International Scholars Journals

Advanced Journal of Microbiology Research ISSN 2241-9837 Vol. 13 (6), pp. 001-008, June, 2019. Available online at www.internationalscholarsjournals.org © International Scholars Journals

Full Length Research Paper

Density functional theory (DFT) study of C_7 Si_5 Ge_3 cluster as a novel material for vitamin C nano carrier

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Accepted 23 April, 2019

In the present study, structural properties of C_7 Si_5 Ge_3 cluster and interaction between this cluster and vitamin C have been studied extensively utilizing density functional theory (DFT) employing B3LYP exchange correlation. Nuclear magnetic resonance (NMR) properties are calculated by using density functional method (B3LYP) with 6-31G, 6-311G* and cc-pvdz as basis sets. Also natural bond orbital (NBO) analysis has been performed for C_7 Si_5 Ge_3 cluster and C_7 Si_5 Ge_3 inside vitamin C. Our results indicate that vitamin C can form stable bindings with C_7 Si_5 Ge_3 cluster through oxygen (O) active site. Thus, we arrive at the prediction that the C_7 Si_5 Ge_3 cluster can be implemented as a novel material for drug delivery applications.

Key words: C_7 Si_5 Ge_3, vitamin, nano, nuclear magnetic resonance, natural bond orbital, density functional theory.

INTRODUCTION

Group-VA cluster such as BN nanomaterials are expected in extensive application due to the good stability at high temperatures with high electronic insulation in air. Despite the carbon nanotubes, BN nanotubes are constant band gap materials and thus provide an attractive opportunity for practical applications (Monajjemi et al., 2010). The wide range of their electronic properties from metallic to wide-gap semiconductors, depending on their chemical composition, makes them suitable candidates for nanosize electronic devices (Monajjemi et al., 2008, 2009). Due to the similarity between B-N and C-C units, a lot of effort has been devoted to BN fullerene-like materials in recent years, which have excellent properties such as heat resistance, insulation, and structural stability (Chopra et al., 1995; Monajjemi et al., 2011). Several studies have been made on BN nanomaterials such as BN nanotubes, BN nanocapsules, and BN clusters since they have excellent properties such as heat resistance in air and insulation, and these nano-particles are expected to be useful as electronic devices, high heat resistance semiconductors, and insulator lubricants (Corso et al., 2004; Golberg et al., 1998; Stephan et al., 1998; Monajjemi et al., 2008). Also extensive research has been focused on group-IVA elemental clusters C_n , Si_n, Ge_n , Sn_n and Pb_n in the past two decades for both fundamental and technological reasons while very limited experimental and theoretical investigations performed on binary A_mB_n or ternary AlB_mC_n clusters (A, B, C=C, Si, and Ge)(Mollaamin et al., 2008, 2011; Monajjemi et al., 2004, 2010; Maiti et al., 2000; Froudakis et al.,1994, 1995; Grev and Schaefer, 1985; Lammertsma and Guner, 1988; Drebov et al., 2010).

Over the past several years, Froudakis et al. (1994) have performed various *ab initio* investigations on Si_mC_n binary microclusters, including the second-order Moller-Plesset (MP2) and coupled cluster singles and doubles (CCSD) calculations on Si_4C, (Monajjemi et al., 2010) MP2 or higher-order perturbation (CASP2) on Si_2C_4, Si_3C_3 and Si_2C_4 (Froudakis et al., 1994; Mollaamin et al., 2008). MP2 and CCSD(T) on Si_3C_2 (Froudakis et al., 1995) and CCSD(T) and tight-binding molecular-dynamics studies on SiGe, Si_2Ge_2, and Si_2Ge_4 (Mollaamin et al., 2011).

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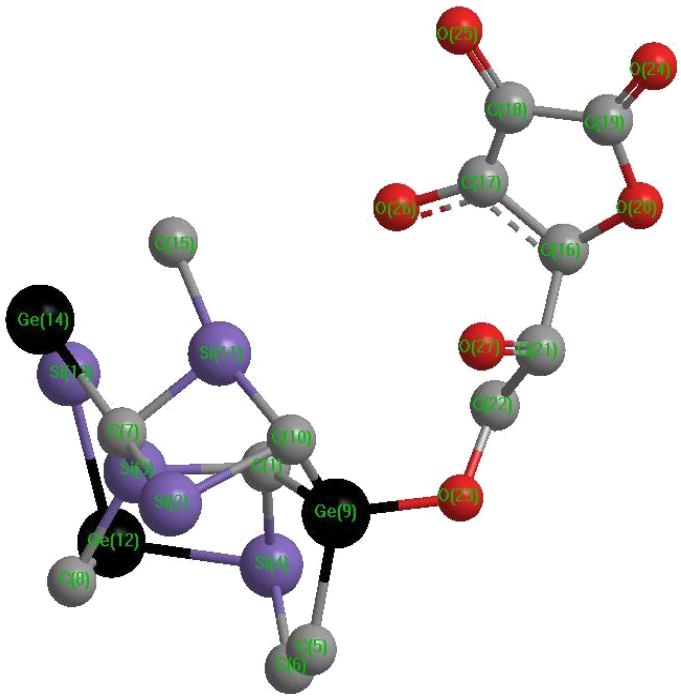

Figure 1. C_7 Si_5 Ge_3 cluster.

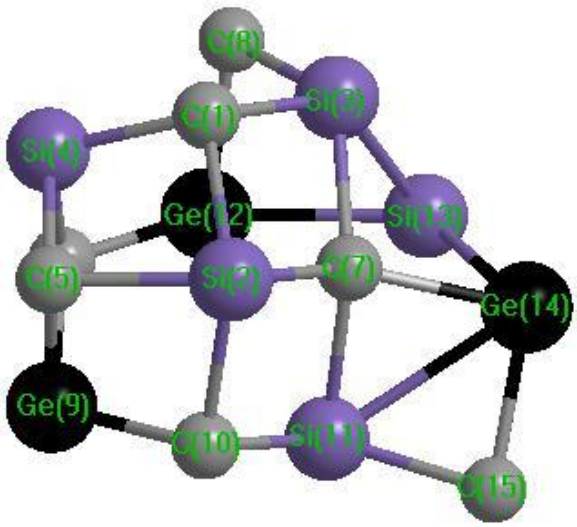

Figure 2. C_7 Si_5 Ge_3 cluster inside vitamin C.

Earlier theoretical and experimental investigations provided detailed structural and bonding characteristics for Si_2C and Si_2C_2 (Lammertsma and Guner, 1988; Drebov et al., 2010). Very recently, we presented a density functional theory (DFT) study on binary microclusters A_mB_n (A, B=Si, Ge; s=m+n≤10) and found that these clusters follow similar structural patterns to corresponding elemental Sis and Ge_s, (Li et al., 2001) and have more isomers with lower symmetries. However, as we know, there have been no theoretical or experimental results reported on $Ge_lSi_mC_n$ ternary clusters to date. In this work, interaction between C_7 Si_5 Ge_3 cluster and vitamin C has been studied by using DFT employing B3LYP exchange correlation.

Computational details

In the present work, we optimized the $C_7Si_5Ge_3$ (Figures 1 and 2) with 3 basis sets, 6–311G, 6–311G* and cc-pvdz and $C_7Si_5Ge_3$ beside vitamin C with 2 basis sets, 6–311G, 6–311G* with the Gaussian 03 by the B3LYP method. The nuclear magnetic resonance (NMR) isotropic shielding constants were calculated using the standard Gauge-Independent Atomic Orbital (GIAO) approach of GAUSSIAN 03 program package (Dichfield, 1974; Zurek and Autschbach, 2004; Osmialowski and Gawinecki, 2001).

