Supporting Information

Vetting Molecular Candidates Posited for the First Diffuse Interstellar Bands (5780 and 5797 Å): A Quantum Chemical Study

Halis Seuret,[a,b] Ailish D. Sullivan,[a] Cercis Morera-Boado,*[b] Tina A. Harriott,*[a,c] Daniel Majaess,*[a,c] Lou Massa,[d] and Chérif F. Matta*[a,e,f]

Figure S1. The UV spectra of 2-cyclopenten-1-one, 2(5H)-furanone, 3(2H)-thiophenone and 3(2H)-selenophenone, potential molecules of interest for the 5797 Å family, calculated

with TD-PBE0/aug-cc-pVTZ level of theory. (*Black line: neutral molecules*) Clearly the only observed lines are in the far UV part of the spectrum. (*Red and blue lines: cations*) the lines fall below 500 nm. The orbitals involved in the transitions marked with a black asterisk (neutral molecules) are shown on the right side of each panel.

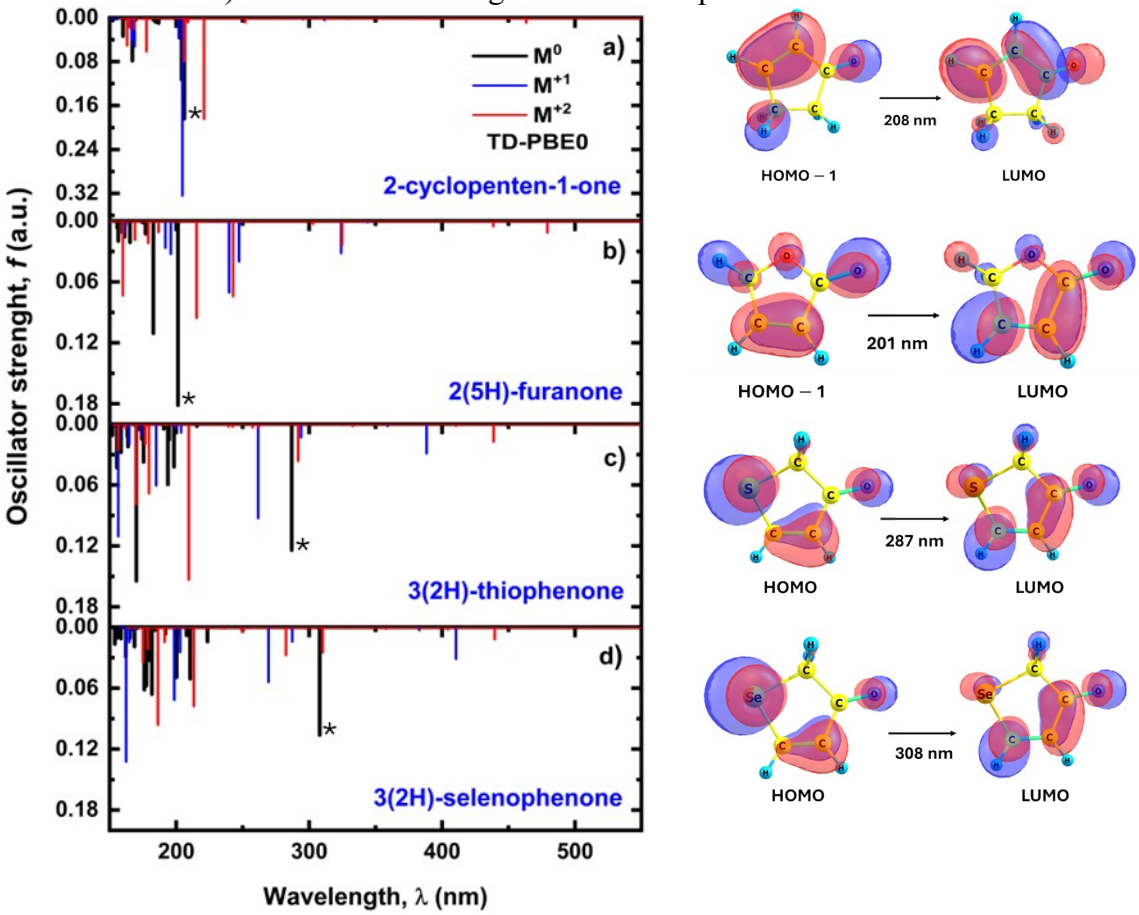

Table S1. Wavelength (λ, nm) and oscillator strength (f, a.u.), of the calculated UV-Vis spectra of glycolamide and lactamide at the PBE0/aug-cc-pVTZ level of theory.

