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Pt Ⅲ离子 $5d^8$-$5d^76p$ 跃迁的极紫外光谱计算

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提　　要

本文运用多组态 Hartree-Fock 加相对论修正方法（MCHFR）计算了 Pt Ⅲ 离子 $5d^8$-$5d^76p$ 跃迁的光谱，得到了有关光谱数据如波长、振子强度和辐射跃迁几率，并就计算结果进行了简要分析．

关键词　光谱，　组态，　能量参数．

1　引　　言

离化态原子的光谱在天体物理，热核聚变及实验室等离子体方面有广泛的应用[1]．过去十多年来，随着几种强有力光源如激光等离子体、托卡马克和束箔技术的应用，以及大型计算机的出现，离化态原子光谱的实验及理论研究已经取得了长足的进展[2~4]．目前，离化态原子光谱研究已转向中到高 Z 元素的电偶极跃迁及禁戒跃迁方面．

Pt Ⅲ 离子属于 OsI 等电子数序列，这个序列的光谱无论是理论计算还是实验都很少[5~10]，仅有基态和最低的几个激发组态被进行了研究，Pt 离子的 $5d^8$-$5d^76p$ 则既无理论预言也无实验观测．为此，本文旨在从理论上分析上述跃迁的光谱特性，为实验提供辨认归类的依据，为保证计算的可靠性，本文采用了多组态 HFR 方法[11]．

2　理论和计算方法

有关组态相互作用理论和多组态 HFR 方法的详细叙述可参见文献〔12,13〕，本文不再赘述，只将与本文计算有关的内容概述如下：

原子序数为 Z 的 N 个电子原子的状态波函数应为原子所有组态（束缚态及连续态）的无微扰态构成的反对称波函数的线性组合

$$\Psi_a = \sum_i C_i \Psi_i(\varphi_1,\ \varphi_2,\ \cdots\cdots,\ \varphi_N), \tag{1}$$

式中，Ψ_i 为由无微扰态波函数构成的反对称（行列式）波函数，C_i 为组态混合系数，原子的无微扰态波函数

$$\varphi_i = (1/r)P_{nl}(r)Y_{lm_l}\chi_{sm_s}, \tag{2}$$

可由 Hartree-Fock 方程加相对论性修正（质量-速度修正和 Darwin 项修正）而求解

$$\Big\{-\frac{d^2}{dr^2} + \frac{l_i(l_i+1)}{r^2} + V^i(r) - \frac{\alpha^2}{4}[\varepsilon_i - V^i(r)]^2$$

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$$-\delta_{io}\frac{\alpha^2}{4}[1+\frac{\alpha^2}{4}(\varepsilon_i+V^i(r)]^{-1}\frac{dV^i}{dr}\left(\frac{dP_i/dr}{P_i}-\frac{1}{r}\right)\Bigg\}P_i(r)=\varepsilon_iP_i(r), \tag{3}$$

$$\left.\begin{aligned}
V^i(r) &= -\frac{2Z}{r}+\sum_{j=1}^{q}(W_j-\delta_{ij})\int_0^\infty\frac{2}{r_>}P_j^2(r_2)dr_2-(W_i-1)A_i(r)\\
&\qquad -\sum_{j(\neq i)=1}^{q}W_j[\delta_{l_il_j}\varepsilon_{ij}+B_{ij}(r)]\frac{P_j(r)}{P_i(r)},\\
A_i(r) &= \frac{2l_i+1}{4l_i+1}\sum_{k>0}\begin{pmatrix} l_i & K & l_j\\ 0 & 0 & 0\end{pmatrix}^2\int_0^\infty\frac{2r_<^k}{r_>^{k+1}}P_i^2(r_2)dr_2,\\
B_{ij}(r) &= (1/r)\sum_k\begin{pmatrix} l_i & k & l_j\\ 0 & 0 & 0\end{pmatrix}^2\int_0^\infty\frac{2r_<^k}{r_>^{k+1}}P_j(r_2)P_i(r_2)dr_2,
\end{aligned}\right\} \tag{4}$$

式中 α 为精细结构常数，V^i 为 HF 势函数. 实际计算中只能考虑有限数目的组态，优先考虑的应是组态相互作用较强的那些组态. 根据分析，本文在计算中选择如下组态：

偶宇称组态：$5d^8$，$5d^76s$，$5d^66s^2$ 和奇宇称组态：$5d^76p$，$5d^66s6p$.

