Supplementary Information

Quantum rotational dynamics of l-C$_4$ ($^3\textstyle\sum_g^-$) by H$_2$ at low temperatures employing machine learning augmented potential energy surface

Pooja Chahal, Apoorv Kushwaha and T.J. Dhilip Kumar
Quantum Dynamics Lab, Department of Chemistry
Indian Institute of Technology Ropar, Rupnagar 140001, India

Table of Contents

Table S1: Data of rate coefficients of excitation transitions for the comparison of *para* H₂ and *ortho* H₂ as a function of temperature.

T (K)	1-3	1-5	*para* -H₂ 1-7	1-9	1-3	*ortho* -H₂ 1-5	1-7	1-9
1	9.31E-12	5.42E-14	4.76E-17	6.67E-21	1.03E-11	7.23E-14	7.89E-17	8.8E-21
2	4.15E-11	2.39E-12	5.87E-14	6.29E-16	4.34E-11	3.22E-12	8.68E-14	7.19E-16
3	6.57E-11	8.55E-12	6.51E-13	2.89E-14	6.93E-11	1.12E-11	9.02E-13	3.24E-14
4	8.07E-11	1.61E-11	2.2E-12	1.98E-13	8.67E-11	2.07E-11	2.91E-12	2.22E-13
5	9E-11	2.36E-11	4.58E-12	6.36E-13	9.87E-11	2.97E-11	5.88E-12	7.14E-13
6	9.61E-11	3.04E-11	7.5E-12	1.39E-12	1.07E-10	3.77E-11	9.41E-12	1.57E-12
7	1E-10	3.63E-11	1.07E-11	2.44E-12	1.13E-10	4.45E-11	1.32E-11	2.76E-12
8	1.03E-10	4.16E-11	1.39E-11	3.74E-12	1.17E-10	5.03E-11	1.7E-11	4.22E-12
9	1.05E-10	4.61E-11	1.71E-11	5.21E-12	1.21E-10	5.53E-11	2.07E-11	5.89E-12
10	1.06E-10	5.01E-11	2.02E-11	6.8E-12	1.23E-10	5.96E-11	2.42E-11	7.7E-12
11	1.07E-10	5.36E-11	2.32E-11	8.46E-12	1.25E-10	6.32E-11	2.75E-11	9.57E-12
12	1.07E-10	5.67E-11	2.59E-11	1.01E-11	1.26E-10	6.63E-11	3.06E-11	1.15E-11
13	1.07E-10	5.94E-11	2.85E-11	1.18E-11	1.27E-10	6.9E-11	3.35E-11	1.33E-11
14	1.07E-10	6.18E-11	3.09E-11	1.34E-11	1.27E-10	7.13E-11	3.61E-11	1.52E-11
15	1.07E-10	6.38E-11	3.3E-11	1.5E-11	1.27E-10	7.32E-11	3.85E-11	1.69E-11
16	1.07E-10	6.56E-11	3.5E-11	1.65E-11	1.28E-10	7.48E-11	4.07E-11	1.86E-11
17	1.07E-10	6.72E-11	3.68E-11	1.8E-11	1.27E-10	7.62E-11	4.26E-11	2.02E-11
18	1.06E-10	6.85E-11	3.84E-11	1.93E-11	1.27E-10	7.73E-11	4.44E-11	2.16E-11
19	1.06E-10	6.96E-11	3.98E-11	2.05E-11	1.26E-10	7.82E-11	4.59E-11	2.3E-11
20	1.05E-10	7.05E-11	4.11E-11	2.17E-11	1.26E-10	7.89E-11	4.73E-11	2.43E-11
21	1.04E-10	7.13E-11	4.23E-11	2.28E-11	1.25E-10	7.95E-11	4.85E-11	2.54E-11
22	1.04E-10	7.19E-11	4.33E-11	2.38E-11	1.24E-10	7.99E-11	4.96E-11	2.65E-11
23	1.03E-10	7.23E-11	4.42E-11	2.47E-11	1.23E-10	8.02E-11	5.05E-11	2.74E-11
24	1.02E-10	7.27E-11	4.5E-11	2.55E-11	1.22E-10	8.03E-11	5.12E-11	2.83E-11
25	1.01E-10	7.29E-11	4.56E-11	2.62E-11	1.21E-10	8.03E-11	5.19E-11	2.9E-11
26	1E-10	7.31E-11	4.62E-11	2.69E-11	1.2E-10	8.03E-11	5.25E-11	2.97E-11
27	9.92E-11	7.31E-11	4.67E-11	2.75E-11	1.19E-10	8.01E-11	5.29E-11	3.03E-11
28	9.82E-11	7.31E-11	4.71E-11	2.81E-11	1.18E-10	7.99E-11	5.33E-11	3.09E-11
29	9.72E-11	7.3E-11	4.74E-11	2.86E-11	1.17E-10	7.96E-11	5.35E-11	3.14E-11
30	9.62E-11	7.28E-11	4.77E-11	2.9E-11	1.15E-10	7.93E-11	5.37E-11	3.18E-11
31	9.52E-11	7.26E-11	4.79E-11	2.94E-11	1.14E-10	7.89E-11	5.39E-11	3.21E-11
32	9.42E-11	7.24E-11	4.8E-11	2.97E-11	1.13E-10	7.84E-11	5.39E-11	3.24E-11
33	9.32E-11	7.21E-11	4.81E-11	3E-11	1.12E-10	7.79E-11	5.39E-11	3.27E-11
34	9.22E-11	7.17E-11	4.82E-11	3.03E-11	1.1E-10	7.74E-11	5.39E-11	3.29E-11
35	9.11E-11	7.13E-11	4.82E-11	3.05E-11	1.09E-10	7.68E-11	5.38E-11	3.31E-11
36	9.01E-11	7.09E-11	4.82E-11	3.07E-11	1.08E-10	7.62E-11	5.37E-11	3.32E-11
37	8.91E-11	7.05E-11	4.81E-11	3.08E-11	1.07E-10	7.56E-11	5.35E-11	3.33E-11
38	8.81E-11	7E-11	4.8E-11	3.09E-11	1.05E-10	7.5E-11	5.33E-11	3.34E-11
39	8.71E-11	6.95E-11	4.79E-11	3.1E-11	1.04E-10	7.44E-11	5.31E-11	3.34E-11
40	8.61E-11	6.91E-11	4.78E-11	3.11E-11	1.03E-10	7.37E-11	5.28E-11	3.34E-11
41	8.51E-11	6.85E-11	4.76E-11	3.12E-11	1.01E-10	7.3E-11	5.26E-11	3.34E-11

