Supplementary material for "Potential energy surface and rovibrational bound states of the H_2–C_3N^- van der Waals complex"

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TABLE S1. Asymptotic form of the leading expansion coefficients for long-range interaction contributions. q is the charge, μ and Θ are the dipole and quadrupole moment respectively. $\alpha = (\alpha_\parallel + 2\alpha_\perp)$ and $\Delta\alpha = (\alpha_\parallel - \alpha_\perp)$ are the isotropic and anisotropic polarizabilities where $\alpha_\parallel$ and $\alpha_\perp$ are dipole polarizabilities. $A_\parallel$ and $A_\perp$ are dipole-quadrupole polarizabilities and U the ionization energies. Subscripts a and b refer to molecules H_2 and C_3N^- respectively.

$v^m_{l_1,l_2}$	Electrostatic	Induction	Dispersion
v^0_{00}		$-\frac{\alpha_a {q_b}^2}{R^4} - \frac{1}{3}\frac{{\mu_b}^2\Delta\alpha_a}{R^6} - \frac{{\mu_b}^2\alpha_a}{R^6} + \dots$	$-3\frac{U_aU_b}{U_a+U_b}\frac{\alpha_a\alpha_b}{R^6} + \dots$
v^0_{01}		$-\frac{4\sqrt{3}}{3}\frac{\alpha_a\mu_b q_b}{R^5} - \frac{12\sqrt{3}}{5}\frac{\alpha_a\mu_b\Theta_b}{R^7} + \dots$	$-\frac{6\sqrt{3}}{5}\frac{U_aU_b}{U_a+U_b}\frac{\alpha_a(A_\parallel+2A_\perp)_b}{R^7} + \dots$
v^0_{02}		$-\frac{6\sqrt{5}}{5}\frac{\alpha_a q_b\Theta_b}{R^6} - \frac{2\sqrt{5}}{5}\frac{\alpha_a\mu_b^2}{R^6} - \frac{\sqrt{5}}{5}\frac{\Delta\alpha_a{\mu_b}^2}{R^6} + \dots$	$-\frac{\sqrt{5}}{5}\frac{U_aU_b}{U_a+U_b}\frac{\alpha_a\Delta\alpha_b}{R^6} + \dots$
v^0_{20}	$\frac{2\sqrt{5}}{5}\frac{q_b\Theta_a}{R^3}$	$-\frac{2\sqrt{5}}{15}\frac{\alpha_a{q_b}^2}{R^4} - \frac{4\sqrt{5}}{15}\frac{\alpha_a q_b\mu_b}{R^5} - \frac{\sqrt{5}}{15}\frac{\Delta\alpha_a{\mu_b}^2}{R^6} + \dots$	$-\frac{\sqrt{5}}{5}\frac{U_aU_b}{U_a+U_b}\frac{\alpha_b\Delta\alpha_a}{R^6} + \dots$
v^0_{21}	$\frac{2\sqrt{15}}{5}\frac{\Theta_a\mu_b}{R^4}$	$-\frac{4\sqrt{15}}{45}\frac{\Delta\alpha_a q_b\mu_b}{R^5} + \dots$	
v^1_{21}	$-\frac{4\sqrt{5}}{5}\frac{\Theta_a\mu_b}{R^4}$	$-\frac{2\sqrt{15}}{15}\frac{\Delta\alpha_a q_b\mu_b}{R^5} + \dots$	
v^0_{22}	$\frac{15}{5}\frac{\Theta_a\Theta_b}{R^5}$	$-\frac{2}{5}\frac{\Delta\alpha_a\mu_b^2}{R^6} - \frac{4}{5}\frac{\Delta\alpha_a q_b\Theta_b}{R^6} + \dots$	
v^1_{22}	$-\frac{16}{5}\frac{\Theta_a\Theta_b}{R^5}$	$\frac{8}{15}\frac{\Delta\alpha_a\mu_b^2}{R^6} + \frac{12}{5}\frac{\Delta\alpha_a q_b\Theta_b}{R^6} + \dots$	
v^2_{22}	$\frac{4}{5}\frac{\Theta_a\Theta_b}{R^5}$	$-\frac{4}{15}\frac{\Delta\alpha_a\mu_b^2}{R^6} + \dots$	

TABLE S2. Character table of the G_4 group .

	E	(12)	E^*	$(12)^*$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	-1	1
B_2	1	-1	1	-1

TABLE S3. Complete list of the H_2–C_3N^- calculated rovibrational energy levels for total angular momentum $J = 0$.

