Abundances of trace constituents in Jupiter's atmosphere inferred from Herschel/PACS observations

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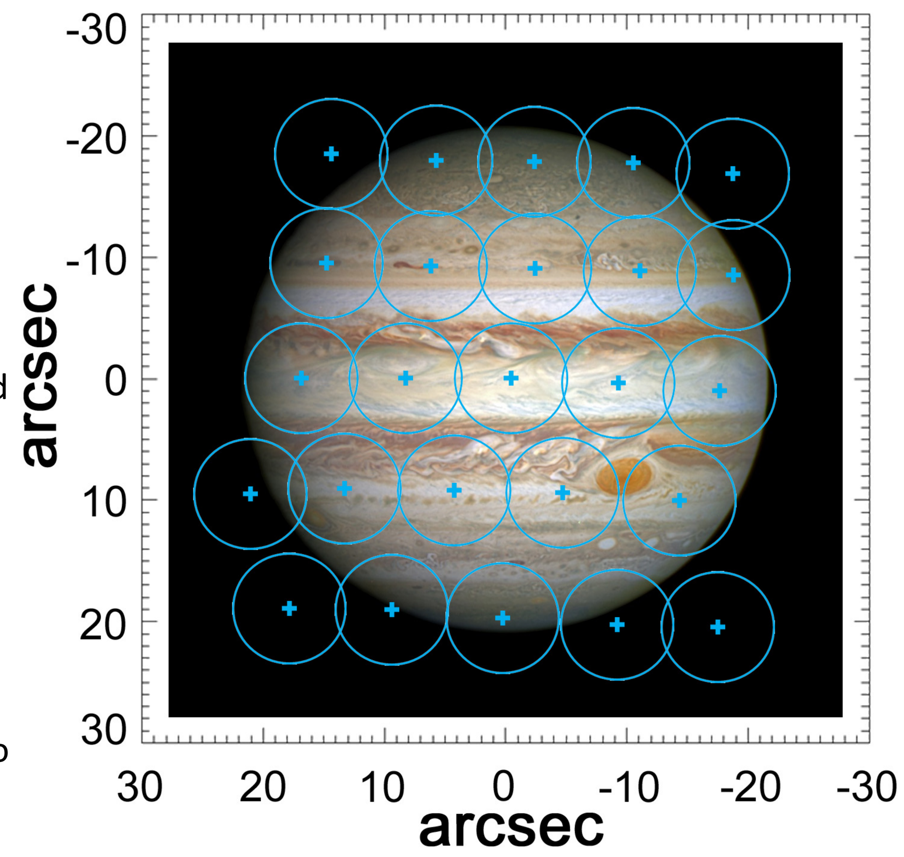
Abstract

Context. On October 31, 2009, the Photodetector Array Camera and Spectrometer (PACS) onboard the Herschel Space Observatory observed far infrared spectra of Jupiter in the wavelength range between 50 and 220 µm as part of the program 'Water and Related Chemistry in the Solar System'. The spectra have an effective spectral resolution between 900 and 3500, depending on wavelength and grating order.
Aims. We investigate the disk-averaged chemical composition of Jupiter's atmosphere as a function of height using these observations.
Methods. We used the Planetary Spectrum Generator (PSG) and the least squares fitting technique to infer the abundances of trace constituents.
Results. The PACS data include numerous spectral lines attributable to ammonia (NH_3), methane (CH_4), phosphine (PH_3), water (H_2O) and deuterated hydrogen (HD) in the Jovian atmosphere and probe the chemical composition from $p \sim 275$ mbar to $p \sim 900$ mbar. From the observations, we infer an ammonia abundance profile that decreases from a mole fraction of $(1.7 \pm 0.8)\times10^{-4}$ at $p \sim 900$ mbar to $(1.7 \pm 0.9)\times10^{-8}$ at $p \sim 275$ mbar, following a fractional scale height of about 0.114. For phosphine, we find a mole fraction of $(7.2 \pm 1.2)\times10^{-7}$ at pressures higher than (550 ± 100) mbar and a decrease of its abundance at lower pressures following a fractional scale height of (0.09 ± 0.02). Our analysis delivers a methane mole fraction of $(1.49 \pm 0.09)\times10^{-3}$. Analyzing the HD R(0) line at 112.1 µm yields a new measurement of Jupiter's D/H ratio, $D/H = (1.5 \pm 0.6)\times10^{-5}$. Finally, the PACS data allow us to put the most stringent 3σ upper limits yet on the mole fractions of hydrogen halides in the Jovian troposphere. These new upper limits are $< 1.1\times10^{-11}$ for hydrogen fluoride (HF), $< 6.0\times10^{-11}$ for hydrogen chloride (HCl), $< 2.3\times10^{-10}$ for hydrogen bromide (HBr) and $< 1.2\times10^{-9}$ for hydrogen iodide (HI) and support the proposed condensation of hydrogen halides into ammonium halide salts in the Jovian troposphere.

