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Excited states of Ne isoelectronic ions: SAC-CI study

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Abstract. Excited states of the *s*, *p*, and *d* symmetries up to principal quantum number $n = 4$ are studied for the first eight members of Ne isoelectronic sequence (Ne to Cl^{7+}) by the SAC-CI (symmetry-adapted-cluster configuration-interaction) method. The valence STO basis sets of Clementi *et al.* and the optimized excited STO are used by the STO-6G expansion method. The calculated transition energies agree well with the experimental values wherever available.

PACS. 31.50.+w Excited states – 31.25.Jf Electron-correlation calculations for atoms and ions: excited states – 34.60.+z Scattering in highly excited states (e.g. Rydberg states)

1 Introduction

In recent years the atomic data for the spectral transitions of neutral atoms and their isoelectronic ions have gained considerable importance because of their significant role in a variety of physical and chemical processes occurring in astrophysics and in the laboratory. The neutral, near-neutral and ionized species of the neon isoelectronic sequence have special interest in plasma research due to their stable closed shell configurations; the corresponding emission lines are essential for diagnostics over a wide range of plasma parameters from those of Tokamak to those for the fusion reactors, in which lower ionic stages released by collision with the walls are more important than the higher ions [1]. The classification of transitions to various excited levels having different symmetries and the determination of energy levels are essential parts of the study of a laboratory spectrum. The excitation energies of the upper level of an emission line or the lower level of an absorption line and the knowledge of connecting paths are extremely necessary for the physical interpretation of any observation [2]. The opacities of the stellar envelope which governed largely by the bound-bound and bound-free transition of the constituent atomic ions, are very useful for theories of stellar structure and stellar pulsations [3–5].

During last few years different theoretical and experimental techniques have been applied to predict the transition energies of the low- and moderately highlying excited states of first few members of Ne sequence. Experimental techniques adopted so far are essentially the spectroscopic [6–8] and reported data are quite extensive. Among different theoretical approaches, the relativistic many body theory of Avgoustoglou *et al.* [1], configuration interaction (CI) approach of Hibbert, La Dourneuf and Mohan [9], coupled cluster with singles, doubles and triples (CCSD+T) by Kaldor and Haque [10], the *R*-matrix with CI wave functions calculation of Hibbert and Scott [5], the relativistic random phase approximation with exchange (RPAE) by Shorer [11] and the time-dependent coupled Hartree-Fock (TDCHF) approach of Das [12] are important. In the previous paper [12], transition energies of optically allowed and optically forbidden excited energy levels up to principal quantum number $n = 4$ have been studied for the first eight members of Ne isoelectronic sequence from Ne to Cl^{7+} using linearized version of TDCHF theory. The TDCHF theory includes the correlation effects partially, namely the radial correlation, through effective summation of hole particle correlation diagrams up to infinite order [13,14].

In this communication, we use SAC (symmetry adapted cluster)/SAC-CI method [15–17] to calculate the transition energies for the $2p^6$: $^1S_0 \rightarrow 2p^5ns$: $^1P_1$; $2p^5np$: $^1D_2$, $^1P_1$, $^1S_0$ and $2p^5nd$: $^1P_1$, $^1F_3$, $^1D_2$ transitions up to principal quantum number $n = 4$ for the first eight members of Ne isoelectronic sequence from Ne to Cl^{7+}. The SAC/SAC-CI method has been successfully applied in the past to various kinds of spectroscopic studies [18] of molecules from the size of water [17] to the size of porphyrin dimers [19,20]. In this paper, we use the SAC-CI SD-*R* method, in which the SAC-CI linked *R* operators consist of singles and doubles, since the excitations are essentially described by the one electron processes [21]. The objective of this paper is two fold, first to show the accuracy of the SAC-CI method for small systems, namely the atomic systems and secondly to show the effect of angular correlation in such systems.

