



SAKARYA ÜNİVERSİTESİ

# FEN BİLİMLERİ ENSTİTÜSÜ DERGİSİ

Sakarya University Journal of Science  
SAUJS

e-ISSN 2147-835X Period Bimonthly Founded 1997 Publisher Sakarya University  
<http://www.saujs.sakarya.edu.tr/>

Title: An Investigation on Electric Dipole Transitions of Pt LXVII

Authors: Gülay GÜNDAY KONAN

Received: 2021-11-08 00:00:00

Accepted: 29.12.2021

Article Type: Research Article

Volume: 26

Issue: 1

Month: February

Year: 2022

Pages: 149-155

How to cite

Gülay GÜNDAY KONAN; (2022), An Investigation on Electric Dipole Transitions of Pt LXVII. Sakarya University Journal of Science, 26(1), 149-155, DOI: 10.16984/saufenbilder.1020582

Access link

<http://www.saujs.sakarya.edu.tr/tr/pub/issue/67934/1020582>

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<http://dergipark.gov.tr/journal/1115/submission/start>

## An Investigation on Electric Dipole Transitions of Pt LXVII

Gülay GÜNDAY KONAN\*<sup>1</sup>

### Abstract

In the present work, we have reported the energy levels, wavelengths, weighted oscillator strengths, and transition probabilities for electric dipole (E1) transitions of magnesium like platinum (Pt LXVII, Z=78). Accurate knowledge of Mg-like ions are of great importance for astrophysics, plasma, and thermonuclear fusion research. The atomic data are calculated with the AUTOSTRUCTURE code, where relativistic corrections are introduced according to the Breit–Pauli distorted wave approach. In the calculations, quantum electrodynamics effects and correlation contributions have been considered. The present results are in good agreement with other available values. There are no experimental works for Pt LXVII in the literature. We predict new theoretical data for several levels will be helpful for future experimental works.

**Keywords:** Energy level, transition probability, oscillator strength, wavefunction

### 1. INTRODUCTION

In fusion research such as International Thermonuclear Experimental Reactor (ITER) project [1], there is a need for more accurate atomic data for energy levels, wavelengths, oscillator strengths, and radiative rates for a wide range of ions. So the interest in highly ionized heavy atoms is a subject of active research. Also, Mg-like ions play an important role in atomic physics, astrophysics, plasma, and thermonuclear fusion research [2-3]. In this framework, we have computed energy levels and radiative parameters for highly ionized Mg-like platinum (Pt LXVII, Z=78). A few works have been reported atomic data of Mg-like platinum.

Hu. et al. reported the transition parameters between the  $3l$  levels for electric dipole transitions for Mg-like ions [4]. The energies of  $3s3p$ ,  $3p^2$ ,

$3s3d$ ,  $3p3d$ , and  $3d^2$  levels in Mg-like Pt have been given by Santana [5,6]. Iorga and Stancalie have studied energy levels and transition parameters for Mg-like Pt using Flexible Atomic Code [7]. There is no experimental data in the literature.

In this paper, the AUTOSTRUCTURE atomic code is performed to calculate the energy levels and electric dipole wavelengths, oscillator strengths, transition probabilities for Mg-like Pt. The present study has been performed as a part of a continuing study on Mg-like ions [8-12].

### 2. METHOD OF CALCULATION

AUTOSTRUCTURE atomic code [13, 14] is a general program for the calculation of atomic and ionic energy levels, radiative and autoionization rates and photoionization cross sections using

\* Corresponding author: ggunday@sakarya.edu.tr

<sup>1</sup> Sakarya University, Faculty of Science and Literature, Department of Physics  
ORCID: <https://orcid.org/0000-0003-1086-995X>

nonrelativistic or semi-relativistic wavefunctions. The program uses Fortran 77/95 programming language and Unix or Windows operating systems. In AUTOSTRUCTURE atomic code, the configuration set is chosen optionally and added new configuration to improve accuracy (a configuration interaction expansion, CI expansion). The CI expansion is related to the choice of radial functions. Each (*nl*) radial function is calculated in Thomas-Fermi or Slater-Type-Orbital potential model. The Hamiltonian in any coupling model (LS, IC or ICR) is diagonalized to obtain eigenvalues and eigenvectors with which to construct the rates. This code makes use of non-relativistic or kappa-averaged relativistic wavefunctions and the full Breit interaction in the Pauli approximation. AUTOSTRUCTURE program steps are summarized in Figure 1.

