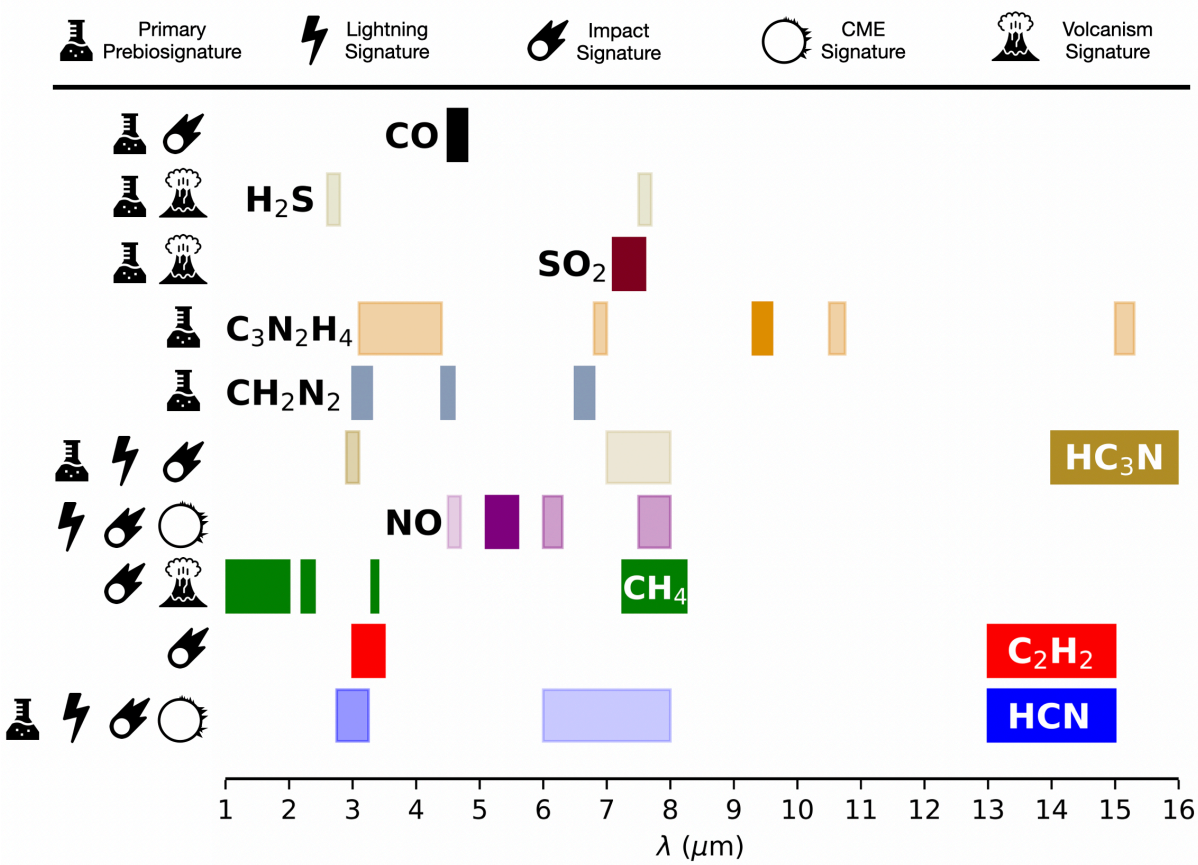
Primary Prebiosignature
Lightning Signature
Impact Signature
CME Signature
Volcanism Signature
CO
H2S
SO2
C3N2H4
CH2N2
HC3N
NO
CH4
C2H2
HCN
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
λ (μm)

# CO

***Cross-Section: EXOMOL***

Chubb, K.L., Rocchetto, M., Yurchenko, S.N., Min, M., Waldmann, I., Barstow, J.K., Molliere, P., Al-Refaie, A.F, Phillips, M.W., Tennyson, J., "The ExoMolOP Database: Cross-sections and k-tables for Molecules of Interest in High-Temperature Exoplanet Atmospheres", Astronomy and Astrophysics Accepted (2020).

Li, G., Gordon, I. E., Rothman, L. S., Tan, Y., Hu, S.-M., Kassi, S., Campargue, A., Medvedev, E. S., "Rovibrational line lists for nine isotopologues of the CO molecule in the X 1Σ+ ground electronic state", Astrophysical Journal Supplement Series 216, 15 (2015).

