Understanding the Parameters Affecting the Photoluminescence of Silicon Nanoparticles.

Supporting information.

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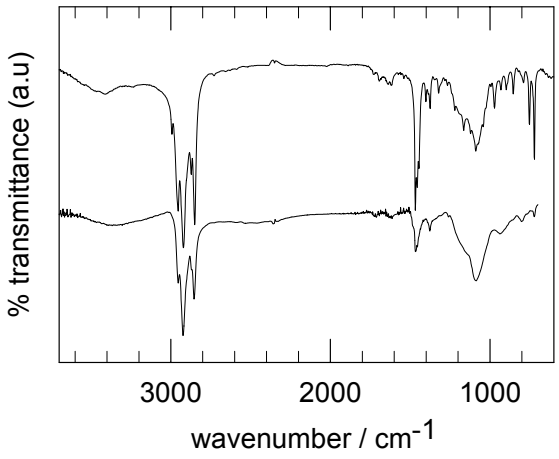
S.I. Particle synthesis

BU approach: The synthesis was performed in a two-necked glass flask with one entrance for the continuous bubbling with Argon gas and the other for the introduction of reactants and gas vent. In a first step, 16 mL of dry toluene and 6.3 g of tetraoctylammonium bromide (TOAB) were introduced and sonicated for 20 minutes to form TOAB reversed micelles. In a second step, 0.6 mL of $SiCl_4$ was added and the mixture sonicated for 20 minutes, followed by the addition of 10 ml of 1M $LiAlH_4$ in ethyl ether. The growth of silicon nanoparticles takes place inside the micelles upon $SiCl_4$ reduction under constant sonication for 30 minutes. Any excess of $LiAlH_4$ is consumed by addition of 30 mL of methanol. The suspension was taken to dryness on a rotary evaporator and re-suspended in cyclohexane to eliminate TOAB by precipitation, cyclohexane was then evaporated and the particles re-suspended in toluene. The particles were allowed to age upon standing for several weeks in an air-saturated toluene suspension in the dark. To further eliminate the remaining surfactant, excess cyclohexane was added to a toluene suspension of the particles, and TOAB extracted in water. Three extraction cycles were needed to minimize TOAB to less than 10% the initial adsorbed amount, as calculated by comparison of the FTIR spectra shown in the following figure, normalizing the TOAB peak at 1468 cm^{-1} to that at 1100 cm^{-1} due to SiO_2.

IR spectra of (from top down) “as obtained” particles and after three TOAB extraction cycles.



***TD approach*:** Clean crystalline Si wafers (p-type, with resistivities between 1.0 and 10.0 Ω cm) were electrochemically etched (20 mA electrical current) in a Teflon cell containing the electrolytic solution (16 % HF, 16 % CH_3OH $^{v}/_{v}$). After anodization, the wafer is rinsed with methanol and toluene, further immersed in toluene, and Si-NPs released by ultrasound (Ney Dental Inc; 50/60 Hz; 100 W). The resulting nanoparticles were purified by filtration through hydrophilic 100-nm PVDF Durapore® VVPP Membrane Filters (Millipore) to eliminate solid residues. These particles exhibit a weak visible PL just after preparation, which strongly increases within a rather short time, evidencing the importance of surface passivation on silicon nanoparticles emission. Therefore, the particles were either allowed to age for two months, or treated thermally at 90 ^{o}C for some hours before use [Llansola Portolés 2009].

When required, the solvent was evaporated, and the particles further dispersed in other solvents of interest.

[Llansola Portolés 2009] Llansola Portolés, M. J.; Rodriguez Nieto, F.; Soria, D. B.; Amalvy, J. I.; Peruzzo, P. J.; Mártire, D. O.; Kotler, M.; Holub, O.; Gonzalez, M. C., Photophysical Properties of Blue-Emitting Silicon Nanoparticles. *J. Phys. Chem. C* **2009,** *113* (31), 13694-13702.

S.I. Bilinear Regression Analysis.

For each excitation wavelength of the particle suspension an emission spectrum is obtained. For a pure substance existing in a unique form, the luminescence spectrum is invariant, remaining the same independent on the excitation wavelength. For low fluorophore absorbance (< 0.05), the steady state emission intensity at a given emission wavelength ($I(\lambda_m)$) is proportional to the absorption coefficient of the fluorophore at a given excitation wavelength ($\varepsilon(\lambda_x)$), the concentration of the fluorophore, and the factor $F(\lambda_m)$ reflecting the distribution of the probability of the various transitions from the lowest vibrational level of the first electronic excited level to the various vibrational levels of the ground state [Valeur 2002]. A bilinear regression analysis taking advantage of the linearity of $I(\lambda_m)$ with both, $\varepsilon(\lambda_x)$ and $F(\lambda_m)$ was applied to the experimental emission matrix in order to retrieve information on the minimum number of species and on their relative emission and absorption spectra. Using the running indexes *x* and *m* for the excitation and emission wavelengths, respectively, in a matrix form $[i_{xm}] = [\varepsilon_{xj}].[\mathbf{f}_{jm}]$, where $[i_{xm}]$, $[\varepsilon_{xj}]$ and $[\mathbf{f}_{jm}]$ represent the emission intensity, absorption coefficients, and $F(\lambda_m)$ matrices, respectively. The procedure is based on the alternating calculus of the matrices $[\varepsilon_{xj}]$ and $[\mathbf{f}_{jm}]$ by multiple linear regression iteratively until convergence is achieved when a least-squares condition is applied in order to minimize the elements of an error matrix. From the error matrix, a corrected emission intensity matrix, $[\boldsymbol{i}_{xm}^{c}]$, is obtained. The number of species is selected as the minimum that shows a reasonable approximation between $[\boldsymbol{i}_{xm}^{c}]$ and $[\boldsymbol{i}_{xm}]$ [Gonzalez 1989].

[Gonzalez 1989] Gonzalez, M. C.; San Roman, E., Photochemistry of aqueous solutions of triphenyltetrazolium chloride. *J. Phys. Chem.* **1989,** *93* (9), 3536-3540.

S.I. XPS Spectra.

In order to investigate the bonding mode and chemical structure in the nanoparticles surface, the peaks are resolved by Gaussian fitting.

Peaks due to contaminating surface adsorbed TOAB were used for internal calibration.

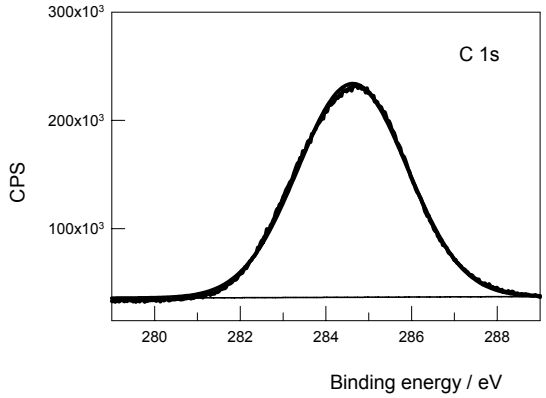
Signals were 2 eV shifted to higher energies with respect to the expected N and C signals in TOAB ($BrN(CH_2(CH_2)_6CH_3)_4$. Therefore, all other peaks were corrected for 2 eV towards lower energies. The C peak may show contamination due to toluene used as solvent of the suspensions as an area relation due to C:N of 44.5:1 is found in comparison with the value 32:1 expected for TOAB.

Peaks at 284.6 and 401.5 are typical for C-C and N in $BrN(CH_3)_4$ environments [Wagner 1979].

C 1s

X0= 284.6 corrected for internal calibration, σ = 3.0,
Area below peak= 630615

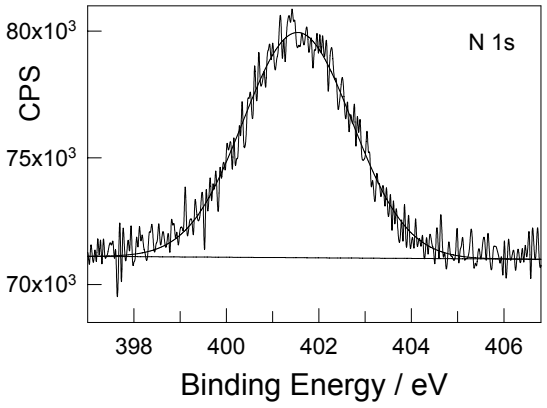
Atomic sensitivity factor= 0.205



N 1s

X0= 401.5 corrected for internal calibration, σ = 2.8,
Area below peak= 26220

Atomic sensitivity factor= 0.38



Calibrated XPS spectra of aged BUSi-NP

In order to investigate the bonding mode and chemical structure in the nanoparticles surface, the peaks are resolved by a 100% Gaussian fitting.

Aged particles

Si 2p

Atomic sensitivity factor= 0.17.

X_{01}= 99.5, σ_1= 1.3, Area below peak= 3000 (8.0%)

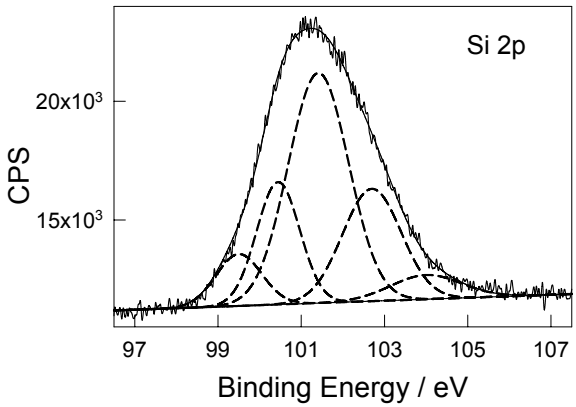
X_{02}= 100.4, σ_2= 1.2, Area below peak= 6696 (17.8 %)

X_{03}= 101.4, σ3= 1.7, Area below peak= 17637 (46.7 %)

X_{04}= 102.7, σ_4= 1.7, Area below peak= 8341 (22 %)

X_{05}= 104.0, σ_5= 2.0, Area below peak= 2168 (5.7%)

Total area: 37773.4



Si 2s

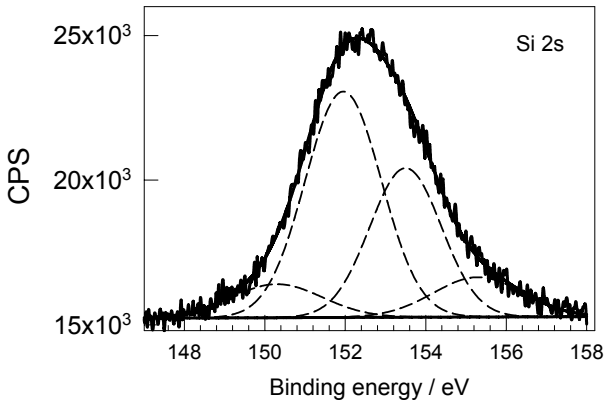
X_{01}= 150.3, σ_1= 2.7, Area below peak= 3278 (8.8%)

X_{043} = 151.95, σ_4 = 2.2, Area below peak= 18535 (49.8%)

X_{03} = 153.5, σ_3 = 2.1, Area below peak= 11520 (31.0%)

X_{02}= 155.3, σ_2= 2.1, Area below peak= 3845.5 (10%)

Total area: 37178.5



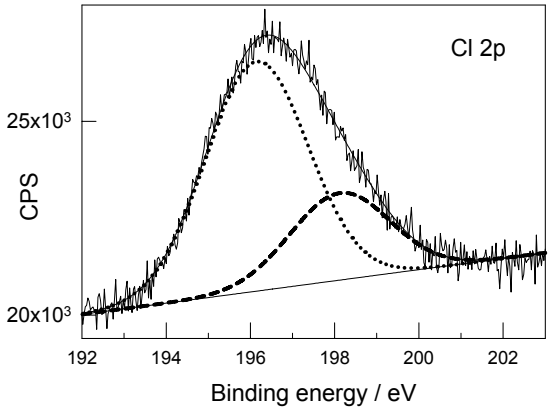
Cl 2p

Atomic sensitivity factor= 0.48

X_{01}= 196.1, σ_1 = 2.9, Area below peak= 18134 (73%)

X_{02}= 198.13, σ_2 = 2.8, Area below peak= 6677 (27%)

Total area: 24811



O 1s

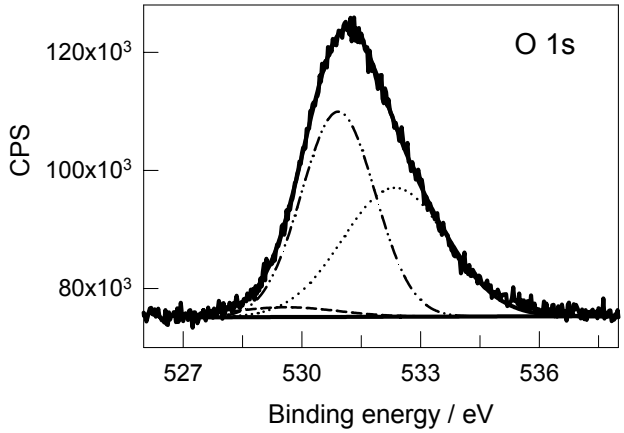
X_{01}= 531.6, σ_1 = 3.1, Area below peak= 5417

X_{02}= 532.9, σ_2 = 2.2, Area below peak= 80882

X_{03}= 534.3, σ_3 = 3.1, Area below peak= 72035.5

Total area: 158334.5

Atomic sensitivity factor= 0.63



S.I Table XPS Literature Assignments

Signal	Structure	B.E. (eV)	Reference
Si 2p	$Si(-O-)_4$	102.8 – 103.6	[David Gara 2012, Ouyang 2000, Wang 1995, Zhu 2001]
	$Si(-O-)_3$	102.0 – 102.8	
	$Si(-O-)_2$	101.4	
	$Si(-O-)_1$	100.6 – 100.0	
	Si-Si	99.2 – 99.0	[Yang 2001] [(a)] [Ouyang 2000, Wang 1995]
	Si-H	99.6	[Hayashi 1988, Nemanick 2006]
	$Si(-H)_2$	100.8	[Nemanick 2006]
	$Si(-H)_3$	101.2	[Nemanick 2006]
	$Si(-Cl)_1$	103.0 100.5	In $SiCl(N(C_2H_4O)_3)$, [Gray 1977, Nemanick 2006]
	$Si(-Cl)_2$	101.0	[Nemanick 2006]
	$Si(-Cl)_3$	102.8	in $C_2H_5SiCl_3$, [Wagner 1979]
Si 2s	Si-Si	150.5	[Pol 2004]
	SiO_2	155.3	
O 1s	O-Si	535 [(a)]	[Yang 2001] [(a)]
	O-Si(H)	531.6[(a)]	
Cl 2p	Cl-Si	199.0	[Szepvolgyi 2001]

(a) Value corrected for the peak of C-C taken as internal standard (found: 280.5 eV, calibrated value: 284.5)

[David Gara 2012] David Gara, P. M.; Garabano, N. I.; Llansola Portolés, M. J.; Moreno, S.; Dodat, D.; Casas, O. R.; Gonzalez, M. C.; Kotler, M. L., ROS enhancement by silicon nanoparticles in X-ray irradiated aqueous suspensions and in glioma C6 cells. *J. Nanopart. Res.* **2012,** 4 (3), 741 - 748.

[Gray 1977] Gray, R. C.; Hercules, D. M., X-ray photoelectron spectroscopic (ESCA) study of bonding in pentacoordinate silicon compounds. *Inorg. Chem.* **1977,** *16* (6), 1426-1427.

[Hayashi 1988] Hayashi, T.; Miyazaki, S.; Hirose, M., *Jpn. J. Appl. Phys.* **1988,** *Part 2* (27), L314

[Nemanick 2006] Nemanick, E. J.; Hurley, P. T.; Webb, L. J.; Knapp, D. W.; Michalak, D. J.; Brunschwig, B. S.; Lewis, N. S., Chemical and Electrical Passivation of Single-Crystal Silicon(100) Surfaces through a Two-Step Chlorination/Alkylation Process. *J. Phys. Chem. B* **2006,** *110* (30), 14770-14778.

