Astrochemistry Does Not (Always) Need Carbon

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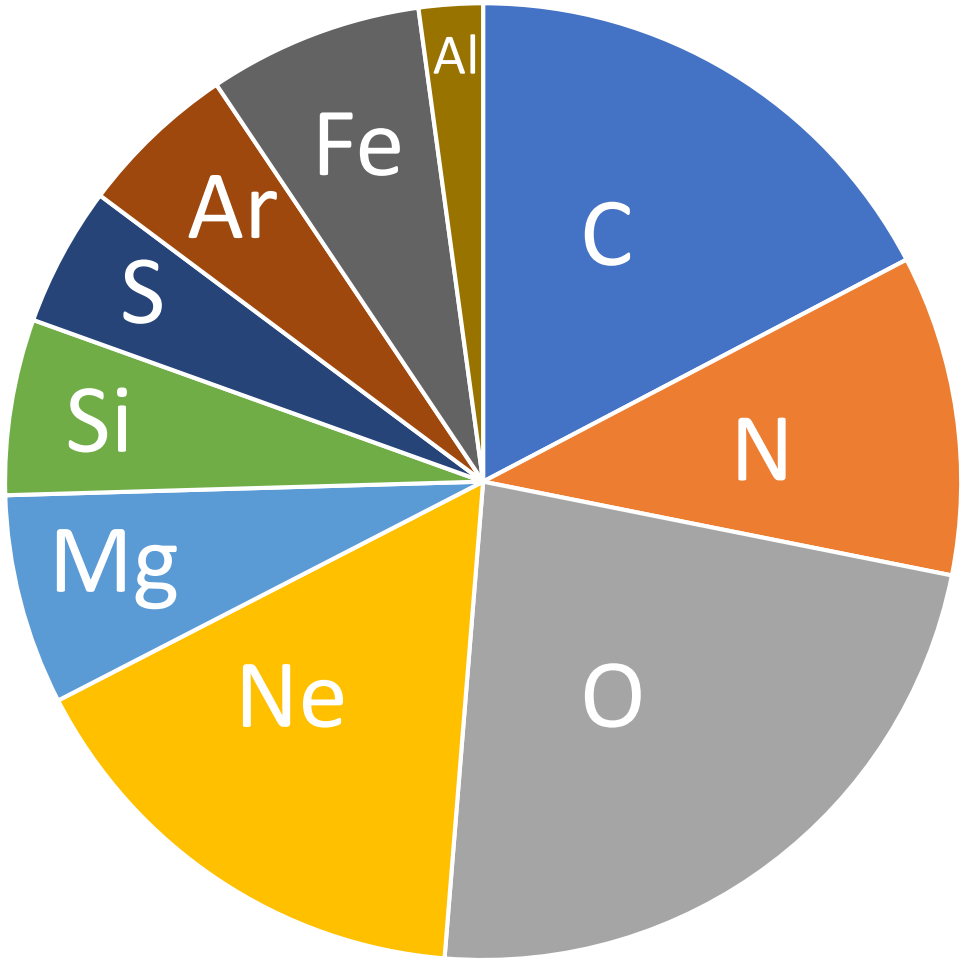
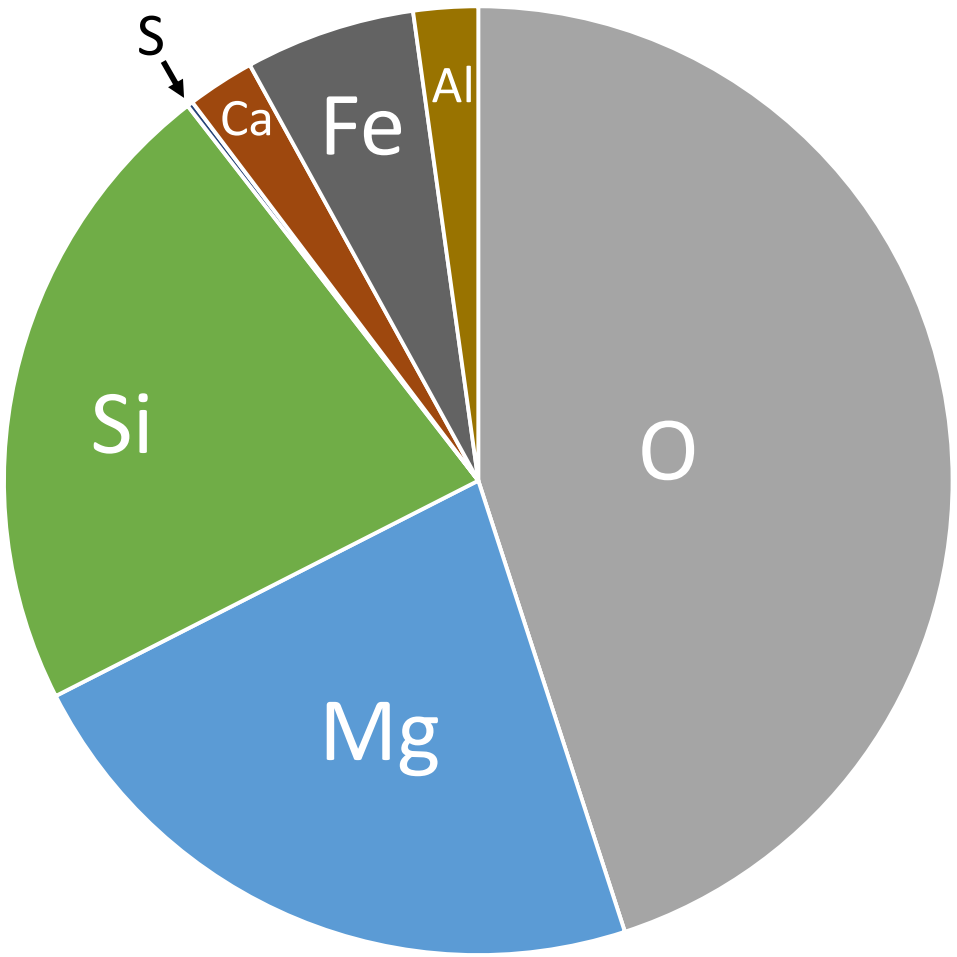
III Chilean Astrochemistry School, November 29, 2022

