

## XYZ coordinates of optimized structures

Optimized structures of alkanes adsorbed on Pt and SrTiO<sub>3</sub> surface models (Figures S5, S7, and S10) using SCAN/rvv10 functional are presented below in VASP-style output (CONTCAR/POSCAR) which contain the unit cell vectors and direct coordinates of all atoms. For information on the structure of these files, we refer to the description given in the VASP online manual ([http://cms.mpi.univie.ac.at/vasp/vasp/POSCAR\\_file.html](http://cms.mpi.univie.ac.at/vasp/vasp/POSCAR_file.html)).

### C<sub>4</sub>H<sub>10</sub>···Pt (111)

Energy: -6773.926147 eV

```
1.0000000000000000
16.5000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 9.5261999999999993 0.0000000000000000
0.0000000000000000 0.0000000000000000 23.7360000000000007
Pt C H
96 4 10
Selective dynamics
Direct
0.16667000000000034 0.33332999999999966 0.00000000000000000 F F F
0.00000000000000000 0.83332999999999966 0.00000000000000000 F F F
0.25000000000000000 0.08332999999999966 0.00000000000000000 F F F
0.08332999999999966 0.58332999999999966 0.00000000000000000 F F F
0.08332999999999966 0.08332999999999966 0.00000000000000000 F F F
0.25000000000000000 0.58332999999999966 0.00000000000000000 F F F
0.00000000000000000 0.33332999999999966 0.00000000000000000 F F F
0.16667000000000034 0.83332999999999966 0.00000000000000000 F F F
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0.33332999999999966 0.83332999999999966 0.00000000000000000 F F F
0.58332999999999966 0.08332999999999966 0.00000000000000000 F F F
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0.41667000000000034 0.08332999999999966 0.00000000000000000 F F F
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0.33332999999999966 0.33332999999999966 0.00000000000000000 F F F
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0.66667000000000034 0.83332999999999966 0.00000000000000000 F F F
0.91667000000000034 0.08332999999999966 0.00000000000000000 F F F
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0.33332999999999966 0.00000000000000000 0.09459999999999998 F F F
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0.83332999999999966 0.00000000000000000 0.09459999999999998 F F F
0.66667000000000034 0.50000000000000000 0.09459999999999998 F F F
0.75000000000000000 0.25000000000000000 0.09459999999999998 F F F
0.91667000000000034 0.75000000000000000 0.09459999999999998 F F F
0.91667000000000034 0.25000000000000000 0.09459999999999998 F F F
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0.0833404071700285	0.4170941276997178	0.1885275763795623	T	T	T
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0.1665435307979193	0.1671733810618876	0.1885746518445102	T	T	T
0.0000411520372839	0.6670308749757592	0.1885735961216664	T	T	T
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0.7053560411513796	0.5000784579291288	0.4193478979962326	T	T	T
0.4146582975613485	0.5666236079289670	0.4579500045788497	T	T	T
0.3672190025638177	0.4316417153972250	0.4182833823631772	T	T	T
0.4166490829529772	0.5720333100767331	0.3836410590854769	T	T	T

**C<sub>6</sub>H<sub>14</sub>···Pt (111)**

**Energy: -6808.970023 eV**

1.0000000000000000

16.500000000000000 0.000000000000000 0.000000000000000  
0.000000000000000 9.526199999999993 0.000000000000000  
0.000000000000000 0.000000000000000 23.736000000000007

Pt C H  
96 6 14

Selective dynamics

Direct

0.1666700000000034	0.3333299999999966	0.0000000000000000	F	F	F
0.0000000000000000	0.8333299999999966	0.0000000000000000	F	F	F
0.2500000000000000	0.0833299999999966	0.0000000000000000	F	F	F
0.0833299999999966	0.5833299999999966	0.0000000000000000	F	F	F
0.0833299999999966	0.0833299999999966	0.0000000000000000	F	F	F
0.2500000000000000	0.5833299999999966	0.0000000000000000	F	F	F
0.0000000000000000	0.3333299999999966	0.0000000000000000	F	F	F
0.1666700000000034	0.8333299999999966	0.0000000000000000	F	F	F
0.5000000000000000	0.3333299999999966	0.0000000000000000	F	F	F
0.3333299999999966	0.8333299999999966	0.0000000000000000	F	F	F
0.5833299999999966	0.0833299999999966	0.0000000000000000	F	F	F
0.4166700000000034	0.5833299999999966	0.0000000000000000	F	F	F
0.4166700000000034	0.0833299999999966	0.0000000000000000	F	F	F
0.5833299999999966	0.5833299999999966	0.0000000000000000	F	F	F
0.3333299999999966	0.3333299999999966	0.0000000000000000	F	F	F
0.5000000000000000	0.8333299999999966	0.0000000000000000	F	F	F
0.8333299999999966	0.3333299999999966	0.0000000000000000	F	F	F
0.6666700000000034	0.8333299999999966	0.0000000000000000	F	F	F
0.9166700000000034	0.0833299999999966	0.0000000000000000	F	F	F
0.7500000000000000	0.5833299999999966	0.0000000000000000	F	F	F
0.7500000000000000	0.0833299999999966	0.0000000000000000	F	F	F
0.9166700000000034	0.5833299999999966	0.0000000000000000	F	F	F
0.6666700000000034	0.3333299999999966	0.0000000000000000	F	F	F
0.8333299999999966	0.8333299999999966	0.0000000000000000	F	F	F
0.1666700000000034	0.0000000000000000	0.0945999999999998	F	F	F
0.0000000000000000	0.5000000000000000	0.0945999999999998	F	F	F
0.0833299999999966	0.2500000000000000	0.0945999999999998	F	F	F
0.2500000000000000	0.7500000000000000	0.0945999999999998	F	F	F
0.2500000000000000	0.2500000000000000	0.0945999999999998	F	F	F
0.0833299999999966	0.7500000000000000	0.0945999999999998	F	F	F
0.0000000000000000	0.0000000000000000	0.0945999999999998	F	F	F
0.1666700000000034	0.5000000000000000	0.0945999999999998	F	F	F
0.5000000000000000	0.0000000000000000	0.0945999999999998	F	F	F
0.3333299999999966	0.5000000000000000	0.0945999999999998	F	F	F
0.4166700000000034	0.2500000000000000	0.0945999999999998	F	F	F
0.5833299999999966	0.7500000000000000	0.0945999999999998	F	F	F
0.5833299999999966	0.2500000000000000	0.0945999999999998	F	F	F
0.4166700000000034	0.7500000000000000	0.0945999999999998	F	F	F
0.3333299999999966	0.0000000000000000	0.0945999999999998	F	F	F
0.5000000000000000	0.5000000000000000	0.0945999999999998	F	F	F
0.8333299999999966	0.0000000000000000	0.0945999999999998	F	F	F
0.6666700000000034	0.5000000000000000	0.0945999999999998	F	F	F
0.7500000000000000	0.2500000000000000	0.0945999999999998	F	F	F
0.9166700000000034	0.7500000000000000	0.0945999999999998	F	F	F
0.9166700000000034	0.2500000000000000	0.0945999999999998	F	F	F
0.7500000000000000	0.7500000000000000	0.0945999999999998	F	F	F
0.6666700000000034	0.0000000000000000	0.0945999999999998	F	F	F
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0.2694387102827902	0.5743368477114303	0.3851611294081334	T	T	T
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**C<sub>8</sub>H<sub>18</sub>···Pt (111)**

**Energy: -6844.029836 eV**

1.0000000000000000  
16.5000000000000000 0.0000000000000000 0.0000000000000000  
0.0000000000000000 9.5261999999999993 0.0000000000000000  
0.0000000000000000 0.0000000000000000 23.7360000000000007

Pt C H  
96 8 18

Selective dynamics

Direct

0.1666700000000034	0.3333299999999966	0.0000000000000000	F	F	F
0.0000000000000000	0.8333299999999966	0.0000000000000000	F	F	F
0.2500000000000000	0.0833299999999966	0.0000000000000000	F	F	F
0.0833299999999966	0.5833299999999966	0.0000000000000000	F	F	F

0.083329999999966	0.083329999999966	0.000000000000000	F F F
0.250000000000000	0.583329999999966	0.000000000000000	F F F
0.000000000000000	0.333329999999966	0.000000000000000	F F F
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0.333329999999966	0.833329999999966	0.000000000000000	F F F
0.583329999999966	0.083329999999966	0.000000000000000	F F F
0.416670000000034	0.583329999999966	0.000000000000000	F F F
0.416670000000034	0.083329999999966	0.000000000000000	F F F
0.583329999999966	0.583329999999966	0.000000000000000	F F F
0.333329999999966	0.333329999999966	0.000000000000000	F F F
0.500000000000000	0.833329999999966	0.000000000000000	F F F
0.833329999999966	0.333329999999966	0.000000000000000	F F F
0.666670000000034	0.833329999999966	0.000000000000000	F F F
0.916670000000034	0.083329999999966	0.000000000000000	F F F
0.750000000000000	0.583329999999966	0.000000000000000	F F F
0.750000000000000	0.083329999999966	0.000000000000000	F F F
0.916670000000034	0.583329999999966	0.000000000000000	F F F
0.666670000000034	0.333329999999966	0.000000000000000	F F F
0.833329999999966	0.833329999999966	0.000000000000000	F F F
0.166670000000034	0.000000000000000	0.094599999999998	F F F
0.000000000000000	0.500000000000000	0.094599999999998	F F F
0.083329999999966	0.250000000000000	0.094599999999998	F F F
0.250000000000000	0.750000000000000	0.094599999999998	F F F
0.250000000000000	0.250000000000000	0.094599999999998	F F F
0.083329999999966	0.750000000000000	0.094599999999998	F F F
0.000000000000000	0.000000000000000	0.094599999999998	F F F
0.166670000000034	0.500000000000000	0.094599999999998	F F F
0.500000000000000	0.000000000000000	0.094599999999998	F F F
0.333329999999966	0.500000000000000	0.094599999999998	F F F
0.416670000000034	0.250000000000000	0.094599999999998	F F F
0.583329999999966	0.750000000000000	0.094599999999998	F F F
0.583329999999966	0.250000000000000	0.094599999999998	F F F
0.416670000000034	0.750000000000000	0.094599999999998	F F F
0.333329999999966	0.000000000000000	0.094599999999998	F F F
0.500000000000000	0.500000000000000	0.094599999999998	F F F
0.833329999999966	0.000000000000000	0.094599999999998	F F F
0.666670000000034	0.500000000000000	0.094599999999998	F F F
0.750000000000000	0.250000000000000	0.094599999999998	F F F
0.916670000000034	0.750000000000000	0.094599999999998	F F F
0.916670000000034	0.250000000000000	0.094599999999998	F F F
0.750000000000000	0.750000000000000	0.094599999999998	F F F
0.666670000000034	0.000000000000000	0.094599999999998	F F F
0.833329999999966	0.500000000000000	0.094599999999998	F F F
0.9990754349202232	0.1699553114550781	0.1887880590342148	T T T
0.1651320189446527	0.6697498316341385	0.1885955350141520	T T T
0.2488086385093723	0.4191423300958669	0.1885155977093860	T T T
0.0820850450388767	0.9200644508851433	0.1887705996861921	T T T
0.0822280810707434	0.4195904977945578	0.1885771805356426	T T T
0.2485714776057395	0.9192909200303182	0.1886307545011650	T T T
0.1657508097778949	0.1690943783510531	0.1886527108131056	T T T
0.9990970604435714	0.6701905722911796	0.1886826893991540	T T T
0.3323853228185205	0.1687217440845308	0.1884836650390403	T T T
0.4990353910955675	0.6698729357255720	0.1882016832900437	T T T
0.5824948791275941	0.4193636326836865	0.1882663401506481	T T T
0.4155173071667636	0.9189707811677277	0.1885074205937954	T T T
0.4154770972814482	0.4195007626247603	0.1884023525093070	T T T
0.5827253902322581	0.9187778364362165	0.1884981681658343	T T T
0.4990504942261375	0.1685456642886714	0.1883926972486452	T T T
0.3317876726594106	0.6698205017884120	0.1884138435472819	T T T
0.6658338833019819	0.1684622638581670	0.1883865704980550	T T T
0.8329988510628867	0.6697641493643476	0.1887830303377393	T T T
0.9159399849812786	0.4197862404572257	0.1887143919697288	T T T
0.7497592452157358	0.9191075669295433	0.1886368321813101	T T T
0.7494408382959663	0.4192975776826577	0.1885402336839542	T T T
0.9160068835769883	0.9201423371741341	0.1887485323518468	T T T
0.8325052956557562	0.1694053490061291	0.1886537955274597	T T T
0.6663899155551556	0.6694213608838893	0.1883991473179264	T T T
0.1637657621964127	0.3385950772542107	0.2842652649294845	T T T
0.9980542375118063	0.8392319802350584	0.2849566639726436	T T T

0.2473069757463521	0.0884753558835980	0.2847264833259138	T	T	T
0.0808843141354944	0.5892700126486664	0.2847296022220593	T	T	T