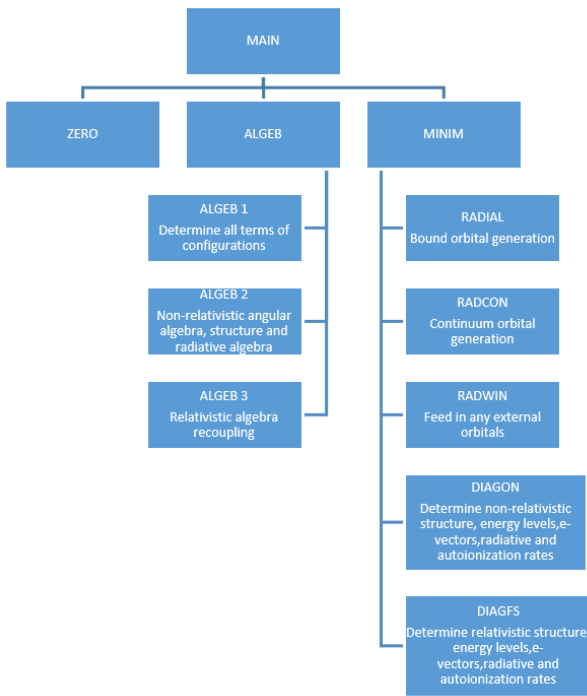


Figure 1 Program Steps of Autostructure [15]

The Hamiltonian can be written as

$$H_{BP} = H_{NR} + H_{RC} \quad (1)$$

where  $H_{NR}$  is the usual nonrelativistic Hamiltonian

$$H_{NR} = \sum_{i=1}^N h(i) + \sum_{j>i=1}^N \frac{1}{r_{ij}} = \sum_{i=1}^N \left( -\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} \right) + \sum_{j>i=1}^N \frac{1}{r_{ij}} \quad (2)$$

and  $H_{RC}$  contains the relativistic correction operators which include one-body relativistic operators (spin-orbit interaction, the non-fine-structure mass variation, and the one-body Darwin corrections) and two-body Breit operators (spin-other-orbit, the mutual spin-spin, the spin-spin contact, the two body Darwin and the orbit-orbit terms). Beside, quantum electrodynamics (QED) contributions (vacuum polarization and self-energy contributions) are treated as a perturbation.

For transitions, code computes Einstein coefficients and associated quantities for multipole transitions of low multipolarity (for electric dipole, E1, radiation). Generally, electric multipole transitions exist in LS coupling. As intermediate coupling wave functions contain admixtures of order  $\alpha^2$ , radiative operators must also be expanded up to Breit contributions order.

In the long wavelength low intensity approximation the probability for spontaneous emission by E1 radiation,

$$A_{i' \rightarrow i} = 2.6774 \times 10^9 \frac{(E_i - E_{i'})^3}{g_i} \cdot S(i, i') \quad (3)$$

where,  $g_i$  is statistical weighted of level,  $E_i$  and  $E_{i'}$  are energies of levels and  $S(i, i')$  is line strengths in form

$$S(i, i') = \left| \langle i' || R^{[k]} || i \rangle \right|^2 \quad (4)$$

where  $R^{[k]}$  is a transition operator and describes each multipole,  $k$  is 1 for electric dipole radiation. In addition weighted absorption or emission oscillator strength ( $gf$ ) value can be written in terms of line strengths

$$(gf)_{i, i'} = (gf)_{i', i} = \frac{|E_i - E_{i'}|}{3} \cdot S(i, i') \quad (5)$$

The method has been described in detail in [13-16].