本文采用的计算程序是基于 Slater-Condon 的理论的原子结构和光谱计算程序库 RCN34/RCN2/RCG9[11]. 此程序首先用 HFR 方法计算各组态的能量参数即组态平均能量 E_{av}，静电相互作用积分 F^K、G^K 自旋-轨道相互作用积分 ζ_i 和组态相互作用积分 R^k，然后用拉卡代数方法求出与上述各参数相联系的角向部分 f_k、g_k、d_j 和 r_k，最后求出原子各状态能量本征值及电偶极跃迁的光谱.

由于理论模型的固有近似，计算中对能量参数 F^k、G^k 和 R^k 作了调整. 文献[11,12]指出大量计算表明，对中性或低电离原子，将上述参数调正为原始计算值的 70% ～ 80% 可得到与实验相符合的结果. Pt Ⅱ 属低电离原子，因此将 F^k、G^k 和 R^k 分别调正至原始计算值的 80%、80% 和 85%，其中 R^k 的百分比稍高的原因是由于考虑的组态已包括了绝大部分组态之间的相互作用，$5d^8$ 及 $5d^76p$ 与本文未考虑的其它组态之间的相互作用均很弱. 自旋-轨道相互作用未调整的原因是它是由精确的 Blume-Waston 方法[12]求得的. 这样的调整可得到较准确的计算结果.

3　结果和讨论

因篇幅所限，表 1 列出了部分 $5d^8$-$5d^76p$ 跃迁的波长、振子强度和跃迁几率，因谱项混合严重，$5d^76p$ 组态的各态能级值难以用 LS 耦合或 JJ 耦合符号标定，因此采用真实能级值及总角动量量子数 J 值标定. 表 2 列出了 $5d^8$ 组态的能级值和 LS 耦合表象下谱项的百分比，N 为同一 J 值下各能级的序号，$N=1$ 对应最低能级值，以此类推. 表 3 列出了 $5d^76p$ 组态的能级值及 JJ 耦合表象下各谱项所占能级的百分比，表中 J 和 N 值的意义同表 2. 由计算结果看出：

1）　由于自旋轨道相互作用较大，使各组态能级能量范围较大，导致 $5d^8$-$5d^76p$ 跃迁占有一很大的波长范围，其中绝大部分处于极紫外波段.

2）　与相互作用的组态平均能量间隔相比，组态相互作用（R^k）不是很大，其中唯有 $5d^8$ 与 $5d^76s$ 间相互作用较强，因此谱项混合主要是同一组态内的混合，不同组态间谱项混合不严重.

3）　对 $5d^8$ 组态来说，较多地倾向于 LS 耦合如对 $J=0$，$N=2$ 能级，^1S 谱占优势，但有少量 $^3P(14\%)$ 与之混合，而 $J=0$，$N=1$ 能级则 ^3P 谱项占优势，少量 $^1S(14\%)$ 与之混合，从而导致它们的能量差别. 除 $J=2$ 的能级外，$5d^8$ 组态各能级值可按占最大百分比的谱项标定.

Table 1 Calculated lines of the $5d^8$-$5d^76p$ transitions of the Pt Ⅲ ion.

