

Supplementary materials

Article

Multiple Pathways for Dissociative Adsorption of SiCl_4 on the $\text{Si}(100)\text{-c}(4\times 2)$ surface

Jianxun Zhang^{1,2}, Quan Zhu^{1,3,4,*} and Jun Li^{2,*}

¹ State Key Laboratory of Chemistry and Utilization of Carbon-Based Energy Resources, School of Chemical Engineering and Technology, Xinjiang University, Urumqi 830017, China

² Department of Chemistry and Chemical Engineering & Chongqing Key Laboratory of Theoretical and Computational Chemistry, Chongqing University, Chongqing 401331, China

³ Department of Chemical Engineering, Sichuan University, Chengdu 610065, China

⁴ Engineering Research Center of Combustion and Cooling for Aerospace Power, Sichuan University, Chengdu 610000, China

* Correspondence: qzhu@scu.edu.cn (Q.Z.); jli15@cqu.edu.cn (J.L.)

Abstract: The adsorption of silicon tetrachloride (STC, SiCl_4) on the silicon surface is a crucial process in polysilicon manufacture. However, the underlying mechanism for the adsorption remains highly uncertain. Here, new dissociative adsorption (DA) reaction pathways involving a flip of a silicon dimer in the first layer and considering physisorption are identified. Different DA patterns, inter-row (IR), inter-dimer (ID), and on-dimer (OD), are confirmed by the density functional theory (DFT) calculations at the PBE-D3(BJ)/TZVP-MOLOPT-GTH level. The stable structures for all minima are searched by global optimization through the artificial bee colony (ABC) algorithm. Findings reveal that the parent molecules dissociate first by breaking one Si-Cl bond, following which the resulting SiCl_3 and Cl fragments are attached to adjacent Si-atom sites. Moreover, dimer flipping significantly reduces the energy barrier for chemisorption, mainly due to the change in electronic structure that enhances the interaction of the site with the SiCl_3 radical. Physisorption may also be accompanied by dimer flipping to form a stable adsorption structure.

Keywords: dissociative adsorption; silicon tetrachloride; density functional theory; dimer flipping

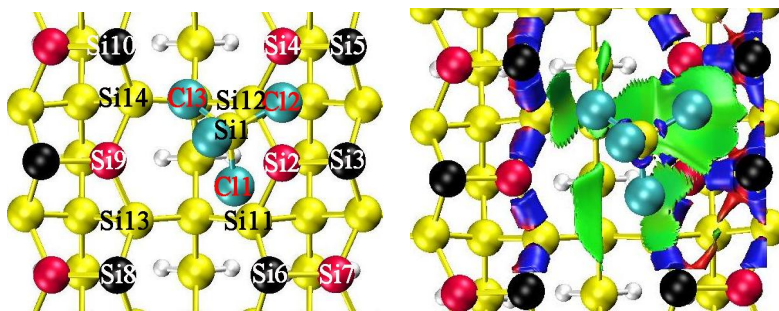


Figure S1. Isosurface map of IRI of VDW2. Isovalue of IRI is chosen to be 1.0.

Table S1. Percentage contribution of several atoms pairs of VDW2 to the physisorption, obtained by IGMH analysis.

Pairs	Percentage
Cl1-Si2	4.8%
Cl3-Si10	4.5%
Cl1-Si6	2.7%
Cl3-Si14	2.4%
Cl1-Si11	2.1%
Cl2-Si5	2.0%
Cl2-Si4	2.0%
Cl2-Si3	2.0%
Cl3-Si12	2.0%

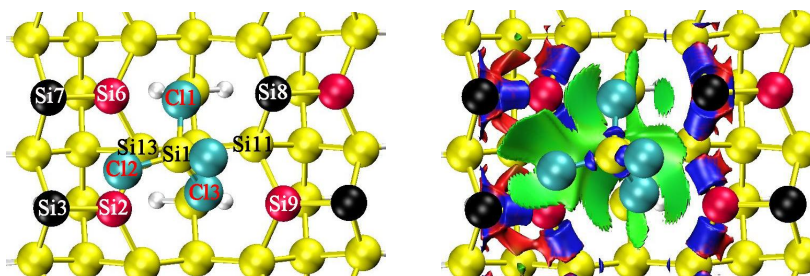
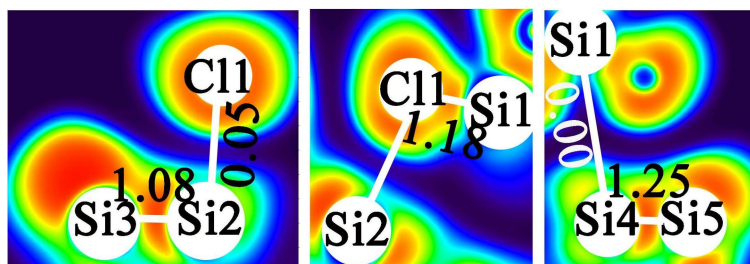


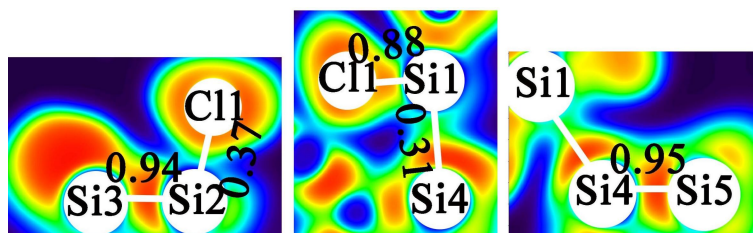
Figure S2. Isosurface map of IRI of VDW3. Isovalue of IRI is chosen to be 1.0.

Table S2. Percentage contribution of several atoms pairs of VDW3 to the physisorption, obtained by IGMH analysis.

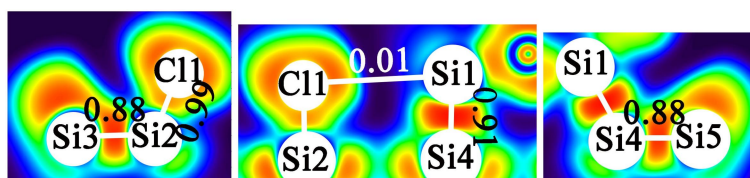
Pairs	Percentage
Cl1-Si6	3.8%
Cl1-Si8	2.9%
Cl3-Si9	2.7%
Cl3-Si13	2.7%
Cl3-Si2	2.6%
Cl3-Si11	2.4%
Cl2-Si3	2.3%
Cl2-Si2	2.0%



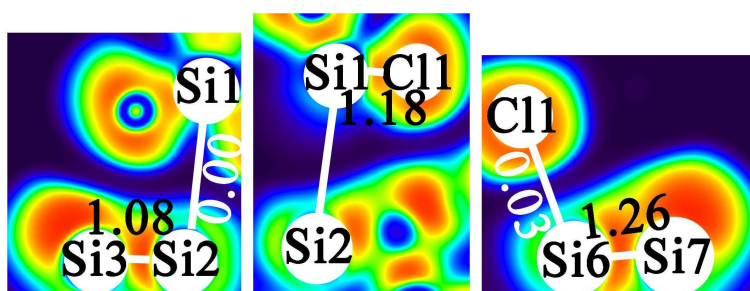
(a) VDW2



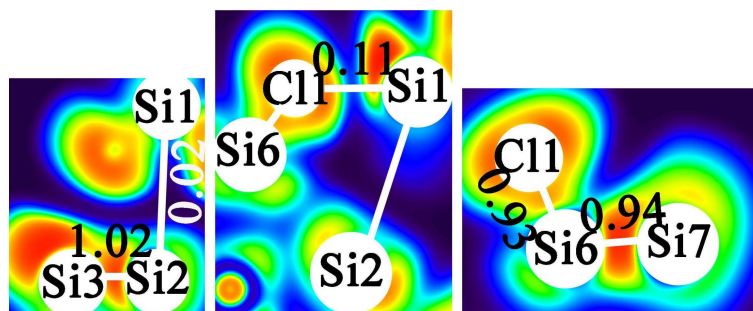
(b) TS4



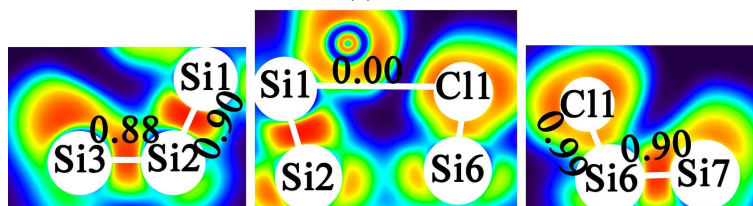
(c) P2



(d) VDW3



(e) TS5



(f) P3

Figure S3. Mayer bond order (MBO) and two-dimensional electron localization function (ELF) color-filled maps for the minima and transition states along the pathway of STC DA at ID site.

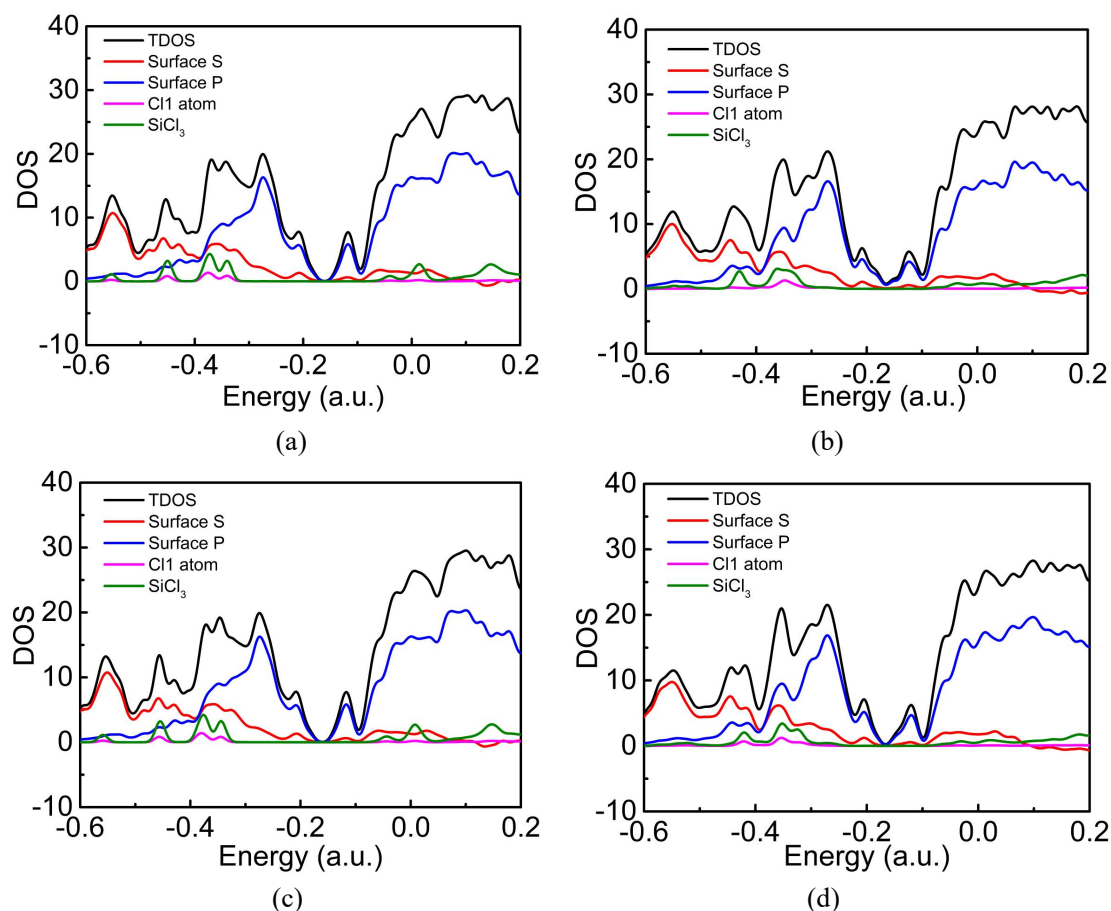


Figure S4. Total and partial densities of states (DOS) for Si(100)-c(4×2) with STC absorption. (a)VDW2; (b) P2; (c) VDW3; (d) P3.

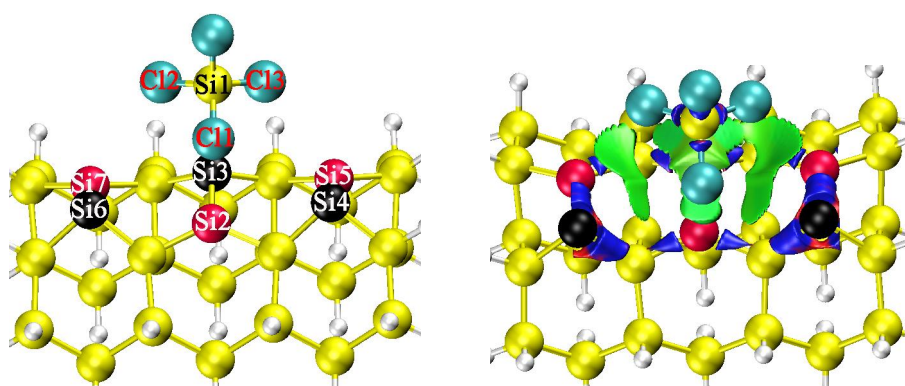


Figure S5. Isosurface map of IRI of VDW4. Isovalue of IRI is chosen to be 1.0.

Table S3. Percentage contribution of several atoms pairs of VDW4 to the physisorption, obtained by IGMH analysis.

Pairs	Percentage
-------	------------

Cl1-Si2	4.5%
Cl2-Si3	3.7%
Cl2-Si3	3.7%
Cl1-Si3	2.5%
Si1-Si3	2.4%

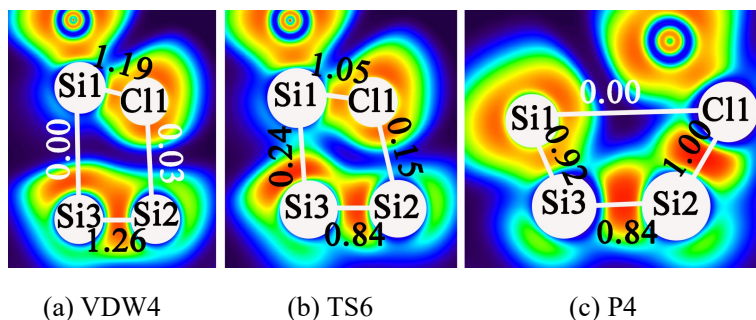


Figure S6. Mayer bond order (MBO) and two-dimensional electron localization function (ELF) color-filled maps for the minima and transition states along the pathway of STC DA at OD site.