***Sources:***

*Impacts*

Kasting, J.F., 1990. Bolide impacts and the oxidation state of carbon in the Earth's early atmosphere. Origins of Life and Evolution of the Biosphere, 20(3-4), pp.199-231.

Ferus, M., Kubelík, P., Knížek, A., Pastorek, A., Sutherland, J. and Civiš, S., 2017. High energy radical chemistry formation of HCN-rich atmospheres on early Earth. Scientific reports, 7(1), pp.1-9.

Zahnle, K.J., Lupu, R., Catling, D.C. and Wogan, N., 2020. Creation and Evolution of Impact-generated Reduced Atmospheres of Early Earth. The Planetary Science Journal, 1(1), p.11.

***Prebiotic Relevance (example references):***

Miyakawa, S., Yamanashi, H., Kobayashi, K., Cleaves, H.J. and Miller, S.L., 2002. Prebiotic synthesis from CO atmospheres: implications for the origins of life. Proceedings of the National Academy of Sciences, 99(23), pp.14628-14631.

# H2S

***Cross-Section: EXOMOL***

Azzam, A. A. A., Tennyson, J., Yurchenko, S. N., Naumenko, O. V., "ExoMol molecular line lists – XVI: The rotation-vibration spectrum of hot H2S", Monthly Notices of the Royal Astronomical Society 460, 4063-4074 (2016).

***Sources:***

*Volcanism*

de Moor, J.M., Fischer, T.P., Sharp, Z.D., King, P.L., Wilke, M., Botcharnikov, R.E., Cottrell, E., Zelenski, M., Marty, B., Klimm, K. and Rivard, C., 2013. Sulfur degassing at Erta Ale (Ethiopia) and Masaya (Nicaragua) volcanoes: Implications for degassing processes and oxygen fugacities of basaltic systems. Geochemistry, Geophysics, Geosystems, 14(10), pp.4076-4108.

***Prebiotic Relevance (example references):***

Keefe, A.D., Miller, S.L., McDonald, G. and Bada, J., 1995. Investigation of the prebiotic synthesis of amino acids and RNA bases from CO2 using FeS/H2S as a reducing agent. Proceedings of the National Academy of Sciences, 92(25), pp.11904-11906.

Patel, B.H., Percivalle, C., Ritson, D.J., Duffy, C.D. and Sutherland, J.D., 2015. Common origins of RNA, protein and lipid precursors in a cyanosulfidic protometabolism. Nature chemistry, 7(4), pp.301-307.

Okamura, H., Becker, S., Tiede, N., Wiedemann, S., Feldmann, J. and Carell, T., 2019. A one-pot, water compatible synthesis of pyrimidine nucleobases under plausible prebiotic conditions. Chemical Communications, 55(13), pp.1939-1942.

# SO2

***Cross-Section: EXOMOL***

Underwood, D. S., Tennyson, J., Yurchenko, S. N., Huang, X., Schwenke, D. W. , Lee, T. J., Clausen, S., Fateev, A., "ExoMol molecular line lists - XIV: The rotation-vibration spectrum of hot SO2", Monthly Notices of the Royal Astronomical Society 459, 3890-3899 (2016).

***Sources:***

*Volcanism*
de Moor, J.M., Fischer, T.P., Sharp, Z.D., King, P.L., Wilke, M., Botcharnikov, R.E., Cottrell, E., Zelenski, M., Marty, B., Klimm, K. and Rivard, C., 2013. Sulfur degassing at Erta Ale (Ethiopia) and Masaya (Nicaragua) volcanoes: Implications for degassing processes and oxygen fugacities of basaltic systems. Geochemistry, Geophysics, Geosystems, 14(10), pp.4076-4108.

***Prebiotic Relevance (example references):***

Xu, J., Ritson, D.J., Ranjan, S., Todd, Z.R., Sasselov, D.D. and Sutherland, J.D., 2018. Photochemical reductive homologation of hydrogen cyanide using sulfite and ferrocyanide. Chemical Communications, 54(44), pp.5566-5569.

# C3N2H4

***Cross-Section: Reference***

Perchard, C. and Novak, A., 1968. Far-Infrared Spectra and Hydrogen-Bond Frequencies of Imidazole. The Journal of Chemical Physics, 48(7), pp.3079-3084.

***Sources:***

No known geochemical source.

***Prebiotic Relevance (example references):***

Lohrmann, R. and Orgel, L.E., 1973. Prebiotic activation processes. Nature, 244(5416), pp.418-420.

