From Adiabatic to Diabatic Representation: An ab initio Investigation of the LiS Molecule

Sana Akkari,[1] Wissem Zrafi,[1,2,*] Mohamed Bejaoui,[1,3] Hela Ladjimi,[1,4]
Jamila Dhiflaoui,[1,3] Józef E. Sienkiewicz,[5] and Hamid Berriche[1,6,†]

[1]*University of Monastir, Faculty of Science of Monastir, Laboratory of Interfaces and Advanced Materials LR11ES55, Physics Department, 5019 Monastir, Tunisia*
[2]*University of Sousse, Electronic Department, Higher Institute of Applied Sciences and Technology of Sousse, 4003 Sousse, Tunisia*
[3]*University of Monastir, Preparatory Institute for Engineering Studies of Monastir, Physics Department, Rue Ibn Eljazzar – 5019 Monastir, Tunisie*
[4]*Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland*
[5]*Gdańsk University of Technology, Faculty of Applied Physics and Mathematics, Narutowicza 11/12, 80-233 Gdańsk, Poland*
[6]*Mathematics and Physics Department, School of Arts and Sciences, American University of Ras Al Khaimah, Ras Al-Khaimah, UAE*

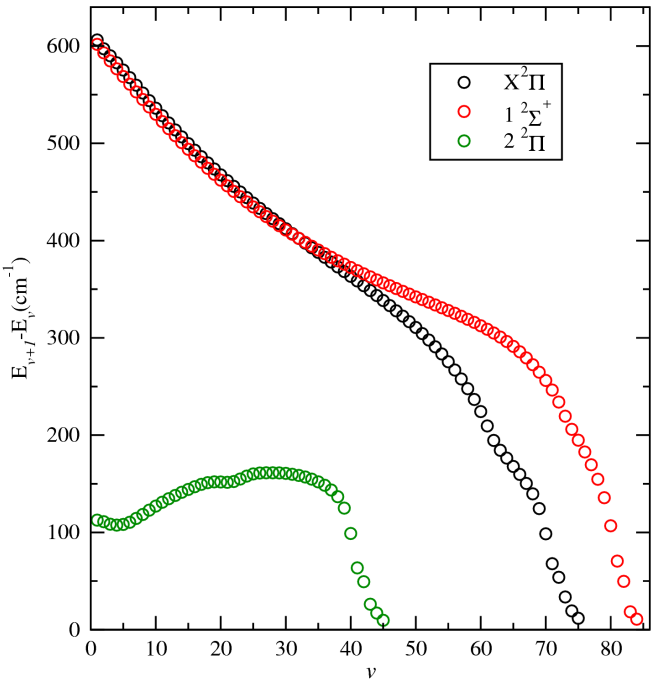

FIG. 1. Vibrational energy levels of LiS.

* wissem.zrafi@issatso.u-sousse.tn

† hamid.berriche@aurak.ac.ae

TABLE I. Vibrational energy levels for the $X^2\Pi$, $A^2\Sigma^+$ and $2^2\Pi$ electronic states of LiS.

