

Reaction network database for fast pyrolysis of vanillyl alcohol based on molecular wavefunction descriptors

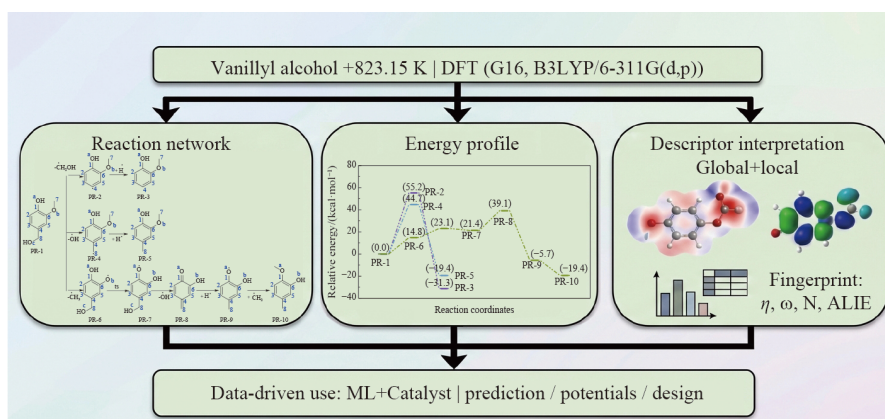
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Abstract: Lignin pyrolysis is a promising avenue for the sustainable production of high-value phenolic chemicals. Nevertheless, unraveling the intricate radical reaction network remains a major bottleneck to optimizing product selectivity. This work constructs a standardized DFT computational database, which systematically describes the

fast pyrolysis of vanillyl alcohol at 823.15 K. The database features out three key components, including primary reaction pathways, thermodynamic energy barriers, and atomic-level electronic fingerprints. Ultimately, the construction of this database not only provides an important reference for data-driven catalyst development, but also lays a theoretical foundation for the precise regulation of lignin depolymerization.

Key words: lignin; vanillyl alcohol; pyrolysis; phenols; DFT



Lignin, the most abundant renewable aromatic polymer in nature, is an ideal feedstock for producing high-value phenolic compounds *via* pyrolysis^[1–2]. However, the pyrolysis process is hindered by extremely low phenolic yields, typically only 10%–20%, thereby limiting its industrial-scale application^[3]. This bottleneck is primarily attributed to the extremely complex radical reaction network during pyrolysis, in which complicated radicals inevitably trigger secondary reactions such as repolymerization^[4]. Although the final product distribution has been extensively studied, there remain significant knowledge gaps regarding the evolution of key radical intermediates and their competitive reaction pathways^[5].

Density Functional Theory (DFT) is a powerful tool for elucidating such complex reaction mechanisms^[6]. However, constructing the potential energy surface of radical network that involves the major reaction pathways poses significant computational challenges. More importantly, single energy

analysis (i.e., energy barriers) is often difficult to reveal the intrinsic driving forces for reactions. And electron-density-based reactivity descriptors, which are crucial for understanding chemical reactivity, remain relatively scarce in the existing databases. At present, there is a lack of a publicly available and standardized database that can systematically document the detailed reaction networks, energetic parameters, and key electronic structure descriptors of lignin model compounds under different reaction conditions of fast pyrolysis.

To address this gap, we constructed a multi-dimensional reaction network database for the fast pyrolysis of vanillyl alcohol^[7], a representative lignin model compound, based on DFT calculations. This dataset covers the reaction pathways of vanillyl alcohol fast pyrolysis at 823.15 K, including the primary reaction pathways, the secondary rearrangements, and the both global and local reactivity indices of key intermediates. The comprehensive dataset

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provided herein not only elucidates the intrinsic limitations of the pyrolysis reactions, but also supplies high-quality descriptors for feature engineering, thereby facilitating the development of machine-learning-based reaction prediction models and the inverse design of novel pyrolysis catalysts.

1 Data summary

1.1 Data profile

The dataset contains raw density functional theory (DFT) calculation data for the fast pyrolysis reaction network of

vanillyl alcohol at 823.15 K (Table 1). It covers optimized geometries, vibrational frequencies, and electronic energies for all stationary points involved in the reaction network, including reactants, intermediates, transition states, and products. In addition, the dataset provides key secondary reaction pathways, initial bond dissociation energies, global reactivity descriptors, atom-resolved electronic fingerprints, spin population analyses of radical species, and molecular wavefunction-based descriptors for characterizing surface reactivity, such as Average Local Ionization Energy (ALIE), Local Electron Affinity Energy (LEAE), and Local Electron Attachment Energy (LEA).