(a) The isotropic value σiso of the shielding tensor which can be defined as (Becke, 1988; Lee et al., 1988):

$$\sigma_{ISO} = \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33})$$

(b) The anisotropy parameter (Δσ) defined as:

$$\text{If } \left|\sigma_{11} - \sigma_{ISO}\right| \geq \left|\sigma_{33} - \sigma_{ISO}\right| \quad \sigma = \sigma^{11} - \frac{\sigma_{22} + \sigma_{33}}{2}$$

$$\text{If } \left|\sigma_{11} - \sigma_{ISO}\right| \leq \left|\sigma_{33} - \sigma_{ISO}\right| \quad \sigma = \sigma^{33} - \frac{\sigma_{22} + \sigma_{11}}{2}$$

(c) The asymmetry parameter (η) which is given by Lee et al. (1988):

$$\text{If } \left|\sigma_{11} - \sigma_{ISO}\right| \geq \left|\sigma_{33} - \sigma_{ISO}\right| \quad \eta = \frac{\sigma_{22} - \sigma_{33}}{\delta}$$

$$\text{If } \left|\sigma_{11} - \sigma_{ISO}\right| \leq \left|\sigma_{33} - \sigma_{ISO}\right| \quad \eta = \frac{\sigma_{22} - \sigma_{11}}{\delta}$$

The calculations of NMR parameters has been shown in Tables 1 and 2 and Plot of σ_{iso}, σ_{aniso}, Δ, δ and η versus atomic charge for $C_7Si_5Ge_3$ cluster and $C_7Si_5Ge_3$ beside vitamin C has been illustrated in Figures 3 and 4. Also NBO analysis has been performed. The results of NBO analysis at different level of theory are listed in Table 3.

RESULTS AND DISCUSSION

Nuclear magnetic resonance (NMR) calculation

We studied about $C_7Si_5Ge_3$ as a novel material for vitamin C carriers. Before and after connecting the vitamin C to $C_7Si_5Ge_3$ NMR calculations were performed

Table 1. Nuclear magnetic resonance parameters of Carbon, Silicon and Germanium atoms in C7 Si5 Ge3 at the level of B3LYP/6-311G, B3LYP/6-311G* and B3LYP/cc-pvdz.

	Atom	σ_{iso}	σ_{aniso}	Determine (NMR)	Distance matrix	ΔE	δ	η	Δσ	Dipole orientation	Atomic charge
B3LYP/6-311G	C(1)	231.7038	201.7217	10361483.58			-123.1349	-0.907854719	201.7217		-1.009404
	Si(2)	437.3231	227.9308	67386975.21			-209.9714	0.447376643	-314.95715		0.867148
	Si(3)	206.9964	294.1195	-4705409.055			-281.7959	0.39164303	-422.6938		1.437836
	Si(4)	209.5199	416.837	-3993017.67			-267.014	-0.959263559	416.837		0.853224
	C(5)	-307.4583	388.5116	-9605090.051			-330.1262	0.569143558	-495.1893		-0.822804
	C(6)	20.9606	314.0346	-1853192.32			-226.5743	0.848014978	-339.8615		-0.978851
	C(7)	-48.551	22.8389	1261262.605			-148.1028	-0.996918357	222.8389		-0.746227
	C(8)	-61.3514	154.2011	260918.8175	8663913.687	7944.729474	-62.3169	-0.350354398	154.2011	2.7151	-1.389715
	Ge(9)	1154.3514	985.7233	981294414.5			-706.1246	0.86128298	-1059.18695		0.879479
	C(10)	-42.0106	205.8843	1021123.58			-129.1728	-0.937421036	205.88425		-1.161014
	Si(11)	31.9291	512.9105	-27366352.95			-469.2204	0.45748288	-703.83055		0.797525
	Ge(12)	795.2434	1612.1652	-109097925.4			-940.3287	-0.857020104	1612.1652		0.655489
	Si(13)	-19.9726	675.703	24649663.86			-273.9452	-0.355624775	675.70305		0.637779
	Ge(14)	782.2023	2476.9529	-147995544			-1075.2836	-0.464310346	2476.95295		0.64898
	C(15)	-117.1535	188.6415	30499.48033			-112.2594	-0.879728557	188.6415		-0.669445
B3LYP/6-311G*	C(1)	216.6532	210.0134	8375401.613			-126.48	-0.893036053	210.0134		-0.767979
	Si(2)	450.7466	232.4786	76296550.03			-200.4019	0.546749307	-300.6028		0.703776
	Si(3)	209.029	268.0837	-3369620.286			-272.1728	0.313301329	-408.25925		0.94453
	Si(4)	233.3558	383.62	-1882069.934			-264.876	0.931067367	-397.314		0.714599
	C(5)	-302.2342	371.8407	-9923881.549			-328.1706	0.510761781	-492.2559		-0.580893
	C(6)	0.9889	306.0146	-1032552.249			-227.5285	0.784477549	-342.2928		-0.68013
	C(7)	-50.2985	237.4117	1601473.617			-150.1999	-0.946241642	237.4117		-0.417008
	C(8)	-62.3578	155.2868	331337.4876	8663913.687	-7944.99425	-60.7854	-0.296883791	155.2868	2.55	-0.835994
	Ge(9)	1201.1183	1030.1901	1102261049			-734.6616	0.869686397	-1101.9924		0.482704
	C(10)	-76.5098	229.6456	1527747.398			-144.4965	-0.940479527	229.6455		-0.773117
	Si(11)	44.9809	467.8052	-26831738.95			-453.5322	0.375294411	-680.29825		0.484356
	Ge(12)	721.7461	1749.9754	-219294325.4			-988.0461	-0.055407941	-482.0691		0.363066
	Si(13)	-7.4712	695.7326	24974460.52			-281.7684	-0.353889932	695.7326		0.43086
	Ge(14)	726.7263	2592.5202	-140648663.3			-1134.928	-0.477130972	2592.52015		0.349979
	C(15)	-116.2643	192.7436	121518.8024			-109.7052	-0.828718238	192.74355		-0.418748
B3LYP/cc-pvdz	C(1)	219.4345	191.1158	9217907.439			-114.0135	-0.882496371	191.11575		-0.421345
	Si(2)	514.7591	206.8696	122762327.9			-180.4345	0.52867772	-270.65175		0.38789
	Si(3)	302.0314	258.8061	12459222.49			-255.8606	0.348682447	-383.79095		0.487941
	Si(4)	321.0828	344.7802	15756607.51	12095331.38	-7944.93099	-244.746	0.878302403	-367.119	2.4172	0.419312
	C(5)	-263.8017	350.1326	-5195149.609			-314.0873	0.486349496	-471.1309		-0.356859
	C(6)	15.9949	298.4917	-1440559.702			-220.0036	0.809010853	-330.00545		-0.459216
	C(7)	-32.4757	22.7183	1105869.528			-146.2138	-0.984508986	222.7182		-0.186287
	C(8)	-42.889	144.3388	330152.1512			-58.5632	-0.356887943	144.33885		-0.390749

Table 1. Contd.