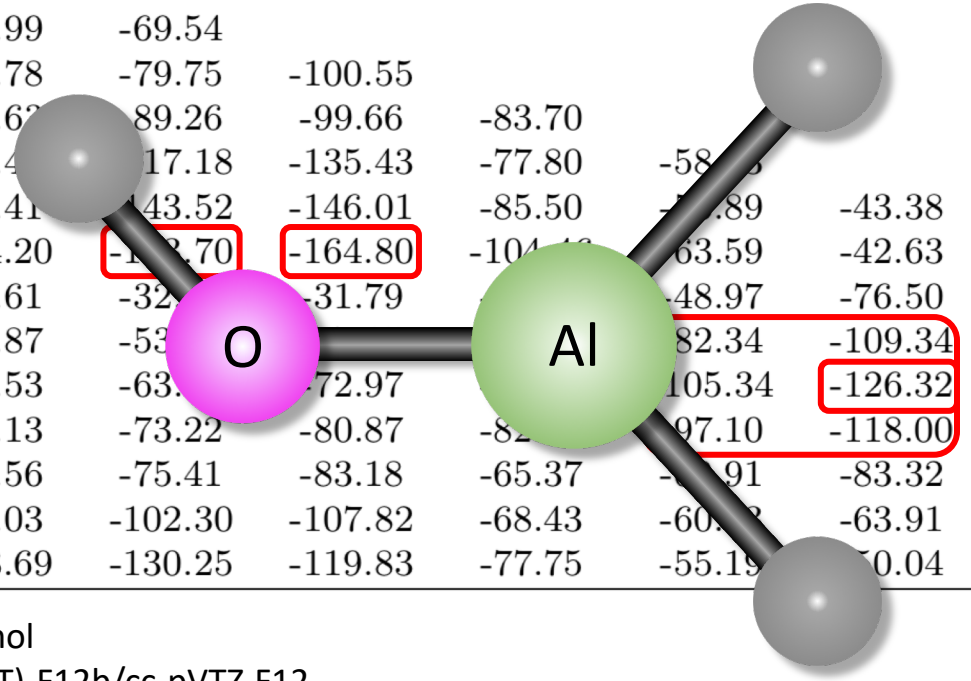
Elemental Abundance



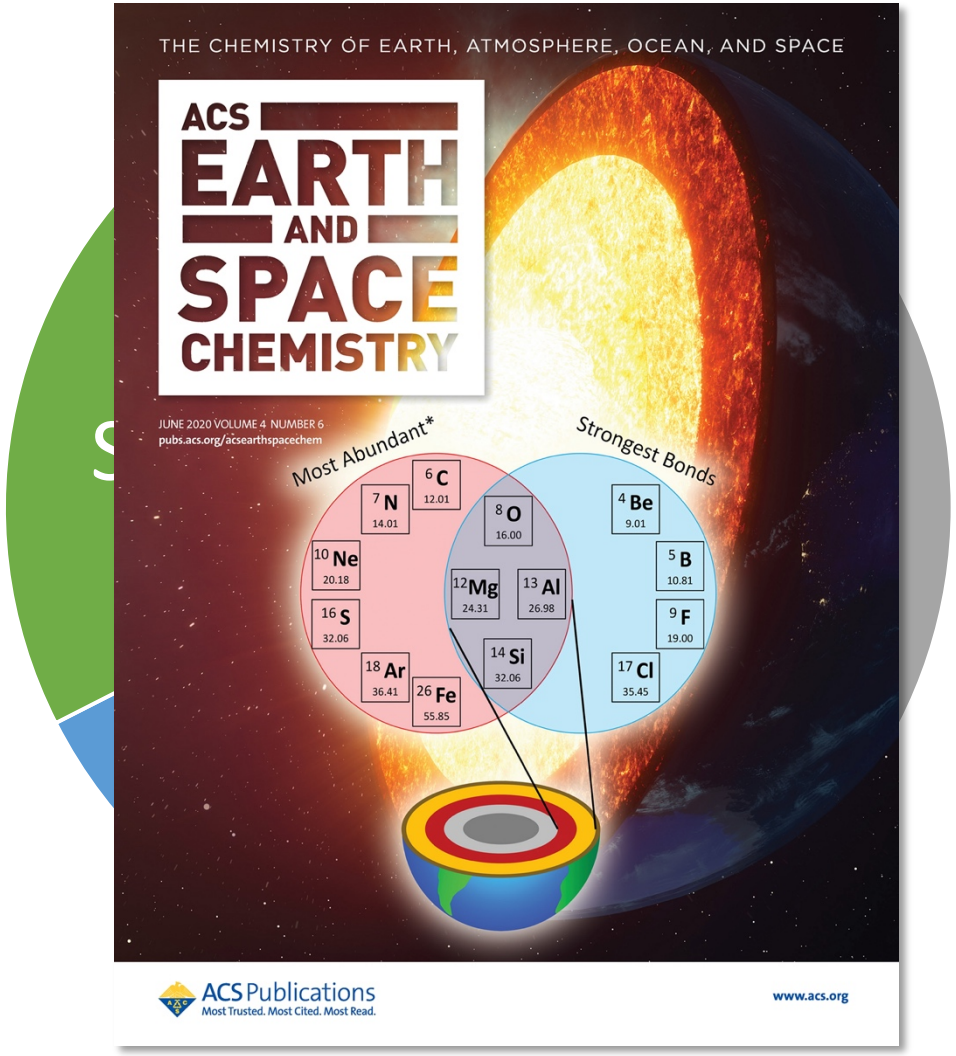


H_nX-YH_m Bond Strengths

	Li	Be	B	C	N	O	F	Na	Cl
Li	-23.54								
Be	-40.99	-69.54							
B	-42.78	-79.75	-100.55						
C	-44.6[illegible]	89.26	-99.66	-83.70					
N	-69.4[illegible]	17.18	-135.43	-77.80	-58[illegible]				
O	-99.41	43.52	-146.01	-85.50	[illegible].89	-43.38			
F	-134.20	-1[illegible].70	-164.80	-104[illegible]	63.59	-42.63	-32.17		
Na	-19.61	-32[illegible]	-31.79	[illegible]	-48.97	-76.50	-111.08	-16.5	
Mg	-33.87	-53[illegible]	[illegible]	[illegible]	82.34	-109.34	-141.50	-28.4	
Al	-40.53	-63.[illegible]	-72.97	[illegible]	105.34	-126.32	-156.00	-33.2	
Si	-48.13	-73.22	-80.87	-82[illegible]	97.10	-118.00	-146.28	-39.2	
P	-49.56	-75.41	-83.18	-65.37	[illegible].91	-83.32	-105.75	-39.6	
S	-77.03	-102.30	-107.82	-68.43	-60[illegible]	-63.91	-77.32	-64.5	
Cl	-108.69	-130.25	-119.83	-77.75	-55.19	[illegible]0.04	-55.62	-95.1	51.79