0.0811017387510519	0.0888879586728726	0.2849436810414099	T	T	T
0.2470229970096624	0.5903069189824147	0.2841200060377044	T	T	T
0.9980999882844835	0.3388501654715049	0.2848223047885462	T	T	T
0.1641958847149111	0.8397377137453950	0.2847978127186663	T	T	T
0.4979212193269556	0.3375480245273981	0.2834764110395798	T	T	T
0.3308770099935636	0.8404834203400645	0.2846350385215281	T	T	T
0.5815974908981429	0.0880082104612842	0.2844815115579491	T	T	T
0.4142368832750515	0.5914524301263915	0.2836534458274074	T	T	T
0.4144105456669147	0.0881002886874401	0.2845390199480940	T	T	T
0.5813266487373796	0.5909974822063490	0.2836504932023978	T	T	T
0.3306424540032504	0.3376197885111721	0.2839149515374933	T	T	T
0.4979560210989101	0.8407480690237885	0.2845603400115980	T	T	T
0.8320608330205863	0.3386560407919183	0.2843617688507794	T	T	T
0.6650468498723320	0.8404461475384046	0.2845281579938002	T	T	T
0.9150772128751742	0.0887228133620520	0.2849333639264443	T	T	T
0.7484839908741312	0.5908623040823385	0.2843731644890197	T	T	T
0.7485492623120626	0.0886584166545494	0.2846492919122482	T	T	T
0.9151118244843198	0.5894553334375477	0.2848166034681419	T	T	T
0.6648924915756459	0.3375219435293777	0.2835715938740630	T	T	T
0.8319408960367681	0.8399750440029429	0.2849090881645146	T	T	T
0.4957924567290234	0.4139215132098309	0.4202796103184464	T	T	T
0.5717500051064921	0.5039404551526662	0.4211207219089676	T	T	T
0.4174171353658194	0.4972811345759959	0.4208658504263359	T	T	T
0.6499770257707658	0.4201474335364589	0.4226392571242646	T	T	T
0.3413252414263286	0.4077910106261325	0.4193444707712297	T	T	T
0.7262337417756626	0.5093518728875922	0.4222685496299524	T	T	T
0.2636138665333352	0.4923676014712497	0.4223962535103320	T	T	T
0.8034565567871750	0.4233826746471146	0.4255680677546596	T	T	T
0.4966800097780615	0.3405979448605259	0.4559992742913607	T	T	T
0.4970019867078672	0.3462309314627779	0.3820049375735808	T	T	T
0.5695823610774658	0.5761541248584141	0.4571742386152499	T	T	T
0.5718852471242990	0.5724834190013827	0.3831280295196011	T	T	T
0.4167305930808756	0.5697357295546351	0.3840940079237581	T	T	T
0.4159474742433286	0.5656673146614812	0.4581135048253397	T	T	T
0.6514984928540800	0.3482192934863390	0.3858051784964516	T	T	T
0.6502335745417296	0.3514479429070216	0.4598157907003934	T	T	T
0.3430740762298167	0.3296870110138111	0.4532864145296308	T	T	T
0.3415955373600431	0.3449162884153981	0.3796429335931802	T	T	T
0.7240355840909564	0.5856665993768245	0.4568380174728165	T	T	T
0.7268274378478785	0.5733922619624258	0.3830848029104318	T	T	T
0.2592410617526854	0.5500800045942608	0.4620844600658468	T	T	T
0.2613280299476929	0.5705896552057476	0.3881686854776137	T	T	T
0.2100492550187056	0.4258823632488007	0.4181603407439198	T	T	T
0.8573840262326700	0.4893578903031286	0.4227408239838797	T	T	T
0.8062383247681090	0.3472227925462040	0.3906970812646277	T	T	T
0.8064028380065059	0.3635098446297418	0.4648068779693984	T	T	T

### C<sub>4</sub>H<sub>10</sub>···Pt (100)

Energy: -6758.763140 eV

1.0000000000000000

11.6672999999999991 0.0000000000000000 0.0000000000000000

0.0000000000000000 15.5564000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 22.8336000000000006

Pt C H

96 4 10

Selective dynamics

Direct

0.0000000000000000 0.1250000000000000 0.0000000000000000 F F F

0.1666700000000003 0.0000000000000000 0.0000000000000000 F F F

0.0000000000000000 0.0000000000000000 0.0851600000000019 F F F

0.1666700000000003 0.1250000000000000 0.0851600000000019 F F F

0.0001378883916429 0.1250266948394504 0.1692840767659526 T T T

0.1666811043224261 0.0001713883616132 0.1693258625748461 T T T

0.0000508221893551 0.0001978015070625 0.2522043947102639 T T T

0.1665943141194408 0.1251190875011387 0.2522049429890707 T T T

0.3333299999999966 0.1250000000000000 0.0000000000000000 F F F

0.5000000000000000 0.0000000000000000 0.0000000000000000 F F F

0.3333299999999966	0.0000000000000000	0.0851600000000019	F	F	F
0.5000000000000000	0.1250000000000000	0.0851600000000019	F	F	F
0.3333397689540622	0.1251131997109369	0.1692257353946965	T	T	T
0.4999949016026504	0.0001821416489561	0.1693085626511036	T	T	T
0.3334303368342624	0.0003551503504360	0.2521605045969111	T	T	T
0.5000281268246478	0.1253704719598202	0.2521236464518086	T	T	T
0.6666700000000034	0.1250000000000000	0.0000000000000000	F	F	F
0.8333299999999966	0.0000000000000000	0.0000000000000000	F	F	F
0.6666700000000034	0.0000000000000000	0.0851600000000019	F	F	F
0.8333299999999966	0.1250000000000000	0.0851600000000019	F	F	F
0.6666093545370512	0.1250647971007091	0.1692359814728042	T	T	T
0.8333640235744310	0.0001397314554754	0.1692930530117555	T	T	T
0.6666008543993668	0.0003431811737637	0.2522239664028858	T	T	T
0.8335692374062665	0.1249968781540843	0.2521332719991868	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1666700000000034	0.2500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.2500000000000000	0.0851600000000019	F	F	F
0.1666700000000034	0.3750000000000000	0.0851600000000019	F	F	F
0.0002206523459035	0.3749714893158556	0.1691817727342474	T	T	T
0.1667725942557497	0.2500853755653438	0.1692550253142177	T	T	T
-0.0002302602101701	0.2500596150633173	0.2521242860466528	T	T	T
0.1662461778915620	0.3747619427813798	0.2522007136084339	T	T	T
0.3333299999999966	0.3750000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3333299999999966	0.2500000000000000	0.0851600000000019	F	F	F
0.5000000000000000	0.3750000000000000	0.0851600000000019	F	F	F
0.3335012092243093	0.3753319831678418	0.1694993086466065	T	T	T
0.4998582367984491	0.2502577792129577	0.1692900734069404	T	T	T
0.3329373514380140	0.2499327337106543	0.2521899094299944	T	T	T
0.5001749012247586	0.3740125064487222	0.2530766070166788	T	T	T
0.6666700000000034	0.3750000000000000	0.0000000000000000	F	F	F
0.8333299999999966	0.2500000000000000	0.0000000000000000	F	F	F
0.6666700000000034	0.2500000000000000	0.0851600000000019	F	F	F
0.8333299999999966	0.3750000000000000	0.0851600000000019	F	F	F
0.6663303013504625	0.3750168118237764	0.1692432229377168	T	T	T
0.8333547639742572	0.2500478348236235	0.1692509798182144	T	T	T
0.6674032294408550	0.2497052283769050	0.2521535827329557	T	T	T
0.8332649336500685	0.3752857988538506	0.2519444090077126	T	T	T
0.0000000000000000	0.6250000000000000	0.0000000000000000	F	F	F
0.1666700000000034	0.5000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.0851600000000019	F	F	F
0.1666700000000034	0.6250000000000000	0.0851600000000019	F	F	F
0.0001518055316356	0.6252060821808765	0.1691316256615799	T	T	T
0.1672594190532169	0.5000635756049931	0.1693358099195915	T	T	T
0.0001940016922633	0.5001410442883090	0.2519016015104462	T	T	T
0.1657806882019361	0.6257437651960627	0.2521589135139822	T	T	T
0.3333299999999966	0.6250000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.3333299999999966	0.5000000000000000	0.0851600000000019	F	F	F
0.5000000000000000	0.6250000000000000	0.0851600000000019	F	F	F
0.3333135737637252	0.6247996024341759	0.1694465858194608	T	T	T
0.4993558268227640	0.4997992925562584	0.1696360886070848	T	T	T
0.3315996240212726	0.4999588815065129	0.2538846502983014	T	T	T
0.5017487989421184	0.6262743274535401	0.2513824561472930	T	T	T
0.6666700000000034	0.6250000000000000	0.0000000000000000	F	F	F
0.8333299999999966	0.5000000000000000	0.0000000000000000	F	F	F
0.6666700000000034	0.5000000000000000	0.0851600000000019	F	F	F
0.8333299999999966	0.6250000000000000	0.0851600000000019	F	F	F
0.6670909651368717	0.6252808986025098	0.1687319572456787	T	T	T
0.8338467929788214	0.4999245613924897	0.1689126190195183	T	T	T
0.6680501262981138	0.5006897949077791	0.2514343100373413	T	T	T
0.8336309312710974	0.6252725041698053	0.2518745427068231	T	T	T
0.0000000000000000	0.8750000000000000	0.0000000000000000	F	F	F
0.1666700000000034	0.7500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.7500000000000000	0.0851600000000019	F	F	F
0.1666700000000034	0.8750000000000000	0.0851600000000019	F	F	F
0.0001456659560851	0.8752937277905245	0.1693072041575571	T	T	T
0.1667688561124188	0.7502078045058361	0.1691860089007164	T	T	T
-0.0000477067989437	0.7504805750556247	0.2521235870685767	T	T	T
0.1667983868504984	0.8752523773216521	0.2521682160539964	T	T	T

0.3333299999999966	0.8750000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.7500000000000000	0.0000000000000000	F	F	F
0.3333299999999966	0.7500000000000000	0.0851600000000019	F	F	F
0.5000000000000000	0.8750000000000000	0.0851600000000019	F	F	F
0.3332405826617412	0.8753616328638723	0.1692035697413591	T	T	T
0.4998937110399362	0.7504981247381325	0.1688928590344431	T	T	T
0.3333498424684233	0.7504477151455657	0.2519691843835082	T	T	T
0.5000438518758769	0.8752319076830014	0.2520490712814176	T	T	T
0.6666700000000034	0.8750000000000000	0.0000000000000000	F	F	F
0.8333299999999966	0.7500000000000000	0.0000000000000000	F	F	F
0.6666700000000034	0.7500000000000000	0.0851600000000019	F	F	F
0.8333299999999966	0.8750000000000000	0.0851600000000019	F	F	F
0.6667876625501352	0.8753416372819932	0.1692966044310419	T	T	T
0.833532559556408	0.7504183156476523	0.1692764226028856	T	T	T
0.6670405927909944	0.7504586329828612	0.2519923306977969	T	T	T
0.8333934687626001	0.8754072968997223	0.2522048172219090	T	T	T
0.5174034081077692	0.5252428739805975	0.3958033689707577	T	T	T
0.3897889818909506	0.5434561494593422	0.3923565809885314	T	T	T
0.5458301694449962	0.4302109776921956	0.3935677198966095	T	T	T
0.3596442914690935	0.6380160655771752	0.3970016419841887	T	T	T
0.5518876992422765	0.5534822119423850	0.4362105027220619	T	T	T
0.5608574682165225	0.5591627736506005	0.3596263231263889	T	T	T
0.3569799647619409	0.5177184650988824	0.3494864090384733	T	T	T
0.3439297613463903	0.5062121182683388	0.4256958140613681	T	T	T
0.5687461187446471	0.3956614189519606	0.4306779217999214	T	T	T
0.5090053678135564	0.4004208015806685	0.3535400961476777	T	T	T
0.6379623090866053	0.4182713609844013	0.3926457346753053	T	T	T
0.3854737002061226	0.6641684256394159	0.4394903925417148	T	T	T
0.2676711146397217	0.6489300297533293	0.3914945738712441	T	T	T
0.4041263673733336	0.6754669109847152	0.3630729751387399	T	T	T

### C<sub>6</sub>H<sub>14</sub>···Pt (100)

Energy: -6793.790327 eV

1.0000000000000000

11.6672999999999991 0.0000000000000000 0.0000000000000000

0.0000000000000000 15.5564000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 22.8336000000000006

Pt C H

96 6 14

Selective dynamics

Direct

0.0000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1666700000000034	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.0000000000000000	0.0851600000000019	F	F	F
0.1666700000000034	0.1250000000000000	0.0851600000000019	F	F	F
0.0000117648038802	0.1247220551664570	0.1692511439477592	T	T	T
0.1667357173436733	-0.0001783634339829	0.1693599403778204	T	T	T
0.0000662442832747	-0.0004634027188262	0.2521238785672065	T	T	T
0.1663453213722229	0.1247141704027777	0.2522335249872686	T	T	T
0.3333299999999966	0.1250000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333299999999966	0.0000000000000000	0.0851600000000019	F	F	F
0.5000000000000000	0.1250000000000000	0.0851600000000019	F	F	F
0.3331749463713626	0.1246891921277690	0.1692097643303090	T	T	T
0.4998766343383514	-0.0002022904785159	0.1692736304765906	T	T	T
0.333298296747108	-0.0002986762952031	0.2522694859192759	T	T	T
0.4992253981068838	0.1245431463094158	0.2521743930661869	T	T	T
0.6666700000000034	0.1250000000000000	0.0000000000000000	F	F	F
0.8333299999999966	0.0000000000000000	0.0000000000000000	F	F	F