### 3. RESULT AND DISCUSSION

The AUTOSTRUCTURE calculations have been performed for the energy levels and electric dipole transitions in Mg-like platinum. Mg-like ions have an electronic structure with ten electrons in the closed shells and two valence electrons ( $1s^2 2s^2 2p^6 3s^2$ ). Since they have been observed in solar plasmas [17,18] and laboratory plasmas [19], accurate data are needed for these ions. In this paper, we have calculated relativistic energies, for the levels of  $3snl$  ( $n = 3-6, l = 0-4$ ),  $3pnl$  ( $n = 3-6, l = 0-4$ ),  $3dnl$  ( $n = 3-6, l = 0-4$ ),  $2p^5 3s^2 3p$ ,  $2p^5 3s 3p^2$ ,  $2p^5 3p^3$ ,  $2p^5 3s^2 3d$ ,  $2p^5 3s^2 4s$ ,  $2p^5 3s 3p 3d$ ,  $2p^5 3p^2 3d$ ,  $2p^5 3d^3$ ,  $2p^5 3s 3d^2$ ,  $2p^5 3s 3p 4s$ ,  $2p^5 3p 3d^2$ ,  $2p^5 3p 3d 4s$ ,  $2p^4 3s^2 3p^2$ ,  $2p^4 3s 3p^3$ ,  $2p^4 3s^2 3d^2$ ,  $2p^4 3s^2 3p 3d$ ,  $2s 2p^5 3s^2 3p 3d$  configurations and the transition parameters such as wavelengths, weighted oscillator strengths and transition probabilities for electric dipole (E1) transitions between these levels. In the calculations QED (self-energy and vacuum polarization) and Breit interaction (magnetic interaction between the electrons and retardation effects of the electron-electron interaction) contributions have been taken into account. Beside various correlation effects (valence-valence (VV), core-valence (CV) and core-core (CC)), have been considered.

Table 1 displays the energies of  $3l3l'$  ( $l, l' = 0, 1, 2$ ) levels relative to  $3s^2 \ ^1S_0$  ground-state level. To assess the accuracy and reliability of our present results, our AUTOSTRUCTURE energies have been compared with the other theoretical results of the relativistic Multi-Reference Møller-Plesset

(MR-MP) theory based on the relativistic Dirac-Coulomb-Breit Hamiltonian [6] and the multi-configuration Dirac-Hartree-Fock (MCDHF) which the Breit interaction and leading quantum electrodynamics effects are included as perturbations [4] and fully relativistic model-potential Flexible Atomic Code [7]. There is no experimental data in the literature. We found the percentage difference to compare our results with these methods. The percent difference is calculated using the formula of  $\left| \frac{E_{tw} - E_{ow}}{E_{ow}} \right| \times 100$ .  $E_{tw}$  and  $E_{ow}$  show our results and other results, respectively. When we evaluate the percentage differences results, the differences (%) are less than 0.59 for MR-MP, less than 0.53 for FAC, and less than 0.58 for MCDHF. Additionally, the energy levels have been compared with other works drawing a graph. Figure 2 shows the comparison for energy levels. Linear correlation coefficient  $R^2$  is 1. The agreement between the presented data is strong evidence for the reliability of the AUTOSTRUCTURE calculations.