42	8.41E-11	6.8E-11	4.74E-11	3.12E-11	1E-10	7.23E-11	5.23E-11	3.33E-11
43	8.31E-11	6.75E-11	4.72E-11	3.12E-11	9.89E-11	7.17E-11	5.2E-11	3.33E-11
44	8.22E-11	6.7E-11	4.7E-11	3.12E-11	9.77E-11	7.1E-11	5.16E-11	3.32E-11
45	8.12E-11	6.64E-11	4.68E-11	3.12E-11	9.65E-11	7.03E-11	5.13E-11	3.31E-11
46	8.03E-11	6.59E-11	4.66E-11	3.12E-11	9.53E-11	6.96E-11	5.09E-11	3.3E-11
47	7.94E-11	6.53E-11	4.63E-11	3.11E-11	9.41E-11	6.89E-11	5.06E-11	3.29E-11
48	7.85E-11	6.48E-11	4.61E-11	3.11E-11	9.29E-11	6.82E-11	5.02E-11	3.27E-11
49	7.76E-11	6.42E-11	4.58E-11	3.1E-11	9.17E-11	6.75E-11	4.98E-11	3.26E-11
50	7.67E-11	6.36E-11	4.55E-11	3.09E-11	9.06E-11	6.68E-11	4.94E-11	3.24E-11
51	7.58E-11	6.31E-11	4.52E-11	3.09E-11	8.95E-11	6.61E-11	4.9E-11	3.23E-11
52	7.5E-11	6.25E-11	4.49E-11	3.08E-11	8.83E-11	6.54E-11	4.86E-11	3.21E-11
53	7.41E-11	6.2E-11	4.47E-11	3.07E-11	8.73E-11	6.47E-11	4.82E-11	3.19E-11
54	7.33E-11	6.14E-11	4.44E-11	3.06E-11	8.62E-11	6.4E-11	4.78E-11	3.17E-11
55	7.25E-11	6.09E-11	4.41E-11	3.04E-11	8.51E-11	6.34E-11	4.74E-11	3.15E-11
56	7.17E-11	6.03E-11	4.38E-11	3.03E-11	8.41E-11	6.27E-11	4.7E-11	3.13E-11
57	7.09E-11	5.98E-11	4.35E-11	3.02E-11	8.3E-11	6.2E-11	4.66E-11	3.11E-11
58	7.01E-11	5.93E-11	4.32E-11	3.01E-11	8.2E-11	6.14E-11	4.61E-11	3.09E-11
59	6.93E-11	5.87E-11	4.29E-11	2.99E-11	8.1E-11	6.07E-11	4.57E-11	3.07E-11
60	6.86E-11	5.82E-11	4.26E-11	2.98E-11	8E-11	6.01E-11	4.53E-11	3.05E-11
61	6.78E-11	5.77E-11	4.23E-11	2.97E-11	7.91E-11	5.94E-11	4.49E-11	3.03E-11
62	6.71E-11	5.72E-11	4.2E-11	2.95E-11	7.81E-11	5.88E-11	4.45E-11	3.01E-11
63	6.64E-11	5.67E-11	4.16E-11	2.94E-11	7.72E-11	5.82E-11	4.41E-11	2.98E-11
64	6.57E-11	5.62E-11	4.13E-11	2.92E-11	7.63E-11	5.76E-11	4.37E-11	2.96E-11
65	6.5E-11	5.57E-11	4.1E-11	2.91E-11	7.54E-11	5.69E-11	4.33E-11	2.94E-11
66	6.43E-11	5.52E-11	4.07E-11	2.9E-11	7.45E-11	5.63E-11	4.29E-11	2.92E-11
67	6.36E-11	5.47E-11	4.04E-11	2.88E-11	7.36E-11	5.57E-11	4.25E-11	2.9E-11
68	6.3E-11	5.42E-11	4.01E-11	2.87E-11	7.28E-11	5.52E-11	4.21E-11	2.87E-11
69	6.23E-11	5.37E-11	3.99E-11	2.85E-11	7.19E-11	5.46E-11	4.17E-11	2.85E-11
70	6.17E-11	5.32E-11	3.96E-11	2.84E-11	7.11E-11	5.4E-11	4.13E-11	2.83E-11
71	6.11E-11	5.28E-11	3.93E-11	2.82E-11	7.03E-11	5.34E-11	4.09E-11	2.81E-11
72	6.04E-11	5.23E-11	3.9E-11	2.81E-11	6.95E-11	5.29E-11	4.05E-11	2.78E-11
73	5.98E-11	5.19E-11	3.87E-11	2.79E-11	6.87E-11	5.23E-11	4.02E-11	2.76E-11
74	5.92E-11	5.14E-11	3.84E-11	2.77E-11	6.79E-11	5.18E-11	3.98E-11	2.74E-11
75	5.87E-11	5.1E-11	3.81E-11	2.76E-11	6.71E-11	5.13E-11	3.94E-11	2.72E-11
76	5.81E-11	5.05E-11	3.78E-11	2.74E-11	6.64E-11	5.07E-11	3.9E-11	2.7E-11
77	5.75E-11	5.01E-11	3.76E-11	2.73E-11	6.57E-11	5.02E-11	3.87E-11	2.67E-11
78	5.7E-11	4.97E-11	3.73E-11	2.71E-11	6.49E-11	4.97E-11	3.83E-11	2.65E-11
79	5.64E-11	4.93E-11	3.7E-11	2.7E-11	6.42E-11	4.92E-11	3.8E-11	2.63E-11
80	5.59E-11	4.88E-11	3.67E-11	2.68E-11	6.35E-11	4.87E-11	3.76E-11	2.61E-11
81	5.53E-11	4.84E-11	3.65E-11	2.67E-11	6.28E-11	4.82E-11	3.73E-11	2.59E-11
82	5.48E-11	4.8E-11	3.62E-11	2.65E-11	6.22E-11	4.77E-11	3.69E-11	2.57E-11
83	5.43E-11	4.76E-11	3.59E-11	2.64E-11	6.15E-11	4.73E-11	3.66E-11	2.55E-11
84	5.38E-11	4.72E-11	3.57E-11	2.62E-11	6.08E-11	4.68E-11	3.63E-11	2.53E-11
85	5.33E-11	4.68E-11	3.54E-11	2.61E-11	6.02E-11	4.63E-11	3.59E-11	2.51E-11
86	5.28E-11	4.65E-11	3.52E-11	2.59E-11	5.96E-11	4.59E-11	3.56E-11	2.49E-11
87	5.23E-11	4.61E-11	3.49E-11	2.58E-11	5.89E-11	4.54E-11	3.53E-11	2.47E-11
88	5.19E-11	4.57E-11	3.47E-11	2.56E-11	5.83E-11	4.5E-11	3.5E-11	2.45E-11