[Ouyang 2000] Ouyang, M.; Yuan, C.; Muisener, R. J.; Boulares, A.; Koberstein, J. T., Conversion of Some Siloxane Polymers to Silicon Oxide by UV/Ozone Photochemical Processes. *Chem. Mater.* **2000,** *12* (6), 1591-1596.

[Pol 2004] Pol, V. G.; Pol, S. V.; Gofer, Y.; Calderon-Moreno, J.; Gedanken, A., Thermal decomposition of tetraethylorthosilicate (TEOS) produces silicon coated carbon spheres. *J. Mater. Chem.* **2004,** *14* (6).

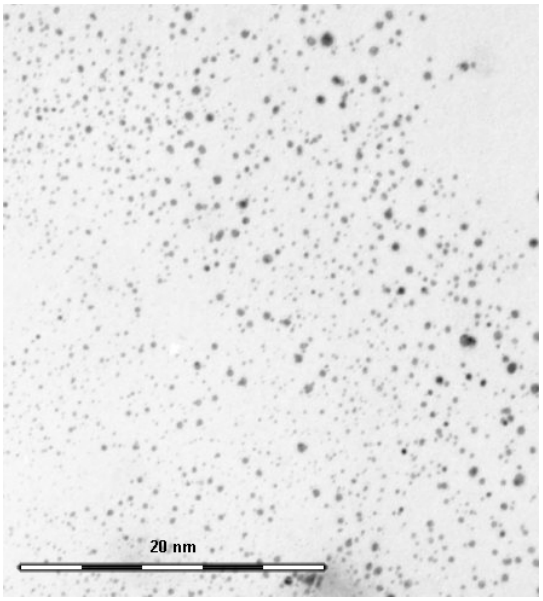
[Szepvolgyi 2001] Szepvolgyi, J.; Mohai, I.; Gubicza, J., Atmospheric ageing of nanosized silicon nitride powders. *J. Mater. Chem.* **2001,** *11* (3), 859-863.

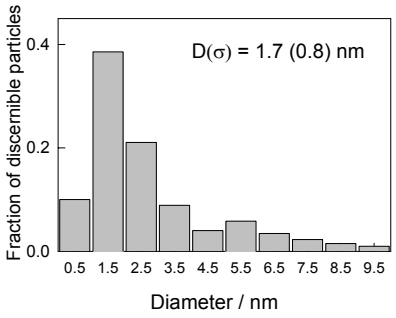
[Wagner 1979] Wagner, C. D.; Riggs, W. M.; Davis, L. E.; Moulder, J. F.; Muilenberg, G. E., *Handbook of x-ray photoelectron spectroscopy*. Perkin Elmer Corporation: 1979.

[Wang 1995] Wang, P. W.; Bater, S.; Zhang, L. P.; Ascherl, M.; Craig, J. H., XPS investigation of electron beam effects on a trimethylsilane dosed Si(100) surface. *Appl. Surf. Sci.* **1995,** *90* (4), 413-417.

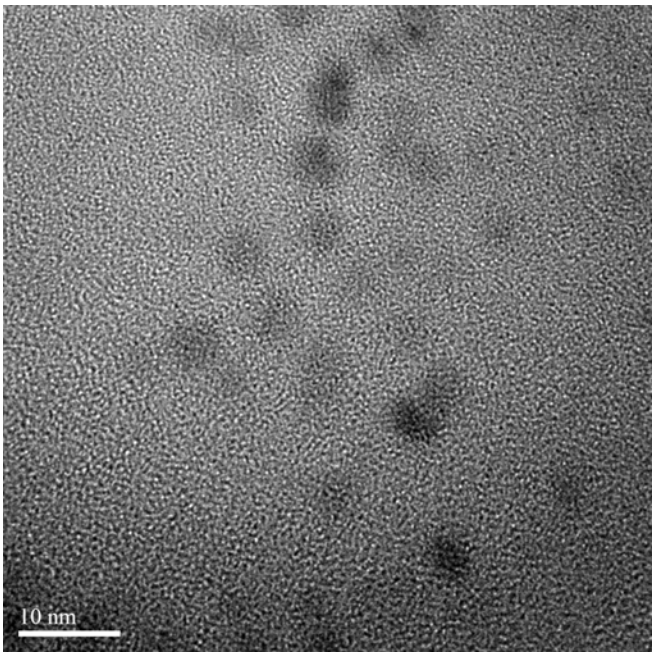
[Yang 2001] Yang, C. S.; Oh, K. S.; Ryu, J. Y.; Kim, D. C.; Shou-Yong, J.; Choi, C. K.; Lee, H. J.; Um, S. H.; Chang, H. Y., A study on the formation and characteristics of the Si-O-C-H composite thin films with low dielectric constant for advanced semiconductor devices. *Thin Solid Films* **2001,** *390*, 113-118.

S.I. TEM Micrographs: Representative TEM micrographs of BUSiNP / BUSINPOX and associated particle size histogram obtained from a total of 450 particles.

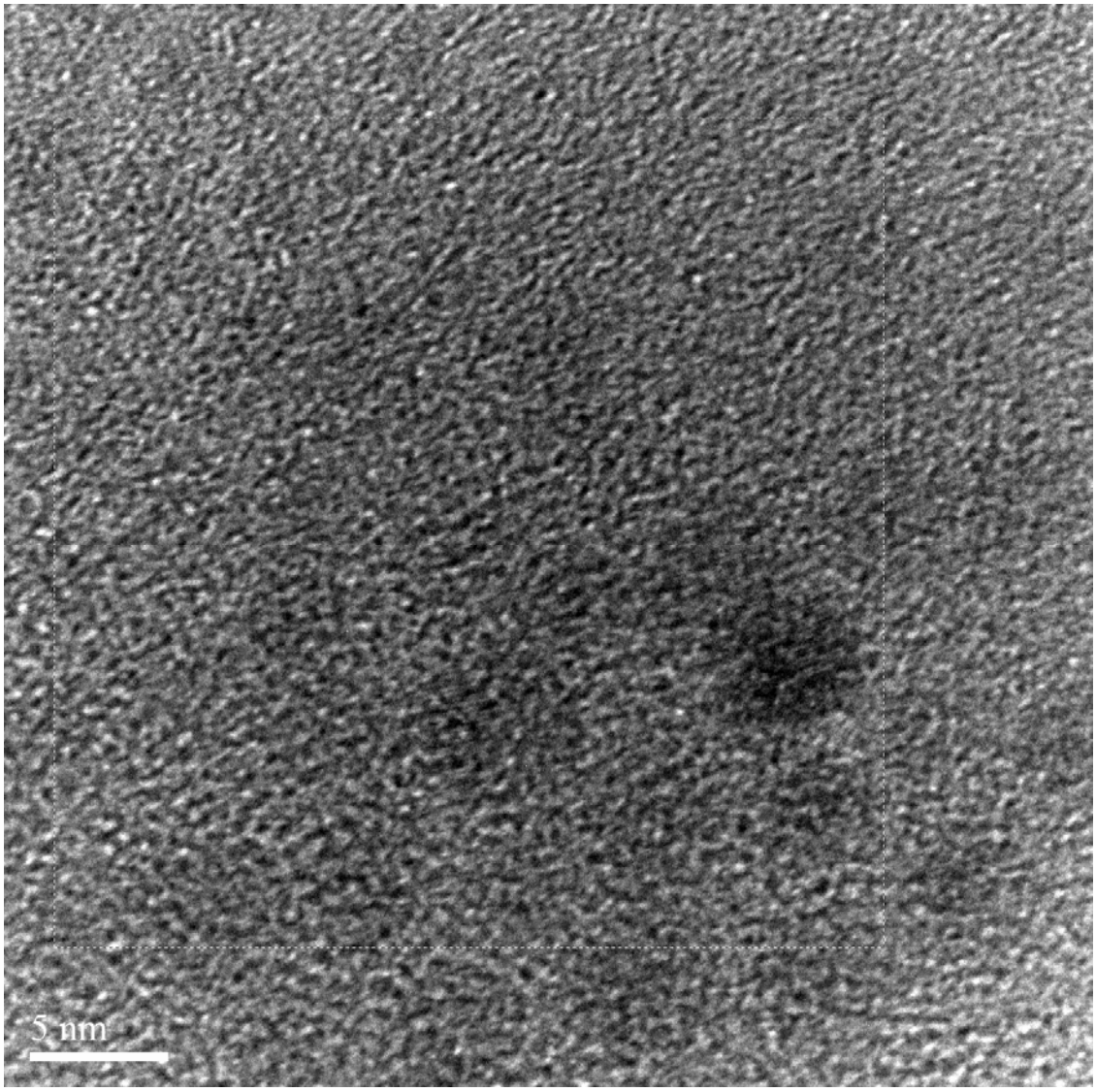




Gaussian distribution is observed with mean diameter of 1.7 nm and 0.8 nm standard deviation.

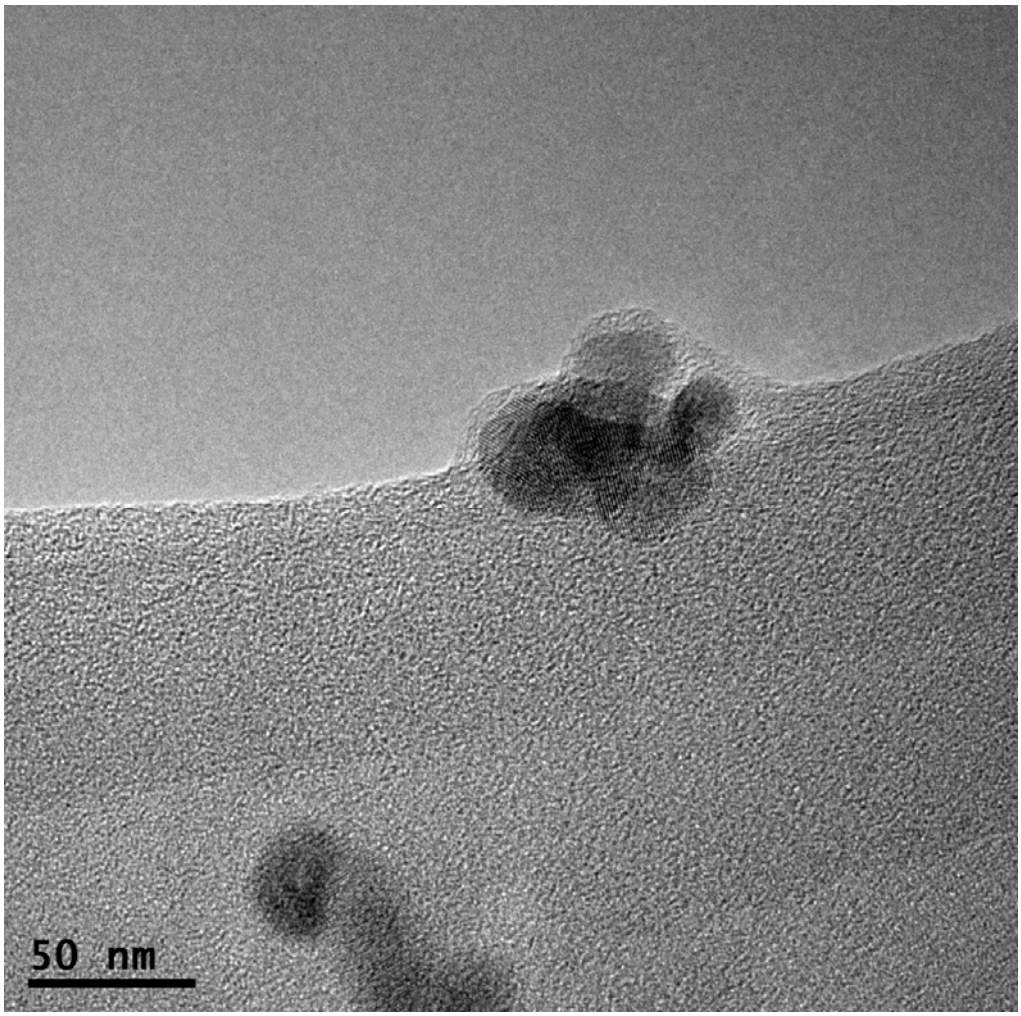


The micrographs show the formation of small agglomerates composed of few particles.



Due to the small atomic mass of Si and the presence of a surface-adsorbed organic layer, the contrast of the nanoparticles against the background is poor and the lattice fringes of the particles are roughly visible. The measured lattice spacing in the 2-3 nm particles seems to be of the order of 2.2 – 1.8 Å. Si nanocrystals fringes with a lattice spacing of 0.19 nm matches well with the (220) plane of diamond cubic silicon reported for some crystalline particles [Barrett 2009, Zou 2004]. Deviations from the bulk lattice constants were reported to depend crucially on their environment [Knipping 2004]. Because the SAED pattern was not clearly observed, information on the Miller indices could not be obtained. Therefore, these observations are not taken as an undeniable evidence of particle crystalline structure.

To improve the contrast between the particles and the substrate, the particles where laser ablated.* Activation of the particle surface upon the elimination of the organic surface envelope leads to the formation of bigger (> 20 nm) crystalline particles, as shown in the micrograph below.



* PC-150 / South Bay Technology Inc. Vacuum 120 mt. Gas 1: Ar, Gas 2: 25,1% Ar,74.9% O_2. 20-30 watts Maximum Forward Power.

[Barrett 2009] Barrett, C. A.; Dickinson, C.; Ahmed, S.; Hantschel, T.; Arstila, K.; Ryan, K. M., The evolution of pseudo-spherical silicon nanocrystals to tetrahedra, mediated by phosphonic acid surfactants. *Nanotechnology* **2009,** *20* (27), 275605.

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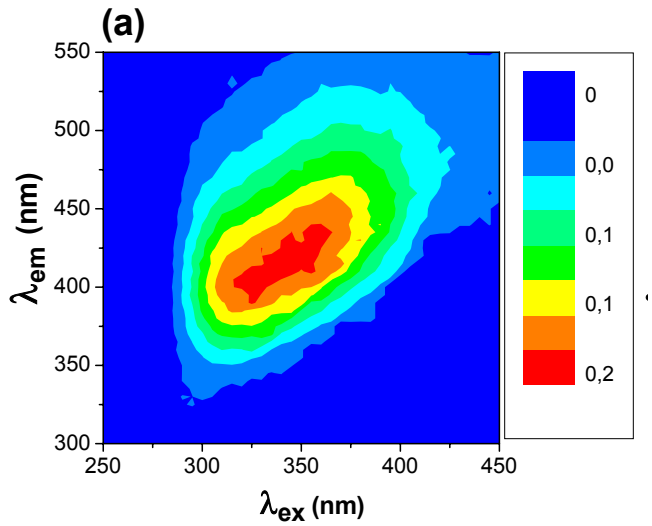
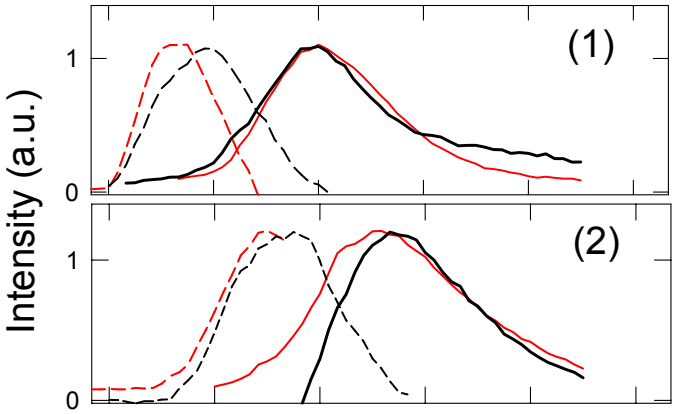
[Zou 2004] Zou, J.; Baldwin, R. K.; Pettigrew, K. A.; Kauzlarich, S. M., Solution Synthesis of Ultrastable Luminescent Siloxane-Coated Silicon Nanoparticles. *Nano Lett.* **2004,** *4* (7), 1181-1186.

