类锂氯离子和钾离子软X射线激光光谱理论计算

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提 要

本文采用 Hartree-Fock 自洽场方法，从理论上计算了类锂氯离子和类锂钾离子可能实现软X射线激光的有关能级能量及跃迁谱线性质：跃迁波长、跃迁几率和振子强度。计算结果表明，类锂钾离子的部分跃迁非常有可能实现软X射线激光，并且其中有三条谱线的波长已进入水窗。

关键词： 类锂钾离子，类锂氯离子，软X射线激光，谱线特性。

一、引 言

在类锂离子复合泵浦机理下，已经在 LF 12# 激光装置上首次实现了以类锂硅离子为增益介质的软X射线自发辐射放大[1,2]，同时在理论上也对类锂硅离子的有关光谱特性作了比较全面的计算和讨论[3]。怎样使软X射线激光的波长更逼近“水窗”(43.8～23.3 Å)，成为很热门的课题。循着复合泵浦机理的线索，对比硅元素稍重的氯和钾元素作进一步探索，但是由于原子序数的提高，同样结构的类锂离子的相同跃迁，就会因跃迁能量的提高而具有较短的波长，从而为实现更短波长的软X射线激光提供可能性。

本文采用美国 Los Alamas 国家实验室 Cowan 博士提供的先进大型计算程序[4~6]，运用 Hartree-Fock 自洽场方法，对类锂氯、钾离子的离子结构和光谱进行了纯理论计算。由计算结果知道，$3p$、$3d$、$4p$、$4d$ 由于跃迁 $3p—2s$, $3d—2p$, $4p—3s$, $2s$, $4d—3p$, $2p$ 的跃迁几率较大，使它们较容易倒空，具有作为激光跃迁下能级的可能性。并给出了类锂氯离子和钾离子可能实现软X射线放大的跃迁的光谱性质：跃迁波长、跃迁几率和振子强度。这些数据对于作进一步的软X射线激光研究，具有重要的意义。

二、计 算 方 法

本文采用著名 Cowan 的计算程序包括三个部分：RCN 34，RCN 2 和 RCG 9。RCN 34 用自洽场方法，逐次迭代逼近求解 Hartree-Fock 方程，考虑了相对论修正和 Breit 修正，从而得出原子或离子状态下各电子轨道的径向波函数及积分参量；RCN 2 求解存在相互作

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用的组态之间的积分参量；RCG 9求解多组态的哈密顿矩阵，从而得出原子或离子组态的能级能量值，本征函数及振子强度。这三个程序相对独立运行，由数据的相互输送相联系。它们的流柱框图可以参见文献[6]。

三、计算结果与讨论

表 1 给出了类锂氯离子及钾离子有关能级的平均相对能量。由此可以估算出各能级之间跃迁波长的理论值。由于跃迁仅发生在宇称不同的组态间，故表 1 中把宇称相同的组态排列在一起。

Table 1　Average relative energy of Cl XV and K XVII. (Unit=1000 cm^{-1})

configuration				energy
CL	XV	1S2	2S	0.000
CL	XV	1S2	3S	3687.562
CL	XV	1S2	3D	3785.312
CL	XV	1S2	4D	4988.168
CL	XV	1S2	5D	5544.739
CL	XV	1S2	6D	5847.008
CL	XV	1S2	2P	255.583
CL	XV	1S2	3P	3758.371
CL	XV	1S2	4P	4976.822
CL	XV	1S2	4F	4989.692
CL	XV	1S2	5F	5545.480
CL	XV	1S2	6F	5847.430
K	XVII	1S2	2S	0.000
K	XVII	1S2	3S	4706.840
K	XVII	1S2	3D	4822.055
K	XVII	1S2	4D	6366.956
K	XVII	1S2	5D	7081.869
K	XVII	1S2	6D	7470.147
K	XVII	1S2	2P	297.229
K	XVII	1S2	3P	4789.411
K	XVII	1S2	4P	6353.212
K	XVII	1S2	4F	6368.923
K	XVII	1S2	5F	7082.836
K	XVII	1S2	6F	7470.700