89	5.14E-11	4.53E-11	3.44E-11	2.55E-11	5.77E-11	4.46E-11	3.46E-11	2.43E-11
90	5.09E-11	4.5E-11	3.42E-11	2.53E-11	5.71E-11	4.41E-11	3.43E-11	2.41E-11
91	5.05E-11	4.46E-11	3.39E-11	2.52E-11	5.65E-11	4.37E-11	3.4E-11	2.39E-11
92	5E-11	4.43E-11	3.37E-11	2.51E-11	5.6E-11	4.33E-11	3.37E-11	2.37E-11
93	4.96E-11	4.39E-11	3.35E-11	2.49E-11	5.54E-11	4.29E-11	3.34E-11	2.35E-11
94	4.92E-11	4.36E-11	3.32E-11	2.48E-11	5.48E-11	4.25E-11	3.31E-11	2.33E-11
95	4.87E-11	4.32E-11	3.3E-11	2.46E-11	5.43E-11	4.21E-11	3.28E-11	2.31E-11
96	4.83E-11	4.29E-11	3.28E-11	2.45E-11	5.37E-11	4.17E-11	3.25E-11	2.29E-11
97	4.79E-11	4.26E-11	3.25E-11	2.43E-11	5.32E-11	4.13E-11	3.23E-11	2.27E-11
98	4.75E-11	4.22E-11	3.23E-11	2.42E-11	5.27E-11	4.09E-11	3.2E-11	2.26E-11
99	4.71E-11	4.19E-11	3.21E-11	2.41E-11	5.22E-11	4.05E-11	3.17E-11	2.24E-11
100	4.67E-11	4.16E-11	3.19E-11	2.39E-11	5.17E-11	4.02E-11	3.14E-11	2.22E-11

