THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS
A JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

pubs.acs.org/JPCL Letter

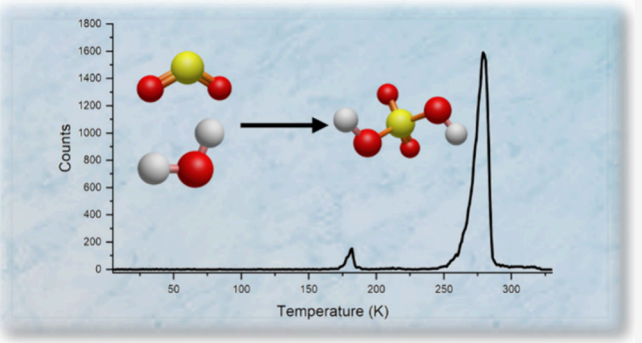
Pre-Accretion Formation of Sulfuric Acid in Interstellar Ice Analogs: Implications for Sulfate in Ryugu and Bennu

Mason McAnally, Xilin Bai, Baoyu Song, Jinghui Lu, Xinxuan Wang, Jiuzhong Yang, Yang Pan,* Tao Yang,* Ryan C. Fortenberry,* and Ralf I. Kaiser*

Cite This: J. Phys. Chem. Lett. 2026, 17, 12713−12718 Read Online

ACCESS | Metrics & More | Article Recommendations | Supporting Information

ABSTRACT: Sulfate-bearing phases and soluble sulfate species, including sodium sulfate (Na_2SO_4), in carbonaceous asteroids are commonly attributed to parent-body aqueous alteration, yet the formation of S(+VI) sulfate under the reducing, low-temperature conditions inferred for primitive bodies remains chemically challenging. Here, we show that sulfuric acid (H_2SO_4) can form before accretion through irradiation of sulfur dioxide/water (SO_2/H_2O) interstellar ice analogs at 5 K. Threshold photoionization, deuterium labeling, and sulfur isotope analysis unambiguously identify sulfuric acid, establishing a route from preaccretion ice chemistry to oxidized sulfur reservoirs. If incorporated into accreting planetesimals, such preaccretion H_2SO_4 could subsequently be mobilized, neutralized, and precipitated during aqueous alteration, providing a potential contribution to sulfate-bearing phases in primitive carbonaceous bodies.



Sulfate-bearing phases and soluble sulfate species—such as sodium (Na_2SO_4) and calcium sulfate ($CaSO_4$)—are critical components of primitive carbonaceous asteroids, including Ryugu and Bennu.[1−7] Classical models invoke the oxidation of iron-bearing sulfides such as troilite (FeS), pyrrhotite ($Fe_{0-0.125}S$), and pentlandite ($(Fe,Ni)_9S_8$) during parent-body aqueous alteration, with liquid water serving as the solvent providing mobility to solvated oxidants.[1,2] However, under the low-temperature and reducing conditions inferred for primitive carbonaceous asteroid parent bodies, sulfate production from FeS-type sulfides is expected to be inefficient because complete oxidation from S(−II) to S(+VI) requires both sufficiently strong oxidants and kinetically favorable mineral-fluid reactions. This is further complicated by chemical analysis of Ryugu samples[3−5] revealing abundant soluble oxygenated sulfur species, including sulfate (SO_4^{2-}), thiosulfate ($S_2O_3^{2-}$), polythionates ($^-O_3S-S_n-SO_3^-$), and organosulfur compounds like alkylsulfonates (RSO_3^-) and alkylthiosulfonates ($RS(S)(O)_2^-$). Moreover, sulfate-bearing grains exhibit anomalous sulfur isotopic signatures consistent with inheritance from molecular cloud chemistries;[8] while their oxygen isotopic compositions point to interaction with parent-body fluids.[1] Preservation of presolar material and primordial organic matter is well established in returned Ryugu samples, while estimates for CI chondrites and interplanetary dust particles indicate preservation of pristine interstellar material at accretion.[9−11] These findings suggest that sulfate formation in primitive bodies does not derive solely from postaccretion chemistry; instead, hitherto poorly explored preaccretion chemistry may provide a critical pathway initializing the synthesis of oxidized sulfur reservoirs in cold clouds that later mobilize during parent-body aqueous alteration (Figure 1).

