Supplementary Information

Case	$P-T$ profile	P_b/bar	Star	Boundary Condition	C_2H_2	C_2H_6	HCN	HC_3N	CH_3OH
1	PT1	100	old	zero flux	3.0E-06	7.5E-05	1.2E-07	9.0E-07	4.3E-06
2	PT2	100	old	zero flux	6.5E-06	1.3E-03	3.4E-07	2.1E-05	9.9E-05
3	PT3	100	old	zero flux	1.6E-05	8.6E-03	4.1E-06	1.3E-04	3.7E-04
4	PT1	1	old	zero flux	3.1E-17	5.9E-11	9.3E-07	3.2E-14	1.2E-08
5	PT3	1	old	zero flux	1.7E-12	8.5E-07	5.5E-08	4.1E-10	2.5E-07
6	PT4	1	old	zero flux	1.3E-06	1.3E-06	2.5E-06	6.7E-07	7.3E-16
7	PT1	100	young	fixed H_2O, CH_4, NH_3	2.8E-07	2.2E-04	3.0E-05	5.8E-05	2.5E-09
8	PT4	1	young	fixed H_2O, CH_4, NH_3	5.8E-03	6.8E-04	2.1E-05	6.7E-07	2.9E-19
9	PT1	100	old	fixed N_2, H_2O; CO_2=1.4E-02	6.0E-17	1.31E-08	8.4E-09	5.7E-13	4.3E-11
10	PT1	100	old	fixed N_2, H_2O; CO_2 = 1.0E-06	6.2E-21	1.2E-11	2.6E-10	6.3E-18	2.9E-15
11	PT4	1	old	fixed N_2, H_2O; CO_2 = 1.0E-01	9.1E-13	1.7E-10	2.0E-12	5.0E-13	2.4E-09

Table S1 Model assumptions and volume mixing ratios at 1 mbar of prominent molecules for Hycean cases explored with the photochemical calculations in this work (see sections 2.2 and 3.2). The initial metallicity is assumed to be 100× solar. P_b is the pressure at the lower boundary. The boundary conditions are those considered at the lower boundary of the atmosphere. The first six cases consider zero-flux boundary conditions, i.e. an unreactive surface, whereas the last five cases consider boundary conditions as discussed in sections 2.2 and 3.2. Cases 7 and 10 compute chemistry at an age of ∼30 Myr in the early evolution of the planet starting with reduced boundary conditions corresponding to an initial equilibrium composition for 100× solar metallicity. The last five columns show the volume mixing ratios at 1 mbar of prominent CNO molecules (C_2H_2, C_2H_6, HCN, HC_3N and CH_3OH) expected in H_2-rich atmospheres.

Case	$P-T$ profile	P_b/bar	Star	Boundary Condition	H_2O	CH_4	NH_3	CO_2	CO
1	PT1	100	old	zero flux	2.4E-02	1.1E-02	4.2E-05	1.3E-02	7.5E-06
2	PT2	100	old	zero flux	1.0E-02	6.7E-03	1.5E-04	4.5E-03	5.1E-05
3	PT3	100	old	zero flux	2.8E-03	2.5E-03	3.3E-04	3.5E-04	2.5E-04
4	PT1	1	old	zero flux	2.4E-02	6.8E-06	3.4E-09	4.1E-02	1.9E-03
5	PT3	1	old	zero flux	2.3E-02	8.2E-05	1.0E-11	4.3E-02	9.3E-04
6	PT4	1	old	zero flux	4.8E-08	7.8E-05	2.2E-07	9.4E-15	3.0E-09
7	PT1	100	young	fixed H_2O, CH_4, NH_3	2.5E-02	5.0E-02	1.5E-02	4.0E-05	2.3E-05
8	PT4	1	young	fixed H_2O, CH_4, NH_3	4.7E-08	4.9E-02	1.4E-02	1.8E-19	2.4E-10
9	PT1	100	old	fixed N_2, H_2O; CO_2=1.4E-02	2.4E-02	1.2E-04	3.7E-10	1.3E-02	2.2E-06
10	PT1	100	old	fixed N_2, H_2O; CO_2 = 1.0E-06	2.4E-02	3.6E-06	6.2E-10	1.0E-06	1.3E-08
11	PT4	1	old	fixed N_2, H_2O; CO_2 = 1.0E-01	4.7E-08	5.6E-08	4.8E-14	1.0E-01	6.4E-03

Table S2 Model assumptions and volume mixing ratios at 10 mbar of prominent molecules for Hycean cases explored with the photochemical calculations in this work (see sections 2.2 and 3.2). The initial metallicity is assumed to be 100× solar. P_b is the pressure at the lower boundary. The boundary conditions are those considered at the lower boundary of the atmosphere. The first six cases consider zero-flux boundary conditions, i.e. an unreactive surface, whereas the last five cases consider boundary conditions as discussed in sectiona 2.2 and 3.2. Cases 7 and 10 compute chemistry at an age of ∼30 Myr in the early evolution of the planet starting with reduced boundary conditions corresponding to an initial equilibrium composition for 100× solar metallicity. The last five columns show the volume mixing ratios at 10 mbar of prominent CNO molecules (H_2O, CH_4, NH_3, CO_2 and CO) expected in H_2-rich atmospheres. The H_2O abundance is controlled by saturation at the lower boundary, that is mixing ratios of $\sim 2\times10^{-2}$ for the 100-bar cases, except when condensation occurs at higher altitudes (e.g., PT2, PT3 and PT4 profiles), where the saturation minimum becomes $\sim 1\times10^{-2}$ for PT2, $\sim 3\times10^{-3}$ for PT3, and lower for PT4. We note that cooler temperature profiles can decrease the H_2O abundance further and affect the abundances of other molecules, especially decrease the CO_2 abundance.