

# 类锂铜离子的振子强度和辐射跃迁几率

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**提要** 本文应用原子结构和光谱的 HFR 程序<sup>[1]</sup>, 结合一个关于原子能量参数的最小二乘优化程序系统计算了高离化态类锂铜离子  $1S^2nl$  ( $n = 2 \sim 6, l = 0 \sim 5$ ) 电偶极跃迁的权重振子强度, 辐射跃迁几率和相应的软 X 射线波长 (30 nm 以下), 将波长计算值与已有的实验值相比较, 二者十分符合。

**关键词** 软 X 射线光谱, 组态, 能量参数

## Theoretical weighted oscillator strengths and radiative transition probabilities of Li-like Cu ion

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**Abstract** Theoretical weighted oscillator strengths and radiative transition probabilities for  $1S^2nl$  ( $n = 2 \sim 6, l = 0 \sim 5$ ) configurations in Li-like Cu ion are computed with the aid of the HFR program developed by R. D. Cowan. The ab initio energy parameters are optimised on the basis of experimental energy levels. The excellent agreement are obtained between the calculated wavelenthgths and the measured ones.

**Key words** soft X-ray spectra, configuration, energy parameter

## 1 引 言

高离化态类锂等电子数序列离子的光谱在软 X 射线激光研究方面有重要应用。以复合机制, 用激光等离子体作为增益介质, 沿类锂等电子数序列将软 X 射线激光跃迁波长推至具有实用意义的“水窗”波段, 在实验上已证明是很有希望的。类锂等电子数序列处于“水窗”波段范围的激光跃迁是原子序数  $Z > 22$  的元素的离子。因此理论上系统提供这些离子的光谱数据是非常必要的。

B. Edlen<sup>[1]</sup> 和 Vainshtein<sup>[2]</sup> 等人先后对类锂等电子系列离子的光谱作了较为系统而准确的计算, 然而他们的计算中没有软 X 射线激光研究需要的振子强度、跃迁几率等数据, 对高主

量子数及高次量子数组态的电偶极跃迁光谱也未作计算。

类锂铜离子作为可实现“水窗”波段软 X 射线激光跃迁的元素,已引起普遍注意<sup>[3,4]</sup>。为此,我们运用 HFR 程序<sup>[5]</sup>,结合一个关于原子组态能量参数的最小二乘优化程序<sup>[6]</sup>,系统计算了类锂铜离子  $1S^2nl(n=2\sim 6, l=0\sim 5)$  组态电偶极跃迁的振子强度,辐射跃迁几率以及相应软 X 射线波长,将我们的计算值与实验值作了比较,二者符合得非常好。

## 2 计算方法

有关运用 HFR 方法计算原子光谱的详细介绍可参看文献<sup>[6]</sup>,这里只将与本文计算有关的内容概述如下:

对形如  $(n_1l_1)^{w_1}(n_2l_2)^{w_2}\cdots(n_q l_q)^{w_q}$ ,  $W_1 + W_2 + \cdots + W_q = N$  的  $N$  个电子的原子体系,首先解 HFR 方程求出上述组态的原子径向波函数及各种相互作用径向积分即组态平均能量  $E_{av}$ ,静电相互作用  $F^k$  和  $G^k$ ,自旋-轨道相互作用  $\xi_{nl}$ ;其次,用 Racah 代数方法<sup>[6]</sup>计算与各相互作用径向积分对应的角系数即  $f_k, g_k$  和  $d_j$ ,然后构造哈密顿矩阵并对角化而求得原子在选定表象下的本征波函数和能量值。

最后,根据已有的实验能级<sup>[7]</sup>,运用最小二乘优化程序,调整各相互作用径向积分(能量参数)以便减小能量计算值与实验值之间的误差,用调整后的能量参数重新求得能量本征值、本征波函数以及电偶极跃迁的振子强度、跃迁几率和相应软 X 射线波长,计算中我们选用了单组态近似,就高电离态类锂铜离子  $1S^2nl$  组态特点而言,这已是非常好的近似。

## 3 计算结果

表 1 列出了我们计算的类锂铜离子  $1S^2nl(n=2\sim 6, l=0\sim 5)$  电偶极跃迁的权重振子强度、辐射跃迁几率和相应软 X 射线波长(30 nm 以下)。表 2 将我们的波长计算值与已有的实验观测值作了比较。