表 2 和表 3 分别给出了类锂氯离子和钾离子有关谱线性质：跃迁波长、跃迁几率和振子强度。程序提供的精度 <1%。计算未考虑经验修正。表中以波长减小的顺序排列。

由计算结果可知，$3p$—$2s$, $3d$—$2p$, $4p$—$3s$, $2s$, $4d$—$3p$, $2p$ 的跃迁振子强度较大，使 $3p$、$3d$、$4p$ 和 $4d$ 能级比较容易倒空，作为 nf-$n'd$, nd-$n'p$ 跃迁的下能级，有利于形成粒子数反转而实现激光输出，这些可能的跃迁为 $3d$—$4f$, $5f$, $6f$, $4d$—$5f$, $6f$, $3p$—$5d$, $6d$, $4p$—$6d$ 等。在相同组态的跃迁中，类锂氯离子的跃迁波长比类锂硅离子小 20～30 Å，已很接近“水窗”，而类锂钾离子则有三条谱线计 9 个跃迁波长已进入水窗：$3p$—$5d$, $3d$—$6f$, $3p$—$6d$。这是一个鼓舞人心的结果，正期望在实验中能使之得到验证。

Table 2 Calculated wavelengths, radiative transition probabilities and oscillator strengths in Cl XV.

No.	j	nl	L	j	nl	L	wavelength, (A)	oscillator strength gf	log gf	radiative probability gA(sec-1)
1	2.5	6d	D	2.5	6f	F	377786.1873	0.0013	-2.873	6.261E+01
2	2.5	6d	D	3.5	6f	F	263503.9239	0.0384	-1.415	3.690E+03
3	2.5	5d	D	2.5	5f	F	212675.4618	0.0010	-3.009	1.444E+02
4	1.5	6d	D	2.5	6f	F	202757.0950	0.0349	-1.457	5.670E+03
5	2.5	5d	D	3.5	5f	F	149554.8522	0.0279	-1.555	8.307E+03
6	1.5	5d	D	2.5	5f	F	115546.6932	0.0252	-1.598	1.261E+04
7	2.5	4d	D	2.5	4f	F	100492.4138	0.0006	-3.236	3.834E+02
8	2.5	4d	D	3.5	4f	F	72421.7325	0.0161	-1.793	2.049E+04
9	1.5	4d	D	2.5	4f	F	56645.9591	0.0144	-1.841	2.997E+04
10	1.5	4d	D	1.5	4p	P	9934.9756	0.0157	-1.804	1.061E+06
11	2.5	4d	D	1.5	4p	P	9228.7523	0.1521	-0.818	1.191E+07
12	1.5	4d	D	0.5	4p	P	7986.0398	0.0976	-1.010	1.021E+07
13	1.5	3d	D	1.5	3p	P	4183.9779	0.0088	-2.058	3.336E+06
14	2.5	3d	D	1.5	3p	P	3886.8233	0.0848	-1.072	3.745E+07
15	1.5	3d	D	0.5	3p	P	3363.0797	0.0545	-1.264	3.212E+07
16	0.5	3s	S	0.5	3p	P	1494.3394	0.0947	-1.024	2.828E+08
17	0.5	3s	S	1.5	3p	P	1374.5109	0.2059	-0.686	7.268E+08
18	0.5	2s	S	0.5	2p	P	412.5105	0.0564	-1.249	2.211E+09
19	0.5	2s	S	1.5	2p	P	381.4392	0.1220	-0.914	5.593E+09
20	1.5	6d	D	2.5	5f	F	331.6704	0.1329	-0.876	8.058E+09
21	2.5	6d	D	3.5	5f	F	331.6374	0.1899	-0.722	1.152E+10
22	2.5	6d	D	2.5	5f	F	331.4193	0.0095	-2.022	5.769E+08
23	2.5	5d	D	2.5	6f	F	330.6140	0.2401	-0.620	1.465E+10
24	2.5	5d	D	3.5	6f	F	330.4886	4.8031	0.682	2.933E+11