0.6666700000000034	0.0000000000000000	0.0851600000000019	F	F	F
0.8333299999999966	0.1250000000000000	0.0851600000000019	F	F	F
0.6663121836287077	0.1248150356171303	0.1692062870551807	T	T	T
0.8332541356333221	-0.0001970161672776	0.1692087645089914	T	T	T
0.6665357217631720	-0.0000613682154404	0.2521366472428562	T	T	T
0.8337176839761600	0.1243051000932828	0.2520945557592627	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1666700000000034	0.2500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.2500000000000000	0.0851600000000019	F	F	F
0.1666700000000034	0.3750000000000000	0.0851600000000019	F	F	F



0.0008850196265446 0.3747704174015712 0.1687874590349405 T T T  
0.1668318572925811 0.2496188535083944 0.1691759872959221 T T T  
-0.0003328006245812 0.2496543516745365 0.2519474654801742 T T T  
0.1661565402041345 0.3740935573606979 0.2521585447733628 T T T  
0.3333299999999966 0.3750000000000000 0.0000000000000000 F F F  
0.5000000000000000 0.2500000000000000 0.0000000000000000 F F F  
0.3333299999999966 0.2500000000000000 0.0851600000000019 F F F  
0.5000000000000000 0.3750000000000000 0.0851600000000019 F F F  
0.3334771892739301 0.3748661247366642 0.1692889631327715 T T T  
0.4998663870721510 0.2498762277353718 0.1691995981496095 T T T  
0.3328196825372507 0.2494198938160045 0.2521509081707905 T T T  
0.4991474690867579 0.3734030721794623 0.2533305733766351 T T T  
0.6666700000000034 0.3750000000000000 0.0000000000000000 F F F  
0.8333299999999966 0.2500000000000000 0.0000000000000000 F F F  
0.6666700000000034 0.2500000000000000 0.0851600000000019 F F F  
0.8333299999999966 0.3750000000000000 0.0851600000000019 F F F  
0.6661874351347771 0.3746111371814254 0.1694958771471082 T T T  
0.8330420659658063 0.2496691118807635 0.1691514827244279 T T T  
0.6668159602058876 0.2482909715634767 0.2527761782318229 T T T  
0.8352659928754554 0.3753840955771155 0.2511036878248043 T T T  
0.0000000000000000 0.6250000000000000 0.0000000000000000 F F F  
0.1666700000000034 0.5000000000000000 0.0000000000000000 F F F  
0.0000000000000000 0.5000000000000000 0.0851600000000019 F F F  
0.1666700000000034 0.6250000000000000 0.0851600000000019 F F F  
0.0004373849379062 0.6250175244772812 0.1691310930031723 T T T  
0.1676834460920502 0.4998903025914686 0.1692612282867794 T T T  
0.0008864896806067 0.4999209222210778 0.2518253626332635 T T T  
0.1663605875663365 0.6252100839348876 0.2521842043800583 T T T  
0.3333299999999966 0.6250000000000000 0.0000000000000000 F F F  
0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F  
0.3333299999999966 0.5000000000000000 0.0851600000000019 F F F  
0.5000000000000000 0.6250000000000000 0.0851600000000019 F F F  
0.3337124749041301 0.6244562414175476 0.1694487762513894 T T T  
0.4995757284205279 0.4994078445437234 0.1696314765811710 T T T  
0.3315529081987362 0.4991880075784321 0.2538050514223241 T T T  
0.5018499552518343 0.6258380395672870 0.2514886752110348 T T T  
0.6666700000000034 0.6250000000000000 0.0000000000000000 F F F  
0.8333299999999966 0.5000000000000000 0.0000000000000000 F F F  
0.6666700000000034 0.5000000000000000 0.0851600000000019 F F F  
0.8333299999999966 0.6250000000000000 0.0851600000000019 F F F  
0.6671290437662201 0.6251882188699608 0.1686762822746193 T T T  
0.8340642590923114 0.5000365643544394 0.1686570147374704 T T T  
0.6684351202714301 0.5008449251637821 0.2513454408147051 T T T  
0.8341570274648321 0.6249924550942397 0.2519407641870903 T T T  
0.0000000000000000 0.8750000000000000 0.0000000000000000 F F F  
0.1666700000000034 0.7500000000000000 0.0000000000000000 F F F  
0.0000000000000000 0.7500000000000000 0.0851600000000019 F F F  
0.1666700000000034 0.8750000000000000 0.0851600000000019 F F F  
0.0002612715008385 0.8748906612575771 0.1692725371062317 T T T  
0.1670807329258553 0.7498399150708589 0.1691613089173037 T T T  
0.0004207558212621 0.7498977986351352 0.2521594176573319 T T T  
0.1670408261719772 0.8746274348749560 0.2521129478594270 T T T  
0.3333299999999966 0.8750000000000000 0.0000000000000000 F F F  
0.5000000000000000 0.7500000000000000 0.0000000000000000 F F F  
0.3333299999999966 0.7500000000000000 0.0851600000000019 F F F  
0.5000000000000000 0.8750000000000000 0.0851600000000019 F F F  
0.3334604347558402 0.8750565126379030 0.1692525138318276 T T T  
0.50007922298029414 0.7502834925827938 0.1689653865665684 T T T  
0.3337151682416721 0.7497920190973746 0.2519770973508872 T T T  
0.5003215122010659 0.8747158930160477 0.2521866684818901 T T T  
0.6666700000000034 0.8750000000000000 0.0000000000000000 F F F  
0.8333299999999966 0.7500000000000000 0.0000000000000000 F F F  
0.6666700000000034 0.7500000000000000 0.0851600000000019 F F F  
0.8333299999999966 0.8750000000000000 0.0851600000000019 F F F  
0.6667679090458041 0.8750139858403397 0.1692621061864163 T T T  
0.8337421794848826 0.7501512446647369 0.1692589421641101 T T T  
0.6674398936471972 0.7500050625150515 0.2520598346305566 T T T  
0.8334528336242132 0.8748616061861150 0.2521257601508893 T T T  
0.5191862444376361 0.5099862483768280 0.3955427055640685 T T T  
0.5541857395824916 0.4161253612538394 0.3928515840891046 T T T

0.3911542098429361	0.5257211503655286	0.3914656397361238	T	T	T
0.6830674543006818	0.4026427474713287	0.3935129967046701	T	T	T
0.3589503431920427	0.6197826573808275	0.3970033284871106	T	T	T
0.7181402864337364	0.3087908351482744	0.3916223277560710	T	T	T
0.5514417221398984	0.5384663692131725	0.4363740838787909	T	T	T
0.5622049861062823	0.5452765451339997	0.3597458810489937	T	T	T
0.5192652070645092	0.3871724176909571	0.3515623440423889	T	T	T
0.5136230820531802	0.3798207048851731	0.4284596018104800	T	T	T
0.3601748024466038	0.5008242805209910	0.3479168950033462	T	T	T
0.3451366121675210	0.4867629370059005	0.4238557356933698	T	T	T
0.7204766799517978	0.4369304438239032	0.3557147965178611	T	T	T
0.7196724876973881	0.4333481274571251	0.4325208641281549	T	T	T
0.3839326698432586	0.6451331355073331	0.4398064429513018	T	T	T
0.2669230285068521	0.6298730334384756	0.3913813090153189	T	T	T
0.4030165563514743	0.6582028958360283	0.3634961357327000	T	T	T
0.6920363584464897	0.2743851011582798	0.4312010132275780	T	T	T
0.6761046738850228	0.2756802566484716	0.3543080476881335	T	T	T
0.8105175628951696	0.3009041850353976	0.3859273375320604	T	T	T

### C<sub>8</sub>H<sub>18</sub>···Pt (100)

Energy: -6828.828548 eV

1.0000000000000000

11.6672999999999991 0.0000000000000000 0.0000000000000000

0.0000000000000000 15.5564000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 22.8336000000000006

Pt C H

96 8 18

Selective dynamics

Direct

0.0000000000000000	0.1250000000000000	0.0000000000000000	F	F	F
0.1666700000000034	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.0000000000000000	0.0851600000000019	F	F	F
0.1666700000000034	0.1250000000000000	0.0851600000000019	F	F	F
0.0003537930286646	0.1250276876014230	0.1692792425886024	T	T	T
0.1668410167064555	0.0001971059829725	0.1691982213102288	T	T	T
0.0008624915790854	0.0000184874260672	0.2522336717575123	T	T	T
0.1672287691411449	0.1251135410385084	0.2520658088082888	T	T	T
0.3333299999999966	0.1250000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333299999999966	0.0000000000000000	0.0851600000000019	F	F	F
0.5000000000000000	0.1250000000000000	0.0851600000000019	F	F	F
0.3338316642187307	0.1251280294917034	0.1691898605052617	T	T	T
0.5004156537603995	0.0002981927843737	0.1692113540137842	T	T	T
0.3337427706847664	0.0001039028014930	0.2520461206007014	T	T	T
0.5001422311489211	0.1250261683695559	0.2521989729171599	T	T	T
0.6666700000000034	0.1250000000000000	0.0000000000000000	F	F	F
0.8333299999999966	0.0000000000000000	0.0000000000000000	F	F	F
0.6666700000000034	0.0000000000000000	0.0851600000000019	F	F	F
0.8333299999999966	0.1250000000000000	0.0851600000000019	F	F	F
0.6669792615612434	0.1251905437044473	0.1693606929578309	T	T	T
0.8337670143891800	0.0001312728608123	0.1693508708842957	T	T	T
0.6671289161594297	0.0004746921665717	0.2521911950690172	T	T	T
0.8346527310864391	0.1248000701880755	0.2522768241131161	T	T	T
0.0000000000000000	0.3750000000000000	0.0000000000000000	F	F	F
0.1666700000000034	0.2500000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.2500000000000000	0.0851600000000019	F	F	F
0.1666700000000034	0.3750000000000000	0.0851600000000019	F	F	F
0.0010691617367758	0.3750413393171714	0.1689380171434052	T	T	T
0.1673711103478818	0.2499932689019283	0.1691629009878574	T	T	T
0.0005488988267849	0.2501405091495020	0.2519510711526980	T	T	T
0.1671447881880324	0.3746254429822419	0.2521353481208570	T	T	T
0.3333299999999966	0.3750000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.2500000000000000	0.0000000000000000	F	F	F
0.3333299999999966	0.2500000000000000	0.0851600000000019	F	F	F
0.5000000000000000	0.3750000000000000	0.0851600000000019	F	F	F
0.3339646742138612	0.3751975528091833	0.1693284356280946	T	T	T
0.5004337844704972	0.2502599127127009	0.1693724847010337	T	T	T
0.3337741342191611	0.2499068641697765	0.2521220765561618	T	T	T
0.5003803489734882	0.3739874022257291	0.2535051229910635	T	T	T

0.66667000000000034	0.3750000000000000	0.0000000000000000	F F F
0.8333299999999996	0.2500000000000000	0.0000000000000000	F F F
0.66667000000000034	0.2500000000000000	0.0851600000000019	F F F
0.8333299999999996	0.3750000000000000	0.0851600000000019	F F F
0.6664945851578850	0.3749281373546725	0.1694777914727713	T T T
0.8335227887914548	0.2499178406242182	0.1691964498588156	T T T
0.6677259173063008	0.2488687661740178	0.2528852328302627	T T T
0.8348489030436012	0.3753719889137749	0.2513453913722369	T T T
0.0000000000000000	0.6250000000000000	0.0000000000000000	F F F
0.16667000000000034	0.5000000000000000	0.0000000000000000	F F F
0.0000000000000000	0.5000000000000000	0.0851600000000019	F F F
0.16667000000000034	0.6250000000000000	0.0851600000000019	F F F
0.0012779101950227	0.6252328811617753	0.1694727181126734	T T T
0.1676245489033826	0.5002665843993414	0.1695417624450949	T T T
0.0003986668615814	0.4995523408028155	0.2520969565421356	T T T
0.1650395262135483	0.6251852293657544	0.2539836342463648	T T T
0.3333299999999996	0.6250000000000000	0.0000000000000000	F F F
0.5000000000000000	0.5000000000000000	0.0000000000000000	F F F
0.3333299999999996	0.5000000000000000	0.0851600000000019	F F F
0.5000000000000000	0.6250000000000000	0.0851600000000019	F F F
0.3328738064969576	0.6247751169114989	0.1697331314810753	T T T
0.4996839802191387	0.4999151710339872	0.1694751299801785	T T T
0.3332456732032990	0.4990680542087564	0.2537565877726143	T T T
0.5014160420990829	0.6262390095796470	0.2514681822364904	T T T
0.66667000000000034	0.6250000000000000	0.0000000000000000	F F F
0.8333299999999996	0.5000000000000000	0.0000000000000000	F F F
0.66667000000000034	0.5000000000000000	0.0851600000000019	F F F
0.8333299999999996	0.6250000000000000	0.0851600000000019	F F F
0.6671916015598585	0.6253253214563801	0.1687675034156548	T T T
0.8342075081164082	0.5002607214696790	0.1687852701418175	T T T
0.6684180234817546	0.5012672102525180	0.2513623384320971	T T T
0.8343424714207309	0.6253960018998892	0.2519435990969168	T T T
0.0000000000000000	0.8750000000000000	0.0000000000000000	F F F
0.16667000000000034	0.7500000000000000	0.0000000000000000	F F F
0.0000000000000000	0.7500000000000000	0.0851600000000019	F F F
0.16667000000000034	0.8750000000000000	0.0851600000000019	F F F
0.0003397640256772	0.8750929043362536	0.1693124676228188	T T T