Table 1 Calculated wavelengths (nm) Oscillator strengths ( $Gf$ ) and transition probability ( $GA$ ) for Li-like Cu ion

$\lambda$ (nm)	$Gf$	$GA$ ( $s^{-1}$ )	Transition			
			( $nl$ )	$^2L - (nl)$	$^2L$	$J - J$
22.47701	0.0321	$4.242E + 09$	( $2s$ )	$2S - (2p)$	$2P$	0.5 - 0.5
15.35080	0.0941	$2.663E + 10$	( $2s$ )	$2S - (2p)$	$2P$	0.5 - 1.5
10.37106	0.3739	$2.319E + 11$	( $6s$ )	$2S - (5p)$	$2P$	0.5 - 1.5
10.32218	0.1840	$1.152E + 11$	( $5d$ )	$2D - (6p)$	$2P$	1.5 - 0.5
10.28589	0.3324	$2.096E + 11$	( $5d$ )	$2D - (6p)$	$2P$	2.5 - 1.5
10.24227	0.0371	$2.358E + 10$	( $5d$ )	$2D - (6p)$	$2P$	1.5 - 1.5
10.24036	0.1354	$8.615E + 10$	( $6d$ )	$2D - (5f)$	$2F$	1.5 - 2.5
10.23694	0.1936	$1.232E + 11$	( $6d$ )	$2D - (5f)$	$2F$	2.5 - 3.5
10.23348	0.0755	$4.810E + 10$	( $5g$ )	$2G - (6f)$	$2F$	4.5 - 3.5
10.23302	0.0583	$3.711E + 10$	( $5g$ )	$2G - (6f)$	$2F$	3.5 - 2.5
10.23225	0.1895	$1.207E + 11$	( $6s$ )	$2S - (5p)$	$2P$	0.5 - 0.5
10.22581	0.3043	$1.941E + 11$	( $5g$ )	$2G - (6h)$	$2H$	4.5 - 4.5
10.22079	6.4393	$1.050E + 13$	( $5g$ )	$2G - (6h)$	$2H$	4.5 - 5.5