v	E($X^2\Pi$)	$\Delta E(X^2\Pi)$	E($A^2\Sigma^+$)	$\Delta E(A^2\Sigma^+)$	E($2^2\Pi$)	$\Delta E(2^2\Pi)$
0	-26730.9		-30456.8		-5770.6	
1	-26124.6	606.3	-29855.1	601.7	-5657.9	112.7
2	-25527.4	597.2	-29262.1	593.0	-5547.0	110.9
3	-24937.4	589.9	-28677.3	584.8	-5438.6	108.4
4	-24354.7	582.8	-28100.7	576.6	-5331.1	107.5
5	-23779.3	575.3	-27532.1	568.6	-5222.9	108.2
6	-23211.8	567.5	-26971.4	560.7	-5112.5	110.4
7	-22652.2	559.6	-26418.5	552.8	-4998.1	114.4
8	-22100.5	551.7	-25873.5	545.0	-4879.6	118.5
9	-21556.6	543.9	-25336.1	537.4	-4756.7	122.9
10	-21020.5	536.1	-24806.3	529.8	-4629.6	127.0
11	-20492.0	528.4	-24283.9	522.3	-4498.7	130.9
12	-19971.0	521.0	-23768.9	515.0	-4364.0	134.7
13	-19457.3	513.7	-23261.1	507.8	-4225.9	138.0
14	-18950.7	506.6	-22760.4	500.8	-4084.7	141.2
15	-18451.0	499.7	-22266.5	493.9	-3940.6	144.2
16	-17958.1	492.9	-21779.3	487.2	-3793.6	146.9
17	-17471.7	486.3	-21298.7	480.6	-3644.2	149.4
18	-16991.9	479.9	-20824.4	474.3	-3493.0	151.2
19	-16518.3	473.6	-20356.3	468.1	-3341.0	152.0
20	-16050.7	467.5	-19894.2	462.1	-3189.2	151.9
21	-15589.1	461.6	-19437.9	456.3	-3037.7	151.5
22	-15133.4	455.7	-18987.4	450.6	-2885.3	152.3
23	-14683.5	449.9	-18542.2	445.1	-2730.4	154.9
24	-14239.3	444.2	-18102.5	439.8	-2572.5	157.9
25	-13800.7	438.5	-17667.9	434.6	-2412.4	160.1
26	-13367.7	433.1	-17238.3	429.6	-2251.3	161.1
27	-12939.9	427.7	-16813.7	424.7	-2090.1	161.3
28	-12517.4	422.5	-16393.7	419.9	-1928.7	161.3
29	-12100.0	417.3	-15978.3	415.4	-1767.5	161.2
30	-11687.8	412.2	-15567.4	410.9	-1606.8	160.7
31	-11280.7	407.1	-15160.9	406.5	-1447.0	159.8
32	-10878.5	402.2	-14758.6	402.3	-1288.4	158.6
33	-10481.0	397.4	-14360.4	398.2	-1131.5	156.9
34	-10088.4	392.6	-13966.2	394.2	-976.7	154.8
35	-9700.6	387.8	-13575.9	390.3	-824.7	152.0
36	-9317.7	382.9	-13189.3	386.5	-676.2	148.5
37	-8939.8	377.9	-12806.5	382.8	-532.6	143.6
38	-8566.8	372.9	-12427.3	379.2	-395.9	136.7
39	-8198.7	368.1	-12051.5	375.8	-270.9	124.9
40	-7835.3	363.3	-11679.1	372.4	-171.9	98.9
41	-7476.8	358.5	-11310.1	369.0	-108.4	63.5
42	-7123.3	353.6	-10944.3	365.8	-59.0	49.4
43	-6774.7	348.6	-10581.6	362.6	-32.9	26.2
44	-6431.1	343.5	-10222.1	359.5	-15.8	17.1
45	-6092.7	338.4	-9865.5	356.5	-6.2	9.6
46	-5759.5	333.2	-9511.9	353.6		
47	-5431.7	327.8	-9161.3	350.7		
48	-5109.3	322.3	-8813.5	347.8		
49	-4792.8	316.6	-8468.5	344.9		

TABLE II. Continued

v	E($X^2\Pi$)	$\Delta E(X^2\Pi)$	E($A^2\Sigma^+$)	$\Delta E(1^2\Sigma^+)$	E($2^2\Pi$)	$\Delta E(2^2\Pi)$
50	-4482.1	310.6	-8126.4	342.2		
51	-4177.7	304.4	-7786.9	339.4		
52	-3879.9	297.8	-7450.4	336.6		
53	-3589.1	290.8	-7116.6	333.8		
54	-3305.7	283.4	-6785.6	330.9		
55	-3030.2	275.5	-6457.5	328.1		
56	-2763.2	266.9	-6132.3	325.2		
57	-2505.5	257.7	-5810.1	322.2		
58	-2257.8	247.7	-5490.9	319.1		
59	-2021.1	236.7	-5175.1	315.9		
60	-1796.9	224.2	-4862.6	312.5		
61	-1587.5	209.4	-4553.7	308.9		
62	-1392.9	194.6	-4248.7	304.9		
63	-1208.4	184.4	-3947.9	300.8		
64	-1032.1	176.4	-3651.7	296.3		
65	-864.3	167.8	-3360.4	291.3		
66	-704.7	159.6	-3074.7	285.7		
67	-554.4	150.3	-2795.3	279.4		
68	-414.8	139.6	-2522.9	272.4		
69	-290.3	124.5	-2258.2	264.7		
70	-191.8	98.5	-2001.9	256.2		
71	-123.9	67.8	-1755.6	246.4		
72	-70.1	53.8	-1521.6	233.9		
73	-36.5	33.6	-1302.2	219.4		
74	-17.2	19.3	-1096.2	206.0		
75	-5.5	11.7	-901.4	194.8		
76			-718.7	182.7		
77			-549.2	169.5		
78			-394.5	154.7		
79			-258.9	135.7		
80			-152.1	106.8		
81			-81.5	70.5		
82			-31.8	49.7		
83			-13.4	18.4		
84			-2.6	10.8		