25	1.5	5d	D	2.5	6f	F	330.1826	3.3653	0.527	2.059E+11
26	1.5	5d	D	2.5	4f	F	180.1705	0.0508	-1.294	1.043E+10
27	2.5	5d	D	3.5	4f	F	180.1674	0.0725	-1.139	1.490E+10
28	2.5	5d	D	2.5	4f	F	180.0422	0.0036	-2.440	7.468E+08
29	2.5	4d	D	2.5	5f	F	179.5685	0.2535	-0.596	5.245E+10
30	2.5	4d	D	3.5	5f	F	179.5045	5.0727	0.705	1.050E+12
31	1.5	4d	D	2.5	5f	F	179.3205	3.5546	0.551	7.373E+11
32	1.5	5d	D	1.5	4p	P	176.4102	0.2270	-0.644	4.866E+10
33	2.5	5d	D	1.5	4p	P	176.2872	2.0448	0.311	4.389E+11
34	1.5	5d	D	0.5	4p	P	175.6490	1.1402	0.057	2.465E+11
35	2.5	6d	D	3.5	4f	F	116.6531	0.0129	-1.888	4.344E+09
36	1.5	6d	D	2.5	4f	F	116.6317	0.0091	-2.043	4.443E+09
37	2.5	6d	D	2.5	4f	F	116.6007	0.0006	-3.189	3.176E+08
38	2.5	4d	D	2.5	6f	F	116.4296	0.0532	-1.274	2.615E+10
39	2.5	4d	D	3.5	6f	F	116.4141	1.0632	0.027	5.233E+11
40	1.5	4d	D	2.5	6f	F	116.3253	0.7448	-0.128	3.671E+11
41	1.5	6d	D	1.5	4p	P	115.0443	0.0573	-1.242	2.887E+10
42	2.5	6d	D	1.5	4p	P	115.0141	0.5158	-0.288	2.601E+11
43	1.5	6d	D	0.5	4p	P	114.7201	0.2873	-0.542	1.456E+11
44	1.5	3d	D	0.5	4p	P	83.9653	0.0443	-1.354	4.188E+10
45	2.5	3d	D	1.5	4p	P	83.9209	0.0797	-1.098	7.551E+10
46	1.5	3d	D	1.5	4p	P	83.7925	0.0089	-2.052	8.429E+09
47	2.5	3d	D	2.5	4f	F	83.0959	0.2905	-0.537	2.806E+11
48	2.5	3d	D	3.5	4f	F	83.0693	5.8118	0.764	5.617E+12
49	1.5	3d	D	2.5	4f	F	82.9699	4.0731	0.610	3.946E+12
50	1.5	4d	D	1.5	3p	P	81.4736	0.2337	-0.631	2.348E+11
51	2.5	4d	D	1.5	3p	P	81.4225	2.1045	0.323	2.117E+12
52	1.5	4d	D	0.5	3p	P	81.0882	1.1740	0.070	1.191E+12
53	0.5	3s	S	0.5	4p	P	77.6625	0.2562	-0.591	2.833E+11
54	0.5	3s	S	1.5	4p	P	77.5147	0.5133	-0.290	5.698E+11
55	2.5	3d	D	2.5	5f	F	56.8400	0.0448	-1.349	9.245E+10
56	2.5	3d	D	3.5	5f	F	56.8336	0.8975	-0.048	1.850E+12
57	1.5	3d	D	2.5	5f	F	56.7810	0.6276	-0.202	1.298E+12
58	1.5	5d	D	1.5	3p	P	56.0480	0.0545	-1.264	1.157E+11
59	2.5	5d	D	1.5	3p	P	56.0355	0.4970	-0.309	1.042E+12
60	1.5	5d	D	0.5	3p	P	55.8653	0.2734	-0.563	5.844E+11

