Theoretical Prediction of the Ionization Potential Using Different Methods AM1, HF and DFT

Ammar Abdulsattar Ibrahim[1], Ghufran Mohammed Abed

[1]Department of Chemistry, College of Science, University of Mosul, Iraq

ABSTRACT

This study is depend on the theoretical calculations for the prediction of the ionization potential for one hundred compounds which were experimentally characterized. All these compounds were evaluated by semi-empirical (AM1) , ab initio (HF/6-31G) and density function theory (B3LYP) in different basis set (DFT/STO-3G, DFT/ 3-21G and DFT/6-31G). The physical properties of ionization potential was computed. The calculations values were correlated with experimental data; a linearity was shown for the different methods (AM1, HF/6-31G, DFT/STO-3G, DFT/3-21G and DFT/6-31G) which has gave an excellent correlation (R=0.898, R=0.902, R=0.519, R=0.864 and R=0.912) respectively. The best method for prediction of the experimental values was found with (DFT/6-31G) even there is a minor error at the calculations. All the calculations have been evaluated by Chem-Bio Office version (11.0. 1) using GAMMESS program.

Keywords: Ionization Potential, Theoretical calculation, AM1, HF, DFT.

INTRODUCTION

One of the most important properties influencing the chemical behavior is the energy required to remove one electron from the valence shell, referred to as the ionization potential. ionization potentials and electron affinities can be calculated as energy differences between the ground state and a state with one electron added or removed[1,2]. Number of substituted indoles were accurate using ab initio calculations of twenty molecules. An increased ionization potential translates to a more positive Gibbs free energy change[3]. Ionization potentials, electron affinities and proton affinities of compounds containing first- (Li-F) and second row atoms (Na-Cl) were evaluated theoretically using (G2) based on ab initio molecular orbital theory[4]. Theoretical estimates of the second to fourth ionization potentials of the actinide elements have been derived from relativistic energy-consistent ab initio pseudo-potential calculations. The quality of the predictions is estimated from related calculations on the lanthanide elements (La) to (Lu), where the experimental values are available[5]. A theoretical treatment is used to perform conformational studies of electron impact ionization of 2 Furanmethanol, Tetrahydro ($C_5H_{10}O_2$) and 3-Furanol, Tetrahydro (C4H8O2), both as important models for more complicated compounds like nucleic acids. These compounds were optimized using DFT level with B3LYPfunctional, and ionization energies were estimated[6]. The ionization potential of aluminum clusters of 2–23 atoms are studied with a total energy method DFT. The calculated properties agree with the data from threshold photoionization measurements[7]. Quantum Monte Carlo methods were used to the calculation of the optical and thermal ionization energies of the F-center defect in magnesium oxide. It is shows a large promise for the quantitative first-principles calculation of point-defect properties[8]. A generalized Kohn-Sham (GKS) approach to density functional theory (DFT) combined with ab initio motivated is used to study properties of water dimer and pentamer cations. The orbital energies are good approximations to the experimental ionization potentials of the system [9]. Ionization potentials and fragmentation dynamics of neutral, singly- and doubly charged small carbon clusters have been theoretically studied with a combination of the density functional theory, the coupled cluster method and the statistical model microcanonical Metropolis Monte Carlo. The second ionization potential decreases with the cluster size and is larger than the first one, which also decreases with the size showing oscillations[10].

MATERIALS AND METHODS

All the calculations have been performed using the GAMMESS package using ChemBio Office (version 11.0.1). The GAMMESS program was employed for the calculation of ionization potential. The correlation coefficient (R), standard error (SE) and Fisher constant (F) were employed to judge the validity of regression equation.

Firstly, MM2 method was used to find the best configuration stable form. Later, (AM1, HF/6-31G, DFT/STO-3G, DFT/3-21G and DFT/6-31G) methods were used to calculate the physical properties of the compounds.

RESULTS AND DISCUSSION

The experimental ionization potential values for the 100 compounds are summarized in Table1.