Table S2: Data of rate coefficients of de-excitation transitions for the comparison of _para_ H$_2$ and He as a function of temperature.

	para -H$_2$					He		
T (K)	3-1	5-1	7-1	9-1	3-1	5-1	7-1	9-1
5	9.58E-11	2.24E-11	4.37E-12	6.43E-13	2.30E-11	1.08E-11	5.63E-12	2.88E-12
6	9.23E-11	2.55E-11	6.27E-12	1.23E-12	2.30E-11	1.09E-11	5.73E-12	2.93E-12
7	8.88E-11	2.77E-11	8.01E-12	1.93E-12	2.30E-11	1.09E-11	5.79E-12	2.98E-12
8	8.54E-11	2.93E-11	9.56E-12	2.68E-12	2.28E-11	1.09E-11	5.84E-12	3.02E-12
9	8.24E-11	3.04E-11	1.09E-11	3.45E-12	2.26E-11	1.08E-11	5.86E-12	3.06E-12
10	7.97E-11	3.12E-11	1.21E-11	4.19E-12	2.25E-11	1.07E-11	5.88E-12	3.09E-12
11	7.73E-11	3.17E-11	1.30E-11	4.89E-12	2.23E-11	1.06E-11	5.88E-12	3.13E-12
12	7.51E-11	3.21E-11	1.39E-11	5.55E-12	2.21E-11	1.05E-11	5.88E-12	3.16E-12
13	7.31E-11	3.24E-11	1.46E-11	6.15E-12	2.19E-11	1.04E-11	5.88E-12	3.19E-12
14	7.12E-11	3.25E-11	1.52E-11	6.70E-12	2.17E-11	1.03E-11	5.87E-12	3.22E-12
15	6.95E-11	3.26E-11	1.57E-11	7.19E-12	2.15E-11	1.02E-11	5.85E-12	3.25E-12
16	6.80E-11	3.26E-11	1.61E-11	7.64E-12	2.14E-11	1.01E-11	5.84E-12	3.28E-12
17	6.65E-11	3.26E-11	1.65E-11	8.03E-12	2.12E-11	9.96E-12	5.82E-12	3.30E-12
18	6.51E-11	3.25E-11	1.67E-11	8.38E-12	2.11E-11	9.86E-12	5.81E-12	3.32E-12
19	6.38E-11	3.23E-11	1.70E-11	8.68E-12	2.09E-11	9.77E-12	5.79E-12	3.34E-12
20	6.25E-11	3.22E-11	1.71E-11	8.95E-12	2.08E-11	9.68E-12	5.77E-12	3.36E-12
21	6.13E-11	3.20E-11	1.72E-11	9.18E-12	2.06E-11	9.60E-12	5.75E-12	3.38E-12
22	6.02E-11	3.17E-11	1.73E-11	9.38E-12	2.05E-11	9.51E-12	5.73E-12	3.40E-12
23	5.91E-11	3.15E-11	1.74E-11	9.54E-12	2.04E-11	9.44E-12	5.71E-12	3.41E-12
24	5.80E-11	3.12E-11	1.74E-11	9.68E-12	2.03E-11	9.36E-12	5.69E-12	3.43E-12
25	5.70E-11	3.09E-11	1.74E-11	9.80E-12	2.02E-11	9.29E-12	5.67E-12	3.44E-12
26	5.60E-11	3.06E-11	1.74E-11	9.89E-12	2.01E-11	9.22E-12	5.66E-12	3.45E-12
27	5.50E-11	3.03E-11	1.73E-11	9.96E-12	2.00E-11	9.15E-12	5.64E-12	3.46E-12
28	5.40E-11	3.00E-11	1.73E-11	1.00E-11	1.99E-11	9.09E-12	5.62E-12	3.47E-12
29	5.31E-11	2.97E-11	1.72E-11	1.01E-11	1.98E-11	9.03E-12	5.60E-12	3.48E-12
30	5.22E-11	2.94E-11	1.71E-11	1.01E-11	1.97E-11	8.97E-12	5.58E-12	3.49E-12
31	5.13E-11	2.90E-11	1.70E-11	1.01E-11	1.96E-11	8.92E-12	5.56E-12	3.50E-12
32	5.04E-11	2.87E-11	1.69E-11	1.01E-11	1.95E-11	8.86E-12	5.55E-12	3.51E-12