S.I. BUSiNP-TOAB



Steady-state excitation – emission matrix of argon-saturated toluene suspensions of BUSINP inside TOAB micelles.

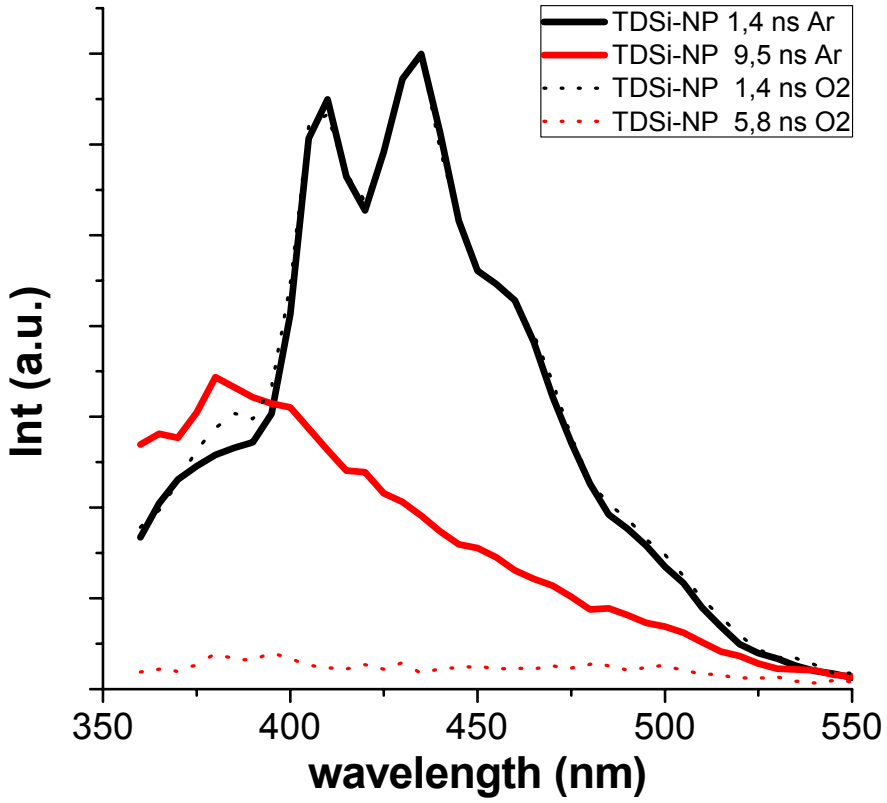


Emission (full lines) and excitation (dashed lines) spectra of species E1 and E2 (graphs **1** and **2**, respectively) contributing to the BUSiNPs excitation-emission matrix, as obtained from the bilinear analysis.

The excitation wavelength used for normalizing the emission spectrum, and the emission wavelength used for the normalization of the excitation spectrum, λ_{exc} / nm and λ_{em}/ nm, respectively, are: (E1) 340, 400; (E2) 380, 440. Despite the intensity units are arbitrary; the scales of the graphs are correlated to show the relative contribution of each species to the overall emission.

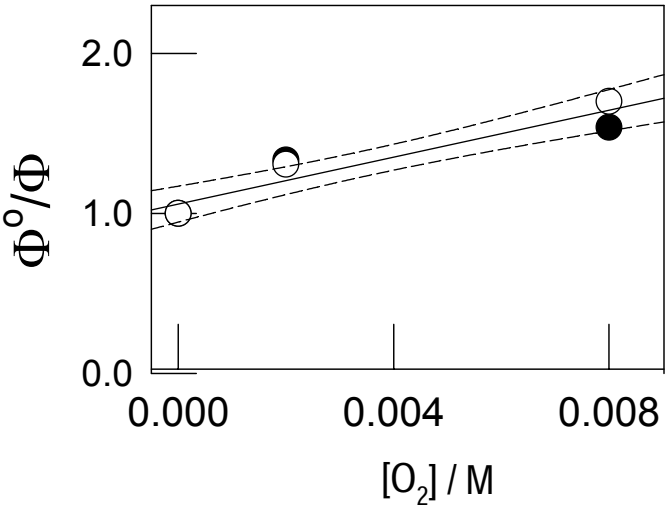
The red traces in graphs **1** and **2** stand for the emission -excitation spectra of the two species contributing to the excitation-emission matrix of argon-saturated toluene suspensions of BUSiNPs inside the TOAB micelles.

S.I. TDSiNP PL: Contribution to the emission spectra obtained upon 340 nm excitation of TDSiNP toluene suspensions of the species with the fast (black lines) and longer (red lines) decay times. The effect of molecular oxygen on the contribution of these species to the overall emission is also shown.

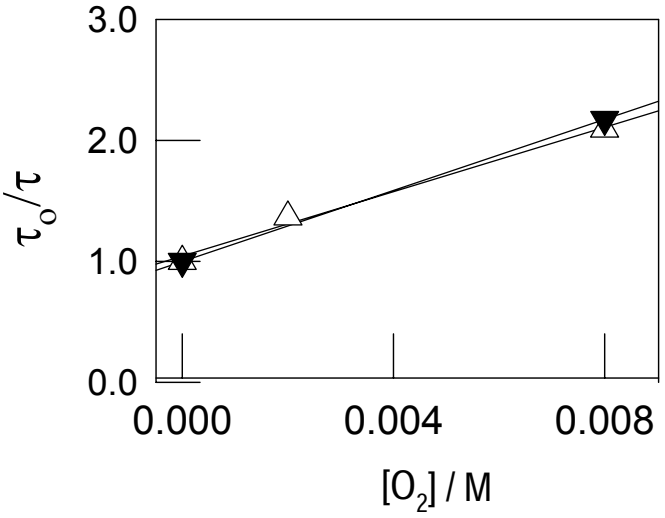


S.I. O_2 effect on PL: (***a***) Plots of the ratio of the luminescence quantum yields in the absence and presence of molecular oxygen (Φ^o/Φ) vs. the dissolved oxygen concentration of toluene suspensions of BUSiNPOX (●) and TDSiNP (○). (***b***) Plots of the inverse of the decay time ($1/\tau$) vs. the dissolved oxygen concentration of toluene suspensions of toluene suspensions of BUSiNPOX (▲) and BUSiNP (Δ).

(a)

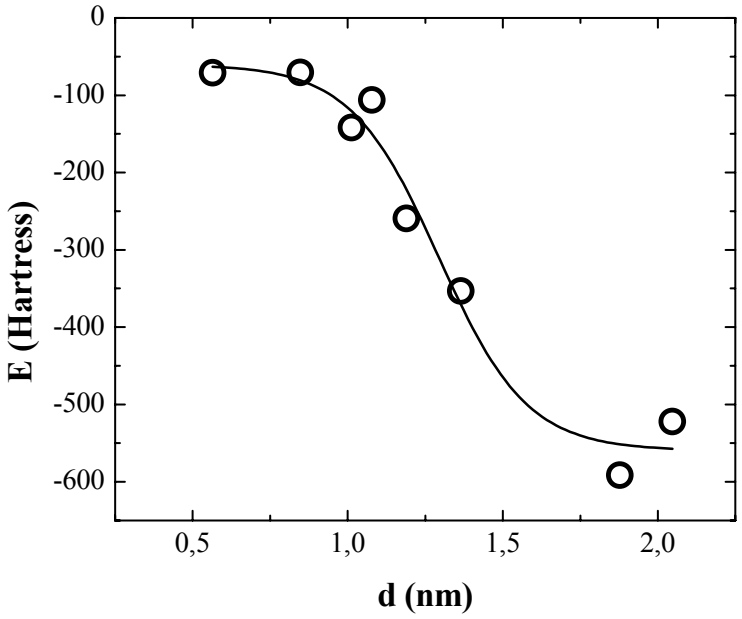


(b)



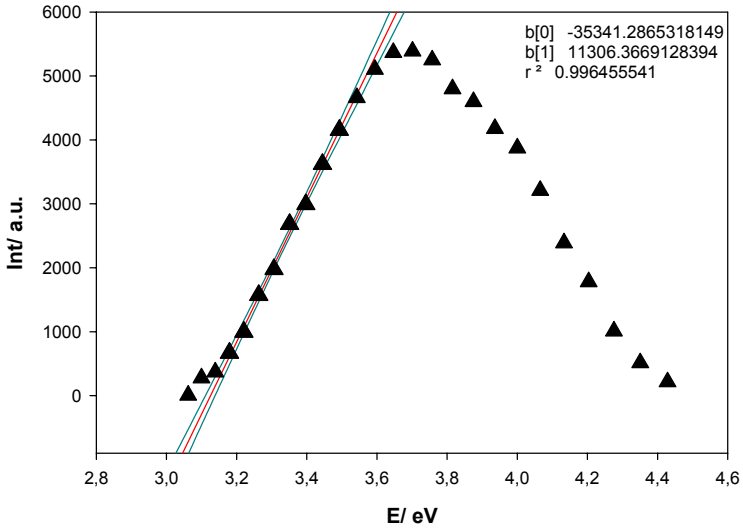
S.I. Energy increment:

Calculated energy increment (in vacuum at 0 K) of the surface oxidation process vs particle diameter

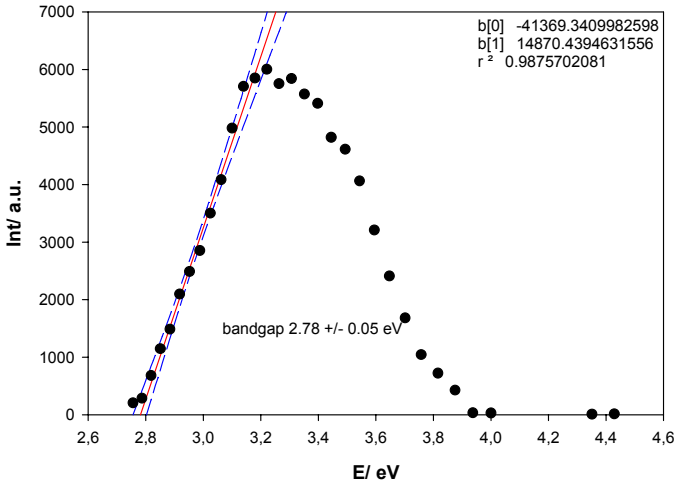


S.I. Band Gap calculation: Plots illustrating the threshold analysis for the bandgap estimation for each species.

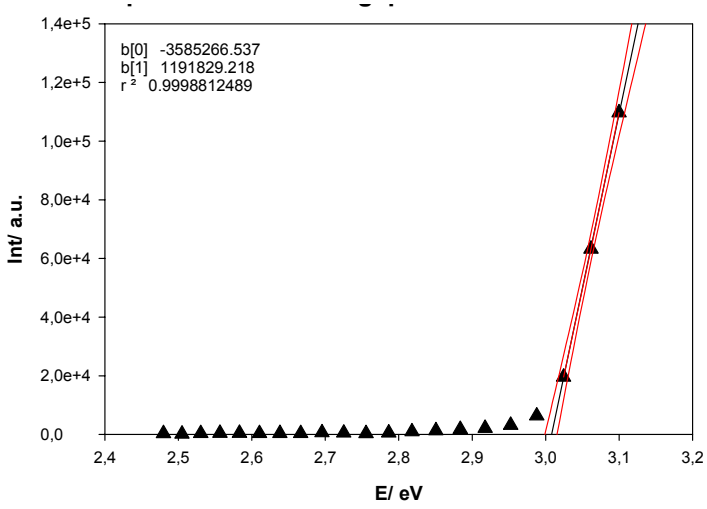
Specie E1: band gap 3.1 ± 0.05 eV.



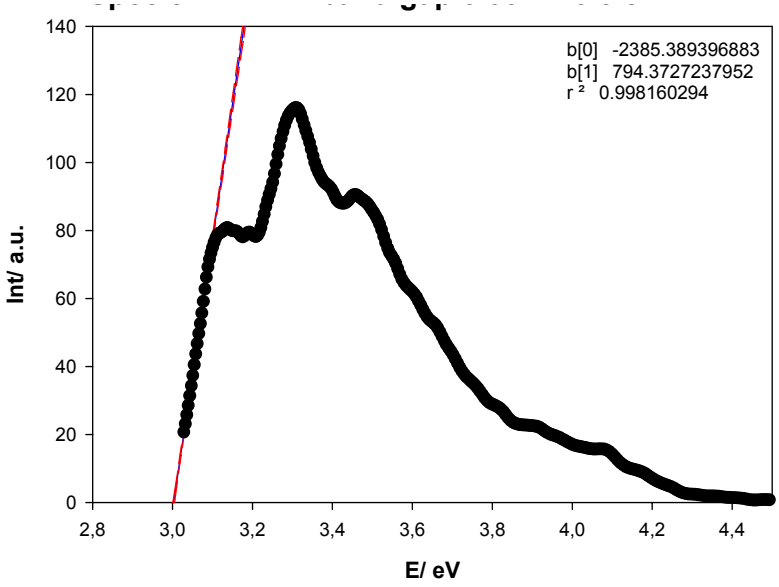
Specie E2: band gap 2.8 ± 0.05 eV.



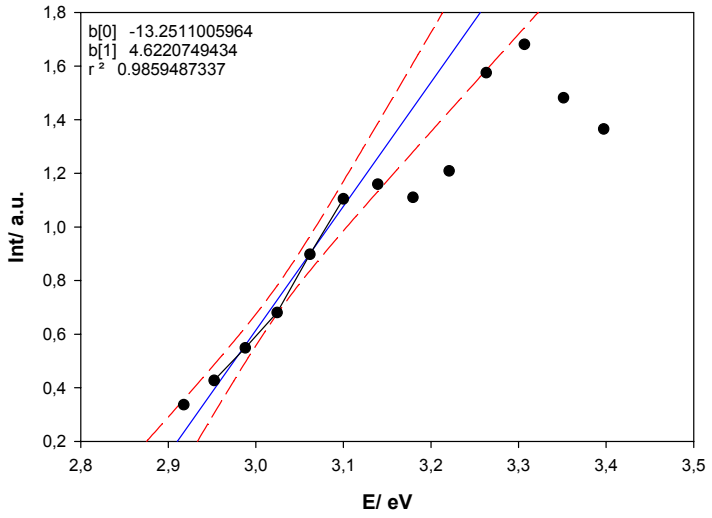
Specie E4: band gap 3.0 ± 0.05 eV.



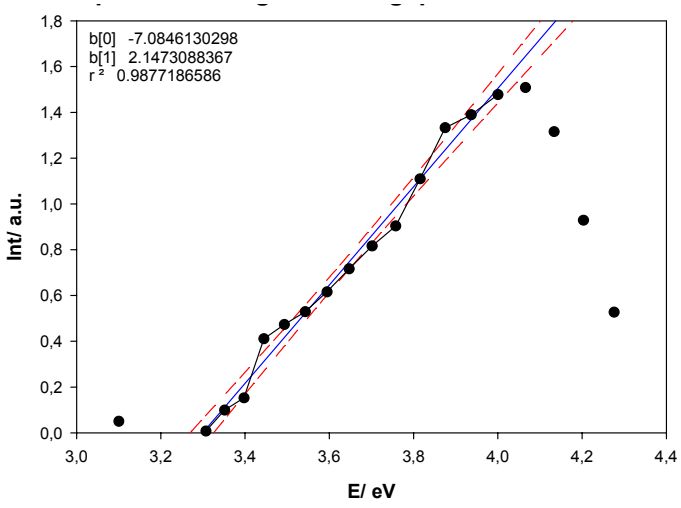
Specie E4´: band gap 3.0 ± 0.5 eV.