Observations

To build up the full **wavelength range between 50 and 220 µm**, two separate observations (ObsIDs 1342186573 and 1342186574) were conducted. During both observations, PACS obtained spectra using its array of 5×5 spaxels with a total field of view (FOV) of 47″ × 47″ on the sky, while Jupiter had an angular diameter of 41″ (see Fig. on the right).

As an **extremely bright infrared source,** Jupiter caused strong fluxes on PACS's detectors. To prevent saturation and persistence effects due to on-and-off transients, the unchopped full resolution up-and-down grating scan with shortened integration time in the time-limited special telemetry burst mode had to be used. These observational modes compromised the signal-to-noise ratio (S/N) of each spaxel substantially and prevented us from carrying out an absolute flux calibration. Thus, we divided all resulting spectra by their local continua for the following analyses. To increase the S/N, we **only analyzed the average spectra of the innermost nine spaxels**, yielding information on the disk-averaged properties of Jupiter's atmosphere.

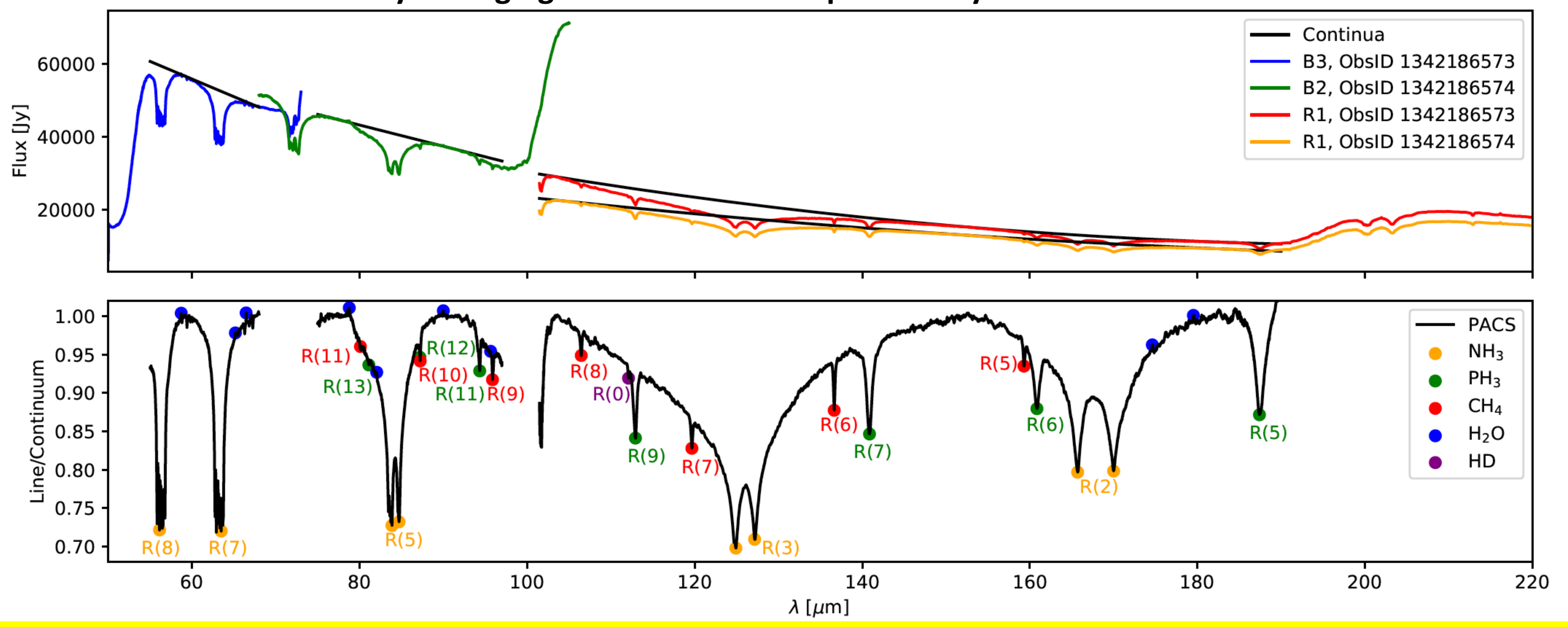


Data & Analysis

The spectral range of the blue spectrometer was covered in grating order 3 (B3, $50 - 73\ \mu m$) for the first observation (ObsID 1342186573) and in grating order 2 (B2, $68 - 105\ \mu m$) for the second observation (ObsID 1342186574). During both observations, the spectra of the red spectrometer were covered using grating order 1 (R1, $101 - 220\ \mu m$) and we **combined both observations by averaging them for all subsequent analyses**.

