INFRARED DETECTION OF DEUTERATED PAHS

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All deuterium (D) formed during Big Bang
D/H_{prim} = 27.5^{+2.4}_{-1.9} \text{ ppm}

17 ppm range in value (Linsky et al. 2006)

Deuterium ”locked-up” in grains or molecules
Polycyclic Aromatic Hydrocarbons (PAHs)

* Typical size of greater than 50 carbon atoms
* Relatively stable against photodissociation
* UV/visible-pumped fluorescence

Peeters et al. 2004: ISO SWS
Spectroscopic Identity

$I_{CH}/I_{CD} = 1.75$

Based on B3LYP/4-31G calculations and matrix isolation experiments (Bauschlicher et al. 1997)
CD str at 4.40 μm
CDH asym str at 4.63 μm
CDH sym str at 4.75 μm

Calculated using B3LYP/4-31G
(Hudgins et al. 2004)
Detected D/H values

Peeters et al. 2004: ISO SWS
Orion Bar: 0.17 ± 0.03
M17: 0.36 ± 0.08

Onaka et al. 2014: AKARI Nh
Orion Bar: 0.029 ± 0.002
M17: 0.023 ± 0.004
* Used the Infrared Camera (IRC)
  2.5 – 5 μm with R ~100 for diffuse sources

* Nh slit (1’ x 3”) with grism disperser – dispersion of 0.0097 μm/px

* Observed HII regions: 7 in LMC; 5 in SMC; 41 in MW
Results

*Observed C-D features in 6/53 sources; 8 observations
-IRAS 12073-6233 obs. 1 and 2
-NGC 3603
-M8
-M17b
-W51 obs. 1 and 2
-G75.783+0.343

Doney et al. 2016: IRAS 12073-6233 obs. 1
Results

* Observed C-D features in 6/53 sources; 8 observations
* In all aliphatic features are stronger than the aromatic feature
* Aromatic is absent in M17b
* Consistent with at least monodeuteration

Doney et al. 2016: IRAS 12073-6233 obs. 1
PAH D/H range

- D/H = 0.44 → 18 ppm
  "locked-up"
- D/H = 0.03 → 1.7 ppm
  "locked-up"

*D enrichment is more than in dark clouds but less than in hot corinos

Linsky et al. 2006: (not corrected for the Local Bubble foreground)
In PAHs in water ices, D substitution to an aromatic position is favored (Sandford et al. 2000)

In gas-phase H interaction with PAHs, H or D aliphatic addition is favored (Ricca et al. 2007, Rassussen et al. 2010, Thrower et al. 2012, and Klaerke et al. 2013)
Conclusion

- Incorporation of D in PAHs is rare and highly dependent on the local conditions of the environment.
- The D is preferentially added to an aliphatic position suggesting gas-phase incorporation.
- PAHs can still explain part of the variation of the galactic gas-phase D/H.
- Need to better constrain PAH size to more accurately determine the amount of D locked up.