

Figure FS1: The spin-orbit splitting  $\Delta E$  for the  $1^3\Sigma^+$  and  $1^3\Phi$  parent states and their corresponding daughter states.

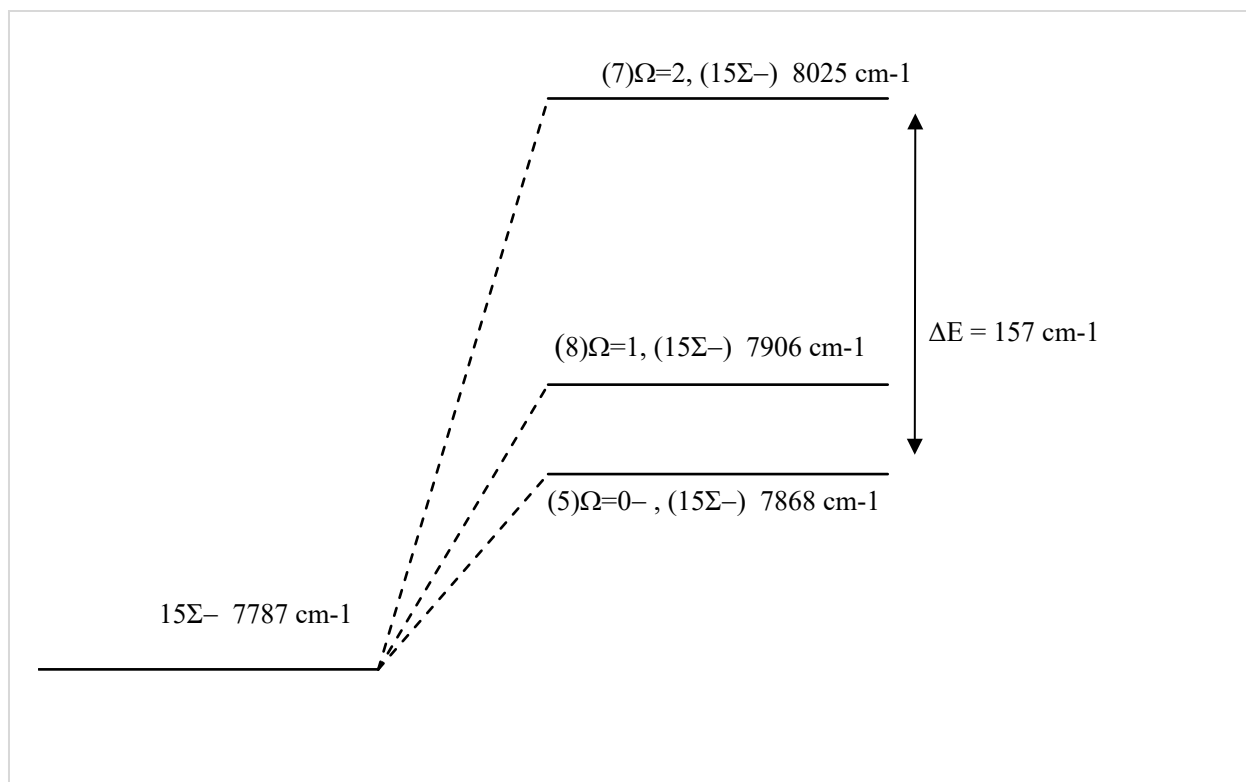


Figure FS2: The spin-orbit splitting  $\Delta E$  for the  $1^5\Sigma^-$  parent states and its corresponding daughter state.