The PACS observations, before and after normalization by the continua, are plotted in the Figure on the right. To approximate the continua for the Line-to-Continuum normalization, we fit second-order polynomials to selected parts of the data far from any absorption or emission features. The spectra show numerous rotational spectral features caused by ammonia, phosphine, methane, water vapor and deuterated hydrogen in the Jovian atmosphere. Except for the water features, **all of these features are absorption lines and thus originate from Jupiter's troposphere**. The water emission lines are generated in Jupiter's stratosphere and are unresolved given PACS's spectral resolution. Therefore, we used their observed line shapes to calibrate PACS's effective spectral resolution rather than analyzing Jupiter's stratospheric water reservoir.

To derive constraints on the observed molecules' abundances from the observed spectra, we computed synthetic spectra using the **Planetary Spectrum Generator** (**PSG,** Villanueva et al. 2018) and compared these spectra to the PACS data in Line-to-Continuum using reduced chi-squares. We used HITRAN for both rotational lines and collision-induced absorption and employed ephemerides taken from the NASA/JPL Horizons Web-Interface for the simulations. We adopted the a priori temperature profile that Nixon (2007) derived from the temperature measurements of the *Galileo* Entry Probe.



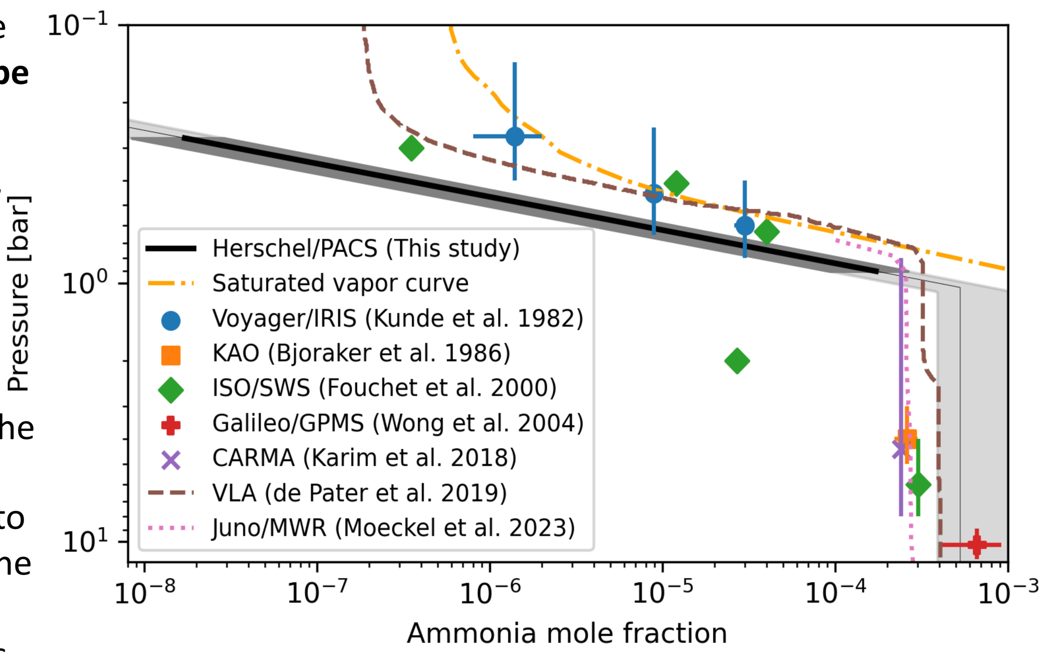
Results: Ammonia (NH_3)