Table 1: The experimental ionization potential of 100 compounds

No.	Form	Name	Ionization Potential (eV)	No.	Form	Name	Ionization Potential (eV)
1	$CBrClF_2$	Bromochlorodi fluoromethane	11.21	**51**	$C_2Cl_2F_4$	1,2-Dichloro tetrafluoroethane	12.20
2	$CBrCl_3$	Bromotri chloromethane	10.60	**52**	$C_2Cl_3F_3$	1,1,1-Trichloro trifluoroethane	11.50
3	$CBrF_3$	Bromotri fluoromethane	11.40	**53**	$C_2Cl_3F_3$	1,1,2-Trichloro trifluoroethane	11.99
4	$CBr2F_2$	Dibromodifluoromethane	11.03	**54**	C_2Cl_4	Tetrachloroethylene	9.326
5	CBr_4	Tetrabromomethane	10.31	**55**	$C_2Cl_4F_2$	1,1,2,2-Tetrachloro-1,2-difluoroethane	11.30
6	$CClF_3$	Chlorotrifluoromethane	12.60	**56**	C_2Cl_4O	Trichloroacetyl chloride	11.00
7	CClN	Cyanogen chloride	12.34	**57**	C_2Cl_6	Hexachloroethane	11.10
8	CCl_2F_2	Dichlorodifluoromethane	12.05	**58**	C_2F_3N	Trifluoroacetonitrile	13.93
9	CCl_2O	Carbonyl chloride	11.50	**59**	C_2HBr	Bromoacetylene	10.31
10	CCl_3F	Trichlorofluoromethane	11.77	**60**	$C_2HBrClF_3$	2-Bromo-2-chloro-1,1,1-trifluoroethane	11.00
11	CCl_4	Tetrachloromethane	11.47	**61**	C_2HCl	Chloroacetylene	10.58
12	CFN	Cyanogen fluoride	13.34	**62**	C_2HClF_2	1-Chloro-2,2-difluoroethylene	9.80
13	CF_2O	Carbonyl fluoride	13.035	**63**	C_2HCl_3	Trichloroethylene	9.46
14	CF_3I	Trifluoroiodomethane	10.23	**64**	C_2HCl_3O	Dichloroacetyl chloride	10.90
15	$CHBrCl_2$	Bromodichloromethane	10.60	**65**	C_2HCl_5	Pentachloroethane	11.00
16	$CHBr_2Cl$	Chlorodibromomethane	10.59	**66**	C_2HF	Fluoroacetylene	11.26
17	$CHBr_3$	Tribromomethane	10.48	**67**	C_2HF_3	Trifluoroethylene	10.14
18	$CHClF_2$	Chlorodifluoromethane	12.20	**68**	$C_2HF_3O_2$	Trifluoroacetic acid	11.46
19	$CHCl_2F$	Dichlorofluoromethane	11.50	**69**	C_2H_2	Acetylene	11.40
20	$CHCl_3$	Trichloromethane	11.37	**70**	$C_2H_2Cl_2$	1,1-Dichloro ethylene	9.81
21	CHF_3	Trifluoromethane	13.86	**71**	$C_2H_2Cl_2$	cis-1,2-Dichloro ethylene	9.66
22	CHI_3	Triiodomethane	9.25	**72**	$C_2H_2Cl_2$	trans-1,2-Dichloro ethylene	9.64
23	CHN	Hydrogen cyanide	13.60	**73**	$C_2H_2Cl_2O$	Chloroacetyl chloride	10.30
24	CHNO	Isocyanic acid	11.595	**74**	$C_2H_2F_2$	cis-1,2-Difluoroethylene	10.23
25	CH_2BrCl	Bromochloromethane	10.77	**75**	C_2H_2O	Ketene	9.617
26	CH_2Br2	Dibromomethane	10.50	**76**	$C_2H_2O_2$	Glyoxal	10.20
27	CH_2ClF	Chlorofluoromethane	11.71	**77**	$C_2H_2S_2$	Thiirene	8.610
28	CH_2Cl_2	Dichloromethane	11.32	**78**	C_2H_3Br	Bromoethylene	9.83
29	CH_2F_2	Difluoromethane	12.71	**79**	C_2H_3Cl	Chloroethylene	9.99
30	CH_2I_2	Diiodomethane	9.46	**80**	$C_2H_3ClF_2$	1-Chloro-1,1-difluoroethane	11.98
31	CH_2N_2	Cyanamide	10.40	**81**	C_2H_3ClO	Acetyl chloride	10.82
32	CH_2O	Formaldehyde	10.88	**82**	C_2H_3ClO	Chloroacetaldehyde	10.48
33	CH_2O_2	Formic acid	11.33	**83**	$C_2H_3ClO_2$	Chloroacetic acid	10.70
34	CH_3Br	Bromomethane	10.541	**84**	$C_2H_3Cl_3$	1,1,1-Trichloro ethane	11.00
35	CH_3Cl	Chloromethane	11.22	**85**	$C_2H_3Cl_3$	1,1,2-Trichloro ethane	11.00
36	CH_3Cl_3Si	Methyltrichlorosilane	11.36	**86**	C_2H_3F	Fluoroethylene	10.36
37	CH_3F	Fluoromethane	12.47	**87**	C_2H_3FO	Acetyl fluoride	11.50
38	CH_3I	Iodomethane	9.538	**88**	$C_2H_3F_3$	1,1,1-Trifluoroethane	13.30
39	CH_3NO	Formamide	10.16	**89**	C_2H_3N	Acetonitrile	12.20
40	CH_4	Methane	12.61	**90**	C_2H_3NO	Methylisocyanate	10.67
41	CH_4N_2O	Urea	9.70	**91**	C_2H_4	Ethylene	10.514
42	CH_4O	Methanol	10.85	**92**	$C_2H_4Br_2$	1,2-Dibromoethane	10.35