Table 1 Specifications of the dataset

Dataset title	Reaction network database for fast pyrolysis of vanillyl alcohol based on molecular wavefunction descriptors
Data version	V1.0 (released in February 2026)
Software version	Gaussian 16
Authors	SHI Jingyuan, LI Chenchen, CHENG Xiaoxue, LING Qifan, MU Mao, WANG Shuang, JIANG Ding
Corresponding author's name	WANG Shuang, JIANG Ding
Data content descriptor	Raw DFT calculation data for the fast pyrolysis of vanillyl alcohol (823.15 K), comprising: (1) Optimized geometries, frequencies, and energies for all stationary points (reactants, intermediates, transition states, and products); (2) Key secondary reaction pathways; (3) Initial bond dissociation energies (BDEs); (4) Global reactivity indices and atomic-level electronic fingerprints; (5) Spin population analysis for free radicals, as well as Average Local Ionization Energy (ALIE), Local Electron Affinity Energy (LEAE), and Local Electron Attachment Energy (LEA) for characterizing molecular surface reactivity
Data Generation time	2022–2025
Data Volume	Approximately 134 MB
Data format	.log, .chk, .wfn, .txt, .xlsx
Data source location	CSTR:31253.11.sciencedb.j00124.00456 https://doi.org/10.57760/sciencedb.j00124.00456 SHI Jingyuan, LI Chenchen, CHENG Xiaoxue, et al. Reaction network database for fast pyrolysis of vanillyl alcohol based on molecular wavefunction descriptors[J]. J Fuel Chem Technol, 2026, 54(7): 20260324.
Citation format of data	SHI Jingyuan, LI Chenchen, CHENG Xiaoxue, et al. Reaction network database for fast pyrolysis of vanillyl alcohol based on molecular wavefunction descriptors[DS/OL]. V1. Science Data Bank, 2026[2026-02-16]. https://doi.org/10.57760/sciencedb.j00124.00456 DOI:10.57760/sciencedb.j00124.00456

1.2 Description of data generation methods and procedures

Database construction consists of two steps: raw data generation from DFT calculations, data extraction and data structuring. The detail workflow is as follows. First, the structures of reactants, key intermediates, transition states, and products involved in the fast pyrolysis of vanillyl alcohol (823.15 K) were built. Subsequently, DFT calculations were performed using Gaussian 16. Finally, the calculation output files were subjected to data extraction and preprocessing to generate the raw data package and the structured data. The operating details are described as follows:

Computational settings: All calculations were performed using the Gaussian 16 package with the B3LYP functional and the 6-311G (d, p) basis set.

All relevant species along the target reaction pathways,

including reactants, intermediates, products, and those involved in secondary reaction pathways, were fully geometry-optimized. All optimized structures were subjected to vibrational frequency analysis to obtain Gibbs free energies at 823.15 K. All stable structures are presented as local minima on the potential energy surface. Each obtained transition state has only one imaginary frequency, indicating that it corresponds to a first-order saddle point. Furthermore, intrinsic reaction coordinate (IRC) calculations were performed to verify that each transition state correctly connects the corresponding reactant and the product on the one-dimensional potential energy profile^[8–9].

Energy and barrier calculations: Free energies were obtained from frequency calculations with zero-point energy corrections. Reaction barriers were determined as the free energy differences between the transition states and the corresponding reactants.

Bond energy calculations: Key bond energies of the

initial vanillyl alcohol species were calculated out based on the electronic energy differences.

Extraction of electronic structures and reactivity descriptors: These parameters were obtained based on the wavefunction analysis using the Multiwfn program. Notably, to keep the scaling consistent with that widely used in the literature, the nucleophilicity index was computed by referencing the energy of tetracyanoethylene (TCE) at the B3LYP/6-31G* level as implemented in Multiwfn program^[10–12].

1.3 Description of data examples

This dataset provides multi-dimensional reactivity data spanning from macroscopic thermodynamic potential

energy surfaces to microscopic electronic structures, in order to characterize the fast pyrolysis behavior of vanillyl alcohol. To facilitate rapid indexing and reusing, this section first describes the file organization of the dataset and the workflow of data generation. Then, the detailed data using key intermediates as examples are presented.