Oró, J., Basile, B., Cortes, S., Shen, C. and Yamrom, T., 1984. The prebiotic synthesis and catalytic role of imidazoles and other condensing agents. Origins of life, 14(1-4), pp.237-242.

Fahrenbach, A.C., Giurgiu, C., Tam, C.P., Li, L., Hongo, Y., Aono, M. and Szostak, J.W., 2017. Common and potentially prebiotic origin for precursors of nucleotide synthesis and activation. Journal of the American Chemical Society, 139(26), pp.8780-8783.

# CH2N2

***Cross-Section: Reference***

Lee, G., Kossowska, D., Lim, J., Kim, S., Han, H., Kwak, K. and Cho, M., 2018. Cyanamide as an infrared reporter: Comparison of vibrational properties between nitriles bonded to N and C atoms. The Journal of Physical Chemistry B, 122(14), pp.4035-4044.

***Sources:***

No known geochemical source.

***Prebiotic Relevance (example references):***

Ibanez, J.D., Kimball, A.P. and Oro, J., 1971. Possible prebiotic condensation of mononucleotides by cyanamide. Science, 173(3995), pp.444-446.

Patel, B.H., Percivalle, C., Ritson, D.J., Duffy, C.D. and Sutherland, J.D., 2015. Common origins of RNA, protein and lipid precursors in a cyanosulfidic protometabolism. Nature chemistry, 7(4), pp.301-307.

Tsanakopoulou, M. and Sutherland, J.D., 2017. Cyanamide as a prebiotic phosphate activating agent–catalysis by simple 2-oxoacid salts. Chemical Communications, 53(87), pp.11893-11896.

# HC3N

***Cross-Section: NIST***

NIST Standard Reference Data Program
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This IR spectrum is from the NIST/EPA Gas-Phase Infrared Database

***Sources:***

*Lightning*
Ferris, J.P., Sanchez, R.A. and Orgel, L.E., 1968. Studies in prebiotic synthesis: III. Synthesis of pyrimidines from cyanoacetylene and cyanate. Journal of molecular biology, 33(3), pp.693-704.

*Impacts*
Ferus, M., Rimmer, P., Cassone, G., Knížek, A., Civiš, S., Šponer, J.E., Ivanek, O., Šponer, J., Saeidfirozeh, H., Kubelík, P. and Dudžák, R., 2020. One-pot hydrogen cyanide-based prebiotic synthesis of canonical nucleobases and glycine initiated by high-velocity impacts on early Earth. Astrobiology, 20(12), pp.1476-1488.

***Prebiotic Relevance (example references):***

Sanchez, R.A., Ferris, J.P. and Orgel, L.E., 1966. Cyanoacetylene in prebiotic synthesis. Science, 154(3750), pp.784-785.

Ferris, J.P., Sanchez, R.A. and Orgel, L.E., 1968. Studies in prebiotic synthesis: III. Synthesis of pyrimidines from cyanoacetylene and cyanate. Journal of molecular biology, 33(3), pp.693-704.

Orgel, L.E., 2002. Is cyanoacetylene prebiotic?. Origins of Life and Evolution of the Biosphere, 32(3), pp.279-281.

Benner, S.A., Bell, E.A., Biondi, E., Brasser, R., Carell, T., Kim, H.J., Mojzsis, S.J., Omran, A., Pasek, M.A. and Trail, D., 2019. When did life likely emerge on Earth in an RNA-first process?. ChemSystemsChem.

# NO

***Cross-Section: EXOMOL***

Wong, A., Yurchenko, S. N., Bernath, P., Mueller, H. S. P., McConkey, S., Tennyson, J., "ExoMol line list XXI: nitric oxide (NO)", Monthly Notices of the Royal Astronomical Society 470, 882-897 (2017).

***Sources:***

*Lightning*
Mvondo, D.N., Navarro-González, R., McKay, C.P., Coll, P. and Raulin, F., 2001. Production of nitrogen oxides by lightning and coronae discharges in simulated early Earth, Venus and Mars environments. Advances in Space Research, 27(2), pp.217-223.

*Stellar Activity*
Airapetian, V.S., Glocer, A., Gronoff, G., Hebrard, E. and Danchi, W., 2016. Prebiotic chemistry and atmospheric warming of early Earth by an active young Sun. Nature Geoscience, 9(6), pp.452-455.

