4	-10.87	-7.20	-0.32	-21.15
C5	3.30	14.51	-1.91	0.78
C6	14.30	-52.11	-24.53	-38.88
H1A	1.87	54.63	22.23	17.05
H1B	16.27	68.22	-11.03	-2.56
H3A	-11.01	134.24	-12.66	32.50
H4A	5.73	28.30	5.27	16.17
H5A	-6.66	71.31	8.49	23.38
H6A	12.26	80.98	23.34	-6.55
H6B	7.33	58.62	6.33	12.19

[%]

From Table 3, the Net Charge variation at the C2 and C5 positions is relatively small (highlighted in yellow). This implies that the Net Charge at these positions is minimally affected by the molecular environment, remaining nearly constant between the D and D,L forms. Accordingly, the C2 and C5 sites can be regarded as electronically stable regions within the ketohexose framework. In contrast, the C3, C4, and C6 positions exhibit relatively larger variations in Net Charge. These positions are therefore

considered to be key sites involved in intramolecular charge redistribution. By modulating their electronic states in response to changes in the surrounding environment, these groups likely contribute to the stabilization of the overall crystal structure.

Notably, although many of the observed variations are small (< 1 %), such differences are not negligible in the context of intramolecular charge distribution. In molecular systems, even subtle changes in atomic charge can significantly influence intermolecular interactions, particularly hydrogen-bonding strength and directionality. Therefore, these small variations are considered to be chemically meaningful, especially when they exhibit systematic trends across different ketohexoses. The consistent minimal variation observed at the C2 and C5 positions strongly supports their identification as electronically stable sites.

3.3. Variation in intramolecular charge distribution

Next, the variation in the proportional contribution of Net Charge was examined. For instance, in D-tagatose, the O1 atom exhibited a Net Charge of -0.62108, which accounted for approximately 8.52 % of the total intramolecular charge. In contrast, in D,L-tagatose, the O1 atom had a Net Charge of -0.61542, corresponding to about 8.35 % of the total. The difference, $8.35 - 8.52 = -0.17\,\%$, indicates that the relative contribution of the O1 atom to molecular polarity decreased by 0.17 % in the racemic form compared to the chiral form. Conversely, positive differences reflect an increase in the relative contribution to overall polarity. A summary of these results is presented in Table 4.

Table 4. Changes in intramolecular charge distribution (D → D,L (#D) or L → D,L (#L)).

	Tagatose	Sorbose	Fructose	Psicose
O1	-0.17	-0.44	-0.13	-0.48
O2	-0.18	0.30	0.41	0.65
O3	0.39	0.61	-0.22	-0.38
O4	-0.01	0.00	0.03	-1.26
O5	-0.07	0.35	0.12	0.88
O6	0.04	-0.82	-0.20	0.58
H1	-0.07	0.04	0.00	-0.16
H2	-0.15	-0.02	0.46	0.45
H3	0.13	0.48	-0.13	-0.21
H4	-0.14	0.02	-0.05	-0.59
H5	0.03	0.34	0.07	0.46
C1	0.05	-1.04	-0.11	-0.75
C2	-0.09	-0.40	0.09	0.72
C3	0.28	-0.05	-0.17	-0.60
C4	-0.37	-0.91	-0.03	-0.48
C5	0.06	-0.02	-0.08	0.24
C6	0.09	-1.03	-0.31	-0.33
H1A	0.01	0.30	0.21	0.26
H1B	0.13	0.54	-0.12	0.06
H3A	-0.11	0.46	-0.15	0.36
H4A	0.04	0.28	0.03	0.18
H5A	-0.08	0.30	0.05	0.19
H6A	0.12	0.39	0.18	0.01
H6B	0.06	0.32	0.06	0.20

[%]

It should be noted that, although most changes are small—on the order of ~1 % or less—the variation observed at the C2 position is comparatively significant (highlighted in yellow in Table 4). This suggests that C2 is a key site where the relative distribution of charge is actively modulated in response to the surrounding molecular environment. In contrast, the C5 position exhibits minimal variation, implying that the proportion of polarization at this site remains essentially constant between the D-chiral and the D,L-racemic form. This finding suggests that each sugar possesses structurally preferred charge distributions that remain invariant at specific atomic positions.