(0.1 nm)	Gf	GA(sec^{-1})	J—J	Transitions
904.3860	0.4998	4.076E+09	2.0-2.0	(^1D) ^1D-116.3615
903.4341	0.6128	5.008E+09	2.0-3.0	(^3F) ^3F-125.9925
900.9882	0.1885	1.549E+09	3.0-3.0	(^3F) ^3F-121.2654
900.4758	0.3603	2.963E+09	4.0-5.0	(^3F) ^3F-111.0510
898.0671	0.0388	3.212E+08	3.0-4.0	(^3F) ^3F-121.6264
897.2147	0.3219	2.667E+09	4.0-3.0	(^3F) ^3F-111.4546
895.5894	0.0904	7.521E+08	0.0-1.0	(^3P) ^3P-127.7786
894.5247	0.0978	8.153E+08	1.0-1.0	(^3P) ^3P-130.1567
893.2961	0.0647	5.410E+08	2.0-2.0	(^1D) ^1D-117.7342
893.1186	0.2514	2.102E+09	1.0-2.0	(^3P) ^3P-130.3327
891.9669	0.8017	6.721E+09	4.0-3.0	(^1G) ^1G-133.9935
891.6422	0.0265	2.225E+08	4.0-3.0	(^3F) ^3F-112.1512
890.6717	0.2488	2.092E+09	2.0-2.0	(^1D) ^1D-137.8326
890.4034	0.0744	6.258E+08	3.0-2.0	(^3F) ^3F-122.5848
890.3549	0.0574	4.831E+08	2.0-3.0	(^1D) ^1D-118.1040
889.0873	0.2479	2.092E+09	2.0-1.0	(^3F) ^3F-127.7786
888.9228	0.1990	1.680E+09	1.0-0.0	(^3P) ^3P-130.8611
884.4136	0.1791	1.527E+09	2.0-2.0	(^3F) ^3F-128.3730
883.0187	0.5614	4.802E+09	4.0-3.0	(^3F) ^3F-113.2465
882.0956	0.1350	1.157E+09	3.0-3.0	(^3F) ^3F-123.6426
880.1524	0.0942	8.110E+08	2.0-3.0	(^1D) ^1D-139.1744
879.1511	0.5669	4.892E+09	4.0-3.0	(^1G) ^1G-135.6278
878.6034	0.0209	1.807E+08	2.0-3.0	(^3F) ^3F-129.1207
877.7714	0.0198	1.710E+08	2.0-3.0	(^1D) ^1D-119.7141
876.9135	0.0925	8.026E+08	0.0-1.0	(^3P) ^3P-130.1567
875.2068	0.0030	2.588E+07	3.0-4.0	(^3F) ^3F-124.5349
871.9002	0.0002	1.396E+06	2.0-1.0	(^1D) ^1D-120.4813

Note: Units of the upper energy levels: 1000 cm^{-1}

Table 2 Engergy levels(in cm^{-1})in the configuration $5d^8$ of Pt Ⅲ

J	N	Energy Level	Percentage Compositions
0	2	46411	79% ^1S + 14% ^3P
	1	16120	75% ^3P + 14% ^1S
1	1	18365	91% ^3P
2	3	25558	46% ^1D + 35% ^3F + 14% ^3P
	2	15304	45% ^3P + 45% ^3F + 4% ^1D
	1	5789	46% ^1D + 34% ^3P + 16% ^3F
3	1	10276	98% ^3F
4	2	21882	90% ^1G + 4% ^3F
	1	-1	95% ^3F + 4% ^1G

Table 3　Energy levels (in cm^{-1}) and percentage of the levels of the $5d^76p$ Configuration of Pt Ⅱ.