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2 Computational details

Presently, we have studied the low- and high-lying single excitations having symmetries s, p and d up to principal quantum number $n = 4$ for the first eight members of the Ne isoelectronic sequence with nuclear charge $Z = 10{-}17$. The STO basis sets for ground states of all the ions have been taken from Clementi and Roetti [22]. The optimized STO basis sets for the excitation spectra of all the ions are obtained from our previous calculations based on the TDCHF theory [12]. The number of STO parameters employed in that calculation [12] is determined by testing the absolute convergence in the static limit of frequency-dependent polarizabilities. The number of STO parameters has been restricted to 15 for all the excitations. The choice of exponents depends on principal quantum number and symmetry of the excited levels. The final basis sets are determined by examining the convergence of static limit of the frequency-dependent polarizabilities and the stability of the SAC-CI excitation energy. The integrals are calculated with the STO-GTO expansion method [23] and the SCF calculations are performed with the GAUSSIAN 98 program [24].

Electron correlations of the ground and excited states are calculated by the SAC/SAC-CI method. In SAC/SAC-CI calculations, $1s$ orbitals of all the ions are fixed as cores. In order to reduce computational effort, we use standard perturbation procedure [25]. For the ground state, the threshold of the linked term is set to $\lambda g = 1\times10^{-6}$ and the unlinked terms are adopted as the products of the important linked terms whose SDCI coefficients are larger than 0.001. For excited state, the threshold of the linked term is set to $\lambda e = 1 \times 10^{-6}$. The thresholds for the unlinked terms in the SAC-CI are set to 0.001 and 0.05 respectively for selecting the important S and R operators, where only doubles: $S(2)$ are used from the SAC linked operators S. The contributions of both $S(2) \times R(1)$ and $S(2) \times R(2)$ unlinked terms *i.e.*, so called "3, 4-excited" terms [25] are included. The SAC-CI calculations are performed with the SAC-CI96 program system [26].

3 Results and discussions

The SAC-CI results are summarized in Table 1 along with the recent compilation of experimental values of Martin *et al.* [6], spectroscopic values of Bashkin and Stoner [7] and Moore [8] and other theoretical values. We used LS-coupling scheme to designate the energy levels and compared them with the experimental values. For the assignment of levels, Moore [8] and Bashkin and Stoner [7] followed jl coupling scheme. The term designations on the assumption of LS-coupling are also available from their work [6–8]. It was also pointed out that the excited configurations are much closer to LS-coupling than to jl-coupling [8]. The deviations are calculated with respect to the experimental values [6–8] and displayed in Table 1. The overall agreement between the SAC-CI results and the experiment is very good, especially for Ne and Na$^+$. For Ne atom, the excitation energies of $2p^5 3p$: $^1\mathrm{D}_2$, $^1\mathrm{P}_1$, $^1\mathrm{S}_0$ and $2p^5 3d$: $^1\mathrm{P}_1$, $^1\mathrm{F}_3$, $^1\mathrm{D}_2$ states calculated by the SAC-CI method agree very well with the experimental values: the deviations are within 3 mhartree. The deviations for the $2p^5 3s$: $^1\mathrm{P}_1$ and $2p^5 4s$: $^1\mathrm{P}_1$ states are also small, 0.7 and 2.6 mhartree, respectively. For $2p^5 4s$: $^1\mathrm{P}_1$ state, the R-matrix method by Hibbert and Scott [5] gave high excitation energy. For Na$^+$, good agreements are also obtained for the $2p^5 np$: $^1\mathrm{D}_2$, $^1\mathrm{P}_1$, $^1\mathrm{S}_0$ with deviation from experimental values ranges from 0.3 mhartree to 5 mhartree and for the $2p^5 nd$: $^1\mathrm{P}_1$, $^1\mathrm{F}_3$, $^1\mathrm{D}_2$ states the deviations are from 0.9 mhartree to 5.4 mhartree. The errors for the $2p^5 ns$: $^1\mathrm{P}_1$ states are also small, of the order of mhartree.