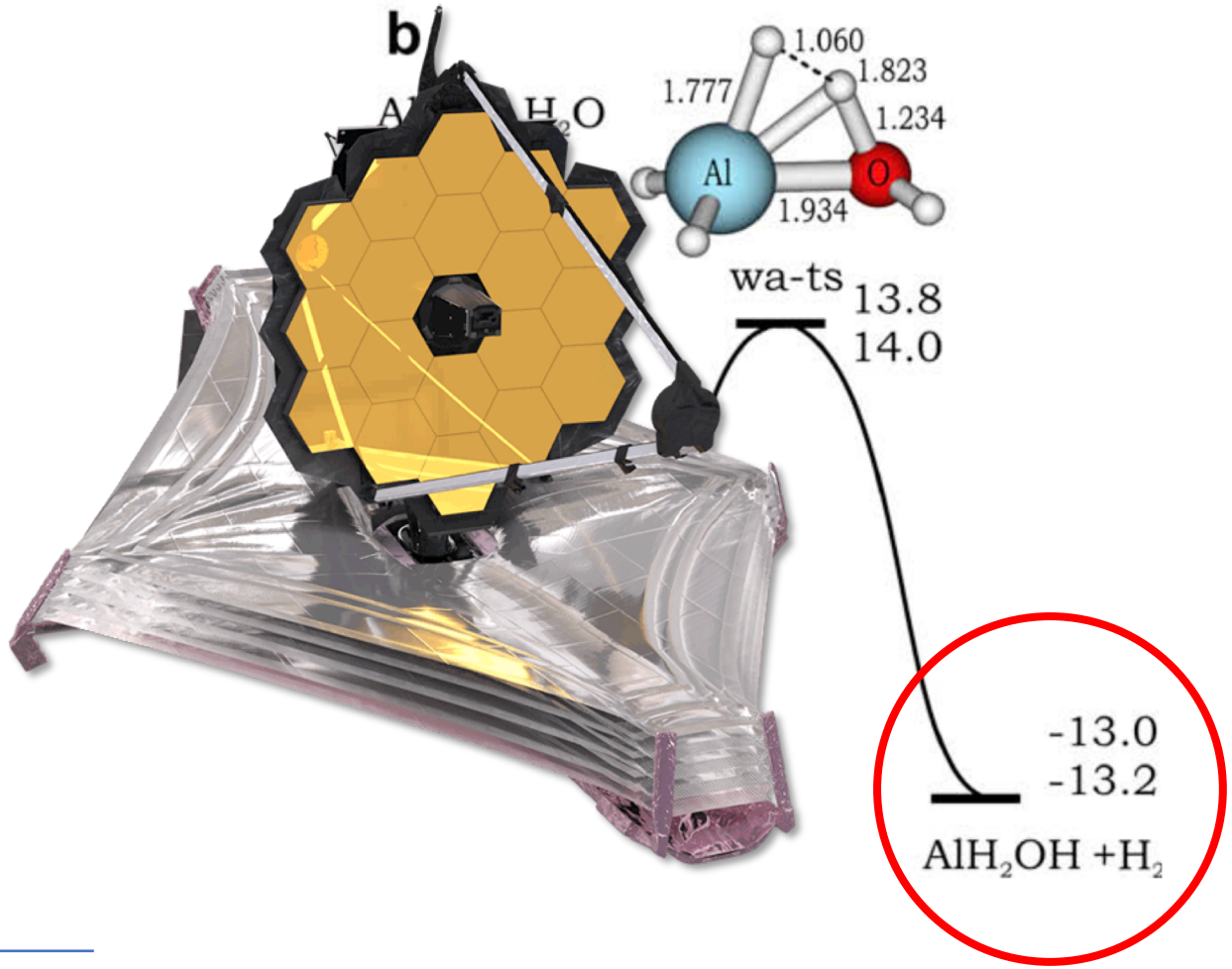


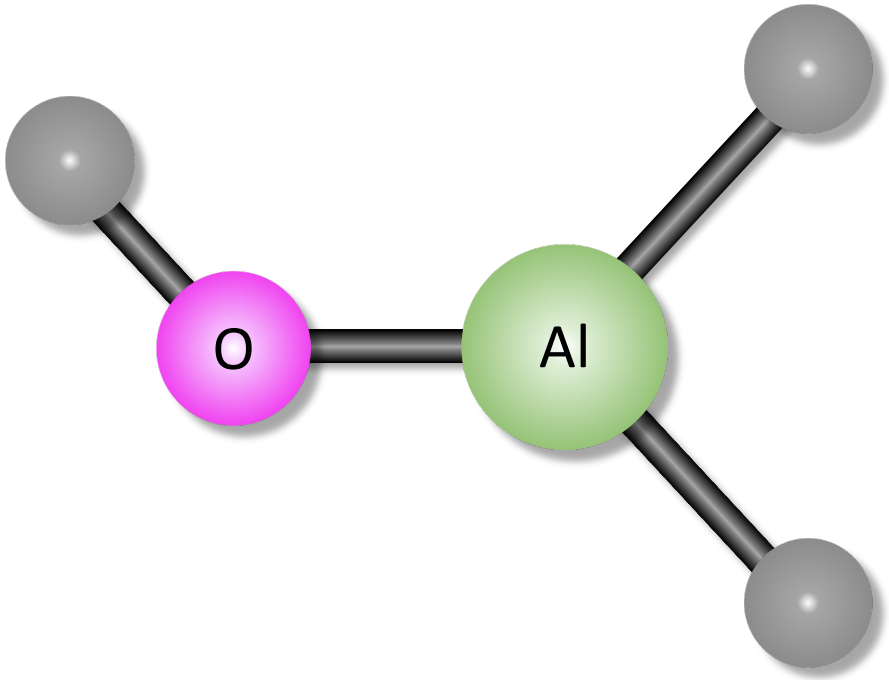
kcal/mol
CCSD(T)-F12b/cc-pVTZ-F12



E. S. Doerksen & R. C. Fortenberry, *ACS Earth Space Chem.*, **4**, 812, (2020).

H_nX-YH_m Molecules





S. Swinnen, V. S. Nguyen, S. Sakai, & M. T. Nguyen, *Chem. Phys. Lett.*, **472**, 175, (2009).

Computing Anharmonic Freqs

$$H = \frac{1}{2}\sum_{\alpha\beta}(J_\alpha - \pi_\alpha)\mu_{\alpha\beta}(J_\beta - \pi_\beta) - \frac{1}{2}\sum_k \frac{\partial^2}{\partial Q_k^2} - \frac{1}{8}\sum_\alpha \mu_{\alpha\alpha} + V(\mathbf{Q})$$

$$V = \frac{1}{2}\sum_{ij} F_{ij}\Delta_i\Delta_j + \frac{1}{6}\sum_{ijk} F_{ikj}\Delta_i\Delta_j\Delta_k + \frac{1}{24}\sum_{ijkl} F_{ikjl}\Delta_i\Delta_j\Delta_k\Delta_l$$

Geometry Optimization (F12-TZ)

Generate Points (0.005 Å or 0.005 rad.)

Calculate Energies (F12-TZ)

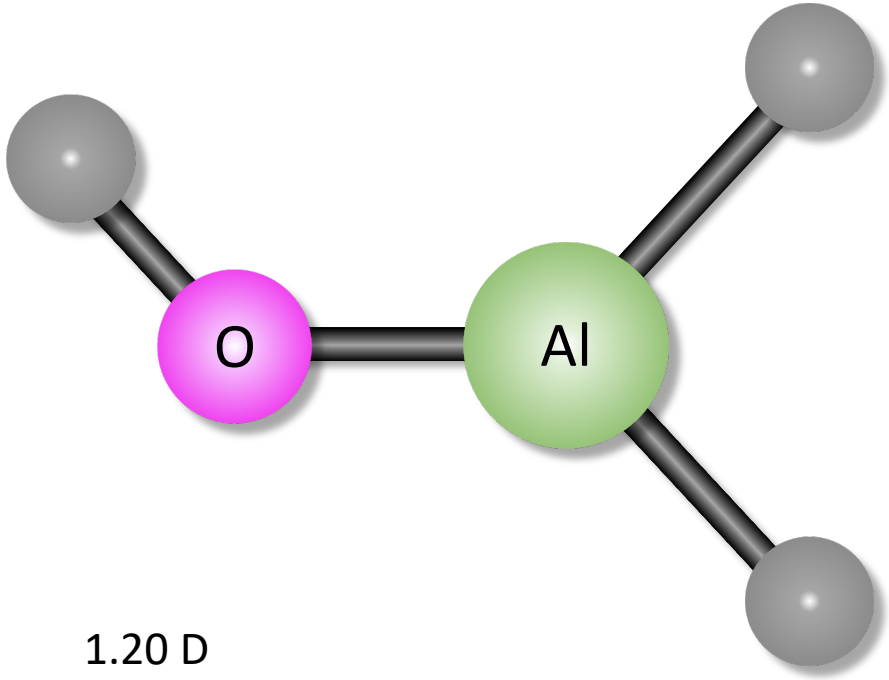
Least-Squares Fit

Transform Coordinates

Compute Frequencies & Rotational Constants (VPT2)

X. Huang & T. J. Lee, *J. Chem. Phys.* **129**, 044312 (2008).
R. C. Fortenberry & T. J. Lee, *Ann. Rep. Comput. Chem.* **15**, 173-202 (2019).