J	N	Energy levels	Percentage composition in J_j
0.0	7	146334	67% $({}^2D_{3/2})_{3/2}$ + 10% $({}^2P_{3/2})_{3/2}$
	6	130861	53% $({}^2D_{3/2})_{3/2}$ + 19% $({}^2P_{3/2})_{3/2}$
	5	124831	48% $({}^4P_{3/2})_{3/2}$ + 21% $({}^2P_{3/2})_{3/2}$
	4	113628	52% $({}^4F_{3/2})_{3/2}$ + 14% $({}^4P_{3/2})_{3/2}$
	3	110734	55% $({}^2P_{1/2})_{1/2}$ + 13% $({}^4F_{3/2})_{1/2}$
	2	103844	35% $({}^2P_{3/2})_{3/2}$ + 24% $({}^4P_{1/2})_{1/2}$
	1	97717	30% $({}^4P_{1/2})_{1/2}$ + 22% $({}^2P_{1/2})_{1/2}$
1.0	19	146886	28% $({}^2D_{5/2})_{3/2}$ + 20% $({}^2D_{3/2})_{1/2}$
	18	140401	67% $({}^2D_{3/2})_{1/2}$ + 15% $({}^2D_{5/2})_{3/2}$
	17	134590	23% $({}^2D_{3/2})_{1/2}$ + 21% $({}^2D_{3/2})_{1/2}$
	16	130157	35% $({}^2D_{3/2})_{1/2}$ + 24% $({}^2P_{3/2})_{1/2}$
	15	127770	35% $({}^2F_{5/2})_{3/2}$ + 11% $({}^4P_{1/2})_{1/2}$
	14	124344	29% $({}^2F_{5/2})_{3/2}$ + 18% $({}^2P_{1/2})_{1/2}$
	13	123188	25% $({}^4P_{1/2})_{1/2}$ + 17% $({}^2D_{5/2})_{3/2}$
	12	120936	16% $({}^2D_{5/2})_{3/2}$ + 14% $({}^4P_{3/2})_{1/2}$
	11	120481	14% $({}^4P_{3/2})_{1/2}$ + 13% $({}^2D_{3/2})_{1/2}$
	10	120144	29% $({}^4P_{1/2})_{1/2}$ + 14% $({}^2P_{1/2})_{1/2}$
	9	114677	37% $({}^4P_{5/2})_{3/2}$ + 19% $({}^2P_{1/2})_{1/2}$
	8	113881	31% $({}^4P_{5/2})_{3/2}$ + 21% $({}^2P_{1/2})_{1/2}$
	7	111285	27% $({}^2P_{3/2})_{1/2}$ + 24% $({}^4P_{3/2})_{1/2}$
	6	109612	25% $({}^4F_{5/2})_{3/2}$ + 22% $({}^4P_{5/2})_{3/2}$
	5	108920	24% $({}^4P_{3/2})_{1/2}$ + 16% $({}^4F_{3/2})_{1/2}$
	4	104018	24% $({}^4F_{3/2})_{1/2}$ + 15% $({}^2D_{3/2})_{1/2}$
	3	101632	45% $({}^4P_{1/2})_{1/2}$ + 23% $({}^2P_{1/2})_{1/2}$
	2	97204	35% $({}^4F_{3/2})_{1/2}$ + 28% $({}^4P_{3/2})_{1/2}$
	1	89932	36% $({}^2P_{1/2})_{1/2}$ + 20% $({}^2D_{3/2})_{1/2}$
2.0	25	150377	41% $({}^2D_{5/2})_{1/2}$ + 22% $({}^2D_{5/2})_{1/2}$
	24	146771	55% $({}^2D_{3/2})_{1/2}$ + 15% $({}^2D_{3/2})_{1/2}$
	23	139174	40% $({}^2D_{5/2})_{1/2}$ + 19% $({}^2D_{5/2})_{1/2}$
	22	137833	45% $({}^2D_{3/2})_{1/2}$ + 12% $({}^2D_{3/2})_{1/2}$
	21	133692	24% $({}^2D_{3/2})_{1/2}$ + 22% $({}^2F_{7/2})_{3/2}$
	20	130333	23% $({}^2F_{7/2})_{3/2}$ + 22% $({}^2D_{3/2})_{1/2}$
	19	128373	30% $({}^2F_{5/2})_{1/2}$ + 12% $({}^2P_{1/2})_{3/2}$
	18	125483	21% $({}^2F_{5/2})_{1/2}$ + 17% $({}^2P_{1/2})_{3/2}$
	17	124943	26% $({}^2P_{1/2})_{3/2}$ + 16% $({}^2G_{7/2})_{3/2}$