For highly ionized atoms, electron correlations should be small in comparison with those of neutral atoms and therefore, agreement between theory and experiment should become better. However, some discrepancies exist between our results and the experimental values, particularly for the $2p^5 3p$: $^1\mathrm{D}_2$ state of P^{5+} and for the $2p^5 3d$: $^1\mathrm{F}_3$ state of S^{6+}: the deviations from the experimental values are about 19 mhartree and 23 mhartree respectively. These discrepancies may be due to the valence basis sets. The stability of all the excited levels of these ions under present consideration has been tested with basis sets having different choice of exponents but in all cases transition energies remain unchanged. It essentially means that our predicted energy levels are very stable. The SAC-CI excitation energies of the $2p^5 3s$: $^1\mathrm{P}_1$ states for Mg^{2+} to P^{5+} agree well with the experimental values and also with the values of the CI method [9]. For the $2p^5 4s$: $^1\mathrm{P}_1$ states, SAC-CI gives good results for these highly ionized atoms: the errors are in the order of mhartree whereas the values of Hibbert and Scott [5] for Ne to Si^{4+} are much higher.

For the $2p^5 3p$: $^1\mathrm{D}_2$, $^1\mathrm{P}_1$ and $^1\mathrm{S}_0$ states of Mg^{2+}, our calculated value is higher than the experimental value [6, 8]. Our SAC-CI value for the $2p^5 3p$: $^1\mathrm{S}_0$ state of Al^{3+} is close to the experimental value of Martin *et al.* [6] and also to the CI value of Hibbert *et al.* [9]. It should be noted that the CI calculation of Hibbert, La Dourneuf and Mohan [9] adopted the semi-empirical fit of the diagonal elements of the CI matrix to reproduce the experimental values. For Si^{4+} and P^{5+}, our SAC-CI results for $2p^5 3p$: $^1\mathrm{P}_1$ and $^1\mathrm{S}_0$ states agree within 4 mhartree with the experimental values while our predicted values for the $2p^5 3p$: $^1\mathrm{D}_2$ state differ from the experimental value. It should be noted here that the SAC-CI value for the $2p^5 3p$: $^1\mathrm{D}_2$ state of P^{5+} is very close to the CI value [9]. The SAC-CI values for $2p^5 4p$: $^1\mathrm{P}_1$ and $^1\mathrm{S}_0$ states of Si^{4+} agree very well with the experimental values; agreement is about 1 mhartree but for the $2p^5 4p$: $^1\mathrm{D}_2$ state, the deviation between our value and the experimental value is large, about 10 mhartree.

The SAC-CI values for the $2p^5 nd$: $^1\mathrm{P}_1$, $^1\mathrm{D}_2$ ($n = 3$, 4) states of Si^{4+} agree within 10 mhartee but for the $2p^5 nd$: $^1\mathrm{F}_3$ ($n = 3$, 4) state, the deviation between our SAC-CI values and the experimental values are about 12 mhartree. It is worth mentioning that from P^{5+} onwards no theoretical and experimental values exist for the $2p^5 4p$: $^1\mathrm{D}_2$, $^1\mathrm{P}_1$ and $^1\mathrm{S}_0$ states and the for the $2p^5 4d$: $^1\mathrm{F}_3$, $^1\mathrm{D}_2$ states.

In Table 1, we also displayed the difference of energy between the transition energies of the TDCHF [12] and

Table 1. Transition energies for the excited levels having *s*, *p* and *d* symmetries of the Ne isoelectronic ions from Ne to Cl^{7+}.