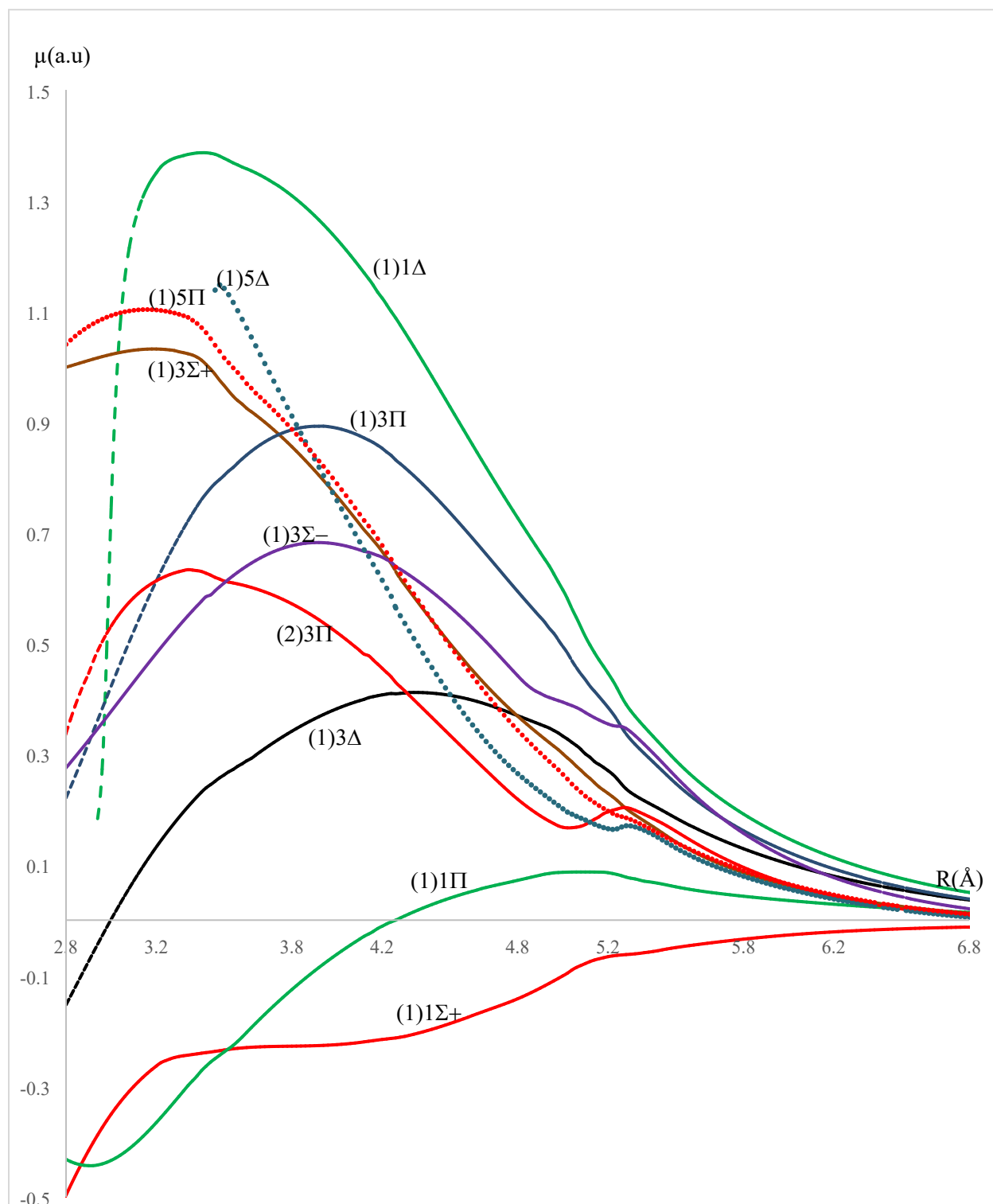


Figure FS3: Permanent dipole moment curves for singlet, triplet and quintet electronic states of LaNa molecule using spin-free MRCI + Q calculation.

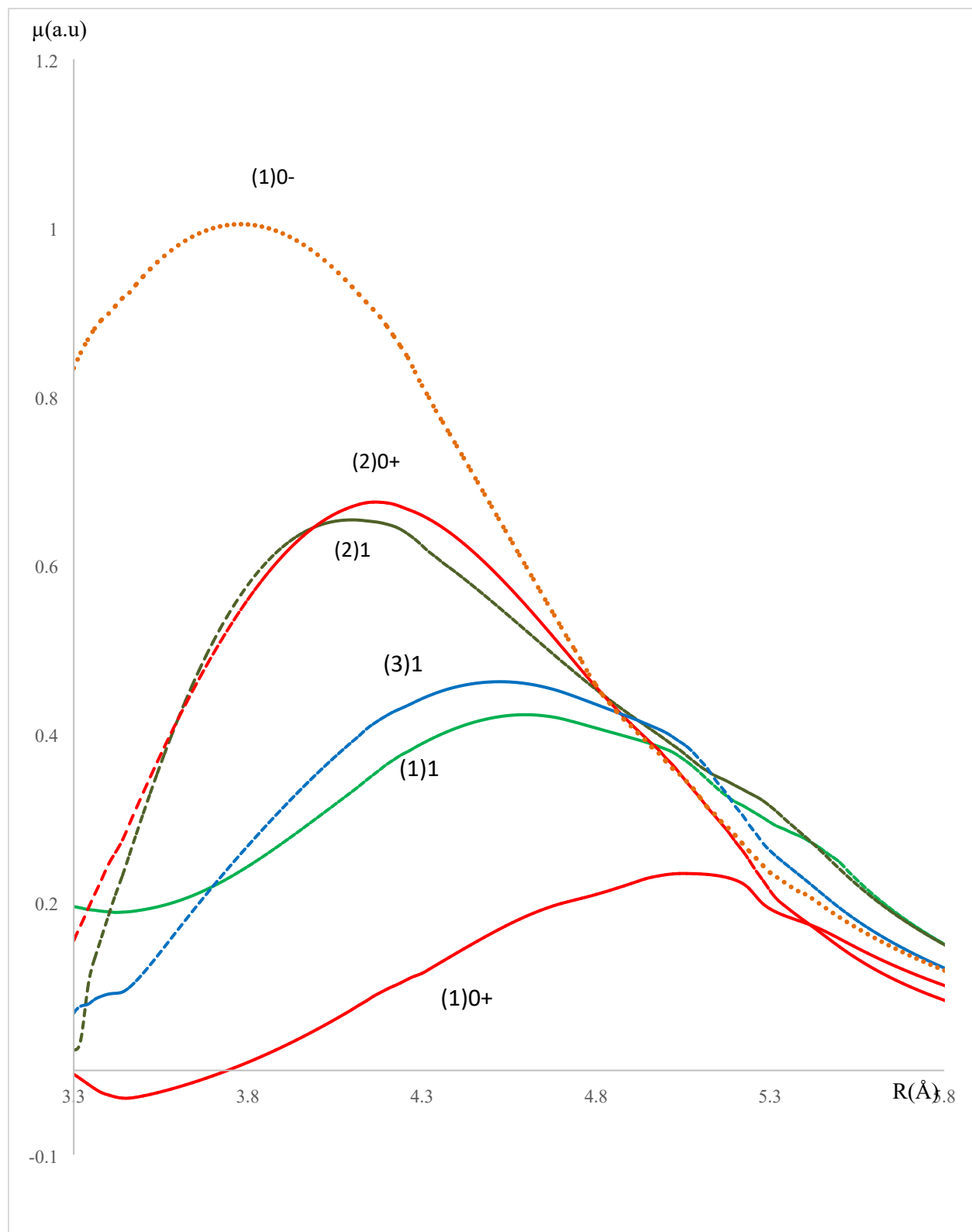


Figure FS4: Permanent dipole moment curves of the electronic states  $\Omega = 0^+, 0^-, 1$  of LaNa molecule.