1.3.1 Dataset generation workflow and organizational structure

Computational workflow: This database uses DFT as the underlying data-generation approach and follows the computational procedure as shown in Figure 1, which mainly consists of the following three core steps.

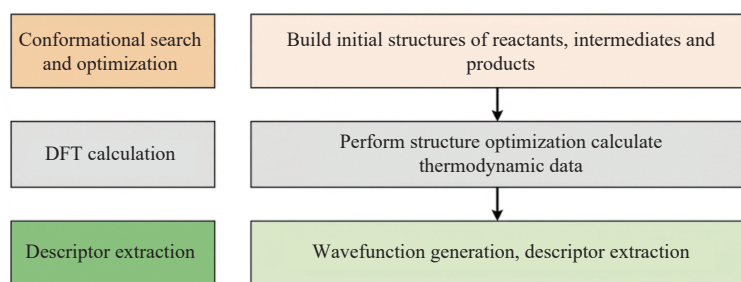


Fig. 1 Dataset generation workflow

Structure search and optimization: Based on the Py-GC/MS data of the fast pyrolysis of vanillyl alcohol, initial structures of key species involved in the reaction network were systematically constructed (as shown in Figure 3(a) and (c)). Subsequently, geometry optimizations and frequency calculations were carried out at the B3LYP/6-311G (d, p) level.

Multi-electronic-state wavefunction generation: Based on the optimized equilibrium geometries, single-point energy calculations were performed for the neutral (N), cationic (N–1) and anionic (N+1) systems, and the corresponding wavefunction files were output.

Descriptor analysis: The wavefunction files were batch processed using Multiwfn to systematically compute (i) the descriptors covering global reactivity and atom-level local electronic-structure, (ii) the spin population analysis for radicals, and (iii) the average local ionization energy (ALIE), local electron affinity energy (LEAE), and local electron attachment energy (LEA) for characterizing molecular surface activity.

Data file organizational structure: This database adopts a standardized hierarchical directory structure for storage to ensure data readability and traceability. As shown in Figure 2, the dataset is organized according to a hierarchical logic of “reaction pathway-species node”. In this framework, each structure (e.g., “SR-1”) is assigned an independent storage unit. The unit specifically includes the following information:

Gaussian calculation records: These files include output log files (.log) and checkpoint files (.chk), which contain

complete molecular geometries and thermodynamic data.

Wavefunction analysis files: These files include wavefunction files (.wfn) for the neutral (N), cationic (N–1) and anionic (N+1) states, which are used for subsequent detailed analysis of electronic properties.

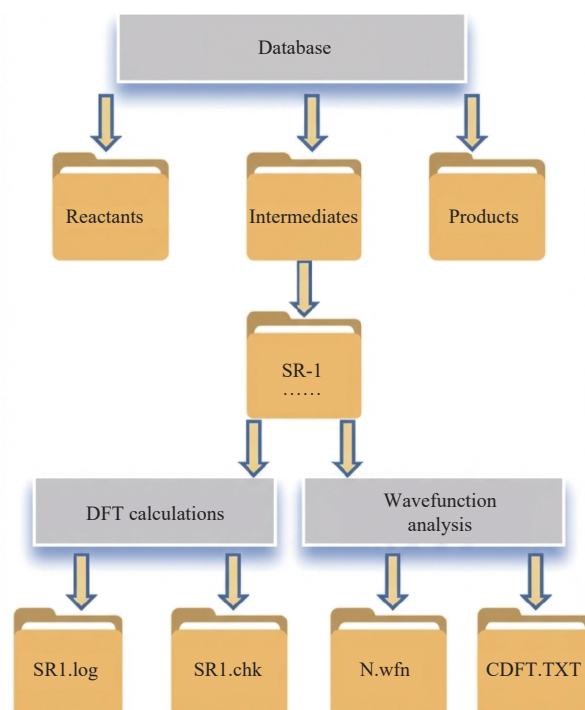


Fig. 2 Data file organization architecture

1.3.2 Secondary cracking reaction network

The final product distribution of vanillyl alcohol pyrolysis largely depends on the secondary evolution of the primary products. To elucidate the complex competition mechanism among radical reaction pathways, this section highlights representative secondary cracking pathways. As shown in Figure 3, this database not only covers the formation pathways of the primary products (Figure 3(a) and (b)) but also emphasizes on the secondary cracking processes of key intermediates. Figure 3(c) constructs a reaction network centered on the consumption of hydrogen radicals, whereas Figure 3(d) provides the corresponding data of potential energy surface. These results systematically document the thermodynamic evolution from the intermediates to the final small-molecule products.