We analyzed four ammonia bands (NH_3 R(2), R(3), R(5), and R(7)) **simultaneously for constraints on the Jovian ammonia abundances**. Out of these four bands, the NH_3 R(3) band consistently showed large deviations from any model spectra between $100 - 110$ µm and we did not identify the origin of this discrepancy. Therefore, we excluded the NH_3 R(3) band from the ammonia analysis and all data between $100 - 110$ µm from all further analyses.

We parameterized ammonia's vertical abundance profile using a **three-parameter model of the shape**

$$a_{NH_3}(p) = \begin{cases} a_{NH_3}(\infty) & \text{if } p \geq p_{NH_3} \\ a_{NH_3}(\infty)\left(\frac{p}{p_{NH_3}}\right)^{(1-f_{NH_3})/f_{NH_3}} & \text{else} \end{cases},$$

where p is pressure and $a_{NH_3}(\infty)$, p_{NH_3} and f_{NH_3} are to be fit for. We used a total of ten thousand different combinations of all three parameters to find the best-fitting parameter combination with the respective error bars by comparing the calculated synthetic spectra of each parameter combination to the observations. The best-fit model profile with the corresponding 1σ interval are shown in the Figure on the right together with previous studies' results.



Our ammonia abundances are lower than the saturated vapor curve in the entire atmosphere, suggesting that our **disk-averaged spectra might be sensitive to dry, cloud-poor parts of the Jovian atmosphere**. This might be caused by the fact that these regions emit more infrared radiation than cloudier parts of the atmosphere where the clouds absorb parts of Jupiter's thermal radiation.

Methane (CH_4)

We used six methane bands (CH_4 R(5), R(6), R(7), R(9), R(10), and R(11)) simultaneously to infer the methane mole fraction in Jupiter's troposphere which we assumed to be vertically constant. We adopted the prescribed temperature, inferred ammonia and phosphine abundance profiles and varied the model's methane abundance to generate synthetic spectra we compared the PACS observations to in line-to-continuum ratios. Our constraints are consistent with the results of the Galileo entry probe (see Table below), but point toward a slightly lower mole fraction that corresponds to a Jovian C/H ratio of 2.4 ± 0.1 times the protosolar value (Lodders 2019). This ratio still represents a **significant enrichment of carbon in Jupiter compared to the primordial composition and is in agreement with the core accretion theory** (Pollack et al. 1996).

Data source	Mole fractions	Sensitivity ranges	Reference
Galileo/GPMS	$(1.81 \pm 0.34)\times10^{-3}$	$p \sim (0.5 - 3.8)$ bar	Niemann et al, 1998
Galileo/GPMS	$(2.04 \pm 0.49)\times10^{-3}$	$p \sim (0.5 - 3.8)$ bar	Wong et al., 2004
Herschel/PACS	$\mathbf{(1.5 \pm 0.1)\times10^{-3}}$	$\mathbf{p \sim (0.35 - 0.8)}$ **bar**	**This study**