This scenario gains further support from recent observations of the James Webb Space Telescope (JWST) revealing infrared signatures congruent with sulfur dioxide (SO_2) on icy grains in the molecular cloud Chamaleon Itoward Ced 110 IRS4A and IRS4B.[12,13] Sulfur dioxide allows a lower redox barrier from S(+IV) to S(+VI) in sulfuric acid. Previous work has demonstrated energetic processing of SO_2/H_2O ices can produce infrared signatures of sulfate, bisulfate, and other sulfur-bearing material.[14,15] However, the overlapping vibrational signatures of sulfur hydroxyanions (HSO_3^-, HSO_4^-, SO_4^{2-}), sulfur oxides (S_xO_y), and hydrated sulfuric acid ($H_2SO_4{\cdot}nH_2O$) prevented the unambiguous identification of neutral H_2SO_4.[16]

Here, we report the direct detection of sulfuric acid **1** formed in sulfur dioxide/water (SO_2/H_2O) interstellar analog ices at 5 K following exposures to proxies of galactic cosmic rays (GCRs) in the form of energetic electrons.[17] These electrons serve as laboratory proxies for secondary electrons

Received: August 27, 2026
Revised: September 21, 2026
Accepted: October 5, 2026
Published: October 22, 2026



Downloaded from pubs.acs.org/jpclcd/article-pdf/17/44/12713/6894707/acs.jpclett.6c02877.pdf by UNIV OF HAWAII user on 06 November 2026

© 2026 American Chemical Society

https://doi.org/10.1021/acs.jpclett.6c02877
J. Phys. Chem. Lett. 2026, 17, 12713−12718

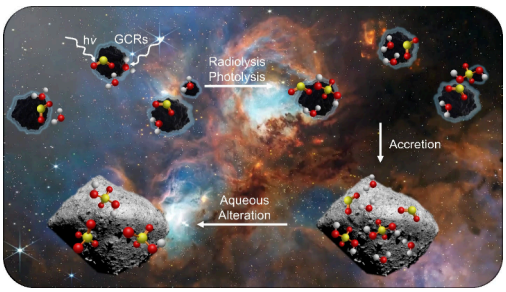


Figure 1. Schematic illustration of the proposed pathway linking preaccretion SO_2/H_2O ice chemistry to sulfate formation in primitive bodies. Vacuum ultraviolet photons and galactic cosmic rays (GCRs) process interstellar and/or protosolar icy grains to form sulfuric acid **1** (H_2SO_4). Following accretion into primitive asteroid parent bodies, sulfuric acid can be mobilized and neutralized during aqueous alteration or hydrothermal processing, yielding bisulfate (HSO_4^-) or sulfate (SO_4^{2-}) that may subsequently precipitate as sulfate-bearing salts.

generated by GCRs and initiate nonequilibrium chemistry within astrophysical ice analogs.[18,19] In this environment, SO_2 provides an oxidized sulfur precursor, while radiolysis of H_2O generates reactive intermediates capable of driving both oxidation and reduction chemistry.

During temperature-programmed desorption (TPD), desorbing products were analyzed using tunable synchrotron vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry (PI-ReToF-MS), enabling isomer-selective identification of sulfuric acid (H_2SO_4) (Figure 2). The formation of H_2SO_4 demonstrates that S(+VI) reservoirs can be generated directly within low-temperature SO_2-bearing ices prior to planetary accretion.

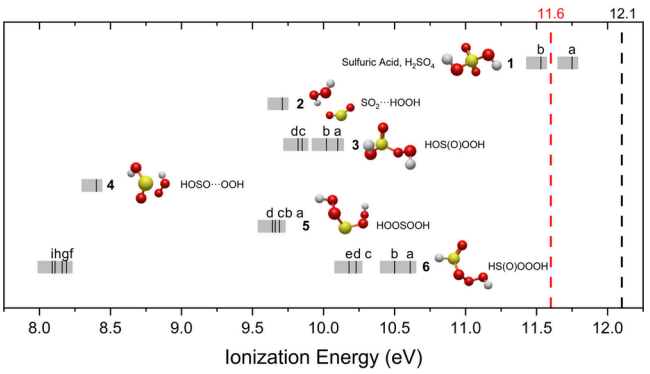


Figure 2. Compilation of experimental photon energies (vertical dashed lines) and calculated adiabatic ionization energies (solid black lines) along with corresponding error ranges (gray boxes) of distinct H_2SO_4 isomers (**1**–**6**) and conformers (**a**–**i**).

Isomer-specific assignment was achieved by tuning the photon energy above and below the calculated adiabatic ionization energies of H_2SO_4 isomers and conformers. The calculated ionization energies utilized here (Figure 2) are estimated to be accurate to ± 0.07 eV;[20−23] for sulfuric acid, the calculated value differs from the experimentally measured adiabatic ionization energy (11.684 ± 0.006 eV) by 0.066 eV.[24]

The 12.10 eV TPD-PI-ReToF-MS overview (Figure 3; Table S1) revealed multiple newly formed sulfur-bearing products including a prominent signal at m/z = 98. Specifically, at 12.10 eV, all H_2SO_4 isomers (**1**–**6**) can be ionized, and a signal at m/z = 98 is observed during TPD, peaking at 273 K, consistent with the mass-to-charge ratio of $H_2SO_4^+$ (Figure 4). When the photon energy is reduced to 11.60 eV, all H_2SO_4 isomers except the **1a** conformer of sulfuric acid remain ionizable. Under these conditions, the m/z = 98 signal at 273 K disappears, indicating that the signal observed at 12.10 eV originates solely from the **1a** conformer of sulfuric acid. A lower temperature sublimation event is observed (179 K) at 11.60 eV, likely originating from fragmentation of higher mass products such as H_2S_4 (m/z = 130) (Figure S1).