43	CH_4S	Methanethiol	9.44	**93**	$C_2H_4Cl_2$	1,1-Dichloroethane	11.04
44	CH_5N	Methylamine	8.80	**94**	$C_2H_4Cl_2$	1,2-Dichloroethane	11.04
45	CH_6N_2	Methylhydrazine	7.70	**95**	$C_2H_4F_2$	1,1-Difluoroethane	11.87
46	CH_6Si	Methylsilane	10.70	**96**	C_2H_4O	Acetaldehyde	10.229
47	$C_2Br_2F_4$	1,2-Dibromotetrafluoroethane	11.10	**97**	C_2H_4O	Ethylene oxide	10.56
48	C_2ClF_3	Chlorotrifluoroethylene	9.81	**98**	$C_2H_4O_2$	Acetic acid	10.65
49	C_2ClF_5	Chloropentafluoroethane	12.60	**99**	$C_2H_4O_2$	Methyl formate	10.835
50	C_2Cl_2	Dichloroacetylene	9.90	**100**	C_2H_5Br	Bromoethane	10.29

While Table2 was showed the calculated ionization potential using different methods of quantum mechanics (AM1, HF/6-31G, DFT/STO-3G, DFT/3-21G and DFT/6-31G).

Table 2: The experimental ionization potential (IP), theoretical calculated and percent error of compounds