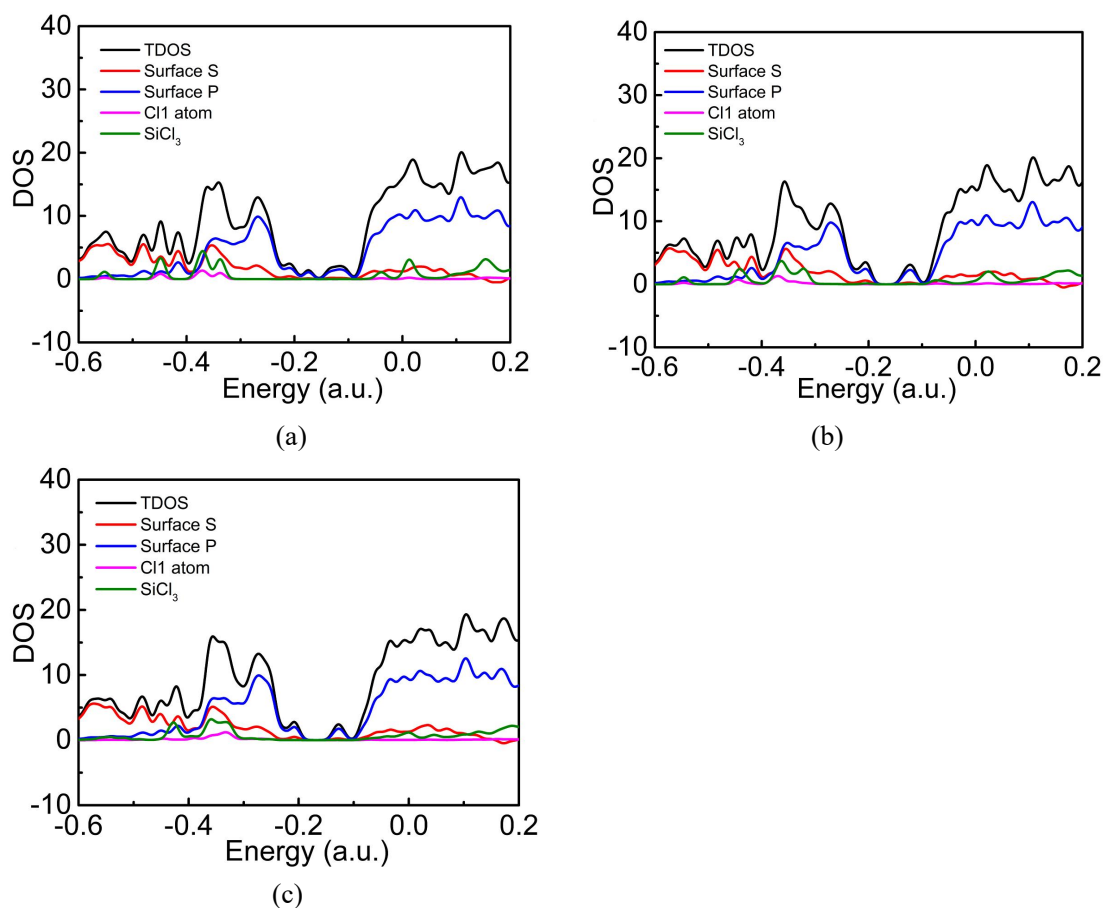


Figure S7. Total and partial densities of states (DOS) for Si(100)-c(4x2) with STC absorption. (a)VDW4; (b) TS6; (c) P4.

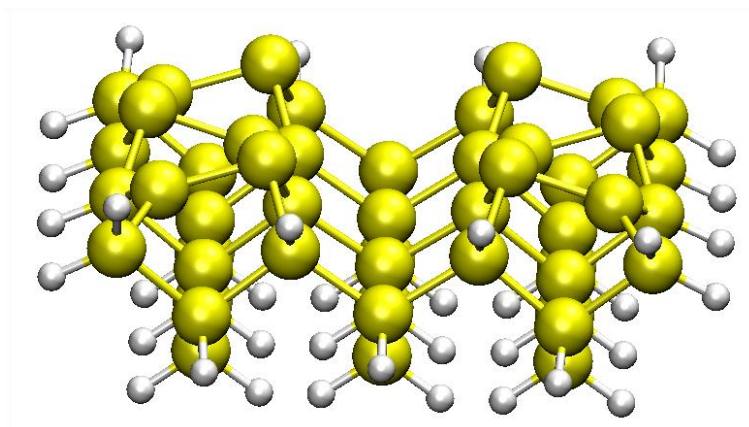


Figure S8. The cluster model used for the single point calculations in ORCA.

The structural coordinates (Å) used in DFT calculations.

1. Si(100) surface.

Si	3.8845136532	-0.1092732147	5.6590287034
Si	1.8870000000	1.9340000000	2.8900000000
Si	1.8869298788	0.0040376766	4.3348357717
Si	3.8070000000	1.9340000000	1.5330000000
Si	4.7707053037	1.9346643911	6.3968206839
Si	7.5684423512	0.1387424550	5.6591239129
Si	5.7260000000	1.9340000000	2.8900000000
Si	5.7263287865	0.0142522235	4.1810195792
Si	7.6460000000	1.9340000000	1.5330000000
Si	7.0113745604	1.9344596829	7.1377719705
Si	3.8843172059	3.9783997496	5.6594000315
Si	1.8870000000	5.7730000000	2.8900000000
Si	1.8868972039	3.8639869795	4.3350229713
Si	3.8070000000	5.7730000000	1.5330000000
Si	4.4418279173	5.7743259097	7.1374947041
Si	7.5682663503	3.7302927217	5.6590888059
Si	5.7260000000	5.7730000000	2.8900000000
Si	5.7262377750	3.8535532921	4.1812154509
Si	7.6460000000	5.7730000000	1.5330000000
Si	6.6820863194	5.7738444823	6.3964203266
Si	11.5636508118	0.1385348974	5.6590472101
Si	9.5660000000	1.9340000000	2.8900000000
Si	9.5659802868	0.0247314020	4.3348430830
Si	11.4860000000	1.9340000000	1.5330000000
Si	12.1207444570	1.9340780770	7.1378268579
Si	15.2476129542	-0.1092289321	5.6588541319
Si	13.4060000000	1.9340000000	2.8900000000
Si	13.4057993629	0.0143816866	4.1809280787

Si	15.3250000000	1.9340000000	1.5330000000
Si	14.3614336473	1.9346367263	6.3967775963
Si	11.5638191750	3.7298493656	5.6591888485
Si	9.5660000000	5.7730000000	2.8900000000
Si	9.5660698086	3.8432401966	4.3350163332
Si	11.4860000000	5.7730000000	1.5330000000
Si	12.4499510764	5.7735519598	6.3964014909
Si	15.2477268286	3.9782923708	5.6592945383
Si	13.4060000000	5.7730000000	2.8900000000
Si	13.4057798175	3.8535577439	4.1813121993
Si	15.3250000000	5.7730000000	1.5330000000
Si	14.6903791818	5.7742639321	7.1375299133
Si	3.8846128244	7.5698451634	5.6587895446
Si	1.8870000000	9.6130000000	2.8900000000
Si	1.8869519206	7.6827622007	4.3345562782
Si	3.8070000000	9.6130000000	1.5330000000
Si	4.7710834716	9.6138148534	6.3964089070
Si	7.5684308277	7.8180021484	5.6587188432
Si	5.7260000000	9.6130000000	2.8900000000
Si	5.7263807358	7.6930759892	4.1808497506
Si	7.6460000000	9.6130000000	1.5330000000
Si	7.0110487312	9.6136822773	7.1369808001
Si	3.8843847889	11.6577501256	5.6592793038
Si	1.8870000000	13.4530000000	2.8900000000
Si	1.8869639291	11.5434426682	4.3347278246
Si	3.8070000000	13.4530000000	1.5330000000
Si	4.4417698395	13.4534076977	7.1376851779
Si	7.5682140536	11.4093586293	5.6587296863
Si	5.7260000000	13.4530000000	2.8900000000
Si	5.7263200519	11.5328527383	4.1809493968
Si	7.6460000000	13.4530000000	1.5330000000
Si	6.6819911989	13.4535578153	6.3963465455
Si	11.5636678553	7.8175017799	5.6585706320
Si	9.5660000000	9.6130000000	2.8900000000
Si	9.5659681248	7.7035106916	4.3346652495
Si	11.4860000000	9.6130000000	1.5330000000
Si	12.1209591756	9.6132169454	7.1371297564
Si	15.2475853647	7.5696623460	5.6586936702
Si	13.4060000000	9.6130000000	2.8900000000
Si	13.4057720149	7.6930450357	4.1807149819
Si	15.3250000000	9.6130000000	1.5330000000
Si	14.3612592383	9.6136880950	6.3962509089
Si	11.5637689423	11.4089998925	5.6587438219
Si	9.5660000000	13.4530000000	2.8900000000

Si	9.5659628715	11.5226874056	4.3347135616
Si	11.4860000000	13.4530000000	1.5330000000
Si	12.4499637895	13.4532610302	6.3962970993
Si	15.2477975417	11.6577566220	5.6591253399
Si	13.4060000000	13.4530000000	2.8900000000
Si	13.4057429852	11.5329732705	4.1809620837
Si	15.3250000000	13.4530000000	1.5330000000
Si	14.6904683793	13.4534208066	7.1376943166
H	3.8070000000	3.1910000000	0.6430000000
H	3.8070000000	0.6760000000	0.6430000000
H	7.6460000000	3.1910000000	0.6430000000
H	7.6460000000	0.6760000000	0.6430000000
H	3.8070000000	7.0310000000	0.6430000000
H	3.8070000000	4.5160000000	0.6430000000
H	7.6460000000	7.0310000000	0.6430000000
H	7.6460000000	4.5160000000	0.6430000000
H	11.4860000000	3.1910000000	0.6430000000
H	11.4860000000	0.6760000000	0.6430000000
H	15.3250000000	3.1910000000	0.6430000000
H	15.3250000000	0.6760000000	0.6430000000
H	11.4860000000	7.0310000000	0.6430000000
H	11.4860000000	4.5160000000	0.6430000000
H	15.3250000000	7.0310000000	0.6430000000
H	15.3250000000	4.5160000000	0.6430000000
H	3.8070000000	10.8700000000	0.6430000000
H	3.8070000000	8.3560000000	0.6430000000
H	7.6460000000	10.8700000000	0.6430000000
H	7.6460000000	8.3560000000	0.6430000000
H	3.8070000000	14.7100000000	0.6430000000
H	3.8070000000	12.1950000000	0.6430000000
H	7.6460000000	14.7100000000	0.6430000000
H	7.6460000000	12.1950000000	0.6430000000
H	11.4860000000	10.8700000000	0.6430000000
H	11.4860000000	8.3560000000	0.6430000000
H	15.3250000000	10.8700000000	0.6430000000
H	15.3250000000	8.3560000000	0.6430000000
H	11.4860000000	14.7100000000	0.6430000000
H	11.4860000000	12.1950000000	0.6430000000
H	15.3250000000	14.7100000000	0.6430000000
H	15.3250000000	12.1950000000	0.6430000000

2. STC

Si	4.8590139051	6.2136802424	13.4868398940
Cl	6.2964832500	7.6908723800	13.4500224000

Cl	4.3539442361	5.8917855049	15.4383678410
Cl	3.1179087800	6.6031905000	12.4531672500
Cl	5.6847667014	4.5262003438	12.6883482443

3. VDW1

Si	2.9535699855	0.2714616615	11.3289670858
Si	0.9597000000	2.3132000000	8.5584014400
Si	0.9580282337	0.3839932284	10.0030570330
Si	2.8797000000	2.3132000000	7.2014014400
Si	3.8354737156	2.3168630635	12.0609656787
Si	6.6441047319	0.5107624713	11.3256017370
Si	4.7997000000	2.3132000000	8.5584014400
Si	4.7979701504	0.3932824214	9.8504114164
Si	6.7187000000	2.3132000000	7.2014014400
Si	6.0778215238	2.3105188890	12.7899838015
Si	2.9547414830	4.3625638900	11.3315555234
Si	0.9597000000	6.1532000000	8.5584014400
Si	0.9601751746	4.2418444811	10.0025178939
Si	2.8797000000	6.1532000000	7.2014014400
Si	3.5102873635	6.1540162140	12.8216917347
Si	6.6408307125	4.1140650983	11.3245032011
Si	4.7997000000	6.1532000000	8.5584014400
Si	4.7970632925	4.2332942298	9.8502116660
Si	6.7187000000	6.1532000000	7.2014014400
Si	5.7586132160	6.1527638115	12.0796486666
Si	10.6346431006	0.5216209365	11.3337543483
Si	8.6387000000	2.3132000000	8.5584014400
Si	8.6414043992	0.4032786268	10.0035426613
Si	10.5587000000	2.3132000000	7.2014014400
Si	11.1927322454	2.3217470375	12.8122797135
Si	14.3196309559	0.2778173126	11.3264993772
Si	12.4787000000	2.3132000000	8.5584014400
Si	12.4762727868	0.3927145114	9.8524727391
Si	14.3987000000	2.3132000000	7.2014014400
Si	13.4335069356	2.3256588821	12.0632431432
Si	10.6387013582	4.1214391389	11.3376332033
Si	8.6387000000	6.1532000000	8.5584014400
Si	8.6420656422	4.2258435025	10.0074978626
Si	10.5587000000	6.1532000000	7.2014014400
Si	11.5342821303	6.1525947680	12.1077188184
Si	14.3284659149	4.3619108662	11.3316946694
Si	12.4787000000	6.1532000000	8.5584014400
Si	12.4788121858	4.2330568805	9.8531516273
Si	14.3987000000	6.1532000000	7.2014014400

Si	13.8111296560	6.1525286789	12.8349140901
Si	2.9549548887	7.9453711385	11.3311732004
Si	0.9597000000	9.9922000000	8.5584014400
Si	0.9601338386	8.0641966622	10.0027576538
Si	2.8797000000	9.9922000000	7.2014014400
Si	3.8354952396	9.9909867353	12.0612646305
Si	6.6407856540	8.1913235617	11.3244490240
Si	4.7997000000	9.9922000000	8.5584014400
Si	4.7971739808	8.0726530191	9.8503909196
Si	6.7187000000	9.9922000000	7.2014014400
Si	6.0778936856	9.9946184888	12.7905445419
Si	2.9535201007	12.0361132533	11.3294253607
Si	0.9597000000	13.8322000000	8.5584014400
Si	0.9582322149	11.9218564899	10.0029326879
Si	2.8797000000	13.8322000000	7.2014014400
Si	3.5097943641	13.8330519746	12.8110151535
Si	6.6442497491	11.7941566100	11.3261778682
Si	4.7997000000	13.8322000000	8.5584014400
Si	4.7980922089	11.9124624135	9.8503733377
Si	6.7187000000	13.8322000000	7.2014014400
Si	5.7507080934	13.8316339146	12.0645037103
Si	10.6385574101	8.1840179624	11.3385836486
Si	8.6387000000	9.9922000000	8.5584014400
Si	8.6421845908	8.0799681304	10.0078926597
Si	10.5587000000	9.9922000000	7.2014014400
Si	11.1932534746	9.9840405391	12.8124238426
Si	14.3286928094	7.9435524291	11.3322794774
Si	12.4787000000	9.9922000000	8.5584014400
Si	12.4787258565	8.0728200494	9.8540008192
Si	14.3987000000	9.9922000000	7.2014014400
Si	13.4338560448	9.9798319029	12.0632343938
Si	10.6347356857	11.7836905867	11.3335737377
Si	8.6387000000	13.8322000000	8.5584014400
Si	8.6413505015	11.9023166516	10.0035405986
Si	10.5587000000	13.8322000000	7.2014014400
Si	11.5192047283	13.8318166424	12.0599306237
Si	14.3195381995	12.0277023258	11.3258635091
Si	12.4787000000	13.8322000000	8.5584014400
Si	12.4761554408	11.9129977697	9.8520169950
Si	14.3987000000	13.8322000000	7.2014014400
Si	13.7566579261	13.8317402465	12.7919896902
H	2.8797000000	3.5702000000	6.3114014300
H	2.8797000000	1.0562000000	6.3114014300
H	6.7187000000	3.5702000000	6.3114014300

H	6.7187000000	1.0562000000	6.3114014300
H	2.8797000000	7.4102000000	6.3114014300
H	2.8797000000	4.8952000000	6.3114014300
H	6.7187000000	7.4102000000	6.3114014300
H	6.7187000000	4.8952000000	6.3114014300
H	10.5587000000	3.5702000000	6.3114014300
H	10.5587000000	1.0562000000	6.3114014300
H	14.3987000000	3.5702000000	6.3114014300
H	14.3987000000	1.0562000000	6.3114014300
H	10.5587000000	7.4102000000	6.3114014300
H	10.5587000000	4.8952000000	6.3114014300
H	14.3987000000	7.4102000000	6.3114014300
H	14.3987000000	4.8952000000	6.3114014300
H	2.8797000000	11.2502000000	6.3114014300
H	2.8797000000	8.7352000000	6.3114014300
H	6.7187000000	11.2502000000	6.3114014300
H	6.7187000000	8.7352000000	6.3114014300
H	2.8797000000	15.0892000000	6.3114014300
H	2.8797000000	12.5742000000	6.3114014300
H	6.7187000000	15.0892000000	6.3114014300
H	6.7187000000	12.5742000000	6.3114014300
H	10.5587000000	11.2502000000	6.3114014300
H	10.5587000000	8.7352000000	6.3114014300
H	14.3987000000	11.2502000000	6.3114014300
H	14.3987000000	8.7352000000	6.3114014300
H	10.5587000000	15.0892000000	6.3114014300
H	10.5587000000	12.5742000000	6.3114014300
H	14.3987000000	15.0892000000	6.3114014300
H	14.3987000000	12.5742000000	6.3114014300
Si	8.9607436762	6.1529398333	15.6182215439
Cl	8.1294245873	7.8190403720	14.7907449762
Cl	8.6915358924	6.1608563055	17.6347983156
Cl	8.1123147927	4.4905080632	14.8004919640
Cl	10.9756780943	6.1409534569	15.2118709501