Ge(9)	1438.9032	863.1021	2448192943	-622.2915	0.849298761	-933.4372	0.374131
C(10)	-57.5232	216.8211	1397515.216	-132.4638	-0.908778096	216.8211	-0.399124
Si(11)	152.4864	416.918	-28077133.16	-399.2861	0.392225024	-598.9264	0.131189
Ge(12)	1008.0843	1558.5175	337456034.6	-862.9395	-0.795962289	1558.51755	0.261685
Si(13)	97.3005	590.2695	3905728.001	-242.0477	-0.374233674	590.2695	0.152828
Ge(14)	989.0263	2292.39	-20826458.59	-1016.4582	-0.496479737	2292.39815	0.207784
C(15)	-95.7853	176.9289	288341.24	-106.8816	-0.896417157	176.92895	-0.209179

Table 2. Nuclear magnetic resonance parameters of Carbon, Silicon, Germanium and Oxygen atoms in C_7 Si_5 Ge_3 inside of vitamin C at the level of B3LYP/6-311G and B3LYP/6-311G*.

Method	Atom	σ_{iso}	σ_{aniso}	σ_{11}	σ_{22}	σ_{33}	Determine (NMR)	Distance matrix	ΔE	δ	η	Δσ	Dipole orientation	Atomic charge
B3LYP/6-311G	C(1)	-645.7465	1260.869	-1863.958	-268.1145	194.8331	-7697806	-9.96E+12	-22620.3	-1218.212	0.380022	-1827.317	10.8001	-1.013667
	Si(2)	328.063	1466.009	-927.0378	605.8245	1305.402	23561661			-1255.101	0.557388	-1882.651		0.883092
	Si(3)	372.5191	467.6201	-90.4508	523.7423	684.2659	-1675060			-462.9699	0.346726	-694.4549		0.518203
	Si(4)	134.1127	764.0834	-380.7592	139.5956	643.5016	-1.16E+08			-514.8719	0.978702	-772.3078		0.703889
	C(5)	-234.8056	190.4396	-363.0613	-233.5097	-107.8459	-9751558			-128.2557	0.979791	-192.3835		-0.290315
	C(6)	-9.7212	288.4426	-230.939	19.2016	182.5739	-4764277			-221.2178	0.738513	-331.8268		-0.372796
	C(7)	-418.5622	1675.224	-1240.455	-713.4853	698.2535	7.07E+08			-821.8925	-0.641166	1675.224		-1.572688
	C(8)	-1138.946	1998.366	-2239.047	-1371.089	193.298	-1.65E+08			-1100.101	-0.78898	1998.366		-0.435397
	Ge(9)	1025.327	844.623	143.0221	1344.55	1588.409	3.73E+08			-882.305	0.276389	-1323.458		1.381945
	C(10)	-122.7659	1010.676	-1118.143	198.8273	551.0178	20595553			-995.377	0.353826	-1493.065		-0.896844
	Si(11)	-680.6575	2385.135	-3092.525	141.1199	909.4324	-4.85E+08			-2411.867	0.318555	-3617.801		1.045512
	Ge(12)	1228.927	2310.215	-25.7599	943.4703	2769.07	7.81E+08			-1254.687	-0.772488	2310.215		0.287004
	Si(13)	-342.2017	1013.021	-1120.188	-239.5625	333.1453	1.64E+08			-777.9861	0.736141	-1166.979		0.333809
	Ge(14)	-523.0917	2921.81	-3255.248	261.1914	1424.782	-8.59E+08			-2732.156	0.425887	-4098.234		0.584703
	C(15)	2813.448	10341.75	-1185.049	-82.5536	9707.948	4.95E+09			-3998.498	-0.275727	10341.75		-0.417952
	C(16)	38.403	325.5507	-220.5401	80.3124	255.4368	-2515844			-258.9431	0.676305	-388.4147		0.160967
	C(17)	-56.1238	259.5801	-228.383	-56.9179	116.9296	1493027			-172.2592	-0.99539	259.5801		0.244959
	C(18)	-5.8769	168.4873	-128.9208	4.8421	106.448	208869.2			-123.0439	0.82577	-184.5659		0.183606
	C(19)	32.8849	124.4213	-73.8826	56.7048	115.8324	-432292.9			-106.7675	0.553798	-160.1512		0.4963
	O(20)	-169.9147	509.8918	-539.3696	-140.3875	170.0132	11686559			-369.4549	0.840159	-554.1825		-0.42876
	C(21)	-34.564	270.5059	-280.1856	30.7203	145.7733	1503192			-245.6216	0.468416	-368.4324		0.182574
	C(22)	-451.7256	732.0889	-1257.82	-133.6903	36.3337	-13074981			-806.0945	0.210923	-1209.142		0.321104
	O(23)	-493.3326	1014.63	-1355.613	-307.4721	183.0872	32035755			-862.2802	0.568909	-1293.42		-0.629221
	O(24)	-238.3456	795.3663	-701.4513	-305.4841	291.8986	58114131			-463.1057	-0.855026	795.3663		-0.261257
	O(25)	-1057.534	2072.535	-2893.651	-603.1073	324.1558	5.98E+08			-1836.117	0.505013	-2754.175		-0.295617
	O(26)	-776.13	2670.099	-3014.352	-317.9741	1003.936	3.83E+08			-2238.222	0.590607	-3357.333		-0.38465
	O(27)	-1073.145	2401.492	-4232.156	484.871	527.8492	7.55E+08			-3159.01	0.013605	-4738.516		-0.328505

Table 2. Contd.

B3LYP/6-311G*	C(1)	-118.8758	1064.804	-1017.154	69.5332	590.9938	-29851317	-9.96E+12	-22621.54	-898.2785	0.580511	-1347.418	10.7691	-0.813643
	Si(2)	236.8509	1593.269	-523.5847	-64.8926	1299.03	3.46E+08			-760.4356	-0.603197	1593.269		0.635962
	Si(3)	300.6817	348.252	-63.4098	432.605	532.8497	-11632059			-364.0915	0.275328	-546.1372		0.728352
	Si(4)	21.0507	876.237	-702.2376	160.1809	605.2087	-84509705			-723.2883	0.615284	-1084.932		0.649518
	C(5)	-220.4648	394.5872	-438.5544	-265.4333	42.5934	-10447115			-218.0896	-0.793807	394.5873		-0.237894
	C(6)	-86.4844	374.4661	-326.6341	-95.9787	163.1596	-5619970			-240.1497	-0.960465	374.466		-0.298431
	C(7)	-476.5998	1136.251	-1444.024	-266.6757	280.9007	1.27E+08			-967.4245	0.566015	-1451.137		-0.973733
	C(8)	-1309.92	1192.982	-2342.165	-1072.996	-514.599	-1.49E+09			-1032.245	0.540954	-1548.368		-0.350904
	Ge(9)	1064.778	613.7112	746.6391	973.776	1473.919	1.17E+09			-318.1389	-0.713955	613.7113		0.997985
	C(10)	-48.7617	798.2597	-487.1442	-142.5523	483.4114	14020943			-438.3825	-0.786053	798.2597		-0.663846
	Si(11)	-475.6232	1416.989	-2279.099	383.1927	469.0364	1.79E+08			-1803.476	0.047599	-2705.213		0.839597
	Ge(12)	-224.5383	3000.414	-2875.418	426.0649	1775.738	-1.58E+09			-2650.88	0.509142	-3976.319		-0.005226
	Si(13)	-446.3191	1582.931	-2127.441	179.5157	608.9679	-5.57E+08			-1681.122	0.255456	-2521.683		0.277576
	Ge(14)	877.5062	5134.5	-2297.612	629.6241	4300.506	-5.4E+09			-3175.118	-0.92193	5134.5		0.252147
	C(15)	2586.425	10266.7	-1601.376	-70.2382	9430.889	2.12E+09			-4187.801	-0.365619	10266.7		-0.348332
	C(16)	-64.7432	244.4591	-170.8905	-121.5686	98.2296	1983842			-106.1473	-0.464655	244.4592		0.107986
	C(17)	-38.151	222.4513	-197.2205	-27.3824	110.1498	1775898			-159.0695	0.864604	-238.6042		0.239571
	C(18)	-53.2916	218.934	-156.2206	-96.3186	92.6644	1671421			-102.929	-0.581974	218.934		0.138587
	C(19)	26.4991	126.9126	-74.5851	42.9748	111.1075	-297103			-101.0842	0.674019	-151.6263		0.415218
	O(20)	209.2108	471.057	-53.3354	157.719	523.2488	-2660776			-262.5462	-0.803875	471.057		-0.299345
	C(21)	-75.4783	462.5502	-323.6846	-135.6388	232.8884	4907655			-248.2063	-0.757619	462.5501		0.180957
	C(22)	-331.9876	658.6004	-1054.323	-48.7194	107.0793	412863.6			-722.335	0.215688	-1083.503		0.168089
	O(23)	-336.8436	654.4009	-1007.089	-102.8651	99.4236	-47992185			-670.2458	0.301813	-1005.369		-0.476587
	O(24)	-229.7163	764.4972	-646.2729	-322.8245	279.9485	58766218			-416.5566	-0.776481	764.4972		-0.242906
	O(25)	-1319.404	2476.629	-3471.12	-818.7743	331.6816	9.43E+08			-2151.716	0.534669	-3227.574		-0.278922
	O(26)	-1258.476	2354.633	-3261.692	-825.0144	311.2794	8.96E+08			-2003.216	0.567235	-3004.825		-0.358456
	O(27)	-647.2325	3206.098	-3169.057	-262.8063	1490.166	7.76E+08			-2521.825	0.695121	-3782.737		-0.283321