	Experimental	**AM1**		**HF/6-31G**		**DFT/STO-3G**		**DFT/3-21G**		**DFT/6-31G**	
No.	**IP (eV)**	**IP (eV)**	**% error**	**IP (eV)**	**% error**	**IP (eV)**	**% error**	**IP (eV)**	**% error**	**IP (eV)**	**% error**
1	11.21	11.82	5.41	12.50	11.47	5.86	-47.71	8.44	-24.75	8.79	-21.57
2	10.60	11.73	10.65	12.21	15.20	6.69	-36.93	8.51	-19.67	8.62	-18.69
3	11.40	12.32	8.10	12.90	13.19	5.24	-54.06	8.43	-26.09	9.04	-20.73
4	11.03	11.31	2.53	11.99	8.74	5.18	-53.07	7.95	-27.89	8.43	-23.61
5	10.31	11.22	8.87	11.49	11.48	5.30	-48.57	7.61	-26.24	8.03	-22.13
6	12.60	13.25	5.13	14.23	12.92	6.49	-48.53	9.38	-25.58	9.88	-21.59
7	12.34	13.04	5.65	13.04	5.65	7.75	-37.17	9.37	-24.09	9.42	-23.69
8	12.05	13.42	11.39	13.42	11.39	6.94	-42.44	9.14	-24.16	9.40	-21.99
9	11.50	13.31	15.70	13.31	15.70	7.23	-37.15	9.15	-20.47	9.21	-19.88
10	11.77	13.15	11.73	13.15	11.73	7.34	-37.63	9.09	-22.76	9.17	-22.12
11	11.47	12.38	7.92	13.05	13.79	7.73	-32.62	9.13	-20.37	9.13	-20.44
12	13.34	13.09	-1.88	14.12	5.87	6.88	-48.40	9.66	-27.56	10.02	-24.87
13	13.035	13.39	2.69	15.56	19.35	5.42	-58.44	9.53	-26.85	10.24	-21.43
14	10.23	11.97	16.99	---	---	---	---	---	---	---	---
15	10.60	11.48	8.30	11.89	12.12	6.24	-41.15	8.21	-22.52	8.35	-21.20
16	10.59	11.17	5.45	11.48	8.44	5.62	-46.91	7.81	-26.29	8.06	-23.91
17	10.48	11.07	5.65	11.27	7.53	5.13	-51.09	7.46	-28.78	7.84	-25.18
18	12.20	12.28	0.69	13.44	10.19	6.32	-48.21	8.90	-27.09	9.32	-23.64
19	11.50	12.87	11.92	12.87	11.92	6.88	-40.16	8.84	-23.11	9.01	-21.69
20	11.37	11.77	3.53	12.70	11.70	7.33	-35.54	8.83	-22.37	8.83	-22.33
21	13.86	13.32	-3.92	16.70	20.50	5.66	-59.15	10.29	-25.76	11.06	-20.22
22	9.25	10.68	15.50	---	---	---	---	---	---	---	---
23	13.60	13.68	0.57	13.64	0.30	8.12	-40.32	9.89	-27.32	9.96	-26.75
24	11.595	11.24	-3.08	12.21	5.26	5.24	-54.84	7.83	-32.43	8.28	-28.60
25	10.77	11.09	2.94	11.47	6.54	5.59	-48.13	7.86	-27.00	8.08	-25.00
26	10.50	10.96	4.37	11.05	5.25	5.04	-51.98	7.44	-29.11	7.77	-26.00
27	11.71	11.58	-1.11	12.57	7.34	6.12	-47.74	8.39	-28.37	8.60	-26.55
28	11.32	11.39	0.61	12.32	8.87	6.89	-39.15	8.60	-24.05	8.62	-23.86
29	12.71	12.02	-5.40	14.98	17.90	4.99	-60.76	8.87	-30.22	9.56	-24.82
30	9.46	10.56	11.66	---	---	---	---	---	---	---	---
31	10.40	10.30	-0.96	10.93	5.07	4.75	-54.29	6.82	-34.45	7.16	-31.20
32	10.88	10.78	-0.89	12.04	10.71	4.45	-59.07	7.07	-35.01	7.37	-32.23
33	11.33	11.50	1.53	12.73	12.37	4.41	-61.05	7.53	-33.57	7.97	-29.65
34	10.541	10.80	2.49	10.89	3.32	4.80	-54.51	7.18	-31.92	7.48	-29.03
35	11.22	11.34	1.05	11.89	6.00	6.33	-43.62	8.08	-27.99	8.10	-27.79
36	11.36	12.07	6.21	12.91	13.61	7.15	-37.02	9.12	-19.72	9.08	-20.09
37	12.47	12.10	-3.00	14.48	16.09	4.95	-60.30	8.54	-31.48	9.07	-27.29
38	9.538	10.51	10.23	---	---	---	---	---	---	---	---
39	10.16	10.67	4.99	11.24	10.63	3.71	-63.51	6.56	-35.48	6.94	-31.70
40	12.61	13.31	5.54	14.83	17.62	9.79	-22.33	10.58	-16.08	10.61	-15.86
41	9.70	10.47	7.91	10.90	12.33	3.34	-65.58	6.28	-35.28	6.72	-30.76
42	10.85	11.13	2.62	12.13	11.75	3.89	-64.16	6.68	-38.44	7.17	-33.95
43	9.44	8.93	-5.36	9.87	4.58	3.18	-66.27	6.52	-30.94	6.54	-30.76
44	8.80	9.76	10.86	9.85	11.97	4.02	-54.27	5.45	-38.03	5.61	-36.30