4. P1

Si	2.9264051492	0.2484592445	11.3215642297
Si	0.9597000000	2.3132000000	8.5584000000
Si	0.9413348343	0.3787216184	9.9993053745
Si	2.8797000000	2.3132000000	7.2014000000
Si	3.6877128254	2.3346073550	12.0020909417
Si	6.6699020553	0.4544603240	11.2848895116
Si	4.7997000000	2.3132000000	8.5584000000
Si	4.7713488334	0.3969145368	9.8531371696

Si	6.7187000000	2.3132000000	7.2014000000
Si	5.9571998710	2.3427928296	12.4406290699
Si	2.9407765817	4.4165412055	11.3295769838
Si	0.9597000000	6.1532000000	8.5584000000
Si	0.9936139622	4.2339040518	9.9704620762
Si	2.8797000000	6.1532000000	7.2014000000
Si	3.4193909116	6.1519552297	12.9060127726
Si	6.6468925189	4.2631705315	11.3082724894
Si	4.7997000000	6.1532000000	8.5584000000
Si	4.7966664808	4.2272827982	9.8710912536
Si	6.7187000000	6.1532000000	7.2014000000
Si	5.8478626006	6.1528772054	12.4950861331
Si	10.6367203479	0.5178532024	11.3416454567
Si	8.6387000000	2.3132000000	8.5584000000
Si	8.6684705414	0.3963886699	9.9869793727
Si	10.5587000000	2.3132000000	7.2014000000
Si	11.1587652598	2.3316512354	12.8066138007
Si	14.3150636559	0.2669466661	11.3380945989
Si	12.4787000000	2.3132000000	8.5584000000
Si	12.4741585609	0.3923980094	9.8553002451
Si	14.3987000000	2.3132000000	7.2014000000
Si	13.3920142520	2.2900153395	12.0668705689
Si	10.6415312090	4.1640432674	11.3582220098
Si	8.6387000000	6.1532000000	8.5584000000
Si	8.6569386050	4.2322685594	10.0126367981
Si	10.5587000000	6.1532000000	7.2014000000
Si	11.2861403186	6.1520106262	12.4765822867
Si	14.3648611593	4.2579350135	11.2644939492
Si	12.4787000000	6.1532000000	8.5584000000
Si	12.4401687863	4.2394912530	9.8597433013
Si	14.3987000000	6.1532000000	7.2014000000
Si	13.6822589560	6.1523252046	12.4318704439
Si	2.9472640725	7.8865075639	11.3271488701
Si	0.9597000000	9.9922000000	8.5584000000
Si	0.9975405642	8.0715978282	9.9732332479
Si	2.8797000000	9.9922000000	7.2014000000
Si	3.6884298142	9.9714439543	12.0005206842
Si	6.6394702946	8.0441560786	11.3037736107
Si	4.7997000000	9.9922000000	8.5584000000
Si	4.7951812733	8.0774357519	9.8631922476
Si	6.7187000000	9.9922000000	7.2014000000
Si	5.9559225020	9.9643949775	12.4407463797
Si	2.9268088845	12.0576327875	11.3227347468
Si	0.9597000000	13.8322000000	8.5584000000

Si	0.9434238247	11.9270605827	9.9987261441
Si	2.8797000000	13.8322000000	7.2014000000
Si	3.4675374578	13.8326956480	12.8347975897
Si	6.6692686556	11.8510793534	11.2834417267
Si	4.7997000000	13.8322000000	8.5584000000
Si	4.7708871144	11.9080499953	9.8528038826
Si	6.7187000000	13.8322000000	7.2014000000
Si	5.6943322066	13.8318992706	12.0526441835
Si	10.6421806008	8.1415443984	11.3593887194
Si	8.6387000000	9.9922000000	8.5584000000
Si	8.6542476880	8.0737905640	10.0155593999
Si	10.5587000000	9.9922000000	7.2014000000
Si	11.1584206632	9.9753483249	12.8078927266
Si	14.3653109497	8.0470174801	11.2641049140
Si	12.4787000000	9.9922000000	8.5584000000
Si	12.4405514891	8.0663515824	9.8595137400
Si	14.3987000000	9.9922000000	7.2014000000
Si	13.3922687358	10.0159583280	12.0675111108
Si	10.6365464657	11.7885760716	11.3407440338
Si	8.6387000000	13.8322000000	8.5584000000
Si	8.6674838464	11.9091456708	9.9860429705
Si	10.5587000000	13.8322000000	7.2014000000
Si	11.5217800682	13.8322862148	12.0631465684
Si	14.3159506991	12.0392437245	11.3368743577
Si	12.4787000000	13.8322000000	8.5584000000
Si	12.4746543225	11.9133600868	9.8549581264
Si	14.3987000000	13.8322000000	7.2014000000
Si	13.7591114037	13.8322094822	12.8092285191
H	2.8797000000	3.5702000000	6.3114000000
H	2.8797000000	1.0562000000	6.3114000000
H	6.7187000000	3.5702000000	6.3114000000
H	6.7187000000	1.0562000000	6.3114000000
H	2.8797000000	7.4102000000	6.3114000000
H	2.8797000000	4.8952000000	6.3114000000
H	6.7187000000	7.4102000000	6.3114000000
H	6.7187000000	4.8952000000	6.3114000000
H	10.5587000000	3.5702000000	6.3114000000
H	10.5587000000	1.0562000000	6.3114000000
H	14.3987000000	3.5702000000	6.3114000000
H	14.3987000000	1.0562000000	6.3114000000
H	10.5587000000	7.4102000000	6.3114000000
H	10.5587000000	4.8952000000	6.3114000000
H	14.3987000000	7.4102000000	6.3114000000
H	14.3987000000	4.8952000000	6.3114000000

H	2.8797000000	11.2502000000	6.3114000000
H	2.8797000000	8.7352000000	6.3114000000
H	6.7187000000	11.2502000000	6.3114000000
H	6.7187000000	8.7352000000	6.3114000000
H	2.8797000000	15.0892000000	6.3114000000
H	2.8797000000	12.5742000000	6.3114000000
H	6.7187000000	15.0892000000	6.3114000000
H	6.7187000000	12.5742000000	6.3114000000
H	10.5587000000	11.2502000000	6.3114000000
H	10.5587000000	8.7352000000	6.3114000000
H	14.3987000000	11.2502000000	6.3114000000
H	14.3987000000	8.7352000000	6.3114000000
H	10.5587000000	15.0892000000	6.3114000000
H	10.5587000000	12.5742000000	6.3114000000
H	14.3987000000	15.0892000000	6.3114000000
H	14.3987000000	12.5742000000	6.3114000000
Si	6.8147176961	6.1544568246	14.6331404515
Cl	7.9791353836	7.8465174368	14.9159918415
Cl	5.4043057043	6.1626781015	16.1444444382
Cl	7.9730030336	4.4601690219	14.9257243359
Cl	10.9446935125	6.1488193290	14.5370444656

5. TS1

Si	2.9587707472	0.2715322164	11.3274746841
Si	0.9597000000	2.3132000000	8.5584005837
Si	0.9702019625	0.3902557483	10.0023873854
Si	2.8797000000	2.3132000000	7.2014005837
Si	3.8406815912	2.3125201765	12.0421865762
Si	6.6373915778	0.5058901854	11.3169204276
Si	4.7997000000	2.3132000000	8.5584005837
Si	4.7940098100	0.3911859730	9.8474160564
Si	6.7187000000	2.3132000000	7.2014005837
Si	6.0738099198	2.3113414114	12.7703156109
Si	2.9820099773	4.3644022289	11.3492863424
Si	0.9597000000	6.1532000000	8.5584005837
Si	1.0409536396	4.2297636753	9.9658059494
Si	2.8797000000	6.1532000000	7.2014005837
Si	3.5028492729	6.1527491504	12.8618818048
Si	6.6309238986	4.1208447709	11.3167305812
Si	4.7997000000	6.1532000000	8.5584005837
Si	4.7964364980	4.2340511105	9.8433038708
Si	6.7187000000	6.1532000000	7.2014005837
Si	5.7530116509	6.1531487905	12.0666797956
Si	10.6048266064	0.5213305084	11.3271898457

Si	8.6387000000	2.3132000000	8.5584005837
Si	8.6266703613	0.4012222476	9.9935349125
Si	10.5587000000	2.3132000000	7.2014005837
Si	11.1157706396	2.3241330047	12.8283607877
Si	14.3324360027	0.2798907941	11.3223610964
Si	12.4787000000	2.3132000000	8.5584005837
Si	12.4594290815	0.3915648861	9.8709569717
Si	14.3987000000	2.3132000000	7.2014005837
Si	13.3427368554	2.2558517575	12.0535158208
Si	10.5978823365	4.1310290799	11.3476721583
Si	8.6387000000	6.1532000000	8.5584005837
Si	8.6242242933	4.2249894978	10.0001498970
Si	10.5587000000	6.1532000000	7.2014005837
Si	11.1875736027	6.1530380377	12.4025472648
Si	14.4068879865	4.1656477936	11.2463540839
Si	12.4787000000	6.1532000000	8.5584005837
Si	12.4143644170	4.2434393330	9.8590516440
Si	14.3987000000	6.1532000000	7.2014005837
Si	13.5203459725	6.1527080080	11.9384428906
Si	2.9822017265	7.9415638567	11.3497947605
Si	0.9597000000	9.9922000000	8.5584005837
Si	1.0410275084	8.0762082215	9.9664026990
Si	2.8797000000	9.9922000000	7.2014005837
Si	3.8427189604	9.9924808012	12.0436757993
Si	6.6302261332	8.1851772190	11.3156902188
Si	4.7997000000	9.9922000000	8.5584005837
Si	4.7960208530	8.0720063601	9.8429747573
Si	6.7187000000	9.9922000000	7.2014005837
Si	6.0766818914	9.9933498185	12.7734595880
Si	2.9593467291	12.0326239332	11.3272777726
Si	0.9597000000	13.8322000000	8.5584005837
Si	0.9703987842	11.9151737016	10.0022594978
Si	2.8797000000	13.8322000000	7.2014005837
Si	3.5165555851	13.8312884946	12.8047099391
Si	6.6375917478	11.7983158570	11.3175154429
Si	4.7997000000	13.8322000000	8.5584005837
Si	4.7944747614	11.9145256564	9.8470471919
Si	6.7187000000	13.8322000000	7.2014005837
Si	5.7526449269	13.8311536013	12.0434921143
Si	10.5976845426	8.1746022932	11.3473749318
Si	8.6387000000	9.9922000000	8.5584005837
Si	8.6239826405	8.0808091413	10.0001460063
Si	10.5587000000	9.9922000000	7.2014005837
Si	11.1150233504	9.9812344749	12.8286570304

Si	14.4068600634	8.1399775897	11.2470234995
Si	12.4787000000	9.9922000000	8.5584005837
Si	12.4144410001	8.0625088896	9.8594404044
Si	14.3987000000	9.9922000000	7.2014005837
Si	13.3422397543	10.0496280662	12.0540278047
Si	10.6047772637	11.7839832487	11.3270407261
Si	8.6387000000	13.8322000000	8.5584005837
Si	8.6265541138	11.9044048428	9.9934126583
Si	10.5587000000	13.8322000000	7.2014005837
Si	11.4608422470	13.8317983555	12.0186067839
Si	14.3324005978	12.0253243705	11.3222616980
Si	12.4787000000	13.8322000000	8.5584005837
Si	12.4594288010	11.9141022012	9.8707204466
Si	14.3987000000	13.8322000000	7.2014005837
Si	13.7022841764	13.8317999140	12.7163417607
H	2.8797000000	3.5702000000	6.3114005797
H	2.8797000000	1.0562000000	6.3114005797
H	6.7187000000	3.5702000000	6.3114005797
H	6.7187000000	1.0562000000	6.3114005797
H	2.8797000000	7.4102000000	6.3114005797
H	2.8797000000	4.8952000000	6.3114005797
H	6.7187000000	7.4102000000	6.3114005797
H	6.7187000000	4.8952000000	6.3114005797
H	10.5587000000	3.5702000000	6.3114005797
H	10.5587000000	1.0562000000	6.3114005797
H	14.3987000000	3.5702000000	6.3114005797
H	14.3987000000	1.0562000000	6.3114005797
H	10.5587000000	7.4102000000	6.3114005797
H	10.5587000000	4.8952000000	6.3114005797
H	14.3987000000	7.4102000000	6.3114005797
H	14.3987000000	4.8952000000	6.3114005797
H	2.8797000000	11.2502000000	6.3114005797
H	2.8797000000	8.7352000000	6.3114005797
H	6.7187000000	11.2502000000	6.3114005797
H	6.7187000000	8.7352000000	6.3114005797
H	2.8797000000	15.0892000000	6.3114005797
H	2.8797000000	12.5742000000	6.3114005797
H	6.7187000000	15.0892000000	6.3114005797
H	6.7187000000	12.5742000000	6.3114005797
H	10.5587000000	11.2502000000	6.3114005797
H	10.5587000000	8.7352000000	6.3114005797
H	14.3987000000	11.2502000000	6.3114005797
H	14.3987000000	8.7352000000	6.3114005797
H	10.5587000000	15.0892000000	6.3114005797

H	10.5587000000	12.5742000000	6.3114005797
H	14.3987000000	15.0892000000	6.3114005797
H	14.3987000000	12.5742000000	6.3114005797
Si	7.8950282866	6.1195664698	15.8245884059
Cl	8.0638644446	7.8273747932	14.6546806710
Cl	5.9714321763	6.0985734857	16.5946606471
Cl	8.1042530262	4.4149590142	14.6576487913
Cl	11.2129904953	6.1557930395	14.5066828645

6. TS2

Si	2.9441476600	0.2407303882	11.3520032325
Si	0.9597000000	2.3132000000	8.5584006327
Si	0.9615706646	0.3855465154	10.0052907429
Si	2.8797000000	2.3132000000	7.2014006327
Si	3.8900576675	2.2324422338	12.0258699122
Si	6.6485829608	0.4887435289	11.3177622225
Si	4.7997000000	2.3132000000	8.5584006327
Si	4.7984020599	0.4004664583	9.8479007047
Si	6.7187000000	2.3132000000	7.2014006327
Si	6.1165787707	2.2777106914	12.8084440807
Si	2.9382225433	4.2357081335	11.2527048163
Si	0.9597000000	6.1532000000	8.5584006327
Si	0.9282295797	4.2355610456	9.9817112397
Si	2.8797000000	6.1532000000	7.2014006327
Si	3.7249512454	6.1529084348	12.3113276572
Si	6.6718678570	4.0681031768	11.3197912218
Si	4.7997000000	6.1532000000	8.5584006327
Si	4.8350089312	4.2472225004	9.8573313405
Si	6.7187000000	6.1532000000	7.2014006327
Si	5.9846331731	6.1528815125	12.0556990308
Si	10.6337979870	0.5209781922	11.3323739625
Si	8.6387000000	2.3132000000	8.5584006327
Si	8.6417274949	0.4001791505	9.9989659397
Si	10.5587000000	2.3132000000	7.2014006327
Si	11.1903159202	2.3203422652	12.8137014774
Si	14.3216141351	0.2762183171	11.3254042228
Si	12.4787000000	2.3132000000	8.5584006327
Si	12.4771071611	0.3926227751	9.8528477226
Si	14.3987000000	2.3132000000	7.2014006327
Si	13.4303104600	2.3198851793	12.0645077773
Si	10.6444388814	4.1209261514	11.3376285849
Si	8.6387000000	6.1532000000	8.5584006327
Si	8.6560840034	4.2196087802	9.9999452282
Si	10.5587000000	6.1532000000	7.2014006327