33	4.96E-11	2.83E-11	1.68E-11	1.01E-11	1.95E-11	8.81E-12	5.53E-12	3.51E-12
34	4.88E-11	2.80E-11	1.66E-11	1.01E-11	1.94E-11	8.76E-12	5.51E-12	3.52E-12
35	4.80E-11	2.76E-11	1.65E-11	1.00E-11	1.93E-11	8.71E-12	5.50E-12	3.53E-12
36	4.72E-11	2.73E-11	1.63E-11	9.98E-12	1.92E-11	8.67E-12	5.48E-12	3.53E-12
37	4.64E-11	2.70E-11	1.62E-11	9.94E-12	1.92E-11	8.62E-12	5.46E-12	3.54E-12
38	4.57E-11	2.66E-11	1.60E-11	9.89E-12	1.91E-11	8.58E-12	5.45E-12	3.54E-12
39	4.49E-11	2.63E-11	1.59E-11	9.83E-12	1.90E-11	8.54E-12	5.43E-12	3.54E-12
40	4.42E-11	2.59E-11	1.57E-11	9.78E-12	1.90E-11	8.50E-12	5.42E-12	3.55E-12
41	4.35E-11	2.56E-11	1.56E-11	9.71E-12	1.89E-11	8.46E-12	5.40E-12	3.55E-12
42	4.28E-11	2.53E-11	1.54E-11	9.65E-12	1.89E-11	8.42E-12	5.39E-12	3.55E-12
43	4.22E-11	2.50E-11	1.52E-11	9.58E-12	1.88E-11	8.38E-12	5.38E-12	3.56E-12
44	4.15E-11	2.46E-11	1.51E-11	9.50E-12	1.88E-11	8.35E-12	5.36E-12	3.56E-12
45	4.09E-11	2.43E-11	1.49E-11	9.43E-12	1.87E-11	8.32E-12	5.35E-12	3.56E-12
46	4.03E-11	2.40E-11	1.47E-11	9.35E-12	1.87E-11	8.28E-12	5.33E-12	3.56E-12
47	3.97E-11	2.37E-11	1.46E-11	9.27E-12	1.86E-11	8.25E-12	5.32E-12	3.56E-12
48	3.91E-11	2.34E-11	1.44E-11	9.20E-12	1.86E-11	8.22E-12	5.31E-12	3.56E-12
49	3.85E-11	2.31E-11	1.43E-11	9.11E-12	1.85E-11	8.19E-12	5.30E-12	3.56E-12
50	3.79E-11	2.28E-11	1.41E-11	9.03E-12	1.85E-11	8.16E-12	5.28E-12	3.56E-12
51	3.74E-11	2.25E-11	1.39E-11	8.95E-12				
52	3.68E-11	2.22E-11	1.38E-11	8.87E-12				
53	3.63E-11	2.19E-11	1.36E-11	8.79E-12				
54	3.58E-11	2.16E-11	1.35E-11	8.70E-12				
55	3.52E-11	2.13E-11	1.33E-11	8.62E-12				
56	3.47E-11	2.11E-11	1.32E-11	8.54E-12				
57	3.43E-11	2.08E-11	1.30E-11	8.46E-12				
58	3.38E-11	2.05E-11	1.29E-11	8.37E-12				
59	3.33E-11	2.03E-11	1.27E-11	8.29E-12				
60	3.29E-11	2.00E-11	1.26E-11	8.21E-12				
61	3.24E-11	1.98E-11	1.24E-11	8.13E-12				
62	3.20E-11	1.95E-11	1.23E-11	8.05E-12				
63	3.15E-11	1.93E-11	1.21E-11	7.97E-12				
64	3.11E-11	1.91E-11	1.20E-11	7.89E-12				
65	3.07E-11	1.88E-11	1.19E-11	7.81E-12				
66	3.03E-11	1.86E-11	1.17E-11	7.73E-12				
67	2.99E-11	1.84E-11	1.16E-11	7.66E-12				
68	2.95E-11	1.82E-11	1.15E-11	7.58E-12				
69	2.91E-11	1.79E-11	1.14E-11	7.50E-12				
70	2.88E-11	1.77E-11	1.12E-11	7.43E-12				
71	2.84E-11	1.75E-11	1.11E-11	7.36E-12				
72	2.80E-11	1.73E-11	1.10E-11	7.28E-12				
73	2.77E-11	1.71E-11	1.09E-11	7.21E-12				
74	2.74E-11	1.69E-11	1.07E-11	7.14E-12				
75	2.70E-11	1.67E-11	1.06E-11	7.07E-12				
76	2.67E-11	1.65E-11	1.05E-11	7.00E-12				
77	2.64E-11	1.63E-11	1.04E-11	6.93E-12				
78	2.60E-11	1.62E-11	1.03E-11	6.86E-12				
79	2.57E-11	1.60E-11	1.02E-11	6.79E-12				