Ions	Level	Transition energy (a.u.)					
		SAC-CI	Observed	Theoretical		Deviation^{h}	Angular correlation^{i} (a.u.)
				Others	TDCHF^{g}	(a.u.)	
Ne	$2p^53s$: $^1\mathrm{P}_1$	0.6199	0.6192^{a,b,c}	0.6192^{d}, 0.6177^{e}	0.6741	0.0007	0.0542
	$2p^53p$: $^1\mathrm{D}_2$	0.6868	0.6849^{a}	0.6849^{d}	0.7387	0.0019	0.0519
	: $^1\mathrm{P}_1$	0.6869	0.6870^{a}	0.6870^{d}		0.0001	
	: $^1\mathrm{S}_0$	0.6978	0.6970^{a}	0.6970^{d}		0.0008	
	$2p^53d$: $^1\mathrm{P}_1$	0.7390	0.7365^{a,b}	0.7365^{d}	0.7943	0.0025	0.0553
	: $^1\mathrm{F}_3$	0.7398	0.7368^{a}	0.7363^{d}		0.0030	
	: $^1\mathrm{D}_2$	0.7401	0.7400^{a}	0.7368^{d}		0.0001	
	$2p^54s$: $^1\mathrm{P}_1$	0.7243	0.7269^{a,b}	0.7638^{f}	0.7818	0.0026	0.0575
	$2p^54p$: $^1\mathrm{D}_2$	0.7449	0.7429^{a}		0.7995	0.0020	0.0546
	: $^1\mathrm{P}_1$	0.7454	0.7457^{a}			0.0003	
	: $^1\mathrm{S}_0$	0.7486	0.7486^{a}			0.0000	
	$2p^54d$: $^1\mathrm{P}_1$	0.7631	0.7610^{a,b}		0.8189	0.0021	0.0558
	: $^1\mathrm{F}_3$	0.7632	0.7611^{a}			0.0021	
	: $^1\mathrm{D}_2$	0.7645	0.7645^{a}			0.0000	
Na^{+}	$2p^53s$: $^1\mathrm{P}_1$	1.2283	1.2246^{a,b}	1.2246^{d}, 1.2233^{e}	1.2793	0.0037	0.0510
	$2p^53p$: $^1\mathrm{D}_2$	1.3688	1.3632^{a}	1.3632^{d}	1.4145	0.0056	0.0457
	: $^1\mathrm{P}_1$	1.3696	1.3664^{a}	1.3664^{d}		0.0032	
	: $^1\mathrm{S}_0$	1.4111	1.4073^{a}	1.4073^{d}		0.0038	
	$2p^53d$: $^1\mathrm{P}_1$	1.5170	1.5116^{a}	1.5116^{d}	1.5724	0.0054	0.0554
	: $^1\mathrm{F}_3$	1.5167	1.5114^{a}	1.5091^{d}		0.0053	
	: $^1\mathrm{D}_2$	1.5173	1.5164^{a}	1.5164^{d}		0.0009	
	$2p^54s$: $^1\mathrm{P}_1$	1.5187	1.5178^{a,b}	1.5580^{f}	1.5723	0.0009	0.0546
	$2p^54p$: $^1\mathrm{D}_2$	1.5629	1.5581^{b}		1.6147	0.0048	0.0518
	: $^1\mathrm{P}_1$	1.5631	1.5617^{b}			0.0014	
	: $^1\mathrm{S}_0$	1.5653	1.5650^{b}			0.0003	
	$2p^54d$: $^1\mathrm{P}_1$	1.6162	1.6111^{a,b}		1.6711	0.0051	0.0549
	: $^1\mathrm{F}_3$	1.6160	1.6106^{b}			0.0054	
	: $^1\mathrm{D}_2$	1.6164	1.6154^{b}			0.0010	
Mg^{2+}	$2p^53s$: $^1\mathrm{P}_1$	1.9751	1.9662^{a,b,c}	1.9662^{d}, 1.9647^{e}	2.0201	0.0089	0.0450
	$2p^53p$: $^1\mathrm{D}_2$	2.1870	2.1754^{a}	2.1753^{d}	2.2254	0.0116	0.0384
	: $^1\mathrm{P}_1$	2.1895	2.1797^{a}	2.1796^{d}		0.0098	
	: $^1\mathrm{S}_0$	2.2687	2.2600^{c}	2.2600^{d}		0.0087	
	$2p^53d$: $^1\mathrm{P}_1$	2.4419	2.4340^{a}	2.4429^{d}	2.5000	0.0079	0.0581
	: $^1\mathrm{F}_3$	2.4400	2.4284^{a}	2.4284^{d}		0.0116	
	: $^1\mathrm{D}_2$	2.4470	2.4367^{a}	2.4365^{d}		0.0104	
	$2p^54s$: $^1\mathrm{P}_1$	2.5087	2.5002^{a,b}	2.5401^{f}	2.5537	0.0085	0.0450
	$2p^54p$: $^1\mathrm{D}_2$	2.5760	2.5649^{b}		2.6225	0.0111	0.0465
	: $^1\mathrm{P}_1$	2.5788	2.5711^{b}			0.0077	
	: $^1\mathrm{S}_0$	2.6059	2.5976^{b}			0.0083	
	$2p^54d$: $^1\mathrm{P}_1$	2.6689	2.6584^{a,c}		2.7222	0.0105	0.0533
	: $^1\mathrm{F}_3$	2.6671	2.6556^{c}			0.0115	
	: $^1\mathrm{D}_2$	2.6702	2.6637^{c}			0.0065	