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61	2.5	3d	D	2.5	6f	F	48.5126	0.0154	-1.812	4.367E+10
62	2,5	3d	D	3.5	6f	F	48.5099	0.3082	-0.511	8.736E+11
63	1.5	3d	D	2.5	6f	F	48.4696	0.2159	-0.666	6.130E+11
64	1.5	6d	D	1.5	3p	P	47.9259	0.0223	-1.653	6.462E+10
65	2.5	6d	D	1.5	3p	P	47.9206	0.2003	-0.698	5.818E+11
66	1.5	6d	D	0.5	3p	P	47.7922	0.1116	-0.952	3.258E+11
67	0.5	3s	S	1.5	2p	P	29.1937	0.0786	-1.105	6.148E+11
68	0.5	3s	S	0.5	2p	P	29.0264	0.0395	-1.403	3.127E+11
69	1.5	3d	D	1.5	2p	P	28.3925	0.2703	-0.568	2.236E+12
70	2.5	3d	D	1.5	2p	P	28.3778	2.4335	0.386	2.016E+13
71	1.5	3d	D	0.5	2p	P	28.2342	1.3588	0.133	1.137E+13
72	0.5	2s	S	0.5	3p	P	26.6348	0.2357	-0.628	2.216E+12
73	0.5	2s	S	1.5	3p	P	26.5935	0.4721	-0.326	4.452E+12
74	1.5	4d	D	1.5	2p	P	21.1616	0.0490	-1.310	7.299E+11
75	2.5	4d	D	1.5	2p	P	21.1581	0.4411	-0.355	6.572E+12
76	1.5	4d	D	0.5	2p	P	21.0735	0.2461	-0.609	3.696E+12
77	0.5	2s	S	0.5	4p	P	20.0998	0.0600	-1.222	9.905E+11
78	0.5	2s	S	1.5	4p	P	20.0898	0.1201	-0.921	1.984E+12
79	1.5	5d	D	1.5	2p	P	18.9310	0.0181	-1.743	3.362E+11
80	2.5	5d	D	1.5	2p	P	18.9296	0.1626	-0.789	3.026E+12
81	1.5	5d	D	0.5	2p	P	18.8605	0.0907	-1.043	1.700E+12
82	1.5	6d	D	1.5	2p	P	17.9060	0.0089	-2.053	1.842E+11
83	2.5	6d	D	1.5	2p	P	17.9053	0.0797	-1.099	1.658E+12
84	1.5	6d	D	0.5	2p	P	17.8430	0.0444	-1.352	9.308E+11

Table 3　Calculated wavelengths, radiative transition probabilities and oscillator strengths in K XVII.

transition, No.	j	nl	L	j	nl	L	wavelength, (A)	oscillator strength gf	Log gf	radiatiy probability gA(sec-1)
1	2.5	6d	D	2.5	6f	F	340831.6408	0.0012	-2.937	6.638E+01
2	2.5	6d	D	3.5	6f	F	206996.0569	0.0381	-1.419	5.926E+03
3	2.5	5d	D	2.5	5f	F	192418.7068	0.0008	-3.074	1.518E+02
4	1.5	6d	D	2.5	6f	F	149053.2903	0.0370	-1.432	1.111E+04
5	2.5	5d	D	3.5	5f	F	118119.3988	0.0275	-1.561	1.313E+04
6	2.5	4d	D	2.5	4f	F	91407.6791	0.0005	-3.304	3.966E+02
7	1.5	5d	D	2.5	5f	F	85309.6021	0.0266	-1.575	2.439E+04
8	2.5	4d	D	3.5	4f	F	57781.7252	0.0157	-1.804	3.140E+04
9	1.5	4d	D	2.5	4f	F	42252.0157	0.0150	-1.823	5.622E+04
10	1.5	4d	D	1.5	4p	P	8597.6761	0.0141	-1.850	1.273E+06
11	2.5	4d	D	1.5	4p	P	7749.6545	0.1409	-0.851	1.565E+07
12	1.5	4d	D	0.5	4p	P	6378.3438	0.0951	-1.022	1.559E+07
13	1.5	3d	D	1.5	3p	P	3619.2544	0.0079	-2.104	4.009E+06
14	2.5	3d	D	1.5	3p	P	3262.8023	0.0786	-1.105	4.925E+07
15	1.5	3d	D	0.5	3p	P	2685.2701	0.0531	-1.275	4.908E+07
16	0.5	2s	S	0.5	3p	P	1312.9597	0.0840	-1.075	3.252E+08
17	0.5	2s	S	1.5	3p	P	1165.8544	0.1893	-0.723	9.290E+08
18	0.5	2s	S	0.5	2p	P	362.9057	0.0501	-1.300	2.535E+09
19	0.5	2s	S	1.5	2p	P	324.6046	0.1119	-0.951	7.086E+09
20	1.5	6d	D	2.5	5f	F	258.2170	0.1332	-0.876	1.332E+10
21	2.5	6d	D	3.5	5f	F	258.1832	0.1903	-0.721	1.904E+10
22	2.5	6d	D	2.5	5f	F	257.9655	0.0095	-2.021	9.544E+08
23	2.5	5d	D	2.5	6f	F	257.4256	0.2399	-0.620	2.414E+10
24	2.5	5d	D	3.5	6f	F	257.2999	4.8000	0.681	4.836E+11
25	1.5	5d	D	2.5	6f	F	256.9939	3.3640	0.527	3.397E+11
26	1.5	5d	D	2.5	4f	F	140.2685	0.0509	-1.293	1.726E+10