Specie E4´ (argón): band gap 2.9 ± 0.1 eV.



Specie E6 (argón): band gap 3.3 ± 0.05 eV.



S.I. Tables with the Cartesian coordinates of theoretical geometries.

Geometry of $Si_{71}H_{60}$

Si	Si1	1.3564	1.35693	1.35729
Si	Si2	0.03386	0.03937	0.03374
Si	Si3	2.67964	0.03997	2.68006
Si	Si4	2.68105	2.67361	0.03222
Si	Si5	0.03256	2.6731	2.68066
Si	Si6	1.34278	-1.33317	4.04149
Si	Si7	1.33986	4.04607	-1.32701
Si	Si8	1.37024	4.04605	4.04283
Si	Si9	4.03271	1.32521	-1.32091
Si	Si10	4.03357	1.38782	4.03221
Si	Si11	4.03945	-1.33275	1.34135
Si	Si12	4.04269	4.04627	1.37023
Si	Si13	-1.32093	1.32579	4.03293
Si	Si14	-1.32725	4.04568	1.33945
Si	Si15	1.37155	-1.33247	-1.32539
Si	Si16	-1.31829	1.38829	-1.31934
Si	Si17	-1.32773	-1.33325	1.36934
Si	Si18	5.51301	0.01299	0.01995
Si	Si19	0.02075	0.01387	5.51122
Si	Si20	0.01857	5.50636	0.01802
Si	Si21	2.69295	2.70124	5.50777
Si	Si22	2.69244	5.5057	2.69263
Si	Si23	5.50814	2.701	2.69258
Si	Si24	2.69108	0.01346	-2.80077
Si	Si25	2.69243	-2.79361	0.02001
Si	Si26	-2.79876	0.01431	2.69023
Si	Si27	-2.79615	2.70343	0.01827
Si	Si28	0.02036	-2.79156	2.69202
Si	Si29	0.01922	2.70332	-2.79637
Si	Si30	1.35768	1.3521	-4.35954
Si	Si31	1.356	1.35305	7.07516
Si	Si32	1.35592	-4.35762	1.35606

Si	Si33	1.35682	7.0771	1.3586
Si	Si34	7.0743	1.35342	1.35431
Si	Si35	-4.35974	1.35115	1.3557
Si	Si36	-0.44825	5.18142	5.18876
Si	Si37	5.1668	-0.47453	5.1634
Si	Si38	5.19252	5.17871	-0.44706
Si	Si39	3.16212	-2.46697	5.19075
Si	Si40	3.1639	5.177	-2.4781
Si	Si41	5.19112	-2.46387	3.16529
Si	Si42	5.16248	3.18813	-2.44999
Si	Si43	-2.45196	3.1857	5.16487
Si	Si44	-2.47381	5.17961	3.1662
Si	Si45	-2.44696	-0.47763	-2.45171
Si	Si46	-2.48025	-2.46617	-0.44614
Si	Si47	-0.45034	-2.46175	-2.48047
Si	Si48	4.34288	-1.63211	-3.31483
Si	Si49	3.86747	-1.13892	6.98972
Si	Si50	4.34768	-3.30262	-1.63552
Si	Si51	3.86055	-4.28259	3.8584
Si	Si52	3.87817	3.86206	-4.27453
Si	Si53	4.34224	4.34963	6.03982
Si	Si54	3.84773	6.99545	-1.13698
Si	Si55	4.34618	6.00671	4.34655
Si	Si56	6.03954	-1.63356	-1.63029
Si	Si57	6.98657	-1.14302	3.87054
Si	Si58	6.98873	3.85577	-1.15982
Si	Si59	6.03754	4.34855	4.34302
Si	Si60	-4.27722	-1.13978	-1.15967
Si	Si61	-3.31527	-1.63125	4.34133
Si	Si62	-3.32646	4.34846	-1.62958
Si	Si63	-4.27523	3.86243	3.87481
Si	Si64	-1.16242	-1.144	-4.27274
Si	Si65	-1.62923	-1.63249	6.03903
Si	Si66	-1.13904	-4.28085	-1.14128
Si	Si67	-1.63393	-3.30346	4.34585
Si	Si68	-1.62965	4.34632	-3.32208
Si	Si69	-1.15593	3.8552	6.98998
Si	Si70	-1.63334	6.0094	-1.63244

Si	Si71	-1.13976	6.99522	3.85034
H	H72	0.76373	0.47334	-5.43026
H	H73	1.95555	2.2316	-5.42878
H	H74	0.47593	2.16527	7.95044
H	H75	2.23954	0.53608	7.93661
H	H76	1.95076	-5.57278	2.01639
H	H77	0.5581	-5.22193	0.47536
H	H78	0.76226	8.2917	2.01999
H	H79	2.14949	7.94509	0.47466
H	H80	8.39023	1.90206	0.88028
H	H81	7.58095	0.4701	2.42929
H	H82	-5.67733	0.79546	0.89617
H	H83	-4.85931	2.24172	2.43087
H	H84	0.59793	5.92058	6.18472
H	H85	5.7872	-1.77318	5.7893
H	H86	6.01037	6.02115	0.69515
H	H87	2.1109	-3.20701	6.18529
H	H88	2.02095	6.02129	-3.30059
H	H89	6.1893	-3.19997	2.11645
H	H90	6.01134	2.08849	-3.33276
H	H91	-3.12693	4.45315	5.83682
H	H92	-3.47311	5.91433	2.12735
H	H93	-3.3215	0.60609	-3.35269
H	H94	-3.29734	-3.30938	0.69377
H	H95	0.69121	-3.30577	-3.29876
H	H96	4.71778	-2.02205	-4.7116
H	H97	2.67322	-1.37789	7.93375
H	H98	4.84486	-2.06698	7.61508
H	H99	4.72034	-4.69983	-2.02168
H	H100	4.53564	-5.46426	4.48974
H	H101	2.91889	-4.42835	2.76205
H	H102	4.62963	4.39697	-5.45001
H	H103	3.13344	2.62828	-4.30764
H	H104	4.72483	4.73063	7.43476
H	H105	3.27136	8.09565	-0.37329
H	H106	4.78547	7.71173	-2.06881
H	H107	4.73042	7.40186	4.72672
H	H108	7.43115	-2.0203	-2.0196

H	H109	7.93923	-1.48342	2.7111
H	H110	7.58958	-2.05249	4.88519
H	H111	8.18357	4.45596	-1.82709
H	H112	7.11996	2.78377	-0.1842
H	H113	7.43293	4.73262	4.72199
H	H114	-5.47607	-1.7228	-1.83489
H	H115	-4.39604	-0.0429	-0.2121
H	H116	-4.71155	-2.01065	4.72333
H	H117	-4.71834	4.73955	-2.01322
H	H118	-5.20456	4.22325	2.69904
H	H119	-4.87791	4.7772	4.88794
H	H120	-1.87563	-1.66465	-5.48534
H	H121	-0.36569	0.08409	-4.24072
H	H122	-2.01971	-2.00784	7.43354
H	H123	-0.55901	-5.38331	-0.3871
H	H124	-2.07741	-4.9973	-2.07366
H	H125	-2.0235	-4.69742	4.72632
H	H126	-2.0023	4.73998	-4.71819
H	H127	0.06174	4.10903	7.90887
H	H128	-2.13567	4.78856	7.62173
H	H129	-2.00675	7.40709	-2.01524
H	H130	-1.79676	8.19342	4.46677
H	H131	-0.19863	7.09748	2.77002

Geometry of $Si_{71}O_{60}$

Si	Si1	1.3564	1.35693	1.35729
Si	Si2	0.03386	0.03937	0.03374
Si	Si3	2.67964	0.03997	2.68006
Si	Si4	2.68105	2.67361	0.03222
Si	Si5	0.03256	2.6731	2.68066
Si	Si6	1.34278	-1.33317	4.04149
Si	Si7	1.33986	4.04607	-1.32701
Si	Si8	1.37024	4.04605	4.04283
Si	Si9	4.03271	1.32521	-1.32091
Si	Si10	4.03357	1.38782	4.03221
Si	Si11	4.03945	-1.33275	1.34135
Si	Si12	4.04269	4.04627	1.37023

Si	Si13	-1.32093	1.32579	4.03293
Si	Si14	-1.32725	4.04568	1.33945
Si	Si15	1.37155	-1.33247	-1.32539
Si	Si16	-1.31829	1.38829	-1.31934
Si	Si17	-1.32773	-1.33325	1.36934
Si	Si18	5.51301	0.01299	0.01995
Si	Si19	0.02075	0.01387	5.51122
Si	Si20	0.01857	5.50636	0.01802
Si	Si21	2.69295	2.70124	5.50777
Si	Si22	2.69244	5.5057	2.69263
Si	Si23	5.50814	2.701	2.69258
Si	Si24	2.69108	0.01346	-2.80077
Si	Si25	2.69243	-2.79361	0.02001
Si	Si26	-2.79876	0.01431	2.69023
Si	Si27	-2.79615	2.70343	0.01827
Si	Si28	0.02036	-2.79156	2.69202
Si	Si29	0.01922	2.70332	-2.79637
Si	Si30	1.35768	1.3521	-4.35954
Si	Si31	1.356	1.35305	7.07516
Si	Si32	1.35592	-4.35762	1.35606
Si	Si33	1.35682	7.0771	1.3586
Si	Si34	7.0743	1.35342	1.35431
Si	Si35	-4.35974	1.35115	1.3557
Si	Si36	-0.44825	5.18142	5.18876
Si	Si37	5.1668	-0.47453	5.1634
Si	Si38	5.19252	5.17871	-0.44706
Si	Si39	3.16212	-2.46697	5.19075
Si	Si40	3.1639	5.177	-2.4781
Si	Si41	5.19112	-2.46387	3.16529
Si	Si42	5.16248	3.18813	-2.44999
Si	Si43	-2.45196	3.1857	5.16487
Si	Si44	-2.47381	5.17961	3.1662
Si	Si45	-2.44696	-0.47763	-2.45171
Si	Si46	-2.48025	-2.46617	-0.44614
Si	Si47	-0.45034	-2.46175	-2.48047
Si	Si48	4.34288	-1.63211	-3.31483
Si	Si49	3.86747	-1.13892	6.98972
Si	Si50	4.34768	-3.30262	-1.63552

Si	Si51	3.86055	-4.28259	3.8584
Si	Si52	3.87817	3.86206	-4.27453
Si	Si53	4.34224	4.34963	6.03982
Si	Si54	3.84773	6.99545	-1.13698
Si	Si55	4.34618	6.00671	4.34655
Si	Si56	6.03954	-1.63356	-1.63029
Si	Si57	6.98657	-1.14302	3.87054
Si	Si58	6.98873	3.85577	-1.15982
Si	Si59	6.03754	4.34855	4.34302
Si	Si60	-4.27722	-1.13978	-1.15967
Si	Si61	-3.31527	-1.63125	4.34133
Si	Si62	-3.32646	4.34846	-1.62958
Si	Si63	-4.27523	3.86243	3.87481
Si	Si64	-1.16242	-1.144	-4.27274
Si	Si65	-1.62923	-1.63249	6.03903
Si	Si66	-1.13904	-4.28085	-1.14128
Si	Si67	-1.63393	-3.30346	4.34585
Si	Si68	-1.62965	4.34632	-3.32208
Si	Si69	-1.15593	3.8552	6.98998
Si	Si70	-1.63334	6.0094	-1.63244
Si	Si71	-1.13976	6.99522	3.85034
O	O72	0.55112	0.60208	-5.64419
O	O73	2.51695	2.53823	-4.04346
O	O74	0.46648	1.9897	8.30741
O	O75	2.46827	0.43247	7.93814
O	O76	2.23875	-4.67027	2.59051
O	O77	0.54318	-5.61159	0.68175
O	O78	0.64753	8.34992	2.2123
O	O79	2.4982	7.74184	0.27991
O	O80	8.26418	2.46095	0.86375
O	O81	8.0787	0.09442	1.7664
O	O82	-5.57857	0.3076	0.78874
O	O83	-5.30488	2.67324	1.73514
O	O84	0.11861	5.17975	6.64703
O	O85	5.40086	-0.54137	6.86661
O	O86	6.66456	5.55507	-0.37924
O	O87	3.12819	-4.06858	5.33639
O	O88	3.88646	5.54138	-3.8017

O	O89	5.71722	-3.56036	4.1191
O	O90	5.32538	3.17867	-4.02676
O	O91	-3.91215	2.60114	5.14319
O	O92	-2.70315	6.67125	2.82392
O	O93	-2.74885	-0.15586	-3.93388
O	O94	-3.95255	-2.81366	-0.1266
O	O95	0.1549	-3.90989	-2.59195
O	O96	4.98249	-1.77215	-4.66859
O	O97	2.93768	0.14311	6.41434
O	O98	3.12154	-2.41879	7.35863
O	O99	5.59334	-3.00781	-0.63858
O	O100	4.45512	-5.57392	3.34678
O	O101	3.52754	-2.62699	3.34097
O	O102	3.60849	4.09458	-5.76548
O	O103	4.19887	4.23624	-1.55145
O	O104	5.54715	4.06237	6.92077
O	O105	2.0742	7.25422	-1.09628
O	O106	4.71758	8.15465	-1.51145
O	O107	4.32749	7.43646	4.32722
O	O108	7.46943	-1.62248	-1.61613
O	O109	7.88016	-0.34473	3.09008
O	O110	7.87393	-1.93136	4.66805
O	O111	8.29339	4.2592	-1.5841
O	O112	7.26627	2.8577	-0.17406
O	O113	7.46741	4.33849	4.3267
O	O114	-5.58301	-1.54078	-1.58277
O	O115	-4.5522	-0.13998	-0.17495
O	O116	-4.74509	-1.61678	4.32385
O	O117	-4.75635	4.33929	-1.61447
O	O118	-5.17334	3.06803	3.09556
O	O119	-5.1581	4.65306	4.67503
O	O120	-1.58749	-1.5484	-5.57684
O	O121	-0.177	-0.14598	-4.55167
O	O122	-1.61509	-1.62116	7.46892
O	O123	-0.34017	-5.16066	-0.3459
O	O124	-1.9248	-5.18074	-1.9272
O	O125	-1.61965	-4.73329	4.32893
O	O126	-1.61343	4.33422	-4.75194

O	O127	-0.37551	3.05661	7.88335
O	O128	-1.95358	4.64312	7.87758
O	O129	-1.61494	7.43917	-1.61423
O	O130	-1.54632	8.30516	4.2549
O	O131	-0.14719	7.25902	2.8553

Geometry of $Si_{185}H_{76}$

Si	Si1	1.37481	1.38996	1.37929
Si	Si2	0.05123	0.05741	0.0535
Si	Si3	2.69249	0.02846	2.704
Si	Si4	2.69246	2.71063	0.01914
Si	Si5	0.03444	2.71766	2.69616
Si	Si6	1.31914	-1.33345	4.03437
Si	Si7	1.31635	4.03795	-1.33531
Si	Si8	1.42636	4.03007	4.03654
Si	Si9	4.0128	1.30975	-1.30412
Si	Si10	4.04457	1.40299	4.02898
Si	Si11	4.0097	-1.29657	1.29529
Si	Si12	4.03884	4.03431	1.39703
Si	Si13	-1.30301	1.33304	4.01134
Si	Si14	-1.30745	4.00388	1.28799
Si	Si15	1.39768	-1.28273	-1.29384
Si	Si16	-1.2794	1.40317	-1.29639
Si	Si17	-1.2847	-1.28825	1.40508
Si	Si18	5.41071	-0.04272	-0.05128
Si	Si19	-0.04369	-0.03424	5.39995
Si	Si20	-0.04471	5.41114	-0.04537
Si	Si21	2.77341	2.74703	5.41409
Si	Si22	2.7653	5.4182	2.74895
Si	Si23	5.41899	2.75884	2.75172
Si	Si24	2.75337	-0.03257	-2.71178
Si	Si25	2.74841	-2.7082	-0.04484
Si	Si26	-2.70272	-0.03216	2.74972
Si	Si27	-2.71027	2.74006	-0.0557
Si	Si28	-0.04248	-2.71009	2.76007