in electric field of charges. The remarkable feature in these calculations is observed in calculations of η. We can see completely symmetrical curves at various methods and basis sets (Figure 3e). This symmetry does not exist after connecting to vitamin C (Figure 4e).

Although the maximum points are various in different methods but the symmetry is observed around the axis of zero charge. In other words, positive and negative areas show the same behaviour. Some minimums are observed for η at zero charge that are -7 and -3 for 6-311G and 6-311G* basis sets respectively but to be positive for cc-pvdz basis set. This symmetry does not exist for σ_{iso} and σ_{aniso} and in positive area is more regular than negative area. But in the case $\Delta\sigma$ that is the result of σiso and σ_{aniso} this symmetry can be seen again (Figure 3C).This symmetry is lower for the cc-pvdz basis set.

We want to examine what changes occur if the vitamin C connect to $C_7Si_5Ge_3$ cluster and under what circumstances the vitamin C establishes a strong connection and in what situation the connection would be weak. The results show that vitamin C connects stronger to $C_7Si_5Ge_3$ cluster in positive charges than negative charge. Thus by creating a positive field vitamin C can be connected to the $C_7Si_5Ge_3$ cluster and delivered easily by using a negative filed. These observations are exactly observed for σiso, σ_{aniso} and $\Delta\sigma$.

Natural bond orbital (NBO) analysis

The concepts of NBO analyses are useful for

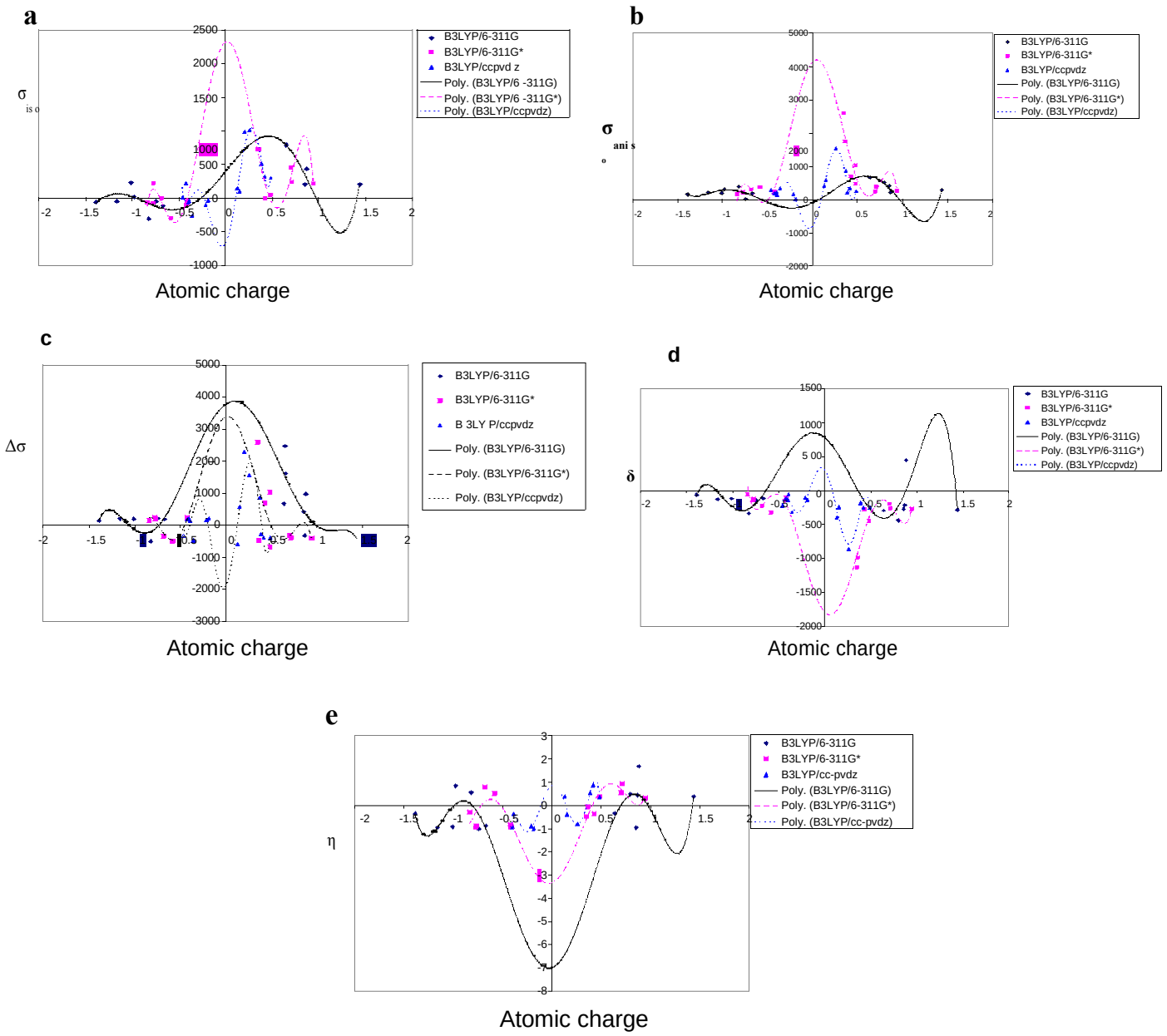

Figure 3. Plot of (a) σ_{iso} (b) σ_{aniso} (c) $\Delta\sigma$ (d) δ and (e) η versus atomic charge for C_7 Si_5 Ge_3 cluster.