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27	2.5	5d	D	3.5	4f	F	140.2654	0.0727	-1.138	2.466E+10
28	2.5	5d	D	2.5	4f	F	140.1403	0.0036	-2.439	1.236E+09
29	2.5	4d	D	2.5	5f	F	139.8241	0.2534	-0.596	8.644E+10
30	2.5	4d	D	3.5	5f	F	139.7602	5.0698	0.705	1.731E+12
31	1.5	4d	D	2.5	5f	F	139.5757	3.5536	0.551	1.217E+12
32	1.5	5d	D	1.5	4p	P	137.5675	0.2280	-0.642	8.034E+10
33	2.5	5d	D	1.5	4p	P	137.4441	2.0534	0.312	7.250E+11
34	1.5	5d	D	0.5	4p	P	136.8058	1.1461	0.059	4.084E+11
35	2.5	6d	D	3.5	4f	F	90.8181	0.0130	-1.887	1.050E+10
36	1.5	6d	D	2.5	4f	F	90.7967	0.0091	-2.042	7.352E+09
37	2.5	6d	D	2.5	4f	F	90.7656	0.0006	-3.188	5.257E+08
38	2.5	4d	D	2.5	6f	F	90.6514	0.0531	-1.275	4.312E+10
39	2.5	4d	D	3.5	6f	F	90.6358	1.0628	0.026	8.629E+11
40	1.5	4d	D	2.5	6f	F	90.5470	0.7447	-0.128	6.058E+11
41	1.5	6d	D	1.5	4p	P	89.6572	0.0574	-1.241	4.763E+10
42	2.5	6d	D	1.5	4p	P	89.6269	0.5168	-0.287	4.291E+11
43	1.5	6d	D	0.5	4p	P	89.3331	0.2880	-0.541	2.407E+11
44	1.5	3d	D	0.5	4p	P	65.3479	0.0438	-1.358	6.847E+10
45	2.5	3d	D	1.5	4p	P	65.3040	0.0790	-1.103	1.235E+11
46	1.5	3d	D	1.5	4p	P	65.1756	0.0088	-2.056	1.380E+10
47	2.5	3d	D	2.5	4f	F	64.7125	0.2903	-0.537	4.624E+11
48	2.5	3d	D	3.5	4f	F	64.6858	5.8085	0.764	9.259E+12
49	1.5	3d	D	2.5	4f	F	64.5863	4.0722	0.610	6.511E+12
50	1.5	4d	D	1.5	3p	P	63.5494	0.2344	-0.630	3.872E+11
51	2.5	4d	D	1.5	3p	P	63.4981	2.1116	0.325	3.493E+12
52	1.5	4d	D	0.5	3p	P	63.1637	1.1793	0.072	1.972E+12
53	0.5	2s	S	0.5	4p	P	60.8393	0.2619	-0.582	4.719E+11
54	0.5	2s	S	1.5	4p	P	60.6899	0.5251	-0.280	9.509E+11
55	2.5	3d	D	2.5	5f	F	44.2598	0.0447	-1.349	1.524E+11
56	2.5	3d	D	3.5	5f	F	44.2534	0.8951	-0.048	3.049E+12
57	1.5	3d	D	2.5	5f	F	44.2007	0.6273	-0.203	2.142E+12
58	1.5	5d	D	1.5	3p	P	43.6898	0.0546	-1.263	1.906E+11
59	2.5	5d	D	1.5	3p	P	43.6774	0.4911	-0.309	1.717E+12
60	1.5	5d	D	0.5	3p	P	43.5071	0.2739	-0.562	9.652E+11
61	2.5	3d	D	2.5	6f	F	37.7739	0.0154	-1.813	7.198E+10