0.1669148862699107	0.7498455636077709	0.1695553585928934	T T T
-0.0002082680697666	0.7509602399599434	0.2524131045111538	T T T
0.1673006363343673	0.8754083797074392	0.2520528478904238	T T T
0.3333299999999996	0.8750000000000000	0.0000000000000000	F F F
0.5000000000000000	0.7500000000000000	0.0000000000000000	F F F
0.3333299999999996	0.7500000000000000	0.0851600000000019	F F F
0.5000000000000000	0.8750000000000000	0.0851600000000019	F F F
0.3334790580351833	0.8754373245649647	0.1689541909838785	T T T
0.5003026404343994	0.7503600586794350	0.1687419514515072	T T T
0.3352432359855557	0.7513952055842174	0.2516059223710280	T T T
0.5007687935433728	0.8755441279431861	0.2519813672678510	T T T
0.66667000000000034	0.8750000000000000	0.0000000000000000	F F F
0.8333299999999996	0.7500000000000000	0.0000000000000000	F F F
0.66667000000000034	0.7500000000000000	0.0851600000000019	F F F
0.8333299999999996	0.8750000000000000	0.0851600000000019	F F F
0.6671439637162428	0.8754072481923775	0.1692751210991869	T T T
0.8338766649847564	0.7502927532582001	0.1692753638808806	T T T
0.6672490581420365	0.7503126100436929	0.2519529986650875	T T T
0.8334712847547071	0.8754706423233362	0.2522567634158931	T T T
0.3913952441262670	0.5323461186204655	0.3934973816370268	T T T
0.5189343826153212	0.5143768425187613	0.3977701347477449	T T T
0.3624658057051435	0.6271891585640821	0.3979893268202944	T T T
0.5508052606216295	0.4199812881936542	0.3942409647643463	T T T
0.236077787769617	0.6483455563868535	0.3920852510952245	T T T
0.6791474415881730	0.4041418822164520	0.3964537137864971	T T T
0.2114602002816025	0.7437528055101928	0.3974983226855411	T T T
0.7110569003869158	0.3096359602834381	0.3950590088762929	T T T
0.3442500946001940	0.4953933272466760	0.4265448799967885	T T T
0.3594421024185553	0.5075087042034656	0.3502826749057297	T T T
0.5517060506926798	0.5410731414475878	0.4390499601186162	T T T
0.5634602604612501	0.5496761975498701	0.3625322667426301	T T T
0.4105375153658402	0.6625556085886446	0.3640683393365124	T T T
0.3935819317000301	0.6520117028502358	0.4401487009641067	T T T

0.5169849530584213	0.3929469589957233	0.3521922000140840	T	T	T
0.5073690334059056	0.3835139566940897	0.4288908416320451	T	T	T
0.1854814070215828	0.6115338070838392	0.4237992721534780	T	T	T
0.2058334387458783	0.6252453172619741	0.3481092112632244	T	T	T
0.7147575794638340	0.4341394477798471	0.4359463463999600	T	T	T
0.7197222340070634	0.4375171120415633	0.3591643550017248	T	T	T
0.2340699056986967	0.7674273431937636	0.4410880946898909	T	T	T
0.2622672827491069	0.7803189408263735	0.3655602572490573	T	T	T
0.1212655361544595	0.7584323536896034	0.3893659777636058	T	T	T
0.8037737958838734	0.3000065451641644	0.3934490393794146	T	T	T
0.6746556947400896	0.2782417753741656	0.3556663235595163	T	T	T
0.6770974217052455	0.2750979383028840	0.4330060109504903	T	T	T

**C<sub>6</sub>H<sub>14</sub>···Pt (111) with 1 ML H (24H)**

**Energy: -6899.905497 eV**

1.0000000000000000		
16.5000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.5261999999999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	23.7360000000000007

Pt H C

96 38 6

Selective dynamics

Direct

0.1666700000000034	0.3333299999999966	0.0000000000000000	F	F	F
0.0000000000000000	0.8333299999999966	0.0000000000000000	F	F	F
0.2500000000000000	0.0833299999999966	0.0000000000000000	F	F	F
0.0833299999999966	0.5833299999999966	0.0000000000000000	F	F	F
0.0833299999999966	0.0833299999999966	0.0000000000000000	F	F	F
0.2500000000000000	0.5833299999999966	0.0000000000000000	F	F	F
0.0000000000000000	0.3333299999999966	0.0000000000000000	F	F	F
0.1666700000000034	0.8333299999999966	0.0000000000000000	F	F	F
0.1666700000000034	0.0000000000000000	0.0945999999999998	F	F	F
0.0000000000000000	0.5000000000000000	0.0945999999999998	F	F	F
0.0833299999999966	0.2500000000000000	0.0945999999999998	F	F	F
0.2500000000000000	0.7500000000000000	0.0945999999999998	F	F	F
0.2500000000000000	0.2500000000000000	0.0945999999999998	F	F	F
0.0833299999999966	0.7500000000000000	0.0945999999999998	F	F	F
0.0000000000000000	0.0000000000000000	0.0945999999999998	F	F	F
0.1666700000000034	0.5000000000000000	0.0945999999999998	F	F	F
0.001942496478747	0.1665560879198682	0.1898454442508636	T	T	T
0.1665434247507767	0.6668203952158970	0.1897357151073645	T	T	T
0.2499621219533887	0.4164110197294582	0.1896017873642355	T	T	T
0.0835342061218982	0.9166389984303547	0.1898464903244493	T	T	T
0.0834376260092130	0.4165629101013120	0.1898918491478229	T	T	T
0.2501927562851177	0.9165421653378230	0.1898989227642736	T	T	T
0.1668566961886818	0.1664846464370136	0.1898753267996197	T	T	T
0.0000844178075485	0.6665730941988249	0.1898712826894854	T	T	T
0.1668628871339110	0.3328545979728687	0.2901630705780273	T	T	T
0.0002084059517230	0.8330134018312679	0.2899245400548852	T	T	T
0.2501264411474113	0.0829840703313181	0.2900288918431195	T	T	T
0.0835830740149863	0.5829740151783492	0.2901024065460893	T	T	T
0.0835352713307098	0.0829905622738170	0.2898750298954809	T	T	T
0.2501941114368302	0.5831094235431049	0.2889050441117939	T	T	T
0.0003037689932831	0.3329703947017250	0.2899439137526263	T	T	T
0.1668393074236963	0.8329891823939970	0.2901045284091311	T	T	T
0.5000000000000000	0.3333299999999966	0.0000000000000000	F	F	F
0.3333299999999966	0.8333299999999966	0.0000000000000000	F	F	F
0.5833299999999966	0.0833299999999966	0.0000000000000000	F	F	F
0.4166700000000034	0.5833299999999966	0.0000000000000000	F	F	F
0.4166700000000034	0.0833299999999966	0.0000000000000000	F	F	F
0.5833299999999966	0.5833299999999966	0.0000000000000000	F	F	F
0.3333299999999966	0.3333299999999966	0.0000000000000000	F	F	F
0.5000000000000000	0.8333299999999966	0.0000000000000000	F	F	F
0.5000000000000000	0.0000000000000000	0.0945999999999998	F	F	F
0.3333299999999966	0.5000000000000000	0.0945999999999998	F	F	F
0.4166700000000034	0.2500000000000000	0.0945999999999998	F	F	F
0.5833299999999966	0.7500000000000000	0.0945999999999998	F	F	F
0.5833299999999966	0.2500000000000000	0.0945999999999998	F	F	F
0.4166700000000034	0.7500000000000000	0.0945999999999998	F	F	F

0.3333299999999966	0.0000000000000000	0.0945999999999998	F	F	F
0.5000000000000000	0.5000000000000000	0.0945999999999998	F	F	F
0.3335475111811756	0.1661499625083875	0.1897664663044066	T	T	T
0.5001813367438330	0.6668514033144196	0.1897541978181546	T	T	T
0.5835049672991601	0.4165640628130793	0.1896215752721535	T	T	T
0.4169219486206774	0.9165414204219666	0.1898953050529016	T	T	T
0.4168522581543043	0.4166376567430078	0.1896389587820027	T	T	T
0.5835451386748268	0.9165171404698813	0.1899026995483378	T	T	T
0.5001528233992901	0.1663003636609677	0.1898368976120425	T	T	T
0.3334917164001917	0.6668709668813839	0.1896770951618146	T	T	T
0.5003738938171578	0.3325732831405476	0.2895162299438053	T	T	T
0.3335291825247206	0.8332200649406859	0.2900763700210331	T	T	T
0.5836005281149660	0.0829456213316176	0.2900914808634374	T	T	T
0.4168967702293874	0.5831183705309683	0.2895407239159061	T	T	T
0.4168972603889378	0.0829128157534642	0.2900879687413113	T	T	T
0.5837425522997943	0.5831628048318436	0.2892730170444194	T	T	T
0.3335259211622930	0.3327529829319106	0.2890369975641029	T	T	T
0.5002763870066947	0.8331859116013461	0.2900680999125921	T	T	T
0.8333299999999966	0.3333299999999966	0.0000000000000000	F	F	F
0.6666700000000034	0.8333299999999966	0.0000000000000000	F	F	F
0.9166700000000034	0.0833299999999966	0.0000000000000000	F	F	F
0.7500000000000000	0.5833299999999966	0.0000000000000000	F	F	F
0.7500000000000000	0.0833299999999966	0.0000000000000000	F	F	F
0.9166700000000034	0.5833299999999966	0.0000000000000000	F	F	F
0.6666700000000034	0.3333299999999966	0.0000000000000000	F	F	F
0.8333299999999966	0.8333299999999966	0.0000000000000000	F	F	F
0.8333299999999966	0.0000000000000000	0.0945999999999998	F	F	F
0.6666700000000034	0.5000000000000000	0.0945999999999998	F	F	F
0.7500000000000000	0.2500000000000000	0.0945999999999998	F	F	F
0.9166700000000034	0.7500000000000000	0.0945999999999998	F	F	F
0.9166700000000034	0.2500000000000000	0.0945999999999998	F	F	F
0.7500000000000000	0.7500000000000000	0.0945999999999998	F	F	F
0.6666700000000034	0.0000000000000000	0.0945999999999998	F	F	F
0.8333299999999966	0.5000000000000000	0.0945999999999998	F	F	F
0.6668128307141350	0.1662791524400746	0.1897807731380112	T	T	T
0.8334755676255415	0.6666061115112404	0.1898977226718727	T	T	T
0.9168292583262196	0.4165066470982363	0.1898537587198630	T	T	T
0.7502067041668518	0.9165788880944052	0.1898625574734223	T	T	T
0.7502869268719419	0.4167232662708204	0.1897985302995778	T	T	T
0.9168399391746659	0.9166190204788840	0.1898330603774269	T	T	T
0.8334645304433523	0.1665749776371738	0.1898547271981555	T	T	T
0.6670022843207288	0.6667107360413804	0.1898134777366544	T	T	T
0.8336641583703489	0.3328810498353015	0.2900424616612705	T	T	T
0.6669644371433819	0.8329924454566748	0.2900465205551789	T	T	T
0.9168918765088017	0.0830477253352877	0.2899127799245660	T	T	T
0.7502957273988065	0.5829021233360764	0.2903067426600494	T	T	T
0.7503029060465766	0.0829325293196888	0.2900128420862142	T	T	T
0.9170017865626486	0.5829240026157056	0.2898580425425048	T	T	T
0.6671379870952923	0.3328311957874884	0.2892223208997197	T	T	T
0.8335970911191209	0.8329199087136132	0.2898983052279425	T	T	T
0.0834948645952919	0.4165184495467512	0.3289968984257450	T	T	T
0.2493782278207190	0.4156755383240801	0.3281275543605216	T	T	T
0.1662578858748040	0.6668429381660436	0.3286616661216908	T	T	T
0.0001832697928916	0.6663868648013086	0.3288368165485832	T	T	T
0.1669852846353817	0.1664216576594217	0.3289578218269172	T	T	T
0.0002477495828050	0.1663385798257973	0.3288258716687857	T	T	T
0.0835261174622552	0.9164398516949491	0.3288949346010883	T	T	T
0.2501457064982049	0.9161376038133884	0.3289649426255238	T	T	T
0.4173771518763561	0.4172944034544352	0.3277717379822171	T	T	T
0.5833745677579181	0.4160607093829083	0.3278708956473758	T	T	T
0.5001175863830152	0.6678193821631068	0.3283063910700042	T	T	T
0.3339162160326705	0.6676184995933084	0.3282043114808833	T	T	T
0.5002137216126369	0.1652317189003801	0.3288306889467730	T	T	T
0.3336117866097563	0.1646185859545173	0.3286172652768830	T	T	T
0.4168617145068154	0.9163207091412068	0.3291002394694434	T	T	T
0.5835376805192048	0.9161478603470763	0.3289850849810514	T	T	T
0.7505890931694010	0.4169824986252680	0.3287876873506656	T	T	T
0.9167975868309907	0.4163020162786633	0.3288831886362076	T	T	T
0.8335619292519123	0.6663325153931230	0.3288741352743252	T	T	T
0.6676062169234280	0.6668470120823743	0.3288011324254628	T	T	T

0.8335328587514476	0.1664299047243666	0.3289048899297236	T	T	T
0.6669763446892966	0.1651157563259150	0.3286612978024053	T	T	T
0.7502302354790292	0.9164453833157374	0.3289283249906427	T	T	T
0.9168591171182986	0.9162903248261023	0.3287660243759237	T	T	T
0.4213275427228336	0.5659008954030905	0.4925683756620474	T	T	T
0.4252533326372943	0.5720298333807035	0.4187781023028577	T	T	T
0.5000949545900951	0.3396806492518514	0.4191648997511875	T	T	T
0.5011871690179754	0.3448118853215464	0.4930299193004692	T	T	T
0.3484298174264713	0.3483718212050194	0.4126336845134955	T	T	T
0.3447603791152843	0.3368549444219254	0.4862151904828261	T	T	T
0.5766721609304311	0.5645925039121402	0.4152584973032657	T	T	T
0.5780357617190018	0.5731518844500070	0.4889943673022087	T	T	T
0.2635404742654728	0.5585537199614670	0.4909945291627931	T	T	T
0.2155734594923531	0.4368968327950444	0.4455948268012417	T	T	T
0.2713841509531574	0.5783595658332465	0.4173097097482395	T	T	T