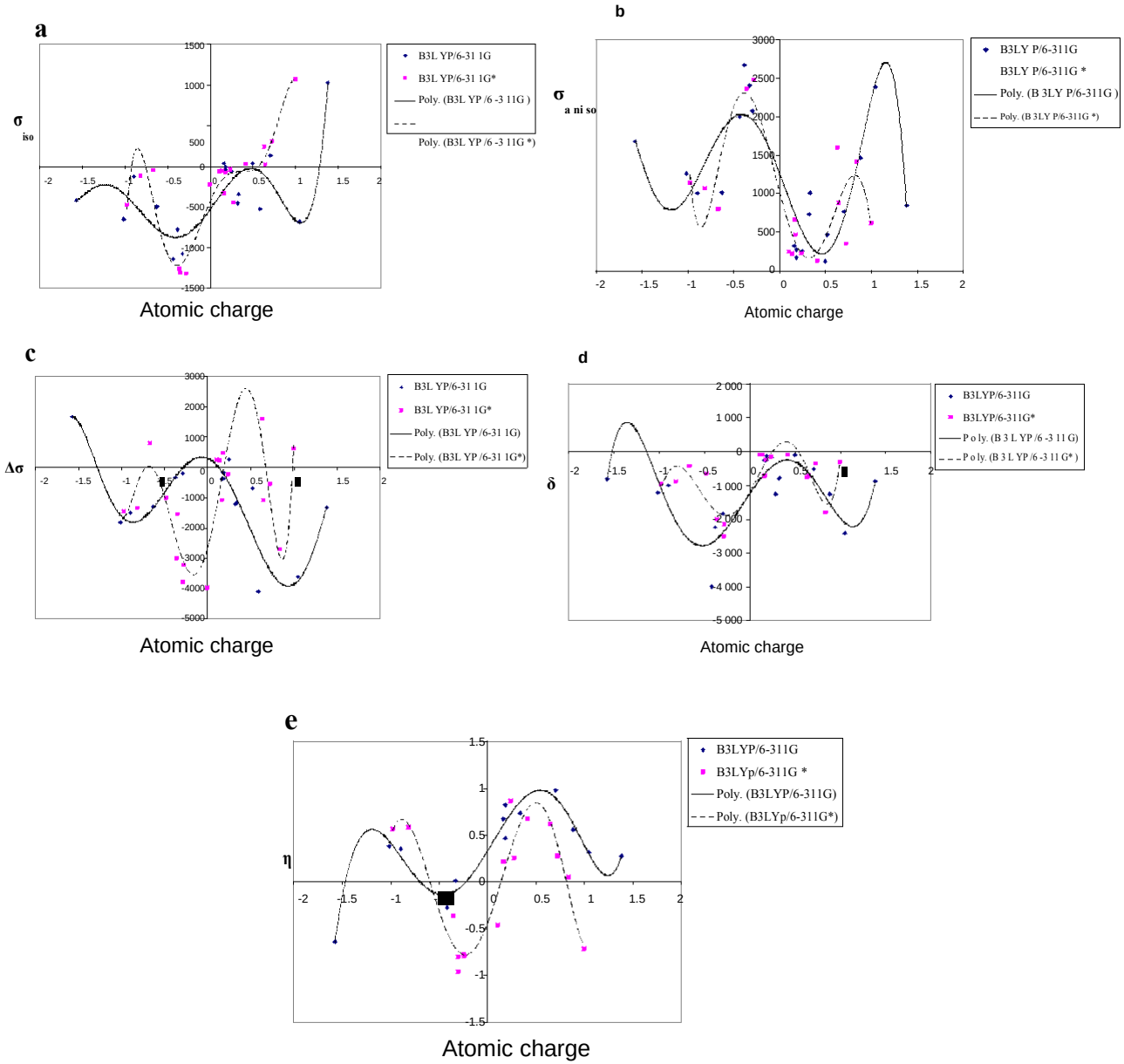

Figure 4. Plot of (a) σ_{iso} (b) σ_{aniso} (c) $\Delta\sigma$ d) δ and (e) η versus atomic charge for $C_7 SI_5 GE_3$ cluster beside to vitamin C.

Table 3a. NBO analysis of C_7 Si_5 Ge_3.