Table 1. *Continued.*

Ions	Level	Transition energy (a.u.)					
		SAC-CI	Observed	Theoretical		Deviation[h]	Angular correlation[i] (a.u.)
				Others	TDCHF[g]	(a.u.)	
Al^{3+}	$2p^53s$: $^1\mathrm{P}_1$	2.8543	2.8464[a,b]	2.8464[d], 2.8448[e]	2.8998	0.0079	0.0455
	$2p^53p$: $^1\mathrm{D}_2$	3.1339	3.1244[a]	3.1243[d]	3.1740	0.0095	0.0401
	: $^1\mathrm{P}_1$	3.1401	3.1323[a]	3.1300[d]		0.0078	
	: $^1\mathrm{S}_0$	3.2580	3.2537[c]	3.2537[d]		0.0043	
	$2p^53d$: $^1\mathrm{P}_1$	3.5194	3.5122[c]	3.5122[d]	3.5714	0.0072	0.0520
	: $^1\mathrm{F}_3$	3.4930	3.4824[c]	3.4824[d]		0.0106	
	: $^1\mathrm{D}_2$	3.5035	3.4949[c]	3.4949[d]		0.0086	
	$2p^54s$: $^1\mathrm{P}_1$	3.6733	3.6735[a,b]	3.7118[f]	3.7248	0.0002	0.0515
	$2p^54p$: $^1\mathrm{D}_2$	3.7719	3.7624[c]		3.8209	0.0095	0.0490
	: $^1\mathrm{P}_1$	3.7749	3.7719[c]			0.0030	
	: $^1\mathrm{S}_0$	3.8161	3.8121[c]			0.0040	
	$2p^54d$: $^1\mathrm{P}_1$	3.9047	3.8970[a,c]		3.9666	0.0078	0.0619
	: $^1\mathrm{F}_3$	3.9011	3.8910[c]			0.0101	
	: $^1\mathrm{D}_2$	3.9151	3.9031[c]			0.0120	
Si^{4+}	$2p^53s$: $^1\mathrm{P}_1$	3.8732	3.8661[c]	3.8661[d], 3.8642[e]	3.9186	0.0071	0.0454
	$2p^53p$: $^1\mathrm{D}_2$	4.2209	4.2114[c]	4.2113[d]	4.2611	0.0095	0.0402
	: $^1\mathrm{P}_1$	4.2226	4.2189[c]	4.2190[d]		0.0037	
	: $^1\mathrm{S}_0$	4.3896	4.3875[c]	4.3875[d]		0.0021	
	$2p^53d$: $^1\mathrm{P}_1$	4.7317	4.7245[c]	4.7245[d]	4.7842	0.0072	0.0525
	: $^1\mathrm{F}_3$	4.6844	4.6727[c]	4.6728[d]		0.0117	
	: $^1\mathrm{D}_2$	4.6996	4.6900[c]	4.6901[d]		0.0096	
	$2p^54s$: $^1\mathrm{P}_1$	5.0347	5.0373[a,b,c]	5.0727[f]	5.0853	0.0026	0.0506
	$2p^54p$: $^1\mathrm{D}_2$	5.1597	5.1491[c]		5.2089	0.0106	0.0492
	: $^1\mathrm{P}_1$	5.1627	5.1638[c]			0.0011	
	: $^1\mathrm{S}_0$	5.2182	5.2168[c]			0.0014	
	$2p^54d$: $^1\mathrm{P}_1$	5.3304	5.3246[c]		5.4016	0.0058	0.0712
	: $^1\mathrm{F}_3$	5.3259	5.3152[c]			0.0107	
	: $^1\mathrm{D}_2$	5.3319	5.3329[c]			0.0010	
P^{5+}	$2p^53s$: $^1\mathrm{P}_1$	5.0306	5.0262[c]	5.0262[d], 5.0235[e]	5.0766	0.0044	0.0460
	$2p^53p$: $^1\mathrm{D}_2$	5.4556	5.4371[c]	5.4580[d]	5.4869	0.0185	0.0313
	: $^1\mathrm{P}_1$	5.4472	5.4476[c]	5.4477[d]		0.0004	
	: $^1\mathrm{S}_0$	5.6613	5.6617[c]	5.6617[d]		0.0004	
	$2p^53d$: $^1\mathrm{P}_1$	6.0835	6.0789[c]	6.0789[d]	6.1371	0.0046	0.0536
	: $^1\mathrm{F}_3$	6.0114	5.9998[c]	5.9999[d]		0.0116	
	: $^1\mathrm{D}_2$	6.0278	6.0230[c]	6.0231[d]		0.0048	
	$2p^54s$: $^1\mathrm{P}_1$	6.5821	6.5918[a,b]		6.6345	0.0098	0.0524
	$2p^54p$: $^1\mathrm{D}_2$	6.7346			6.7859		0.0513
	: $^1\mathrm{P}_1$	6.7384					
	: $^1\mathrm{S}_0$	6.8067					
	$2p^54d$: $^1\mathrm{P}_1$	6.9395	6.9414[a,b,c]		7.0259	0.0019	0.0864
	: $^1\mathrm{F}_3$	6.9387					
	: $^1\mathrm{D}_2$	6.9445					