Si	Si29	-0.03984	2.76125	-2.71334
Si	Si30	1.38712	1.39338	-3.97314
Si	Si31	1.36192	1.35101	6.61369
Si	Si32	1.37894	-3.96753	1.38361
Si	Si33	1.34513	6.61998	1.3615
Si	Si34	6.61721	1.35416	1.34748
Si	Si35	-3.95556	1.38097	1.37842
Si	Si36	0.10494	5.33932	5.38005
Si	Si37	5.34925	0.03018	5.33201
Si	Si38	5.34503	5.32407	0.01496
Si	Si39	2.66515	-2.66782	5.36588
Si	Si40	2.66862	5.36222	-2.66967
Si	Si41	5.32606	-2.60386	2.64853
Si	Si42	5.32762	2.661	-2.6161
Si	Si43	-2.59274	2.73669	5.32113
Si	Si44	-2.62462	5.31007	2.6367
Si	Si45	-2.59242	0.06455	-2.60641
Si	Si46	-2.60317	-2.61416	0.07987
Si	Si47	0.0774	-2.60965	-2.60751
Si	Si48	4.10142	-1.42756	-4.06432
Si	Si49	4.04971	-1.3456	6.72504
Si	Si50	4.0978	-4.06243	-1.44132
Si	Si51	4.04009	-4.07375	3.99556
Si	Si52	4.0429	4.00953	-4.08579
Si	Si53	4.14481	4.11425	6.79988
Si	Si54	4.03801	6.72497	-1.33785
Si	Si55	4.14969	6.79936	4.10797
Si	Si56	6.79703	-1.4106	-1.41552
Si	Si57	6.75478	-1.32441	4.02313
Si	Si58	6.76179	4.02577	-1.33292
Si	Si59	6.81297	4.12467	4.11307
Si	Si60	-4.03017	-1.25324	-1.24772
Si	Si61	-4.07072	-1.42636	4.09333
Si	Si62	-4.07595	4.08674	-1.44875
Si	Si63	-4.07091	4.06148	4.0249
Si	Si64	-1.22549	-1.24071	-4.05649
Si	Si65	-1.45748	-1.34373	6.79617

Si	Si66	-1.24411	-4.04611	-1.24242
Si	Si67	-1.43535	-4.05877	4.12412
Si	Si68	-1.42998	4.12847	-4.05822
Si	Si69	-1.3	4.07855	6.78211
Si	Si70	-1.45487	6.80206	-1.35909
Si	Si71	-1.28456	6.63756	4.02519
Si	Si72	5.52215	5.50009	5.49882
Si	Si73	-5.45788	0.10419	0.11724
Si	Si74	0.10776	-5.47044	0.11795
Si	Si75	0.12307	0.12671	-5.47558
Si	Si76	2.66396	2.66548	-5.48659
Si	Si77	2.65568	-5.4783	2.65592
Si	Si78	-5.43497	2.66187	2.65813
Si	Si79	2.63729	8.04425	0.0473
Si	Si80	8.05657	2.63974	0.0578
Si	Si81	0.06004	8.05688	2.68419
Si	Si82	2.64919	0.03995	8.04605
Si	Si83	8.05384	0.06492	2.63962
Si	Si84	0.08279	2.66003	8.04308
Si	Si85	5.49222	-2.78441	-2.79015
Si	Si86	-2.80215	-2.76825	5.50493
Si	Si87	-2.79893	5.50516	-2.77515
Si	Si88	1.06744	-4.08497	-4.08502
Si	Si89	1.45206	-3.97377	6.90544
Si	Si90	1.45855	6.90268	-3.97233
Si	Si91	1.20301	6.8345	6.81313
Si	Si92	6.83131	1.50287	-3.98837
Si	Si93	6.80202	1.13311	6.77494
Si	Si94	6.82909	-3.97882	1.50142
Si	Si95	6.79122	6.77534	1.10725
Si	Si96	-4.06711	1.06048	-4.07194
Si	Si97	-4.02358	1.60559	6.75889
Si	Si98	-4.08463	-4.08661	1.07417
Si	Si99	-4.06556	6.80857	1.56584
Si	Si100	0.03625	-5.37534	5.46696
Si	Si101	0.03929	5.47318	-5.37163
Si	Si102	-5.38782	0.07414	5.40913

Si	Si103	5.43192	0.04751	-5.37864
Si	Si104	5.42681	-5.3707	0.04207
Si	Si105	-5.38236	5.41315	0.04422
Si	Si106	2.59569	-2.72379	-5.42378
Si	Si107	2.59287	-5.42251	-2.73354
Si	Si108	-5.43539	-2.73684	2.59945
Si	Si109	-5.43304	2.57513	-2.73756
Si	Si110	-2.71884	2.60354	-5.407
Si	Si111	-2.73645	-5.41474	2.61639
Si	Si112	2.68661	5.44177	8.16758
Si	Si113	2.69905	8.16774	5.44078
Si	Si114	5.45407	2.61889	8.16466
Si	Si115	5.45441	8.1675	2.61042
Si	Si116	8.17059	2.63998	5.43098
Si	Si117	8.16792	5.44067	2.62184
Si	Si118	-0.03494	8.19608	-2.6366
Si	Si119	8.17538	0.03438	-2.68131
Si	Si120	8.17402	-2.6752	0.03242
Si	Si121	-2.72648	0.1402	8.18126
Si	Si122	-2.73222	8.17641	0.11306
Si	Si123	-0.04371	-2.63871	8.19143
Si	Si124	0.83783	3.63981	-6.62552
Si	Si125	1.84352	3.53737	9.30092
Si	Si126	0.83059	-6.62809	3.62701
Si	Si127	1.83857	9.31486	3.55643
Si	Si128	3.60905	0.83973	-6.65155
Si	Si129	3.5575	1.79265	9.30406
Si	Si130	3.59986	-6.64204	0.82862
Si	Si131	3.54446	9.30055	1.79857
Si	Si132	9.31136	1.81387	3.53855
Si	Si133	9.31109	3.54066	1.8066
Si	Si134	-6.64053	0.85168	3.57226
Si	Si135	-6.62601	3.58033	0.84092
Si	Si136	0.88049	-0.81364	9.32515
Si	Si137	0.86851	9.32434	-0.79804
Si	Si138	9.31816	0.89229	-0.82651
Si	Si139	9.32094	-0.83022	0.90137

Si	Si140	-0.82487	0.9385	9.31608
Si	Si141	-0.85009	9.32491	0.94588
Si	Si142	5.82569	-5.23889	4.99671
Si	Si143	5.84268	5.00063	-5.24401
Si	Si144	-5.63664	5.51321	5.16547
Si	Si145	-5.62947	-2.54405	-2.53347
Si	Si146	-2.51386	-2.51868	-5.64454
Si	Si147	-2.53663	-5.63434	-2.53262
Si	Si148	5.33386	-2.7157	8.19342
Si	Si149	5.28349	8.23629	-2.7109
Si	Si150	8.27485	-2.64057	5.37075
Si	Si151	8.30256	5.3303	-2.66705
Si	Si152	-2.36501	5.53412	8.38501
Si	Si153	-2.78693	7.72597	5.5046
Si	Si154	6.82292	-4.14432	-4.14954
Si	Si155	6.756	-4.00063	6.78188
Si	Si156	6.73851	6.79484	-3.97958
Si	Si157	6.84422	6.86122	6.8699
Si	Si158	-3.56548	-3.568	-3.58282
Si	Si159	-4.1655	-4.14092	6.82455
Si	Si160	-4.16632	6.81817	-4.15255
Si	Si161	-4.17132	6.42229	6.96346
Si	Si162	11.22408	0.52112	0.51996
Si	Si163	0.5193	0.54572	11.22767
Si	Si164	0.51289	11.22723	0.56055
Si	Si165	-1.42235	-4.62171	-4.63389
Si	Si166	-4.60673	-1.41766	-4.63392
Si	Si167	2.21307	11.22455	2.19227
Si	Si168	2.21434	2.19096	11.22208
Si	Si169	-4.62293	-4.63621	-1.41533
Si	Si170	11.22792	2.19187	2.19032
Si	Si171	3.58468	-4.48183	7.91481
Si	Si172	3.57411	7.92718	-4.51252
Si	Si173	-4.66664	4.04856	7.34258
Si	Si174	7.69664	3.69386	-4.56567
Si	Si175	7.68384	-4.56305	3.70348
Si	Si176	-4.72759	7.49739	3.85863

Si	Si177	-0.86242	-6.66529	1.89773
Si	Si178	1.88417	-0.85169	-6.68954
Si	Si179	1.87125	-6.67856	-0.86384
Si	Si180	-6.68382	-0.86257	1.87784
Si	Si181	-6.67922	1.86678	-0.8618
Si	Si182	-0.84828	1.90635	-6.67484
Si	Si183	-1.10028	7.52553	7.47522
Si	Si184	7.46404	-1.28909	7.39367
Si	Si185	7.41213	7.36079	-1.37474
H	H186	-0.81698	-6.26419	6.32995
H	H187	-0.8061	6.34751	-6.2504
H	H188	-6.22241	-0.76175	6.32996
H	H189	6.32546	-0.80229	-6.23859
H	H190	6.3278	-6.23196	-0.80104
H	H191	-6.22934	6.3191	-0.79111
H	H192	3.37144	-3.69602	-6.29738
H	H193	3.3565	-6.30394	-3.71206
H	H194	-6.30746	-3.69956	3.37779
H	H195	-6.33226	3.31601	-3.72837
H	H196	-3.70413	3.36888	-6.28773
H	H197	-3.69606	-6.28527	3.40078
H	H198	3.48915	6.32539	9.08137
H	H199	3.4877	9.07637	6.33334
H	H200	6.37563	3.40686	9.07021
H	H201	6.37234	9.06629	3.39963
H	H202	9.07342	3.43491	6.35053
H	H203	9.07228	6.3513	3.4198
H	H204	-0.83904	9.12526	-3.51825
H	H205	9.08418	-0.76904	-3.58725
H	H206	9.08662	-3.59285	-0.75366
H	H207	-3.62515	-0.675	9.06365
H	H208	-3.61813	9.07875	-0.68374
H	H209	-0.83867	-3.53561	9.11955
H	H210	1.2219	4.03271	-8.03433
H	H211	1.21997	-8.03856	4.0097
H	H212	4.01598	1.21465	-8.05537
H	H213	4.00261	-8.04859	1.20257

H	H214	-8.0407	1.23223	3.99349
H	H215	-8.03165	3.989	1.22462
H	H216	5.53183	-6.72186	5.17793
H	H217	5.58464	5.1783	-6.73518
H	H218	7.73593	-3.28391	-4.96517
H	H219	5.97169	-4.96445	-5.06574
H	H220	7.64385	-5.05522	-3.29216
H	H221	7.69539	-4.87028	7.59948
H	H222	7.67234	7.62074	-4.83729
H	H223	7.71468	7.74692	6.04938
H	H224	7.71075	6.03466	7.75331
H	H225	5.98213	7.71928	7.73018
H	H226	-2.69798	-2.69716	-2.70975
H	H227	-5.07338	-4.95572	5.96201
H	H228	-4.98423	-3.27862	7.73034
H	H229	-3.31261	-5.05246	7.64473
H	H230	-4.97633	5.95422	-5.05932
H	H231	-3.31453	7.72981	-4.97319
H	H232	-5.08101	7.63537	-3.29909
H	H233	-5.01561	7.3533	7.75005
H	H234	12.52992	0.00045	0.01592
H	H235	0.02287	0.0132	12.53747
H	H236	0.02511	12.54186	0.03225
H	H237	-1.7182	-5.66988	-5.6808
H	H238	-5.66574	-1.69359	-5.67575
H	H239	2.73053	12.53139	2.71713
H	H240	2.7366	2.70549	12.53114
H	H241	-5.67319	-5.67812	-1.69964
H	H242	12.5306	2.71583	2.7134
H	H243	4.21455	-4.96485	6.6154
H	H244	3.68104	-5.71018	8.78159
H	H245	3.54069	9.03971	-5.52579
H	H246	4.24545	6.76062	-5.21914
H	H247	-5.7532	4.06917	8.42552
H	H248	8.76452	3.62597	-5.64479
H	H249	8.76015	-5.6385	3.67203
H	H250	-5.77789	8.60543	3.79235

H	H251	-1.2145	-8.10319	1.54042
H	H252	1.52126	-1.21145	-8.1197
H	H253	1.51379	-8.10875	-1.22599
H	H254	-8.1156	-1.21625	1.52075
H	H255	-8.10737	1.51485	-1.21882
H	H256	-1.19836	1.55181	-8.10519
H	H257	-1.01008	8.66384	8.50249
H	H258	8.56218	-1.36429	8.45857
H	H259	8.48032	8.45455	-1.48105

Geometry of $Si_{185}O_{76}$

Si	Si1	-0.13855	24.96912	-0.05654
Si	Si2	-1.49168	23.63109	-1.40234
Si	Si3	1.22854	23.66423	1.3141
Si	Si4	1.22566	26.33953	-1.36329
Si	Si5	-1.44809	26.33763	1.3086
Si	Si6	-0.14736	22.34624	2.66482
Si	Si7	-0.14958	27.69781	-2.68155
Si	Si8	-0.03605	27.66022	2.63365
Si	Si9	2.57808	24.95934	-2.66882
Si	Si10	2.55259	25.06494	2.63238
Si	Si11	2.58343	22.36783	-0.06632
Si	Si12	2.55132	27.65706	0.03959
Si	Si13	-2.76381	24.95254	2.66131
Si	Si14	-2.75557	27.69807	-0.075
Si	Si15	-0.06286	22.30813	-2.72722
Si	Si16	-2.8052	25.04326	-2.736
Si	Si17	-2.80912	22.29161	0.00796
Si	Si18	3.9904	23.57621	-1.4557
Si	Si19	-1.5407	23.56873	4.07392
Si	Si20	-1.548	29.11171	-1.46758
Si	Si21	1.29179	26.393	4.06136
Si	Si22	1.29014	29.09012	1.36695
Si	Si23	3.97642	26.39332	1.36887
Si	Si24	1.30094	23.64386	-4.06365
Si	Si25	1.29951	20.97453	-1.37887

Si	Si26	-4.15579	23.62375	1.37739
Si	Si27	-4.14779	26.41109	-1.39877
Si	Si28	-1.47159	20.9557	1.37545
Si	Si29	-1.47637	26.41143	-4.07424
Si	Si30	-0.04586	25.07051	-5.33119
Si	Si31	-0.12055	24.97709	5.28458
Si	Si32	-0.04144	19.69723	0.03524
Si	Si33	-0.13053	30.30762	-0.04735
Si	Si34	5.19133	24.9794	-0.03626
Si	Si35	-5.41197	25.05882	0.02289
Si	Si36	-1.39412	28.99738	3.96627
Si	Si37	3.88	23.70266	3.96401
Si	Si38	3.87748	28.99813	-1.32377
Si	Si39	1.17381	20.94493	3.96274
Si	Si40	1.17464	28.99851	-4.08146
Si	Si41	3.87497	20.95681	1.24338
Si	Si42	3.87431	26.28519	-4.06944
Si	Si43	-4.16824	26.28282	3.96025
Si	Si44	-4.16745	28.99578	1.24795
Si	Si45	-4.11861	23.67622	-4.05532
Si	Si46	-4.12704	20.97845	-1.35017
Si	Si47	-1.41907	20.98768	-4.05616
Si	Si48	2.70766	22.35164	-5.49051
Si	Si49	2.57542	22.27301	5.30353
Si	Si50	2.7037	19.54432	-2.67601
Si	Si51	2.58333	19.56754	2.65864
Si	Si52	2.57647	27.69865	-5.45712
Si	Si53	2.62707	27.7138	5.51708
Si	Si54	2.56981	30.33738	-2.75074
Si	Si55	2.62759	30.54946	2.67734
Si	Si56	5.45839	22.23931	-2.779
Si	Si57	5.22549	22.27914	2.65151
Si	Si58	5.22006	27.6904	-2.74285
Si	Si59	5.45687	27.71739	2.67565
Si	Si60	-5.48324	22.3816	-2.65138
Si	Si61	-5.5705	22.35095	2.78258
Si	Si62	-5.57081	27.79279	-2.67704
Si	Si63	-5.54848	27.68981	2.6493