Si	11.5381727680	6.1530278725	12.1068852009
Si	14.3212314506	4.3596758667	11.3384152278
Si	12.4787000000	6.1532000000	8.5584006327
Si	12.4808451350	4.2337056149	9.8519067867
Si	14.3987000000	6.1532000000	7.2014006327
Si	13.8173905698	6.1524867346	12.8446421302
Si	2.9381624212	8.0703397032	11.2531741819
Si	0.9597000000	9.9922000000	8.5584006327
Si	0.9281996623	8.0702797583	9.9821912810
Si	2.8797000000	9.9922000000	7.2014006327
Si	3.8901704477	10.0737063652	12.0260051641
Si	6.6718570776	8.2378095536	11.3201620294
Si	4.7997000000	9.9922000000	8.5584006327
Si	4.8349656662	8.0586259421	9.8578353772
Si	6.7187000000	9.9922000000	7.2014006327
Si	6.1167205772	10.0283586477	12.8087749062
Si	2.9442029666	12.0653608637	11.3517690221
Si	0.9597000000	13.8322000000	8.5584006327
Si	0.9616550250	11.9202011985	10.0049490708
Si	2.8797000000	13.8322000000	7.2014006327
Si	3.4955131176	13.8321590669	12.8601291163
Si	6.6485615760	11.8170130401	11.3174932445
Si	4.7997000000	13.8322000000	8.5584006327
Si	4.7984220298	11.9053155923	9.8475756340
Si	6.7187000000	13.8322000000	7.2014006327
Si	5.7413213834	13.8320707839	12.0442863017
Si	10.6442762398	8.1853065962	11.3385362920
Si	8.6387000000	9.9922000000	8.5584006327
Si	8.6561311563	8.0862716374	10.0004470512
Si	10.5587000000	9.9922000000	7.2014006327
Si	11.1904790534	9.9863498940	12.8138293741
Si	14.3214039719	7.9456902565	11.3391424918
Si	12.4787000000	9.9922000000	8.5584006327
Si	12.4808374134	8.0721160876	9.8526668858
Si	14.3987000000	9.9922000000	7.2014006327
Si	13.4304632786	9.9856582795	12.0645265239
Si	10.6339288727	11.7852570690	11.3317737244
Si	8.6387000000	13.8322000000	8.5584006327
Si	8.6417031951	11.9056043027	9.9986027857
Si	10.5587000000	13.8322000000	7.2014006327
Si	11.5205200398	13.8322900717	12.0580530465
Si	14.3215895796	12.0293012447	11.3248405955
Si	12.4787000000	13.8322000000	8.5584006327
Si	12.4771655924	11.9131287195	9.8523781021

Si	14.3987000000	13.8322000000	7.2014006327
Si	13.7585575041	13.8317834993	12.7915091994
H	2.8797000000	3.5702000000	6.3114006283
H	2.8797000000	1.0562000000	6.3114006283
H	6.7187000000	3.5702000000	6.3114006283
H	6.7187000000	1.0562000000	6.3114006283
H	2.8797000000	7.4102000000	6.3114006283
H	2.8797000000	4.8952000000	6.3114006283
H	6.7187000000	7.4102000000	6.3114006283
H	6.7187000000	4.8952000000	6.3114006283
H	10.5587000000	3.5702000000	6.3114006283
H	10.5587000000	1.0562000000	6.3114006283
H	14.3987000000	3.5702000000	6.3114006283
H	14.3987000000	1.0562000000	6.3114006283
H	10.5587000000	7.4102000000	6.3114006283
H	10.5587000000	4.8952000000	6.3114006283
H	14.3987000000	7.4102000000	6.3114006283
H	14.3987000000	4.8952000000	6.3114006283
H	2.8797000000	11.2502000000	6.3114006283
H	2.8797000000	8.7352000000	6.3114006283
H	6.7187000000	11.2502000000	6.3114006283
H	6.7187000000	8.7352000000	6.3114006283
H	2.8797000000	15.0892000000	6.3114006283
H	2.8797000000	12.5742000000	6.3114006283
H	6.7187000000	15.0892000000	6.3114006283
H	6.7187000000	12.5742000000	6.3114006283
H	10.5587000000	11.2502000000	6.3114006283
H	10.5587000000	8.7352000000	6.3114006283
H	14.3987000000	11.2502000000	6.3114006283
H	14.3987000000	8.7352000000	6.3114006283
H	10.5587000000	15.0892000000	6.3114006283
H	10.5587000000	12.5742000000	6.3114006283
H	14.3987000000	15.0892000000	6.3114006283
H	14.3987000000	12.5742000000	6.3114006283
Si	9.0088913953	6.1525121658	15.6605404799
Cl	8.1785585678	7.8213853284	14.8397029783
Cl	8.7458900221	6.1599127394	17.6791647986
Cl	8.1638515772	4.4862837129	14.8493599134
Cl	11.0220558628	6.1424911274	15.2482097702

7. TS3

Si	2.9415720335	0.2514119471	11.3262565053
Si	0.9597000000	2.3132000000	8.5584000000
Si	0.9491186786	0.3825181116	10.0021484677

Si	2.8797000000	2.3132000000	7.2014000000
Si	3.8959280219	2.2589232394	12.0174807125
Si	6.6584018783	0.5025832889	11.3029343443
Si	4.7997000000	2.3132000000	8.5584000000
Si	4.7977272905	0.3904683135	9.8501119567
Si	6.7187000000	2.3132000000	7.2014000000
Si	6.1068016891	2.3278557645	12.7089346307
Si	2.9127445188	4.2413058040	11.2932391977
Si	0.9597000000	6.1532000000	8.5584000000
Si	0.9104332551	4.2422502867	9.9859991765
Si	2.8797000000	6.1532000000	7.2014000000
Si	3.9828028454	6.1525879742	12.0859936858
Si	6.6494560365	4.2069269623	11.3398864297
Si	4.7997000000	6.1532000000	8.5584000000
Si	4.8498575295	4.2406772864	9.8586834812
Si	6.7187000000	6.1532000000	7.2014000000
Si	6.2641122929	6.1530966720	12.6656494952
Si	10.6371327930	0.5208230210	11.3285783731
Si	8.6387000000	2.3132000000	8.5584000000
Si	8.6518132381	0.4015008878	9.9916154180
Si	10.5587000000	2.3132000000	7.2014000000
Si	11.1986251754	2.3247336104	12.7866216778
Si	14.3154888865	0.2763002896	11.3257987211
Si	12.4787000000	2.3132000000	8.5584000000
Si	12.4788704681	0.3907936082	9.8489434616
Si	14.3987000000	2.3132000000	7.2014000000
Si	13.4309507784	2.3272862471	12.0503888642
Si	10.6483316413	4.1453240287	11.3429886079
Si	8.6387000000	6.1532000000	8.5584000000
Si	8.6449343926	4.2275173877	10.0156281020
Si	10.5587000000	6.1532000000	7.2014000000
Si	11.4728245271	6.1528910514	12.2869427785
Si	14.3069738812	4.3752402143	11.3520560819
Si	12.4787000000	6.1532000000	8.5584000000
Si	12.4681136681	4.2363723651	9.8589456172
Si	14.3987000000	6.1532000000	7.2014000000
Si	13.8345929153	6.1523924248	12.8926701086
Si	2.9126396263	8.0640440048	11.2938564319
Si	0.9597000000	9.9922000000	8.5584000000
Si	0.9103949433	8.0635517877	9.9865586130
Si	2.8797000000	9.9922000000	7.2014000000
Si	3.8957308244	10.0467679187	12.0173027242
Si	6.6493499697	8.0993253709	11.3401361958
Si	4.7997000000	9.9922000000	8.5584000000

Si	4.8496160994	8.0652846145	9.8592560543
Si	6.7187000000	9.9922000000	7.2014000000
Si	6.1063671438	9.9785871341	12.7084358554
Si	2.9415938259	12.0542954070	11.3258266193
Si	0.9597000000	13.8322000000	8.5584000000
Si	0.9491347608	11.9231930580	10.0017699549
Si	2.8797000000	13.8322000000	7.2014000000
Si	3.5275689919	13.8319353566	12.7898949692
Si	6.6582058016	11.8036607766	11.3023382868
Si	4.7997000000	13.8322000000	8.5584000000
Si	4.7976770837	11.9151676472	9.8497269993
Si	6.7187000000	13.8322000000	7.2014000000
Si	5.7679866332	13.8323830971	12.0463079074
Si	10.6482879336	8.1608881422	11.3437907826
Si	8.6387000000	9.9922000000	8.5584000000
Si	8.6449775009	8.0784542264	10.0161677425
Si	10.5587000000	9.9922000000	7.2014000000
Si	11.1990489795	9.9820768207	12.7862076545
Si	14.3070665396	7.9300077002	11.3527644124
Si	12.4787000000	9.9922000000	8.5584000000
Si	12.4681126561	8.0695248780	9.8596855382
Si	14.3987000000	9.9922000000	7.2014000000
Si	13.4312281017	9.9782157795	12.0503658840
Si	10.6372854083	11.7856059229	11.3278353088
Si	8.6387000000	13.8322000000	8.5584000000
Si	8.6517496668	11.9042650874	9.9912379967
Si	10.5587000000	13.8322000000	7.2014000000
Si	11.5187245033	13.8324121581	12.0543729794
Si	14.3154218125	12.0291825368	11.3252206794
Si	12.4787000000	13.8322000000	8.5584000000
Si	12.4789076007	11.9148724269	9.8484706342
Si	14.3987000000	13.8322000000	7.2014000000
Si	13.7561050241	13.8317862395	12.7928164258
H	2.8797000000	3.5702000000	6.3114000000
H	2.8797000000	1.0562000000	6.3114000000
H	6.7187000000	3.5702000000	6.3114000000
H	6.7187000000	1.0562000000	6.3114000000
H	2.8797000000	7.4102000000	6.3114000000
H	2.8797000000	4.8952000000	6.3114000000
H	6.7187000000	7.4102000000	6.3114000000
H	6.7187000000	4.8952000000	6.3114000000
H	10.5587000000	3.5702000000	6.3114000000
H	10.5587000000	1.0562000000	6.3114000000
H	14.3987000000	3.5702000000	6.3114000000

H	14.3987000000	1.0562000000	6.3114000000
H	10.5587000000	7.4102000000	6.3114000000
H	10.5587000000	4.8952000000	6.3114000000
H	14.3987000000	7.4102000000	6.3114000000
H	14.3987000000	4.8952000000	6.3114000000
H	2.8797000000	11.2502000000	6.3114000000
H	2.8797000000	8.7352000000	6.3114000000
H	6.7187000000	11.2502000000	6.3114000000
H	6.7187000000	8.7352000000	6.3114000000
H	2.8797000000	15.0892000000	6.3114000000
H	2.8797000000	12.5742000000	6.3114000000
H	6.7187000000	15.0892000000	6.3114000000
H	6.7187000000	12.5742000000	6.3114000000
H	10.5587000000	11.2502000000	6.3114000000
H	10.5587000000	8.7352000000	6.3114000000
H	14.3987000000	11.2502000000	6.3114000000
H	14.3987000000	8.7352000000	6.3114000000
H	10.5587000000	15.0892000000	6.3114000000
H	10.5587000000	12.5742000000	6.3114000000
H	14.3987000000	15.0892000000	6.3114000000
H	14.3987000000	12.5742000000	6.3114000000
Si	8.5964345215	6.1530632435	14.9250177936
Cl	8.4051936691	8.1477175689	14.3919752865
Cl	8.1487570684	6.1581531776	16.9236657860
Cl	8.3983032155	4.1570881571	14.3998099135
Cl	10.7950061097	6.1494305697	14.7136795003

8. IM1

Si	2.9467191478	0.2352304975	11.3532369172
Si	0.9597000000	2.3132000000	8.5584000000
Si	0.9634224102	0.3861769487	10.0069049347
Si	2.8797000000	2.3132000000	7.2014000000
Si	3.9310284763	2.2114886402	12.0028149933
Si	6.6540168173	0.4880599004	11.3099798869
Si	4.7997000000	2.3132000000	8.5584000000
Si	4.7983973267	0.4000143144	9.8460597660
Si	6.7187000000	2.3132000000	7.2014000000
Si	6.1463446526	2.2946692381	12.7800343152
Si	2.9213730621	4.1765180896	11.2496661914
Si	0.9597000000	6.1532000000	8.5584000000
Si	0.9186908873	4.2319973769	9.9731417789
Si	2.8797000000	6.1532000000	7.2014000000
Si	3.8671647209	6.1528021649	11.9877498548
Si	6.6747410359	4.1169582349	11.3165187044

Si	4.7997000000	6.1532000000	8.5584000000
Si	4.8445189798	4.2469169421	9.8588453311
Si	6.7187000000	6.1532000000	7.2014000000
Si	6.1097919829	6.1528810730	12.2767639285
Si	10.6341312815	0.5210076521	11.3314878207
Si	8.6387000000	2.3132000000	8.5584000000
Si	8.6443942426	0.3994229127	9.9946514144
Si	10.5587000000	2.3132000000	7.2014000000
Si	11.1886379291	2.3205025673	12.8145218826
Si	14.3226578730	0.2756680579	11.3258280732
Si	12.4787000000	2.3132000000	8.5584000000
Si	12.4782677525	0.3925069405	9.8530088942
Si	14.3987000000	2.3132000000	7.2014000000
Si	13.4286196417	2.3178299486	12.0661377327
Si	10.6458327400	4.1214502423	11.3369771554
Si	8.6387000000	6.1532000000	8.5584000000
Si	8.6571764391	4.2227497715	9.9988622094
Si	10.5587000000	6.1532000000	7.2014000000
Si	11.5417221545	6.1531956530	12.1054805527
Si	14.3204697855	4.3578066252	11.3402772848
Si	12.4787000000	6.1532000000	8.5584000000
Si	12.4826090755	4.2337468771	9.8515565281
Si	14.3987000000	6.1532000000	7.2014000000
Si	13.8212586896	6.1524655068	12.8454566879
Si	2.9212730097	8.1292565895	11.2502951381
Si	0.9597000000	9.9922000000	8.5584000000
Si	0.9186589700	8.0738491641	9.9736928101
Si	2.8797000000	9.9922000000	7.2014000000
Si	3.9310754756	10.0943672358	12.0029908923
Si	6.6746525513	8.1889794729	11.3168601799
Si	4.7997000000	9.9922000000	8.5584000000
Si	4.8443882523	8.0589588326	9.8593844818
Si	6.7187000000	9.9922000000	7.2014000000
Si	6.1463914472	10.0114663091	12.7801399067
Si	2.9467849921	12.0704947367	11.3528765989
Si	0.9597000000	13.8322000000	8.5584000000
Si	0.9634643773	11.9195086957	10.0065379256
Si	2.8797000000	13.8322000000	7.2014000000
Si	3.5055721879	13.8319376903	12.8543344259
Si	6.6539404701	11.8177455523	11.3095932153
Si	4.7997000000	13.8322000000	8.5584000000
Si	4.7983976068	11.9057209775	9.8456522046
Si	6.7187000000	13.8322000000	7.2014000000
Si	5.7442722636	13.8320700521	12.0349832396