H_nX-YH_m Molecules

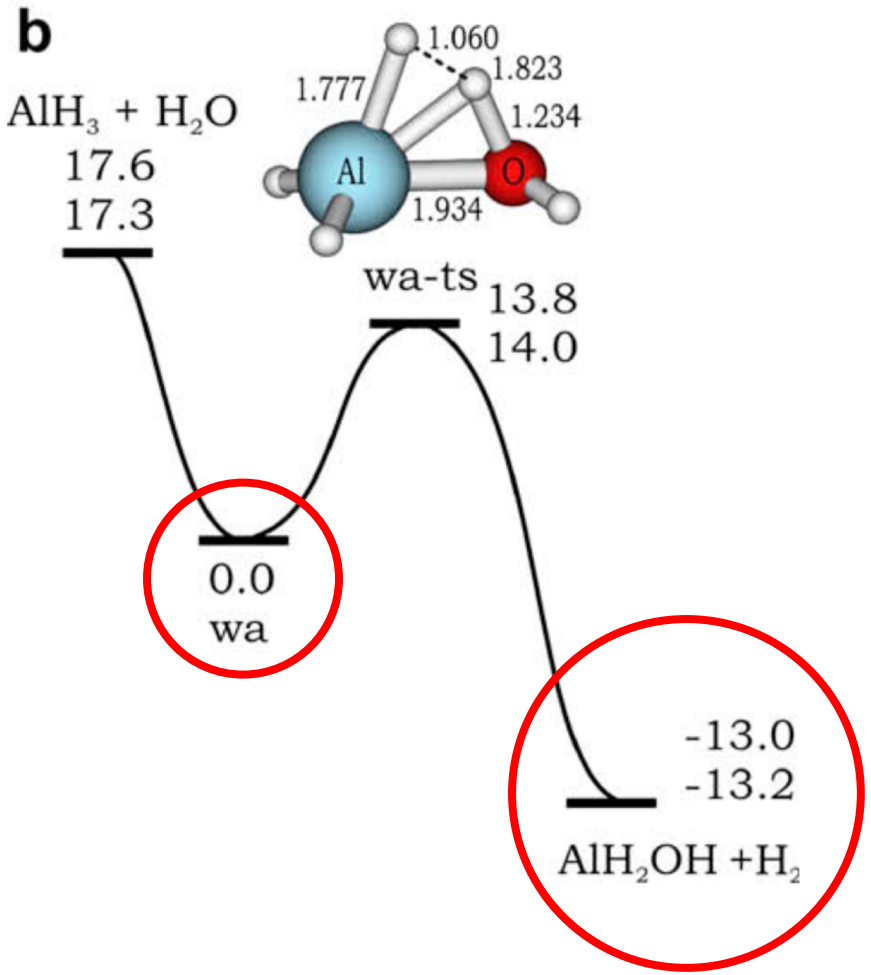


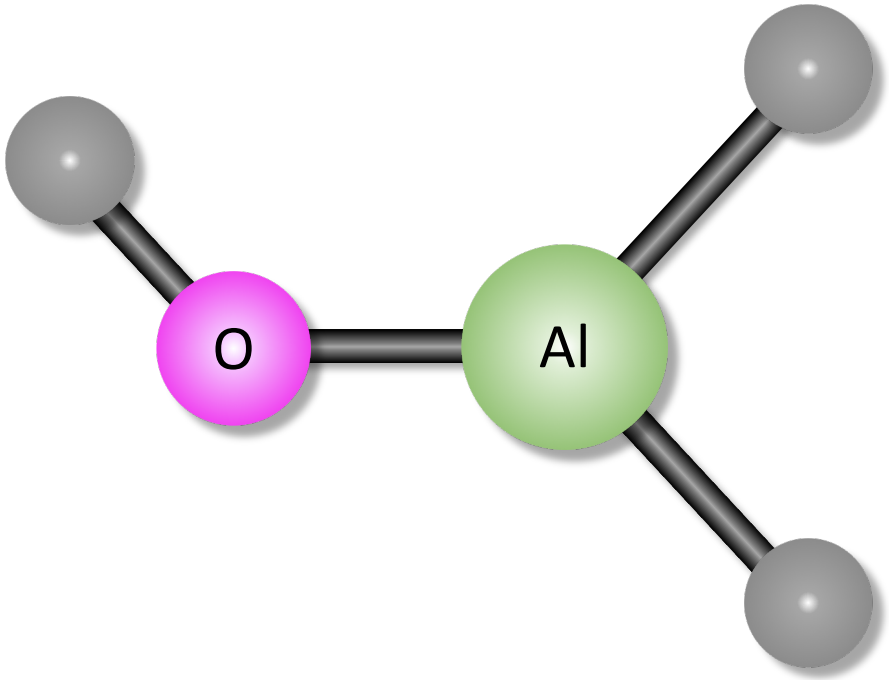
1.20 D

AlH_2OH	*f*	F12-TZ
ν_1 cm^{-1}	83	3768.7
ν_2 cm^{-1}	170	1918.4
ν_3 cm^{-1}	179	1892.5
ν_4 cm^{-1}	203	855.7
ν_5 cm^{-1}	76	766.3
ν_6 cm^{-1}	260	621.9
ν_7 cm^{-1}	218	616.1
ν_8 cm^{-1}	84	486.3
ν_9 cm^{-1}	104	424.1