45	7.70	8.97	16.44	9.89	28.40	4.16	-46.00	5.63	-26.85	5.70	-26.03
46	10.70	11.62	8.60	12.17	13.70	7.30	-31.78	8.85	-17.28	8.84	-17.38
47	11.10	11.91	7.31	12.55	13.03	5.13	-53.79	8.34	-24.87	8.84	-20.38
48	9.81	10.09	2.88	11.45	16.70	4.09	-58.36	7.35	-25.05	7.76	-20.92
49	12.60	12.75	1.23	14.33	13.72	5.63	-55.32	9.48	-24.78	9.97	-20.88
50	9.90	10.23	3.30	11.01	11.20	6.30	-36.36	7.77	-21.47	7.65	-22.69
51	12.20	12.45	2.08	13.87	13.70	6.39	-47.59	---	---	---	---
52	11.50	12.43	8.09	13.26	15.33	6.65	-42.21	9.13	-20.57	9.25	-19.59
53	11.99	12.37	3.18	13.31	11.04	6.85	-42.90	9.16	-23.61	9.33	-22.20
54	9.326	9.90	6.16	10.78	15.61	6.16	-33.92	7.72	-17.24	7.62	-18.29
55	11.30	12.30	8.82	12.91	14.22	7.18	-36.49	8.91	-21.18	9.03	-20.13
56	11.00	11.91	8.25	13.05	18.59	7.04	-35.97	8.98	-18.32	9.05	-17.72
57	11.10	12.18	9.75	12.78	15.17	7.63	-31.30	8.89	-19.87	8.90	-19.83
58	13.93	14.19	1.84	15.08	8.25	6.91	-50.42	10.73	-22.99	11.08	-20.50
59	10.31	10.61	2.96	10.57	2.53	5.20	-49.53	7.32	-28.99	7.40	-28.22
60	11.00	11.75	6.84	12.14	10.38	5.55	-49.56	8.27	-24.86	8.58	-22.02
61	10.58	10.70	1.17	11.04	4.34	6.30	-40.50	7.84	-25.92	7.71	-27.10
62	9.80	10.05	2.51	11.08	13.03	4.60	-53.10	7.35	-24.97	7.61	-22.36
63	9.46	9.96	5.24	10.69	12.97	6.04	-36.10	7.65	-19.15	7.55	-20.21
64	10.90	11.68	7.12	12.96	18.91	6.75	-38.10	9.00	-17.39	9.08	-16.70
65	11.00	11.87	7.90	12.53	13.94	7.39	-32.82	8.74	-20.51	8.76	-20.38
66	11.26	11.15	-0.98	11.63	3.25	5.33	-52.63	7.86	-30.20	7.98	-29.13
67	10.14	10.09	-0.47	11.47	13.09	3.42	-66.28	7.07	-30.32	7.65	-24.57
68	11.46	12.49	8.96	14.18	23.72	---	---	8.38	-26.90	9.05	-21.03
69	11.40	11.50	0.87	11.08	-2.85	6.28	-44.91	7.90	-30.73	7.77	-31.85
70	9.81	10.19	3.88	10.63	8.38	6.07	-38.12	6.07	-38.12	7.57	-22.86
71	9.66	9.97	3.24	10.53	9.02	5.83	-39.61	7.51	-22.31	7.41	-23.28
72	9.64	10.01	3.89	10.58	9.72	5.87	-39.09	7.55	-21.68	7.45	-22.73
73	10.30	11.60	12.62	12.64	22.76	6.44	-37.48	8.81	-14.47	8.89	-13.69
74	10.23	9.99	-2.39	11.01	7.66	3.71	-63.75	6.99	-31.69	7.40	-27.62
75	9.617	9.60	-0.17	9.91	3.00	4.15	-56.83	6.49	-32.46	6.68	-30.55
76	10.20	10.66	4.52	12.10	18.59	4.11	-59.67	7.12	-30.18	7.56	-25.89
77	8.610	---	---	8.73	1.38	2.03	-76.39	5.63	-34.62	5.59	-35.11
78	9.83	10.15	3.28	9.99	1.63	4.71	-52.10	6.86	-30.17	7.04	-28.39
79	9.99	10.21	2.20	10.42	4.27	5.77	-42.21	7.43	-25.63	7.36	-26.34
80	11.98	12.18	1.71	13.07	9.10	6.06	-49.43	8.60	-28.18	8.98	-25.06
81	10.82	11.59	7.09	12.26	13.28	5.86	-45.82	8.17	-24.50	8.34	-22.93
82	10.48	11.01	5.03	12.15	15.96	4.92	-53.01	7.50	-28.47	7.74	-26.16
83	10.70	11.64	8.76	12.32	15.14	4.85	-54.68	7.94	-25.79	8.28	-22.61
84	11.00	11.99	9.02	12.44	13.13	7.04	-35.97	8.56	-22.16	8.58	-22.03
85	11.00	11.57	5.15	12.39	12.60	6.92	-37.12	8.57	-22.06	8.62	-21.65
86	10.36	10.24	-1.18	10.65	2.78	4.56	-55.97	7.16	-30.93	7.36	-28.97
87	11.50	11.99	4.28	13.43	16.82	4.63	-59.74	8.12	-29.43	8.62	-25.07
88	13.30	13.12	-1.39	15.79	18.72	5.39	-59.45	9.94	-25.25	10.66	-19.87
89	12.20	12.46	2.16	12.67	3.86	7.25	-40.58	8.95	-26.67	9.03	-26.00
90	10.67	10.51	-1.46	11.31	6.04	4.77	-55.25	7.25	-32.05	7.58	-28.98
91	10.514	10.55	0.36	10.19	-3.05	5.86	-44.23	7.36	-29.95	7.30	-30.58
92	10.35	11.01	6.40	11.14	7.66	4.90	-52.62	7.42	-28.31	7.76	-25.00
93	11.04	11.42	3.46	12.05	9.14	6.67	-39.60	8.30	-24.79	8.35	-24.39
94	11.04	11.42	3.41	12.19	10.39	6.58	-40.41	8.46	-23.40	8.47	-23.24
95	11.87	11.93	0.47	14.39	21.23	4.80	-59.53	8.71	-26.64	9.34	-21.29
96	10.229	10.72	4.80	11.59	13.35	4.13	-59.66	6.74	-34.15	7.02	-31.41
97	10.56	11.33	7.32	12.31	16.59	4.29	-59.38	6.89	-34.77	7.21	-31.70
98	10.65	11.62	9.15	12.41	16.52	4.15	-61.06	7.23	-32.11	7.65	-28.15
99	10.835	11.27	4.02	12.39	14.35	4.38	-59.58	7.42	-31.50	7.76	-28.40
100	10.29	10.69	3.91	10.73	4.29	4.67	-54.60	7.05	-31.47	7.34	-28.66