Si	10.6456049645	8.1850821549	11.3379663240
Si	8.6387000000	9.9922000000	8.5584000000
Si	8.6571823100	8.0831860095	9.9994128558
Si	10.5587000000	9.9922000000	7.2014000000
Si	11.1887551222	9.9864927670	12.8145793439
Si	14.3205973086	7.9475323706	11.3410513178
Si	12.4787000000	9.9922000000	8.5584000000
Si	12.4825365041	8.0721200415	9.8523382803
Si	14.3987000000	9.9922000000	7.2014000000
Si	13.4286803580	9.9876252110	12.0662115243
Si	10.6342484854	11.7854817343	11.3308070951
Si	8.6387000000	13.8322000000	8.5584000000
Si	8.6443366644	11.9063553896	9.9942682827
Si	10.5587000000	13.8322000000	7.2014000000
Si	11.5210731232	13.8324144200	12.0574247041
Si	14.3225624573	12.0296726705	11.3251797844
Si	12.4787000000	13.8322000000	8.5584000000
Si	12.4782747293	11.9132110699	9.8525144116
Si	14.3987000000	13.8322000000	7.2014000000
Si	13.7590720011	13.8316927456	12.7918835574
H	2.8797000000	3.5702000000	6.3114000000
H	2.8797000000	1.0562000000	6.3114000000
H	6.7187000000	3.5702000000	6.3114000000
H	6.7187000000	1.0562000000	6.3114000000
H	2.8797000000	7.4102000000	6.3114000000
H	2.8797000000	4.8952000000	6.3114000000
H	6.7187000000	7.4102000000	6.3114000000
H	6.7187000000	4.8952000000	6.3114000000
H	10.5587000000	3.5702000000	6.3114000000
H	10.5587000000	1.0562000000	6.3114000000
H	14.3987000000	3.5702000000	6.3114000000
H	14.3987000000	1.0562000000	6.3114000000
H	10.5587000000	7.4102000000	6.3114000000
H	10.5587000000	4.8952000000	6.3114000000
H	14.3987000000	7.4102000000	6.3114000000
H	14.3987000000	4.8952000000	6.3114000000
H	2.8797000000	11.2502000000	6.3114000000
H	2.8797000000	8.7352000000	6.3114000000
H	6.7187000000	11.2502000000	6.3114000000
H	6.7187000000	8.7352000000	6.3114000000
H	2.8797000000	15.0892000000	6.3114000000
H	2.8797000000	12.5742000000	6.3114000000
H	6.7187000000	15.0892000000	6.3114000000
H	6.7187000000	12.5742000000	6.3114000000

H	10.5587000000	11.2502000000	6.3114000000
H	10.5587000000	8.7352000000	6.3114000000
H	14.3987000000	11.2502000000	6.3114000000
H	14.3987000000	8.7352000000	6.3114000000
H	10.5587000000	15.0892000000	6.3114000000
H	10.5587000000	12.5742000000	6.3114000000
H	14.3987000000	15.0892000000	6.3114000000
H	14.3987000000	12.5742000000	6.3114000000
Si	9.0497314032	6.1522161699	15.6998283886
Cl	8.2231007830	7.8250557908	14.8827716948
Cl	8.7861566630	6.1598018650	17.7172035859
Cl	8.2096818837	4.4812113709	14.8928978682
Cl	11.0610260895	6.1429626213	15.2796257123

9. VDW2

Si	2.9572603127	0.2724611354	11.0360469604
Si	0.9597000000	2.3132000000	8.2630408300
Si	0.9663878545	0.3877871951	9.6998487576
Si	2.8797000000	2.3132000000	6.9060408300
Si	3.8505155060	2.3145609274	11.7693554676
Si	6.6466721095	0.5258314201	11.0395611015
Si	4.7997000000	2.3132000000	8.2630408300
Si	4.8027980336	0.3939326400	9.5579438367
Si	6.7187000000	2.3132000000	6.9060408300
Si	6.0923519813	2.3237457235	12.5157057740
Si	2.9595310231	4.3551350264	11.0333083267
Si	0.9597000000	6.1532000000	8.2630408300
Si	0.9673176608	4.2396108040	9.6986800692
Si	2.8797000000	6.1532000000	6.9060408300
Si	3.5093386986	6.1536942636	12.5170391503
Si	6.6493943856	4.1206823125	11.0366673857
Si	4.7997000000	6.1532000000	8.2630408300
Si	4.8057692642	4.2331657194	9.5577224457
Si	6.7187000000	6.1532000000	6.9060408300
Si	5.7535684547	6.1584203145	11.7809886812
Si	10.6318031140	0.5431504925	11.0545415024
Si	8.6387000000	2.3132000000	8.2630408300
Si	8.6425832318	0.4026552423	9.7145853381
Si	10.5587000000	2.3132000000	6.9060408300
Si	11.1910073210	2.3272676731	12.5322891397
Si	14.3328827279	0.2953899568	11.0163634343
Si	12.4787000000	2.3132000000	8.2630408300
Si	12.4770077134	0.3915540452	9.5532328022
Si	14.3987000000	2.3132000000	6.9060408300

Si	13.4370032941	2.3227324018	11.7540915928
Si	10.6441227436	4.0932459598	11.0302939408
Si	8.6387000000	6.1532000000	8.2630408300
Si	8.6452239740	4.2270926309	9.7108593565
Si	10.5587000000	6.1532000000	6.9060408300
Si	11.6154068807	6.0729842597	11.7481893921
Si	14.3363993848	4.3458377056	11.0157983007
Si	12.4787000000	6.1532000000	8.2630408300
Si	12.4869749920	4.2334922867	9.5431234901
Si	14.3987000000	6.1532000000	6.9060408300
Si	13.8435484599	6.1538592730	12.4864469699
Si	2.9545605907	7.9468222652	11.0312192362
Si	0.9597000000	9.9922000000	8.2630408300
Si	0.9549283551	8.0627177599	9.7098916234
Si	2.8797000000	9.9922000000	6.9060408300
Si	3.8381876226	9.9912933029	11.7605072460
Si	6.6356325242	8.2007660641	11.0431934591
Si	4.7997000000	9.9922000000	8.2630408300
Si	4.8009050819	8.0730264646	9.5554248224
Si	6.7187000000	9.9922000000	6.9060408300
Si	6.0796417370	10.0064851491	12.5082815210
Si	2.9555371566	12.0344127959	11.0257492417
Si	0.9597000000	13.8322000000	8.2630408300
Si	0.9570879390	11.9216413982	9.7066652652
Si	2.8797000000	13.8322000000	6.9060408300
Si	3.5074929794	13.8287005456	12.5124821408
Si	6.6354735242	11.8042101062	11.0359759366
Si	4.7997000000	13.8322000000	8.2630408300
Si	4.8009510719	11.9120726545	9.5521958132
Si	6.7187000000	13.8322000000	6.9060408300
Si	5.7475997743	13.8468413915	11.7716003383
Si	10.6083907419	8.0388637503	10.9969169088
Si	8.6387000000	9.9922000000	8.2630408300
Si	8.6093251633	8.0766061771	9.6923769874
Si	10.5587000000	9.9922000000	6.9060408300
Si	11.6486464373	9.9883829295	11.7155053983
Si	14.3354157721	8.0171039996	11.0526484263
Si	12.4787000000	9.9922000000	8.2630408300
Si	12.5326322570	8.0754442011	9.5690299964
Si	14.3987000000	9.9922000000	6.9060408300
Si	13.8718874775	9.9908014128	12.2687666083
Si	10.6093351906	11.9380891398	10.9867627427
Si	8.6387000000	13.8322000000	8.2630408300
Si	8.6092309841	11.9087142174	9.6867430610

Si	10.5587000000	13.8322000000	6.9060408300
Si	11.6074792246	13.9099039184	11.7336390265
Si	14.3374868905	11.9585934390	11.0482196696
Si	12.4787000000	13.8322000000	8.2630408300
Si	12.5319276073	11.9081821168	9.5662303636
Si	14.3987000000	13.8322000000	6.9060408300
Si	13.8275025483	13.8293755995	12.4593626462
H	2.8797000000	3.5702000000	6.0160408400
H	2.8797000000	1.0562000000	6.0160408400
H	6.7187000000	3.5702000000	6.0160408400
H	6.7187000000	1.0562000000	6.0160408400
H	2.8797000000	7.4102000000	6.0160408400
H	2.8797000000	4.8952000000	6.0160408400
H	6.7187000000	7.4102000000	6.0160408400
H	6.7187000000	4.8952000000	6.0160408400
H	10.5587000000	3.5702000000	6.0160408400
H	10.5587000000	1.0562000000	6.0160408400
H	14.3987000000	3.5702000000	6.0160408400
H	14.3987000000	1.0562000000	6.0160408400
H	10.5587000000	7.4102000000	6.0160408400
H	10.5587000000	4.8952000000	6.0160408400
H	14.3987000000	7.4102000000	6.0160408400
H	14.3987000000	4.8952000000	6.0160408400
H	2.8797000000	11.2502000000	6.0160408400
H	2.8797000000	8.7352000000	6.0160408400
H	6.7187000000	11.2502000000	6.0160408400
H	6.7187000000	8.7352000000	6.0160408400
H	2.8797000000	15.0892000000	6.0160408400
H	2.8797000000	12.5742000000	6.0160408400
H	6.7187000000	15.0892000000	6.0160408400
H	6.7187000000	12.5742000000	6.0160408400
H	10.5587000000	11.2502000000	6.0160408400
H	10.5587000000	8.7352000000	6.0160408400
H	14.3987000000	11.2502000000	6.0160408400
H	14.3987000000	8.7352000000	6.0160408400
H	10.5587000000	15.0892000000	6.0160408400
H	10.5587000000	12.5742000000	6.0160408400
H	14.3987000000	15.0892000000	6.0160408400
H	14.3987000000	12.5742000000	6.0160408400
Si	9.9430840793	7.2466642479	15.4515038115
Cl	11.7436205699	8.1779628070	15.2643928836
Cl	10.0717476331	5.3566106238	14.6711904808
Cl	9.4105512255	7.1260790775	17.4118744214
Cl	8.5282683082	8.2951166460	14.4151698715

10. VDW3

Si	2.9455849484	0.2928948965	11.5184546796
Si	0.9597000000	2.3132000000	8.7670985100
Si	0.9534941490	0.3877756359	10.2029707394
Si	2.8797000000	2.3132000000	7.4100985100
Si	3.8437469321	2.3182097337	12.2581367772
Si	6.6450066673	0.5387831146	11.5566118777
Si	4.7997000000	2.3132000000	8.7670985100
Si	4.8011599240	0.3910256278	10.0564202944
Si	6.7187000000	2.3132000000	7.4100985100
Si	6.0855630652	2.3158770494	13.0445060470
Si	2.9407474976	4.3397801233	11.5213874790
Si	0.9597000000	6.1532000000	8.7670985100
Si	0.9519205387	4.2393606497	10.2032894586
Si	2.8797000000	6.1532000000	7.4100985100
Si	3.4337552777	6.1569250983	12.9782342829
Si	6.6420248337	4.0911803616	11.5566086115
Si	4.7997000000	6.1532000000	8.7670985100
Si	4.7971308110	4.2354959299	10.0559304048
Si	6.7187000000	6.1532000000	7.4100985100
Si	5.6587797280	6.0761259137	12.2403749590
Si	10.6324568328	0.5146235459	11.5387672271
Si	8.6387000000	2.3132000000	8.7670985100
Si	8.6345114890	0.4014305384	10.2174198360
Si	10.5587000000	2.3132000000	7.4100985100
Si	11.1860358412	2.3115395562	13.0194384614
Si	14.3196355040	0.2770191451	11.5357779342
Si	12.4787000000	2.3132000000	8.7670985100
Si	12.4750933420	0.3937268114	10.0602041419
Si	14.3987000000	2.3132000000	7.4100985100
Si	13.4277917621	2.3188482851	12.2735490099
Si	10.6311609955	4.1100163221	11.5436874563
Si	8.6387000000	6.1532000000	8.7670985100
Si	8.6335482212	4.2265006312	10.2191355418
Si	10.5587000000	6.1532000000	7.4100985100
Si	11.5350192759	6.1471454315	12.2782675102
Si	14.3210148365	4.3592612170	11.5419054742
Si	12.4787000000	6.1532000000	8.7670985100
Si	12.4753329285	4.2329770778	10.0618988468
Si	14.3987000000	6.1532000000	7.4100985100
Si	13.7757798668	6.1599802904	13.0229214659
Si	2.9385350357	8.0246235263	11.5534092578
Si	0.9597000000	9.9922000000	8.7670985100

Si	0.9616998527	8.0641096059	10.2118437312
Si	2.8797000000	9.9922000000	7.4100985100
Si	3.4069271159	9.9881651203	12.7830075028
Si	6.6603501447	8.0356466633	11.4744697222
Si	4.7997000000	9.9922000000	8.7670985100
Si	4.7363631090	8.0770899004	10.0639128643
Si	6.7187000000	9.9922000000	7.4100985100
Si	5.6278224010	9.9820947280	12.2107217570
Si	2.9412785910	11.9523697668	11.5543323928
Si	0.9597000000	13.8322000000	8.7670985100
Si	0.9619978002	11.9211176855	10.2129021721
Si	2.8797000000	13.8322000000	7.4100985100
Si	3.4535968597	13.8263804178	12.9593746351
Si	6.6697481734	11.9333453795	11.4877067632
Si	4.7997000000	13.8322000000	8.7670985100
Si	4.7455448235	11.9080575021	10.0703604947
Si	6.7187000000	13.8322000000	7.4100985100
Si	5.6729776253	13.9037013397	12.2351790532
Si	10.6444579066	8.1887066587	11.5437271979
Si	8.6387000000	9.9922000000	8.7670985100
Si	8.6702482050	8.0750187351	10.1927420426
Si	10.5587000000	9.9922000000	7.4100985100
Si	11.1942405038	9.9831583076	13.0252594566
Si	14.3214137139	7.9526843183	11.5309155964
Si	12.4787000000	9.9922000000	8.7670985100
Si	12.4759136551	8.0743222567	10.0566463063
Si	14.3987000000	9.9922000000	7.4100985100
Si	13.4319753657	9.9930087028	12.2645796436
Si	10.6422271595	11.7856082750	11.5514107727
Si	8.6387000000	13.8322000000	8.7670985100
Si	8.6722068564	11.9067927113	10.1930063790
Si	10.5587000000	13.8322000000	7.4100985100
Si	11.5281073398	13.8333464291	12.2751235577
Si	14.3221140609	12.0356387552	11.5344660721
Si	12.4787000000	13.8322000000	8.7670985100
Si	12.4754500426	11.9117503291	10.0601317697
Si	14.3987000000	13.8322000000	7.4100985100
Si	13.7674489005	13.8338262153	13.0126709229
H	2.8797000000	3.5702000000	6.5200985100
H	2.8797000000	1.0562000000	6.5200985100
H	6.7187000000	3.5702000000	6.5200985100
H	6.7187000000	1.0562000000	6.5200985100
H	2.8797000000	7.4102000000	6.5200985100
H	2.8797000000	4.8952000000	6.5200985100

H	6.7187000000	7.4102000000	6.5200985100
H	6.7187000000	4.8952000000	6.5200985100
H	10.5587000000	3.5702000000	6.5200985100
H	10.5587000000	1.0562000000	6.5200985100
H	14.3987000000	3.5702000000	6.5200985100
H	14.3987000000	1.0562000000	6.5200985100
H	10.5587000000	7.4102000000	6.5200985100
H	10.5587000000	4.8952000000	6.5200985100
H	14.3987000000	7.4102000000	6.5200985100
H	14.3987000000	4.8952000000	6.5200985100
H	2.8797000000	11.2502000000	6.5200985100
H	2.8797000000	8.7352000000	6.5200985100
H	6.7187000000	11.2502000000	6.5200985100
H	6.7187000000	8.7352000000	6.5200985100
H	2.8797000000	15.0892000000	6.5200985100
H	2.8797000000	12.5742000000	6.5200985100
H	6.7187000000	15.0892000000	6.5200985100
H	6.7187000000	12.5742000000	6.5200985100
H	10.5587000000	11.2502000000	6.5200985100
H	10.5587000000	8.7352000000	6.5200985100
H	14.3987000000	11.2502000000	6.5200985100
H	14.3987000000	8.7352000000	6.5200985100
H	10.5587000000	15.0892000000	6.5200985100
H	10.5587000000	12.5742000000	6.5200985100
H	14.3987000000	15.0892000000	6.5200985100
H	14.3987000000	12.5742000000	6.5200985100
Si	7.7127165835	8.0316620180	15.7085991743
Cl	8.5926555878	7.9671725995	17.5389709742
Cl	8.6301650837	6.6809136760	14.4702707231
Cl	5.7388613908	7.5630585396	15.8369862773
Cl	7.9047160612	9.9112078064	14.9281600359