A. Watrous, M. C. Davis, & R. C. Fortenberry, *Frontiers Astron. Space Sci.*, **8**, 643348 (2021).

H_nX-YH_m Molecules





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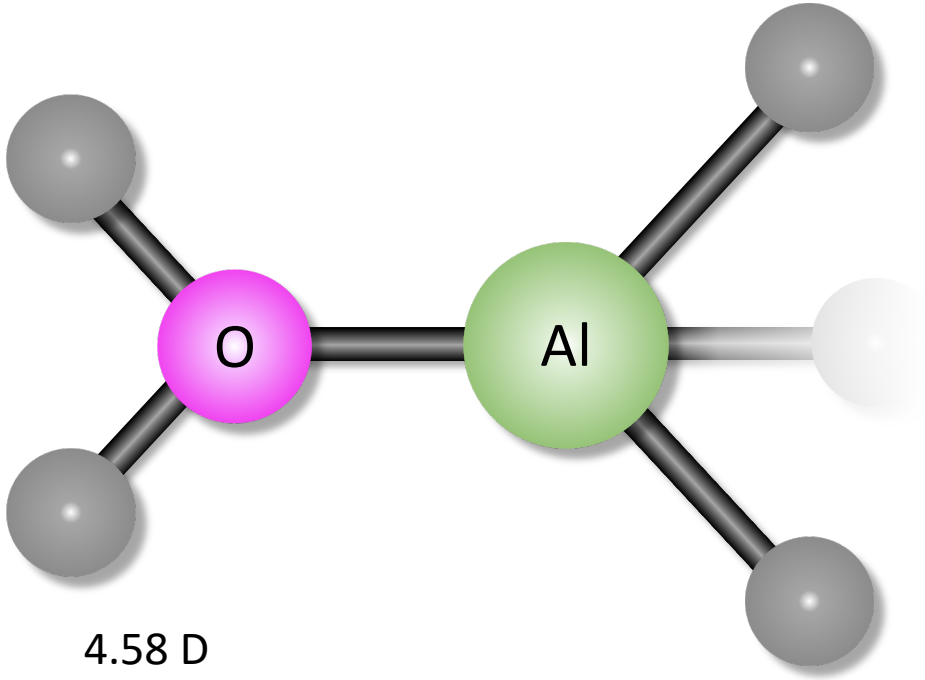
AlH_3OH_2