0.6592017174356457	0.3520377922293963	0.4937973134547416	T	T	T
0.6537954025215715	0.3341375113516371	0.4199150033260245	T	T	T
0.7086949499769186	0.4748663678421174	0.4497906332802845	T	T	T
0.4234254051307805	0.4993814835822575	0.4548229112938503	T	T	T
0.5005262649041420	0.4117877595373513	0.4554031413742092	T	T	T
0.3464304298824419	0.4120029532176409	0.4512533140181441	T	T	T
0.5775553817028085	0.4994929561822710	0.4534897801973520	T	T	T
0.2699281708212661	0.5009043920549686	0.4514171473016795	T	T	T
0.6541410407958386	0.4107049793056421	0.4543627578576661	T	T	T

### C<sub>6</sub>H<sub>14</sub>···Pt (111) with 16H

Energy: -6870.986720 eV

1.0000000000000000

16.5000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 9.5261999999999993 0.0000000000000000

0.0000000000000000 0.0000000000000000 23.7360000000000007

Pt H C

96 30 6

Selective dynamics

Direct

0.1666700000000034	0.3333299999999966	0.0000000000000000	F	F	F
0.0000000000000000	0.8333299999999966	0.0000000000000000	F	F	F
0.2500000000000000	0.0833299999999966	0.0000000000000000	F	F	F
0.0833299999999966	0.5833299999999966	0.0000000000000000	F	F	F
0.0833299999999966	0.0833299999999966	0.0000000000000000	F	F	F
0.2500000000000000	0.5833299999999966	0.0000000000000000	F	F	F
0.0000000000000000	0.3333299999999966	0.0000000000000000	F	F	F
0.1666700000000034	0.8333299999999966	0.0000000000000000	F	F	F
0.1666700000000034	0.0000000000000000	0.0945999999999998	F	F	F
0.0000000000000000	0.5000000000000000	0.0945999999999998	F	F	F
0.0833299999999966	0.2500000000000000	0.0945999999999998	F	F	F
0.2500000000000000	0.7500000000000000	0.0945999999999998	F	F	F
0.2500000000000000	0.2500000000000000	0.0945999999999998	F	F	F
0.0833299999999966	0.7500000000000000	0.0945999999999998	F	F	F
0.0000000000000000	0.0000000000000000	0.0945999999999998	F	F	F
0.1666700000000034	0.5000000000000000	0.0945999999999998	F	F	F
0.0003546557834575	0.1698069757002170	0.1908197264907529	T	T	T
0.1633751840643158	0.6716154786162917	0.1883134321929724	T	T	T
0.2479348812057837	0.4186214094110323	0.1873929292668706	T	T	T
0.0841555868568137	0.9224318237838954	0.1908205232022539	T	T	T
0.0818737301416662	0.4178312846949653	0.1900633779728004	T	T	T
0.2515967471083990	0.9205477153040615	0.1908699775914177	T	T	T
0.1683761465900002	0.1679010579160763	0.1904909573544108	T	T	T
0.9991876436806658	0.6718347514885782	0.1904512285098024	T	T	T
0.170553884039162	0.3484575960694581	0.2885197279209574	T	T	T
0.0022170755529142	0.8433198721317859	0.2900337074354624	T	T	T
0.2547552543637241	0.1025221159788311	0.2885887735248609	T	T	T
0.0867518370587556	0.5936945529328853	0.2879811410574473	T	T	T
0.0872896687151494	0.0947447938235922	0.2920319109354731	T	T	T
0.2517150413619073	0.5922105595200310	0.2816722979001063	T	T	T
0.0006642071813524	0.3434498873065700	0.2920083027717126	T	T	T
0.1710950719526876	0.8408812319938267	0.2878543702358216	T	T	T
0.5000000000000000	0.3333299999999966	0.0000000000000000	F	F	F
0.3333299999999966	0.8333299999999966	0.0000000000000000	F	F	F

0.5833299999999966 0.0833299999999966 0.0000000000000000 F F F  
0.4166700000000034 0.5833299999999966 0.0000000000000000 F F F  
0.4166700000000034 0.0833299999999966 0.0000000000000000 F F F  
0.5833299999999966 0.5833299999999966 0.0000000000000000 F F F  
0.3333299999999966 0.3333299999999966 0.0000000000000000 F F F  
0.5000000000000000 0.8333299999999966 0.0000000000000000 F F F  
0.5000000000000000 0.0000000000000000 0.0945999999999998 F F F  
0.3333299999999966 0.5000000000000000 0.0945999999999998 F F F  
0.4166700000000034 0.2500000000000000 0.0945999999999998 F F F  
0.5833299999999966 0.7500000000000000 0.0945999999999998 F F F  
0.5833299999999966 0.2500000000000000 0.0945999999999998 F F F  
0.4166700000000034 0.7500000000000000 0.0945999999999998 F F F  
0.3333299999999966 0.0000000000000000 0.0945999999999998 F F F  
0.5000000000000000 0.5000000000000000 0.0945999999999998 F F F  
0.3362369002382517 0.1674118564593645 0.1895264989041596 T T T  
0.5004332709150917 0.6745805568344667 0.1877944540794917 T T T  
0.5841375195371818 0.4212811360758397 0.1863161694126924 T T T  
0.4167189603171199 0.9192698490931892 0.1923458501240609 T T T  
0.4165555099946440 0.4227140746264972 0.1863310363358720 T T T  
0.5816892685025361 0.9199095376769904 0.1912843374292962 T T T  
0.4998574300406474 0.1668168845696430 0.1906212983144018 T T T  
0.3316748984049080 0.6733847027058758 0.1875640505529944 T T T  
0.4998629864844639 0.3545551516615360 0.2826200275995971 T T T  
0.3352202320741410 0.8433712450237232 0.2908984727147245 T T T  
0.5806652895984096 0.1086931069415270 0.2917030180974970 T T T  
0.4170838850978710 0.5933623667368582 0.2827098918088125 T T T  
0.4177929175585242 0.1079819337636248 0.2925973434362599 T T T  
0.5826623963006020 0.5935809541156560 0.2820606561020504 T T T  
0.3350915446696657 0.3532381665440272 0.2823475366571313 T T T  
0.4989800659742983 0.8448884490617203 0.2913676386560854 T T T  
0.8333299999999966 0.3333299999999966 0.0000000000000000 F F F  
0.6666700000000034 0.8333299999999966 0.0000000000000000 F F F  
0.9166700000000034 0.0833299999999966 0.0000000000000000 F F F  
0.7500000000000000 0.5833299999999966 0.0000000000000000 F F F  
0.7500000000000000 0.0833299999999966 0.0000000000000000 F F F  
0.9166700000000034 0.5833299999999966 0.0000000000000000 F F F  
0.6666700000000034 0.3333299999999966 0.0000000000000000 F F F  
0.8333299999999966 0.8333299999999966 0.0000000000000000 F F F  
0.8333299999999966 0.0000000000000000 0.0945999999999998 F F F  
0.6666700000000034 0.5000000000000000 0.0945999999999998 F F F  
0.7500000000000000 0.2500000000000000 0.0945999999999998 F F F  
0.9166700000000034 0.7500000000000000 0.0945999999999998 F F F  
0.9166700000000034 0.2500000000000000 0.0945999999999998 F F F  
0.7500000000000000 0.7500000000000000 0.0945999999999998 F F F  
0.6666700000000034 0.0000000000000000 0.0945999999999998 F F F  
0.8333299999999966 0.5000000000000000 0.0945999999999998 F F F  
0.6648377682840377 0.1654357809435027 0.1904424437032414 T T T  
0.8362043477898982 0.6728055509030190 0.1896966270815646 T T T  
0.9174242408659639 0.4188144053322584 0.1905752074257683 T T T  
0.7495643474605020 0.9208349193458721 0.1912744203559689 T T T  
0.7523425294446723 0.4192775568502239 0.1878442184944486 T T T  
0.9170434813702777 0.9231071491927620 0.1907551017024669 T T T  
0.8310903065174556 0.1676875530119754 0.1908501593294023 T T T  
0.6693912307574728 0.6728832181190263 0.1877053118363265 T T T  
0.8296201437669090 0.3453161263100189 0.2884836246711218 T T T  
0.6626811371563140 0.8417162962376812 0.2877324600316850 T T T  
0.9149239874930694 0.0940435870033263 0.2895508803905472 T T T  
0.7467485283856464 0.5908075493225078 0.2845988170731125 T T T  
0.7442875035189538 0.0996942493976615 0.2948559668254629 T T T  
0.9156034526989214 0.5928236369954558 0.2911015950073102 T T T  
0.6654444065567110 0.3518327312769331 0.2822284402338029 T T T  
0.8301272754209064 0.8426038697930881 0.2905176667455986 T T T  
0.0880129499301349 0.4280360535251466 0.3280691863563179 T T T  
0.0028414203305631 0.6720984562550922 0.3271739805563612 T T T  
0.1709289785274468 0.1707395531848001 0.3295173703754800 T T T  
0.0006371343177305 0.1748598789144274 0.3286663289517199 T T T  
0.0874051992900767 0.9217780941042079 0.3280737314255504 T T T  
0.2509361002226807 0.8332266013760082 0.3354442166608298 T T T  
0.4995546185053631 0.1067411848761234 0.3387642577811889 T T T  
0.3344626233851544 0.1030387337898425 0.3371137419881471 T T T

0.4172576043796662	0.8291066694560582	0.3370244726903188	T	T	T
0.5827948961595162	0.8339905980082406	0.3356786749200958	T	T	T
0.9141840794822993	0.4229059038115618	0.3283890463534289	T	T	T
0.8291501473031065	0.6711996888261526	0.3268290764156794	T	T	T
0.8310066591994987	0.1788814360227180	0.3294196892897924	T	T	T
0.6601717549356565	0.1157134415867900	0.3390637516282143	T	T	T
0.7489418070951595	0.9193525416714210	0.3285294165729835	T	T	T
0.9168268686203415	0.9235005686298510	0.3271202526432614	T	T	T
0.4168642298484316	0.6061996547354095	0.4601607090022934	T	T	T
0.4180937259763868	0.5838665800569370	0.3866764590689883	T	T	T
0.5014237549949637	0.3656727633207181	0.3977392469198541	T	T	T
0.5015242105499570	0.3886418895512962	0.4712286175158564	T	T	T
0.3463348168375414	0.3578272821692605	0.3947877675246992	T	T	T
0.3477582243803538	0.3681940420873007	0.4686800231725095	T	T	T
0.5724477960604409	0.5913182867171989	0.3843326366583787	T	T	T
0.5702631847918861	0.6248482469465259	0.4570186580922738	T	T	T
0.2617970352703890	0.5865305975722803	0.4649773145004294	T	T	T
0.2132633228115352	0.4458707277108641	0.4295744961265417	T	T	T
0.2623314410730849	0.5788329719422596	0.3905986868162525	T	T	T
0.6574874551157648	0.4116591377349744	0.4742128870721216	T	T	T
0.6575087820988034	0.3759608297462320	0.4010690672589496	T	T	T
0.7052376201760321	0.5289985971436473	0.4267947338075516	T	T	T
0.4196203043996936	0.5255489720977755	0.4271421059697784	T	T	T
0.4992521264905107	0.4461853096506967	0.4311579318834399	T	T	T
0.3449981072193378	0.4324358051854608	0.4303583953124604	T	T	T
0.5736412722128774	0.5394134517960025	0.4261047076841886	T	T	T
0.2661763186202638	0.5148104150478237	0.4291291302038266	T	T	T
0.6529138901188350	0.4600637877869821	0.4325445440671399	T	T	T

### C<sub>6</sub>H<sub>14</sub>···Pt (100) with 1 ML H

Energy: -10285.746588 eV

1.0000000000000000

23.3345999999999982 0.0000000000000000 0.0000000000000000

0.0000000000000000 11.6672999999999991 0.0000000000000000

0.0000000000000000 0.0000000000000000 22.8336000000000006

Pt H C

144 50 6

Selective dynamics

Direct

0.0000000000000000	0.1666700000000034	0.0000000000000000	F	F	F
0.0833299999999966	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.0000000000000000	0.0851600000000019	F	F	F
0.0833299999999966	0.1666700000000034	0.0851600000000019	F	F	F
0.0000102453854511	0.1666005593059137	0.1696995300897067	T	T	T
0.0833387849293577	-0.0000275451547538	0.1696857554411256	T	T	T
0.0000037941087112	-0.0000947382775816	0.2566902557886625	T	T	T
0.0832985761470835	0.1666375627254923	0.2567810288940751	T	T	T
0.1666700000000034	0.1666700000000034	0.0000000000000000	F	F	F
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.1666700000000034	0.0000000000000000	0.0851600000000019	F	F	F
0.2500000000000000	0.1666700000000034	0.0851600000000019	F	F	F
0.1666224869897136	0.1665884839534396	0.1697178825502696	T	T	T
0.2498983109758027	0.0000483721586266	0.1697590639779723	T	T	T
0.1666197826054856	0.0000577264446341	0.2568741679533946	T	T	T
0.2499038137358921	0.1668212456179400	0.2568539336628283	T	T	T
0.3333299999999966	0.1666700000000034	0.0000000000000000	F	F	F
0.4166700000000034	0.0000000000000000	0.0000000000000000	F	F	F
0.3333299999999966	0.0000000000000000	0.0851600000000019	F	F	F
0.4166700000000034	0.1666700000000034	0.0851600000000019	F	F	F
0.3332030218320413	0.1664660453567192	0.1696728349087767	T	T	T
0.4165748372192190	-0.0000357666217913	0.1697371028131675	T	T	T
0.3332641846146852	0.0001492877419086	0.2569114396614779	T	T	T
0.4165410717228314	0.1666670453908695	0.2567587198301920	T	T	T
0.5000000000000000	0.1666700000000034	0.0000000000000000	F	F	F
0.5833299999999966	0.0000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.0000000000000000	0.0851600000000019	F	F	F
0.5833299999999966	0.1666700000000034	0.0851600000000019	F	F	F
0.4999701730226900	0.1662216131386045	0.1695787159735491	T	T	T