1.3.3 Electronic-structure characteristics of key species

To facilitate an in-depth investigation of the intrinsic factors governing reaction kinetics, this database provides global electronic fingerprints for all key species along the pathways as shown in Figure 3. Tables 2 and 3 present an example for the pathway in Figure 3(c). These features (including energy, chemical hardness, electrophilicity and nucleophilicity indices, average local ionization energy, local electron affinity energy, and local electron attachment energy, etc.) constitute the basis for understanding molecular reactivity. Based on these standardized data, users can not only evaluate the thermodynamic stability of intermediates but also quantitatively interpret the electronic origin for the competitive advantages among different reaction pathways (e.g., why SR-1 tends to follow a specific rearrangement pathway).

1.3.4 Analysis of the local active sites

To facilitate mechanistic analysis of radical reactions at the microscopic level, this database further provides atom-resolved electronic descriptors. Table 4 takes the intermediate SR-1 as an example. The atomic numbering is shown on the left of Figure 4, and the table presents a multi-dimensional local feature matrix that includes Fukui indices and atomic charges. Table 5 reports the spin populations for intermediate SR-2, whose atomic numbering is displayed on the right of Figure 4. These data enable effective identification of intramolecular active sites and help to explain the regioselectivity rules of radical attacks. In addition, these standardized features also provide essential training data for constructing high-accuracy machine-learning potentials.

1.4 Data quality control statement

The quality control of this dataset is ensured through the

following measures:

Standardized computational workflow: All calculations in this database strictly follow unified computational parameters and procedures to ensure the comparability of data across all the species. Specifically, all calculations were performed using the Gaussian 16 package at the B3LYP/6-311G (d, p) level of theory. All thermodynamic parameters were obtained at 823.15 K.

Structure and convergence verification: All the computational tasks were confirmed to be converged. All stationary points were validated by frequency calculations. Stable structures were confirmed as minima, and transition states were confirmed as first-order saddle points.

Based on the IRC calculations verification, each transition state correctly connected the corresponding reactant and product on the one-dimensional potential energy profile, thereby ensuring the accuracy of the computational results.

Data consistency and scaling validation: All key data in this dataset were extracted from the original computational output files, either automatically or manually, and were cross-checked to ensure consistency between the summarized data and the raw data, which effectively avoided transcription errors. For electronic-structure descriptors, a specific clarification was provided. To maintain consistency with the scaling widely adopted in the literature, the TCE at the B3LYP/6-31G* level was used as the reference when calculating the nucleophilicity index.

2 Value and potential applications of the dataset

This dataset establishes the first multi-dimensional database for the fast pyrolysis of lignin model compounds that integrates thermodynamic barriers and electronic-structure descriptors, addressing the lack of a systematic “reaction network-electronic property” correlation map in existing resources. The core value and specific application scenarios of this database can be summarized in the following four aspects:

A theoretical benchmark for fast pyrolysis mechanistic studies: This dataset systematically provides thermodynamic data for vanillyl alcohol under fast pyrolysis conditions. It can serve as a benchmark dataset for mechanistic studies of lignin model compound pyrolysis, enabling the comparisons of reaction pathways across different catalytic systems. It also allows quantitative evaluation of the catalytic efficiencies for specific elementary reactions, thereby assisting in an in-depth elucidation of catalytic mechanisms.

Reactivity analysis based on electronic effects: Unlike traditional databases that contain only energetic parameters, this dataset integrates key electronic descriptors such as chemical hardness and nucleophilicity/electrophilicity indices, which provides a new perspective for understanding the competition mechanism among radical pathways.

