

10. Supplementary material

Tab. I: Assignment of the $\tilde{C}' \leftarrow \tilde{X} 2_{0+}^0$ band of NH_3 [$^{\Delta K} \Delta J_{K''} (J'')$]

experimental	simulation	transition	experimental	simulation	transition
63796.8	63796.45	$^q Q_9(9)$	63868.4	63867.93	$^q Q_0(1)$
63804.6	63804.46	$^q P_2(3)$	63869.4	63869.02	$^q Q_2(3)$
63812.4	63811.84	$^q Q_8(8)$	63869.6	63869.43	$^q Q_1(2)$
63813.6	63812.77	$^q Q_9(10)$	63872.6	63872.27	$^q Q_4(6)$
63825.6	63825.32	$^q Q_7(7)$	63875	63874.32	$^q Q_1(3)$
63826.6	63826.52	$^q Q_8(9)$	63875.4	63874.86	$^q Q_3(5)$
63831.2	63830.73	$^q Q_9(11)$	63876.6	63876.09	$^q Q_0(3)$
63837.2	63836.89	$^q Q_6(6)$	63881.4	63880.85	$^q Q_1(4)$
63838.6	63838.37	$^q Q_7(8)$	63884.2	63883.7	$^q Q_2(5)$
63844	63842.84	$^q Q_8(10)$	63885.6	63884.65	$^q Q_3(6)$
63846.8	63846.56	$^q Q_5(5)$	63889.6	63889.01	$^q Q_1(5)$
63848.6	63848.31	$^q Q_6(7)$	63891.2	63890.78	$^q Q_0(5)$
63854.8	63854.32	$^q Q_4(4)$	63894	63864.12	$^q Q_2(6)$
63856.8	63856.35	$^q Q_5(6)$	63896.6	63896.75	$^q Q_4(8)$
63860.4	63860.17	$^q Q_3(3)$	63899.4	63898.8	$^q Q_1(6)$
63862	63862.48	$^q Q_4(5)$	63905.2	63904.92	$^q Q_2(7)$
63864.6	63864.12	$^q Q_2(2)$	63910.6	63910.23	$^q Q_1(7)$
63866.8	63866.16	$^q Q_1(1)$	63912.2	63912	$^q Q_0(7)$
63867.2	63866.7	$^q Q_3(4)$	63928.8	63928.68	$^q R_2(3)$

Tab. II: Assignment of the $\tilde{C}' \leftarrow \tilde{X} 2_{0+}^0$ band of NH_2D (J_{K_a, K_c})

experimental	simulation	transition	experimental	simulation	transition
63826.23	63826.06	$10_{0/1,10} \leftarrow 10_{0/1,10}$	63885.76	63885.54	$2_{0/1,2} \leftarrow 2_{0/1,2}$
63832.02	63838.01	$9_{0/1,9} \leftarrow 9_{0/1,9}$	63887.7	63887.89	$1_{1,1} \leftarrow 1_{1,1}$
63848.84	63848.72	$8_{0/1,8} \leftarrow 8_{0/1,8}$	63888.3	63888.7	$1_{1,0} \leftarrow 1_{1,0}$
63858.1	63858.16	$7_{0/1,7} \leftarrow 7_{0/1,7}$	63891.06	63891.56	$2_{2,0/1} \leftarrow 2_{2,0/1}$
63866.26	63866.32	$6_{0/1,6} \leftarrow 6_{0/1,6}$	63896.38	63896.57	$3_{3,0/1} \leftarrow 3_{3,0/1}$
63873.2	63873.17	$5_{0/1,5} \leftarrow 5_{0/1,5}$	63903.92	63903.8	$4_{4,0/1} \leftarrow 4_{4,0/1}$
63878.6	63878.7	$4_{0/1,4} \leftarrow 4_{0/1,4}$	63913.22	63913.21	$5_{5,0/1} \leftarrow 5_{5,0/1}$
63882.9	63882.84	$3_{0/1,3} \leftarrow 3_{0/1,3}$			

Tab. III: Assignment of the $\tilde{C}' \leftarrow \tilde{X} 2_{0+}^0$ band of NHD_2 (J_{K_a, K_c})

experimental	simulation	transition	experimental	simulation	transition
63877.18	63876.95	$9_{0/1,9} \leftarrow 9_{0/1,9}$	63917.42	63917.15	$0_{0,0} \leftarrow 0_{0,0}$
63885.66	63885.62	$8_{0/1,8} \leftarrow 8_{0/1,8}$	63918.32	63918.49	$1_{1,0/1} \leftarrow 1_{1,0/1}$
63893	63893.25	$7_{0/1,7} \leftarrow 7_{0/1,7}$	63920.16	63920.32	$2_{2,0/1} \leftarrow 2_{2,0/1}$
63899.22	63899.86	$6_{0/1,6} \leftarrow 6_{0/1,6}$	63924.06	63924.21	$3_{3,0/1} \leftarrow 3_{3,0/1}$
63905.36	63905.41	$5_{0/1,5} \leftarrow 5_{0/1,5}$	63929.78	63929.49	$4_{4,0/1} \leftarrow 4_{4,0/1}$
63909.94	63909.89	$4_{0/1,4} \leftarrow 4_{0/1,4}$	63937.02	63936.98	$5_{5,0/1} \leftarrow 5_{5,0/1}$
63913.32	63913.27	$3_{0/1,3} \leftarrow 3_{0/1,3}$	63945.82	63945.9	$6_{6,0/1} \leftarrow 6_{6,0/1}$
63915.36	63915.53	$2_{0/1,2} \leftarrow 2_{0/1,2}$	63956.46	63956.48	$7_{7,0/1} \leftarrow 7_{7,0/1}$
63916.7	63916.81	$1_{0/1,1} \leftarrow 1_{0/1,1}$			

Tab. IV: Assignment of the $\tilde{C}' \leftarrow \tilde{X} 2_{0+}^0$ band of ND_3 [$^{\Delta K} \Delta J_{K''}$ (J'')]

experimental	simulation	transition	Experimental	simulation	transition
63918	63917.82	$^q Q_9(9)$	63948.6	63948.12	$^q Q_4(4)$
63922	63921.96	$^q Q_9(10)$	63950	63950.19	$^q Q_4(5)$
36926	63925.81	$^q Q_8(8)$	63950.8	63951.28	$^q Q_3(3)$
63929.8	63929.53	$^q Q_8(9)$	63951.4	63952.94	$^q Q_3(4)$
63933.4	63932.83	$^q Q_7(7)$	63953.4	63953.49	$^q Q_2(2)$
63936.2	63936.14	$^q Q_7(8)$	63956.8	63955	$^q Q_0(0)$
63939	63938.89	$^q Q_6(6)$	63959	63956.38	$^q Q_2(4)$
63942	63941.79	$^q Q_6(7)$	63961.2	63961.21	$^q Q_0(5)$
63944.4	63943.99	$^q Q_5(5)$	63964.4	63959.14	$^q Q_1(4)$
63946	63945.1	$^q Q_6(8)$	63966.6	63958.45	$^q Q_2(5)$
63947	63946.47	$^q Q_5(6)$	63970	63960.52	$^q Q_1(5)$