0.5834115330895129	-0.0003369193173466	0.1697118081047183	T	T	T



0.4999659016989789	0.0000427477395044	0.2568568525670272	T	T	T
0.5834206703903321	0.1663603025300627	0.2564683301525662	T	T	T
0.6666700000000034	0.1666700000000034	0.0000000000000000	F	F	F
0.7500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6666700000000034	0.0000000000000000	0.0851600000000019	F	F	F
0.7500000000000000	0.1666700000000034	0.0851600000000019	F	F	F
0.6668321879798772	0.1661496425957298	0.1695715078376566	T	T	T
0.7500776039990524	-0.0003019766698752	0.1697302610491829	T	T	T
0.6667128630961211	-0.0002427492844320	0.2568832169934609	T	T	T
0.7501234057493521	0.1663835768813144	0.2566986703533228	T	T	T
0.8333299999999966	0.1666700000000034	0.0000000000000000	F	F	F
0.9166700000000034	0.0000000000000000	0.0000000000000000	F	F	F
0.8333299999999966	0.0000000000000000	0.0851600000000019	F	F	F
0.9166700000000034	0.1666700000000034	0.0851600000000019	F	F	F
0.8334013822227870	0.1664155990626972	0.1696889889217569	T	T	T
0.9166720296519477	-0.0001268585737242	0.1696722065864055	T	T	T
0.8333795428256568	-0.0002496048364103	0.2568097075936954	T	T	T
0.9166990158155334	0.1664862287500909	0.2567336351283712	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0833299999999966	0.3333299999999966	0.0000000000000000	F	F	F
0.0000000000000000	0.3333299999999966	0.0851600000000019	F	F	F
0.0833299999999966	0.5000000000000000	0.0851600000000019	F	F	F
-0.0000284137978737	0.4999870323714319	0.1697093245382462	T	T	T
0.0833001871520929	0.3332684620574177	0.1697065664611489	T	T	T
-0.0000168195957352	0.3332185568960749	0.2567495173941268	T	T	T
0.0832349409028593	0.5000130853233732	0.2567381410812015	T	T	T
0.1666700000000034	0.5000000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.3333299999999966	0.0000000000000000	F	F	F
0.1666700000000034	0.3333299999999966	0.0851600000000019	F	F	F
0.2500000000000000	0.5000000000000000	0.0851600000000019	F	F	F
0.1665711466569433	0.5000736047871424	0.1696972679408813	T	T	T
0.2498278833165984	0.3332961248104557	0.1696459986642777	T	T	T
0.1665672776134684	0.3334041326775573	0.2567498702464810	T	T	T
0.2499283828354530	0.5001280319536020	0.2566431757908924	T	T	T
0.3333299999999966	0.5000000000000000	0.0000000000000000	F	F	F
0.4166700000000034	0.3333299999999966	0.0000000000000000	F	F	F
0.3333299999999966	0.3333299999999966	0.0851600000000019	F	F	F
0.4166700000000034	0.5000000000000000	0.0851600000000019	F	F	F
0.3331047602300249	0.5001732202525042	0.1695216984058191	T	T	T
0.4164948184601281	0.3330865034178902	0.1694626131928923	T	T	T
0.3331626479098244	0.3334170219289470	0.2564456711731798	T	T	T
0.4166528382033801	0.5001556063977518	0.2558432657034602	T	T	T
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5833299999999966	0.3333299999999966	0.0000000000000000	F	F	F
0.5000000000000000	0.3333299999999966	0.0851600000000019	F	F	F
0.5833299999999966	0.5000000000000000	0.0851600000000019	F	F	F
0.5000104762847768	0.5002259734890897	0.1693036286578816	T	T	T
0.5834593973778851	0.3330253953467313	0.1693806478521184	T	T	T
0.4999819841490123	0.3331188364985904	0.2559580068401364	T	T	T
0.5832989846765448	0.5001010011076258	0.2559451210592780	T	T	T
0.6666700000000034	0.5000000000000000	0.0000000000000000	F	F	F
0.7500000000000000	0.3333299999999966	0.0000000000000000	F	F	F
0.6666700000000034	0.3333299999999966	0.0851600000000019	F	F	F
0.7500000000000000	0.5000000000000000	0.0851600000000019	F	F	F
0.6668641641874817	0.5001993197889443	0.1695348146572185	T	T	T
0.7502161603941015	0.3331655314481497	0.1695849240557938	T	T	T
0.6668091746925673	0.3330999395261542	0.2560530256812161	T	T	T
0.7500652560958208	0.4998406455613312	0.2568275625595212	T	T	T
0.8333299999999966	0.5000000000000000	0.0000000000000000	F	F	F
0.9166700000000034	0.3333299999999966	0.0000000000000000	F	F	F
0.8333299999999966	0.3333299999999966	0.0851600000000019	F	F	F
0.9166700000000034	0.5000000000000000	0.0851600000000019	F	F	F
0.8333522645000910	0.5000333833008630	0.1697308314816262	T	T	T
0.9166730003013899	0.3332548148527752	0.1697165382468054	T	T	T
0.8333997781398533	0.3331620864624549	0.2567224865085743	T	T	T
0.9166727045019361	0.4998513731415926	0.2567707708287178	T	T	T
0.0000000000000000	0.8333299999999966	0.0000000000000000	F	F	F
0.0833299999999966	0.6666700000000034	0.0000000000000000	F	F	F
0.0000000000000000	0.6666700000000034	0.0851600000000019	F	F	F
0.0833299999999966	0.8333299999999966	0.0851600000000019	F	F	F

-0.0000228832667944	0.8333014234246146	0.1696649741842100	T	T	T
0.0832933501880914	0.6667080972231249	0.1697015384602690	T	T	T
-0.0000558147470018	0.6665837427472538	0.2567143302548127	T	T	T
0.0832769312744820	0.8332934892590613	0.2567381222278647	T	T	T
0.1666700000000034	0.8333299999999966	0.0000000000000000	F	F	F
0.2500000000000000	0.6666700000000034	0.0000000000000000	F	F	F
0.1666700000000034	0.6666700000000034	0.0851600000000019	F	F	F
0.2500000000000000	0.8333299999999966	0.0851600000000019	F	F	F
0.1666230671875000	0.8334306541444439	0.1697111504208415	T	T	T
0.2498513753536694	0.6669209923818196	0.1696792028038144	T	T	T
0.1665772763223813	0.6666999592040598	0.2567534051618864	T	T	T
0.2498851016436935	0.8334910679889883	0.2569039984652280	T	T	T
0.3333299999999966	0.8333299999999966	0.0000000000000000	F	F	F
0.4166700000000034	0.6666700000000034	0.0000000000000000	F	F	F
0.3333299999999966	0.6666700000000034	0.0851600000000019	F	F	F
0.4166700000000034	0.8333299999999966	0.0851600000000019	F	F	F
0.3331732016548796	0.8337420284235693	0.1696842472436958	T	T	T
0.4165343974513548	0.6672194194009315	0.1694938764488853	T	T	T
0.3332306606720880	0.6670697357329209	0.2564419071722610	T	T	T
0.4166076545170477	0.8336019304232875	0.2568345445020297	T	T	T
0.5000000000000000	0.8333299999999966	0.0000000000000000	F	F	F
0.5833299999999966	0.6666700000000034	0.0000000000000000	F	F	F
0.5000000000000000	0.6666700000000034	0.0851600000000019	F	F	F
0.5833299999999966	0.8333299999999966	0.0851600000000019	F	F	F
0.4999710519969340	0.8336385242749317	0.1697160270369203	T	T	T
0.5834048393024729	0.6671146796489508	0.1695780113513342	T	T	T
0.4999007987116891	0.6669375764411780	0.2564781839038278	T	T	T
0.5833158840386468	0.8332179959652889	0.2569092909147276	T	T	T
0.6666700000000034	0.8333299999999966	0.0000000000000000	F	F	F
0.7500000000000000	0.6666700000000034	0.0000000000000000	F	F	F
0.6666700000000034	0.6666700000000034	0.0851600000000019	F	F	F
0.7500000000000000	0.8333299999999966	0.0851600000000019	F	F	F
0.6667542227107043	0.8332567846868255	0.1698105524701997	T	T	T
0.7500481453899189	0.6667261016108902	0.1697735405233891	T	T	T
0.6666749677421605	0.6664704457212551	0.2569531860730815	T	T	T
0.7499721258299864	0.8330510504426017	0.2569703914023563	T	T	T
0.8333299999999966	0.8333299999999966	0.0000000000000000	F	F	F
0.9166700000000034	0.6666700000000034	0.0000000000000000	F	F	F
0.8333299999999966	0.6666700000000034	0.0851600000000019	F	F	F
0.9166700000000034	0.8333299999999966	0.0851600000000019	F	F	F
0.8333151190762830	0.8332034761969929	0.1697245082155809	T	T	T
0.9166207250220235	0.6666370345074023	0.1697029324431931	T	T	T
0.8333177608869552	0.6664351093761630	0.2568767865555625	T	T	T
0.9166507910985308	0.8331689531379182	0.2567267316446212	T	T	T
0.1249039633017615	0.8333313193080033	0.3034909068561089	T	T	T
0.2915829794974313	0.8335542663076848	0.3035379903613276	T	T	T
0.0416245449384047	0.2499198665344242	0.3033974448214695	T	T	T
0.2082244598538554	0.2501796549911586	0.3034226504620124	T	T	T
0.4584189185836159	0.8337165710738358	0.3034623791114635	T	T	T
0.6250852388119200	0.8334109708789359	0.3033887880724674	T	T	T
0.3743657973609317	0.2495105033406390	0.3031078994768846	T	T	T
0.5415869599222025	0.2490917434787068	0.3025786875148708	T	T	T
0.7917550158791070	0.8331333141747614	0.3034296780483734	T	T	T
0.9583824203768881	0.8332335419871444	0.3033539942451674	T	T	T
0.7086517625659344	0.2500600270696524	0.3030041150742592	T	T	T
0.8750755386580662	0.2499059773949921	0.3033638626717148	T	T	T
0.1248629045763061	0.4166588016478682	0.3033992296874883	T	T	T
0.2915802738857509	0.4168541449899966	0.3031675702189189	T	T	T
0.0415618081423922	0.5833039374760297	0.3033699769576492	T	T	T
0.2082685678974411	0.5833598324057010	0.3033506481103005	T	T	T
0.4583631107134811	0.4168863174399122	0.3021512011713652	T	T	T
0.6252506912080055	0.4170668449070717	0.3020831563140764	T	T	T
0.3756969307589183	0.5853426715186368	0.3024616633535094	T	T	T
0.5413459846302734	0.5835981907877872	0.3026057756725113	T	T	T
0.7916482434179065	0.4163419636915150	0.3033975268093961	T	T	T
0.9583499924195849	0.4166196112821268	0.3034043980043009	T	T	T
0.7081481585861944	0.5827035082414894	0.3035060965746363	T	T	T
0.875050375130695	0.5832671182710932	0.3034522381273593	T	T	T
0.1248956692738083	0.7499829466534902	0.3033988202005720	T	T	T
0.2916015667568732	0.7500135412447834	0.3034016291367093	T	T	T

0.0416222042263309	0.9166284865224548	0.3033738104998637	T	T	T
0.2082170080566974	0.9167859383735597	0.3035912844975052	T	T	T
0.4581575803747823	0.7499153528294070	0.3033670578655187	T	T	T
0.6248338741174997	0.7495668785092584	0.3035727825021301	T	T	T
0.3749459654856688	0.9168669555489987	0.3035557288009612	T	T	T
0.5416389939255881	0.9166728744841122	0.3035026553912507	T	T	T
0.7917132691737817	0.7498501847399170	0.3035874082152155	T	T	T
0.9583203865226529	0.7499651345819121	0.3033684205126549	T	T	T
0.7083406946427613	0.9165178453211351	0.3036059157682943	T	T	T
0.8750704090548077	0.9164854053961891	0.3034613244437372	T	T	T
0.4732263195472688	0.5052694276506510	0.4675134555208379	T	T	T
0.4752436077256115	0.5096402022407487	0.3907888120686684	T	T	T
0.5326727235690786	0.3263491265138293	0.3907230425473208	T	T	T
0.5332725355371012	0.3283296701462954	0.4674239671942171	T	T	T
0.4267500016834646	0.3189572514061080	0.3862166019335278	T	T	T
0.4244477114324200	0.3133963906897782	0.4627947143712384	T	T	T
0.5839869640335383	0.5130966575916803	0.3879777025351401	T	T	T
0.5851519036652906	0.5178835072398913	0.4646303741168836	T	T	T
0.3616916753884578	0.4878924370031584	0.4651660499654090	T	T	T
0.3305024598825100	0.3800548288266800	0.4210176945724941	T	T	T
0.3654049671666897	0.4977564338561488	0.3882501297582621	T	T	T
0.6447037021845767	0.3405377066944147	0.4683251286650074	T	T	T
0.6398298534139024	0.3255374168999356	0.3917280371120633	T	T	T
0.6782310135365203	0.4418451207057836	0.4219233057704677	T	T	T
0.4758562624635830	0.4507564258261402	0.4284130895340386	T	T	T
0.5318860171829645	0.3841643633081793	0.4287474557783081	T	T	T
0.4235763661176578	0.3728439966508285	0.4255717721286489	T	T	T
0.5853433967602333	0.4588141646453908	0.4272833395547481	T	T	T
0.3671289677941557	0.4379000737729684	0.4250802074203648	T	T	T
0.6401646776127938	0.3883135827271483	0.4273932601289099	T	T	T

**C<sub>4</sub>H<sub>10</sub>···SrTiO<sub>3</sub> (001)**

**Energy: -5310.140219 eV**

1.0000000000000000

23.3760000000000012 0.0000000000000000 0.0000000000000000

0.0000000000000000 11.6880000000000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 28.6878999999999991

Sr Ti O C H

54 88 230 4 10

Selective dynamics

Direct

0.0833299999999966	0.1666700000000034	0.0679000000000016	F	F	F
0.0837497188757101	0.1673409239037983	0.2033887100742426	T	T	T
0.0821643396391831	0.1622275216709538	0.3408482577696957	T	T	T
0.2500000000000000	0.1666700000000034	0.0679000000000016	F	F	F
0.2499249271238669	0.1671369118070774	0.2037658997218028	T	T	T