Hydrogen halides

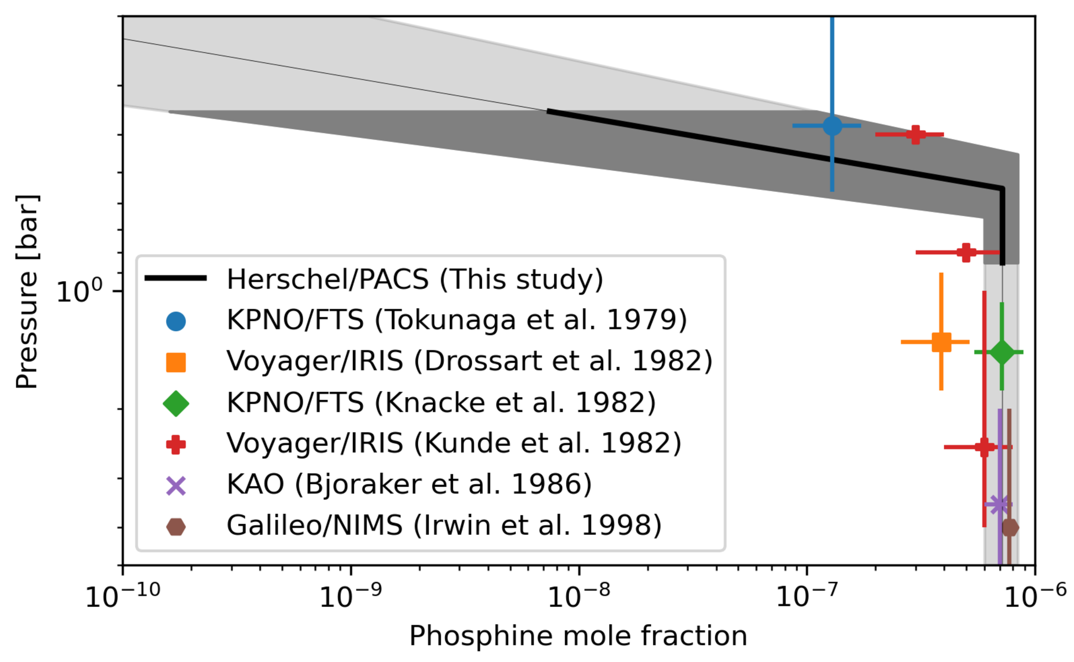
Several rotational lines of hydrogen fluoride (HF), hydrogen chloride (HCl), hydrogen bromide (HBr), and hydrogen iodide (HI) lie in the spectral range of PACS. However, **we detected none of them** and instead inferred upper limits on their mole fractions by varying each molecule's vertically constant mole fraction one-by-one. All spectral lines the hydrogen halides would have caused in the PACS spectra, if they had been present in observable quantities in the atmosphere, would have been absorption lines. Thus, **this analysis constrains the occurrence of hydrogen halides in the Jovian troposphere**. Our 3σ upper limits, their previously most stringent upper limits inferred from Cassini/CIRS and their mole fractions, if the halogen abundances were equal to their Solar abundances, are summarized in the Table below.

Molecule	Herschel/PACS upper limits	Cassini/CIRS upper limits (Fouchet et al., 2004)	Proto-Solar composition mole fractions (Lodders, 2019)
HF	$< 1.1 \times 10^{-11}$	$< 2.7 \times 10^{-11}$	$(1.1 \pm 0.2) \times 10^{-7}$
HCl	$< 6.0 \times 10^{-11}$	$< 2.3 \times 10^{-9}$	$(3.6 \pm 0.5) \times10^{-7}$
HBr	$< 2.3 \times 10^{-10}$	$< 1.0 \times 10^{-9}$	$(8.4 \pm 1.7) \times10^{-10}$
HI	$< 1.2 \times 10^{-9}$	$< 7.6 \times 10^{-9}$	$(1.1 \pm 0.4) \times10^{-10}$

Phosphine (PH_3)

We used the PH_3 R(6), R(7), R(9), R(11), and R(13) bands simultaneously for the analysis of phosphine in Jupiter's atmosphere and **parameterized phosphine's abundance profile using the same formula as for ammonia**. For the comparison with synthetic spectra, we ran the forward model simulations of the observed phosphine bands using the previously determined ammonia profile and calculated line-to-continuum ratios in both the observations and models with respect to the pseudo-continuum around the phosphine bands created by ammonia.