TABLE III. Radiative lifetimes of the vibrational states (j=0) of $X^2\Pi$ of LiS molecule.

v	τ_v(s) ($X^2\Pi$)	τ_v(ms) ($A^2\Sigma$)	τ_v(ns) ($2^2\Pi$)
0	14.537	0.4817	74.552
1	0.7209	0.3336	70.314
2	0.3960	0.2560	65.933
3	0.2887	0.2043	62.059
4	0.2314	0.1688	58.662
5	0.1944	0.1434	56.136
6	0.1694	0.1245	54.510
7	0.1508	0.1101	53.362
8	0.1365	0.0987	52.658
9	0.1253	0.0895	52.149
10	0.1164	0.0820	51.779
11	0.1090	0.0757	51.524
12	0.1028	0.0703	51.343
13	0.0973	0.0657	51.230
14	0.0924	0.0617	51.159
15	0.0880	0.0582	51.121
16	0.0839	0.0552	51.134
17	0.0799	0.0524	51.251
18	0.0762	0.0500	51.551
19	0.0726	0.0478	52.094
20	0.0690	0.0458	52.799
21	0.0655	0.0440	53.357
22	0.0620	0.0422	53.452
23	0.0587	0.0406	53.210
24	0.0555	0.0389	53.065
25	0.0524	0.0374	53.266
26	0.0495	0.0361	53.683
27	0.0466	0.0349	54.204
28	0.0439	0.0338	55.016
29	0.0415	0.0326	55.746
30	0.0392	0.0315	56.719
31	0.0371	0.0304	58.334
32	0.0351	0.0293	60.171
33	0.0333	0.0282	61.872
34	0.0316	0.0272	64.772
35	0.0301	0.0260	67.565
36	0.0287	0.0249	70.652
37	0.0275	0.0237	74.705
38	0.0263	0.0226	80.605
39	0.0253	0.0216	93.482
40	0.0243	0.0207	139.47
41	0.0234	0.0198	191.70
42	0.0226	0.0189	321.93
43	0.0218	0.0181	576.85
44	0.0211	0.0172	816.92
45	0.0205	0.0164	1191.2
46	0.0199	0.0156	
47	0.0193	0.0148	
48	0.0188	0.0141	
49	0.0184	0.0133	

TABLE IV. Continued

v	τ_v(s) ($X^2\Pi$)	τ_v(ms) ($A^2\Sigma$)	τ_v(s) ($2^2\Pi$)
50	0.0179	0.0126	
51	0.0176	0.0119	
52	0.0173	0.0112	
53	0.0170	0.0106	
54	0.0168	0.0099	
55	0.0167	0.0093	
56	0.0166	0.0087	
57	0.0167	0.0082	
58	0.0168	0.0077	
59	0.0171	0.0072	
60	0.0177	0.0067	
61	0.0185	0.0063	
62	0.0193	0.0059	
63	0.0197	0.0056	
64	0.0203	0.0052	
65	0.0209	0.0049	
66	0.0217	0.0047	
67	0.0229	0.0042	
68	0.0248	0.0039	
69	0.0285	0.0042	
70	0.0398	0.0045	
71	0.0534	0.0047	
72	0.0739	0.0059	
73	0.1309	0.0069	
74	0.1875	0.0079	
75	0.3884	0.0099	
		0.0121	
		0.0163	
		0.0223	
		0.0339	
		0.0734	
		0.1312	
		0.2419	
		0.8401	
		2.0052	