Since other chemical formulas potentially contribute to this signal (H_2S_3, $H_2S_2O_2$), additional experiments were performed to verify the molecular formula. Exploiting isotopically labeled water (D_2O), the mass-to-charge signal shifts by 1 m/z for each H atom replaced with D. Consistent with this expectation, the SO_2/D_2O experiment at 12.10 eV revealed a corresponding TPD feature at m/z = 100, coincident with D_2SO_4 (Figure 5).

This mass shift confirms that the carrier contains two H/D atoms and is, therefore, consistent with the sulfuric acid isotopologue D_2SO_4. Next, the sulfur composition was evaluated using the natural abundance of sulfur isotopes, particularly ^{34}S. The theoretical M: M+2 ratios for H_2SO_4, $H_2S_2O_2$, and H_2S_3 are 19.23:1, 10.77:1, and 7.50:1, respectively. The measured ratios of 16.8 ± 1.9:1 for SO_2/H_2O and 17.5 ± 1.5:1 for SO_2/D_2O are consistent with a single sulfur atom; at high dose, the ratio of 19.2 ± 0.7:1 matches the theoretical value for H_2SO_4 (Figure 5, Table 1). Together with the threshold ionization behavior, these results identify the m/z = 98 carrier as sulfuric acid (H_2SO_4, **1a**).

Since we detected H_2SO_4 **1a** during TPD, we now discuss the possible formation mechanism in cryogenic ices. Here, we consider a targeted sequence of oxidation steps involving the reagent material and major radiolysis products known to form in interstellar ice analogs.[25] This sequence is not intended to represent an exhaustive mechanism, but rather a plausible pathway for successive oxidation toward H_2SO_4. First, impinging electrons can initiate bond cleavage of water to produce a hydrogen atom $H(^2S)$ and hydroxyl radical $OH(X^2\Pi)$ (reaction 1).

$$H_2O \rightarrow H(^2S) + OH(X^2\Pi) \quad \Delta_r G = +492 \text{ kJ mol}^{-1} \tag{1}$$

This dissociation is endoergic by 492 kJ mol^{-1} and thus cannot proceed thermally at 5 K; instead, it requires energy deposition from the impinging electrons. Once formed, OH radicals can add to sulfur in SO_2 ($X\ ^1A_1$) forming the hydroxysulfonyl radical ($HOSO_2$). High-level calculations show that OH addition to SO_2 is highly exoergic by 111 kJ mol^{-1} and proceeds through a small entrance barrier on the order of 1 kJ mol^{-1}; however, kinetic experiments reveal that reaction 2 is barrierless.[26,27]

$$OH(X^2\Pi) + SO_2(X^1A_1) \rightarrow HOSO_2(X^2A') \quad \Delta_r G = -111 \text{ kJ mol}^{-1} \tag{2}$$

The hydroxysulfonyl radical can then undergo further oxidation to S(+VI) via addition of a second hydroxyl radical to the central sulfur atom (reaction 3) and is highly exoergic at − 386 kJ mol^{-1}.[28]

Downloaded from pubs.acs.org/jpclcd/article-pdf/17/44/12713/6894370/acs.jpclett.6c02877.pdf by UNIV OF HAWAII user on 06 November 2026

https://doi.org/10.1021/acs.jpclett.6c02877
J. Phys. Chem. Lett. 2026, 17, 12713−12718