Si	Si64	-2.7052	22.39763	-5.4147
Si	Si65	-2.86969	22.23491	5.5342
Si	Si66	-2.70751	19.6227	-2.63827
Si	Si67	-2.74408	19.52844	2.78462
Si	Si68	-2.74802	27.80876	-5.50483
Si	Si69	-2.8226	27.67759	5.30227
Si	Si70	-2.88365	30.55765	-2.80542
Si	Si71	-2.82555	30.4053	2.68427
Si	Si72	3.96276	29.05682	3.96824
Si	Si73	-6.81204	23.98606	-1.55437
Si	Si74	-1.13849	18.24661	-1.50448
Si	Si75	-1.13029	23.54687	-6.77018
Si	Si76	1.10839	26.48403	-6.91384
Si	Si77	1.19971	18.09616	1.34932
Si	Si78	-6.95313	26.41143	1.21831
Si	Si79	1.09486	31.73276	-1.44549
Si	Si80	6.60662	26.35629	-1.27405
Si	Si81	-1.36722	31.77422	1.31415
Si	Si82	1.16003	23.58899	6.73167
Si	Si83	6.63415	23.62264	1.22318
Si	Si84	-1.37943	26.35667	6.72276
Si	Si85	3.75433	20.35298	-4.56429
Si	Si86	-4.64355	20.3206	3.85063
Si	Si87	-4.64892	28.84782	-4.6674
Si	Si88	-0.5681	19.48504	-5.56319
Si	Si89	0.02732	19.52766	5.48034
Si	Si90	0.06795	30.5113	-5.57156
Si	Si91	-0.19156	30.50166	5.33952
Si	Si92	5.4436	25.02197	-5.25997
Si	Si93	5.39211	24.96181	5.30715
Si	Si94	5.43392	19.47054	0.19095
Si	Si95	5.2523	30.5003	-0.2076
Si	Si96	-5.62757	24.53538	-5.53994
Si	Si97	-5.6105	25.25903	5.49281
Si	Si98	-5.60746	19.3895	-0.54896
Si	Si99	-5.55021	30.58914	0.12926
Si	Si100	-1.6111	18.2255	4.35803
Si	Si101	-1.651	29.3928	-6.81115

Si	Si102	-6.9363	23.5082	4.45089
Si	Si103	4.4323	23.4246	-6.79012
Si	Si104	4.3408	18.3224	-1.52626
Si	Si105	-6.8043	29.6533	-1.64913
Si	Si106	0.7252	21.9281	-6.81162
Si	Si107	0.7177	18.2328	-3.11427
Si	Si108	-7.1479	21.5931	1.19986
Si	Si109	-6.934	25.8457	-3.13438
Si	Si110	-3.875	26.6160	-7.32556
Si	Si111	-3.8197	17.6837	1.55218
Si	Si112	1.5471	29.5533	6.79295
Si	Si113	1.3108	32.0012	4.25152
Si	Si114	4.2816	26.5147	6.72152
Si	Si115	4.0434	31.9906	1.27260
Si	Si116	6.9562	26.3939	4.10935
Si	Si117	6.7831	29.4818	1.31268
Si	Si118	-1.5763	31.7360	-4.38238
Si	Si119	7.0061	23.5897	-4.07703
Si	Si120	6.6572	20.6533	-1.45332
Si	Si121	-4.3047	23.7449	6.92516
Si	Si122	-4.2563	32.0323	-1.41621
Si	Si123	-1.5366	20.7421	6.77162
Si	Si124	-0.4937	27.1469	-8.66520
Si	Si125	0.7529	27.1170	7.42434
Si	Si126	-0.4016	16.3878	2.09549
Si	Si127	0.586	32.8054	2.16958
Si	Si128	2.1074	24.8367	-8.36478
Si	Si129	1.9963	25.2718	8.27200
Si	Si130	2.0991	16.5046	-0.29471
Si	Si131	2.0737	33.0788	0.28375
Si	Si132	7.9738	25.4127	2.13293
Si	Si133	7.5727	27.3217	0.67978
Si	Si134	-8.4241	24.6433	1.79306
Si	Si135	-8.5557	27.3238	-0.36917
Si	Si136	-0.6271	22.6067	8.02005
Si	Si137	-0.7788	32.8748	-2.40987
Si	Si138	8.0317	24.5985	-2.11456
Si	Si139	7.7505	22.6645	-0.67320

Si	Si140	-2.1759	24.5076	8.07179
Si	Si141	-2.2502	33.1211	-0.48774
Si	Si142	4.6338	17.1622	3.67776
Si	Si143	4.6721	28.9687	-7.65789
Si	Si144	-6.8027	28.9893	4.13053
Si	Si145	-6.4939	20.8351	-4.18844
Si	Si146	-4.1534	21.3632	-7.03486
Si	Si147	-4.3977	18.5569	-3.97122
Si	Si148	3.813	20.6434	6.56909
Si	Si149	3.7761	31.7935	-4.20800
Si	Si150	6.5804	20.9001	4.11500
Si	Si151	6.5469	29.0850	-4.13950
Si	Si152	-4.4886	29.2199	6.00765
Si	Si153	-3.9902	31.2877	4.58594
Si	Si154	6.231	18.6290	-3.86080
Si	Si155	4.8674	19.3976	4.82912
Si	Si156	4.7539	30.0240	-5.39481
Si	Si157	4.3913	29.3608	6.67615
Si	Si158	-4.9953	19.2309	-6.24356
Si	Si159	-3.8796	18.5946	6.31106
Si	Si160	-3.9655	31.3093	-6.44078
Si	Si161	-6.2603	31.5336	4.70700
Si	Si162	10.1421	24.4701	-1.01518
Si	Si163	-1.2536	24.4682	10.27666
Si	Si164	-1.1481	35.2194	-0.63312
Si	Si165	-2.6322	18.6757	-6.41966
Si	Si166	-6.3051	22.2773	-6.29957
Si	Si167	1.0048	35.1965	0.40500
Si	Si168	0.9502	25.4545	10.46337
Si	Si169	-6.5482	18.7829	-2.73332
Si	Si170	10.1178	25.4938	1.12292
Si	Si171	2.0629	18.9410	6.59617
Si	Si172	2.1108	31.7694	-5.96950
Si	Si173	-6.3286	27.5273	6.20578
Si	Si174	6.5989	27.8401	-6.28000
Si	Si175	6.2138	18.0353	2.11408
Si	Si176	-6.9163	30.5199	2.17039
Si	Si177	-2.0475	16.6052	0.23603

Si	Si178	1.2013	22.6749	-9.02649
Si	Si179	1.0528	15.9657	-2.41276
Si	Si180	-8.5289	23.0548	-0.11078
Si	Si181	-9.1912	26.2348	-2.45048
Si	Si182	-2.1149	25.2453	-8.37980
Si	Si183	-2.9423	31.2525	6.77287
Si	Si184	5.7876	22.0406	6.08254
Si	Si185	6.2902	31.5149	-3.08962
O	O186	-2.7099	17.7542	5.40290
O	O187	-2.758	30.4353	-7.26482
O	O188	-7.527	22.5363	5.43157
O	O189	5.4069	22.5023	-7.46380
O	O190	5.2793	17.8123	-2.70169
O	O191	-7.2658	30.5241	-2.78581
O	O192	0.2986	20.3220	-6.70408
O	O193	0.2856	18.3387	-4.71960
O	O194	-6.6092	20.3435	0.39219
O	O195	-6.8251	25.3188	-4.70039
O	O196	-4.7044	25.5012	-6.43360
O	O197	-4.6392	18.4910	0.39414
O	O198	0.8541	28.6724	8.02630
O	O199	2.2604	32.6419	5.24215
O	O200	3.5565	25.7829	7.99392
O	O201	4.9443	32.9633	1.99681
O	O202	7.7799	27.1838	5.10229
O	O203	7.5912	30.3198	2.26768
O	O204	-2.9198	31.9811	-5.21099
O	O205	7.9802	22.8633	-4.97664
O	O206	6.8765	19.8547	-2.81820
O	O207	-5.0861	23.0305	8.00305
O	O208	-5.1274	33.0596	-2.09770
O	O209	-2.8582	19.8571	6.93315
O	O210	-1.111	28.5074	-8.07840
O	O211	-1.034	17.0133	3.44018
O	O212	3.4687	24.5078	-7.61425
O	O213	3.4585	17.0717	-0.89577
O	O214	-7.8658	24.0070	3.11889
O	O215	-7.9498	28.6907	-0.83539

O	O216	3.9468	15.8917	3.32988
O	O217	4.4623	28.2916	-8.96483
O	O218	4.3015	21.5647	-3.59251
O	O219	4.9915	19.3740	-4.81672
O	O220	7.2362	17.8503	-4.64064
O	O221	5.3543	17.8074	5.04991
O	O222	5.3044	30.3255	-6.99715
O	O223	4.862	29.8258	5.21084
O	O224	4.9854	27.9946	7.26511
O	O225	3.0988	30.0746	7.33184
O	O226	-4.9203	20.1141	-4.66913
O	O227	-4.8596	19.2952	5.06265
O	O228	-3.7818	21.5895	4.44486
O	O229	-4.6392	17.8293	7.34452
O	O230	-4.904	30.0389	-5.70798
O	O231	-4.7697	32.3103	-7.21268
O	O232	-3.9345	29.5172	-3.33602
O	O233	-6.9902	31.6977	6.00208
O	O234	11.1758	23.4655	-1.43081
O	O235	-1.5809	23.4999	11.37251
O	O236	-1.5082	36.2873	-1.61773
O	O237	-2.5719	17.5697	-7.44217
O	O238	-7.5099	22.2960	-7.21529
O	O239	1.3051	36.1977	1.47801
O	O240	1.4009	26.7243	11.12754
O	O241	-7.602	17.7012	-2.72982
O	O242	11.1362	26.5326	1.48537
O	O243	3.7118	18.7933	3.63933
O	O244	2.5931	17.5554	6.40603
O	O245	2.4685	32.0323	-7.40154
O	O246	3.7248	28.7341	-6.19737
O	O247	-7.4168	27.7395	7.22058
O	O248	6.2036	26.3467	-5.89998
O	O249	7.7117	18.0847	2.14948
O	O250	-6.6988	31.8398	3.08193
O	O251	-2.3283	15.2683	-0.40255
O	O252	0.5342	22.5105	-10.35292
O	O253	0.3345	14.6819	-2.66588

O	O254	-9.8912	22.6393	-0.60806
O	O255	-10.4632	25.4604	-2.56174
O	O256	-2.3826	24.6164	-9.72377
O	O257	-1.3798	30.9316	6.37671
O	O258	5.7585	23.6195	6.29475
O	O259	5.9448	31.1251	-1.58636

Geometry of $Si_{240}H_{88}$

Si	Si1	1.31454	1.28132	1.2815
Si	Si2	2.65268	-0.05249	2.65332
Si	Si3	1.32816	-1.35163	4.03554
Si	Si4	2.67784	-2.64949	5.40187
Si	Si5	1.38775	-4.04413	6.7959
Si	Si6	0.0576	-2.63423	8.16175
Si	Si7	1.67084	-1.53193	9.49517
Si	Si8	0.62092	0.47921	10.36811
Si	Si9	1.89276	1.70895	11.94199
H	H10	0.92699	2.40913	12.85985
H	H11	2.7265	0.77656	12.76159
Si	Si12	3.09869	3.1661	10.54906
Si	Si13	4.87622	4.8959	10.8616
H	H14	5.20973	5.23918	12.29872
Si	Si15	6.84776	3.87573	9.48981
Si	Si16	8.56106	2.31534	8.55408
H	H17	9.66306	2.31684	9.65606
Si	Si18	7.99799	0.08252	8.0174
Si	Si19	6.28248	-0.31269	9.83249
H	H20	6.81395	-0.54255	11.22036
Si	Si21	5.37764	-2.07742	8.40849
Si	Si22	6.84309	-3.33652	6.95699
Si	Si23	7.20315	-5.62261	7.10322
H	H24	6.94383	-6.2261	8.4499
H	H25	8.1741	-6.39271	6.28166
Si	Si26	5.07704	-4.94285	6.20367
Si	Si27	8.31784	-2.27777	5.30418
Si	Si28	6.71465	-1.23579	3.97324
Si	Si29	5.31658	0.03959	5.29576

Si	Si30	8.12156	0.09649	2.69184
Si	Si31	9.42843	1.25116	4.30741
Si	Si32	8.00232	2.75133	5.38986
Si	Si33	6.68791	4.03838	4.03851
Si	Si34	5.29717	5.31566	5.31411
Si	Si35	4.01696	4.02388	6.69475
Si	Si36	2.72327	5.38008	7.99809
Si	Si37	1.38835	6.62805	6.62096
Si	Si38	0.0544	8.00374	8.00134
Si	Si39	-0.41266	6.24351	9.76085
H	H40	-0.65246	6.76385	11.15092
Si	Si41	-2.2015	5.28093	8.37446
Si	Si42	-3.13904	3.46483	9.77345
H	H43	-3.75552	3.72442	11.11769
Si	Si44	-4.54241	3.63889	7.86995
H	H45	-5.99814	3.89215	8.21461
Si	Si46	-4.12466	1.45615	6.86355
Si	Si47	-2.62807	0.06833	8.07964
Si	Si48	-3.56744	-2.05629	8.39626
H	H49	-4.18739	-1.97052	9.80421
Si	Si50	-5.67666	-2.21498	7.28128
H	H51	-6.92248	-2.51947	8.04558
Si	Si52	-4.28958	-3.99858	6.26643
Si	Si53	-2.21695	-4.82874	7.05851
H	H54	-2.57503	-6.30652	7.43808
Si	Si55	-2.51786	-2.64617	5.35289
Si	Si56	-4.0708	-1.41104	4.04453
Si	Si57	-5.33957	-3.16818	2.96996
H	H58	-6.83864	-2.96542	2.83923
Si	Si59	-4.11756	-4.08415	1.16876
Si	Si60	-3.20533	-5.29114	2.97102
H	H61	-2.97953	-6.75773	2.78976
Si	Si62	-2.68358	-2.69309	-0.03752
Si	Si63	-1.34972	-1.35882	1.32805
Si	Si64	-1.31327	-4.16845	-1.3376
Si	Si65	0.14239	-5.38904	0.09998
Si	Si66	-0.30012	-7.0592	1.77848
Si	Si67	1.09739	-6.66399	3.73536