80	2.54E-11	1.58E-11	1.01E-11	6.73E-12
81	2.51E-11	1.56E-11	9.96E-12	6.66E-12
82	2.48E-11	1.54E-11	9.86E-12	6.60E-12
83	2.45E-11	1.53E-11	9.75E-12	6.53E-12
84	2.43E-11	1.51E-11	9.65E-12	6.47E-12
85	2.40E-11	1.49E-11	9.55E-12	6.41E-12
86	2.37E-11	1.48E-11	9.45E-12	6.35E-12
87	2.34E-11	1.46E-11	9.36E-12	6.29E-12
88	2.32E-11	1.45E-11	9.26E-12	6.23E-12
89	2.29E-11	1.43E-11	9.17E-12	6.17E-12
90	2.27E-11	1.42E-11	9.08E-12	6.11E-12
91	2.24E-11	1.40E-11	8.99E-12	6.05E-12
92	2.22E-11	1.39E-11	8.90E-12	6.00E-12
93	2.19E-11	1.37E-11	8.81E-12	5.94E-12
94	2.17E-11	1.36E-11	8.72E-12	5.89E-12
95	2.15E-11	1.34E-11	8.64E-12	5.83E-12
96	2.12E-11	1.33E-11	8.55E-12	5.78E-12
97	2.10E-11	1.32E-11	8.47E-12	5.72E-12
98	2.08E-11	1.30E-11	8.39E-12	5.67E-12
99	2.06E-11	1.29E-11	8.31E-12	5.62E-12
100	2.04E-11	1.28E-11	8.23E-12	5.57E-12

Table S3: Python program for generating PES.

Program for generating PES	Analytical expression
``# Import math Library
import math;
import os;
path = os.getcwd()
print(path)
for l in range (0,1,30):
    phi = int(l)
    directory2 = path+ "/" + "%s"%(str(l))
    if not os.path.exists(directory2):
        os.makedirs(directory2)
    os.chdir(directory2)
    for k in range (0,1,30):
        theta2 = int(k)
        directory1 = directory2+ "/" + "%s"%(str(k))
        if not os.path.exists(directory1):
            os.makedirs(directory1)
        os.chdir(directory1)
        for j in range (0,1,15):
            theta1 = int(j)
            directory = path+ "/" + "%s"%(str(j))
            if not os.path.exists(directory):
                os.makedirs(directory)
            os.chdir(directory)
            for i in range (76):
                R=i/10.0+2.5
                r1 = 1.9534
                r2 = 0.6445
                rh = 0.3714
                a1 = math.sin(math.radians(theta1))*math.sin(math.radians(phi))
                a2 = math.sin(math.radians(theta1))*math.cos(math.radians(phi))
                a3 = math.cos(math.radians(theta1))
                b1 = math.sin(math.radians(theta2))
                b2 = math.cos(math.radians(theta2))
                r11= R-rh*b2
                r21= R+rh*b2
                f= open("%d.gjf" %(i),"w+") # w+=write/r=read
                f.write("""%%nprocshared=4
%%mem=10GB
%%chk=%d_%d_%d.chk
CCSD=(T,SaveAmplitudes,ReadAmplitudes)/aug-cc-pVTZ

R = %d, phi=%d, theta2=%d, theta1=%d,

0 3
C   %.4f   %.4f   %.4f
C   %.4f   %.4f   %.4f
C   %.4f   %.4f   %.4f
C   %.4f   %.4f   %.4f
H   0.0000   %.4f   %.4f
H   0.0000   %.4f   %.4f``` | *General Experssion:*

C	$r1{*}sin(\theta1){*}sin(\phi)$	$r1{*}sin(\theta1){*}cos(\phi)$	$r1{*}cos(\theta1)$
C	$r2{*}sin(\theta1){*}sin(\phi)$	$r2{*}sin(\theta1){*}cos(\phi)$	$r2{*}cos(\theta1)$
C	$-r2{*}sin(\theta1){*}sin(\phi)$	$-r2{*}sin(\theta1){*}cos(\phi)$	$-r2{*}cos(\theta1)$
C	$-r1{*}sin(\theta1){*}sin(\phi)$	$-r1{*}sin(\theta1){*}cos(\phi)$	$-r1{*}cos(\theta1)$
H	0.0000	$rh{*}sin(\theta2)$	$R + rh{*}cos(\theta2)$
H	0.0000	$rh{*}sin(\theta2)$	$R - rh{*}cos(\theta2)$

Stationary point (Global Minimum)
ϕ, θ_2, θ_1 = 0°, 90°, 90° and R = 3.4 Å

C	0.0000	1.9534	0.0000
C	0.0000	0.6445	0.0000
C	0.0000	-0.6445	0.0000
C	0.0000	-1.9534	0.0000
H	0.0000	0.3714	3.4000
H	0.0000	-0.3714	3.4000	

```
      """ %(phi,theta2,theta1,R,phi,theta2,theta1,
r1*a1,r1*a2,r1*a3,    r2*a1,r2*a2,r2*a3,    -r2*a1,-r2*a2,-r2*a3,    -r1*a1,-r1*a2,-r1*a3,rh*b1,r11,-
rh*b1,r21))

      f.close()
    os.chdir(directory)
  os.chdir(directory1)
os.chdir(directory2)
```

Table S4: *Ab initio* energies (C_4-H_2) at various geometries compared to recreated PES (from radial terms).