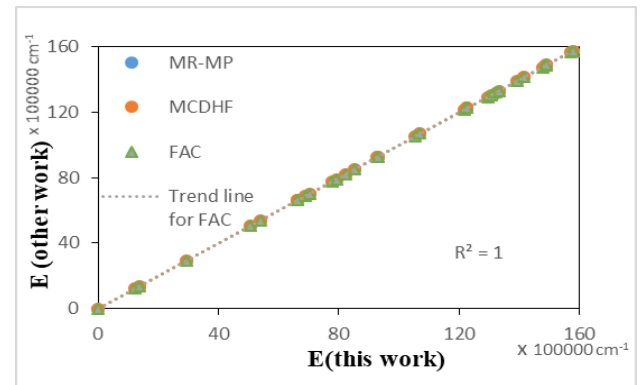


Figure 2 The comparison for energy levels between present AUTOSTRUCTURE results and other MR-MP [6] and MCDHF [4] and FAC [7] results

Table 1 Energy levels ( $\text{cm}^{-1}$ ) and differences (%) in energies for Pt LXVII

Index	Levels	Energy Levels					Diff. %		
		This work A.S.	Other Works			MR-MP <sup>a</sup>	MCDHF <sup>b</sup>	FAC <sup>c</sup>	
			MR-MP <sup>a</sup>	MCDHF <sup>b</sup>	FAC <sup>c</sup>				
1	$3s^2 \ ^1S_0$	0	0	0	0	0.00	0.00		
2	$3s3p \ ^3P_0$	1225050	1227195	1224802.1	1226702.5	0.17	0.02	0.13	
3	$3s3p \ ^3P_1$	1369147	1363754	1361799.7	1364076.39	0.40	0.54	0.37	
4	$3p^2 \ ^3P_0$	2927825	2921397	2918146.63	2925339.9	0.22	0.33	0.08	
5	$3s3p \ ^3P_2$	5057707	5050746	5054646.66	5054114.98	0.14	0.06	0.07	
6	$3s3p \ ^1P_1$	5379831	5369075	5373970.93	5374991.19	0.20	0.11	0.09	

7	3p <sup>2</sup>	<sup>1</sup> D <sub>2</sub>	6616898	6603313	6604114.46	6606939.52	0.21	0.19	0.15
8	3p <sup>2</sup>	<sup>3</sup> P <sub>1</sub>	6632746	6622421	6624625.98	6628428.54	0.16	0.12	0.07
9	3s3d	<sup>3</sup> D <sub>1</sub>	6902987	6896371	6895334.73	6900009.79	0.10	0.11	0.04
10	3s3d	<sup>3</sup> D <sub>2</sub>	7027544	7015382	7016204.56	7021734.91	0.17	0.16	0.08
11	3s3d	<sup>3</sup> D <sub>3</sub>	7795847	7754192	7753843.2	7756145.08	0.54	0.54	0.51
12	3s3d	<sup>1</sup> D <sub>2</sub>	7946414	7899749	7900846.29	7904214.68	0.59	0.58	0.53
13	3p3d	<sup>3</sup> F <sub>2</sub>	8225287	8217167	8214111.06	8218841.72	0.10	0.14	0.08
14	3p3d	<sup>3</sup> D <sub>1</sub>	8523303	8516747	8514797.93	8521718.88	0.08	0.10	0.02
15	3p3d	<sup>3</sup> P <sub>2</sub>	9276423	9237871	9235690.69	9239301.91	0.42	0.44	0.40
16	3p3d	<sup>3</sup> F <sub>3</sub>	9313664	9266005	9264352.53	9268160.41	0.51	0.53	0.49
17	3p <sup>2</sup>	<sup>3</sup> P <sub>2</sub>	10524747	10505626	10514459.09	10516028.5	0.18	0.10	0.08
18	3p <sup>2</sup>	<sup>1</sup> S <sub>0</sub>	10688467	10672224	10681784.45	10684558	0.15	0.06	0.04
19	3p3d	<sup>3</sup> D <sub>2</sub>	12166079	12155328	12158656.26	12161963.2	0.09	0.06	0.03
20	3p3d	<sup>3</sup> P <sub>0</sub>	12245423	12241460	12244988.02	12249071.1	0.03	0.00	0.03
21	3p3d	<sup>1</sup> F <sub>3</sub>	12252878	12241637	12245796.14	12249788.9	0.09	0.06	0.03
22	3p3d	<sup>3</sup> P <sub>1</sub>	12260695	12245435	12249013.68	12253015.1	0.12	0.10	0.06
23	3p3d	<sup>3</sup> F <sub>4</sub>	12962287	12913890	12917870.27	12918083.4	0.37	0.34	0.34
24	3p3d	<sup>1</sup> D <sub>2</sub>	13055335	13013743	13017773.21	13018717.2	0.32	0.29	0.28
25	3p3d	<sup>3</sup> D <sub>3</sub>	13220603	13170344	13175365.53	13177430.9	0.38	0.34	0.33
26	3p3d	<sup>1</sup> P <sub>1</sub>	13322750	13279799	13285634.92	13288267.5	0.32	0.28	0.26
27	3d <sup>2</sup>	<sup>3</sup> F <sub>2</sub>	13916827	13913209	13911729.51	13921985.1	0.03	0.04	0.04
28	3d <sup>2</sup>	<sup>3</sup> P <sub>0</sub>	14137651	14144256	14144095.48	14156950.4	0.05	0.05	0.14
29	3d <sup>2</sup>	<sup>3</sup> F <sub>3</sub>	14773827	14734119	14733014	14739629.2	0.27	0.28	0.23
30	3d <sup>2</sup>	<sup>3</sup> P <sub>2</sub>	14869267	14837565	14836947.5	14844932.9	0.21	0.22	0.16
31	3d <sup>2</sup>	<sup>1</sup> G <sub>4</sub>	14911425	14857585	14857576.42	14864903.1	0.36	0.36	0.31
32	3d <sup>2</sup>	<sup>3</sup> P <sub>1</sub>	14911979	14885502	14884787.64	14893382.6	0.18	0.18	0.12
33	3d <sup>2</sup>	<sup>3</sup> F <sub>4</sub>	15710577	15631219	15631221.75	15635041.2	0.51	0.51	0.48
34	3d <sup>2</sup>	<sup>1</sup> D <sub>2</sub>	15788150	15722082	15722410.12	15727520.7	0.42	0.42	0.39
35	3d <sup>2</sup>	<sup>1</sup> S <sub>0</sub>	16028288	15966090	15968778.42	15976528.1	0.39	0.37	0.32