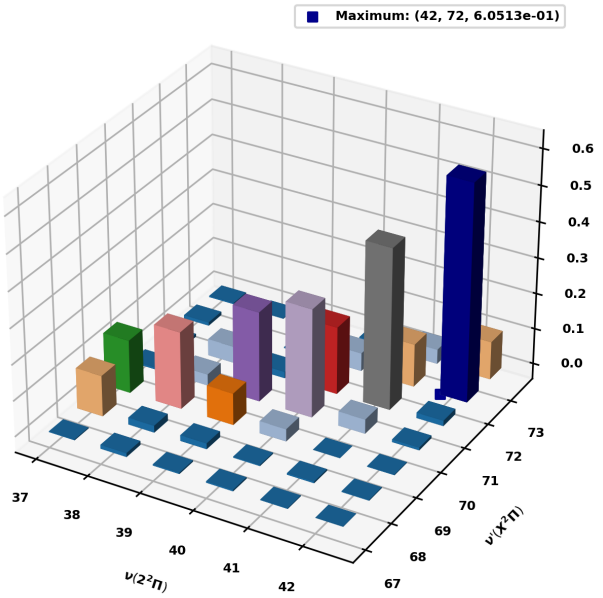

FIG. 2. Franck–Condon Factor diagram of the LiS $2^2\Pi \rightarrow X^2\Pi$ Vibrational Levels.

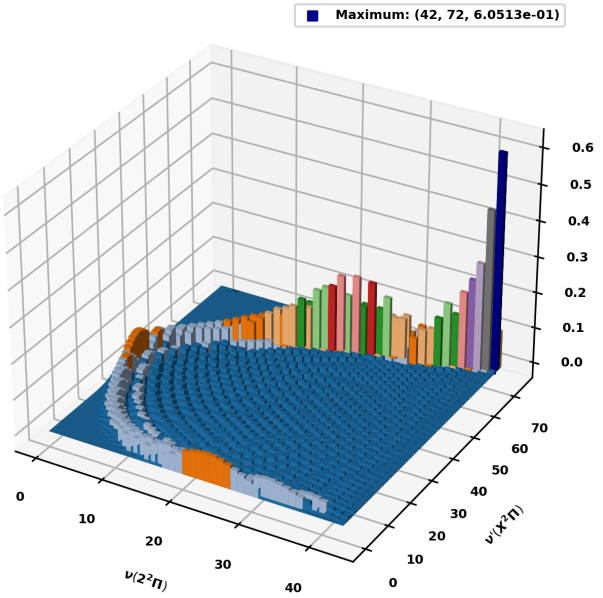

FIG. 3. 3D Visualization of Franck–Condon Factors for LiS $2^2\Pi \rightarrow X^2\Pi$ Vibrational Transitions

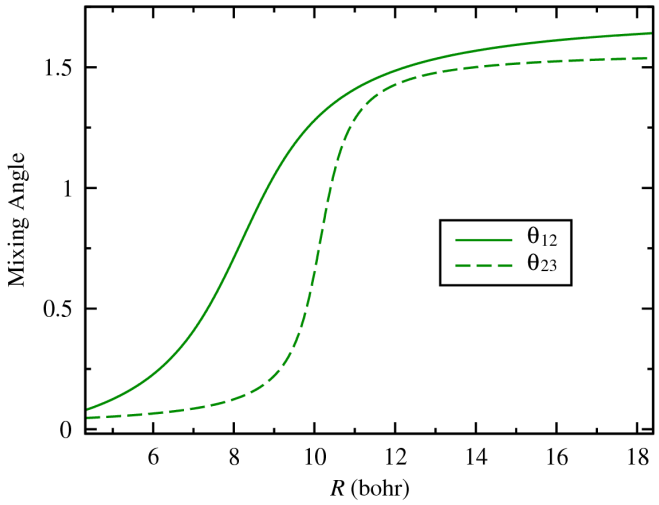

FIG. 4. Mixing Angle of LiS