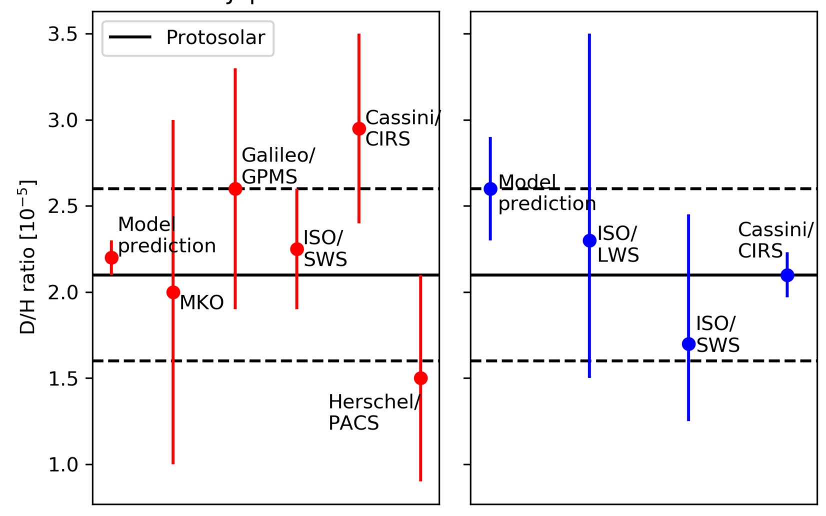
Our result for phosphine's mole fractions between $p \sim 550$ mbar and $p \sim 850$ mbar agrees very well with the mole fractions in the lower troposphere determined previously (see Fig. on the right). However, the **depletion of phosphine with height above 550 mbar we find is faster than what was inferred before** (corresponding to a lower f_{PH_3}). We observed that the best-fitting value for f_{PH_3} is positively correlated with p_{PH_3}, for which we also fit. In some previous studies (such as Irwin et al. 1998), the value for p_{PH_3} was held fixed at 1 bar and thus, f_{PH_3} might be lower than previously thought.



Deuterated Hydrogen (HD)

PACS's spectral range includes the HD R(0) line which we used to infer Jupiter's atmospheric D/H ratio. Our forward model consisted of the adopted temperature profile, the ammonia, phosphine and methane abundances determined before and varying D/H ratios. Our analysis delivered a Jovian atmospheric **D/H ratio of** $\mathbf{(1.5 \pm 0.6)\times10^{-5}}$ which is plotted together with previous studies' results below.

Within the error bars, the Jovian D/H ratio inferred from the PACS data is compatible with the protosolar ratio and all its previous determinations in Jupiter's atmosphere, except for the result of the Cassini/CIRS analysis. Our result demonstrates that the **Jovian D/H ratio could fall into the lower range of possible primordial D/H ratios** and that it could be lower than Saturn's D/H ratio. This suggests that icy planetesimals which were greatly enriched in deuterium and probably played a vital role during Jupiter's formation did not accumulate deuterium in its atmosphere to a measurable degree.



Conclusions

1. The disk-averaged FIR spectra obtained with Herschel/PACS are **sensitive to Jupiter's troposphere** between $p \sim 275$ mbar and $p \sim 900$ mbar.
2. Our inferred ammonia abundance profile suggests a dry atmosphere, hinting at the **observations being sensitive to cloud-poor parts of the atmosphere** that emit more thermal radiation.
3. For **phosphine**, we found lower tropospheric ($p \gtrsim 550$ mbar) abundances in agreement with previous studies, but a **faster depletion in the upper troposphere than previously reported**. This might be driven by the knee pressure we inferred, which was held fixed at higher values in previous studies.
4. The **methane abundance we derive is consistent with previous works**, but points toward a slightly lower, but still super-solar carbon abundance in Jupiter.
5. By analyzing the HD R(0) line, we present a new measurement of Jupiter's **D/H ratio**, $D/H = (1.5 \pm 0.6)\times10^{-5}$. This value lies within the lower range of possible values of the protosolar D/H raios and suggests that **Jupiter is a good approximation of the protosolar D/H ratio** despite the accretion of icy planetesimals during its formation.
6. **Hydrogen halides remain undetected in Jupiter.** Using PACS, however, we can rule out near- or super-Solar abundances for hydrogen fluoride, hydrogen chloride and, for the first time, hydrogen bromide in the Jovian troposphere.

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