<sup>a</sup>[6]. <sup>b</sup>[4] <sup>c</sup>[7]

In Table 2, the energy levels above the ionization level ( $2p^53s^23p$  and  $2p^53s^23d$  levels) are presented as new data. The core  $1s^22s^22p^6$  or  $1s^22s^2$  is omitted in the tables.

Table 2 Energy levels (cm<sup>-1</sup>) for the levels of  $2p^53s^23p$  and  $2p^53s^23d$  for Pt LXVII

Levels	Energy Levels	Levels	Energy Levels
$2p^53s^23p$	<sup>3</sup> S <sub>1</sub> 75642112	$2p^53s^23d$	<sup>3</sup> P <sub>1</sub> 81203100
$2p^53s^23p$	<sup>3</sup> D <sub>2</sub> 75666263	$2p^53s^23d$	<sup>1</sup> F <sub>3</sub> 81277389
$2p^53s^23p$	<sup>3</sup> D <sub>3</sub> 79269022	$2p^53s^23d$	<sup>3</sup> D <sub>2</sub> 81318928
$2p^53s^23p$	<sup>1</sup> P <sub>1</sub> 79269634	$2p^53s^23d$	<sup>3</sup> F <sub>4</sub> 81952173
$2p^53s^23p$	<sup>3</sup> P <sub>2</sub> 79377445	$2p^53s^23d$	<sup>1</sup> D <sub>2</sub> 81993492
$2p^53s^23p$	<sup>1</sup> S <sub>0</sub> 79941286	$2p^53s^23d$	<sup>3</sup> D <sub>3</sub> 82080818
$2p^53s^23d$	<sup>3</sup> P <sub>0</sub> 80969439	$2p^53s^23d$	<sup>1</sup> P <sub>1</sub> 82379269

Here, electric dipole transitions parameters comparisons have been made graphically. Figure 3 presents the comparison of weighted oscillator strengths. As shown from Figure 3, there is a qualitative agreement with the results of MCDHF

[4] and FAC [7]. Linear correlation coefficient R<sup>2</sup> is 0.9992 for MCDHF.