glycolamide		lactamide	
M^0	M^{1+}	M^0	M^{1+}

209.23, 0.0002	870.21, 0.0003	221.47, 0.0004	748.02, 0.0002
193.22, 0.0006	435.35, 0.1089	201.14, 0.0058	405.88, 0.0912
187.80, 0.0136	376.58, 0.0052	191.51, 0.0039	379.41, 0.0168
185.29, 0.0302	257.69, 0.0040	187.00, 0.0323	317.84, 0.0011
179.79, 0.0158	243.41, 0.0087		309.79, 0.0146
173.15, 0.0053	195.72, 0.0066		239.03, 0.0031
167.82, 0.0846	189.61, 0.0030		220.12, 0.0107
167.2, 0.0076	186.18, 0.0077		216.04, 0.0001
162.58, 0.0225	172.55, 0.0006		199.28, 0.0004
161.13, 0.0282	151.19, 0.0781		192.45, 0.0091
158.00, 0.0046			
156.25, 0.0089			
155.27, 0.0006			
152.42, 0.0004			

Table S2. Wavelength (λ, nm) and oscillator strength (f, a.u.), of the calculated UV-Vis spectra of 3- hydroxypropanamide and oxamic acid at the PBE0/aug-cc-pVTZ level of theory.

3- hydroxypropanamide			**oxamic acid**	
M^0	**M^{1+}**	**M^{2+}**	**M^0**	**M^{1+}**
220.72, 0.0001	733.63, 0.0002	255.00, 0.0017	202.27, 0.0538	456.47, 0.1067
196.89, 0.0073	499.12, 0.0999	209.96, 0.0018	184.86, 0.0080	456.47, 0.1067
195.92, 0.0204	392.94, 0.0314	172.84, 0.0199	177.59, 0.1007	304.04, 0.0010
192.90, 0.0090	288.66, 0.0012	167.05, 0.0242	169.96, 0.0095	235.98, 0.0002
186.62, 0.0133	263.11, 0.0111	161.20, 0.0388	167.45, 0.0297	219.26, 0.0001
179.18, 0.0058	230.59, 0.0028	157.40, 0.1423	159.27, 0.0345	214.13, 0.0116
176.51, 0.0125	225.36, 0.0138	154.56, 0.0709	159.26, 0.0024	197.78, 0.0160
172.17, 0.0074	210.10, 0.0178		154.42, 0.0003	193.64, 0.0012
169.74, 0.0085	195.25, 0.0110		152.35, 0.0025	184.93, 0.0493
168.90, 0.0473	189.25, 0.0003			157.73, 0.0650
168.10, 0.1315	175.59, 0.0206			156.55, 0.0046
165.60, 0.0270	170.40, 0.0072			154.91, 0.0366
164.18, 0.0068	161.76, 0.0419			151.74, 0.0005
162.44, 0.0078	157.74, 0.1013			
159.54, 0.0039	154.16, 0.0091			
159.01, 0.0012	152.69, 0.0063			
158.39, 0.0005	151.2, 0.0220			
155.21, 0.0168				
153.76, 0.0020				
153.09, 0.0069				
151.50, 0.0045				
151.07, 0.0072				
150.65, 0.0455				

Table S3. Wavelength (λ, nm) and oscillator strength (f, a.u.), of the calculated UV-Vis spectra of 2-cyclopenten-1-one and 2(5H)-furanone at the PBE0/aug-cc-pVTZ level of theory.

2-cyclopenten-1-one			**2(5H)-furanone**		
M^0	**M^{1+}**	**M^{2+}**	**M^0**	**M^{1+}**	**M^{2+}**
329.33, 0.0002	366.62, 0.0002	570.49, 0.0001	259.16, 0.0001	439.87, 0.0001	479.36, 0.0114

206.21, 0.1840	365.64, 0.0001	463.42, 0.0086	201.34, 0.1814	343.89, 0.0013	398.36, 0.0003
204.03, 0.1127	311.67, 0.0040	382.43, 0.0005	182.86, 0.1107	324.17, 0.0317	366.45, 0.0001
186.78, 0.0097	295.42, 0.0024	365.74, 0.0001		248.55, 0.0005	352.59, 0.0003
184.51, 0.0078	278.30, 0.0001	360.07, 0.0009		247.38, 0.0398	324.88, 0.0236
183.05, 0.0044	265.57, 0.0010	313.93, 0.0017		239.90, 0.0703	303.03, 0.0028
	252.51, 0.0010	294.24, 0.0006		230.19, 0.0009	246.20, 0.0004
	218.98, 0.0006	273.45, 0.0009		196.01, 0.0324	242.83, 0.0740
	204.74, 0.3238	252.00, 0.0085		191.98, 0.0001	228.26, 0.0001
	202.02, 0.0374	245.14, 0.0003		191.88, 0.0263	218.85, 0.0003
	186.38, 0.0006	220.97, 0.1842			215.47, 0.0955
	181.91, 0.0002	216.17, 0.0004			204.36, 0.0011
		208.94, 0.0081			186.81, 0.0110
		206.11, 0.0795			181.98, 0.0004
		194.81, 0.0002			
		186.38, 0.0004			

Table S4. Wavelength (λ, nm) and oscillator strength (f, a.u.), of the calculated UV-Vis spectra of 3(2H)-thiophenone and 3(2H)-selenophenone at the PBE0/aug-cc-pVTZ level of theory.