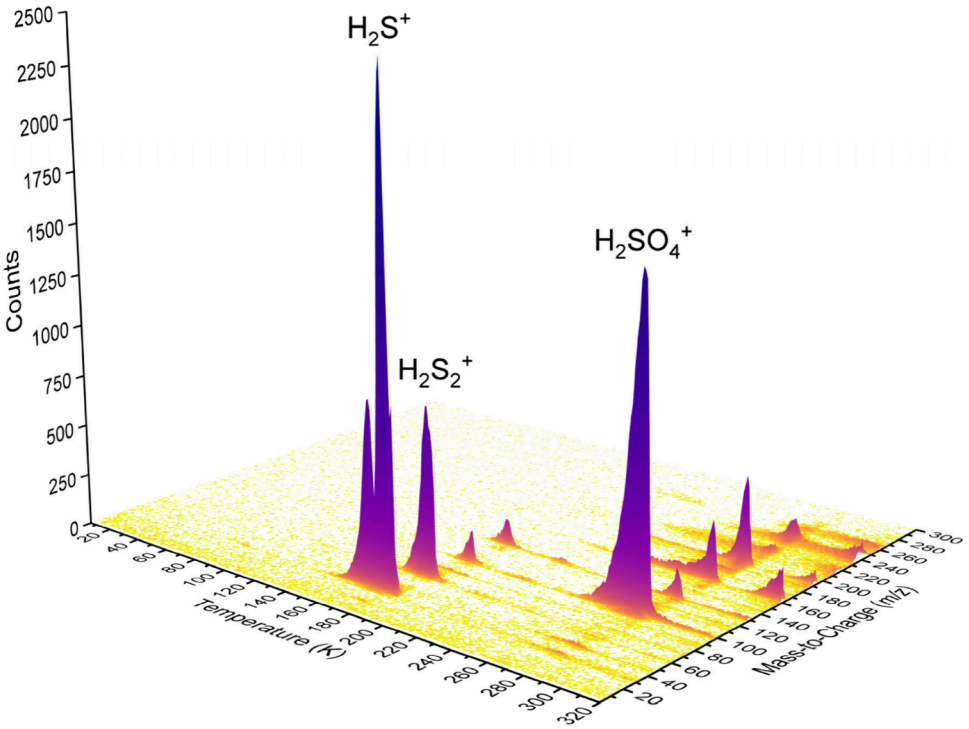


Figure 3. TPD-PI-ReToF-MS data of the processed sulfur dioxide/water (SO_2/H_2O) ice recorded using 12.10 eV photoionization. Major product channels are labeled; a complete list of detected mass-to-charge ratios and possible assignments is provided in Table S1.

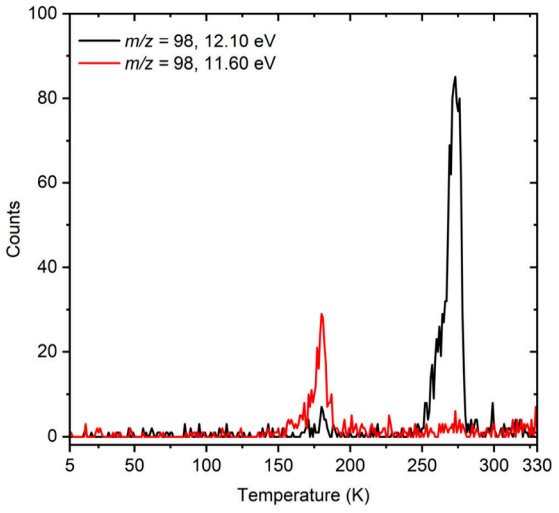


Figure 4. TPD-PI-ReToF-MS of sulfur dioxide/water (SO_2/H_2O) ices collected at 12.10 eV (black) and 11.60 eV (red). Sulfuric acid ($H_2{}^{32}SO_4$) corresponds to m/z = 98.

$$HOSO_2(X^2A') + OH(X^2\Pi) \rightarrow H_2SO_4 \quad \Delta_r G = -386\ \text{kJ mol}^{-1} \tag{3}$$

Preservation of presolar material, organic matter, and inherited interstellar ice through disk evolution and planetesimal accretion is independently established.[29,30] Therefore, if H_2SO_4 or related S(+VI) material forms in SO_2/H_2O ices, this material can be inherited by primitive bodies, where subsequent aqueous processing could mobilize the oxidized sulfur reservoirs as bisulfate and sulfate depending on the pH of the mobilized fluid (reactions 4 and 5).[5,9−11]

$$H_2SO_{4(aq)} + H_2O_{(l)} \rightarrow HSO^-_{4(aq)} + H_3O^+_{(aq)} \quad \text{pH} < 2 \tag{4}$$

$$HSO^-_{4(aq)} + H_2O_{(l)} \rightleftharpoons SO^{2-}_{4\ (aq)} + H_3O^+_{(aq)} \quad \text{pH} \geq 2 \tag{5}$$

In the case of Ryugu's alkaline conditions (pH ≅ 8−10),[7,31,32] the sulfuric acid would be mobilized in the parent-body fluids and modified toward sulfate. During late-stage brine concentration, freezing, or water loss, this sulfate could precipitate with available cations such as Na^+, Mg^{2+} or Ca^{2+}, forming sulfate-bearing salts (reaction 6).[31]

$$SO^{2-}_{4\ (aq)} + 2Na^+ \text{ or } Mg^{2+}/Ca^{2+}_{(aq)} \rightleftharpoons Na_2SO_4 \text{ or } MgSO_4/CaSO_{4(s)} \tag{6}$$

These results suggest that preaccretion formation of sulfuric acid in irradiated SO_2-bearing ices provides a plausible pathway toward sulfate production in primitive asteroid materials such as Ryugu and Bennu. Although parent-body oxidation of reduced sulfides during aqueous alteration may also contribute to sulfate formation, producing abundant S(+VI) sulfate from reduced sulfur under comparatively low-redox, low-temperature conditions remains chemically challenging. In contrast, SO_2 already contains sulfur in the + IV oxidation state and therefore requires only a two-electron oxidation to reach S(+VI).