11. P2

Si	2.9462575972	0.2964931188	11.0183668743
Si	0.9597000000	2.3132000000	8.2630000000
Si	0.9557888464	0.3905749045	9.7002263630
Si	2.8797000000	2.3132000000	6.9060000000
Si	3.8588509544	2.3116190055	11.7503819561
Si	6.6464277717	0.5495646721	11.0569743698
Si	4.7997000000	2.3132000000	8.2630000000
Si	4.7992349025	0.3887942667	9.5512817446
Si	6.7187000000	2.3132000000	6.9060000000
Si	6.0989066460	2.3155299537	12.5578220239
Si	2.9570987549	4.3320486328	11.0233039774

Si	0.9597000000	6.1532000000	8.2630000000
Si	0.9838699367	4.2339224145	9.6856385146
Si	2.8797000000	6.1532000000	6.9060000000
Si	3.4412507897	6.1441099993	12.4958723002
Si	6.6512400918	4.0819372417	11.0585137015
Si	4.7997000000	6.1532000000	8.2630000000
Si	4.8047502699	4.2378790336	9.5521110096
Si	6.7187000000	6.1532000000	6.9060000000
Si	5.6622059817	6.0548774988	11.7344549675
Si	10.6213833948	0.5249044190	11.0505170052
Si	8.6387000000	2.3132000000	8.2630000000
Si	8.6326284880	0.3995940125	9.7155081163
Si	10.5587000000	2.3132000000	6.9060000000
Si	11.1512866947	2.3412312267	12.4983566709
Si	14.3223142617	0.2840644745	11.0339216166
Si	12.4787000000	2.3132000000	8.2630000000
Si	12.4679357185	0.3910954893	9.5693694943
Si	14.3987000000	2.3132000000	6.9060000000
Si	13.3863668920	2.3004976231	11.7663340775
Si	10.6351954484	4.1365306643	11.0119916917
Si	8.6387000000	6.1532000000	8.2630000000
Si	8.6340356747	4.2240323103	9.7112397845
Si	10.5587000000	6.1532000000	6.9060000000
Si	11.2198593457	6.0989293056	12.1670714391
Si	14.3462907362	4.2839954227	10.9940919745
Si	12.4787000000	6.1532000000	8.2630000000
Si	12.4484570561	4.2359694421	9.5514711781
Si	14.3987000000	6.1532000000	6.9060000000
Si	13.6421216115	6.1639323394	12.1970090939
Si	2.9435195722	7.9855390338	11.0380675692
Si	0.9597000000	9.9922000000	8.2630000000
Si	0.9769035728	8.0647206031	9.6941616876
Si	2.8797000000	9.9922000000	6.9060000000
Si	3.4553748677	9.9954669449	12.1188159705
Si	6.6657539988	8.0196635598	10.9789731862
Si	4.7997000000	9.9922000000	8.2630000000
Si	4.7545571211	8.0805586633	9.5649120025
Si	6.7187000000	9.9922000000	6.9060000000
Si	5.6925123636	9.9919524553	11.7056103771
Si	2.9324002290	12.0007150050	11.0335064910
Si	0.9597000000	13.8322000000	8.2630000000
Si	0.9523057073	11.9242650445	9.7049782334
Si	2.8797000000	13.8322000000	6.9060000000
Si	3.4423865332	13.8422724585	12.4847550998

Si	6.6670956410	11.9648878783	10.9809853392
Si	4.7997000000	13.8322000000	8.2630000000
Si	4.7521705130	11.9035051816	9.5675104106
Si	6.7187000000	13.8322000000	6.9060000000
Si	5.6608382952	13.9321660981	11.7286933434
Si	10.6162842663	8.0521420182	11.0062643757
Si	8.6387000000	9.9922000000	8.2630000000
Si	8.6486902381	8.0720844116	9.6745000550
Si	10.5587000000	9.9922000000	6.9060000000
Si	11.3144137253	9.9791305379	12.1693439344
Si	14.3449937507	8.0650863785	11.0059966778
Si	12.4787000000	9.9922000000	8.2630000000
Si	12.4721562087	8.0688579702	9.5708081737
Si	14.3987000000	9.9922000000	6.9060000000
Si	13.7163075701	10.0211691082	12.1167032234
Si	10.6255524995	11.8842836759	10.9693864698
Si	8.6387000000	13.8322000000	8.2630000000
Si	8.6438355157	11.9157348765	9.6644331015
Si	10.5587000000	13.8322000000	6.9060000000
Si	11.5502118253	13.8683862861	11.7834392967
Si	14.3177365214	12.0093798002	11.0243074968
Si	12.4787000000	13.8322000000	8.2630000000
Si	12.5071501089	11.9067600728	9.5490905135
Si	14.3987000000	13.8322000000	6.9060000000
Si	13.7891108105	13.8271611579	12.4807550496
H	2.8797000000	3.5702000000	6.0160000000
H	2.8797000000	1.0562000000	6.0160000000
H	6.7187000000	3.5702000000	6.0160000000
H	6.7187000000	1.0562000000	6.0160000000
H	2.8797000000	7.4102000000	6.0160000000
H	2.8797000000	4.8952000000	6.0160000000
H	6.7187000000	7.4102000000	6.0160000000
H	6.7187000000	4.8952000000	6.0160000000
H	10.5587000000	3.5702000000	6.0160000000
H	10.5587000000	1.0562000000	6.0160000000
H	14.3987000000	3.5702000000	6.0160000000
H	14.3987000000	1.0562000000	6.0160000000
H	10.5587000000	7.4102000000	6.0160000000
H	10.5587000000	4.8952000000	6.0160000000
H	14.3987000000	7.4102000000	6.0160000000
H	14.3987000000	4.8952000000	6.0160000000
H	2.8797000000	11.2502000000	6.0160000000
H	2.8797000000	8.7352000000	6.0160000000
H	6.7187000000	11.2502000000	6.0160000000

H	6.7187000000	8.7352000000	6.0160000000
H	2.8797000000	15.0892000000	6.0160000000
H	2.8797000000	12.5742000000	6.0160000000
H	6.7187000000	15.0892000000	6.0160000000
H	6.7187000000	12.5742000000	6.0160000000
H	10.5587000000	11.2502000000	6.0160000000
H	10.5587000000	8.7352000000	6.0160000000
H	14.3987000000	11.2502000000	6.0160000000
H	14.3987000000	8.7352000000	6.0160000000
H	10.5587000000	15.0892000000	6.0160000000
H	10.5587000000	12.5742000000	6.0160000000
H	14.3987000000	15.0892000000	6.0160000000
H	14.3987000000	12.5742000000	6.0160000000
Si	10.3952616716	10.1221058476	14.3090110123
Cl	11.5363851894	9.1773082113	15.7354400719
Cl	10.4589057031	6.0377621384	14.1119261791
Cl	10.1924962350	12.1055835277	14.8806968581
Cl	8.4945134292	9.2936563859	14.3016204160

12. P3

Si	2.9498687926	0.2808465727	11.5382548020
Si	0.9597000000	2.3132000000	8.7671000000
Si	0.9587573025	0.3845636494	10.2106794885
Si	2.8797000000	2.3132000000	7.4101000000
Si	3.8822031553	2.2976164545	12.2594928268
Si	6.6597047568	0.5256055798	11.5387405646
Si	4.7997000000	2.3132000000	8.7671000000
Si	4.8024467511	0.3910865177	10.0707254358
Si	6.7187000000	2.3132000000	7.4101000000
Si	6.1129774196	2.3373719152	12.9652908767
Si	2.9451561182	4.2927903276	11.5028872149
Si	0.9597000000	6.1532000000	8.7671000000
Si	0.9407806769	4.2415660399	10.2011044428
Si	2.8797000000	6.1532000000	7.4101000000
Si	3.6362283399	6.1680367799	12.7383974016
Si	6.6410836742	4.1597925975	11.5205973369
Si	4.7997000000	6.1532000000	8.7671000000
Si	4.8325460283	4.2365736850	10.0563719201
Si	6.7187000000	6.1532000000	7.4101000000
Si	6.0623068447	6.1332497475	12.6994953166
Si	10.6383782838	0.5187946244	11.5380085281
Si	8.6387000000	2.3132000000	8.7671000000
Si	8.6461828128	0.4016985575	10.2096785519
Si	10.5587000000	2.3132000000	7.4101000000

Si	11.2038266794	2.3242723043	12.9970072107
Si	14.3251472772	0.2663517847	11.5380829511
Si	12.4787000000	2.3132000000	8.7671000000
Si	12.4819670267	0.3927196487	10.0613964072
Si	14.3987000000	2.3132000000	7.4101000000
Si	13.4400829802	2.3132691734	12.2640924824
Si	10.6481537537	4.1193439220	11.5203553908
Si	8.6387000000	6.1532000000	8.7671000000
Si	8.6421692152	4.2256571077	10.2142294557
Si	10.5587000000	6.1532000000	7.4101000000
Si	11.5321987489	6.1516176352	12.2900104840
Si	14.3207353224	4.3609236735	11.5450821285
Si	12.4787000000	6.1532000000	8.7671000000
Si	12.4892367657	4.2319358543	10.0535801220
Si	14.3987000000	6.1532000000	7.4101000000
Si	13.7826341849	6.1507515418	13.0461545505
Si	2.9328589932	8.0576041400	11.5164605329
Si	0.9597000000	9.9922000000	8.7671000000
Si	0.9351275380	8.0639415609	10.2056610546
Si	2.8797000000	9.9922000000	7.4101000000
Si	3.5694011394	10.0227195504	12.5829709175
Si	6.6837905963	8.0923884067	11.5495784718
Si	4.7997000000	9.9922000000	8.7671000000
Si	4.8214903542	8.0759545081	10.0938035506
Si	6.7187000000	9.9922000000	7.4101000000
Si	5.9636758072	10.0433793447	12.6774085764
Si	2.9381181160	12.0106968602	11.5260218971
Si	0.9597000000	13.8322000000	8.7671000000
Si	0.9467571391	11.9224076397	10.2105150584
Si	2.8797000000	13.8322000000	7.4101000000
Si	3.4926142350	13.8251790003	12.9789552320
Si	6.6533449022	11.9003917563	11.4270844511
Si	4.7997000000	13.8322000000	8.7671000000
Si	4.7487309062	11.9092559066	10.0442367454
Si	6.7187000000	13.8322000000	7.4101000000
Si	5.7239574575	13.8731015947	12.2544130550
Si	10.6437008840	8.1918161279	11.5526551249
Si	8.6387000000	9.9922000000	8.7671000000
Si	8.6637285753	8.0792046806	10.2118220262
Si	10.5587000000	9.9922000000	7.4101000000
Si	11.1701149259	9.9909370960	13.0400213251
Si	14.3135082313	7.9483823123	11.5546916134
Si	12.4787000000	9.9922000000	8.7671000000
Si	12.4786317315	8.0724047606	10.0626457154

Si	14.3987000000	9.9922000000	7.4101000000
Si	13.4132124478	9.9873191124	12.2802428667
Si	10.6357676765	11.7889003268	11.5504463307
Si	8.6387000000	13.8322000000	8.7671000000
Si	8.6725695919	11.9115838076	10.1832458784
Si	10.5587000000	13.8322000000	7.4101000000
Si	11.5255203411	13.8341804151	12.2738098719
Si	14.3113710679	12.0258842859	11.5361379661
Si	12.4787000000	13.8322000000	8.7671000000
Si	12.4708289680	11.9125984564	10.0601687256
Si	14.3987000000	13.8322000000	7.4101000000
Si	13.7644637970	13.8259052300	13.0128323576
H	2.8797000000	3.5702000000	6.5201000000
H	2.8797000000	1.0562000000	6.5201000000
H	6.7187000000	3.5702000000	6.5201000000
H	6.7187000000	1.0562000000	6.5201000000
H	2.8797000000	7.4102000000	6.5201000000
H	2.8797000000	4.8952000000	6.5201000000
H	6.7187000000	7.4102000000	6.5201000000
H	6.7187000000	4.8952000000	6.5201000000
H	10.5587000000	3.5702000000	6.5201000000
H	10.5587000000	1.0562000000	6.5201000000
H	14.3987000000	3.5702000000	6.5201000000
H	14.3987000000	1.0562000000	6.5201000000
H	10.5587000000	7.4102000000	6.5201000000
H	10.5587000000	4.8952000000	6.5201000000
H	14.3987000000	7.4102000000	6.5201000000
H	14.3987000000	4.8952000000	6.5201000000
H	2.8797000000	11.2502000000	6.5201000000
H	2.8797000000	8.7352000000	6.5201000000
H	6.7187000000	11.2502000000	6.5201000000
H	6.7187000000	8.7352000000	6.5201000000
H	2.8797000000	15.0892000000	6.5201000000
H	2.8797000000	12.5742000000	6.5201000000
H	6.7187000000	15.0892000000	6.5201000000
H	6.7187000000	12.5742000000	6.5201000000
H	10.5587000000	11.2502000000	6.5201000000
H	10.5587000000	8.7352000000	6.5201000000
H	14.3987000000	11.2502000000	6.5201000000
H	14.3987000000	8.7352000000	6.5201000000
H	10.5587000000	15.0892000000	6.5201000000
H	10.5587000000	12.5742000000	6.5201000000
H	14.3987000000	15.0892000000	6.5201000000
H	14.3987000000	12.5742000000	6.5201000000

Si	7.0342983675	5.7852274343	14.8102196768
Cl	7.5317124030	7.4213560041	15.9420356155
Cl	8.8207597730	4.7563285386	14.5019113567
Cl	5.8076023681	4.5796439503	15.9552679615
Cl	6.6234563972	10.3822900307	14.6297624471

13. TS4

Si	2.9541829991	0.2755349162	11.0381319112
Si	0.9597000000	2.3132000000	8.2630261349
Si	0.9602438495	0.3834073307	9.7077306058
Si	2.8797000000	2.3132000000	6.9060261349
Si	3.8495409390	2.3144240845	11.7738323613
Si	6.6427014936	0.5270568682	11.0449088279
Si	4.7997000000	2.3132000000	8.2630261349
Si	4.7983311346	0.3923797555	9.5575487068
Si	6.7187000000	2.3132000000	6.9060261349
Si	6.0935051463	2.3213836700	12.5312131811
Si	2.9529407355	4.3501244660	11.0313279088
Si	0.9597000000	6.1532000000	8.2630261349
Si	0.9500123390	4.2420303500	9.7118016718
Si	2.8797000000	6.1532000000	6.9060261349
Si	3.5056573267	6.1442148282	12.5184328505
Si	6.6445751096	4.1139353305	11.0406739374
Si	4.7997000000	6.1532000000	8.2630261349
Si	4.7999497171	4.2345709684	9.5568593139
Si	6.7187000000	6.1532000000	6.9060261349
Si	5.7502724558	6.1497542005	11.7782465404
Si	10.6310926520	0.5025698375	11.0269929689
Si	8.6387000000	2.3132000000	8.2630261349
Si	8.6335927708	0.4020236730	9.7085846524
Si	10.5587000000	2.3132000000	6.9060261349
Si	11.2050873660	2.3108547702	12.4785726730
Si	14.3173441907	0.2774433200	11.0232501857
Si	12.4787000000	2.3132000000	8.2630261349
Si	12.4745984373	0.3922678242	9.5575376573
Si	14.3987000000	2.3132000000	6.9060261349
Si	13.4384912307	2.3333436278	11.7514652282
Si	10.6411766089	4.1335345191	11.0441880361
Si	8.6387000000	6.1532000000	8.2630261349
Si	8.6433429984	4.2274234294	9.7168827797
Si	10.5587000000	6.1532000000	6.9060261349
Si	11.4727353404	6.1698562293	11.9224123170
Si	14.3225092117	4.3790689925	11.0589163198
Si	12.4787000000	6.1532000000	8.2630261349