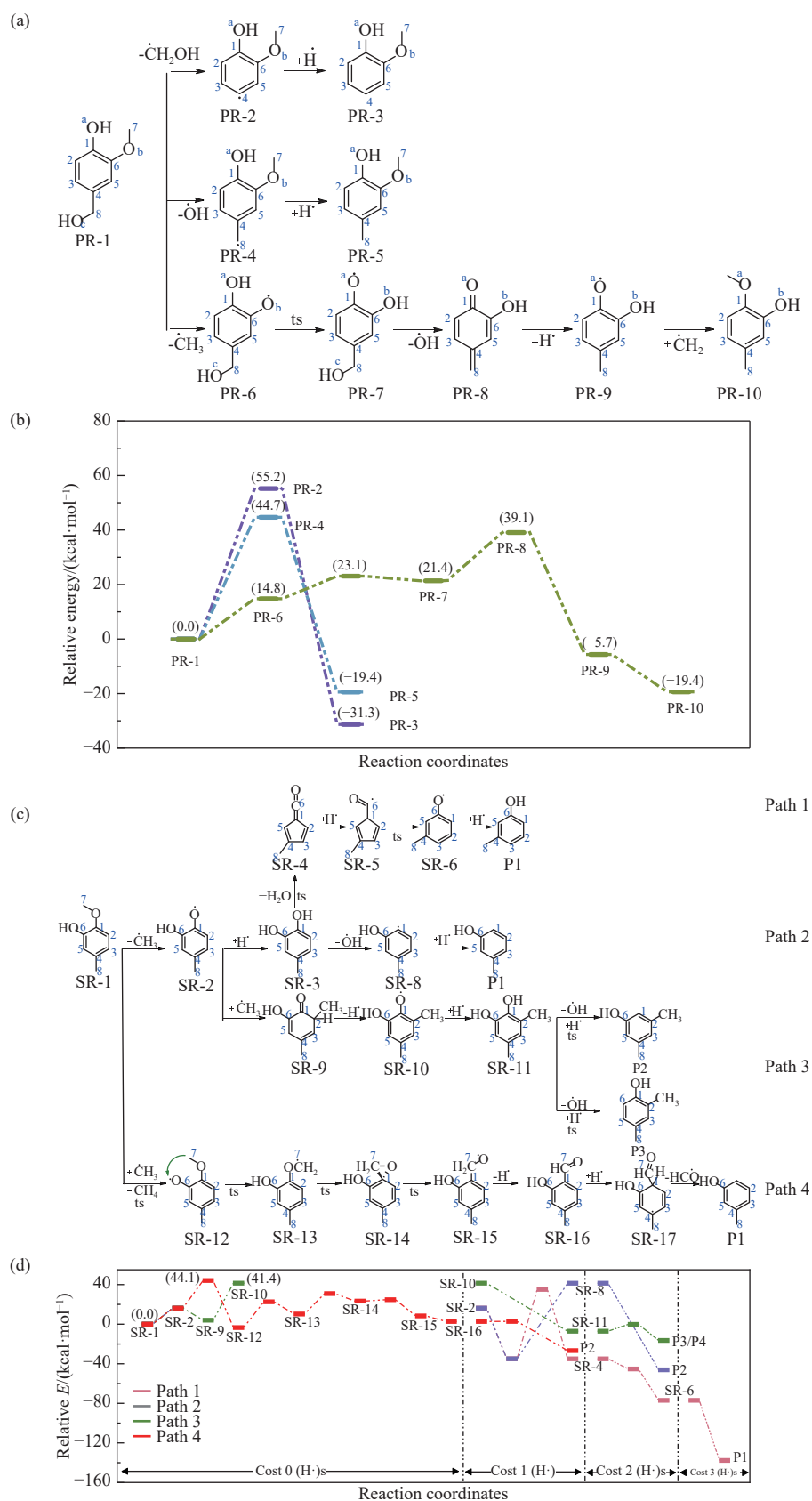


Fig. 3 Reaction pathways and thermodynamic energy barriers for vanillyl alcohol fast pyrolysis^[13]: (a) Primary product formation network, (b) Primary product reaction potential energy curves, (c) Secondary cracking pathways of key intermediates, (d) Reaction potential energy curves of key intermediates

Note: “Cost (H)” represents the number of hydrogen atoms/radicals consumed in the corresponding elementary reaction.