Table 1. *Continued.*

Ions	Level	Transition energy (a.u.)					
		SAC-CI	Observed	Theoretical		Deviation[h]	Angular correlation[i] (a.u.)
				Others	TDCHF[g]	(a.u.)	
S^{6+}	$2p^5 3s$: $^1P_1$	6.3367	6.3257[a,b]	6.3259[d], 6.3232[e]	6.3738	0.0110	0.0371
	$2p^5 3p$: $^1D_2$	6.8326	6.8303[c]	6.8305[d]	6.8516	0.0023	0.0190
	: $^1P_1$	6.8209	6.8156[c]	6.8160[d]		0.0053	
	: $^1S_0$	7.0831	7.0747[c]	7.0749[d]		0.0084	
	$2p^5 3d$: $^1P_1$	7.5866	7.5735[c]	7.5738[d]	7.6293	0.0131	0.0427
	: $^1F_3$	7.4860	7.4629[c]	7.4632[d]		0.0231	
	: $^1D_2$	7.5049	7.4937[c]	7.4941[d]		0.0112	
	$2p^5 4s$: $^1P_1$	8.3317	8.3370[a,b]		8.3721	0.0053	0.0404
	$2p^5 4p$: $^1D_2$	8.5107			8.5516		0.0409
	: $^1P_1$	8.5139					
	: $^1S_0$	8.5167					
	$2p^5 4d$: $^1P_1$	8.7520	8.7459[a,c]		8.8380	0.0061	0.0860
	: $^1F_3$	8.7513					
	:$^1D_1$	8.7595					
Cl^{7+}	$2p^5 3s$: $^1P_1$	7.7777	7.7656[a]	7.7660[d], 7.7637[e]	7.8102	0.0121	0.0325
	$2p^5 3p$: $^1D_2$	8.3405		8.3438[d]	8.3552		0.0147
	: $^1P_1$	8.3290		8.3240[d]			
	: $^1S_0$	8.6383		8.6274[d]			
	$2p^5 3d$: $^1P_1$	9.1144	9.0992[a]	9.2071[d]	9.2607	0.0152	0.0463
	: $^1F_3$	9.0934		9.0633[d]			
	: $^1D_2$	9.2241		9.1035[d]			
	$2p^5 4s$: $^1P_1$	10.2738	10.2709[a]		10.2979	0.0029	0.0241
	$2p^5 4p$: $^1D_2$	10.4682			10.5056		0.0374
	: $^1P_1$	10.4739					
	: $^1S_0$	10.5859					
	$2p^5 4d$: $^1P_1$	10.7483	10.7385[a]		10.8253	0.0098	0.0770
	: $^1F_3$	10.7459					
	: $^1D_2$	10.7538					