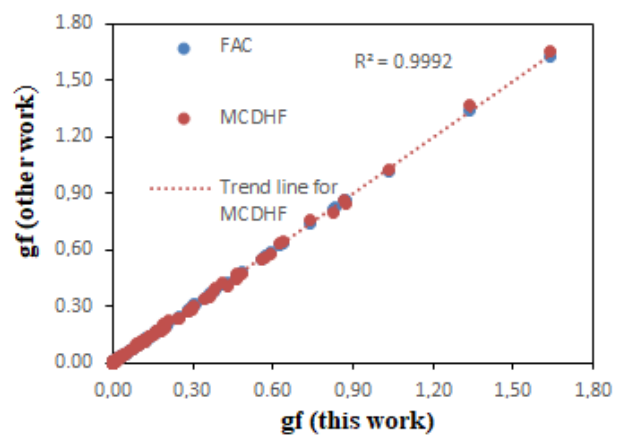


Figure 3 The comparison of weighted oscillator strengths between present AUTOSTRUCTURE results and other MCDHF [4] and FAC [7] results for E1 transitions

In figure 4 the transition probabilities have been presented and compared. Linear correlation

coefficient  $R^2$  is 0.9994 for MCDHF. From this figure, one can see that our calculated transition probabilities match well with the theoretically calculated MCDHF [4] and FAC [7] results.

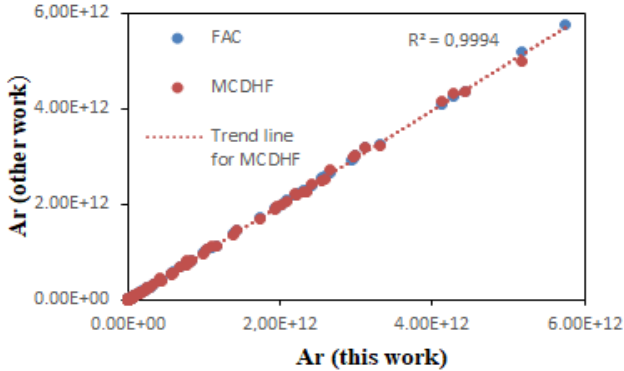


Figure 4 The comparison of transition probabilities between present AUTOSTRUCTURE results and other MCDHF [4] and FAC [7] results for E1 transitions

Table 3 shows the transition probabilities, weighted oscillator strengths, and wavelengths, for some electric dipole (E1) transitions between  $2p^5 3s^2 3l$  ( $l=1,2$ ) and  $3l3l'$  ( $l, l'=0,1,2$ ) levels in Mg-like Pt. In the table, the number in brackets represents the power of 10. These data on E1 transitions for this ion have been presented for the first time. In the table, the number in brackets represents the power of 10.

Table 3 Transition probabilities,  $A_r$  ( $s^{-1}$ ), weighted oscillator strengths, ( $gf$ ), and wavelengths,  $\lambda$  ( $\text{\AA}$ ), for some electric dipole (E1) transitions between  $2p^5 3s^2 3l$  ( $l=1,2$ ) and  $3l3l'$  ( $l, l'=0,1,2$ ) levels in Pt LXVII