More specifically, the origin of sulfate-bearing evaporites, including sodium sulfate (Na_2SO_4) identified in Bennu, remains poorly understood.[33] In general, if sulfuric acid or related S(+VI) species were inherited by accreting planetesimals, subsequent interaction with Na-, Mg-, or Ca-bearing fluids could contribute to the sulfate component of primitive-body evaporites without requiring complete oxidation of

Downloaded from pubs.acs.org/jpclcd/article-pdf/17/44/12713/6894370/acs.jpclett.6c02877.pdf by UNIV OF HAWAII user on 06 November 2026

https://doi.org/10.1021/acs.jpclett.6c02877
J. Phys. Chem. Lett. 2026, 17, 12713−12718

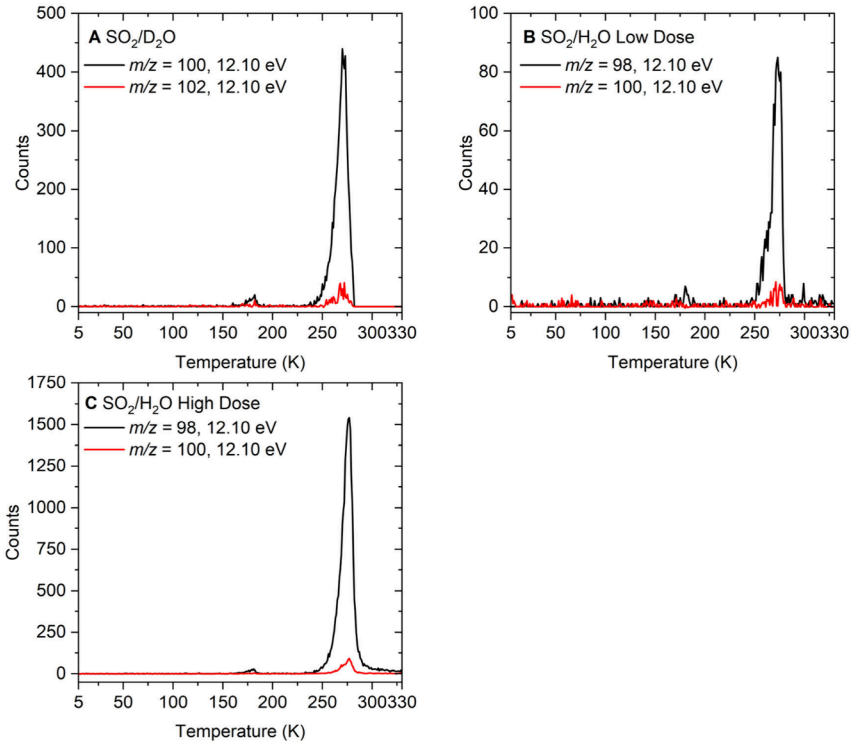


Figure 5. TPD-PI-ReToF-MS of sulfur dioxide/deuterium oxide (SO_2/D_2O) and sulfur dioxide/water (SO_2/H_2O) ices recorded using 12.10 eV photons. Each mass channel correlates to the parent ion of $D_2{}^{32}SO_4$ (A, black) and $H_2{}^{32}SO_4$ (B and C, black) as well as the corresponding ^{34}S isotopologue channel (red).

Table 1. Integrated PI-ReToF-MS of m/z = 98, 100, and 102 associated with H_2SO_4 and D_2SO_4 and their respective sulfur (^{34}S) isotopologues

Mass (m/z)	Integrated Counts	Experimental Ratio (M:M+2)	Theoretical Ratio	Error (%)
		SO_2/H_2O		
98	1088 ± 33	16.8 ± 1.9	19.2	12.6
100	65 ± 8			
		SO_2/H_2O (High Dose)		
98	22484 ± 150	19.2 ± 0.7	19.2	0
100	1172 ± 34			
		SO_2/D_2O		
100	6180 ± 79	17.5 ± 1.5	19.2	9.0
102	353 ± 29			
			Average Low Dose Error	10.8%

sulfide minerals during aqueous alteration alone. In the context of Bennu and Ryugu, this decouples the initial formation of S(+VI) sulfur reservoirs from the final precipitation of sulfate salts, providing a hybrid model in which interstellar or protosolar ice chemistry supplies oxidized sulfur, while parent-body aqueous alteration controls its redistribution, neutralization, and mineralogical preservation.

Overall, our experiments demonstrate that energetic processing of SO_2/H_2O ices can generate sulfuric acid **1** through redox chemistry initiated by reactive oxidants, such as hydroxyl radicals. When considered together with the preservation of presolar and interstellar material during planetesimal accretion and evidence for both molecular-cloud inheritance and subsequent fluid processing in Ryugu,[8] these results establish a chemically viable preaccretion source of S(+VI) sulfur. If inherited by primitive bodies, such oxidized sulfur species could subsequently be redistributed, neutralized, and precipitated during parent-body aqueous alteration, providing an additional pathway consistent with the hybrid chemical history inferred for asteroids, such as Ryugu.