$\lambda$ (nm)	$Gf$	$GA$ ( $s^{-1}$ )	Transition			
			( $nl$ )	${}^2L - (nl)$	${}^2L$	$J - J$
10.22049	0.0022	$1.380E + 09$	(5g)	$2G - (6f)$	$2F$	3.5 - 3.5
10.22015	0.2625	$1.676E + 11$	(6g)	$2G - (5f)$	$2F$	3.5 - 3.5
10.21530	0.0097	$6.199E + 09$	(6d)	$2D - (5f)$	$2F$	2.5 - 2.5
10.21284	3.4054	$8.572E + 12$	(5g)	$2G - (6h)$	$2H$	3.5 - 4.5
10.21264	9.1943	$5.880E + 12$	(6g)	$2G - (5f)$	$2F$	4.5 - 3.5
10.20444	0.2386	$1.528E + 11$	(5d)	$2D - (6f)$	$2F$	2.5 - 2.5
10.19858	7.1025	$4.555E + 12$	(6g)	$2G - (5f)$	$2F$	3.5 - 2.5
10.19198	4.7773	$3.067E + 12$	(5d)	$2D - (6f)$	$2F$	2.5 - 3.5
10.16151	3.3541	$2.167E + 12$	(5d)	$2D - (6f)$	$2F$	1.5 - 2.5
10.09791	0.2319	$1.517E + 11$	(6d)	$2D - (5p)$	$2P$	1.5 - 1.5
10.07354	2.0923	$1.375E + 12$	(6d)	$2D - (5p)$	$2P$	2.5 - 1.5
9.96627	1.1749	$7.890E + 11$	(6d)	$2D - (5p)$	$2P$	1.5 - 0.5
9.85629	0.3355	$2.303E + 11$	(5s)	$2S - (6p)$	$2P$	0.5 - 0.5
9.78340	0.6760	$4.711E + 11$	(5s)	$2S - (6p)$	$2P$	0.5 - 1.5
5.61104	0.2682	$5.681E + 11$	(5s)	$2S - (4p)$	$2P$	0.5 - 1.5
5.60562	0.1080	$2.291E + 11$	(4d)	$2D - (5p)$	$2P$	1.5 - 0.5
5.58658	0.1950	$4.167E + 11$	(4d)	$2D - (5p)$	$2P$	2.5 - 1.5
5.57416	0.0519	$1.113E + 11$	(5d)	$2D - (4f)$	$2F$	1.5 - 2.5
5.57372	0.0741	$1.591E + 11$	(5d)	$2D - (4f)$	$2F$	2.5 - 3.5
5.56523	0.2977	$6.410E + 11$	(5g)	$2G - (4f)$	$2F$	3.5 - 3.5
5.56482	0.0217	$4.684E + 10$	(4d)	$2D - (5p)$	$2P$	1.5 - 1.5
5.56139	0.4253	$2.248E + 13$	(5g)	$2G - (4f)$	$2F$	4.5 - 3.5
5.56132	0.0037	$8.008E + 09$	(5d)	$2D - (4f)$	$2F$	2.5 - 2.5
5.55287	8.0547	$1.742E + 13$	(5g)	$2G - (4f)$	$2F$	3.5 - 2.5
5.54391	0.2522	$5.473E + 11$	(4d)	$2D - (5f)$	$2F$	2.5 - 2.5
5.53924	0.1358	$2.952E + 11$	(5s)	$2S - (4p)$	$2P$	0.5 - 0.5
5.53756	5.0502	$1.098E + 13$	(4d)	$2D - (5f)$	$2F$	2.5 - 3.5
5.52248	3.5448	$7.752E + 12$	(4d)	$2D - (5f)$	$2F$	1.5 - 2.5
5.47048	0.2285	$5.093E + 11$	(5d)	$2D - (4p)$	$2P$	1.5 - 1.5
5.45812	2.0614	$4.615E + 12$	(5d)	$2D - (4p)$	$2P$	2.5 - 1.5
5.40221	1.1571	$2.644E + 12$	(5d)	$2D - (4p)$	$2P$	1.5 - 0.5
5.32926	0.3030	$7.116E + 11$	(4s)	$2S - (5p)$	$2P$	0.5 - 0.5
5.29237	0.6103	$1.453E + 12$	(4s)	$2S - (5p)$	$2P$	0.5 - 1.5
3.60529	0.0132	$6.786E + 10$	(6d)	$2D - (4f)$	$2F$	2.5 - 3.5
3.60389	0.0223	$1.146E + 11$	(4d)	$2D - (6p)$	$2P$	1.5 - 0.5
3.60320	0.0093	$4.758E + 10$	(6d)	$2D - (4f)$	$2F$	1.5 - 2.5
3.60320	0.0404	$2.073E + 11$	(6g)	$2G - (4f)$	$2F$	3.5 - 3.5
3.60316	0.0402	$2.065E + 11$	(4d)	$2D - (6p)$	$2P$	2.5 - 1.5
3.60227	1.4127	$7.261E + 12$	(6g)	$2G - (4f)$	$2F$	4.5 - 3.5
3.60010	0.0007	$3.408E + 09$	(6d)	$2D - (4f)$	$2F$	2.5 - 2.5
3.59802	1.0911	$5.621E + 12$	(6g)	$2G - (4f)$	$2F$	3.5 - 2.5
3.59410	0.0045	$2.311E + 10$	(4d)	$2D - (6p)$	$2P$	1.5 - 1.5
3.59312	0.0530	$2.737E + 11$	(4d)	$2D - (6f)$	$2F$	2.5 - 2.5
3.59295	0.0599	$3.097E + 11$	(6s)	$2S - (4p)$	$2P$	0.5 - 1.5