0.2506106769897403	0.1631908224536480	0.3399824744088946	T	T	T
0.4166600000000003	0.1666700000000034	0.0679000000000016	F	F	F
0.4163230111989093	0.1673888235851855	0.2033787253137541	T	T	T
0.4186100632107663	0.1628372608284239	0.3400868986530274	T	T	T
0.0833299999999966	0.5000000000000000	0.0679000000000016	F	F	F
0.0836237798140304	0.5000956883288790	0.2037827978978770	T	T	T
0.0808540351297308	0.4986105713065867	0.3400508231620747	T	T	T
0.2500000000000000	0.5000000000000000	0.0679000000000016	F	F	F
0.2499484941784635	0.5001721331393688	0.2041187857940976	T	T	T
0.2495392989461921	0.5010819786094525	0.3361092013574656	T	T	T
0.4166600000000003	0.5000000000000000	0.0679000000000016	F	F	F
0.4164123237651717	0.5002016211606375	0.2037878680100093	T	T	T
0.4184429801944147	0.4987784986587732	0.3399135884604460	T	T	T
0.0833299999999966	0.8333299999999966	0.0679000000000016	F	F	F
0.0837669119412631	0.8325788701785855	0.2034081389191022	T	T	T
0.0821527486649026	0.8357157995224896	0.3414476107850906	T	T	T
0.2500000000000000	0.8333299999999966	0.0679000000000016	F	F	F
0.2499576218657999	0.8328285512801168	0.2038126062518997	T	T	T
0.2506649645950887	0.8384799498406399	0.3401681655022844	T	T	T
0.4166600000000003	0.8333299999999966	0.0679000000000016	F	F	F
0.4163411894791391	0.8326230982584667	0.2034104032660753	T	T	T
0.4188661460640855	0.8357375851111472	0.3409373289896561	T	T	T
0.5833299999999966	0.1666700000000034	0.0679000000000016	F	F	F

0.5837663236898039 0.1672967302337317 0.2034105903367612 T T T  
0.5822899303668643 0.1622010256542979 0.3409130032360513 T T T  
0.7500000000000000 0.16667000000000034 0.06790000000000016 F F F  
0.7499378999745542 0.1671216796662325 0.2037424715970195 T T T  
0.7506998525984805 0.1632449628651099 0.3398920774470633 T T T  
0.9166600000000003 0.16667000000000034 0.06790000000000016 F F F  
0.9163217986367646 0.1673799466197824 0.2033404581839122 T T T  
0.9186507983918486 0.1628113746976609 0.3399767055274908 T T T  
0.5833299999999966 0.5000000000000000 0.06790000000000016 F F F  
0.5836082992059167 0.5001058552075359 0.2037945258800583 T T T  
0.5808209444061768 0.4986972536136673 0.3400608638071864 T T T  
0.7500000000000000 0.5000000000000000 0.06790000000000016 F F F  
0.7499452607903996 0.5001142073312419 0.2041080812178363 T T T  
0.7495331080900459 0.5010937472109132 0.3360757302186516 T T T  
0.9166600000000003 0.5000000000000000 0.06790000000000016 F F F  
0.9164489612658324 0.5001641608134638 0.2037526710823256 T T T  
0.9184737498960790 0.4986745169837358 0.3398908245451069 T T T  
0.5833299999999966 0.8333299999999966 0.06790000000000016 F F F  
0.5837432165700471 0.8326181601426953 0.2034220125401948 T T T  
0.5822600060677768 0.8357623043101740 0.3415114589436350 T T T  
0.7500000000000000 0.8333299999999966 0.06790000000000016 F F F  
0.7499636109293435 0.8328199302162080 0.2037945521688119 T T T  
0.7507426120183739 0.8383710248549383 0.3400889889139701 T T T  
0.9166600000000003 0.8333299999999966 0.06790000000000016 F F F  
0.9163410233040125 0.8325495389592475 0.2033843219240890 T T T  
0.9189325572282198 0.8356560235082364 0.3408333060241898 T T T  
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F  
0.0000000000000000 0.0000000000000000 0.1358099999999993 F F F  
0.0002390768482763 0.9996186116490202 0.2698619706011521 T T T  
0.0029594683033612 0.9940672937545186 0.4033851897385167 T T T  
0.16667000000000034 0.0000000000000000 0.0000000000000000 F F F  
0.16667000000000034 0.0000000000000000 0.1358099999999993 F F F  
0.1665513601072758 0.9999327497098739 0.2716323281981330 T T T  
0.1700630660977137 0.0012449172070319 0.4092658747014972 T T T  
0.3333399999999997 0.0000000000000000 0.0000000000000000 F F F  
0.3333399999999997 0.0000000000000000 0.1358099999999993 F F F  
0.3336206798179576 0.9999848280706480 0.2715052037763831 T T T  
0.3376550729026232 0.0014852898199832 0.4094420263879828 T T T  
0.0000000000000000 0.3333299999999966 0.0000000000000000 F F F  
0.0000000000000000 0.3333299999999966 0.1358099999999993 F F F  
0.0000415601381476 0.3328030493455100 0.2714728173638207 T T T  
0.4993509401406184 0.3246261231990559 0.4093896538249852 T T T  
0.16667000000000034 0.3333299999999966 0.0000000000000000 F F F  
0.16667000000000034 0.3333299999999966 0.1358099999999993 F F F  
0.1655960502922041 0.3312001449799571 0.2733195778140652 T T T  
0.170992530041553 0.3441415438793945 0.4076367010791087 T T T  
0.3333399999999997 0.3333299999999966 0.0000000000000000 F F F  
0.3333399999999997 0.3333299999999966 0.1358099999999993 F F F  
0.3343194739067943 0.3313775293917443 0.2732726874990135 T T T  
0.3277345377430717 0.3444871113054158 0.4075029124405746 T T T  
0.0000000000000000 0.66667000000000034 0.0000000000000000 F F F  
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0.8296918594405767	0.8355878581606694	0.4178055951564693	T	T	T
0.8321256343525916	0.6644503297940030	0.2046218650836004	T	T	T
0.8413975568404084	0.6851932730350738	0.3408139350975810	T	T	T
0.9170689807901825	0.6666650362730359	0.2703837776064831	T	T	T
0.9156696024857798	0.6640903403181008	0.4179121361118345	T	T	T
0.8315222263456303	0.0020307229140107	0.4781253407443741	T	T	T
0.6673430606497173	0.0019192470649276	0.4781664334891638	T	T	T
0.6687916678386192	0.3415059439756189	0.4723419115202039	T	T	T
0.6041944037167171	0.2133637694665645	0.5126939266032782	T	T	T
0.8293809630236764	0.6628532643837493	0.4722998424463087	T	T	T
0.8935826472648678	0.7921260703621970	0.5125255623619851	T	T	T
0.8292554029179579	0.3415959715541306	0.4721052460627999	T	T	T
0.8934675700882307	0.2133063871294804	0.5124404173808317	T	T	T
0.6688982372855219	0.6629438352643764	0.4724645421233484	T	T	T
0.6045263435909306	0.7921789084706278	0.5128980625838266	T	T	T
0.7488582813292334	0.1769998706951663	0.5051773701784085	T	T	T
0.7490705194290127	0.8273475819610883	0.5055792143632524	T	T	T
0.9115372003804990	0.502680772092189	0.5051508969139379	T	T	T
0.5868148477088887	0.5031406465990528	0.5044509889718325	T	T	T
0.9990351408124212	0.3373854862015922	0.4781707485398362	T	T	T
0.9991424829739229	0.6657674055814851	0.4781714536879683	T	T	T
0.5099720575084364	0.5371698979384893	0.6059094863798982	T	T	T
0.4553130463911124	0.4672693915391744	0.6100542331508125	T	T	T
0.5636004731041387	0.4652767722742341	0.6121270399362742	T	T	T
0.4017344822200680	0.5409033579351299	0.6119477211596693	T	T	T
0.5094584616430111	0.6063386793570799	0.6317200360906984	T	T	T
0.5103981183397548	0.5789103380851059	0.5716137967884730	T	T	T



0.4532319424655060	0.4080266319856907	0.5804046121994597	T	T	T
0.4575217841194385	0.4130532703440175	0.6411875929739224	T	T	T
0.5662759760489687	0.4319590816267995	0.6476626756972783	T	T	T
0.5633395058584882	0.3913008152871179	0.5886861308605484	T	T	T
0.6024814507718048	0.5139450194996399	0.6049760705864888	T	T	T
0.3984876578106363	0.5848332672695239	0.6454705175897576	T	T	T
0.3628750139747086	0.4905910687810951	0.6068148339297346	T	T	T
0.4023917924684693	0.6070824121936356	0.5849914840213609	T	T	T

**C<sub>6</sub>H<sub>14</sub>··· SrTiO<sub>3</sub> (001)**

**Energy: -5345.010766 eV**

1.0000000000000000  
 23.3760000000000012 0.0000000000000000 0.0000000000000000  
 0.0000000000000000 11.6880000000000006 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 28.6878999999999991

Sr Ti O C H

54 88 230 6 14

Selective dynamics

Direct

0.0833299999999966	0.1666700000000034	0.0679000000000016	F	F	F
0.0837614027549050	0.1674032593855012	0.2033715749629177	T	T	T
0.0821176410591150	0.1623044721098305	0.3408170624715325	T	T	T
0.2500000000000000	0.1666700000000034	0.0679000000000016	F	F	F
0.2499362282226406	0.1672631025791302	0.2037930669072812	T	T	T
0.2505234719066741	0.1632218863056062	0.3401192328440829	T	T	T
0.4166600000000003	0.1666700000000034	0.0679000000000016	F	F	F
0.4162999399260682	0.1673929096125976	0.2033507803793914	T	T	T
0.4184426187658667	0.1626512417615427	0.3401160815317418	T	T	T
0.0833299999999966	0.5000000000000000	0.0679000000000016	F	F	F
0.0836779149781644	0.5001277577595573	0.2037756148068403	T	T	T
0.0808607342391011	0.4986745957899748	0.3400695139446839	T	T	T
0.2500000000000000	0.5000000000000000	0.0679000000000016	F	F	F
0.2499867291551648	0.5000958303469712	0.2041758649243096	T	T	T
0.2495868322349973	0.5009776561372216	0.3361906612759682	T	T	T
0.4166600000000003	0.5000000000000000	0.0679000000000016	F	F	F
0.4164376344870998	0.5002250917183724	0.2038590229293534	T	T	T
0.4182641470805408	0.4988345912240337	0.3400364481087139	T	T	T
0.0833299999999966	0.8333299999999966	0.0679000000000016	F	F	F
0.0837574719235292	0.8326554520880961	0.2033992374264310	T	T	T
0.0820728661320808	0.8357749446477861	0.3413945801740685	T	T	T
0.2500000000000000	0.8333299999999966	0.0679000000000016	F	F	F
0.2499681611503960	0.8329758592220436	0.2038230199892826	T	T	T
0.2506347019523625	0.8386237373068726	0.3401959898472712	T	T	T
0.4166600000000003	0.8333299999999966	0.0679000000000016	F	F	F
0.4163494835531745	0.8326496299778425	0.2034361649512096	T	T	T
0.4188429089183708	0.8355546565875963	0.3409866518393977	T	T	T
0.5833299999999966	0.1666700000000034	0.0679000000000016	F	F	F
0.5837434544561726	0.1672492676696447	0.2034066327053025	T	T	T
0.5821959696118453	0.1622143457741921	0.3409720360436416	T	T	T
0.7500000000000000	0.1666700000000034	0.0679000000000016	F	F	F
0.7499022802981415	0.1670814168254335	0.2037560889345237	T	T	T
0.7506241421601662	0.1632130976340743	0.3399493589592066	T	T	T
0.9166600000000003	0.1666700000000034	0.0679000000000016	F	F	F
0.9162653998113622	0.1674406720694995	0.2033064710573953	T	T	T
0.9185720163459168	0.1626827598641704	0.3399165493410676	T	T	T
0.5833299999999966	0.5000000000000000	0.0679000000000016	F	F	F
0.5836116136017307	0.5001809968287220	0.2038578428248145	T	T	T
0.5807932361482320	0.4984761622855456	0.3400958483461057	T	T	T
0.7500000000000000	0.5000000000000000	0.0679000000000016	F	F	F
0.7499610393380196	0.5001760747335523	0.2040922493477363	T	T	T
0.7494989419642474	0.5011063828448779	0.3360491855172784	T	T	T
0.9166600000000003	0.5000000000000000	0.0679000000000016	F	F	F
0.9164563944005919	0.5001524254829232	0.2037298710488254	T	T	T
0.9184935133459747	0.4987463375725520	0.3398069655606758	T	T	T
0.5833299999999966	0.8333299999999966	0.0679000000000016	F	F	F
0.5837339832727225	0.8325393404053445	0.2034262063406451	T	T	T
0.5820795303140863	0.8354373349401820	0.3416354807934056	T	T	T
0.7500000000000000	0.8333299999999966	0.0679000000000016	F	F	F
0.7499396554685733	0.8328106324561524	0.2037796694510188	T	T	T

0.7506466171273948	0.8382123736260189	0.3401405727115900	T	T	T
0.9166600000000003	0.8333299999999966	0.0679000000000016	F	F	F
0.9163182905395386	0.8325819187816981	0.2033776258593120	T	T	T
0.9188877049806166	0.8357088881691072	0.3407518624438413	T	T	T
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.0000000000000000	0.1358099999999993	F	F	F
0.0001839747974637	0.9996910937537496	0.2698133039247639	T	T	T
0.0028712180955260	0.9940377063837244	0.4033476185263560	T	T	T
0.1666700000000034	0.0000000000000000	0.0000000000000000	F	F	F
0.1666700000000034	0.0000000000000000	0.1358099999999993	F	F	F
0.1665176008095336	-0.0000319767603437	0.2716252296219439	T	T	T
0.1698477485293211	0.0012042102314237	0.4092775410896478	T	T	T
0.3333399999999997	0.0000000000000000	0.0000000000000000	F	F	F
0.3333399999999997	0.0000000000000000	0.1358099999999993	F	F	F