MATERIALS AND METHODS

Photoionization Reflectron Time-of-Flight Mass Spectrometry

Sulfur dioxide/water (SO_2/H_2O) and sulfur dioxide/deuterium oxide (SO_2/D_2O) ices were deposited under ultrahigh-vacuum conditions onto a silver substrate maintained at 5 K.[34,35] The ices were irradiated with 5 keV electrons and subsequently heated from 5 to 330 K at 1 K min^{-1} during temperature-programmed desorption. Subliming products were analyzed by tunable synchrotron vacuum-ultraviolet photoionization reflectron time-of-flight mass spectrometry (PI-ReToF-MS). Complete experimental procedures, irradiation doses, ice characterization, and instrumental parameters are provided in the Supporting Information.

Computational Methods

Adiabatic ionization energies and relative energies were calculated at the CCSD(T)-F12/cc-pVTZ-F12//B3LYP/aug-cc-pVTZ level, including zero-point vibrational energies using MOLPRO quantum chemical software.[23,36−38] Complete computational details are provided in the Supporting Information.

ASSOCIATED CONTENT

Data Availability Statement

All data generated in this study are available in the main text and Supporting Information.

https://doi.org/10.1021/acs.jpclett.6c02877
J. Phys. Chem. Lett. 2026, 17, 12713−12718

Downloaded from pubs.acs.org/jpclcd/article-pdf/17/44/12713/6894370/acs.jpclett.6c02877.pdf by UNIV OF HAWAII user on 06 November 2026

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.jpclett.6c02877.

Possible identified products (Table S1), fragmentation data (Figure S1), physical ice parameters (Tables S2 and S3), quantum-chemical calculations including ionization energies (Table S4), Cartesian coordinates (Table S5), vibrational frequencies (Table S6), and supporting references (PDF)

AUTHOR INFORMATION

Corresponding Authors

Yang Pan − *National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, P. R. China;* orcid.org/0000-0002-9360-3809; Email: panyang@ustc.edu.cn

Tao Yang − *State Key Laboratory of Precision Spectroscopy, East China Normal University, Shanghai 200062, P. R. China; Xinjiang Key Laboratory of Radio Astrophysics, Urumqi, Xinjiang 830011, P. R. China; Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan, Shanxi 030006, P. R. China;* orcid.org/0000-0003-4101-2385; Email: tyang@lps.ecnu.edu.cn

Ryan C. Fortenberry − *Department of Chemistry & Biochemistry, University of Mississippi, University, Mississippi 38677, United States;* orcid.org/0000-0003-4716-8225; Email: r410@olemiss.edu

Ralf I. Kaiser − *Department of Chemistry, University of Hawaii at Mānoa, Honolulu, Hawaii 96822, United States; W.M. Keck Laboratory in Astrochemistry, University of Hawaii at Mānoa, Honolulu, Hawaii 96822, United States;* orcid.org/0000-0002-7233-7206; Email: ralfk@hawaii.edu

Authors

Mason McAnally − *Department of Chemistry, University of Hawaii at Mānoa, Honolulu, Hawaii 96822, United States; W.M. Keck Laboratory in Astrochemistry, University of Hawaii at Mānoa, Honolulu, Hawaii 96822, United States;* orcid.org/0009-0000-7799-9914

Xilin Bai − *State Key Laboratory of Precision Spectroscopy, East China Normal University, Shanghai 200062, P. R. China*

Baoyu Song − *National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, P. R. China*

Jinghui Lu − *National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, P. R. China*

Xinxuan Wang − *National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, P. R. China*

Jiuzhong Yang − *National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, P. R. China;* orcid.org/0000-0002-7076-3412

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jpclett.6c02877

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

This work was conducted under a Memorandum of Understanding between the East China Normal University (ECNU), the University of Hawaii at Manoa (UHM), and the National Synchrotron Radiation Laboratory (NSRL) at the University of Science and Technology of China (USTC). The UHM team was supported by the US National Science Foundation (NSF) Division for Astronomy (NSF-AST 2403867). T.Y. thanks the support from the National Natural Science Foundation of China (Grants Nos. 92461301, 12034008, 12250003, and 12274140), the Xinjiang Tianchi Talent Program (2023), and the Program for Professor of Special Appointment (Eastern Scholar) at Shanghai Institutions of Higher Learning. R.C.F. acknowledges funding from NSF Grant AST-2407815 and computing resources as provided by the Mississippi Center for Supercomputing Research.

REFERENCES

(1) Airieau, S. A.; Farquhar, J.; Thiemens, M. H.; Leshin, L. A.; Bao, H.; Young, E. Planetesimal sulfate and aqueous alteration in CM and CI carbonaceous chondrites. *Geochim. Cosmochim. Acta* **2005**, *69*, 4167−4172.

(2) Singerling, S. A.; Corrigan, C. M.; Brearley, A. J. The fate of primary iron sulfides in the CM1 carbonaceous chondrites: Effects of advanced aqueous alteration on primary components. *Meteorit. Planet. Sci.* **2024**, *59*, 475−501.