Table 2 Global reactivity descriptors of key intermediates

Name	Energy/Hartree	Chemical hardness/eV	Electrophilicity index/eV	Nucleophilicity index/eV
SR-1	-461.306522	9.7620	0.3339	3.6995
SR-2	-421.364970	6.4665	1.4377	3.6707
SR-3	-421.999101	9.9146	0.3560	3.6094
SR-4	-345.526761	8.7745	0.6876	3.3954
SR-5	-346.083985	8.2511	0.7314	4.0184
SR-6	-346.146234	6.8707	1.7245	2.9849
SR-8	-346.094347	8.7009	1.2989	3.1726
SR-9	-461.300406	8.0207	0.8845	3.3911
SR-10	-460.702161	6.2769	1.5213	3.6679
SR-11	-461.317781	9.7110	0.3411	3.7287
SR-12	-460.670323	6.3406	1.4708	3.6699
SR-13	-460.632012	8.4702	0.4220	4.7049
SR-14	-460.626006	6.0727	0.8750	4.7729
SR-15	-460.648820	6.9490	1.9666	3.1836
SR-16	-460.122735	8.5591	0.9669	2.8295
SR-17	-460.650170	6.1603	0.7383	4.9809
P1	-346.782849	10.2272	0.4159	3.2550
P2	-386.100893	9.9501	0.4234	3.3294
P3	-386.100808	9.9238	0.3732	3.4908

Table 3 Selected surface reactivity descriptors for key intermediates

Name	Average local ionization energy/eV	Local electron affinity energy/eV	Local electron attachment energy/eV
SR-1	8.49028	-0.01312	-42.24867
SR-2	9.06915	-0.86047	-43.17636
SR-3	8.56807	-0.09143	-42.35322
SR-4	8.08924	-3.13961	-39.65641
SR-5	7.74846	-1.90041	-39.38563
SR-6	9.27811	-1.20499	-40.83675
SR-8	8.10993	-3.22907	-41.6531
SR-9	8.3827	-1.95717	-41.58555
SR-10	9.09017	-0.86788	-42.71372
SR-11	8.46774	-7.00E-05	-42.07113
SR-12	8.95109	-0.92821	-44.13936
SR-13	6.75532	-0.70355	-42.32281
SR-14	8.40005	-0.69247	-42.12875
SR-15	8.74201	-2.01104	-46.24571
SR-16	9.00363	-2.09037	-45.11871
SR-17	8.03565	-4.05501	-43.75225
P1	8.54923	-0.17562	-41.33117
P2	8.40451	-0.14836	-41.67931
P3	8.67962	-0.11472	-40.80582

In practical applications, researchers can use these data to interpret regioselectivity rules, and such electron-density-based analysis can reveal out the kinetic phenomena that cannot be clarified by conventional thermodynamic analysis. This knowledge provides a microscopic basis for tuning reaction pathways.

Data-driven machine-learning model development: With a standardized data structure and atom-level feature labels, this dataset is an ideal resource for training high-accuracy machine-learning models. First, this dataset can be used to develop reactivity prediction models, enabling predictions

for lignin oligomer systems with more complex structure. Second, based on the provided high-fidelity configurations and energy data, machine-learning potentials can be trained, thereby enabling reactive molecular dynamics simulations at the nanosecond timescale. Finally, by integrating the multi-dimensional electronic descriptors in this dataset, researchers can build quantitative models to reveal out the relationship between structure and property of “electronic microenvironment-product selectivity”, which provides key theoretical criteria for the rational screening and inverse design of efficient lignin depolymerization catalysts.

Table 4 Descriptors of SR-1

Atom	q(N)	f ⁻	f ⁺	f0	CDD
C1	-0.0059	0.0807	0.0729	0.0768	-0.0078
C2	-0.0662	0.0443	0.1267	0.0855	0.0824
C3	0.0617	0.0796	0.0566	0.0681	-0.0230
C4	0.0457	0.0823	0.0838	0.0830	0.0016
C5	-0.0718	0.0453	0.1243	0.0848	0.0790
C6	-0.0651	0.1061	0.0530	0.0795	-0.0531
H7	0.0446	0.0363	0.0595	0.0479	0.0231
H8	0.0389	0.0343	0.0552	0.0448	0.0209
O9	-0.1388	0.0810	0.0353	0.0581	-0.0457
C10	0.0105	0.0250	0.0186	0.0218	-0.0064
H11	0.0481	0.0290	0.0284	0.0287	-0.0006
H12	0.0386	0.0265	0.0176	0.0220	-0.0089
H13	0.0386	0.0265	0.0176	0.0220	-0.0089
O14	-0.2019	0.1077	0.0480	0.0779	-0.0598
H15	0.1632	0.0329	0.0245	0.0287	-0.0084
H16	0.0367	0.0468	0.0405	0.0436	-0.0063
C17	-0.0818	0.0249	0.0305	0.0277	0.0056
H18	0.0355	0.0336	0.0394	0.0365	0.0058
H19	0.0355	0.0336	0.0394	0.0365	0.0058
H20	0.0338	0.0236	0.0283	0.0260	0.0047