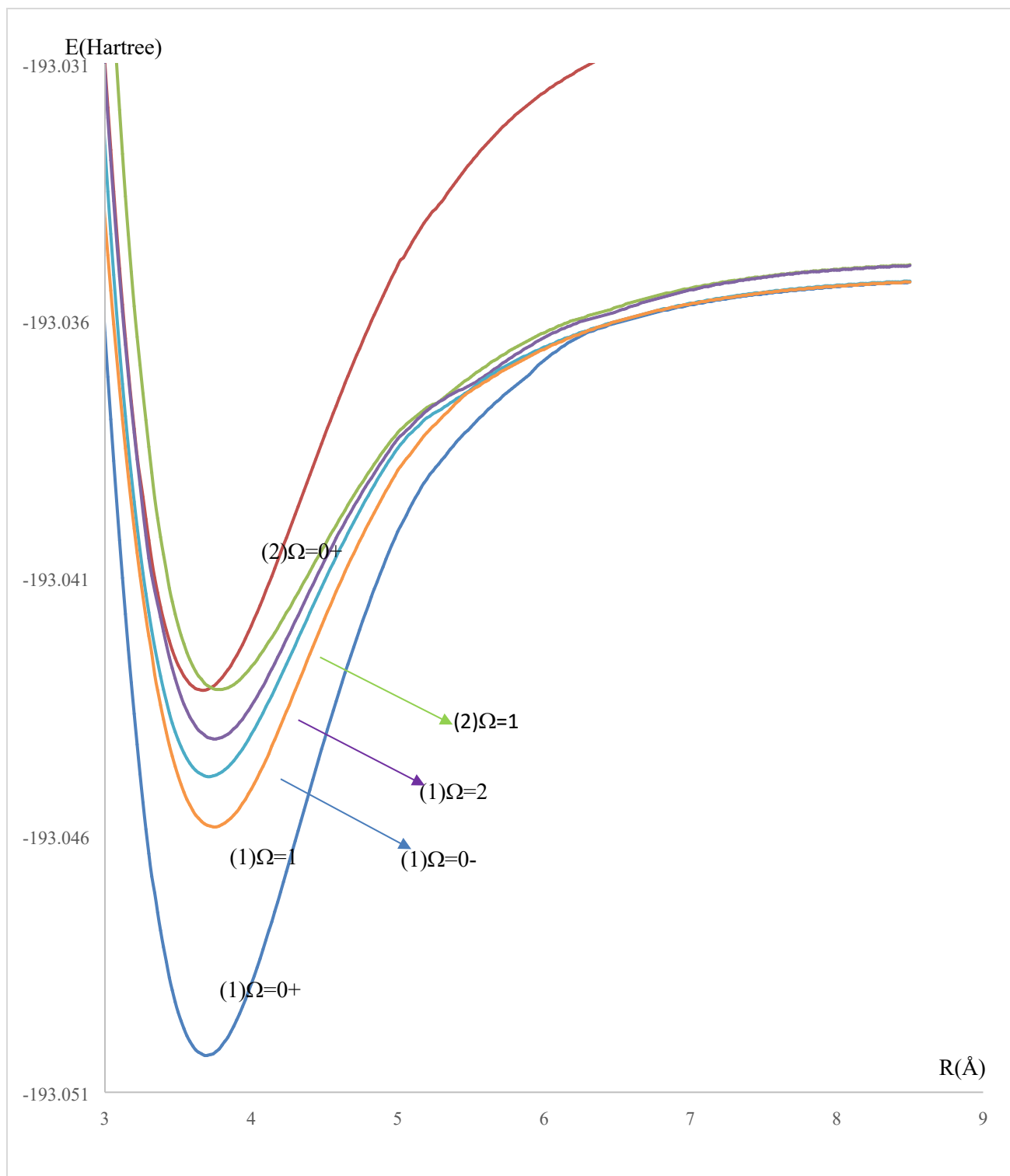


Fig. FS5: potential energy curves of the  $\Omega$  states  $(1)0^+$ ,  $(1)1$ ,  $(1)2$ ,  $(1)0^-$ ,  $(2)1$ ,  $(2)0^+$ .