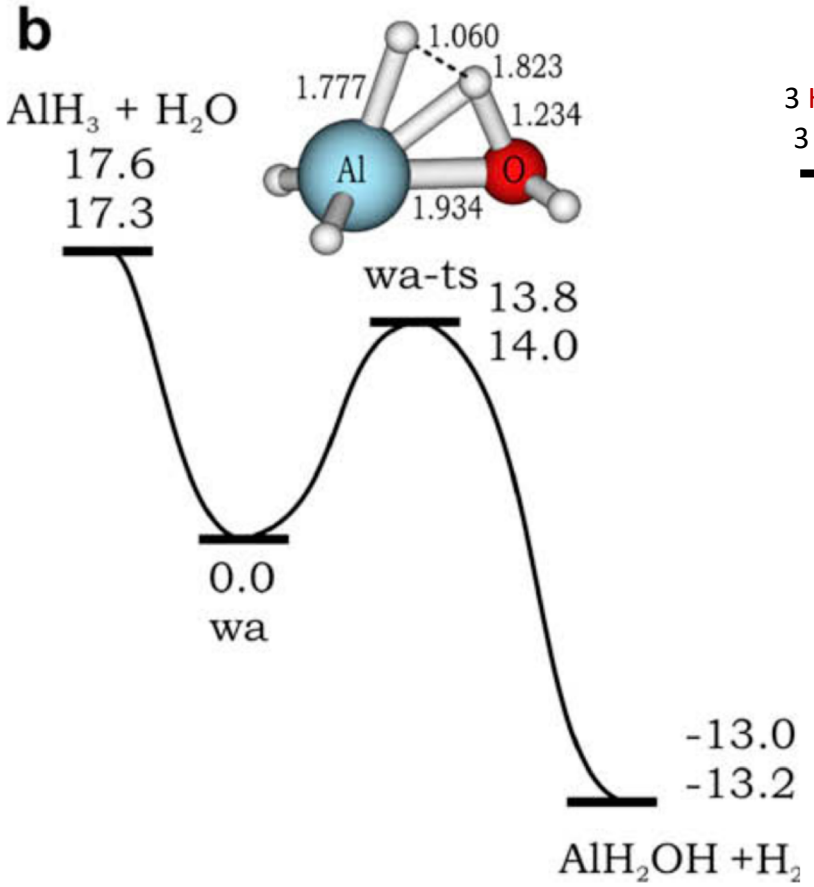


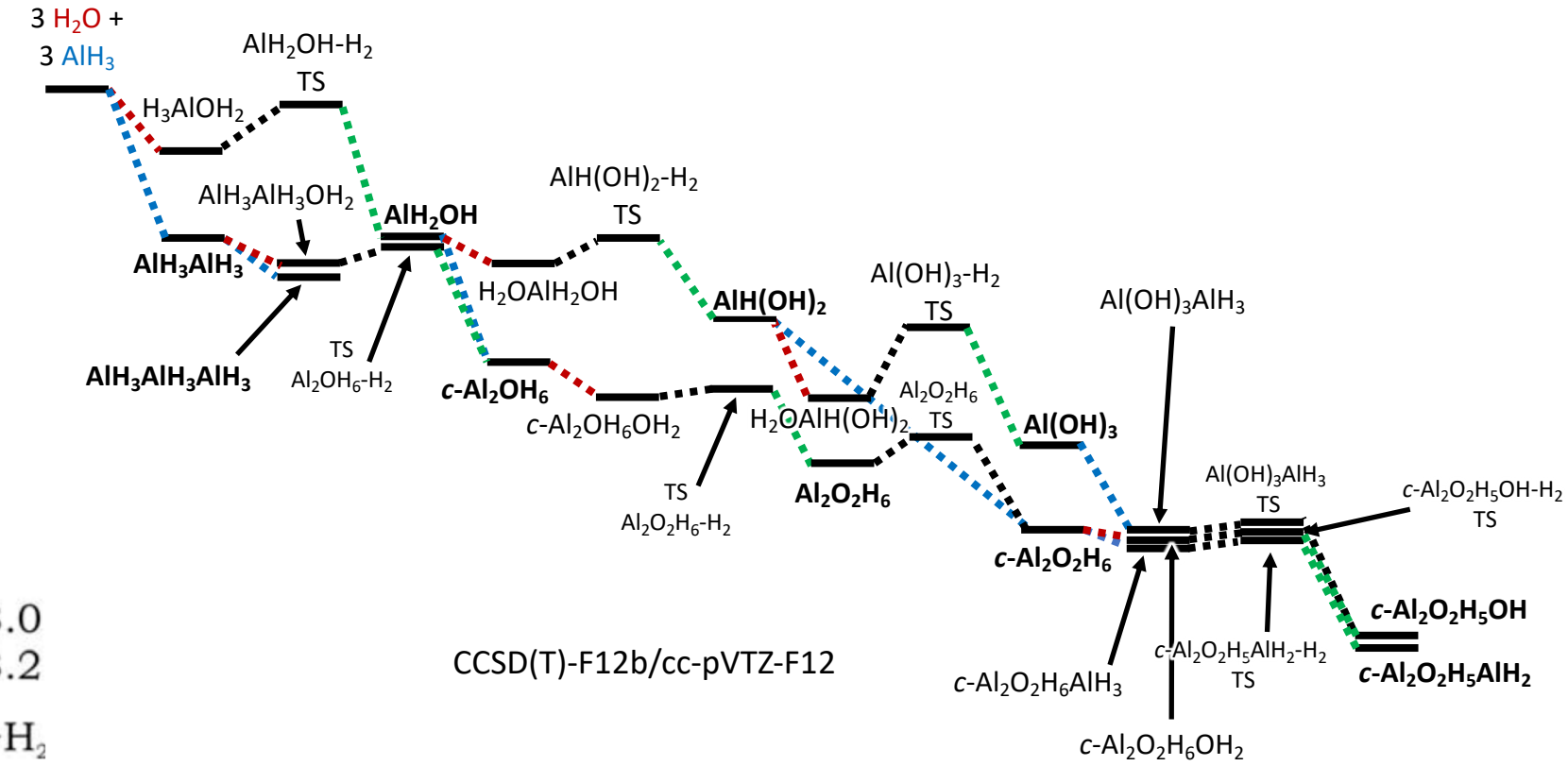
4.58 D

	f	F12-TZ
v_1 cm^{-1}	142	3715.0
v_2 cm^{-1}	62	3624.5
v_3 cm^{-1}	168	1854.5
v_4 cm^{-1}	194	1819.3
v_5 cm^{-1}	367	1809.0
v_6 cm^{-1}	91	1607.4
v_7 cm^{-1}	261	785.1
v_8 cm^{-1}	297	778.9
v_9 cm^{-1}	412	775.3
v_{10} cm^{-1}	5	664.0
v_{11} cm^{-1}	153	487.9
v_{12} cm^{-1}	148	319.7

A. Watrous, B. R. Westbrook, M. C. Davis, & R410, *MNRAS*, **508**, 2613 (2021).

H_nX-YH_m Molecules





D. Grosselin & R. C. Fortenberry, *ACS Earth Space Chem.*, **6**, 18-24, (2022).

H_nX-YH_m Molecules

$Al_2O_3H_6$

c-$Al_2O_2H_5OH$

D. Grosselin & R. C. Fortenberry, *ACS Earth Space Chem.*, **6**, 18-24, (2022).

H_nX-YH_m Bond Strengths

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O	-99.41	-143.52	-146.01	-85.50	-56.89	-43.38								
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Na	-19.61	-32.97	-31.79	-30.30	-48.97	-76.50	-111.08	-16.56						
Mg	-33.87	-53.32	-57.15	-60.64	-82.34	-109.34	-141.50	-28.42	-43.05					
Al	-40.53	-63.91	-72.97	-78.01	-105.34	-126.32	-156.00	-33.27	-49.73	-58.64				
Si	-48.13	-73.22	-80.87	-82.87	-97.10	-118.00	-146.28	-39.25	-56.67	-65.72	-71.18			
P	-49.56	-75.41	-83.18	-65.37	-69.91	-83.32	-105.75	-39.62	-57.80	-67.13	-65.44	-51.26		
S	-77.03	-102.30	-107.82	-68.43	-60.33	-63.91	-77.32	-64.50	-82.61	-92.54	-82.21	-60.19	-57.55	
Cl	-108.69	-130.25	-119.83	-77.75	-55.19	-50.04	-55.62	-95.16	-111.41	-116.10	-103.40	-71.83	-58.22	-51.79

kcal/mol
CCSD(T)-F12b/cc-pVTZ-F12

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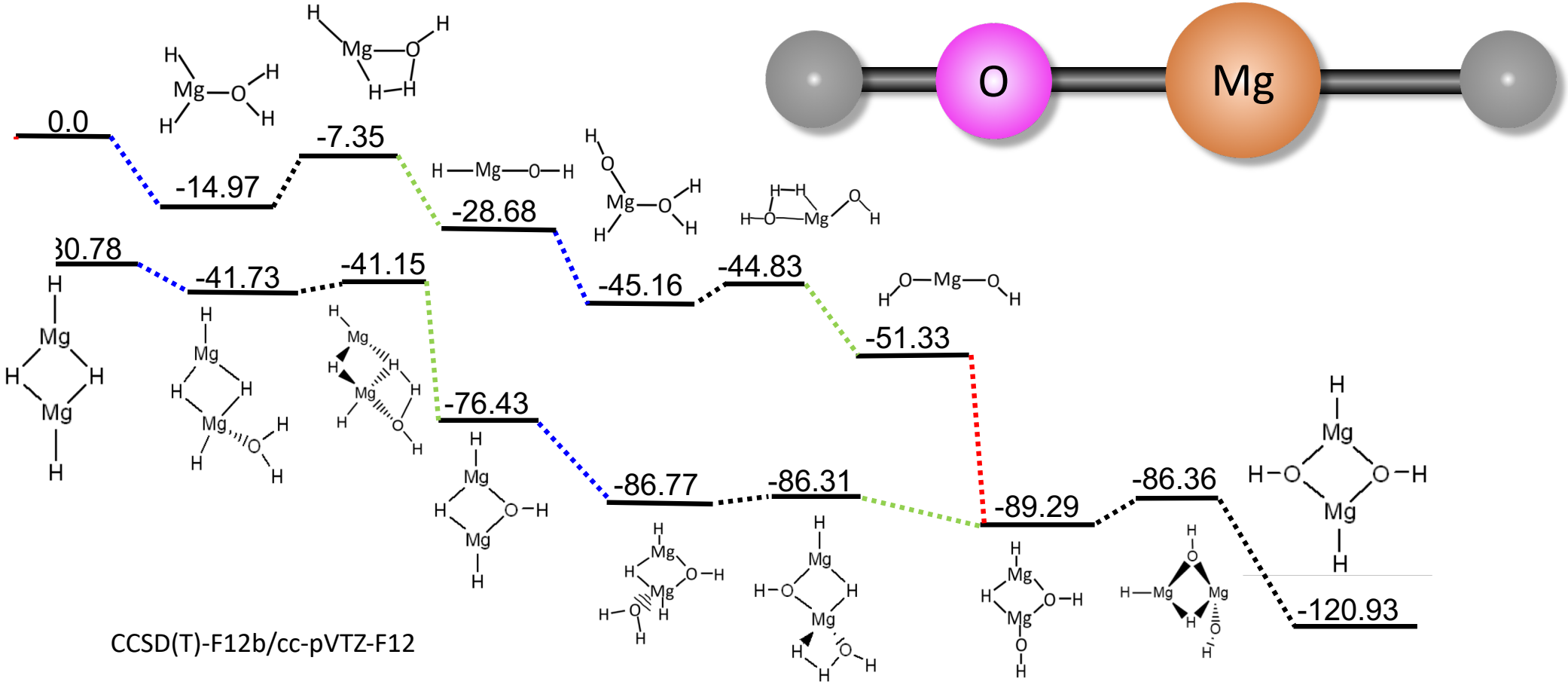
H_nX-YH_m Molecules