Furthermore, the C3, C4, and C6 positions, similar to C2, appear to act as responsive sites where the relative distribution of intramolecular charge can be flexibly adjusted. Such adaptability likely plays an important role in stabilizing the overall electronic and crystal structure of ketohexoses. From a theoretical perspective, the coexistence of stable and adaptive electronic sites suggests that ketohexoses achieve structural stability through a balance between rigidity and flexibility in charge distribution. Stable sites maintain the fundamental electronic framework of the molecule, while adaptive sites allow fine-tuning of intermolecular interactions in response to the crystal environment.

3.4. General Discussion

The most important finding of this study is the clear distinction between two types of electronic behavior in ketohexoses: (i) electronically stable sites, where absolute charge values remain nearly constant, and (ii) adaptive sites, where both absolute and relative charge distributions vary in response to the molecular environment. This dual characterization provides a new framework for understanding how electronic structure governs both molecular stability and crystal packing in rare sugars.

Synthesizing the results from Sections 3.2 and 3.3, it was revealed that the C2 position exhibits only minor variation in absolute Net Charge values, yet shows relatively large changes in proportional contribution. This indicates that the C2 site tends to maintain a nearly constant absolute charge value, even if this requires adjustment of its relative contribution to the total intramolecular charge. Thus, C2 can be identified as an electronically stable site, whose polarity remains robust despite changes in the surrounding molecular or crystalline environment.

In contrast, the C5 position exhibited minimal variation in both absolute values and relative proportions. This dual stability suggests that C5 represents a characteristic feature of ketohexoses: a position inherently resistant to perturbations in charge distribution, both in magnitude and in proportion. On the other hand, the C3, C4, and C6 positions showed substantial variations in both absolute and proportional charge values. These findings imply that these sites function as electronically adaptive regions, capable of modulating their charge states in response to environmental influences. Such flexibility likely contributes not only to the stabilization of the individual molecules but also to the cooperative stability of the crystalline lattice as a whole.

4. **Conclusion**

This study demonstrates that molecular orbital calculations based on the DV-Xα method were performed to elucidate the intramolecular electronic structures of ketohexoses in both D-chiral and D,L-racemic forms. The most significant finding is the clear distinction between two types of electronic behavior: (i) electronically stable sites, represented by the C2 and C5 positions, where absolute charge values remain nearly invariant, and (ii) adaptive sites, represented by the C3, C4, and C6 positions, where charge distribution flexibly responds to changes in the molecular environment. This classification provides a new conceptual framework for understanding how electronic structure governs both molecular stability and crystal packing in rare sugars. From an application perspective, these findings offer important implications for crystal engineering and the design of functional sugar-based materials. In particular, stable sites can be regarded as structural anchors that maintain electronic robustness, while adaptive sites may serve as tunable regions that modulate intermolecular interactions, such as hydrogen bonding, thereby influencing crystal packing and material properties. Furthermore, this framework may

contribute to the rational design and functionalization of rare sugars in fields such as pharmaceuticals, food science, and sustainable agrochemicals, where precise control of molecular and crystal structures is essential. Future work will involve quantitative analysis of intermolecular interactions, including hydrogen-bond distances and energies, as well as comparative studies using alternative computational methods. Experimental validation through detailed crystallographic analysis will also be important to further establish the relationship between electronic structure and crystal stability.

Acknowledgements
I would like to thank Ms. M. Matsumoto, Mr. R. Motoyasu and Mr. R. Ishikawa for their valuable guidance in this study. I also thank the members of our laboratory for their kind support and discussions.

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