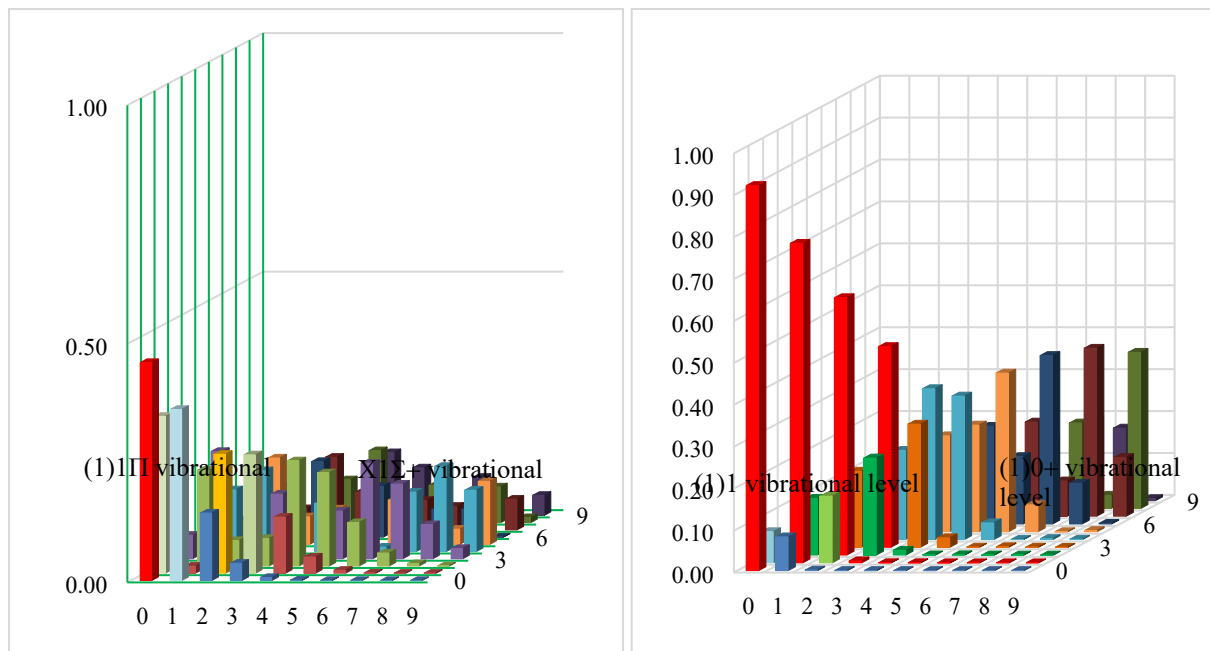


Fig. FS6: The FCF plotting of the considered transitions LaNa  $X^1\Sigma^+ - (1)^1\Pi$  and  $(1)0^+ - (1)1$  of LaNa molecule.

Table TS1: Positions of the avoided crossings  $R_{AC}$  of  $\Omega$  states of LaNa molecule.

$\Omega$	$(n+1) \Omega / n\Omega$	$R_{AC}$ (Å)
$0^+$	4/2	2.76
	5/4	2.80
		4.80
	5/3	4.96
1	3/2	2.72
	5/4	2.76
		3.22
		3.42
	7/5	2.82
	7/6	5.66
	8/6	2.88
	8/7	4.94
2	4/3	3.08
		3.22
	5/3	2.82
	6/4	2.90
	6/5	2.88
		4.70
	7/6	5.00
	6/5	5.66
3	2/1	2.80
	3/2	2.90
		5.60

Table TS2: The radiative lifetimes  $\tau$  and vibrational branching ratio of the spin orbit vibrational Transitions of the molecule LaNa:

LaNa _ spin orbit transition (1) $\Omega=1 \rightarrow$ (2) $\Omega=0^+$								
		$v'((2)\Omega=0^+)=0$	1	2	3	4	5	6
$v((1)\Omega=1)=0$	Av $v'$	464.4728036	118.0982974	5.73743034	0.000949279	0.004402833	2.5096E-05	2.95825E-06
	Rv $v'$	0.88220504	0.22571986	0.01110528	0.00000187	0.00000895	0.00000006	0.00000001
$v=1$	Av $v'$	57.74968714	305.2267057	192.4783961	13.92589029	6.1581E-05	0.021134957	9.0847E-05
	Rv $v'$	0.10968794	0.58337615	0.37255815	0.02745865	0.00000013	0.00004764	0.00000027
$v=2$	Av $v'$	4.100764067	89.28948863	196.8944367	236.9272309	22.30575356	0.006917491	0.064420502
	Rv $v'$	0.00778886	0.17065793	0.38110577	0.46716601	0.04534783	0.00001559	0.00019465
$v=3$	Av $v'$	0.16564654	10.02315561	103.9830484	124.210911	260.8337352	29.12700876	0.070412219
	Rv $v'$	0.00031462	0.01915714	0.20126795	0.24491535	0.53027770	0.06565237	0.00021275
$v=4$	Av $v'$	0.001373222	0.561676381	16.3356809	107.787844	76.38222935	270.9716667	33.77570996
	Rv $v'$	0.00000261	0.00107353	0.03161909	0.21253284	0.15528587	0.61077103	0.10205250
$v=5$	Av $v'$	0.000303561	0.00663598	1.191106438	22.24593139	104.7056944	45.01959597	272.7386862
	Rv $v'$	0.00000058	0.00001268	0.00230549	0.04386386	0.21286777	0.10147432	0.82407345
$v=6$	Av $v'$	0.000181489	0.001421326	0.019775379	2.05978389	27.64951916	98.50872688	24.31472551
	Rv $v'$	0.00000034	0.00000272	0.00003828	0.00406142	0.05621176	0.22203899	0.07346636
Sum( $s^{-1}$ ) = $A_{v'v}$		526.4907596	523.207381	516.6398742	507.1585407	491.8813961	443.6550759	330.9640482
$\tau:(s) = 1/A_{v'v}$		0.001899369	0.001911288	0.001935584	0.00197177	0.00203301	0.002254003	0.003021476
LaNa _ spin orbit transition (1) $\Omega=2 \rightarrow$ (2) $\Omega=0^+$								
		$v'((2)\Omega=0^+)=0$	1	2	3	4	5	6
$v((1)\Omega=2)=0$	Av $v'$	711.6676537	169.0936721	7.065103303	0.000262996	0.005699466	7.01134E-07	3.08787E-06
	Rv $v'$	0.83006417	0.21250722	0.00960745	0.00000039	0.00000944	0.00000000	0.00000001
$v=1$	Av $v'$	133.8450155	392.9475154	256.588478	16.94731597	0.004296194	0.027068581	0.000108473
	Rv $v'$	0.15611213	0.49383388	0.34892062	0.02503748	0.00000712	0.00006271	0.00000042
$v=2$	Av $v'$	11.42133696	201.7680194	191.4588327	288.3545279	26.93243232	0.027800967	0.082393599
	Rv $v'$	0.01332145	0.25357047	0.26035438	0.42600673	0.04460578	0.00006441	0.00032014
$v=3$	Av $v'$	0.424880082	30.03701751	223.2527773	74.2413107	282.4601013	35.17756357	0.11393255
	Rv $v'$	0.00049557	0.03774880	0.30358922	0.10968199	0.46781345	0.08149930	0.00044268
$v=4$	Av $v'$	8.94124E-05	1.836743882	52.10615241	213.1380823	16.77150577	251.9570139	40.89899661
	Rv $v'$	0.00000010	0.00230831	0.07085630	0.31488411	0.02777715	0.58373348	0.15891078
$v=5$	Av $v'$	0.004172899	0.008873234	4.833325622	74.32605736	183.4310321	0.066893112	208.2669985
	Rv $v'$	0.00000487	0.00001115	0.00657257	0.10980719	0.30380044	0.00015498	0.80920987