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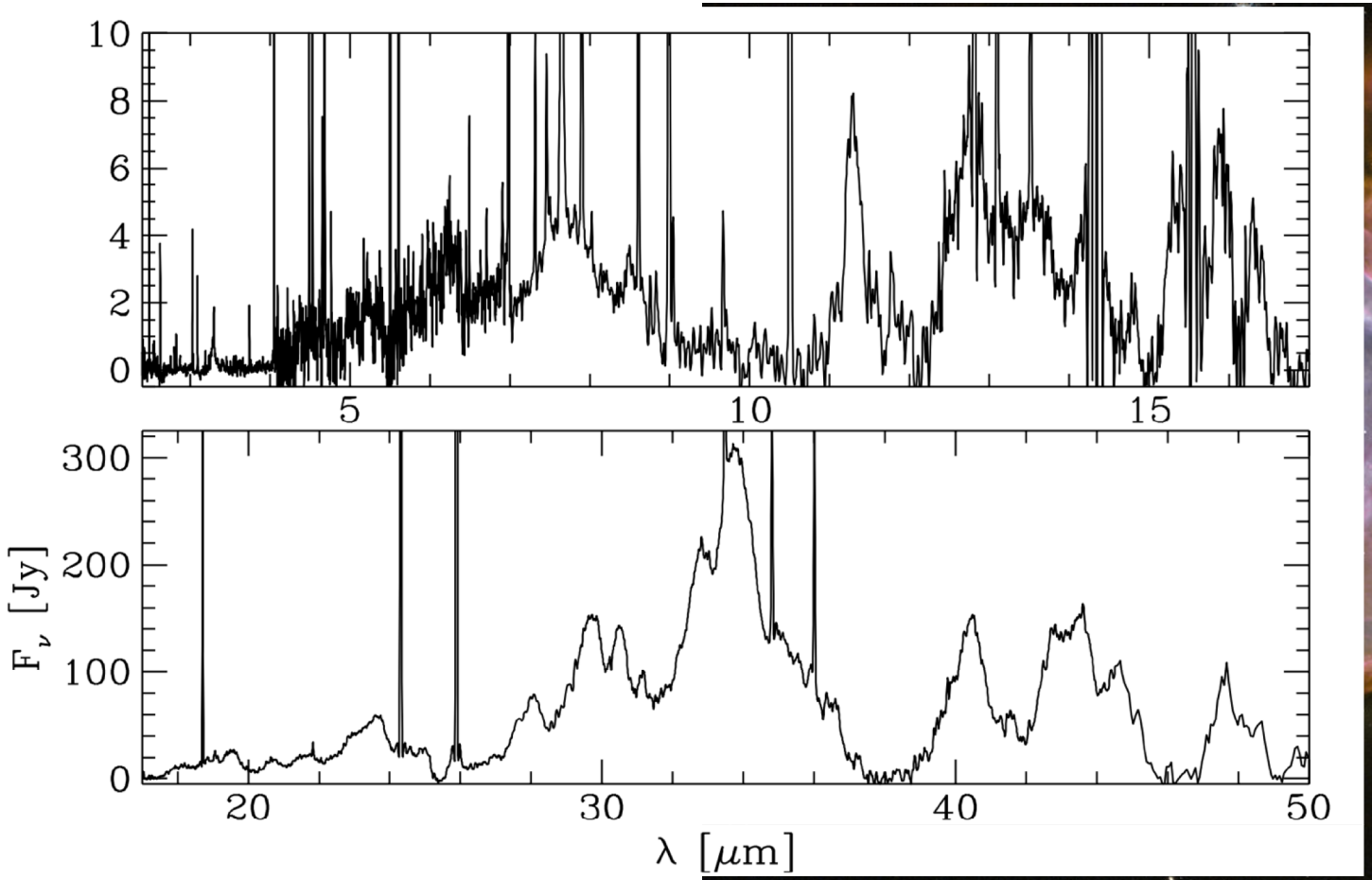
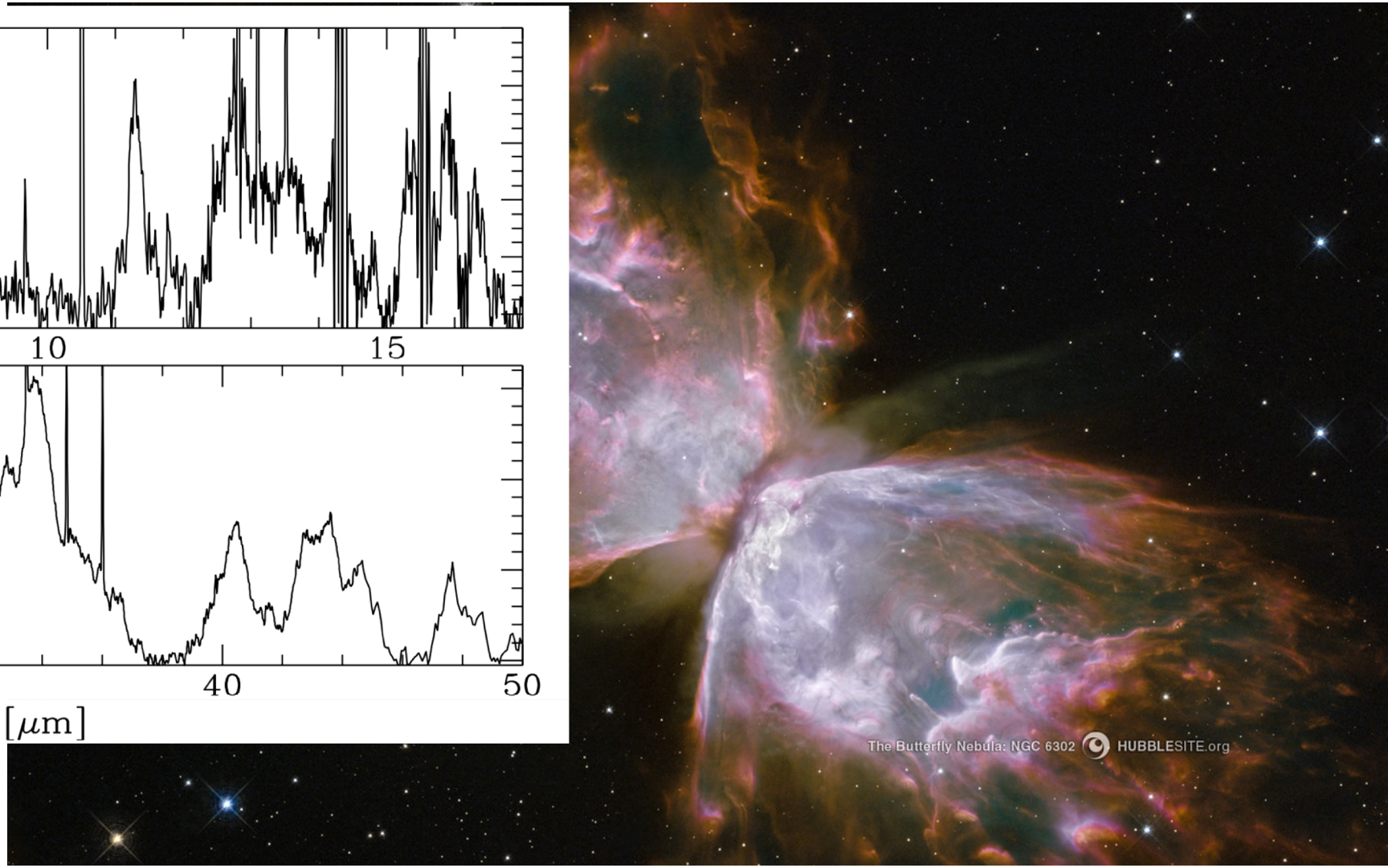
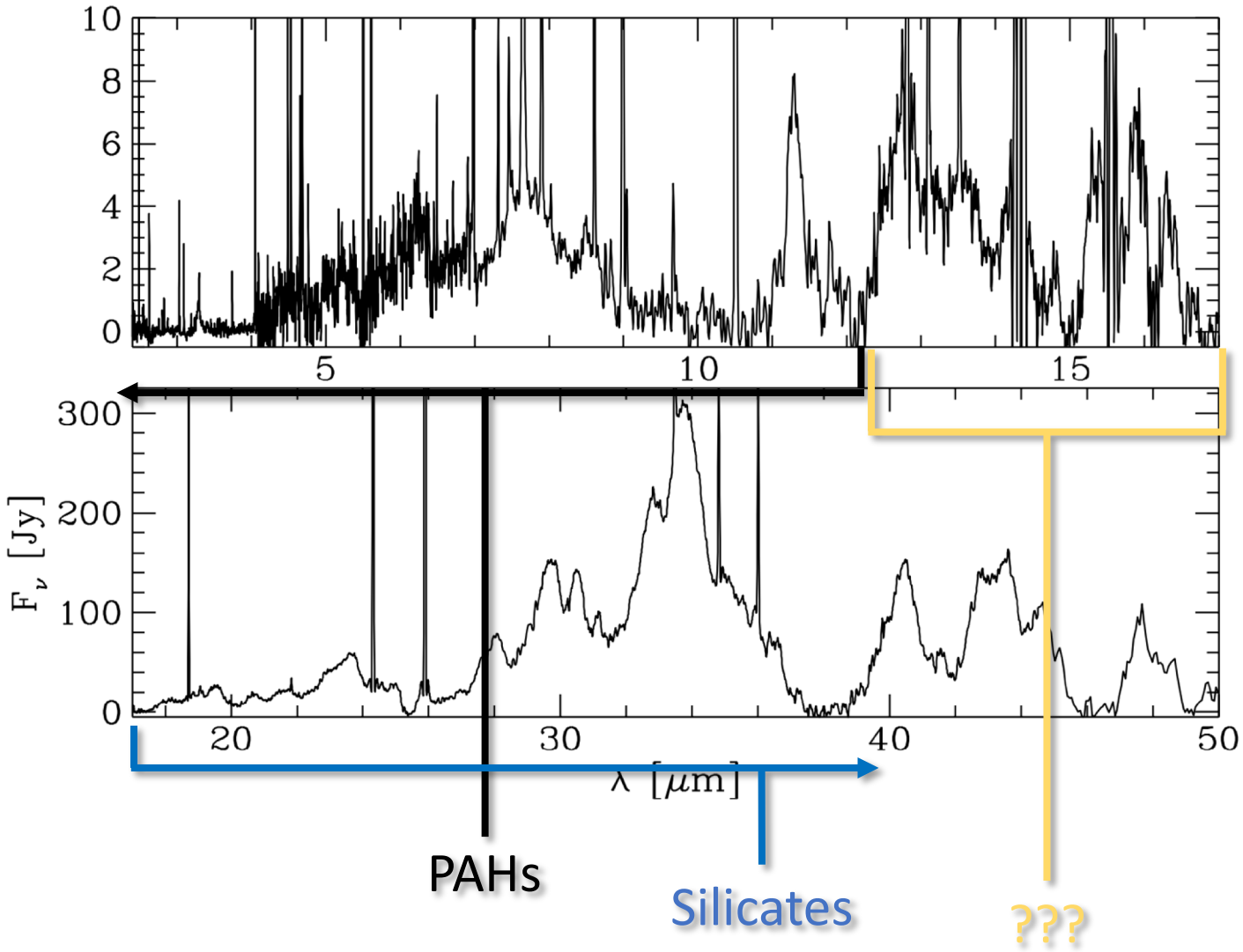