Si	Si68	2.73612	-5.23159	2.74783
Si	Si69	3.7642	-6.57655	1.03651
Si	Si70	5.61889	-5.36764	-0.21949
Si	Si71	6.8772	-4.08992	1.40321
Si	Si72	8.04956	-4.62715	3.46938
H	H73	7.03048	-4.47381	4.53922
H	H74	8.50773	-6.06972	3.53693
Si	Si75	8.07101	-2.61148	-0.02586
Si	Si76	6.66068	-1.14667	-1.1894
Si	Si77	5.30253	0.12693	0.13853
Si	Si78	4.03725	1.35734	-1.35388
Si	Si79	5.46577	2.63223	-2.66434
Si	Si80	6.72301	3.96782	-1.21645
Si	Si81	8.15351	2.66749	0.09641
Si	Si82	9.43449	4.30191	1.26151
Si	Si83	9.76964	6.25909	-0.38167
Si	Si84	8.00591	8.00949	0.07344
Si	Si85	8.55569	8.55656	2.30936
Si	Si86	9.48673	6.84865	3.87978
Si	Si87	7.84221	7.84581	5.14647
H	H88	8.71048	8.71392	6.10042
Si	Si89	10.86611	4.89866	4.89721
H	H90	12.30207	5.23863	5.23486
Si	Si91	6.84513	9.48934	3.8774
Si	Si92	4.88682	10.85677	4.89756
Si	Si93	3.86318	9.4789	6.84506
Si	Si94	5.12988	7.84149	7.8503
H	H95	6.07234	8.71373	8.72473
H	H96	5.22471	12.2928	5.24027
Si	Si97	3.12692	10.54235	3.1479
Si	Si98	1.23747	9.4306	4.296
Si	Si99	0.09354	8.11528	2.68596
Si	Si100	-1.2289	6.70539	3.97194
Si	Si101	-2.15333	8.38567	5.31409
Si	Si102	-3.19971	9.77474	3.56605
Si	Si103	-4.48277	7.72886	3.69219
Si	Si104	-4.9031	5.93472	5.32815
Si	Si105	-5.57058	7.1942	7.26721

H	H106	-6.3924	6.57764	8.34741
H	H107	-6.12521	8.48386	6.75261
Si	Si108	-3.93895	4.14028	4.16496
Si	Si109	-5.17842	2.75778	2.7599
Si	Si110	-6.54898	1.04373	3.75622
Si	Si111	-8.07591	2.48721	2.48937
H	H112	-9.07588	3.33138	3.34793
Si	Si113	-8.91531	0.86035	0.89441
H	H114	-10.30197	0.49224	0.50667
Si	Si115	-7.0268	1.79767	-0.29685
Si	Si116	-5.37636	0.11995	0.12019
H	H117	-7.50522	2.0341	-1.68415
Si	Si118	-7.00346	-0.34075	1.81463
H	H119	-7.59994	-1.73682	1.99534
Si	Si120	-3.88691	1.37402	1.36986
Si	Si121	-2.67954	2.72655	-0.06175
Si	Si122	-1.34355	4.03341	1.33683
Si	Si123	0.06535	5.36077	0.06972
Si	Si124	-1.22759	6.73699	-1.24034
Si	Si125	-2.66972	8.0706	0.08676
Si	Si126	-3.56437	8.40181	-2.06001
H	H127	-4.21478	9.7903	-1.97441
Si	Si128	-5.65701	7.27298	-2.24219
Si	Si129	-5.38604	5.62576	-0.23019
H	H130	-6.89885	8.04508	-2.54641
Si	Si131	-4.27676	6.25	-3.99808
Si	Si132	-2.21436	7.10374	-4.79177
Si	Si133	-0.1802	5.58784	-5.27841
Si	Si134	1.47566	6.89093	-4.07947
Si	Si135	2.65904	5.46763	-2.64103
Si	Si136	3.98307	6.73305	-1.19513
Si	Si137	2.69417	8.15805	0.12556
Si	Si138	1.63782	9.50955	-1.5025
Si	Si139	0.60098	10.36481	0.50195
H	H140	-0.17501	11.50117	-0.18341
Si	Si141	3.61643	9.7843	-3.19456
H	H142	3.94652	11.05666	-3.92608
Si	Si143	5.35968	8.3564	-2.17295

Si	Si144	6.90503	6.89665	-3.27691
Si	Si145	5.60579	5.62584	-4.87837
H	H146	5.36212	5.04856	-6.48568
Si	Si147	7.2222	7.24149	-5.62794
H	H148	8.44866	6.51471	-6.07218
H	H149	7.06241	8.56747	-6.32342
Si	Si150	3.73916	7.74518	-4.51733
H	H151	4.47272	6.77424	-3.70791
H	H152	4.10381	7.90874	-5.97591
Si	Si153	-1.3536	3.91527	-4.08357
Si	Si154	-0.01281	2.68475	-2.66997
Si	Si155	1.38302	1.38093	-3.92626
Si	Si156	2.72537	2.7246	-5.22133
Si	Si157	3.77379	1.04889	-6.60361
Si	Si158	5.64316	-0.18359	-5.43956
Si	Si159	4.00834	-1.30457	-4.13293
Si	Si160	3.09019	-3.20691	-5.2752
Si	Si161	1.24926	-4.13051	-4.11554
Si	Si162	3.11197	-5.27864	-3.23161
H	H163	3.01548	-6.75664	-3.00351
Si	Si164	-1.14517	-4.56714	-4.43198
H	H165	-1.3297	-5.73829	-5.42385
Si	Si166	-2.68856	-2.74772	-5.60439
Si	Si167	-4.03902	-4.06166	-3.97072
Si	Si168	-5.66123	-2.71701	-2.65033
Si	Si169	-5.30315	-5.28216	-5.39084
H	H170	-6.22798	-6.18312	-4.66099
H	H171	-4.4464	-6.11926	-6.26075
H	H172	-6.11855	-4.40442	-6.26135
Si	Si173	-1.32553	-1.35131	-4.15838
Si	Si174	-2.67521	-0.04035	-2.68374
Si	Si175	-4.08111	1.16368	-4.09391
Si	Si176	-5.29311	3.01096	-3.27017
H	H177	-6.7418	2.82593	-2.98453
Si	Si178	-4.52627	-1.26662	-4.51687
H	H179	-5.62988	-1.44461	-5.60939
Si	Si180	4.66254	-5.0381	-5.09131
Si	Si181	6.42633	-3.82832	-3.84146

H	H182	4.76225	-6.07136	-6.16781
H	H183	2.76988	-2.75749	-6.59441
Si	Si184	7.15366	-2.28475	-5.75788
Si	Si185	8.4634	-2.09714	-3.76127
H	H186	9.95766	-2.15686	-4.19615
H	H187	7.80082	-2.6882	-7.04478
Si	Si188	1.8014	-0.33688	-7.02714
H	H189	2.00056	-1.71747	-7.58465
Si	Si190	0.79752	0.78251	-8.90017
Si	Si191	-0.36606	1.80599	-7.04324
H	H192	-1.76168	2.01716	-7.60573
H	H193	0.40656	0.35842	-10.2694
Si	Si194	2.4447	2.37844	-8.17624
H	H195	3.25675	3.14778	-9.27255
Si	Si196	0.09642	0.11781	-5.39892
Si	Si197	-3.19569	2.97463	-5.32786
H	H198	-2.99648	2.82073	-6.81834
Si	Si199	1.05539	3.75228	-6.63509
H	H200	-2.54098	7.48341	-6.27736
Si	Si201	-5.17164	4.40425	-5.22916
H	H202	-6.19758	4.52469	-6.28756
Si	Si203	-1.85465	9.16818	-3.69843
H	H204	-1.95422	10.49915	-4.34379
Si	Si205	0.06036	8.15912	-2.61721
Si	Si206	-2.52107	5.34024	-2.63523
Si	Si207	1.3315	4.06671	-1.35619
Si	Si208	-1.3457	1.33899	-1.35137
Si	Si209	-4.07875	4.01646	-1.42632
Si	Si210	-6.54438	3.7577	1.04886
H	H211	-5.89791	8.36953	3.69599
Si	Si212	-4.12504	6.80222	1.47403
H	H213	-3.91248	11.1242	3.67337
Si	Si214	-2.67198	5.40096	2.66438
Si	Si215	-1.4671	9.48191	1.54832
H	H216	-1.84018	10.89972	1.32235
Si	Si217	1.39337	6.73504	1.38718
Si	Si218	2.69272	5.34864	2.69508
Si	Si219	1.34414	3.96477	3.97087

Si	Si220	3.96913	3.97339	1.35177
Si	Si221	1.83731	11.94631	1.77164
H	H222	0.92954	12.88518	2.50677
H	H223	2.72163	12.76475	0.87031
Si	Si224	4.30478	9.45585	1.26823
Si	Si225	5.38116	8.00482	2.74319
H	H226	9.65891	9.65933	2.30915
Si	Si227	6.63107	6.63235	1.40857
Si	Si228	6.25891	9.78486	-0.38016
H	H229	6.7821	11.17424	-0.65148
H	H230	11.16051	6.76515	-0.67317
Si	Si231	9.49357	1.56319	-1.53418
Si	Si232	10.35511	0.60558	0.53611
Si	Si233	11.96808	1.82136	1.81233
H	H234	12.75193	0.81115	2.59712
H	H235	12.90157	2.54599	0.89459
H	H236	11.53578	-0.1274	-0.12707
Si	Si237	9.77342	3.60533	-3.21021
H	H238	11.06522	3.86145	-3.94414
Si	Si239	7.74609	3.68942	-4.52369
H	H240	6.74379	4.60481	-3.98543
H	H241	8.01417	3.93816	-5.99951
Si	Si242	5.30681	5.30004	0.0429
Si	Si243	8.35832	5.34638	-2.1762
Si	Si244	4.08475	4.0796	-3.89063
Si	Si245	6.84981	1.44683	-4.13434
Si	Si246	2.72969	-0.01569	-2.71393
Si	Si247	1.40154	-1.36767	-1.39167
Si	Si248	2.73169	-2.68371	-0.03315
Si	Si249	5.22773	-2.42468	-2.49312
Si	Si250	8.06015	0.01738	-2.66399
Si	Si251	8.59078	-3.77939	-2.05596
H	H252	10.07643	-4.17802	-2.11585
Si	Si253	4.00859	-4.0587	-1.37118
Si	Si254	7.13474	-5.69181	-2.29531
H	H255	7.70081	-7.00475	-2.73955
Si	Si256	2.49757	-8.19928	2.38629
H	H257	3.32298	-9.28707	3.15086

H	H258	-1.69674	-7.56144	2.00126
Si	Si259	0.85903	-8.90681	0.77753
H	H260	0.44212	-10.26951	0.35529
Si	Si261	1.4143	-3.92792	1.36729
Si	Si262	1.82293	-7.03502	-0.38206
H	H263	2.04694	-7.49471	-1.78043
Si	Si264	-2.72032	-5.67564	-2.62147
Si	Si265	0.00572	-2.7002	-2.70888
Si	Si266	-4.14308	-1.35174	-1.34276
Si	Si267	-4.53908	-4.58405	-1.18023
H	H268	-5.63987	-5.68556	-1.33386
Si	Si269	-2.67966	-0.06302	2.7227
Si	Si270	-1.36179	1.34357	4.0436
Si	Si271	-1.34465	-4.09314	3.91169
Si	Si272	-5.17999	-5.13541	4.34314
H	H273	-6.20067	-6.204	4.44397
Si	Si274	-5.38673	-0.2069	5.64003
Si	Si275	-2.69664	2.6555	5.44672
H	H276	-4.15095	4.56886	6.80876
Si	Si277	-3.28694	6.93019	6.92146
Si	Si278	-1.23179	3.96369	6.71175
Si	Si279	0.09352	2.66905	8.12683
Si	Si280	1.38492	1.37441	6.72906
Si	Si281	2.29177	8.55532	8.55561
H	H282	2.28054	9.65799	9.66103
Si	Si283	-0.38132	9.78751	6.25425
H	H284	-0.62227	11.18063	6.76685
Si	Si285	2.72955	8.00463	5.3778
Si	Si286	0.01812	5.29086	5.30105
Si	Si287	2.69215	2.68723	5.34735
Si	Si288	6.64045	6.64508	6.64746
Si	Si289	4.02029	6.69385	4.0241
Si	Si290	7.99953	5.38701	2.74832
Si	Si291	5.34065	2.71174	2.71141
Si	Si292	10.5476	3.14301	3.14648
Si	Si293	9.46963	-1.44373	1.49302
Si	Si294	6.73525	1.41934	1.41862
Si	Si295	5.47506	-2.72177	2.67775

Si	Si296	9.80824	-3.07297	3.4448
H	H297	11.19019	-3.5858	3.7249
Si	Si298	6.63151	1.41268	6.63362
Si	Si299	9.70777	-0.44377	6.24057
H	H300	11.09773	-0.70041	6.76193
Si	Si301	9.48916	3.88914	6.84584
Si	Si302	5.37916	2.74283	8.0123
Si	Si303	7.84114	5.14945	7.84839
H	H304	8.70894	6.10162	8.71824
Si	Si305	3.85706	6.83821	9.48149
Si	Si306	4.29144	1.28137	9.46885
Si	Si307	1.22982	4.30291	9.41609
H	H308	-0.09658	-0.24275	11.51126
Si	Si309	-1.44211	1.50821	9.51274
Si	Si310	3.68895	-3.1379	9.89629
H	H311	3.93043	-3.80133	11.20671
Si	Si312	2.70597	0.11999	8.14509
Si	Si313	-1.87271	-3.73536	9.11254
H	H314	-1.96191	-4.39565	10.43832
Si	Si315	-1.20777	-1.25506	6.73194
Si	Si316	3.46135	-4.34034	7.87873
H	H317	3.36562	-5.7884	8.4675
Si	Si318	-0.18479	-5.34817	5.55507
Si	Si319	3.98936	-1.20484	6.72313
Si	Si320	4.14227	-3.99702	4.18086
Si	Si321	0.06022	0.06045	5.34748
Si	Si322	-0.00541	-2.68162	2.6605
Si	Si323	3.96762	1.34508	3.96878
Si	Si324	4.0619	-1.38683	1.38309
Si	Si325	-0.02636	2.62954	2.63993
Si	Si326	2.64176	2.66831	-0.04407
Si	Si327	-0.01436	-0.07178	-0.07156

Geometry of $Si_{240}O_{88}$

Si	Si1	1.31454	1.28132	1.2815
Si	Si2	-0.01436	-0.07178	-0.07156
Si	Si3	2.65268	-0.05249	2.65332

Si	Si4	2.64176	2.66831	-0.04407
Si	Si5	-0.02636	2.62954	2.63993
Si	Si6	1.32816	-1.35163	4.03554
Si	Si7	1.3315	4.06671	-1.35619
Si	Si8	1.34414	3.96477	3.97087
Si	Si9	4.03725	1.35734	-1.35388
Si	Si10	3.96762	1.34508	3.96878
Si	Si11	4.0619	-1.38683	1.38309
Si	Si12	3.96913	3.97339	1.35177
Si	Si13	-1.36179	1.34357	4.0436
Si	Si14	-1.34355	4.03341	1.33683
Si	Si15	1.40154	-1.36767	-1.39167
Si	Si16	-1.3457	1.33899	-1.35137
Si	Si17	-1.34972	-1.35882	1.32805
Si	Si18	5.30253	0.12693	0.13853
Si	Si19	0.06022	0.06045	5.34748
Si	Si20	0.06535	5.36077	0.06972
Si	Si21	2.69215	2.68723	5.34735
Si	Si22	2.69272	5.34864	2.69508
Si	Si23	5.34065	2.71174	2.71141
Si	Si24	2.72969	-0.01569	-2.71393
Si	Si25	2.73169	-2.68371	-0.03315
Si	Si26	-2.67966	-0.06302	2.7227
Si	Si27	-2.67954	2.72655	-0.06175
Si	Si28	-0.00541	-2.68162	2.6605
Si	Si29	-0.01281	2.68475	-2.66997
Si	Si30	1.38302	1.38093	-3.92626
Si	Si31	1.38492	1.37441	6.72906
Si	Si32	1.4143	-3.92792	1.36729
Si	Si33	1.39337	6.73504	1.38718
Si	Si34	6.73525	1.41934	1.41862
Si	Si35	-3.88691	1.37402	1.36986
Si	Si36	0.01812	5.29086	5.30105
Si	Si37	5.31658	0.03959	5.29576
Si	Si38	5.30681	5.30004	0.0429
Si	Si39	2.67784	-2.64949	5.40187
Si	Si40	2.65904	5.46763	-2.64103
Si	Si41	5.47506	-2.72177	2.67775