Percent error factor was measured using the following equation:

$$\%error = \frac{Calculated - Experimental}{Experimental} \times 100$$

Comparing between the experimental values with the predicted of compounds Table 3, there is a correlation between the observed and that predicted by all the methods calculations. Later, there are many equations which were used to predict the ionization potential of these values of 100 compounds in different methods.

AM1:
IP (exp.) = 0.488 + 0.915 × (IP Calc.)
(R= 0.898 , SE= 0.491, F= 401.77)

HF/6-31G:
IP (exp.) = 2.511 + 0.694 × (IP Calc.)
(R= 0.902 , SE= 0.483, F= 412.70)

DFT/STO-3G:
IP (exp.) = 8.448 + 0.448 × (IP Calc.)
(R= 0.519 , SE= 0.962, F= 34.31)

DFT/3-21G:
IP (exp.) = 3.778 + 0.894 × (IP Calc.)
(R= 0.864 , SE= 0.563, F= 275.08)

DFT/6-31G:
IP (exp.) = 3.296 + 0.925 × (IP Calc.)
(R= 0.912 , SE= 0.460, F= 459.30)

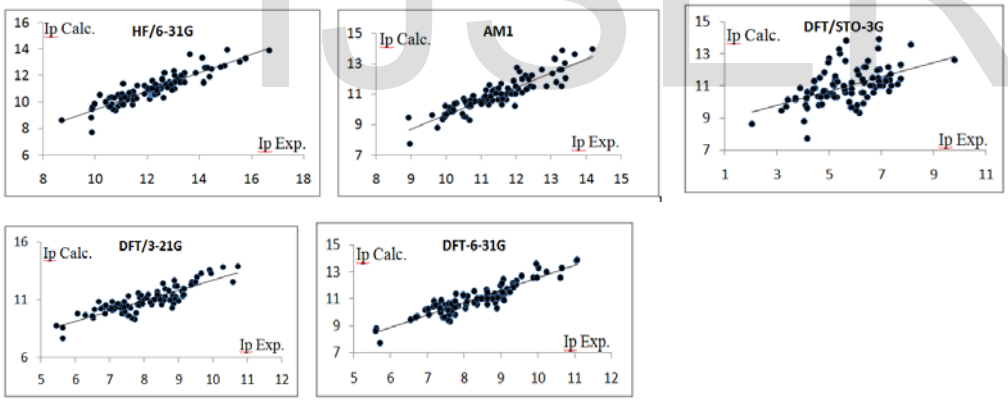

Figure 1. Correlation between experimental and calculated ionization potential

Table 3: The correlation between the experimental and predicted values of 100 compounds

	Experimental	AM1	HF/6-31G	DFT/STO 3G	DFT/3-21G	DFT/6-31G
Name	**IP**	**Predicted**	**Predicted**	**Predicted**	**Predicted**	**Predicted**
1	11.21	11.30	11.18	11.08	11.32	11.43
2	10.60	11.22	10.98	11.45	11.39	11.27
3	11.40	11.76	11.46	10.80	11.31	11.66
4	11.03	10.84	10.83	10.77	10.88	11.10
5	10.31	10.75	10.48	10.82	10.58	10.73
6	12.60	12.61	12.38	11.36	12.16	12.44
7	12.34	12.42	11.56	11.92	12.15	12.01
8	12.05	12.77	11.82	11.56	11.95	11.99
9	11.50	12.67	11.75	11.69	11.96	11.82
10	11.77	12.52	11.64	11.74	11.90	11.78
11	11.47	11.81	11.57	11.91	11.94	11.74

12	13.34	12.46	12.31	11.53	12.41	12.57
13	13.04	12.74	13.31	10.88	12.30	12.77
14	10.23	11.44	---	---	---	---
15	10.60	10.99	10.76	11.25	11.12	11.02
16	10.59	10.71	10.48	10.97	10.76	10.75
17	10.48	10.62	10.33	10.75	10.45	10.55
18	12.20	11.72	11.84	11.28	11.73	11.92
19	11.50	12.26	11.44	11.53	11.68	11.63