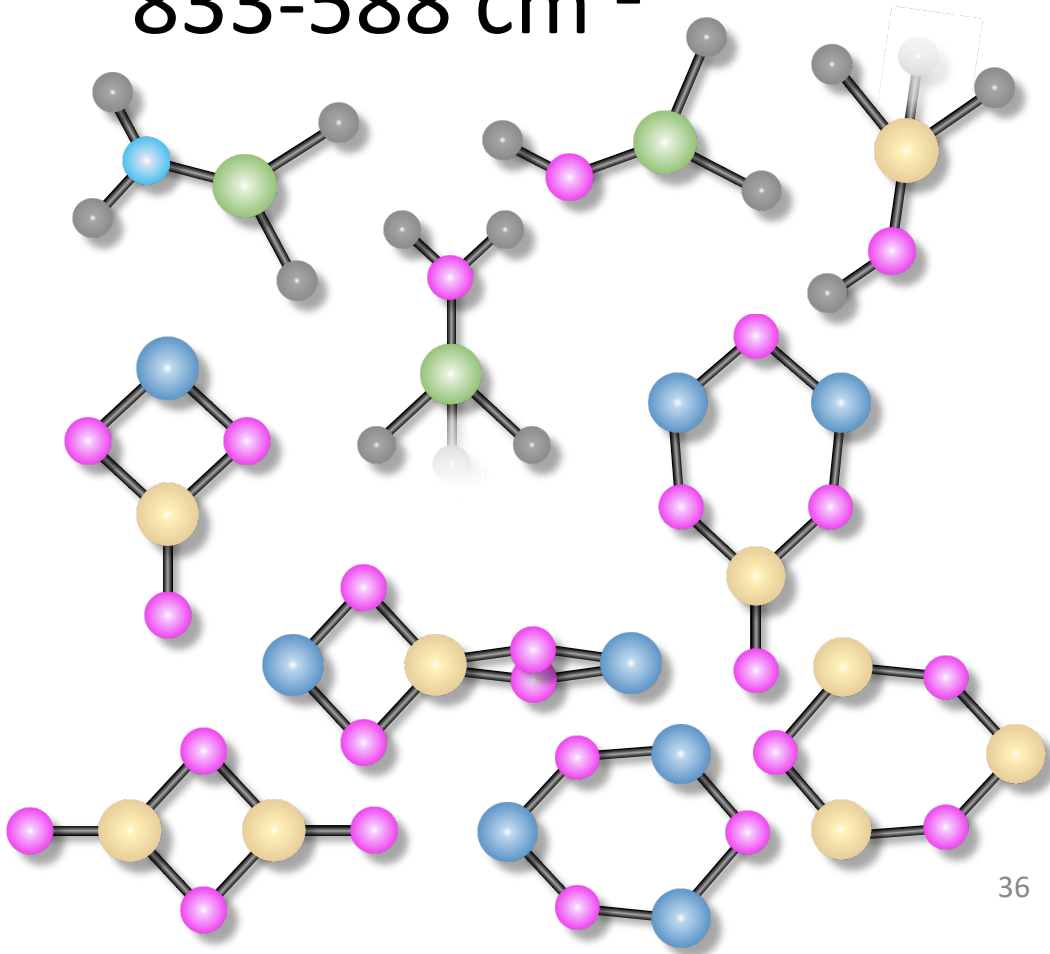


F. J. Molster, et al., *Astron. Astrophys.*, **372**, 165 (2001).



12-17 μm

833-588 cm^{-1}



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- Noah Garrett*
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