	16	122585	18% $({}^4P_{3/2})_{1/2}$ + 13% $({}^2F_{5/2})_{1/2}$
	15	120207	15% $({}^2D_{5/2})_{1/2}$ + 11% $({}^2G_{7/2})_{3/2}$
	14	117734	28% $({}^2D_{3/2})_{3/2}$ + 16% $({}^2G_{7/2})_{1/2}$
	13	116362	28% $({}^4P_{1/2})_{3/2}$ + 14% $({}^2P_{1/2})_{3/2}$
	12	114975	66% $({}^2F_{7/2})_{1/2}$ + 15% $({}^2D_{5/2})_{1/2}$
	11	113494	25% $({}^4P_{5/2})_{1/2}$ + 14% $({}^2D_{5/2})_{1/2}$
	10	111259	20% $({}^4P_{1/2})_{3/2}$ + 19% $({}^4P_{5/2})_{1/2}$
	9	109662	17% $({}^4F_{7/2})_{3/2}$ + 16% $({}^4P_{3/2})_{1/2}$
	8	107705	36% $({}^4F_{3/2})_{1/2}$ + 10% $({}^4P_{3/2})_{1/2}$
	7	105571	33% $({}^4P_{3/2})_{1/2}$ + 17% $({}^4F_{7/2})_{3/2}$
	6	103809	33% $({}^4F_{5/2})_{1/2}$ + 11% $({}^4P_{5/2})_{1/2}$
	5	102193	22% $({}^4F_{7/2})_{3/2}$ + 21% $({}^2P_{3/2})_{1/2}$
	4	96506	41% $({}^4F_{3/2})_{1/2}$ + 23% $({}^4P_{3/2})_{1/2}$
	3	95800	48% $({}^4P_{5/2})_{1/2}$ + 22% $({}^4F_{5/2})_{1/2}$
	2	91346	24% $({}^4F_{5/2})_{1/2}$ + 16% $({}^2P_{3/2})_{1/2}$
	1	90291	24% $({}^2P_{3/2})_{1/2}$ + 17% $({}^4P_{3/2})_{1/2}$
3.0	24	151939	41% $({}^2D_{5/2})_{1/2}$ + 15% $({}^2D_{5/2})_{1/2}$
	23	147772	64% $({}^2D_{3/2})_{3/2}$ + 14% $({}^2P_{3/2})_{3/2}$
	22	140592	42% $({}^2D_{5/2})_{1/2}$ + 17% $({}^2D_{5/2})_{1/2}$
	21	135628	38% $({}^2F_{7/2})_{1/2}$ + 21% $({}^2F_{5/2})_{1/2}$
	20	133993	36% $({}^2D_{3/2})_{3/2}$ + 17% $({}^2P_{3/2})_{3/2}$
	19	129121	25% $({}^2H_{9/2})_{3/2}$ + 22% $({}^2F_{5/2})_{1/2}$
	18	125992	37% $({}^2F_{3/2})_{3/2}$ + 9% $({}^2H_{9/2})_{3/2}$
	17	123643	38% $({}^2F_{7/2})_{1/2}$ + 13% $({}^2D_{5/2})_{1/2}$
	16	121256	17% $({}^2G_{7/2})_{1/2}$ + 15% $({}^2H_{9/2})_{3/2}$
	15	119714	15% $({}^4P_{3/2})_{3/2}$ + 13% $({}^4F_{3/2})_{3/2}$
	14	118104	58% $({}^2G_{7/2})_{1/2}$ + 13% $({}^2D_{5/2})_{5/2}$
	13	115460	29% $({}^2F_{5/2})_{1/2}$ + 21% $({}^2G_{9/2})_{3/2}$
	12	113246	17% $({}^4P_{5/2})_{1/2}$ + 17% $({}^2F_{5/2})_{1/2}$
	11	112151	16% $({}^4F_{5/2})_{1/2}$ + 16% $({}^2F_{5/2})_{1/2}$
	10	111455	58% $({}^2D_{5/2})_{1/2}$ +9% $({}^4P_{5/2})_{1/2}$
	9	108772	30% $({}^4F_{3/2})_{3/2}$ + 22% $({}^4P_{3/2})_{3/2}$
	8	108167	30% $({}^2G_{7/2})_{1/2}$ + 21% $({}^2D_{5/2})_{1/2}$
	7	106063	19% $({}^4F_{4/2})_{1/2}$ + 18% $({}^2G_{7/2})_{1/2}$
	6	103253	22% $({}^4F_{5/2})_{1/2}$ + 21% $({}^2P_{3/2})_{3/2}$