3(2H)-thiophenone			3(2H)-selenophenone		
M^0	**M^{1+}**	**M^{2+}**	**M^0**	**M^{1+}**	**M^{2+}**
325.12, 0.0002	388.44, 0.0289	438.80, 0.0173	328.75, 0.0001	410.50, 0.0311	439.62, 0.0119
286.90, 0.1242	359.04, 0.0019	410.46, 0.0017	307.93, 0.1061	382.87, 0.0028	404.52, 0.0020
215.55, 0.0021	336.51, 0.0006	335.81, 0.0003	223.56, 0.0141	343.64, 0.0001	394.03, 0.0005
198.36, 0.0422	293.99, 0.0132	332.72, 0.0017	210.59, 0.0508	287.32, 0.0142	357.76, 0.0016
194.69, 0.0155	322.51, 0.0003	322.51, 0.0003	207.89, 0.0082	278.14, 0.0001	337.13, 0.0001
193.76, 0.0596	250.53, 0.0003	291.85, 0.0362	200.48, 0.0080	269.49, 0.0540	325.38, 0.0001
192.26, 0.0027	222.89, 0.0001	262.17, 0.0028	200.43, 0.0493	222.59, 0.0001	310.15, 0.0248
190.74, 0.0047	214.73, 0.0001	260.06, 0.0001	191.86, 0.0068	218.27, 0.0002	282.66, 0.0275
	203.71, 0.0083	257.55, 0.0032	186.06, 0.0001	212.44, 0.0014	259.36, 0.0005
	201.27, 0.0009	242.57, 0.0025	184.40, 0.0029	208.67, 0.0002	249.85, 0.0048
	199.23, 0.0038	239.39, 0.0024	181.81, 0.0660	203.09, 0.0245	236.22, 0.0013
	184.98, 0.0605	209.51, 0.1532		198.62, 0.0714	213.27, 0.0777
		206.68, 0.0002		181.89, 0.0001	210.14, 0.0002
		201.33, 0.0002			206.79, 0.0001
		192.27, 0.0010			202.32, 0.0004
		192.12, 0.0004			194.26, 0.0002
		182.52, 0.0001			191.39, 0.0146
		180.96, 0.0001			186.32, 0.0960

Table S5. Calculated EOM-CCSD spectra of glycolamide, 2-cyclopente-1-one, 2(5H)-furanone, 3(2H)-thiophenone, and 3(2H)-selenophenone as neutral species.

glycolamide	**2-cyclopenten-1-one**	**2(5H)-furanone**	**32(H)-thiophenone**	**32(H)-selenophene**
205.9, 0.0001	306.9, 0.0002	236.2, 0.0001	306.5, 0.0002	310.2, 0.0001
179.5, 0.0116	189.7, 0.2316	182.8, 0.2679	270.3, 0.1627	285.3, 0.1393
171.9, 0.0344	187.5, 0.1519	168.4, 0.1061	208.7, 0.0040	216.4, 0.0196
166.5, 0.1650	171.4, 0.0113	163.1, 0.0042	186.9, 0.0156	201.2, 0.0068
165.4, 0.0007	170.8, 0.0100	162.1, 0.0324	185.4, 0.0466	191.5, 0.0660

157.7, 0.0231	168.2, 0.0010	153.7, 0.0016	183.8, 0.0066	189.7, 0.0115
154.4, 0.0527	165.2, 0.0004	152.0, 0.0140	182.9, 0.0398	187.4, 0.0260
152.2, 0.0052	156.5, 0.0011	150.5, 0.0167	172.4, 0.0114	177.8, 0.0004
152.0, 0.0524	155.9, 0.0036	150.2, 0.0201		174.9, 0.0018

Table S6. Second ionization potentials (I2) and second electron affinities (A2) of the eight molecules identified as possibly DIBs carrier, in electron volts (eV) at DFT (PBE) level of computational theory.

Molecule*	I_2 (eV) Adiab./ZPE/Vert.	A_2 (eV) Adiab./ZPE/Vert.
glycolamide	-	2.74/2.72/2.85
lactamide	-	2.52/2.49/2.71
3-hydroxypropanamide	23.38/23.42/24.80	2.48/2.47/2.50
Oxamic acid	-	2.50/2.43/2.61
2-cyclopente-1-one	24.85/24.64/25.15	2.65/2.60/2.87
2(5H)-furanone	26.57/26.40/27.06	2.64/2.59/2.67
3(2H)-thiophenone	23.90/23.82/26.60	2.57/2.50/2.98
3(2H)-selenophenone	23.34/23.27/23.48	2.47/2.41/2.53