$\lambda$ (nm)	$Gf$	$GA$ ( $s^{-1}$ )	Transition			
			( $nl$ )	${}^2L - (nl)$	${}^2L$	$J - J$
3.59157	1.0600	$5.481E + 12$	(4d)	2D - (6f)	2F	2.5 - 3.5
3.58410	0.7435	$3.861E + 12$	(4d)	2D - (6f)	2F	1.5 - 2.5
3.56338	0.0302	$1.587E + 11$	(6s)	2S - (4p)	2P	0.5 - 0.5
3.55960	0.0574	$3.022E + 11$	(6d)	2D - (4p)	2P	1.5 - 1.5
3.55656	0.5172	$2.727E + 12$	(6d)	2D - (4p)	2P	2.5 - 1.5
3.53056	0.2894	$1.549E + 12$	(6d)	2D - (4p)	2P	1.5 - 0.5
3.48761	0.0815	$4.469E + 11$	(4s)	2S - (6p)	2P	0.5 - 0.5
3.47844	0.1634	$9.008E + 11$	(4s)	2S - (6p)	2P	0.5 - 1.5
2.59438	0.1656	$1.641E + 12$	(4s)	2S - (3p)	2P	0.5 - 1.5
2.59208	0.0436	$4.332E + 11$	(3d)	2D - (4p)	2P	1.5 - 0.5
2.59000	0.0786	$7.817E + 11$	(3d)	2D - (4p)	2P	2.5 - 1.5
2.57666	0.0088	$8.821E + 10$	(3d)	2D - (4p)	2P	1.5 - 1.5
2.56739	0.2892	$2.926E + 12$	(3d)	2D - (4f)	2F	2.5 - 2.5
2.56476	5.7901	$5.871E + 13$	(3d)	2D - (4f)	2F	2.5 - 3.5
2.55428	4.0697	$4.160E + 13$	(3d)	2D - (4f)	2F	1.5 - 2.5
2.55331	0.0841	$8.606E + 11$	(4s)	2S - (3p)	2P	0.5 - 0.5
2.53357	0.2345	$2.437E + 12$	(4d)	2D - (3p)	2P	1.5 - 1.5
2.52908	2.1145	$2.205E + 13$	(4d)	2D - (3p)	2P	2.5 - 1.5
2.49439	1.1910	$1.277E + 13$	(4d)	2D - (3p)	2P	1.5 - 0.5
2.44266	0.2743	$3.066E + 12$	(3s)	2S - (4p)	2P	0.5 - 0.5
2.42895	0.5516	$6.236E + 12$	(3s)	2S - (4p)	2P	0.5 - 1.5
1.76056	0.0156	$3.352E + 11$	(3d)	2D - (5p)	2P	2.5 - 1.5
1.75842	0.0087	$1.869E + 11$	(3d)	2D - (5p)	2P	1.5 - 0.5
1.75630	0.0446	$9.634E + 11$	(3d)	2D - (5f)	2F	2.5 - 2.5
1.75566	0.8914	$1.929E + 13$	(3d)	2D - (5f)	2F	2.5 - 3.5
1.75438	0.0017	$3.764E + 10$	(3d)	2D - (5p)	2P	1.5 - 1.5
1.75217	0.0366	$7.954E + 11$	(5s)	2S - (3p)	2P	0.5 - 1.5
1.75015	0.6260	$1.363E + 13$	(3d)	2D - (5f)	2F	1.5 - 2.5
1.73823	0.0544	$1.201E + 12$	(5d)	2D - (3p)	2P	1.5 - 1.5
1.73698	0.4898	$1.083E + 13$	(5d)	2D - (3p)	2P	2.5 - 1.5
1.73334	0.0185	$4.108E + 11$	(5s)	2S - (3p)	2P	0.5 - 0.5
1.71969	0.2749	$6.199E + 12$	(5d)	2D - (3p)	2P	1.5 - 0.5
1.68836	0.0724	$1.693E + 12$	(3s)	2S - (5p)	2P	0.5 - 0.5
1.68463	0.1450	$3.408E + 12$	(3s)	2S - (5p)	2P	0.5 - 1.5
1.50030	0.0059	$1.752E + 11$	(3d)	2D - (6p)	2P	2.5 - 1.5
1.49855	0.0153	$4.550E + 11$	(3d)	2D - (6f)	2F	2.5 - 2.5
1.49829	0.3065	$9.106E + 12$	(3d)	2D - (6f)	2F	2.5 - 3.5
1.49750	0.0033	$9.788E + 10$	(3d)	2D - (6p)	2P	1.5 - 0.5
1.49581	0.0007	$1.964E + 10$	(3d)	2D - (6p)	2P	1.5 - 1.5
1.49408	0.2151	$6.428E + 12$	(3d)	2D - (6f)	2F	1.5 - 2.5
1.49071	0.0148	$4.431E + 11$	(6s)	2S - (3p)	2P	0.5 - 1.5
1.48493	0.0221	$6.697E + 11$	(6d)	2D - (3p)	2P	1.5 - 1.5
1.48441	0.1993	$6.034E + 12$	(6d)	2D - (3p)	2P	2.5 - 1.5
1.47706	0.0074	$2.277E + 11$	(6s)	2S - (3p)	2P	0.5 - 0.5