Transitions	$A_r(s^{-1})$	$gf$	$\lambda(\text{\AA})$
$2p^5 3s^2 3p^3 S_1 - 3s 3p^3 P_0$	1.10(14)	8.89(2)	1.34
$2p^5 3s^2 3p^3 S_1 - 3s 3p^3 P_1$	5.09(13)	4.15(2)	1.34
$2p^5 3s^2 3p^3 S_1 - 3s 3p^3 P_2$	2.64(10)	2.38(5)	1.41
$2p^5 3s^2 3p^3 S_1 - 3s 3p^3 P_1$	4.70(08)	4.29(7)	1.42
$2p^5 3s^2 3p^3 S_1 - 3p 3d^3 F_2$	7.57(08)	7.49(7)	1.48
$2p^5 3s^2 3p^3 S_1 - 3p 3d^3 D_1$	5.37(09)	5.36(6)	1.48
$2p^5 3s^2 3p^3 S_1 - 3p 3d^3 P_2$	8.45(10)	8.62(5)	1.50
$2p^5 3s^2 3p^3 D_2 - 3s 3p^3 P_1$	1.69(14)	2.29(1)	1.34
$2p^5 3s^2 3p^3 D_2 - 3s 3p^3 P_2$	1.15(10)	1.73(5)	1.41
$2p^5 3s^2 3p^3 D_2 - 3s 3p^3 P_1$	5.18(11)	7.87(4)	1.42
$2p^5 3s^2 3p^3 D_2 - 3p 3d^3 F_2$	3.93(09)	6.48(6)	1.48
$2p^5 3s^2 3p^3 D_2 - 3p 3d^3 D_1$	1.18(09)	1.97(6)	1.48
$2p^5 3s^2 3p^3 D_2 - 3p 3d^3 P_2$	5.53(09)	9.40(6)	1.50
$2p^5 3s^2 3d^3 P_0 - 3p^2^3 P_1$	1.11(14)	3.01(2)	1.34
$2p^5 3s^2 3d^3 P_0 - 3s 3d^3 D_1$	9.40(13)	2.57(2)	1.35

$2p^5 3s^2 3d^3 P_1 - 3s^2^1 S_0$	7.94(12)	5.41(3)	1.23
$2p^5 3s^2 3d^3 P_1 - 3p^2^3 P_0$	4.77(11)	3.50(4)	1.27
$2p^5 3s^2 3d^3 P_1 - 3p^2^1 D_2$	2.27(13)	1.83(2)	1.34
$2p^5 3s^2 3d^3 P_1 - 3p^2^3 P_1$	2.75(13)	2.22(2)	1.34
$2p^5 3s^2 3d^3 P_1 - 3s 3d^3 D_1$	4.91(13)	4.00(2)	1.34
$2p^5 3s^2 3d^3 P_1 - 3s 3d^3 D_2$	3.25(13)	2.66(2)	1.34
$2p^5 3s^2 3d^3 P_1 - 3s 3d^3 D_2$	2.06(10)	1.73(5)	1.36

#### 4. CONCLUSION

Employing the AUTOSTRUCTURE code, the excitation energies, wavelengths, transition probabilities, and oscillator strengths for the electric dipole transitions of Mg-like Pt have been calculated. Comparisons with three independent atomic structure codes, show that the present AUTOSTRUCTURE results are highly accurate: the differences (%) for the energy levels, oscillator strengths and transition probabilities are around 0.5, 6.2 and 6.0 respectively. We can say that, good agreement has been found with other available theoretical results. The new results reported in this work considerably increase the amount of data available in Mg-like ions. In the end, we believe that our detailed discussion of these data could serve as benchmarks in future experimental work. Further, they will be helpful in plasma physics.

#### Funding

The author has no received any financial support for the research, authorship or publication of this study.

#### The Declaration of Conflict of Interest/ Common Interest

No conflict of interest or common interest has been declared by the author.

#### The Declaration of Ethics Committee Approval

This study does not require ethics committee permission or any special permission.

#### The Declaration of Research and Publication Ethics

The authors of the paper declare that they comply with the scientific, ethical and quotation rules of SAUJS in all processes of the paper and that they

do not make any falsification on the data collected. In addition, they declare that Sakarya University Journal of Science and its editorial board have no responsibility for any ethical violations that may be encountered, and that this study has not been evaluated in any academic publication environment other than Sakarya University Journal of Science.

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