(3) Takano, Y.; et al. Primordial aqueous alteration recorded in water-soluble organic molecules from the carbonaceous asteroid (162173) Ryugu. *Nat. Commun.* **2024**, *15*, 5708.

(4) Yoshimura, T.; et al. Chemical evolution of primordial salts and organic sulfur molecules in the asteroid 162173 Ryugu. *Nat. Commun.* **2023**, *14*, 5284.

(5) Nguyen, A. N.; et al. Abundant presolar grains and primordial organics preserved in carbon-rich exogenous clasts in asteroid Ryugu. *Sci. Adv.* **2023**, *9*, No. eadh1003.

(6) Schrader, D. L.; Zega, T. J.; Benner, M. C.; Davidson, J. Hydrothermal alteration of Ryugu from a disruptive impact recorded in a returned sample. *Nat. Commun.* **2026**, *17*, 466.

(7) Zolotov, M. Y. Aqueous fluid composition in CI chondritic materials: Chemical equilibrium assessments in closed systems. *Icarus* **2012**, *220*, 713−729.

(8) Bose, M.; Root, R. A.; Guan, Y.; Eaton, J.; Wittmann, A.; Skrmetti, T.; Desch, S. J. Evidence of both molecular cloud and fluid chemistry in Ryugu regolith. *Sci. Adv.* **2024**, *10*, No. eadp3037.

(9) Van Kooten, E. M. M. E.; Wielandt, D.; Schiller, M.; Nagashima, K.; Thomen, A.; Larsen, K. K.; Olsen, M. B.; Nordlund, Å.; Krot, A. N.; Bizzarro, M. Isotopic evidence for primordial molecular cloud material in metal-rich carbonaceous chondrites. *Proc. Natl. Acad. Sci. U.S.A.* **2016**, *113*, 2011−2016.

(10) Alexander, C. M. O. D.; Nittler, L. R.; Davidson, J.; Ciesla, F. J. Measuring the level of interstellar inheritance in the solar protoplanetary disk. *Meteorit. Planet. Sci.* **2017**, *52*, 1797−1821.

(11) Cleeves, L. I.; Bergin, E. A.; Alexander, C. M.; Du, F.; Graninger, D.; Öberg, K. I.; Harries, T. J. The ancient heritage of water ice in the solar system. *Science* **2014**, *345*, 1590−3.

(12) McClure, M. K.; et al. An Ice Age JWST inventory of dense molecular cloud ices. *Nat. Astron.* **2023**, *7*, 431−443.

(13) Rocha, W. R. M.; et al. Ice inventory towards the protostar Ced 110 IRS4 observed with the James Webb Space Telescope. *A&A* **2025**, *693*, A288.

(14) Moore, M. H.; Hudson, R. L.; Carlson, R. W. The radiolysis of SO_2 and H_2S in water ice: Implications for the icy jovian satellites. *Icarus* **2007**, *189*, 409−423.

(15) Kaňuchová, Z.; Boduch, P.; Domaracka, A.; Palumbo, M. E.; Rothard, H.; Strazzulla, G. Thermal and energetic processing of astrophysical ice analogues rich in SO_2. *A&A* **2017**, *604*, A68.

Downloaded from pubs.acs.org/jpclcd/article-pdf/17/44/12713/6894370/acs.jpclett.6c02877.pdf by UNIV OF HAWAII user on 06 November 2026