$\lambda$ (nm)	$Gf$	$GA$ ( $s^{-1}$ )	Transition			
			( $nl$ )	$^2L - (nl)$	$^2L$	$J - J$
1.47139	0.1117	$3.442E + 12$	(6d)	$2D - (3p)$	$2P$	1.5 - 0.5
1.44639	0.0313	$9.978E + 11$	(3s)	$2S - (6p)$	$2P$	0.5 - 0.5
1.44481	0.0627	$2.002E + 12$	(3s)	$2S - (6p)$	$2P$	0.5 - 1.5
0.90419	0.0720	$5.876E + 12$	(3s)	$2S - (2p)$	$2P$	0.5 - 1.5
0.88762	0.0367	$3.106E + 12$	(3s)	$2S - (2p)$	$2P$	0.5 - 0.5
0.88530	0.2700	$2.298E + 13$	(3d)	$2D - (2p)$	$2P$	1.5 - 1.5
0.88374	2.4347	$2.079E + 14$	(3d)	$2D - (2p)$	$2P$	2.5 - 1.5
0.86941	1.3749	$1.213E + 14$	(3d)	$2D - (2p)$	$2P$	1.5 - 0.5
0.84452	0.2514	$2.351E + 13$	(2s)	$2S - (3p)$	$2P$	0.5 - 0.5
0.84012	0.5054	$4.776E + 13$	(2s)	$2S - (3p)$	$2P$	0.5 - 1.5
0.66199	0.0155	$2.360E + 12$	(4s)	$2S - (2p)$	$2P$	0.5 - 1.5
0.65796	0.0484	$7.463E + 12$	(4d)	$2D - (2p)$	$2P$	1.5 - 1.5
0.65765	0.4362	$6.726E + 13$	(4d)	$2D - (2p)$	$2P$	2.5 - 1.5
0.65306	0.0079	$1.229E + 12$	(4s)	$2S - (2p)$	$2P$	0.5 - 0.5
0.64914	0.2455	$3.886E + 13$	(4d)	$2D - (2p)$	$2P$	1.5 - 0.5
0.63272	0.0625	$1.041E + 13$	(2s)	$2S - (4p)$	$2P$	0.5 - 0.5
0.63179	0.1251	$2.091E + 13$	(2s)	$2S - (4p)$	$2P$	0.5 - 1.5
0.58967	0.0061	$1.169E + 12$	(5s)	$2S - (2p)$	$2P$	0.5 - 1.5
0.58808	0.0178	$3.428E + 12$	(5d)	$2D - (2p)$	$2P$	1.5 - 1.5
0.58793	0.1600	$3.087E + 13$	(5d)	$2D - (2p)$	$2P$	2.5 - 1.5
0.58257	0.0031	$6.062E + 11$	(5s)	$2S - (2p)$	$2P$	0.5 - 0.5
0.58102	0.0899	$1.777E + 13$	(5d)	$2D - (2p)$	$2P$	1.5 - 0.5
0.56709	0.0259	$5.367E + 12$	(2s)	$2S - (5p)$	$2P$	0.5 - 0.5
0.56667	0.0518	$1.076E + 13$	(2s)	$2S - (5p)$	$2P$	0.5 - 1.5
0.55680	0.0031	$6.632E + 11$	(6s)	$2S - (2p)$	$2P$	0.5 - 1.5
0.55599	0.0087	$1.875E + 12$	(6d)	$2D - (2p)$	$2P$	1.5 - 1.5
0.55592	0.0782	$1.688E + 13$	(6d)	$2D - (2p)$	$2P$	2.5 - 1.5
0.55047	0.0016	$3.432E + 11$	(6s)	$2S - (2p)$	$2P$	0.5 - 0.5
0.54968	0.0440	$9.702E + 12$	(6d)	$2D - (2p)$	$2P$	1.5 - 0.5
0.53692	0.0134	$3.110E + 12$	(2s)	$2S - (6p)$	$2P$	0.5 - 0.5
0.53670	0.0269	$6.228E + 12$	(2s)	$2S - (6p)$	$2P$	0.5 - 1.5