B3LYP/6-311G		B3LYP/6-311G*		B3LYP/cc-pvdz	
BD (1) C 1 -Si 2	0.8232* ($sp^{2.86}$)C+0.5678* ($sp^{2.17}$) Si	BD (1) C 1 -Si 2	0.8246*($sp^{2.80}d^{0.01}$)C+ 0.5657* ($sp^{2.20}d^{0.02}$)Si	BD (1) C 1 -Si 2	($sp^{2.78}d^{0.01}$)+0.5545*($sp^{2.23}d^{0.02}$) *0.8322
BD (1) C 1 -Si 3	0.8462* ($sp^{1.46}$)C+0.5329*($sp^{2.01}$)Si	BD (1) C 1 -Si 3	0.8493*($sp^{1.43}d^{0.01}$)C+ 0.5278* ($sp^{1.99}d^{0.02}$)Si	BD (1) C 1 -Si 3	($sp^{1.48}d^{0.01}$)+0.5234* ($sp^{1.93}d^{0.02}$) *0.8521
BD (2) C 1 -Si 3	0.9047* ($sp^{15.34}$)C+0.4261* ($sp^{33.38}$)Si	BD (2) C 1 -Si 3	0.9246*($sp^{19.10}d^{0.07}$)C+ 0.3810* ($sp^{24.30}d^{0.37}$)Si	BD (2) C 1 -Si 3	*($sp^{17.94}d^{0.10}$)+0.3868* ($sp^{27.67}d^{0.49}$)0.9222
BD (1) C 1 -Si 4	0.8264* ($sp^{2.67}$)C+ 0.5631* ($sp^{2.06}$)Si	BD (1) C 1 -Si 4	0.8279*($sp^{2.56}d^{0.01}$)C+ 0.5609* ($sp^{2.11}d^{0.02}$)Si	BD (1) C 1 -Si 4	*($sp^{2.55}d^{0.01}$)+0.5487*($sp^{2.12}d^{0.02}$) 0.8360
BD (1)Si 2 - C 5	0.5627* ($sp^{2.39}$)Si+ 0.8267* ($sp^{2.18}$)C	BD (1)Si 2 - C 5	0.5621*($sp^{2.32}d^{0.03}$)Si+ 0.8271* ($sp^{2.17}d^{0.01}$)C	BD (1)Si 2 - C 5	*($sp^{2.37}d^{0.03}$)+0.8327* ($sp^{2.21}d^{0.01}$) 0.55378
BD (1)Si 2 - C 10	0.5480* ($sp^{1.83}$)Si+ 0.8364($sp^{2.20}$)C	BD (1)Si 2 - C 10	0.5448*($sp^{1.83}d^{0.02}$)Si+ 0.8386*($sp^{2.24}$)C	BD (1)Si 2 - C 10	0.5328* ($sp^{1.85}d^{0.02}$)+0.8462* ($sp^{2.24}$)
BD (1)Si 3 - C 7	0.5202* ($sp^{2.25}$)Si+0.8540*($sp^{1.34}$)C	BD (1)Si 3 - C 7	0.5092*($sp^{2.27}d^{0.02}$)Si+ 0.8606* ($sp^{1.35}$)C	BD (1)Si 3 - C 7	0.5052* ($sp^{2.29}d^{0.03}$)+0.5487* ($sp^{1.31}$)
BD (1)Si 3 - C 8	0.5097*($sp^{1.99}$)Si+0.8604*($sp^{1.49}$)C	BD (1)Si 3 - C 8	0.5007*($sp^{2.01}d^{0.02}$)Si+)* 0.8656$sp^{1.43}$)C	BD (1)Si 3 - C 8	0.4948* ($sp^{2.01}d^{0.03}$)+0.8690* ($sp^{1.44}$)
BD (1)Si 4 - C 5	0.5527* ($sp^{2.52}$)Si+0.8334* ($sp^{1.85}$)C	BD (1)Si 4 - C 5	0.5497*($sp^{2.48}d^{0.03}$)Si+ 0.8354* ($sp^{1.84}d^{0.01}$)C	BD (1)Si 4 - C 5	*($sp^{2.51}d^{0.03}$)+0.8414*($sp^{1.84}d^{0.01}$) 0.5404
BD (1)Si 4 - C 6	0.5772* ($sp^{1.81}$)Si+ 0.8166* ($sp^{2.72}$)C	BD (1)Si 4 - C 6	0.5799*($sp^{1.81}d^{0.02}$)Si+ 0.8147* ($sp^{2.55}$)C	BD (1)Si 4 - C 6	0.5653* ($sp^{1.83}d^{0.02}$)+0.8249* ($sp^{2.59}d^{0.01}$)
BD (1) C 5 -Ge 9	0.8412* ($sp^{2.06}$)C+0.5407* ($sp^{1.59}$)Ge	BD (1) C 5 -Ge 9	0.8421*($sp^{2.14}d^{0.01}$)C+ 0.5393* ($sp^{1.66}d^{0.01}$)Ge	BD (1) C 5 -Ge 9	0.8458*($sp^{2.18}d^{0.01}$)+0.5336* ($sp^{1.57}d^{0.01}$)
BD (1) C 6 -Ge 9	0.7777* ($sp^{3.47}$)C+ 0.6287* ($sp^{0.93}$)Ge	BD (1) C 6 -Ge 9	0.7716*($sp^{3.35}$)C+ 0.6361*($sp^{0.94}d^{0.01}$)Ge	BD (1) C 6 -Ge 9	0.7790* ($sp^{3.42}d^{0.01}$)+0.6271*($sp^{0.94}$)
BD (1) C 6 -Ge 12	0.8840* ($sp^{0.99}$)C+0.4676* ($sp^{8.21}$)Ge	BD (1) C 6 -Ge 12	0.8868*($sp^{1.05}$)C+ 0.4621* ($sp^{7.62}d^{0.04}$)Ge	BD (1) C 6 -Ge 12	0.8896*($sp^{1.02}$)+0.4568*($sp^{8.45}d^{0.04}$)
BD (2) C 6 -Ge 12	0.8926* ($sp^{99.99}$)C+ 0.4509* ($sp^{28.28}$)Ge	BD (2) C 6 -Ge 12	0.9004*($sp^{99.99}d^{0.56}$)C+ 0.4350* ($sp^{19.59}d^{0.17}$)Ge	BD (2) C 6 -Ge 12	0.8975* ($sp^{99.99}d^{4.24}$)+0.4410* ($sp^{20.38}d^{0.16}$)
BD (1) C 7 -Ge 14	0.8803*($sp^{3.50}$)C+0.4744* ($sp^{15.56}$)Ge	BD (1) C 7 -Ge 14	0.8760*($sp^{3.66}$)C+ 0.4823* ($sp^{12.36}d^{0.03}$)Ge	BD (1) C 7 -Ge 14	0.8803* ($sp^{3.69}d^{0.01}$)+0.4744*($sp^{14.18}d^{0.05}$)
BD(1)C7-C15	0.7150* ($sp^{1.87}$)C+ 0.6992* ($sp^{1.79}$)C	BD(1)C7-C15	0.7177*($sp^{1.80}d^{0.01}$)C+ 0.6963* ($sp^{1.73}$)C	BD(1)C7-C15	0.7157*($sp^{1.85}d^{0.01}$)+0.6984* ($sp^{1.77}$)
BD(2)C7-C15	0.7296* ($sp^{99.99}$)C+0.6839*($sp^{99.99}$)C	BD(2)C7-C15	0.7300*($sp^{99.99}d^{0.93}$)C+ 0.6834* ($sp^{99.99}d^{2.08}$)C	BD(2)C7-C15	0.7284*($sp^{99.99}d^{0.03}$)+0.6852* ($sp^{99.99}d^{2.23}$)
BD (1) C 8 -Ge 12	0.8929* ($sp^{4.70}$)C+0.4502*($sp^{19.95}$)Ge	BD (1) C 8 -Ge 12	0.8953*($sp^{5.84}$)C+ 0.4455* ($sp^{16.14}d^{0.08}$)Ge	BD (1) C 8 -Ge 12	0.8956* ($sp^{5.26}$)+0.4449* ($sp^{17.70}d^{0.09}$)
BD (1) C 8 -Si 13	0.8916* ($sp^{1.37}$)C+0.4528*($sp^{5.41}$)Si	BD (1) C 8 -Si 13	0.8900*($sp^{1.27}$)C+ 0.4559* ($sp^{4.24}d^{0.05}$)Si	BD (1) C 8 -Si 13	0.8940*($sp^{1.33}$)+0.4481* ($sp^{4.72}d^{0.06}$)
BD (2) C 8 -Si 13	0.8600* ($sp^{99.99}$)C+0.5103* ($sp^{99.99}$)Si	BD (2) C 8 -Si 13	0.8775*($sp^{99.99}d^{0.2}$)C+ 0.4796* ($sp^{99.99}d^{42.84}$)Si	BD (2) C 8 -Si 13	0.8717* ($sp^{99.99}d^{0.29}$)+0.4901* ($sp^{99.99}d^{51.51}$)
BD (1) C 10 -Si 11	0.8886* ($sp^{1.02}$)+ 0.4586* ($sp^{5.55}$)	BD (1) C 10 -Si 11	0.8875*($sp^{1.03}$)C+ 0.4608* ($sp^{4.48}d^{0.06}$)Si	BD (1) C 10 -Si 11	0.8919*($sp^{1.8}$)+0.4522* ($sp^{4.99}d^{0.07}$)
BD (1)Si 11 - C 15	0.4591* ($sp^{7.60}$)Si+0.8884* ($sp^{1.29}$)C	BD (1)Si 11 - C 15	0.4590*($sp^{6.39}d^{0.09}$)Si+ 0.8884* ($sp^{1.34}$)C	BD (1)Si 11 - C 15	0.4512* ($sp^{6.97}d^{0.1}$)+0.8924* ($sp^{1.29}$)
BD (1)Ge 14 - C 15	0.4959* ($sp^{14.97}$)Ge+ 0.8684* ($sp^{3.86}$)C	BD (1)Ge 14 - C 15	0.5047*($sp^{11.71}d^{0.04}$)Ge+ 0.8633* ($sp^{3.81}$)C	BD (1)Ge 14 - C 15	0.4958*($sp^{13.51}d^{0.06}$)+0.8685* ($sp^{3.91}$)

Table 3b. C_7 Si_5 Ge_3 inside of vitamin C at different level of theory.