20	11.37	11.26	11.32	11.73	11.67	11.47
21	13.86	12.67	14.10	10.99	12.98	13.53
22	9.25	10.26	---	---	---	---
23	13.60	13.00	11.98	12.09	12.62	12.51
24	11.60	10.77	10.98	10.80	10.78	10.96
25	10.77	10.63	10.47	10.95	10.80	10.77
26	10.50	10.52	10.18	10.71	10.43	10.49
27	11.71	11.08	11.23	11.19	11.28	11.25
28	11.32	10.91	11.06	11.54	11.47	11.27
29	12.71	11.49	12.90	10.69	11.71	12.14
30	9.46	10.15	---	---	---	---
31	10.40	9.91	10.09	10.58	9.87	9.92
32	10.88	10.35	10.86	10.44	10.10	10.12
33	11.33	11.01	11.34	10.43	10.51	10.67
34	10.54	10.37	10.07	10.60	10.20	10.22
35	11.22	10.86	10.76	11.29	11.00	10.79
36	11.36	11.53	11.47	11.65	11.93	11.70
37	12.47	11.56	12.56	10.67	11.41	11.69
38	9.54	10.10	---	---	---	---
39	10.16	10.25	10.31	10.11	9.64	9.72
40	12.61	12.67	12.80	12.84	13.24	13.11
41	9.70	10.07	10.07	9.95	9.39	9.51
42	10.85	10.67	10.93	10.19	9.75	9.93
43	9.44	8.66	9.36	9.87	9.61	9.35
44	8.80	9.42	9.35	10.25	8.65	8.49
45	7.70	8.69	9.37	10.31	8.81	8.57
46	10.70	11.12	10.96	11.72	11.69	11.48
47	11.10	11.38	11.22	10.75	11.23	11.48
48	9.81	9.72	10.46	10.28	10.35	10.48
49	12.60	12.15	12.45	10.97	12.25	12.52
50	9.90	9.85	10.15	11.27	10.72	10.37
51	12.20	11.88	12.13	11.31	---	---
52	11.50	11.86	11.71	11.43	11.94	11.85
53	11.99	11.81	11.75	11.52	11.97	11.93
54	9.33	9.55	9.99	11.21	10.68	10.35
55	11.30	11.74	11.47	11.67	11.74	11.65
56	11.00	11.38	11.57	11.60	11.81	11.67
57	11.10	11.63	11.38	11.87	11.72	11.53
58	13.93	13.47	12.97	11.55	13.37	13.55
59	10.31	10.20	9.85	10.78	10.32	10.14
60	11.00	11.24	10.93	10.94	11.17	11.23
61	10.58	10.28	10.17	11.27	10.79	10.43
62	9.80	9.68	10.20	10.51	10.35	10.34
63	9.46	9.60	9.93	11.16	10.62	10.28
64	10.90	11.17	11.50	11.47	11.82	11.70
65	11.00	11.35	11.20	11.76	11.59	11.40
66	11.26	10.69	10.58	10.84	10.80	10.68
67	10.14	9.72	10.47	9.98	10.10	10.37
68	11.46	11.92	12.35	9.98	11.27	11.67
69	11.40	11.01	10.20	11.26	10.84	10.49
70	9.81	9.81	9.89	11.17	9.20	10.30
71	9.66	9.61	9.82	11.06	10.49	10.15
72	9.64	9.65	9.85	11.08	10.53	10.19