[a] Spectroscopic values of Moore [8]. [b] Spectroscopic values of Bashkin and Stoner [7]. [c] Experimental values of Martin *et al.* [6]. [d] Empirical CI values of Hibbert *et al.* [9]. [e] Relativistic many-body calculation of Avgoustoglou *et al.* [1]. [f] R-matrix calculation of Hibbert and Scott [5]. [g] Das [12]. [h] Difference between SAC-CI and observed values. [i] Difference between SAC-CI and TDCHF values.

those of the SAC-CI to show the effect of the angular correlation in the excited state. The amount of angular correlation is large, about 45 mhartree, for the all excited states of Ne. The correlation energy decreases as we move towards the higher members of the sequence. It is generally true that with the increase of nuclear charge, nuclear potential dominates over the inter-electronic coulomb potential and the effect of electron correlations becomes small for highly ionized atoms. As seen from the table, the effect of angular correlation is still large for some higher excited states having principal quantum number $n = 4$ even for the higher Z members of the sequence. This is due to the effect of higher configurations in high lying states which is not taken into account in my previous calculation [12].

In Figure 1, we have plotted the SAC-CI excitation energies with respect to nuclear charge for the $2p^6$: $^1S_0 \rightarrow 2p^5 4s$: $^1P_1$, $2p^6$: $^1S_0 \rightarrow 2p^5 4p$: $^1S_0$ and $2p^6$: $^1S_0 \rightarrow 2p^5 4d$: $^1D_2$ transitions. Very smooth behaviour is observed indicating the consistency of our calculated values.

The present calculations showed that the deviations from the experimental values are mainly attributed to the quality of the basis set used. In comparison with the previous TDCHF calculations for these atoms [12], the improvement of the results due to the inclusion of electron correlation is remarkable.

The studies of the two- and higher electron processes using general-R method and on the relativistic effects are under progress and results will be reported in due time.

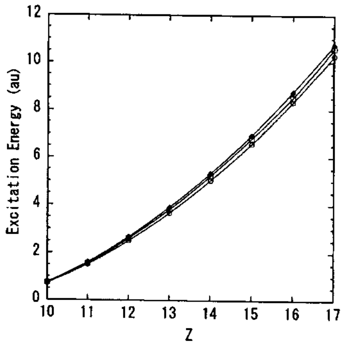

Fig. 1. Plot of transition energies (a.u.) *vs.* nuclear charge (Z) for the $2p^6$: $^1S_0 \rightarrow 2p^5 4s$: $^1P_1$, $2p^5 4p$: $^1S_0$ and $2p^5 4d$: $^1D_2$ transitions.

4 Summary

The SAC-CI method is applied to the excited states ($n = 3$, 4) of the s, p, and d symmetries of Ne to Cl^{7+}. The STO basis sets expanded by the STO-6G method, in which excited STOs are optimized, are used. In view of satisfactory the agreement between our results and the spectroscopic values and lack of accurate reference data for the $2p^5 4p$: $^1D_2$, $^1P_1$, $^1S_0$ and $2p^5 4d$: $^1P_1$, $^1F_3$, $^1D_2$ states from P^{5+} onwards, our accurate results may serve as a reliable set of atomic data for future reference.

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