B3LYP/6-311G		B3LYP/6-311G*		B3LYP/cc-pvdz	
BD(1) C 1 -Si 3	0.8419* ($sp^{1.65}$)C+ 0.5396* ($sp^{2.72}$)Si	BD(1) C 1 -Si 3	0.8419* ($sp^{1.65}$)C+ 0.5396* ($sp^{2.72}$)Si	BD(1) C 1 -Si 3	0.8533* ($sp^{1.62}$)C+ 0.5214* ($sp^{2.09}d^{0.02}$)Si
(1)BD 4Si - 1C	0.8539*(s p $^{2.26}$)C+ 0.5205*($sp^{2.13}$)Si	(1)BD 4Si - 1C	0.8539*(s p $^{2.26}$)C+ 0.5205*($sp^{2.13}$)Si	(1)BD 4Si - 1C	0.8652* ($sp^{2.26}d^{0.01}$)C+0.5014* ($sp^{2.08}d^{0.02}$)Si
BD(2) C 1 -Si 4	0.8339* ($sp^{48.1}$)C+ 0.5520*($sp^{8.04}$)Si	BD(2) C 1 -Si 4	0.8339* ($sp^{48.1}$)C+ 0.5520*($sp^{8.04}$)Si	BD(2) C 1 -Si 4	0.8087* ($sp^{62.65}d^{0.20}$)C+0.5882* ($sp^{5.95}d^{0.03}$)Si
BD(1) C 1 -Ge 9	0.8454* ($sp^{2.35}$)C+ 0.5341* ($sp^{1.81}$)Ge	BD(1) C 1 -Ge 9	0.8454* ($sp^{2.35}$)C+ 0.5341* ($sp^{1.81}$)Ge	BD(1) C 1 -Ge 9	0.8584* ($sp^{2.35}d^{0.01}$)C+0.5130* ($sp^{2.33}d^{0.01}$)Ge
BD (1)Si 2 - C 7	0.4212* ($sp^{6.28}$)Si+ 0.9070* ($sp^{2.03}$)C	BD (1)Si 2 - C 7	0.4212* ($sp^{6.28}$)Si+ 0.9070* ($sp^{2.03}$)C	BD (1)Si 2 - C 7	0.3974*($sp^{6.80}d^{0.10}$)Si+0.9176* ($sp^{1.97}d^{0.01}$)C
BD (1)Si 2 - C 10	0.4824* ($sp^{8.53}$)Si+ 0.8760* ($sp^{1.89}$)C	BD (1)Si 2 - C 10	0.4824* ($sp^{8.53}$)Si+ 0.8760* ($sp^{1.89}$)C	BD (1)Si 2 - C 10	0.4518*($sp^{9.00}d^{0.08}$)Si+0.8921* ($sp^{1.67}d^{0.01}$)C
BD (1)Si 3 - C 7	0.5150* ($sp^{3.00}$)Si+ 0.8572* ($sp^{2.37}$)C	BD (1)Si 3 - C 7	0.5150* ($sp^{3.00}$)Si+ 0.8572* ($sp^{2.37}$)C	BD (1)Si 3 - C 8	0.4937*($sp^{2.98}d^{0.02}$)Si+0.8696* ($sp^{2.29}d^{0.01}$)C
BD (1)Si 3 - C 8	0.6091*($sp^{2.38}$)Si+ 0.7931*($sp^{8.22}$)C	BD (1)Si 3 - C 8	0.6091*($sp^{2.38}$)Si+ 0.7931*($sp^{8.22}$)C	BD (1)Si 3 -Si 13	0.6284*($sp^{1.81}d^{0.01}$)Si+ 0.7779* ($sp^{9.89}d^{0.04}$)C
BD (1)Si 3 -Si 13	0.7978* ($sp^{4.29}$)Si+ *0.6030($sp^{13.63}$)Si	BD (1)Si 3 -Si 13	0.7978* ($sp^{4.29}$)Si+ *0.6030($sp^{13.63}$)Si	BD (1)Si 4 - C 6	0.5123*($sp^{2.59}d^{0.03}$)Si+0.8588* ($sp^{1.00}$)Si
BD (1)Si 4 - C 6	0.5275*($sp^{2.79}$)Si+* 0.8496 ($sp^{1.05}$)C	BD (1)Si 4 - C 6	0.5275*($sp^{2.79}$)Si+* 0.8496 ($sp^{1.05}$)C	BD (1)Si 4 -Ge 12	0.6774*($sp^{2.84}d^{0.02}$)Si+0.7356* ($sp^{2.18}d^{0.02}$)C
BD (1)Si 4 -Ge 12	0.7495*($sp^{2.23}$)Si+ 0.6621*($sp^{34.28}$)Ge	BD (1)Si 4 -Ge 12	0.7495*($sp^{2.23}$)Si+ 0.6621*($sp^{34.28}$)Ge	BD (1)Si 4 -Ge 12	0.7055* ($sp^{1.30}$)Si+0.7087* ($sp^{1.24}$)Ge

Table 3b. Contd.