J	N	Energy levels	Percentage composition in J_j
	5	102705	$38\%\ ({}^4F_{7/2})_{1/2} + 13\%\ ({}^4P_{5/2})_{1/2}$
	4	98674	$35\%\ ({}^4F_{9/2})_{3/2} + 28\%\ ({}^4P_{5/2})_{1/2}$
	3	97309	$30\%\ ({}^4F_{5/2})_{1/2} + 19\%\ ({}^4P_{5/2})_{1/2}$
	2	91656	$36\%\ ({}^4F_{5/2})_{1/2} + 12\%\ ({}^4P_{5/2})_{1/2}$
	1	89595	$59\%\ ({}^4F_{7/2})_{1/2} + 11\%\ ({}^4F_{9/2})_{3/2}$
4.0	18	147919	$40\%\ ({}^2D_{5/2})_{3/2} + 17\%\ ({}^2D_{5/2})_{3/2}$
	17	131952	$50\%\ ({}^2F_{7/2})_{1/2} + 12\%\ ({}^2G_{7/2})_{1/2}$
	16	127739	$47\%\ ({}^2H_{9/2})_{1/2} + 13\%\ ({}^2F_{5/2})_{3/2}$
	15	125985	$45\%\ ({}^2F_{5/2})_{3/2} + 11\%\ ({}^2H_{9/2})_{1/2}$
	14	124535	$24\%\ ({}^2H_{11/2})_{3/2} + 19\%\ ({}^2G_{7/2})_{1/2}$
	13	121626	$18\%\ ({}^2D_{5/2})_{3/2} + 17\%\ ({}^2F_{7/2})_{1/2}$
	12	120532	$31\%\ ({}^2F_{7/2})_{1/2} + 27\%\ ({}^2D_{5/2})_{3/2}$
	11	116978	$50\%\ ({}^2G_{7/2})_{1/2} + 16\%\ ({}^2H_{9/2})_{1/2}$
	10	115849	$44\%\ ({}^2H_{11/2})_{3/2} + 21\%\ ({}^2H_{9/2})_{1/2}$
	9	110514	$50\%\ ({}^2G_{9/2})_{1/2} + 14\%\ ({}^2H_{9/2})_{1/2}$
	8	108394	$53\%\ ({}^4P_{5/2})_{3/2} + 23\%\ ({}^4P_{5/2})_{3/2}$
	7	106185	$66\%\ ({}^2G_{7/2})_{1/2} + 14\%\ ({}^2F_{7/2})_{1/2}$
	6	103618	$31\%\ ({}^4F_{5/2})_{3/2} + 16\%\ ({}^4P_{5/2})_{3/2}$
	5	102504	$44\%\ ({}^4F_{7/2})_{1/2} + 12\%\ ({}^4F_{9/2})_{1/2}$
	4	100107	$39\%\ ({}^4F_{7/2})_{1/2} + 24\%\ ({}^2G_{9/2})_{1/2}$
	3	94954	$52\%\ ({}^4F_{9/2})_{1/2} + 19\%\ ({}^2G_{9/2})_{1/2}$
	2	91296	$72\%\ ({}^4F_{7/2})_{1/2} + 11\%\ ({}^4F_{9/2})_{1/2}$
	1	80320	$77\%\ ({}^4F_{9/2})_{1/2} + 16\%\ ({}^2G_{9/2})_{1/2}$
5.0	11	131993	$64\%\ ({}^2F_{7/2})_{3/2} + 13\%\ ({}^2H_{9/2})_{1/2}$
	10	129111	$59\%\ ({}^2H_{9/2})_{1/2} + 16\%\ ({}^2G_{9/2})_{1/2}$
	9	119493	$71\%\ ({}^2H_{11/2})_{1/2} + 13\%\ ({}^2G_{7/2})_{3/2}$
	8	117348	$60\%\ ({}^2G_{7/2})_{3/2} + 23\%\ ({}^2F_{7/2})_{3/2}$
	7	115712	$46\%\ ({}^2H_{9/2})_{1/2} + 25\%\ ({}^2G_{9/2})_{1/2}$
	6	111051	$54\%\ ({}^2G_{9/2})_{1/2} + 24\%\ ({}^2H_{9/2})_{1/2}$
	5	106529	$86\%\ ({}^2H_{11/2})_{1/2} + 4\%\ ({}^2H_{11/2})_{1/2}$
	4	101821	$88\%\ ({}^4F_{7/2})_{3/2} + 6\%\ ({}^2G_{7/2})_{3/2}$
	3	100102	$50\%\ ({}^2G_{9/2})_{1/2} + 22\%\ ({}^2H_{9/2})_{1/2}$
	2	91496	$77\%\ ({}^4F_{9/2})_{1/2} + 13\%\ ({}^2G_{9/2})_{1/2}$
	1	81860	$78\%\ ({}^4F_{9/2})_{1/2} + 15\%\ ({}^2G_{9/2})_{1/2}$
6.0	5	125848	$71\%\ ({}^2H_{9/2})_{3/2} + 27\%\ ({}^2G_{9/2})_{3/2}$
	4	117490	$95\%\ ({}^2H_{11/2})_{1/2} + 2\%\ ({}^2H_{11/2})_{1/2}$
	3	109560	$54\%\ ({}^2G_{9/2})_{3/2} + 29\%\ ({}^2H_{9/2})_{3/2}$
	2	105561	$95\%\ ({}^2H_{11/2})_{1/2}$
	1	91140	$81\%\ ({}^4F_{9/2})_{3/2} + 15\%\ ({}^2G_{9/2})_{3/2}$
7.0	1	114613	$100\%\ ({}^2H_{11/2})_{3/2}$