Table 2 A comparison of the calculated wavelengths with the observed ones of Li-like Cu ion

$\lambda$ (Calc.) (nm)	$\lambda$ (Obs.) (nm)	$Gf$	$GA$ ( $s^{-1}$ )	Transition			
				( $nl$ )	$^2L - (nl)$	$^2L$	$J - J$
22.47701	22.4795	0.0321	$4.242E + 09$	(2s)	$2S - (2p)$	$2P$	0.5 - 0.5
15.35080	15.3507	0.0941	$2.663E + 10$	(2s)	$2S - (2p)$	$2P$	0.5 - 1.5
2.59000	2.5893	0.0786	$7.817E + 11$	(3d)	$2D - (4p)$	$2P$	2.5 - 1.5
2.56476	2.5646	5.7901	$5.871E + 13$	(3d)	$2D - (4f)$	$2F$	2.5 - 3.5
2.55428	2.5543	4.0697	$4.160E + 13$	(3d)	$2D - (4f)$	$2F$	1.5 - 2.5
2.52908	2.5291	2.1145	$2.205E + 13$	(4d)	$2D - (3p)$	$2P$	2.5 - 1.5
2.49439	2.4943	1.1910	$1.277E + 13$	(4d)	$2D - (3p)$	$2P$	1.5 - 0.5
2.42895	2.4291	0.5516	$6.236E + 12$	(3s)	$2S - (4p)$	$2P$	0.5 - 1.5
0.90419	0.9042	0.0720	$5.876E + 12$	(3s)	$2S - (2p)$	$2P$	0.5 - 1.5

$\lambda$ (Calc. ), (nm)	$\lambda$ (Obs. ) (nm)	$Gf$	$GA$ ( $s^{-1}$ )	Transition			
				( $nl$ )	$^2L - (nl)$	$^2L$	$J - J$
0.88762	0.8876	0.0367	$3.106E + 12$	(3s)	$2S - (2p)$	2P	0.5 - 0.5
0.88530	0.8848	0.2700	$2.298E + 13$	(3d)	$2D - (2p)$	2P	1.5 - 1.5
0.88374	0.8837	2.4347	$2.079E + 14$	(3d)	$2D - (2p)$	2P	2.5 - 1.5
0.86941	0.8691	1.3749	$1.213E + 14$	(3d)	$2D - (2p)$	2P	1.5 - 0.5
0.84452	0.8445	0.2514	$2.351E + 13$	(2s)	$2S - (3p)$	2P	0.5 - 0.5
0.84012	0.8401	0.5054	$4.776E + 13$	(2s)	$2S - (3p)$	2P	0.5 - 1.5
0.65765	0.6575	0.4362	$6.726E + 13$	(4d)	$2D - (2p)$	2P	2.5 - 1.5
0.64914	0.6490	0.2455	$3.886E + 13$	(4d)	$2D - (2p)$	2P	1.5 - 0.5
0.63179	0.6320	0.1251	$2.091E + 13$	(2s)	$2S - (4p)$	2P	0.5 - 1.5

从表 1 的结果及文献[8]的结果看出,类锂等电子数序列离子的  $4f \rightarrow 3d$  跃迁沿等电子数序列具有稳定的自发辐射跃迁几率和较大的振子强度,且下能级具有更大的自发辐射跃迁几率,因而非常有可能形成粒子数反转而实现自发辐射放大(ASE),其中类锂铜离子的  $4f \rightarrow 3d$  跃迁波长已全部处于“水窗”波段。这是今后软 X 射线激光研究努力的一个方向。

从表 2 看出,我们的波长计算值比 B. Edlen<sup>[2]</sup> 和 Vainshtein<sup>[3]</sup> 等人的预言值均好,与实验观测值<sup>[4,9]</sup>十分符合,说明本文的计算是准确可靠的。而 Sureau<sup>[5]</sup> 等人的计算与我们的结果及实验结果相比,其误差明显较大。

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