Geometry (ϕ, θ_2, θ_1, R)	Ab initio energy	Recreated PES (from radial terms)
0°, 90°, 90°, 3.4 Å	-147.79	-147.47
0°, 0°, 0°, 5.4 Å	-144.83	-144.49
0°, 90°, 0°, 5.9 Å	-18.78	-17.89

Table S5: Computed properties of C_4 compared to previous literature.

Properties (C_4)	Current work	Previous Literature
Vibrational Frequencies (cm^{-1})	CCSD(T)/aug-cc-pVQZ (Harmonic) No. Freq in cm^{-1} [D] (mode) 1. 2107 [1] (stretching Σ_g) 2. 1596 [1] (stretching Σ_u) 3. 942 [1] (stretching Σ_g) 4. 369 [2] (bending Π_g) 5. 168 [2] (bending Π_u) [D]: Degeneracy	Experimental [1]: No. Freq in cm^{-1} 1. 2057 2. 1549 3. N.A. 4. 323 5. 160
Bond lengths (Å)	1.2890 (inner) 1.3089 (outer) (CCSD(T)/CBS(DTQ))	Experimental: 1.304 (all same)[1] 1.3167 (inner) 1.2960 (outer)[2] 1.2840 (inner) 1.3060 (outer)[3]

1. *"National Institute of Standards and Technology | NIST." NIST, 22 Dec. 2023, www.nist.gov.*
2. *Lique, François, et al., Phys. Chem. Chem. Phys.,12, 15672-15680 (2010).*
3. *Van Orden, Alan, et al., Chem. Rev., 98, 2313-2358 (1998).*

Figure S1: Cross-sections for the rotational excitation (1-N) transitions of collision of C_4 with *ortho* $- H_2$ till energy range of 300 cm^{-1}.
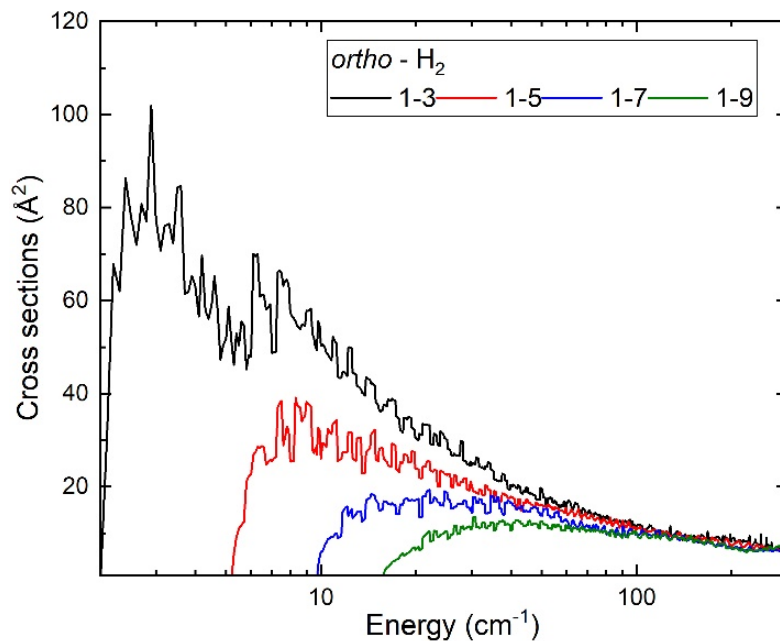