Si	12.4738413580	4.2345859809	9.5714592314
Si	14.3987000000	6.1532000000	6.9060261349
Si	13.8096795857	6.1563735427	12.5998019977
Si	2.9496437416	7.9324942566	11.0306582993
Si	0.9597000000	9.9922000000	8.2630261349
Si	0.9627626722	8.0589557432	9.7005524536
Si	2.8797000000	9.9922000000	6.9060261349
Si	3.8021037813	9.9912472860	11.7420576630
Si	6.6457021299	8.1887368580	11.0358019429
Si	4.7997000000	9.9922000000	8.2630261349
Si	4.7999411408	8.0737626330	9.5599314177
Si	6.7187000000	9.9922000000	6.9060261349
Si	6.0355492404	10.0048958787	12.4538085240
Si	2.9425320292	12.0484583079	11.0306174977
Si	0.9597000000	13.8322000000	8.2630261349
Si	0.9555451958	11.9242066135	9.7012646525
Si	2.8797000000	13.8322000000	6.9060261349
Si	3.5017721275	13.8367688187	12.5214385409
Si	6.6306710484	11.8099795968	11.0195737691
Si	4.7997000000	13.8322000000	8.2630261349
Si	4.7865313173	11.9121923996	9.5525905810
Si	6.7187000000	13.8322000000	6.9060261349
Si	5.7435341929	13.8502686523	11.7714103316
Si	10.6576188103	8.1291951695	10.9194528111
Si	8.6387000000	9.9922000000	8.2630261349
Si	8.6277284820	8.0761141332	9.6888815657
Si	10.5587000000	9.9922000000	6.9060261349
Si	11.2201150265	9.8682660768	12.4167158235
Si	14.3487852263	7.9060749738	11.0426928005
Si	12.4787000000	9.9922000000	8.2630261349
Si	12.5121895616	8.0772524127	9.5297586513
Si	14.3987000000	9.9922000000	6.9060261349
Si	13.4974161423	9.9455741009	11.7413737482
Si	10.6008566844	11.7602854848	11.0782456324
Si	8.6387000000	13.8322000000	8.2630261349
Si	8.6313420200	11.8997837979	9.7103760433
Si	10.5587000000	13.8322000000	6.9060261349
Si	11.5081398260	13.8092575530	11.7753046528
Si	14.3207821724	12.0198563299	11.0273563652
Si	12.4787000000	13.8322000000	8.2630261349
Si	12.4551713087	11.9025334975	9.5754549802
Si	14.3987000000	13.8322000000	6.9060261349
Si	13.7474763798	13.8251983336	12.4849165224
H	2.8797000000	3.5702000000	6.0160261413

H	2.8797000000	1.0562000000	6.0160261413
H	6.7187000000	3.5702000000	6.0160261413
H	6.7187000000	1.0562000000	6.0160261413
H	2.8797000000	7.4102000000	6.0160261413
H	2.8797000000	4.8952000000	6.0160261413
H	6.7187000000	7.4102000000	6.0160261413
H	6.7187000000	4.8952000000	6.0160261413
H	10.5587000000	3.5702000000	6.0160261413
H	10.5587000000	1.0562000000	6.0160261413
H	14.3987000000	3.5702000000	6.0160261413
H	14.3987000000	1.0562000000	6.0160261413
H	10.5587000000	7.4102000000	6.0160261413
H	10.5587000000	4.8952000000	6.0160261413
H	14.3987000000	7.4102000000	6.0160261413
H	14.3987000000	4.8952000000	6.0160261413
H	2.8797000000	11.2502000000	6.0160261413
H	2.8797000000	8.7352000000	6.0160261413
H	6.7187000000	11.2502000000	6.0160261413
H	6.7187000000	8.7352000000	6.0160261413
H	2.8797000000	15.0892000000	6.0160261413
H	2.8797000000	12.5742000000	6.0160261413
H	6.7187000000	15.0892000000	6.0160261413
H	6.7187000000	12.5742000000	6.0160261413
H	10.5587000000	11.2502000000	6.0160261413
H	10.5587000000	8.7352000000	6.0160261413
H	14.3987000000	11.2502000000	6.0160261413
H	14.3987000000	8.7352000000	6.0160261413
H	10.5587000000	15.0892000000	6.0160261413
H	10.5587000000	12.5742000000	6.0160261413
H	14.3987000000	15.0892000000	6.0160261413
H	14.3987000000	12.5742000000	6.0160261413
Si	10.2937473421	8.3666191925	15.0222833898
Cl	12.2329668287	8.8611308658	15.5412049839
Cl	10.2843342736	6.4031607366	14.0445636499
Cl	9.5988694749	7.6880778417	16.8627110043
Cl	8.5998560131	9.4051002605	14.4052059214

14. TS5

Si	2.9488634273	0.2874299987	11.5321375274
Si	0.9597000000	2.3132000000	8.7670982436
Si	0.9570075991	0.3858600141	10.2090108473
Si	2.8797000000	2.3132000000	7.4100982436
Si	3.8444251199	2.3162507058	12.2524169739
Si	6.6471587777	0.5336528677	11.5510808412

Si	4.7997000000	2.3132000000	8.7670982436
Si	4.8004670174	0.3923316738	10.0651159471
Si	6.7187000000	2.3132000000	7.4100982436
Si	6.0822844111	2.3178620957	13.0348174849
Si	2.9454656002	4.3415883327	11.5299051357
Si	0.9597000000	6.1532000000	8.7670982436
Si	0.9550440467	4.2400369315	10.2075941740
Si	2.8797000000	6.1532000000	7.4100982436
Si	3.4568129312	6.1409102814	13.0242734467
Si	6.6442042569	4.1029637436	11.5512460309
Si	4.7997000000	6.1532000000	8.7670982436
Si	4.7992196692	4.2339498791	10.0637430238
Si	6.7187000000	6.1532000000	7.4100982436
Si	5.7004136200	6.0990310023	12.2761453532
Si	10.6334691681	0.5209480470	11.5388121898
Si	8.6387000000	2.3132000000	8.7670982436
Si	8.6365721884	0.4017578224	10.2157724487
Si	10.5587000000	2.3132000000	7.4100982436
Si	11.1909176650	2.3185964784	13.0144911516
Si	14.3214583565	0.2718037291	11.5388737942
Si	12.4787000000	2.3132000000	8.7670982436
Si	12.4775841850	0.3938179750	10.0609569694
Si	14.3987000000	2.3132000000	7.4100982436
Si	13.4302167945	2.3147297595	12.2710181750
Si	10.6328313918	4.1172584965	11.5394112773
Si	8.6387000000	6.1532000000	8.7670982436
Si	8.6356489403	4.2271364489	10.2164445152
Si	10.5587000000	6.1532000000	7.4100982436
Si	11.5231746082	6.1562417360	12.2906633683
Si	14.3202367345	4.3575870074	11.5390997284
Si	12.4787000000	6.1532000000	8.7670982436
Si	12.4757272315	4.2329719288	10.0615551856
Si	14.3987000000	6.1532000000	7.4100982436
Si	13.7694760054	6.1521462014	13.0277363653
Si	2.9211066839	7.9380425862	11.5249287118
Si	0.9597000000	9.9922000000	8.7670982436
Si	0.9388140767	8.0610491534	10.2038463838
Si	2.8797000000	9.9922000000	7.4100982436
Si	3.5648340094	9.9894256163	12.3816070432
Si	6.6695020763	8.0788332536	11.5110021635
Si	4.7997000000	9.9922000000	8.7670982436
Si	4.7742285326	8.0885432874	10.0764469115
Si	6.7187000000	9.9922000000	7.4100982436
Si	5.9293081111	10.0192081630	12.6192933454

Si	2.9195176432	12.0398576345	11.5192053825
Si	0.9597000000	13.8322000000	8.7670982436
Si	0.9369543612	11.9241251972	10.2014433771
Si	2.8797000000	13.8322000000	7.4100982436
Si	3.4792925236	13.8365179618	13.0073210778
Si	6.6607470510	11.9130587286	11.4473114668
Si	4.7997000000	13.8322000000	8.7670982436
Si	4.7568405090	11.9025180884	10.0549546367
Si	6.7187000000	13.8322000000	7.4100982436
Si	5.7092917988	13.8853075312	12.2456096812
Si	10.6379417782	8.1977868728	11.5550484173
Si	8.6387000000	9.9922000000	8.7670982436
Si	8.6659181746	8.0752127948	10.2021870007
Si	10.5587000000	9.9922000000	7.4100982436
Si	11.1732001907	9.9967796245	13.0387288837
Si	14.3115238230	7.9496713432	11.5434902973
Si	12.4787000000	9.9922000000	8.7670982436
Si	12.4710797236	8.0729261309	10.0616949501
Si	14.3987000000	9.9922000000	7.4100982436
Si	13.4169594789	9.9916327559	12.2750502663
Si	10.6389786507	11.7941718682	11.5488455791
Si	8.6387000000	13.8322000000	8.7670982436
Si	8.6734020390	11.9109341649	10.1862779842
Si	10.5587000000	13.8322000000	7.4100982436
Si	11.5268271417	13.8385937920	12.2749641152
Si	14.3101061593	12.0322865991	11.5386382883
Si	12.4787000000	13.8322000000	8.7670982436
Si	12.4714705552	11.9123868895	10.0579275951
Si	14.3987000000	13.8322000000	7.4100982436
Si	13.7667449313	13.8320106295	13.0189025185
H	2.8797000000	3.5702000000	6.5200982436
H	2.8797000000	1.0562000000	6.5200982436
H	6.7187000000	3.5702000000	6.5200982436
H	6.7187000000	1.0562000000	6.5200982436
H	2.8797000000	7.4102000000	6.5200982436
H	2.8797000000	4.8952000000	6.5200982436
H	6.7187000000	7.4102000000	6.5200982436
H	6.7187000000	4.8952000000	6.5200982436
H	10.5587000000	3.5702000000	6.5200982436
H	10.5587000000	1.0562000000	6.5200982436
H	14.3987000000	3.5702000000	6.5200982436
H	14.3987000000	1.0562000000	6.5200982436
H	10.5587000000	7.4102000000	6.5200982436
H	10.5587000000	4.8952000000	6.5200982436

H	14.3987000000	7.4102000000	6.5200982436
H	14.3987000000	4.8952000000	6.5200982436
H	2.8797000000	11.2502000000	6.5200982436
H	2.8797000000	8.7352000000	6.5200982436
H	6.7187000000	11.2502000000	6.5200982436
H	6.7187000000	8.7352000000	6.5200982436
H	2.8797000000	15.0892000000	6.5200982436
H	2.8797000000	12.5742000000	6.5200982436
H	6.7187000000	15.0892000000	6.5200982436
H	6.7187000000	12.5742000000	6.5200982436
H	10.5587000000	11.2502000000	6.5200982436
H	10.5587000000	8.7352000000	6.5200982436
H	14.3987000000	11.2502000000	6.5200982436
H	14.3987000000	8.7352000000	6.5200982436
H	10.5587000000	15.0892000000	6.5200982436
H	10.5587000000	12.5742000000	6.5200982436
H	14.3987000000	15.0892000000	6.5200982436
H	14.3987000000	12.5742000000	6.5200982436
Si	7.5368567524	7.9838558193	16.4162494711
Cl	8.2526199450	7.5538266890	18.3197256828
Cl	8.9114293441	7.3225045189	14.9910765430
Cl	5.7703668998	6.9427919391	16.0823675667
Cl	6.5483195162	10.2431157518	14.6347130278

15. VDW4

Si	3.8701676583	-0.1335117720	5.6822914357
Si	1.8870000000	1.9340000000	2.8900000000
Si	1.8872590249	0.0070837899	4.3373710134
Si	3.8070000000	1.9340000000	1.5330000000
Si	4.8174784019	1.8580380817	6.3640242734
Si	7.5696408855	0.1169642318	5.6589813341
Si	5.7260000000	1.9340000000	2.8900000000
Si	5.7245334410	0.0211150376	4.1825408437
Si	7.6460000000	1.9340000000	1.5330000000
Si	7.0432068666	1.9057139288	7.1674606095
Si	3.8549538257	3.8465434595	5.5771193761
Si	1.8870000000	5.7730000000	2.8900000000
Si	1.8471080817	3.8557073595	4.3116839103
Si	3.8070000000	5.7730000000	1.5330000000
Si	4.6304161135	5.7731110492	6.6107779231
Si	7.5996322854	3.6797805414	5.6539491939
Si	5.7260000000	5.7730000000	2.8900000000
Si	5.7600817338	3.8653239440	4.1864053579
Si	7.6460000000	5.7730000000	1.5330000000

Si	6.8977549365	5.7738720620	6.3328767422
Si	11.5574006360	0.1356306975	5.6604680777
Si	9.5660000000	1.9340000000	2.8900000000
Si	9.5615734932	0.0211862484	4.3327238217
Si	11.4860000000	1.9340000000	1.5330000000
Si	12.1118795680	1.9326738696	7.1424197043
Si	15.2480472994	-0.1083112074	5.6601246735
Si	13.4060000000	1.9340000000	2.8900000000
Si	13.4033933356	0.0140706636	4.1836033400
Si	15.3250000000	1.9340000000	1.5330000000
Si	14.3520690147	1.9295931731	6.3973268145
Si	11.5656757865	3.7319850210	5.6625001525
Si	9.5660000000	5.7730000000	2.8900000000
Si	9.5795485516	3.8376106745	4.3268141160
Si	11.4860000000	5.7730000000	1.5330000000
Si	12.4573495114	5.7735885305	6.3971802431
Si	15.2384837054	3.9752923837	5.6719334314
Si	13.4060000000	5.7730000000	2.8900000000
Si	13.4057468285	3.8539145458	4.1819747597
Si	15.3250000000	5.7730000000	1.5330000000
Si	14.7022913044	5.7739275522	7.1609483138
Si	3.8554950889	7.6997476201	5.5767539800
Si	1.8870000000	9.6130000000	2.8900000000
Si	1.8475795060	7.6909270100	4.3112662953
Si	3.8070000000	9.6130000000	1.5330000000
Si	4.8186095332	9.6879317961	6.3647596895
Si	7.5996737809	7.8678845741	5.6532601263
Si	5.7260000000	9.6130000000	2.8900000000
Si	5.7602716303	7.6812696280	4.1855978360
Si	7.6460000000	9.6130000000	1.5330000000
Si	7.0452755746	9.6417555607	7.1676777712
Si	3.8706151942	11.6793697520	5.6823837266
Si	1.8870000000	13.4530000000	2.8900000000
Si	1.8875608236	11.5400790367	4.3372330318
Si	3.8070000000	13.4530000000	1.5330000000
Si	4.4229346875	13.4521862450	7.1834221169
Si	7.5701383071	11.4297312738	5.6581539669
Si	5.7260000000	13.4530000000	2.8900000000
Si	5.7248423775	11.5260261594	4.1821737466
Si	7.6460000000	13.4530000000	1.5330000000
Si	6.6677534787	13.4523571080	6.3708735227
Si	11.5657513836	7.8149604244	5.6617009937
Si	9.5660000000	9.6130000000	2.8900000000
Si	9.5794680309	7.7090125887	4.3262518117