$v = 6$	Av v'	0.001470776	0.016041932	0.073135682	9.870310966	94.18283397	144.373887	8.00837435
	Rv v'	0.00000172	0.00002016	0.00009945	0.01458212	0.15598662	0.33448512	0.03111609
Sum( $s^{-1}$ ) = $A_{v,v}$		857.3646193	795.7078835	735.3778051	676.8778682	603.7879011	431.6302278	257.3708072
$\tau:(s) = 1/A_{v,v}$		0.001166365	0.001256743	0.001359845	0.001477371	0.001656211	0.002316798	0.003885445

LaNa \_ spin orbit transition (1) $\Omega=0 \rightarrow$  (2) $\Omega=1$

		$v'((2)\Omega=1) = 0$	1	2	3	4	5	6
$v((1)\Omega=0) = 0$	Av v'	2.375276154	0.781117331	0.189755	0.044409856	0.010457442	0.002512119	0.000618588
	Rv v'	0.96039894	0.30306163	0.07102404	0.01621829	0.00373401	0.00088492	0.00023898
$v = 1$	Av v'	0.097398916	1.61284771	1.230303	0.474880297	0.153142054	0.045982283	0.013602742
	Rv v'	0.03938145	0.62576034	0.46049427	0.17342430	0.05468205	0.01619768	0.00525509
$v = 2$	Av v'	0.000532904	0.181657587	1.001016	1.386694178	0.766758001	0.321328191	0.118943149
	Rv v'	0.00021547	0.07048038	0.37467366	0.50641492	0.27378436	0.11319079	0.04595083
$v = 3$	Av v'	1.01E-05	0.001759468	0.246785	0.538341678	1.326058634	0.996649542	0.515319961
	Rv v'	0.00000410	0.00068265	0.09236999	0.19660013	0.47349243	0.35107890	0.19908149
$v = 4$	Av v'	9.47E-08	3.82E-05	0.003752	0.287230417	0.232271005	1.107180662	1.116777951
	Rv v'	0.00000004	0.00001481	0.00140435	0.10489535	0.08293643	0.39001449	0.43144033
$v = 5$	Av v'	9.25E-11	4.91E-07	9.01E-05	0.006518865	0.301860042	0.065826946	0.820065232
	Rv v'	0.00000000	0.00000019	0.00003372	0.00238066	0.10778441	0.02318814	0.31681250
$v = 6$	Av v'	7.84E-12	1.10E-09	1.24E-06	0.000181641	0.010043789	0.299339539	0.003159977
	Rv v'	0.00000000	0.00000000	0.00000046	0.00006633	0.00358631	0.10544508	0.00122078
Sum( $s^{-1}$ ) = $A_{v,v}$		2.473218217	2.57742077	2.671701	2.738256934	2.800590967	2.838819282	2.588487599
$\tau:(s) = 1/A_{v,v}$		0.404331487	0.387984768	0.374293	0.365195825	0.357067495	0.352259126	0.386325977

LaNa \_ spin orbit transition (1) $\Omega=1 \rightarrow$  (2) $\Omega=1$

		$v'((2)\Omega=1)=0$	1	2	3	4	5	6
$v(1)\Omega=1)=0$	Av v'	0.000501103	1.86717E-05	6.40436E-08	3.42175E-07	1.41852E-07	7.20429E-10	4.68134E-08
	Rv v'	0.72493305	0.01392082	0.00002627	0.00008117	0.00002370	0.00000014	0.00004598
$v = 1$	Av v'	0.000161962	0.000734954	2.43243E-05	7.72584E-07	2.01735E-07	3.25454E-07	2.51649E-07
	Rv v'	0.23430657	0.54795118	0.00997716	0.00018326	0.00003371	0.00006445	0.00024718
$v = 2$	Av v'	2.59536E-05	0.000454497	0.000993891	2.23175E-05	2.08368E-06	5.23986E-07	4.47995E-09
	Rv v'	0.03754638	0.33885419	0.40766614	0.00529386	0.00034817	0.00010376	0.00000440
$v = 3$	Av v'	2.03075E-06	0.000114347	0.000973598	0.0012884	9.4765E-06	1.0936E-05	2.93426E-06
	Rv v'	0.00293784	0.08525242	0.39934231	0.30561645	0.00158348	0.00216552	0.00288213
$v = 4$	Av v'	1.49673E-07	1.65139E-05	0.000363735	0.001816568	0.001456297	3.16861E-06	3.78145E-05
	Rv v'	0.00021653	0.01231205	0.14919365	0.43090130	0.24334078	0.00062744	0.03714272
$v = 5$	Av v'	3.87183E-08	2.09167E-06	7.4026E-05	0.000887415	0.002844737	0.001311257	8.39832E-05
	Rv v'	0.00005601	0.00155946	0.03036339	0.21050039	0.47534292	0.25965159	0.08249119
$v = 6$	Av v'	2.50314E-09	2.01044E-07	8.36497E-06	0.000199926	0.001671661	0.003723852	0.000893052
	Rv v'	0.00000362	0.00014989	0.00343107	0.04742358	0.27932723	0.73738711	0.87718640
Sum( $s^{-1}$ ) = $A_{v,v}$		0.00069124	0.001341276	0.002438003	0.00421574	0.005984599	0.005050064	0.001018087