Figure S2: Comparison between the cross-sections ($\Delta j = 2$) computed for C_4 molecule due to its collision with *para* and *ortho* $- H_2$ for different transitions as shown: Solid corresponds to *ortho* $- H_2$ while dotted corresponds to para $- H_2$.
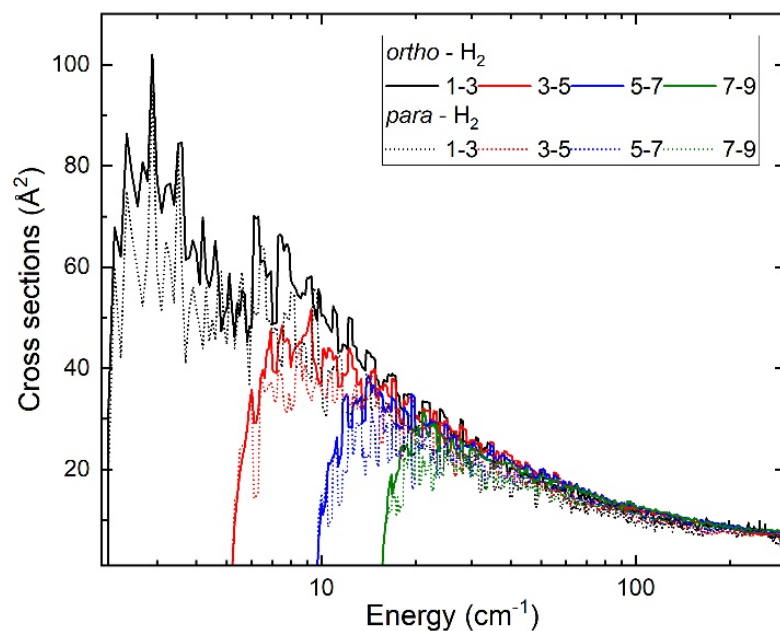
Figure S3: Cross-sections for the rotational excitation transitions ($\Delta j = 2$) of collision of C_4 with *ortho* $- H_2$ till energy range of 300 cm^{-1}.
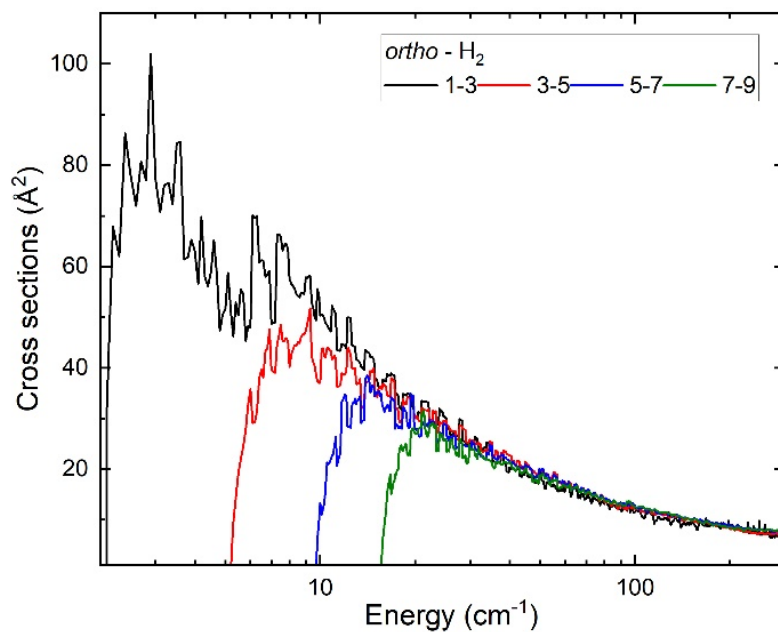

Figure S4: Cross-sections for the rotational excitation transitions (1-N) of collision of C_4 with *para* $-$ H_2 till energy range of 300 cm^{-1}.
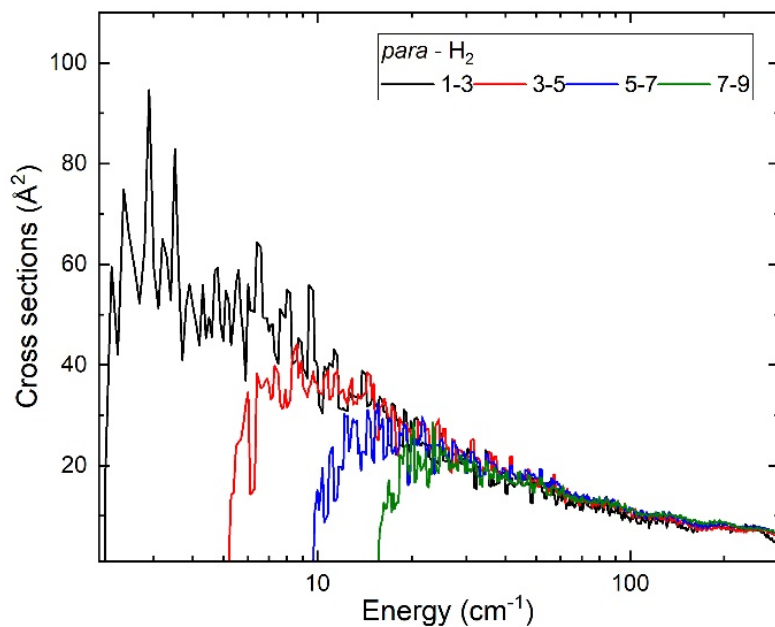
Figure S5: PES at various angular coordinates (ϕ, $\boldsymbol{\theta}_2$, $\boldsymbol{\theta}_1$, R) with respect to R.

Figure S6: Variation of R (optimised) with respect to $\boldsymbol{\theta}_2$ vs $\boldsymbol{\theta}_1$ at ϕ =0°.