对 $5d^8$ 组态 $J=2$ 的三个能级由于谱项混合严重(百分比不大于50%)，因此能级值的标定是按等电子数序列的类比而标定的[7]. 即 ${}^3F_2$ 代表能级值为 25558 的能级，${}^3P_2$ 和 ${}^1D_2$ 分别代表 15304 和 5789 两能级.

4) 对 $5d^76p$ 组态来说，LS 耦合和 JJ 耦合都不是好的耦合表象，但从整个情形看来，稍稍倾向于 JJ 耦合. 因此这里给出了 JJ 耦合表象下各谱项所占能级的百分比. 就某一 J 值而言，由于强烈的自旋轨道相互作用使各谱项之间混合严重，混合比例的不同导致能量上的差别，如前所述，这种情况下能级难以用 LS 耦合或 JJ 耦合的符号标定，只能用真实能级值和总角动量量子数 J 值标定. 对 $5d^76p$ 组态，静电相互作用与自旋轨道相互作用强烈竞争，且自旋轨道相互作用有占优势的趋向.

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A Calculation of XUV spectra of $5d^8$-$5d^76p$ transition array of Pt Ⅲ ion

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Abstract

The XUV spectra of $5d^8$-$5d^76p$ transition array of Pt Ⅲ ion is predicted with the aid of the multi-configurations HFR method. The wavelengths, energy levels, oscillator strengths and radiative transition probability are obtained and these results are analysed.

Key words XUV spectra, configuration, energy parameter.