Si	Si42	5.46577	2.63223	-2.66434
Si	Si43	-2.69664	2.6555	5.44672
Si	Si44	-2.67198	5.40096	2.66438
Si	Si45	-2.67521	-0.04035	-2.68374
Si	Si46	-2.68358	-2.69309	-0.03752
Si	Si47	0.00572	-2.7002	-2.70888
Si	Si48	4.00834	-1.30457	-4.13293
Si	Si49	3.98936	-1.20484	6.72313
Si	Si50	4.00859	-4.0587	-1.37118
Si	Si51	4.14227	-3.99702	4.18086
Si	Si52	4.08475	4.0796	-3.89063
Si	Si53	4.01696	4.02388	6.69475
Si	Si54	3.98307	6.73305	-1.19513
Si	Si55	4.02029	6.69385	4.0241
Si	Si56	6.66068	-1.14667	-1.1894
Si	Si57	6.71465	-1.23579	3.97324
Si	Si58	6.72301	3.96782	-1.21645
Si	Si59	6.68791	4.03838	4.03851
Si	Si60	-4.14308	-1.35174	-1.34276
Si	Si61	-4.0708	-1.41104	4.04453
Si	Si62	-4.07875	4.01646	-1.42632
Si	Si63	-3.93895	4.14028	4.16496
Si	Si64	-1.32553	-1.35131	-4.15838
Si	Si65	-1.20777	-1.25506	6.73194
Si	Si66	-1.31327	-4.16845	-1.3376
Si	Si67	-1.34465	-4.09314	3.91169
Si	Si68	-1.3536	3.91527	-4.08357
Si	Si69	-1.23179	3.96369	6.71175
Si	Si70	-1.22759	6.73699	-1.24034
Si	Si71	-1.2289	6.70539	3.97194
Si	Si72	5.29717	5.31566	5.31411
Si	Si73	-5.37636	0.11995	0.12019
Si	Si74	0.14239	-5.38904	0.09998
Si	Si75	0.09642	0.11781	-5.39892
Si	Si76	2.72537	2.7246	-5.22133
Si	Si77	2.73612	-5.23159	2.74783
Si	Si78	-5.17842	2.75778	2.7599
Si	Si79	2.69417	8.15805	0.12556

Si	Si80	8.15351	2.66749	0.09641
Si	Si81	0.09354	8.11528	2.68596
Si	Si82	2.70597	0.11999	8.14509
Si	Si83	8.12156	0.09649	2.69184
Si	Si84	0.09352	2.66905	8.12683
Si	Si85	5.22773	-2.42468	-2.49312
Si	Si86	-2.51786	-2.64617	5.35289
Si	Si87	-2.52107	5.34024	-2.63523
Si	Si88	1.24926	-4.13051	-4.11554
Si	Si89	1.38775	-4.04413	6.7959
Si	Si90	1.47566	6.89093	-4.07947
Si	Si91	1.38835	6.62805	6.62096
Si	Si92	6.84981	1.44683	-4.13434
Si	Si93	6.63151	1.41268	6.63362
Si	Si94	6.8772	-4.08992	1.40321
Si	Si95	6.63107	6.63235	1.40857
Si	Si96	-4.08111	1.16368	-4.09391
Si	Si97	-4.12466	1.45615	6.86355
Si	Si98	-4.11756	-4.08415	1.16876
Si	Si99	-4.12504	6.80222	1.47403
Si	Si100	-0.18479	-5.34817	5.55507
Si	Si101	-0.1802	5.58784	-5.27841
Si	Si102	-5.38673	-0.2069	5.64003
Si	Si103	5.64316	-0.18359	-5.43956
Si	Si104	5.61889	-5.36764	-0.21949
Si	Si105	-5.38604	5.62576	-0.23019
Si	Si106	3.09019	-3.20691	-5.2752
Si	Si107	3.11197	-5.27864	-3.23161
Si	Si108	-5.33957	-3.16818	2.96996
Si	Si109	-5.29311	3.01096	-3.27017
Si	Si110	-3.19569	2.97463	-5.32786
Si	Si111	-3.20533	-5.29114	2.97102
Si	Si112	2.72327	5.38008	7.99809
Si	Si113	2.72955	8.00463	5.3778
Si	Si114	5.37916	2.74283	8.0123
Si	Si115	5.38116	8.00482	2.74319
Si	Si116	8.00232	2.75133	5.38986
Si	Si117	7.99953	5.38701	2.74832

Si	Si118	0.06036	8.15912	-2.61721
Si	Si119	8.06015	0.01738	-2.66399
Si	Si120	8.07101	-2.61148	-0.02586
Si	Si121	-2.62807	0.06833	8.07964
Si	Si122	-2.66972	8.0706	0.08676
Si	Si123	0.0576	-2.63423	8.16175
Si	Si124	1.05539	3.75228	-6.63509
Si	Si125	1.22982	4.30291	9.41609
Si	Si126	1.09739	-6.66399	3.73536
Si	Si127	1.23747	9.4306	4.296
Si	Si128	3.77379	1.04889	-6.60361
Si	Si129	4.29144	1.28137	9.46885
Si	Si130	3.7642	-6.57655	1.03651
Si	Si131	4.30478	9.45585	1.26823
Si	Si132	9.42843	1.25116	4.30741
Si	Si133	9.43449	4.30191	1.26151
Si	Si134	-6.54898	1.04373	3.75622
Si	Si135	-6.54438	3.7577	1.04886
Si	Si136	1.67084	-1.53193	9.49517
Si	Si137	1.63782	9.50955	-1.5025
Si	Si138	9.49357	1.56319	-1.53418
Si	Si139	9.46963	-1.44373	1.49302
Si	Si140	-1.44211	1.50821	9.51274
Si	Si141	-1.4671	9.48191	1.54832
Si	Si142	5.07704	-4.94285	6.20367
Si	Si143	5.60579	5.62584	-4.87837
Si	Si144	-4.9031	5.93472	5.32815
Si	Si145	-5.66123	-2.71701	-2.65033
Si	Si146	-2.68856	-2.74772	-5.60439
Si	Si147	-2.72032	-5.67564	-2.62147
Si	Si148	5.37764	-2.07742	8.40849
Si	Si149	5.35968	8.3564	-2.17295
Si	Si150	7.9302	-2.86692	5.1467
Si	Si151	8.33837	5.37707	-2.28461
Si	Si152	-2.13126	5.17775	8.56208
Si	Si153	-2.94858	7.70463	5.35053
Si	Si154	6.82341	-3.74874	-3.71077
Si	Si155	6.71677	-3.43859	7.064

Si	Si156	7.29565	7.42785	-3.34096
Si	Si157	6.6588	6.76449	6.55393
Si	Si158	-4.83648	-2.8341	-4.75815
Si	Si159	-3.66843	-4.04759	6.92716
Si	Si160	-3.65381	6.90843	-4.05752
Si	Si161	-3.85373	6.58803	7.65734
Si	Si162	11.01585	0.17286	0.86156
Si	Si163	0.96028	0.03887	11.06597
Si	Si164	0.46772	11.64836	0.5535
Si	Si165	-1.6751	-4.58553	-4.46866
Si	Si166	-4.27756	-0.47262	-6.1167
Si	Si167	3.2377	10.54837	3.24253
Si	Si168	3.15998	3.21039	10.52419
Si	Si169	-5.38502	-4.58506	-1.1721
Si	Si170	10.51752	3.17876	3.19869
Si	Si171	3.30678	-4.86575	7.68047
Si	Si172	2.94536	8.72296	-4.78968
Si	Si173	-4.84188	3.53774	7.68792
Si	Si174	7.82102	3.34149	-5.0596
Si	Si175	8.44165	-5.08078	3.05897
Si	Si176	-4.18085	8.45577	3.33278
Si	Si177	-0.70925	-6.63146	2.01723
Si	Si178	2.01794	-0.70705	-6.6168
Si	Si179	2.06208	-6.5848	-0.73964
Si	Si180	-6.56407	-0.77227	2.04071
Si	Si181	-6.59283	2.02124	-0.74524
Si	Si182	-0.77774	2.04953	-6.60138
Si	Si183	0.04081	8.05817	7.97447
Si	Si184	8.32138	0.09483	7.701
Si	Si185	8.1487	8.08555	0.35331
Si	Si186	3.65816	-2.87612	10.02216
Si	Si187	3.90784	6.86409	9.40926
Si	Si188	3.57957	9.95772	-2.83771
Si	Si189	4.09658	9.30014	6.81272
Si	Si190	6.26377	-0.19674	9.51885
Si	Si191	6.81284	4.02951	9.38472
Si	Si192	6.36737	9.66709	-0.16211
Si	Si193	6.89655	9.36893	3.91601

Si	Si194	9.23815	-1.80457	-3.75017
Si	Si195	10.52712	-0.33025	5.78774
Si	Si196	8.73316	-3.67829	-2.12959
Si	Si197	9.73176	-2.50876	3.6324
Si	Si198	9.84247	3.58794	-2.94877
Si	Si199	9.30301	4.12865	6.80699
Si	Si200	9.66633	6.13583	-0.43799
Si	Si201	9.44862	6.88426	3.8567
Si	Si202	-3.71201	-1.84728	9.15749
Si	Si203	-2.84121	3.45445	10.12815
Si	Si204	-3.71507	9.16427	-1.83023
Si	Si205	-2.7966	10.8174	4.07904
Si	Si206	-2.04936	-3.76647	8.79788
Si	Si207	-0.363	6.14668	9.72066
Si	Si208	-2.06114	8.80383	-3.73841
Si	Si209	-0.89249	9.15293	5.77845
Si	Si210	5.37714	-5.24406	-5.30518
Si	Si211	-5.356	-5.3292	5.0967
Si	Si212	-5.25438	5.1758	-5.40493
Si	Si213	-6.16893	-1.81898	7.13309
Si	Si214	7.05553	-2.06636	-5.90063
Si	Si215	6.31801	-5.87551	-2.58541
Si	Si216	-6.16191	7.12324	-1.83235
Si	Si217	-2.18672	-5.92867	6.78678
Si	Si218	-2.16514	6.77541	-5.93052
Si	Si219	5.62721	8.02609	8.23258
Si	Si220	8.01442	5.7058	8.13661
Si	Si221	8.27751	8.14568	5.51441
Si	Si222	1.48384	12.94204	2.17027
Si	Si223	2.13484	1.26234	12.69059
Si	Si224	0.71965	0.8077	-8.9604
Si	Si225	0.8063	-8.96805	0.71427
Si	Si226	12.50281	1.07165	2.42457
Si	Si227	-8.92673	0.73709	0.81529
Si	Si228	5.05363	10.69726	4.95104
Si	Si229	4.88403	4.98497	10.7686
Si	Si230	2.58539	2.58334	-8.30689
Si	Si231	2.64574	-8.32395	2.51872

Si	Si232	10.75534	5.01619	4.86339
Si	Si233	-8.25812	2.60995	2.60947
Si	Si234	2.85807	9.17734	8.9957
Si	Si235	9.07712	2.94612	8.98734
Si	Si236	8.98396	8.96059	2.42358
Si	Si237	-5.01499	-5.54901	-4.29805
Si	Si238	7.48402	-5.73156	5.95673
Si	Si239	-6.09622	7.86105	7.1236
Si	Si240	5.89768	8.13337	-5.96883
O	O241	4.28176	-4.13697	-5.83466
O	O242	4.64446	-5.72544	-3.81182
O	O243	-5.91907	-4.06804	4.18512
O	O244	-5.83467	4.22677	-4.17606
O	O245	-3.94291	4.29329	-5.92494
O	O246	-4.03864	-5.846	4.24227
O	O247	-0.84347	10.97961	1.18668
O	O248	4.16136	5.12103	-5.22293
O	O249	10.67865	0.96406	-0.46878
O	O250	-0.3464	0.74538	10.5396
O	O251	1.12617	10.86656	-0.63012
O	O252	-0.08158	-4.87591	-4.81335
O	O253	-5.42919	-1.50946	-5.55693
O	O254	-6.24559	-5.79205	-1.0188
O	O255	3.44358	-4.29696	9.15605
O	O256	4.33021	8.16001	-5.41296
O	O257	5.7445	6.70295	-3.552
O	O258	-4.19302	3.29058	9.08388
O	O259	-4.60387	5.04972	6.96703
O	O260	6.70367	4.42901	-4.59578
O	O261	8.96532	3.52137	-6.00667
O	O262	8.63348	-6.54004	2.81467
O	O263	7.63307	-4.55101	4.59176
O	O264	-5.47431	9.2056	3.42951
O	O265	-0.42447	-8.13216	1.38211
O	O266	1.41382	-0.41196	-8.12202
O	O267	1.46726	-8.10595	-0.51319
O	O268	-8.08952	-0.51015	1.46015
O	O269	-8.09768	1.41978	-0.41862

O	O270	-0.53507	1.436	-8.12342
O	O271	4.02683	-2.80391	11.47868
O	O272	3.95612	11.41389	-3.00181
O	O273	7.17029	-0.12916	10.71393
O	O274	6.60685	11.02528	-0.76595
O	O275	8.48321	-1.71888	-5.20185
O	O276	10.60253	-1.54466	4.65979
O	O277	9.80858	-4.73149	-2.13712
O	O278	9.82469	-4.06329	3.1873
O	O279	11.15085	3.69149	-3.67881
O	O280	11.06802	6.67047	-0.59987
O	O281	-5.14671	-1.83479	8.37429
O	O282	-3.02615	3.60048	11.61168
O	O283	-5.13636	8.36448	-1.86886
O	O284	-3.70832	11.97391	4.07147
O	O285	-2.65263	9.69291	2.79338
O	O286	-2.02158	-4.66403	10.00638
O	O287	-0.44304	6.86785	11.04085
O	O288	-2.01503	10.01044	-4.64537
O	O289	-1.665	10.49009	5.18396
O	O290	6.26274	-6.09949	-6.1304
O	O291	-6.12984	-6.10549	6.09646
O	O292	-6.0374	6.13014	-6.22845
O	O293	-7.42371	-2.59111	6.94376
O	O294	6.7488	-2.87715	-7.12308
O	O295	6.84932	-7.25921	-2.80347
O	O296	-7.39007	6.90974	-2.63893
O	O297	-2.33422	-7.32972	7.2894
O	O298	-2.29625	7.28267	-7.3329
O	O299	6.4714	8.96665	9.06116
O	O300	8.91875	6.54868	9.01349
O	O301	9.05235	9.05259	6.4384
O	O302	0.85125	14.22098	2.5572
O	O303	2.64596	12.03582	2.71434
O	O304	2.33146	0.73353	14.06245
O	O305	2.67163	2.59756	11.99293
O	O306	0.97243	1.06914	-10.40928
O	O307	1.07258	-10.41816	0.94631

O	O308	12.03624	2.54601	2.80341
O	O309	13.46772	0.09551	2.99308
O	O310	-10.37396	0.98788	1.07805
O	O311	5.32091	12.12429	5.3618
O	O312	5.29322	5.34321	12.17669
O	O313	3.49463	3.46851	-9.10427
O	O314	3.51216	-9.14152	3.42459
O	O315	12.14564	5.29422	5.38741
O	O316	-8.94359	3.53174	3.57255
O	O317	1.41138	8.86441	8.39352
O	O318	8.77913	1.46476	8.44841
O	O319	9.9726	10.07382	2.62603
O	O320	-4.97907	-6.98741	-4.65109
O	O321	-5.50196	-4.30462	-5.19807
O	O322	-4.26903	-4.87188	-2.90011
O	O323	7.84055	-7.16217	5.79561
O	O324	7.69577	-4.7863	7.33121
O	O325	-7.07326	6.93615	7.79139
O	O326	-5.42067	9.00966	6.45355
O	O327	6.79935	9.29209	-6.2143
O	O328	6.26526	6.55367	-6.09525

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