Si	11.4860000000	9.6130000000	1.5330000000
Si	12.1122468936	9.6144369285	7.1413388988
Si	15.2387941953	7.5720345789	5.6713694916
Si	13.4060000000	9.6130000000	2.8900000000
Si	13.4060035369	7.6926529636	4.1814594851
Si	15.3250000000	9.6130000000	1.5330000000
Si	14.3524753805	9.6179204142	6.3966563519
Si	11.5575930945	11.4118221509	5.6599458795
Si	9.5660000000	13.4530000000	2.8900000000
Si	9.5618235517	11.5261499788	4.3321764716
Si	11.4860000000	13.4530000000	1.5330000000
Si	12.4507410796	13.4529201544	6.3927913548
Si	15.2483529722	11.6560506603	5.6600543573
Si	13.4060000000	13.4530000000	2.8900000000
Si	13.4036998620	11.5331903147	4.1833460377
Si	15.3250000000	13.4530000000	1.5330000000
Si	14.6913745854	13.4530047512	7.1376800782
H	3.8070000000	3.1910000000	0.6430000000
H	3.8070000000	0.6760000000	0.6430000000
H	7.6460000000	3.1910000000	0.6430000000
H	7.6460000000	0.6760000000	0.6430000000
H	3.8070000000	7.0310000000	0.6430000000
H	3.8070000000	4.5160000000	0.6430000000
H	7.6460000000	7.0310000000	0.6430000000
H	7.6460000000	4.5160000000	0.6430000000
H	11.4860000000	3.1910000000	0.6430000000
H	11.4860000000	0.6760000000	0.6430000000
H	15.3250000000	3.1910000000	0.6430000000
H	15.3250000000	0.6760000000	0.6430000000
H	11.4860000000	7.0310000000	0.6430000000
H	11.4860000000	4.5160000000	0.6430000000
H	15.3250000000	7.0310000000	0.6430000000
H	15.3250000000	4.5160000000	0.6430000000
H	3.8070000000	10.8700000000	0.6430000000
H	3.8070000000	8.3560000000	0.6430000000
H	7.6460000000	10.8700000000	0.6430000000
H	7.6460000000	8.3560000000	0.6430000000
H	3.8070000000	14.7100000000	0.6430000000
H	3.8070000000	12.1950000000	0.6430000000
H	7.6460000000	14.7100000000	0.6430000000
H	7.6460000000	12.1950000000	0.6430000000
H	11.4860000000	10.8700000000	0.6430000000
H	11.4860000000	8.3560000000	0.6430000000
H	15.3250000000	10.8700000000	0.6430000000

H	15.3250000000	8.3560000000	0.6430000000
H	11.4860000000	14.7100000000	0.6430000000
H	11.4860000000	12.1950000000	0.6430000000
H	15.3250000000	14.7100000000	0.6430000000
H	15.3250000000	12.1950000000	0.6430000000
Si	5.1421198125	6.0022175338	10.6248146555
Cl	5.1570200090	6.0914545450	12.6582963648
Cl	4.1412220866	7.6205491529	9.8867931558
Cl	7.0665225486	6.0117431287	9.9446809024
Cl	4.2067399143	4.2888426171	10.0304878377

16. P4

Si	3.8860343404	-0.1062425688	5.6700041198
Si	1.8870000000	1.9340000000	2.8900000000
Si	1.8883027316	0.0064391632	4.3402028059
Si	3.8070000000	1.9340000000	1.5330000000
Si	4.8210019546	1.9112897771	6.4111972928
Si	7.5782568100	0.1336458006	5.6619753487
Si	5.7260000000	1.9340000000	2.8900000000
Si	5.7297017144	0.0139692078	4.1894372077
Si	7.6460000000	1.9340000000	1.5330000000
Si	7.0571519208	1.9551533689	7.1167064016
Si	3.8811925080	3.9028057859	5.6286372993
Si	1.8870000000	5.7730000000	2.8900000000
Si	1.8677294263	3.8630425347	4.3324332165
Si	3.8070000000	5.7730000000	1.5330000000
Si	4.6328165318	5.7844782117	6.8419940720
Si	7.5718076412	3.7635345110	5.6373153477
Si	5.7260000000	5.7730000000	2.8900000000
Si	5.7562762859	3.8582461574	4.1760363812
Si	7.6460000000	5.7730000000	1.5330000000
Si	7.0816812835	5.7740603561	6.7658300935
Si	11.5652924899	0.1373085106	5.6633441414
Si	9.5660000000	1.9340000000	2.8900000000
Si	9.5709992554	0.0235544772	4.3340265913
Si	11.4860000000	1.9340000000	1.5330000000
Si	12.1158732142	1.9357239118	7.1440373583
Si	15.2494981290	-0.1071030426	5.6633571881
Si	13.4060000000	1.9340000000	2.8900000000
Si	13.4080252986	0.0138546696	4.1828243969
Si	15.3250000000	1.9340000000	1.5330000000
Si	14.3575150141	1.9340760045	6.4032559784
Si	11.5628054237	3.7324515170	5.6628639467
Si	9.5660000000	5.7730000000	2.8900000000

Si	9.5712951247	3.8406259416	4.3311783180
Si	11.4860000000	5.7730000000	1.5330000000
Si	12.4527863750	5.7728216537	6.3966738618
Si	15.2457189120	3.9779479342	5.6787942540
Si	13.4060000000	5.7730000000	2.8900000000
Si	13.4099547397	3.8535735965	4.1864359345
Si	15.3250000000	5.7730000000	1.5330000000
Si	14.6910893513	5.7720184474	7.1601515445
Si	3.8892641605	7.6544478590	5.6100567082
Si	1.8870000000	9.6130000000	2.8900000000
Si	1.8686007732	7.6844625311	4.3297713043
Si	3.8070000000	9.6130000000	1.5330000000
Si	4.8239056492	9.6408898876	6.4095151299
Si	7.5753785537	7.7845508835	5.6385876942
Si	5.7260000000	9.6130000000	2.8900000000
Si	5.7654217556	7.6892317297	4.1698072710
Si	7.6460000000	9.6130000000	1.5330000000
Si	7.0603834288	9.5898646750	7.1236892341
Si	3.8861830049	11.6574356064	5.6722378273
Si	1.8870000000	13.4530000000	2.8900000000
Si	1.8893463540	11.5410157475	4.3404555470
Si	3.8070000000	13.4530000000	1.5330000000
Si	4.4499787590	13.4551681345	7.1362802937
Si	7.5797169110	11.4102013622	5.6661943337
Si	5.7260000000	13.4530000000	2.8900000000
Si	5.7310496163	11.5333727241	4.1903690885
Si	7.6460000000	13.4530000000	1.5330000000
Si	6.6905154673	13.4508621828	6.3985984682
Si	11.5650345043	7.8137742471	5.6617041847
Si	9.5660000000	9.6130000000	2.8900000000
Si	9.5732055293	7.7060762465	4.3310485213
Si	11.4860000000	9.6130000000	1.5330000000
Si	12.1183106928	9.6106520561	7.1420121472
Si	15.2490391569	7.5670435961	5.6808040867
Si	13.4060000000	9.6130000000	2.8900000000
Si	13.4130399171	7.6927754178	4.1869485381
Si	15.3250000000	9.6130000000	1.5330000000
Si	14.3600142395	9.6111764564	6.4028735115
Si	11.5659005553	11.4093845086	5.6624870158
Si	9.5660000000	13.4530000000	2.8900000000
Si	9.5706859246	11.5233169034	4.3345537692
Si	11.4860000000	13.4530000000	1.5330000000
Si	12.4546139201	13.4525294278	6.3951611401
Si	15.2501624923	11.6532300087	5.6627670222

Si	13.4060000000	13.4530000000	2.8900000000
Si	13.4087675754	11.5333625415	4.1824116029
Si	15.3250000000	13.4530000000	1.5330000000
Si	14.6948255694	13.4520812171	7.1401420864
H	3.8070000000	3.1910000000	0.6430000000
H	3.8070000000	0.6760000000	0.6430000000
H	7.6460000000	3.1910000000	0.6430000000
H	7.6460000000	0.6760000000	0.6430000000
H	3.8070000000	7.0310000000	0.6430000000
H	3.8070000000	4.5160000000	0.6430000000
H	7.6460000000	7.0310000000	0.6430000000
H	7.6460000000	4.5160000000	0.6430000000
H	11.4860000000	3.1910000000	0.6430000000
H	11.4860000000	0.6760000000	0.6430000000
H	15.3250000000	3.1910000000	0.6430000000
H	15.3250000000	0.6760000000	0.6430000000
H	11.4860000000	7.0310000000	0.6430000000
H	11.4860000000	4.5160000000	0.6430000000
H	15.3250000000	7.0310000000	0.6430000000
H	15.3250000000	4.5160000000	0.6430000000
H	3.8070000000	10.8700000000	0.6430000000
H	3.8070000000	8.3560000000	0.6430000000
H	7.6460000000	10.8700000000	0.6430000000
H	7.6460000000	8.3560000000	0.6430000000
H	3.8070000000	14.7100000000	0.6430000000
H	3.8070000000	12.1950000000	0.6430000000
H	7.6460000000	14.7100000000	0.6430000000
H	7.6460000000	12.1950000000	0.6430000000
H	11.4860000000	10.8700000000	0.6430000000
H	11.4860000000	8.3560000000	0.6430000000
H	15.3250000000	10.8700000000	0.6430000000
H	15.3250000000	8.3560000000	0.6430000000
H	11.4860000000	14.7100000000	0.6430000000
H	11.4860000000	12.1950000000	0.6430000000
H	15.3250000000	14.7100000000	0.6430000000
H	15.3250000000	12.1950000000	0.6430000000
Si	3.5980763296	5.8627186593	8.9439217775
Cl	4.8979593961	6.0246540394	10.5245263877
Cl	2.3294785955	7.5042446273	9.0135272636
Cl	7.9604062164	5.7649785779	8.6609899864
Cl	2.4479693188	4.1633510832	9.2236791857

17. TS6

Si	3.8849033464	-0.0959205358	5.6555537475
----	--------------	---------------	--------------

Si	1.8870000000	1.9340000000	2.8900000000
Si	1.8863285733	0.0059182916	4.3357744278
Si	3.8070000000	1.9340000000	1.5330000000
Si	4.7676670134	1.9491384296	6.4115178279
Si	7.5715536442	0.1465391070	5.6684906664
Si	5.7260000000	1.9340000000	2.8900000000
Si	5.7306674894	0.0131222183	4.1880530304
Si	7.6460000000	1.9340000000	1.5330000000
Si	7.0146100922	1.9452134293	7.1573839265
Si	3.8503387615	3.9553691105	5.6554927873
Si	1.8870000000	5.7730000000	2.8900000000
Si	1.8711172429	3.8570153591	4.3263872854
Si	3.8070000000	5.7730000000	1.5330000000
Si	4.4089231560	5.7754809213	7.0789548807
Si	7.5726422345	3.7352542453	5.6694734635
Si	5.7260000000	5.7730000000	2.8900000000
Si	5.7233641530	3.8564863525	4.1909478560
Si	7.6460000000	5.7730000000	1.5330000000
Si	6.7189244680	5.7747510753	6.4485994786
Si	11.5622341396	0.1368568258	5.6624435373
Si	9.5660000000	1.9340000000	2.8900000000
Si	9.5651183852	0.0253515686	4.3374167325
Si	11.4860000000	1.9340000000	1.5330000000
Si	12.1176738849	1.9334463784	7.1426893696
Si	15.2495002178	-0.1077216021	5.6628611745
Si	13.4060000000	1.9340000000	2.8900000000
Si	13.4059425479	0.0142482258	4.1834974157
Si	15.3250000000	1.9340000000	1.5330000000
Si	14.3573166221	1.9337905271	6.3969371631
Si	11.5628622810	3.7331788710	5.6659689586
Si	9.5660000000	5.7730000000	2.8900000000
Si	9.5671893510	3.8452657577	4.3382509210
Si	11.4860000000	5.7730000000	1.5330000000
Si	12.4593544005	5.7734334431	6.4011649542
Si	15.2443321155	3.9764174735	5.6628382253
Si	13.4060000000	5.7730000000	2.8900000000
Si	13.4029642158	3.8536604971	4.1829703894
Si	15.3250000000	5.7730000000	1.5330000000
Si	14.7027983384	5.7738563523	7.1482154926
Si	3.8528604213	7.5907508750	5.6499818228
Si	1.8870000000	9.6130000000	2.8900000000
Si	1.8716452106	7.6896939801	4.3251914654
Si	3.8070000000	9.6130000000	1.5330000000
Si	4.7690808141	9.5946425222	6.4143451937

Si	7.5712462544	7.8117975566	5.6633992833
Si	5.7260000000	9.6130000000	2.8900000000
Si	5.7239500997	7.6914233190	4.1864743985
Si	7.6460000000	9.6130000000	1.5330000000
Si	7.0185382637	9.5977084468	7.1587486090
Si	3.8854920673	11.6405633495	5.6573483869
Si	1.8870000000	13.4530000000	2.8900000000
Si	1.8870627738	11.5411133584	4.3361907874
Si	3.8070000000	13.4530000000	1.5330000000
Si	4.4607512148	13.4522309591	7.1030694029
Si	7.5720976068	11.3970471178	5.6693331750
Si	5.7260000000	13.4530000000	2.8900000000
Si	5.7307468342	11.5338961210	4.1884964613
Si	7.6460000000	13.4530000000	1.5330000000
Si	6.6960595558	13.4506455959	6.3883900762
Si	11.5627168399	7.8132877281	5.6649156053
Si	9.5660000000	9.6130000000	2.8900000000
Si	9.5672522513	7.7012479465	4.3366990596
Si	11.4860000000	9.6130000000	1.5330000000
Si	12.1182474329	9.6131933300	7.1410746964
Si	15.2451117199	7.5707417989	5.6623809365
Si	13.4060000000	9.6130000000	2.8900000000
Si	13.4033984578	7.6929123175	4.1826555919
Si	15.3250000000	9.6130000000	1.5330000000
Si	14.3578680231	9.6134177818	6.3962170890
Si	11.5622745558	11.4102163600	5.6618357469
Si	9.5660000000	13.4530000000	2.8900000000
Si	9.5648462944	11.5217159980	4.3372906526
Si	11.4860000000	13.4530000000	1.5330000000
Si	12.4529067879	13.4526894237	6.3959078009
Si	15.2498147853	11.6552580626	5.6626990965
Si	13.4060000000	13.4530000000	2.8900000000
Si	13.4062167996	11.5329999811	4.1832547435
Si	15.3250000000	13.4530000000	1.5330000000
Si	14.6937672166	13.4528506686	7.1412542277
H	3.8070000000	3.1910000000	0.6430000000
H	3.8070000000	0.6760000000	0.6430000000
H	7.6460000000	3.1910000000	0.6430000000
H	7.6460000000	0.6760000000	0.6430000000
H	3.8070000000	7.0310000000	0.6430000000
H	3.8070000000	4.5160000000	0.6430000000
H	7.6460000000	7.0310000000	0.6430000000
H	7.6460000000	4.5160000000	0.6430000000
H	11.4860000000	3.1910000000	0.6430000000

H	11.4860000000	0.6760000000	0.6430000000
H	15.3250000000	3.1910000000	0.6430000000
H	15.3250000000	0.6760000000	0.6430000000
H	11.4860000000	7.0310000000	0.6430000000
H	11.4860000000	4.5160000000	0.6430000000
H	15.3250000000	7.0310000000	0.6430000000
H	15.3250000000	4.5160000000	0.6430000000
H	3.8070000000	10.8700000000	0.6430000000
H	3.8070000000	8.3560000000	0.6430000000
H	7.6460000000	10.8700000000	0.6430000000
H	7.6460000000	8.3560000000	0.6430000000
H	3.8070000000	14.7100000000	0.6430000000
H	3.8070000000	12.1950000000	0.6430000000
H	7.6460000000	14.7100000000	0.6430000000
H	7.6460000000	12.1950000000	0.6430000000
H	11.4860000000	10.8700000000	0.6430000000
H	11.4860000000	8.3560000000	0.6430000000
H	15.3250000000	10.8700000000	0.6430000000
H	15.3250000000	8.3560000000	0.6430000000
H	11.4860000000	14.7100000000	0.6430000000
H	11.4860000000	12.1950000000	0.6430000000
H	15.3250000000	14.7100000000	0.6430000000
H	15.3250000000	12.1950000000	0.6430000000
Si	4.8852810038	5.9362081528	10.1455795339
Cl	5.2470673787	6.0588062987	12.1821539525
Cl	3.8348743556	7.6781461630	9.8106149567
Cl	6.8749493098	5.9314585084	9.4538063631
Cl	3.8927287564	4.1379311702	10.0048265782