*Impacts*
Heays et al. Impact production of nitrogen oxides in the Hadean atmosphere. Submitted to JGR: Planets

***Prebiotic Relevance (example references):***

Indirect prebiotic relevance, see:

Ranjan, S., Todd, Z.R., Rimmer, P.B., Sasselov, D.D. and Babbin, A.R., 2019. Nitrogen oxide concentrations in natural waters on early Earth. Geochemistry, Geophysics, Geosystems, 20(4), pp.2021-2039.

Mariani, A., Russell, D.A., Javelle, T. and Sutherland, J.D., 2018. A light-releasable potentially prebiotic nucleotide activating agent. Journal of the American Chemical Society, 140(28), pp.8657-8661.

# CH4

***Cross-Section: EXOMOL***

Hill, C., Yurchenko, S. N., Tennyson, J., "Temperature-dependent molecular absorption cross sections for exoplanets and other atmospheres", Icarus 226, 1673-1677 (2013).

Tennyson, J., Yurchenko, S. N., "ExoMol: molecular line lists for exoplanet and other atmospheres", Monthly Notices of the Royal Astronomical Society 425, 21-33 (2012).

***Sources:***

*Volcanoes*
Dimitrov, L.I., 2003. Mud volcanoes—a significant source of atmospheric methane. Geo-Marine Letters, 23(3-4), pp.155-161.

***Prebiotic Relevance (example references):***

No direct prebiotic relevance.

# C2H2

***Cross-Section: EXOMOL***

Chubb, K. L., Tennyson, J., Yurchenko, S.N., "ExoMol molecular line lists - XXXVII: spectra of acetylene", Monthly Notices of the Royal Astronomical Society 493, 1531-1545 (2020).

***Sources:***

*Impacts*
Rimmer, P.B., Ferus, M., Waldmann, I.P., Knížek, A., Kalvaitis, D., Ivanek, O., Kubelík, P., Yurchenko, S.N., Burian, T., Dostál, J. and Juha, L., 2019. Identifiable Acetylene Features Predicted for Young Earth-like Exoplanets with Reducing Atmospheres Undergoing Heavy Bombardment. The Astrophysical Journal, 888(1), p.21.

***Prebiotic Relevance (example references):***

Indirect prebiotic relevance, see:

Patel, B.H., Percivalle, C., Ritson, D.J., Duffy, C.D. and Sutherland, J.D., 2015. Common origins of RNA, protein and lipid precursors in a cyanosulfidic protometabolism. Nature chemistry, 7(4), pp.301-307.

# HCN

***Cross-Section: EXOMOL***

Hill, C., Yurchenko, S. N., Tennyson, J., "Temperature-dependent molecular absorption cross sections for exoplanets and other atmospheres", Icarus 226, 1673-1677 (2013).

Tennyson, J., Yurchenko, S. N., "ExoMol: molecular line lists for exoplanet and other atmospheres", Monthly Notices of the Royal Astronomical Society 425, 21-33 (2012).

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***Sources:***

*Lightning*
Chameides, W.L. and Walker, J.C., 1981. Rates of fixation by lightning of carbon and nitrogen in possible primitive atmospheres. Origins of life, 11(4), pp.291-302.

*Stellar Activity*
Airapetian, V.S., Glocer, A., Gronoff, G., Hebrard, E. and Danchi, W., 2016. Prebiotic chemistry and atmospheric warming of early Earth by an active young Sun. Nature Geoscience, 9(6), pp.452-455.

*Impacts*
Ferus, M., Kubelík, P., Knížek, A., Pastorek, A., Sutherland, J. and Civiš, S., 2017. High energy radical chemistry formation of HCN-rich atmospheres on early Earth. Scientific reports, 7(1), pp.1-9.

Rimmer, P.B., Ferus, M., Waldmann, I.P., Knížek, A., Kalvaitis, D., Ivanek, O., Kubelík, P., Yurchenko, S.N., Burian, T., Dostál, J. and Juha, L., 2019. Identifiable Acetylene Features Predicted for Young Earth-like Exoplanets with Reducing Atmospheres Undergoing Heavy Bombardment. The Astrophysical Journal, 888(1), p.21.

***Prebiotic Relevance (example references):***

Extensive, many dozens of references (including many of the above references). We list one early reference as an example.

Oró, J. and Kimball, A.P., 1961. Synthesis of purines under possible primitive earth conditions. I. Adenine from hydrogen cyanide. Archives of biochemistry and biophysics, 94(2), pp.217-227.