73	10.30	11.10	11.28	11.34	11.65	11.52
74	10.23	9.63	10.15	10.11	10.03	10.14
75	9.62	9.27	9.39	10.31	9.58	9.48
76	10.20	10.24	10.91	10.29	10.14	10.29
77	8.61	---	8.57	9.36	8.81	8.47
78	9.83	9.77	9.44	10.56	9.91	9.81
79	9.99	9.83	9.74	11.03	10.42	10.11
80	11.98	11.63	11.58	11.16	11.47	11.61
81	10.82	11.09	11.02	11.08	11.08	11.01
82	10.48	10.56	10.94	10.65	10.48	10.46
83	10.70	11.14	11.06	10.62	10.88	10.96
84	11.00	11.46	11.14	11.60	11.43	11.23
85	11.00	11.07	11.11	11.55	11.44	11.27
86	10.36	9.86	9.90	10.49	10.18	10.11
87	11.50	11.46	11.83	10.52	11.04	11.27
88	13.30	12.49	13.47	10.86	12.66	13.16
89	12.20	11.89	11.30	11.70	11.78	11.65
90	10.67	10.10	10.36	10.59	10.26	10.31
91	10.51	10.14	9.58	11.08	10.36	10.05
92	10.35	10.56	10.24	10.64	10.41	10.48
93	11.04	10.94	10.87	11.44	11.20	11.02
94	11.04	10.94	10.97	11.40	11.34	11.13
95	11.87	11.40	12.50	10.60	11.56	11.94
96	10.23	10.30	10.55	10.30	9.80	9.79
97	10.56	10.85	11.05	10.37	9.94	9.97
98	10.65	11.12	11.12	10.31	10.24	10.37
99	10.84	10.80	11.11	10.41	10.41	10.48
100	10.29	10.27	9.96	10.54	10.08	10.09
R		0.898	0.902	0.519	0.864	0.912
F		401.7	412.70	34.31	275.08	459.30

CONCLUSION

At comparing between all the percent error for all 100 compounds using different methods were shown an increasing in error by increased in the basis set of calculations:

AM1 < HF/6-31G < DFT/6-31G < DFT/3-21G < DFT/STO-3G

While at comparing between the correlation coefficient (R) and the Fisher constant (F) between all the methods are shown below:

DFT/6-31G > HF/6-31G > AM1 > DFT/3-21G > DFT/STO-3G

The regression statistics of these compounds are given different values in correlation coefficient (R). The best method for prediction of the experimental values are found with (DFT/6-31G) about (R=0.912) even there is a somewhat percent error at the calculations. On the other side, (DFT/STO-3G) method was given a bad correlation with an experimental data (R=0.519) with larger percent error. While (HF/6-31G) and (AM1) give a correlation (R=0.902) and (R=0.898) respectively with small error value for (AM1) compare with the other.

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