$\tau:(s) = 1/A_{v'v}$		1446.6758	745.5584357	410.1717007	237.2062613	167.0955868	198.0172906	982.2347464
<b>LaNa _ spin orbit transition (1)<math>\Omega=2 \rightarrow</math> (2)<math>\Omega=1</math></b>								
		$v((2)\Omega=1)=0$	1	2	3	4	5	6
$v((1)\Omega=2)=0$	Av v'	125.5427814	7.54785346	0.051166867	0.00732867	0.001800919	2.9353E-05	2.18865E-05
	Rv v'	0.98604202	0.06681109	0.00051217	0.00008270	0.00002271	0.00000041	0.00000040
v = 1	Av v'	1.721800856	101.7020502	16.00483102	0.37411557	0.008035339	0.007270752	0.000546636
	Rv v'	0.01352342	0.90023280	0.16020461	0.00422188	0.00010132	0.00010190	0.00000988
v = 2	Av v'	0.054915932	3.574036428	78.23537515	24.4451134	1.306054687	8.07613E-05	0.011328581
	Rv v'	0.00043132	0.03163618	0.78311779	0.27586190	0.01646921	0.00000113	0.00020470
v = 3	Av v'	0.000391417	0.148633024	5.338364122	56.5466222	31.55646188	3.21268159	0.027280339
	Rv v'	0.00000307	0.00131565	0.05343578	0.63812585	0.39792359	0.04502690	0.00049294
v = 4	Av v'	6.58094E-06	0.000412186	0.272667057	6.82149296	37.8815313	35.65638805	6.379526728
	Rv v'	0.00000005	0.00000365	0.00272933	0.07698021	0.47768204	0.49973721	0.11527528
v = 5	Av v'	1.18238E-05	2.94618E-05	2.32146E-05	0.41867253	7.982794274	23.58327578	36.02367923
	Rv v'	0.00000009	0.00000026	0.00000023	0.00472470	0.10066218	0.33052816	0.65093226
v = 6	Av v'	2.33354E-06	4.13972E-05	8.77161E-06	0.00024413	0.566139158	8.890550558	12.89928795
	Rv v'	0.00000002	0.00000037	0.00000009	0.00000275	0.00713895	0.12460429	0.23308454
Sum( $s^{-1}$ ) = $A_{v'v}$		127.3199103	112.9730561	99.9024362	88.6135894	79.30281756	71.35027684	55.34167135
$\tau:(s) = 1/A_{v'v}$		0.007854231	0.008851668	0.010009766	0.01128495	0.012609892	0.014015363	0.018069566

Table TS3: Variation of the laser slowing distance (L) in function of the number of the lasers needed (Laser  $N^\circ$ ), the number of cycles (N) for photon absorption/emission and the total decay channels involved ( $\eta$ ) for cooling LaNa molecular beam for the transitions (1) $\Omega=0^+$  - (2) $\Omega=1$  and (1) $\Omega=0^+$  - (2) $\Omega=1b$ .

<b>Transition (1)<math>\Omega=0^+</math> - (2)<math>\Omega=1</math></b>				
	Lasers $N^\circ$	N	Total decay channels involved ( $\eta$ )	L
a	4	687.66	$(R_{00}+R_{01})+(R_{02}+R_{03})(R_{10}+R_{11}+R_{12}+R_{13})$	8.75 cm
b	4	1617.24	$(R_{00}+R_{01}+R_{02})+(R_{03})(R_{10}+R_{11}+R_{12}+R_{13})$	48.40 cm
c	4	1956.72	$R_{00}+R_{01}+R_{02}+R_{03}$	70.80 cm
d	3	191.16	$R_{00}+R_{01}+R_{02}$	0.68 cm
e	3	164.82	$(R_{00}+R_{01})+(R_{02})(R_{10}+R_{11}+R_{12}+R_{14})$	0.50 cm
f	4	37.20	$(R_{00}+R_{02})+(R_{01}+R_{04})(R_{10}+R_{11}+R_{12}+R_{14})$	0.03 cm
<b>Transition (1)<math>\Omega=0^+</math> - (2)<math>\Omega=0^+</math></b>				
a	4	142005.4	$(R_{00}+R_{01})+(R_{02}+R_{03})(R_{10}+R_{11}+R_{12}+R_{13})$	4320 m
b	4	142712.4	$(R_{00}+R_{01}+R_{02})+(R_{03})(R_{10}+R_{11}+R_{12}+R_{13})$	4740 m
c	3	627.9	$(R_{01})(R_{10}+R_{11}+R_{12})$	8.46 cm

d	3	13504.5	$R_{00}+R_{01}+R_{02}$	39.10 m
e	4	4587.6	$(R_{02}+R_{03})+(R_{00}+R_{01})(R_{20}+R_{21}+R_{22}+R_{23})$	4.51 m
f	2	634.7	$R_{00}+R_{01}$	8.64 cm

Table TS4: The vibrational energy  $E_v$ , the rotational constant  $B_v$ , the centrifugal distortion constant  $D_v$ , and the abscissas of the turning points  $R_{\min}$  and  $R_{\max}$  for the vibrational levels of the  $(1)0^+$  and  $(1)1$  states of LaNa molecule.