BD(1)C5-C6	0.7050* ($sp^{1.27}$)C+ 0.7092* ($sp^{1.17}$)C	BD(1)C5-C6	0.7050* ($sp^{1.27}$)C+ 0.7092* ($sp^{1.17}$)C	BD(1)C5-C6	0.6910*($sp^{62.32}$)C+0.7228* ($sp^{33.57}d^{0.09}$)C
BD(2)C5-C6	0.6963* ($sp^{30.54}$)+ 0.7178* ($sp^{30.09}$)	BD(2)C5-C6	0.6963* ($sp^{30.54}$)+ 0.7178* ($sp^{30.09}$)	BD(2)C5-C6	0.7207* ($sp^{18.90}d^{0.05}$)C+0.6932* ($sp^{40.03}d^{0.13}$)C
BD(3)C5-C6	0.7117* (sp22.30)C+ 0.7025* ($sp^{48.47}$)C	BD(3)C5-C6	0.7117* (sp22.30)C+ 0.7025* ($sp^{48.47}$)C	BD(3)C5-C6	0.8571*($sp^{1.01}$)C+0.5151* ($sp^{3.17}d^{0.02}$)C
BD (1) C 5 -Ge 9	0.8471* ($sp^{1.06}$)C+ 0.5314* ($sp^{2.78}d^{0.01}$)Ge	BD (1) C 5 -Ge 9	0.8471* ($sp^{1.06}$)C+ 0.5314* ($sp^{2.78}d^{0.01}$)Ge	BD (1) C 5 -Ge 9	0.8876* ($sp^{3.06}d^{0.01}$)C+0.4607* ($sp^{3.47}d^{0.04}$)Ge
BD (1) C 7 -Si 11	0.8671* ($sp^{3.23}$)C+ 0.4982*($sp^{3.42}$)Si	BD (1) C 7 -Si 11	0.8671* ($sp^{3.23}$)C+ 0.4982*($sp^{3.42}$)Si	BD (1) C 7 -Si 11	0.9102* ($sp^{7.81}d^{0.01}$)C+0.4141* ($sp^{18.44}d^{0.11}$)Si
BD (1) C 7 -Ge 14	0.9087* ($sp^{6.35}$)C+ 0.4174*($sp^{17.08}d^{0.03}$)Ge	BD (1) C 7 -Ge 14	0.9087* ($sp^{6.35}$)C+ 0.4174*($sp^{17.08}d^{0.03}$)Ge	BD (1) C 7 -Ge 14	0.7842* ($sp^{13.20}d^{0.02}$)C+0.6205* ($sp^{1.69}d^{0.01}$)Ge
BD (1) C 8 -Ge 12	0.8183* ($sp^{10.10}$)C+ 0.5747*($sp^{9.47}d^{0.01}$)Ge	BD (1) C 8 -Ge 12	0.8183* ($sp^{10.10}$)C+ 0.5747*($sp^{9.47}d^{0.01}$)Ge	BD (1) C 8 -Ge 12	0.5775* ($sp^{16.49}d^{0.11}$)C+0.8164* ($sp^{2.54}d^{0.02}$)Ge
BD (1)Ge 9 - C 10	0.5624*($sp^{2.13}$)Ge+ 0.8268* ($sp^{2.00}$)C	BD (1)Ge 9 - C 10	0.5624*($sp^{2.13}$)Ge+ 0.8268* ($sp^{2.00}$)C	BD (1)Ge 9 - C 10	0.5372*($sp^{3.21}d^{0.02}$)Ge+0.8434* ($sp^{2.07}d^{0.01}$)C
BD (1) C 10 -Si 11	0.8132* ($sp^{2.33}$)C+ 0.5820*($sp^{1.85}$)Si	BD (1) C 10 -Si 11	0.8132* ($sp^{2.33}$)C+ 0.5820*($sp^{1.85}$)Si	BD (1) C 10 -Si 11	0.3675*($sp^{3.38}d^{0.04}$)C+0.9300* ($sp^{6.77}$)Si
BD (1)Si 11 - C 15	0.6309*($sp^{1.41}$)Si+ 0.7759* ($sp^{8.77}$)C	BD (1)Si 11 - C 15	0.6309*($sp^{1.41}$)Si+ 0.7759* ($sp^{8.77}$)C	BD (1)Si 11 - C 15	0.8314* ($sp^{2.39}d^{0.01}$)Si+0.5557* ($sp^{1.83}d^{0.01}$)C
BD(1)C16-C17	0.7063* ($sp^{1.64}$)C+ 0.7079* ($sp^{2.31}$)C	BD(1)C16-C17	0.7063* ($sp^{1.64}$)C+ 0.7079* ($sp^{2.31}$)C	BD(1)C16-C17	0.6047*($sp^{1.42}$)C+0.7965* ($sp^{7.95}d^{0.03}$)C
BD(1)C16-O20	0.5472($sp^{3.75}$)+ 0.8370* ($sp^{2.83}$)O	BD(1)C16-O20	0.5472($sp^{3.75}$)+ 0.8370* ($sp^{2.83}$)O	BD(1)C16-O20	0.7124* ($sp^{1.56}$)C+ 0.7018* ($sp^{2.33}$)C
BD(1)C16-C21	0.7192* ($sp^{1.55}$)C+ 0.6948* ($sp^{2.16}$)C	BD(1)C16-C21	0.7192* ($sp^{1.55}$)C+ 0.6948* ($sp^{2.16}$)C	BD(1)C16-C21	0.5464* ($sp^{3.78}d^{0.01}$)C+0.8375* ($sp^{2.82}$)C
BD(1)C17-C18	0.7041* ($sp^{1.52}$)C+ 0.7101* ($sp^{1.54}$)C	BD(1)C17-C18	0.7041* ($sp^{1.52}$)C+ 0.7101* ($sp^{1.54}$)C	BD(1)C17-C18	0.7204* ($sp^{1.57}$)C+0.6936* ($sp^{2.12}$)C
BD(1)C17-O26	0.6162* ($sp^{2.37}$)C+ 0.7876* ($sp^{2.90}$)O	BD(1)C17-O26	0.6162* ($sp^{2.37}$)C+ 0.7876* ($sp^{2.90}$)O	BD(1)C17-O26	0.7066* ($sp^{1.47}$)C+0.7077* ($sp^{1.55}$)O
BD(2)C17-O26	0.5849* ($sp^{1.00}$)C+ 0.8111* ($sp^{1.00}$)O	BD(2)C17-O26	0.5849* ($sp^{1.00}$)C+ 0.8111* ($sp^{1.00}$)O	BD(2)C17-O26	0.6084* ($sp^{2.44}$)C+0.7936* ($sp^{2.58}$)O
BD(1)C18-C19	0.7120* ($sp^{2.26}$)C+ 0.7022* ($sp^{1.64}$)C	BD(1)C18-C19	0.7120* ($sp^{2.26}$)C+ 0.7022* ($sp^{1.64}$)C	BD(1)C18-C19	0.5839* ($sp^{1.00}$)C+0.8118* ($sp^{1.00}$)C
BD(1)C18-O25	0.6175* ($sp^{2.37}$)C+ 0.7866* ($sp^{2.92}$)O	BD(1)C18-O25	0.6175* ($sp^{2.37}$)C+ 0.7866* ($sp^{2.92}$)O	BD(1)C18-O25	0.7161* ($sp^{2.20}$)C+0.6980* ($sp^{1.56}$)O
BD(2)C18-O25	0.6248* ($sp^{99.99}$)C+ 0.7808* ($sp^{1.00}$)O	BD(2)C18-O25	0.6248* ($sp^{99.99}$)C+ 0.7808* ($sp^{1.00}$)O	BD(2)C18-O25	0.6083* ($sp^{2.43}$)C+0.7937* ($sp^{2.58}$)O
BD(1)C19-O20	0.5651* ($sp^{2.75}$)C+ 0.8250*($sp^{2.69}$)O	BD(1)C19-O20	0.5651* ($sp^{2.75}$)C+ 0.8250*($sp^{2.69}$)O	BD(1)C19-O20	0.6242* ($sp^{99.99}d^{1.79}$)C+0.7813* ($sp^{1.00}$)O
BD(1)C19-O24	0.5974* ($sp^{1.84}$)C+ 0.8019* ($sp^{1.72}$)O	BD(1)C19-O24	0.5974* ($sp^{1.84}$)C+ 0.8019* ($sp^{1.72}$)O	BD(1)C19-O24	0.5491* ($sp^{2.78}d^{0.01}$)C+0.8357* ($sp^{2.41}$)O
BD(2)C19-O24	0.5988* ($sp^{99.99}$)C+ 0.8009* ($sp^{99.99}$)O	BD(2)C19-O24	0.5988* ($sp^{99.99}$)C+ 0.8009* ($sp^{99.99}$)O	BD(2)C19-O24	0.5811* ($sp^{1.92}$)C+ 0.8138* ($sp^{1.47}$)O
BD(1)C21-C22	0.7449* ($sp^{1.60}$)C+ 0.6671* ($sp^{4.09}$)C	BD(1)C21-C22	0.7449* ($sp^{1.60}$)C+ 0.6671* ($sp^{4.09}$)C	BD(1)C21-C22	0.5872* ($sp^{99.99}d^{16.07}$)C+0.8095* ($sp^{99.99}d^{5.92}$)C
BD(1)C21-O27	0.6097* ($sp^{2.37}$)C+ 0.7926* ($sp^{4.73}$)O	BD(1)C21-O27	0.6097* ($sp^{2.37}$)C+ 0.7926* ($sp^{4.73}$)O	BD(1)C21-O27	0.7443* ($sp^{1.59}$)C+ 0.6678* ($sp^{4.04}d^{0.01}$)O
BD(2)C21-O27	0.5979* ($sp^{1.00}$)C+ 0.8016* ($sp^{42.71}$)O	BD(2)C21-O27	0.5979* ($sp^{1.00}$)C+ 0.8016* ($sp^{42.71}$)O	BD(2)C21-O27	0.6063* ($sp^{2.42}$)C+0.7952* ($sp^{4.26}d^{0.01}$)O
BD(1)C22-O23	0.5216* ($sp^{5.39}$)C+ 0.8532* ($sp^{3.41}$)O	BD(1)C22-O23	0.5216* ($sp^{5.39}$)C+ 0.8532* ($sp^{3.41}$)O	BD(1)C22-O23	0.5966* ($sp^{99.99}d^{16.54}$)C+ 0.8025* ($sp^{37.20}d^{0.03}$)O

distributing electrons into molecular orbitals used for the one electron density matrix to define the shape of the atomic orbitals in molecular environ-ment and then derive molecular bonds from electron density between atoms. At each considered coordination, the bonding and antibonding coefficients of s and p orbital of Si-C were 0.5 and 0.8 for $C_7Si_5Ge_3$ cluster at B3LYP/6-311G, B3LYP/6-311G* and B3LYP/cc-pvdz level of theory. But this order does not exist for $C_7Si_5Ge_3$ cluster inside vitamin C.

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