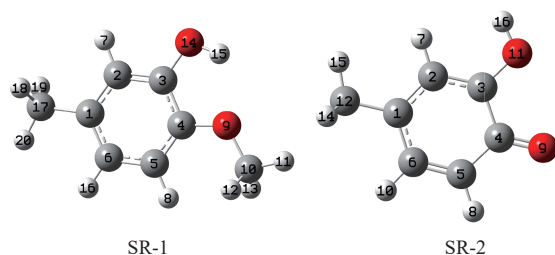


Fig. 4 Atom numbering of SR-1 and SR-2

Table 5 Spin population of SR-2

Atom	Value	Of sum/%
C1	0.21172007	21.172019
C2	-0.03758873	-3.758875
C3	0.18349317	18.349327
C4	0.04149332	4.149334
C5	0.14485804	14.485813
C6	-0.00746581	-0.746581
H7	-0.00394826	-0.394826
H8	0.00769970	0.769971
O9	0.33695409	33.695429
H10	-0.00178741	-0.178741
O11	0.08024134	8.024139
C12	0.01594602	1.594603
H13	0.01263771	1.263772
H14	0.01265549	1.265550
H15	0.00061536	0.061536
H16	0.00247530	0.247530

Catalyst design: The electrophilicity/nucleophilicity indices in this database can be used to guide the design of catalyst active sites for the pyrolysis of lignin model compounds. Taking the vanillyl alcohol pyrolysis system as an example, it is highly dependent on a hydrogen-radical-mediated chain reaction network, and an ideal catalyst design should promote specific pathways while minimizing disturbances to the hydrogen radical concentration in the system or the excessive consumption of key intermediates. Using the electrophilicity/nucleophilicity indices provided by the database, researchers can predict the adsorption tendencies of intermediates on the active sites of catalyst surface. For example, for radical intermediates with high nucleophilicity indices, catalyst materials featuring strongly electrophilic surface active sites should be avoided in the design process to prevent radical quenching or non-selective deep cracking caused by overly strong adsorption.

3 Conclusion

Based on DFT, this work establishes a multi-dimensional reaction network database for the fast pyrolysis of the lignin model compound vanillyl alcohol at 823.15 K. This database not only involves complex radical reaction pathways and thermodynamic energy barriers, but also innovatively integrates electronic-structure fingerprints of key intermediates, which fills the gap in “reaction network-electronic property” correlation data in this field. Standardized computational workflows and rigorous quality control were employed to ensure the accuracy, consistency, and reproducibility of the data. The public release of this dataset will not only provide a reliable theoretical benchmark for mechanistic studies of lignin pyrolysis, but

also offer valuable foundational data support for the rational design of new catalysts and the refinement of reaction kinetic models.

Declaration of Competing Interest

The authors declare no conflict of interest.

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基于分子波函数描述符的香草醇快速热解反应网络数据库

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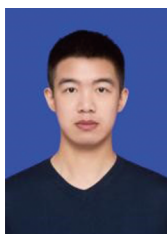
摘 要: 木质素热解作为一种极具前景的途径, 在生产高价值酚类化学品的可持续性方面表现突出。然而, 阐明错综复杂的自由基反应网络仍然是优化产物选择性的主要瓶颈。本工作构建了一个标准化的 DFT 计算数据库。该数据集描绘了香草醇在 823.15 K 下的快速热解。它包含三个核心要素: 主要反应路径、热力学能垒以及原子级电子指纹。该数据库的构建不仅为数据驱动的催化剂开发提供了重要参考, 同时也为精准调控木质素解聚奠定了理论基础。

关键词: 木质素; 香草醇; 热解; 酚类; DFT

中图分类号: TK6

文献标识码: A

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