62	2.5	3d	D	3.5	6f	F	37.7712	0.3080	-0.511	1.440E+12
63	1.5	3d	D	2.5	6f	F	37.7309	0.2158	-0.666	1.011E+12
64	1.5	6d	D	1.5	3p	P	37.3510	0.0223	-1.653	1.064E+11
65	2.5	6d	D	1.5	3p	P	37.3457	0.2003	-0.698	9.578E+11
66	1.5	6d	D	0.5	3p	P	37.2174	0.1117	-0.952	5.376E+11
67	0.5	2s	S	1.5	2p	P	22.7336	0.0763	-1.118	9.843E+11
68	0.5	2s	S	0.5	2p	P	22.5668	0.0384	-1.415	5.031E+11
69	1.5	3d	D	1.5	2p	P	22.1623	0.2706	-0.568	3.674E+12
70	2.5	3d	D	1.5	2p	P	22.1474	2.4367	0.387	3.313E+13
71	1.5	3d	D	0.5	2p	P	22.0037	1.3626	0.134	1.877E+13
72	0.5	2s	S	0.5	3p	P	20.9074	0.2405	-0.619	3.670E+12
73	0.5	2s	S	1.5	3p	P	20.8654	0.4820	-0.317	7.385E+12
74	1.5	4d	D	1.5	2p	P	16.5068	0.0489	-1.311	1.197E+12
75	2.5	4d	D	1.5	2p	P	16.5033	0.4403	-0.356	1.078E+13
76	1.5	4d	D	0.5	2p	P	16.4186	0.2459	-0.609	6.084E+12
77	0.5	2s	S	0.5	4p	P	15.7468	0.0608	-1.216	1.635E+12
78	0.5	2s	S	1.5	4p	P	15.7367	0.1217	-0.915	3.277E+12
79	1.5	5d	D	1.5	2p	P	14.7636	0.0180	-1.744	5.512E+11
80	2.5	5d	D	1.5	2p	P	14.7622	0.1621	-0.790	4.962E+12
81	1.5	5d	D	0.5	2p	P	14.6931	0.0905	-1.043	2.796E+12
82	1.5	6d	D	1.5	2p	P	13.9629	0.0088	-2.054	3.019E+11
83	2.5	6d	D	1.5	2p	P	13.9621	0.0794	-1.100	2.718E+12
84	1.5	6d	D	0.5	2p	P	13.8998	0.0443	-1.353	1.530E+12

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Theoretical calculation of Li-like Cl XV and K XVII soft X-ray laser spectra

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Abstract

Transition wavelengths of $4d-3p$, $4f-3d$, $5d-3p$, $5f-3d$, $6d-3p$ and $6f-3d$ of Cl XV and K XVII are reported. Corresponding transition probabilities and oscillator strengths are given. These transitions are of potential interest for X-ray lasers with shorter wavelengths towards the "water window". Among them, wavelengths of three KXVII transitions are in the range of the "water window". They are $3p-5d$, $3d-6f$, $3p-6d$.

Key words: Li-like Cl XV, Li-like K XVII, soft X-ray laser, atomic spectra.