Γ_i	Energy (cm^{-1})							
	-257.22	-232.95	-216.34	-203.00	-189.93	-174.95	-174.76	-160.57
	-157.08	-153.89	-146.80	-137.43	-134.08	-125.76	-120.79	-113.17
	-109.80	-99.17	-98.14	-85.24	-84.18	-83.73	-80.74	-74.97
A_1	-70.38	-67.58	-66.14	-61.66	-56.92	-52.83	-50.61	-48.28
	-42.22	-38.52	-34.73	-33.05	-32.10	-30.46	-29.16	-25.80
	-24.16	-20.47	-19.33	-17.55	-13.91	-13.50	-11.01	-10.26
	-8.96	-7.47	-6.43	-5.92	-3.85	-2.83	-1.33	
	-242.50	-214.84	-193.29	-174.67	-156.44	-141.71	-137.29	-125.74
	-120.00	-116.38	-101.76	-101.45	-95.02	-84.47	-82.69	-71.89
B_2	-66.53	-59.89	-51.15	-45.22	-39.41	-35.86	-33.47	-33.16
	-26.59	-17.30	-15.93	-15.81	-10.40	-8.41	-4.45	-0.85

TABLE S4. Complete list of the H_2–C_3N^- calculated rovibrational energy levels for total angular momentum $J = 1$.

Γ_i	Energy (cm^{-1})							
A1	-242.83	-223.06	-208.68	-195.80	-181.75	-166.14	-164.81	-153.36
	-146.75	-141.94	-135.81	-125.96	-124.16	-114.41	-110.69	-103.42
	-95.94	-90.43	-80.05	-77.96	-75.99	-71.58	-68.35	-61.83
	-60.69	-60.17	-52.03	-50.92	-43.09	-41.82	-39.71	-32.49
	-28.83	-28.50	-27.64	-23.40	-22.31	-22.10	-17.94	-16.33
	-13.91	-11.10	-8.60	-7.77	-6.94	-5.01	-3.33	-1.74
	-0.48							
A2	-256.89	-242.84	-232.60	-223.07	-215.96	-208.72	-202.58	-195.85
	-189.46	-181.81	-174.42	-174.17	-166.13	-164.96	-159.46	-157.26
	-153.43	-152.30	-148.90	-143.57	-141.96	-139.17	-133.60	-132.71
	-127.83	-125.98	-120.29	-120.21	-115.08	-114.38	-109.34	-106.18
	-103.48	-100.72	-97.43	-91.22	-89.96	-85.42	-83.68	-83.41
	-80.24	-78.19	-77.05	-74.12	-72.53	-71.59	-71.16	-67.46
	-66.28	-65.61	-63.35	-60.33	-57.68	-56.38	-54.35	-54.02
	-52.02	-49.65	-48.15	-46.95	-44.10	-42.70	-37.84	-35.83
	-34.76	-34.29	-32.72	-32.36	-31.21	-29.21	-29.18	-28.84
	-26.83	-25.45	-25.31	-23.45	-22.42	-20.96	-20.70	-19.72
	-18.48	-16.35	-15.23	-13.78	-12.48	-11.91	-9.99	-9.93
	-9.22	-8.67	-8.38	-8.23	-7.88	-6.60	-6.47	-6.23
	-5.35	-4.73	-4.08	-3.28	-3.12	-1.15	-0.97	-0.36
B1	-242.15	-226.67	-214.46	-202.63	-192.86	-182.99	-174.13	-164.63
	-155.64	-145.80	-141.02	-135.96	-129.45	-125.20	-125.07	-119.43
	-113.96	-111.62	-109.40	-103.09	-100.82	-100.21	-94.30	-90.48
	-89.29	-84.97	-81.92	-77.33	-73.36	-72.89	-65.58	-64.03
	-59.08	-57.28	-49.78	-49.40	-45.20	-40.80	-39.56	-37.08
	-35.14	-31.99	-31.32	-28.72	-23.89	-23.83	-23.24	-21.85
	-15.85	-15.06	-12.96	-11.84	-9.12	-8.22	-7.02	-6.70
	-4.88	-3.37	-2.21					
B2	-226.66	-202.62	-182.98	-164.61	-145.79	-129.45	-125.08	-111.61
	-109.44	-102.53	-92.32	-90.48	-80.63	-73.35	-68.85	-57.41
	-54.49	-41.55	-39.83	-34.64	-23.83	-23.27	-21.85	-17.33
	-9.72	-7.72	-6.71	-2.99	-2.81	-2.26		