(16) McAnally, M.; Bocková, J.; Herath, A.; Turner, A. M.; Meinert, C.; Kaiser, R. I. Abiotic formation of alkylsulfonic acids in interstellar analog ices and implications for their detection on Ryugu. *Nat. Commun.* **2024**, *15*, 4409.
(17) Bennett, C. J.; Jamieson, C. S.; Osamura, Y.; Kaiser, R. I. A Combined Experimental and Computational Investigation on the Synthesis of Acetaldehyde [$CH_3CHO(X^1A')$] in Interstellar Ices. *Astrophys. J.* **2005**, *624*, 1097.
(18) Kaiser, R. I.; Roessler, K. Theoretical and laboratory studies on the interaction of cosmic-ray particles with interstellar ices. III. Suprathermal chemistry-induced formation of hydrocarbon molecules in solid methane (CH_4), ethylene (C_2H_4), and acetylene (C_2H_2). *Astrophys. J.* **1998**, *503*, 959.
(19) Bennett, C. J.; Jamieson, C. S.; Kaiser, R. I. Mechanistical studies on the formation and destruction of carbon monoxide (CO), carbon dioxide (CO_2), and carbon trioxide (CO_3) in interstellar ice analog samples. *Phys. Chem. Chem. Phys.* **2010**, *12*, 4032−4050.
(20) McAnally, M.; Wang, Z.; Zhang, C.; Wang, J.; Fortenberry, R.; Kaiser, R. I. Interstellar Ice Chemistry Yields Elusive Sulfinothioic Acid (HS(O)SH). *Angew. Chem.* **2026**, *65*, No. e8731327.
(21) Wang, J.; Herath, A.; Turner, A. M.; McAnally, M.; Fortenberry, R. C.; Eckhardt, A. K.; Kaiser, R. I. Bottom-Up Formation of the Simplest Geminal Thiol−Methanedithiol ($CH_2(SH)_2$)−and the Methyl Hydrodisulfide (H_3CSSH) Isomer in Interstellar Analogue Ices. *J. Phys. Chem. Lett.* **2026**, *17*, 8090−8097.
(22) McAnally, M.; Zhang, C.; Wang, J.; Herath, A.; Turner, A. M.; Kaiser, R. I. Origin of sulfur allotropes on the carbonaceous asteroid Ryugu and implications to the sulfur chemistry in the interstellar medium. *Sci. Adv.* **2026**, *12*, No. eaeb3358.
(23) Knizia, G.; Adler, T. B.; Werner, H.-J. Simplified CCSD(T)-F12 Methods: Theory and Benchmarks. *J. Chem. Phys.* **2009**, *130*, 054104.
(24) Zhang, C.; Lin, X.; Tang, X.; Fittschen, C.; Hartweg, S.; Garcia, G. A.; Long, B.; Zhang, W.; Nahon, L. Vacuum ultraviolet photochemistry of sulfuric acid vapor: a combined experimental and theoretical study. *Phys. Chem. Chem. Phys.* **2022**, *24*, 2015−2021.
(25) Zheng, W.; Jewitt, D.; Kaiser, R. I. Formation of Hydrogen, Oxygen, and Hydrogen Peroxide in Electron-irradiated Crystalline Water Ice. *Astrophys. J.* **2006**, *639*, 534.
(26) Medeiros, D. J.; Blitz, M. A.; Seakins, P. W. Exploring the features on the OH + SO_2 potential energy surface using theory and testing its accuracy by comparison to experimental data. *Phys. Chem. Chem. Phys.* **2018**, *20*, 8984−8990.
(27) Long, B.; Bao, J. L.; Truhlar, D. G. Reaction of SO_2 with OH in the atmosphere. *Phys. Chem. Chem. Phys.* **2017**, *19*, 8091−8100.
(28) Chase, M. W. NIST-JANAF thermochemical tables. *J. Phys. Chem. Ref. Data* **1998**, *28*, 1951.
(29) Bergner, J. B.; Ciesla, F. Ice Inheritance in Dynamical Disk Models. *Astrophys. J.* **2021**, *919*, 45.
(30) Hoppe, P.; Leitner, J.; Kodolányi, J. The stardust abundance in the local interstellar cloud at the birth of the Solar System. *Nat. Astron.* **2017**, *1*, 617−620.
(31) Matsumoto, T.; et al. Sodium carbonates on Ryugu as evidence of highly saline water in the outer Solar System. *Nat. Astron.* **2024**, *8*, 1536−1543.
(32) Nakamura, T.; Matsumoto, M.; Amano, K.; Enokido, Y.; Zolensky, M.; Mikouchi, T.; Genda, H.; Tanaka, S.; Zolotov, M.; Kurosawa, K.; et al. Formation and evolution of carbonaceous asteroid Ryugu: Direct evidence from returned samples. *Science* **2023**, *379*, No. eabn8671.
(33) McCoy, T. J.; et al. An evaporite sequence from ancient brine recorded in Bennu samples. *Nature* **2025**, *637*, 1072−1077.
(34) Bai, X.; Gong, Q.; Lu, J.; Yang, J.; Pan, Y.; Sun, Z.; Kaiser, R. I.; Yang, T. Non-Equilibrium Growth Processes to Glyceraldehyde and Glycerol as Building Blocks of Interstellar Sugars and Phospholipids. *J. Am. Chem. Soc.* **2026**, *148*, 22979−22989.
(35) Bai, X.; et al. Formation of hydrogen trioxide (HOOOH) in extraterrestrial ice analogs and its role as an oxidizer in prebiotic chemistry. *Sci. Adv.* **2025**, *11*, No. eadw5720.
(36) Adler, T. B.; Knizia, G.; Werner, H.-J. A Simple and Efficient CCSD(T)-F12 Approximation. *J. Chem. Phys.* **2007**, *127*, 221106.
(37) Peterson, K. A.; Adler, T. B.; Werner, H.-J. Systematically Convergent Basis Sets for Explicitly Correlated Wavefunctions: The Atoms H, He, B-Ne, and Al-Ar. *J. Chem. Phys.* **2008**, *128*, 084102.
(38) Werner, H. J.; Knowles, P. J.; Knizia, G.; Manby, F. R.; Schütz, M. Molpro: A General-Purpose Quantum Chemistry Program Package. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2*, 242−253.

Downloaded from pubs.acs.org/jpclcd/article-pdf/17/44/12713/6894707/acs.jpclett.6c02877.pdf by UNIV OF HAWAII user on 06 November 2026

https://doi.org/10.1021/acs.jpclett.6c02877
J. Phys. Chem. Lett. 2026, 17, 12713−12718