(1) $0^+$					
$v$	$E_v$ ( $\text{cm}^{-1}$ )	$B_v \times 10^2$ ( $\text{cm}^{-1}$ )	$D_v \times 10^8$ ( $\text{cm}^{-1}$ )	$R_{\min}$ ( $\text{\AA}$ )	$R_{\max}$ ( $\text{\AA}$ )
0	59.66	6.2414	6.8980	3.581	3.820
1	177.94	6.2023	7.0014	3.503	3.921
2	294.73	6.1614	7.0831	3.453	3.995
3	410.06	6.1185	7.2142	3.416	4.058
4	523.83	6.0750	7.5318	3.383	4.116
5	635.74	6.0336	8.0342	3.354	4.171
6	745.51	5.9962	8.4090	3.325	4.223
7	853.19	5.9596	8.4146	3.301	4.272
8	959.02	5.9150	8.2052	3.281	4.320
9	1063.14	5.8610	7.8603	3.263	4.368
10	1165.76	9.0835	0.3771	3.245	4.415
11	1266.83	8.9436	3.9880	3.229	4.462
12	1366.01	9.0685	2.3300	3.214	4.509
(1) 1					
$v$	$E_v$ ( $\text{cm}^{-1}$ )	$B_v \times 10^2$ ( $\text{cm}^{-1}$ )	$D_v \times 10^8$ ( $\text{cm}^{-1}$ )	$R_{\min}$ ( $\text{\AA}$ )	$R_{\max}$ ( $\text{\AA}$ )
0	50.72	6.0739	8.8323	3.621	3.881
1	151.02	6.0314	9.1028	3.538	3.991
2	249.60	5.9879	9.3393	3.484	4.073
3	346.52	5.9440	9.5461	3.441	4.142
4	441.85	5.8979	9.9958	3.406	4.207
5	535.26	5.8438	10.664	3.375	4.270
6	626.37	5.7866	10.575	3.347	4.329
7	715.63	5.7338	10.77	3.326	4.387
8	803.07	5.6726	11.644	3.303	4.444
9	888.33	9.0138	4.0396	3.282	4.501
10	971.61	9.0031	12.227	3.262	4.558
11	1052.52	9.1270	8.8831	3.244	4.615
12	1131.19	9.2530	5.9979	3.227	4.673

Table TS5: The values of the vibrational energy  $E_v$ , the rotational constants  $B_v$ , the centrifugal distortion constant  $D_v$  and the abscissas of the turning points for the different vibrational levels of the ground state  $X^1\Sigma^+$  of LaNa molecule.

$X^1\Sigma^+$					
$v$	$E_v$ ( $\text{cm}^{-1}$ )	$B_v \times 10^2$ ( $\text{cm}^{-1}$ )	$D_v \times 10^8$ ( $\text{cm}^{-1}$ )	$R_{\min}$ ( $\text{\AA}$ )	$R_{\max}$ ( $\text{\AA}$ )
0	61.21	6.2069	6.4397	3.592	3.829
1	182.58	6.1668	6.4996	3.516	3.928
2	302.56	6.1247	6.5208	3.467	4.002
3	421.21	6.0800	6.5412	3.430	4.065
4	538.48	6.0327	6.6821	3.399	4.122
5	654.14	5.9857	6.9615	3.372	4.176
6	880.06	5.9052	7.4314	3.325	4.277
7	990.31	5.8617	7.5525	3.304	4.324
8	1098.64	5.8116	7.1697	3.286	4.371
9	1205.44	5.7617	7.2954	3.269	4.417
10	1310.64	8.8995	5.4798	3.253	4.462
11	1413.92	9.0230	2.9575	3.238	4.508
12	1515.33	9.1473	1.4658	3.224	4.553
13	1614.74	9.1411	3.6411	3.210	4.599
14	1712.41	9.1301	8.4827	3.198	4.644
15	1808.14	9.2631	3.7194	3.186	4.691
16	1901.96	9.2525	8.2586	3.175	4.737
17	1993.67	9.3888	3.2678	3.165	4.784
18	2083.41	9.3799	6.8476	3.155	4.832
19	2171.22	9.6563	0.3755	3.145	4.880
20	2257.15	9.5115	4.8394	3.136	4.928
21	2341.13	9.6507	1.5577	3.128	4.978

Table TS6: The values of the vibrational energies  $E_v$ , the rotational constants  $B_v$ , the centrifugal distortion constant  $D_v$  and the abscissas of the turning points for the different vibrational levels of states  $1^3\Pi$  and  $1^3\Delta$  of LaNa molecule.

$1^3\Pi$						$1^3\Delta$					
$v$	$E_v$ ( $\text{cm}^{-1}$ )	$B_v \times 10^2$ ( $\text{cm}^{-1}$ )	$D_v \times 10^8$ ( $\text{cm}^{-1}$ )	$R_{\min}$ ( $\text{\AA}$ )	$R_{\max}$ ( $\text{\AA}$ )	$v$	$E_v$ ( $\text{cm}^{-1}$ )	$B_v \times 10^2$ ( $\text{cm}^{-1}$ )	$D_v \times 10^8$ ( $\text{cm}^{-1}$ )	$R_{\min}$ ( $\text{\AA}$ )	$R_{\max}$ ( $\text{\AA}$ )
0	51.65	6.3049	9.5191	3.553	3.810	0	51.63	5.9058	7.8393	3.675	3.932
1	153.71	6.2503	9.7184	3.472	3.921	1	153.55	5.8532	8.0253	3.594	4.044
2	253.98	6.1941	9.9491	3.420	4.004	2	253.57	5.7992	8.2162	3.543	4.128
3	352.40	6.1364	10.2140	3.380	4.077	3	351.67	5.7425	8.5601	3.503	4.201
4	448.91	6.0770	10.4994	3.347	4.143	4	447.50	5.6783	9.0795	3.470	4.273
5	543.46	6.0156	10.8021	3.318	4.206	5	540.67	5.6117	8.8997	3.442	4.336
6	635.97	5.9506	11.1666	3.293	4.268	6	631.89	5.5545	8.6672	3.420	4.398
7	726.35	8.8266	10.2902	3.271	4.327	7	721.54	5.4909	9.7691	3.397	4.459
8	814.72	8.9480	7.6832	3.250	4.385	8	808.74	8.2881	3.5867	3.377	4.520
9	901.34	9.0721	5.1857	3.232	4.443	9	893.67	8.3973	2.3550	3.359	4.580
10	985.94	9.1981	3.2378	3.215	4.500	10	976.32	8.3865	6.0096	3.342	4.641
11	1068.37	9.3259	1.8101	3.199	4.558	11	1056.33	8.6212	0.7884	3.327	4.702
12	1148.89	9.3183	4.2766	3.185	4.616	12	1133.99	8.4874	7.8922	3.313	4.764
13	1227.23	9.3045	9.3157	3.171	4.674	13	1209.05	8.7324	0.8669	3.299	4.827
14	1303.56	9.4425	4.5324	3.159	4.733	14	1281.92	8.5933	7.9112	3.288	4.891
15	1377.72	9.4283	9.0224	3.147	4.793	15	1352.42	8.7195	3.5062	3.276	4.955
16	1449.82	9.5715	3.8673	3.136	4.854	16	1420.26	8.7054	6.4842	3.266	5.020
17	1519.68	9.5586	7.0372	3.126	4.915	17	1484.73	8.8352	2.6503	3.256	5.103
18	1587.18	9.7050	2.7379	3.116	4.979	18	1545.54	8.8238	3.7210	3.247	5.176
19	1651.53	9.6945	4.8794	3.107	5.063	19	1604.11	8.9554	1.1582	3.239	5.263
20	1711.77	9.8426	1.6339	3.099	5.136	20	1659.65	8.9471	1.6662	3.231	5.348

Table TS7: The values of the vibrational energies  $E_v$ , the rotational constants  $B_v$ , the centrifugal distortion constant  $D_v$ , and the abscissas of the turning points for the different vibrational levels of states  $(1)^1\Pi$  and  $1^3\Sigma^+$  of LaNa molecule.

$1^1\Pi$						$1^3\Sigma^+$					
$v$	$E_v$ ( $\text{cm}^{-1}$ )	$B_v \times 10^2$ ( $\text{cm}^{-1}$ )	$D_v \times 10^7$ ( $\text{cm}^{-1}$ )	$R_{\min}$ ( $\text{\AA}$ )	$R_{\max}$ ( $\text{\AA}$ )	$v$	$E_v$ ( $\text{cm}^{-1}$ )	$B_v \times 10^2$ ( $\text{cm}^{-1}$ )	$D_v \times 10^7$ ( $\text{cm}^{-1}$ )	$R_{\min}$ ( $\text{\AA}$ )	$R_{\max}$ ( $\text{\AA}$ )
0	41.24	5.6963	1.1125	3.727	4.016	0	42.51	5.5941	0.9920	3.765	4.049
1	122.03	5.6219	1.1655	3.641	4.147	1	125.74	5.5201	1.0434	3.680	4.178
2	200.30	5.5429	1.2299	3.587	4.249	2	206.23	5.4380	1.1317	3.627	4.283
3	275.93	5.4608	1.2557	3.546	4.340	3	283.46	5.3529	1.1188	3.587	4.372
4	349.33	5.3872	1.2111	3.512	4.422	4	358.50	5.2808	1.1483	3.555	4.456
5	421.19	5.3120	1.3419	3.483	4.502	5	431.36	5.1915	1.2841	3.527	4.537
6	490.72	5.2247	1.3201	3.458	4.579	6	501.35	5.1070	1.2379	3.503	4.617
7	558.30	8.2552	1.7793	3.436	4.655	7	634.07	7.8733	1.4184	3.463	4.777
8	623.81	8.2383	5.0863	3.419	4.731	8	696.60	7.9781	0.9503	3.445	4.859
9	687.35	8.3519	3.5208	3.401	4.806	9	756.30	7.9632	2.1506	3.432	4.943
10	748.76	8.4663	2.2306	3.384	4.882	10	812.63	8.1903	0.3318	3.422	5.047
11	807.93	8.4513	5.5064	3.368	4.959	11	864.42	8.0575	3.1154	3.411	5.146
12	863.68	8.5716	3.5941	3.355	5.066	12	911.23	8.2945	0.3915	3.399	5.278
13	914.69	8.5543	8.8443	3.342	5.155	13	954.44	8.1620	3.2518	3.390	5.390
14	961.80	8.5271	17.1513	3.332	5.274	14	995.02	8.2842	1.2656	3.381	5.496
15	1006.13	8.8062	2.2396	3.322	5.384	15	1034.94	8.3994	0.5465	3.373	5.612
16	1046.20	8.6466	17.5346	3.313	5.498	16	1071.31	8.2604	3.8826	3.366	5.731
17	1086.03	8.7907	7.7900	3.305	5.606	17	1106.10	8.2396	6.6185	3.359	5.857

Table TS8: The values of the vibrational energies  $E_v$ , the rotational constants  $B_v$ , the centrifugal distortion constant  $D_v$  and the abscissas of the turning points for the different vibrational levels of state  $1^1\Delta$  of LaNa molecule.

$1^1\Delta$					
$v$	$E_v$ ( $\text{cm}^{-1}$ )	$B_v \times 10^2$ ( $\text{cm}^{-1}$ )	$D_v \times 10^7$ ( $\text{cm}^{-1}$ )	$R_{\min}$ ( $\text{\AA}$ )	$R_{\max}$ ( $\text{\AA}$ )
0	38.32	5.3390	1.0811	3.849	4.148
1	112.38	5.2457	1.1756	3.762	4.296
2	183.04	5.1602	1.1117	3.709	4.402
3	252.38	5.0892	1.2168	3.668	4.499
4	383.55	4.9102	1.3402	3.607	4.680
5	445.32	4.8085	1.3957	3.583	4.770
6	504.67	7.5427	4.9939	3.561	4.857
7	561.40	7.6433	3.6974	3.542	4.943
8	615.19	7.7445	2.6838	3.526	5.010
9	664.14	7.7289	6.6058	3.511	5.156
10	709.81	7.8385	3.4401	3.499	5.270
11	754.19	7.8243	7.5333	3.487	5.377