0.3335969863629627	-0.0001069003575113	0.2715468979303367	T	T	T
0.3375221329609510	0.0014803049973738	0.4095057563772641	T	T	T
0.0000000000000000	0.3333299999999966	0.0000000000000000	F	F	F
0.0000000000000000	0.3333299999999966	0.1358099999999993	F	F	F
0.0000788021980056	0.3328684147859628	0.2714608948453653	T	T	T
0.4990689104133903	0.3241247064131105	0.4092931456456822	T	T	T
0.1666700000000034	0.3333299999999966	0.0000000000000000	F	F	F
0.1666700000000034	0.3333299999999966	0.1358099999999993	F	F	F
0.1656277144090282	0.3312302167812551	0.2733434909150858	T	T	T
0.1709253232541589	0.3442144301179731	0.4076553416782679	T	T	T
0.3333399999999997	0.3333299999999966	0.0000000000000000	F	F	F
0.3333399999999997	0.3333299999999966	0.1358099999999993	F	F	F
0.3343436014110850	0.3312569188992204	0.2733163932999802	T	T	T
0.3276356703766771	0.3445944343569832	0.4075915781632194	T	T	T
0.0000000000000000	0.6666700000000034	0.0000000000000000	F	F	F
0.0000000000000000	0.6666700000000034	0.1358099999999993	F	F	F
0.0000734503427857	0.6670314809019490	0.2715809670357039	T	T	T
0.4993126189997552	0.6591463671900135	0.4091532934485115	T	T	T
0.1666700000000034	0.6666700000000034	0.0000000000000000	F	F	F
0.1666700000000034	0.6666700000000034	0.1358099999999993	F	F	F
0.1655738798891504	0.6689515777287930	0.2733503433485527	T	T	T
0.1710321126237166	0.6578410330146238	0.4076759278805664	T	T	T
0.3333399999999997	0.6666700000000034	0.0000000000000000	F	F	F
0.3333399999999997	0.6666700000000034	0.1358099999999993	F	F	F
0.3343525716433497	0.6688131684936223	0.2733300968929238	T	T	T
0.3277816236157189	0.6582065090817846	0.4076999410473659	T	T	T
0.1730976235248994	0.1712350183855325	0.4852542990385833	T	T	T
0.3237210237111494	0.8330964181301465	0.4853892863567838	T	T	T
0.4143984530145817	0.3515175197527263	0.4850093658315004	T	T	T
0.0836291727823906	0.6531487099446602	0.4853766878731348	T	T	T
0.1733026745066976	0.8326438194787495	0.4854045723787682	T	T	T
0.3238277171996641	0.1713849916109329	0.4852092467574233	T	T	T
0.4144200892179323	0.6541586699424310	0.4851162630408736	T	T	T
0.0834676979626105	0.3523447767421215	0.4851926263999355	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.0000000000000000	0.1358099999999993	F	F	F
0.5001884937485581	-0.0002886296843980	0.2699526437109457	T	T	T
0.5029512008819287	0.9938354796883425	0.4035056452329769	T	T	T
0.6666700000000034	0.0000000000000000	0.0000000000000000	F	F	F
0.6666700000000034	0.0000000000000000	0.1358099999999993	F	F	F
0.6664723597611206	-0.0001309786422728	0.2716136954731835	T	T	T
0.6701680721820017	0.0011318494101376	0.4091159005217592	T	T	T
0.8333399999999997	0.0000000000000000	0.0000000000000000	F	F	F
0.8333399999999997	0.0000000000000000	0.1358099999999993	F	F	F
0.8335440705687651	-0.0000373104430777	0.2714721582219512	T	T	T
0.8375918830628741	0.0014034876660060	0.4094156993195001	T	T	T
0.5000000000000000	0.3333299999999966	0.0000000000000000	F	F	F
0.5000000000000000	0.3333299999999966	0.1358099999999993	F	F	F
0.5000227791674597	0.3328808583852268	0.2714713459573883	T	T	T
0.9992145030464821	0.3245764339624014	0.4093897771229144	T	T	T
0.6666700000000034	0.3333299999999966	0.0000000000000000	F	F	F
0.6666700000000034	0.3333299999999966	0.1358099999999993	F	F	F
0.6655936367434525	0.3311825829533612	0.2733176310970353	T	T	T
0.6711479973633305	0.3442188485256742	0.4075823647713813	T	T	T
0.8333399999999997	0.3333299999999966	0.0000000000000000	F	F	F
0.8333399999999997	0.3333299999999966	0.1358099999999993	F	F	F

0.8343201010023824	0.3313704002286690	0.2732366862633192	T	T	T
0.8278502149593463	0.3444513711510767	0.4074483676595097	T	T	T
0.5000000000000000	0.6666700000000034	0.0000000000000000	F	F	F
0.5000000000000000	0.6666700000000034	0.1358099999999993	F	F	F
0.4999808839039794	0.6670333434200920	0.2716506701885289	T	T	T
0.9993867289753166	0.6596059463722055	0.4092085551461834	T	T	T
0.6666700000000034	0.6666700000000034	0.0000000000000000	F	F	F
0.6666700000000034	0.6666700000000034	0.1358099999999993	F	F	F
0.6655328738882882	0.6688862685073396	0.2733153607614283	T	T	T
0.6712592604449450	0.6578276192620268	0.4076587924929906	T	T	T
0.8333399999999997	0.6666700000000034	0.0000000000000000	F	F	F
0.8333399999999997	0.6666700000000034	0.1358099999999993	F	F	F
0.8343829336034976	0.6688897036825182	0.2732782486080593	T	T	T
0.8281215746499935	0.6578872657887836	0.4075605268183149	T	T	T
0.6733443067669507	0.1711441972051493	0.4851020333336548	T	T	T
0.8238657671114225	0.8327980959355191	0.4851907992032954	T	T	T
0.9143393666894558	0.3521517665279803	0.4850868488488562	T	T	T
0.5835960601603439	0.6543736546469362	0.4849211214182910	T	T	T
0.6736386059310594	0.8329392429099358	0.4853016567865956	T	T	T
0.8239703221103589	0.1713484378164983	0.4850774392065744	T	T	T
0.9143571382825240	0.6536464235056385	0.4852661361170340	T	T	T
0.5832681174651899	0.3513921937878738	0.4846551974862330	T	T	T
0.0000000000000000	0.1666700000000034	0.0000000000000000	F	F	F
0.0000000000000000	0.1666700000000034	0.1358099999999993	F	F	F
0.0000000000000000	0.0000000000000000	0.0679000000000016	F	F	F
0.0833299999999966	0.0000000000000000	0.0000000000000000	F	F	F
0.0833299999999966	0.0000000000000000	0.1358099999999993	F	F	F
0.4996701065278424	0.1668143918280590	0.2713707178897519	T	T	T
0.4985582363164807	0.1679296174780285	0.4045233317608232	T	T	T
0.4996418062960304	0.0004173410249005	0.2033823435161819	T	T	T
0.4997643520125157	0.0005026498287786	0.3386510020659702	T	T	T
0.0828632430041456	0.0005806547419244	0.2708322040888547	T	T	T
0.0818348362828961	0.0022682696956721	0.4043405332996259	T	T	T
0.1666700000000034	0.1666700000000034	0.0000000000000000	F	F	F
0.1666700000000034	0.1666700000000034	0.1358099999999993	F	F	F
0.1666700000000034	0.0000000000000000	0.0679000000000016	F	F	F
0.2500000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.2500000000000000	0.0000000000000000	0.1358099999999993	F	F	F
0.1667429074111176	0.1659947251802710	0.2704380774259381	T	T	T
0.1678488458086589	0.1688952983251354	0.4179928617983882	T	T	T
0.1668135508062890	0.0003749310796956	0.2034829117874919	T	T	T
0.1638470878770708	0.0005244492628264	0.3404503266672834	T	T	T
0.2497601820365039	0.0004173015372437	0.2725545517731367	T	T	T
0.2479828051462681	0.0017347472819136	0.4010723440123116	T	T	T
0.3333399999999997	0.1666700000000034	0.0000000000000000	F	F	F
0.3333399999999997	0.1666700000000034	0.1358099999999993	F	F	F
0.3333399999999997	0.0000000000000000	0.0679000000000016	F	F	F
0.4166600000000003	0.0000000000000000	0.0000000000000000	F	F	F
0.4166600000000003	0.0000000000000000	0.1358099999999993	F	F	F
0.3328405816334582	0.1659547901757114	0.2703954903948262	T	T	T
0.3293540822722194	0.1680840257148888	0.4179691835641297	T	T	T
0.3331086890833840	0.0004195413119265	0.2035487913616758	T	T	T
0.3340829042411724	0.0008309844567090	0.3408103397328920	T	T	T
0.4165925996445704	0.0007578923592253	0.2714744057355607	T	T	T
0.4157184863988381	0.0025265047626624	0.4044614460644005	T	T	T
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.1358099999999993	F	F	F
0.0000000000000000	0.3333299999999966	0.0679000000000016	F	F	F
0.0833299999999966	0.3333299999999966	0.0000000000000000	F	F	F
0.0833299999999966	0.3333299999999966	0.1358099999999993	F	F	F
-0.0001180940440197	0.5004647471352622	0.2724513600993252	T	T	T
0.4992401277881404	0.5032155040637013	0.4012867360851998	T	T	T
0.9998881446312844	0.3337557984914646	0.2035039043270084	T	T	T
0.4994582681300092	0.3314984548166418	0.3408443686521889	T	T	T
0.0825610294316416	0.3343592651528784	0.2702111309698392	T	T	T
0.0821615318454782	0.3408727777505526	0.4178765475287536	T	T	T
0.1666700000000034	0.5000000000000000	0.0000000000000000	F	F	F
0.1666700000000034	0.5000000000000000	0.1358099999999993	F	F	F
0.1666700000000034	0.3333299999999966	0.0679000000000016	F	F	F
0.2500000000000000	0.3333299999999966	0.0000000000000000	F	F	F

0.2500000000000000 0.3333299999999966 0.1358099999999993 F F F  
0.1662201034926998 0.5005186562539894 0.2761028031906206 T T T  
0.1662663762684746 0.5012314104569178 0.3964160695992999 T T T  
0.1678467840221290 0.3358742510435633 0.2046476335966048 T T T  
0.1573767943616086 0.3174182480882132 0.3408737314323309 T T T  
0.2497735508337974 0.3334259682841227 0.2763191938782539 T T T  
0.2492509212511066 0.3353723404707199 0.3961989476286876 T T T  
0.3333399999999997 0.5000000000000000 0.0000000000000000 F F F  
0.3333399999999997 0.5000000000000000 0.1358099999999993 F F F  
0.3333399999999997 0.3333299999999966 0.0679000000000016 F F F  
0.4166600000000003 0.3333299999999966 0.0000000000000000 F F F  
0.4166600000000003 0.3333299999999966 0.1358099999999993 F F F  
0.3333794854269702 0.5005118398713126 0.2763633982753328 T T T  
0.3323808649384626 0.5014428633818864 0.3962539400077432 T T T  
0.3320526491016214 0.3360408870193361 0.2046760215960795 T T T  
0.3416575522115773 0.3165915280398290 0.3409452346691723 T T T  
0.4170276857666814 0.3344004298212129 0.2704280394171851 T T T  
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0.0000000000000000 0.8333299999999966 0.0000000000000000 F F F  
0.0000000000000000 0.8333299999999966 0.1358099999999993 F F F  
0.0000000000000000 0.6666700000000034 0.0679000000000016 F F F  
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0.9997563987283046	0.6720029158320492	0.3404419813988975	T	T	T
0.5825501119270829	0.6666472147898479	0.2704979942441417	T	T	T
0.5827182925568617	0.6649054194587606	0.4178037588759264	T	T	T
0.6666700000000034	0.8333299999999966	0.0000000000000000	F	F	F
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0.6666700000000034	0.6666700000000034	0.0679000000000016	F	F	F
0.7500000000000000	0.6666700000000034	0.0000000000000000	F	F	F
0.7500000000000000	0.6666700000000034	0.1358099999999993	F	F	F
0.6666466302876368	0.8347737834881716	0.2701878483805816	T	T	T
0.6683151404137931	0.8344516689623616	0.4178896434545483	T	T	T
0.6676271297654147	0.6643950534906344	0.2046075016384717	T	T	T
0.6582151460428768	0.6841457266155095	0.3408478105558598	T	T	T
0.7497943882844857	0.6676147776685347	0.2759856490092087	T	T	T
0.7495115202021607	0.6668892223608411	0.3964912070685100	T	T	T
0.8333399999999997	0.8333299999999966	0.0000000000000000	F	F	F
0.8333399999999997	0.8333299999999966	0.1358099999999993	F	F	F
0.8333399999999997	0.6666700000000034	0.0679000000000016	F	F	F
0.9166600000000003	0.6666700000000034	0.0000000000000000	F	F	F
0.9166600000000003	0.6666700000000034	0.1358099999999993	F	F	F
0.8328630404436697	0.8349333105507679	0.2701722095875206	T	T	T
0.8294947858349274	0.8354584314092132	0.4178193697421923	T	T	T
0.8320994407418250	0.6644177965954250	0.2046073925773962	T	T	T
0.8413723845457076	0.6852479403130595	0.3407925705431685	T	T	T
0.9170657702280683	0.6665516683852177	0.2703518686347241	T	T	T
0.9155734576411072	0.6641872891440920	0.4179881640486722	T	T	T
0.8313499230004289	0.0020085119951722	0.4781085793928875	T	T	T
0.6673849836252886	0.0018576964723214	0.4780462947625923	T	T	T
0.6687360922127029	0.3413431826455942	0.4722382338350044	T	T	T
0.6041850372910541	0.2124011398400787	0.5123466541326375	T	T	T
0.8292599616051777	0.6626622723275714	0.4723030758129508	T	T	T
0.8932912771149638	0.7919098803045183	0.5127351997862366	T	T	T
0.8292447262176311	0.3416712345941512	0.4720541898098780	T	T	T
0.8934089703413280	0.2133702401186009	0.5124267352544433	T	T	T
0.6687369719672527	0.6629896526882501	0.4725589730765006	T	T	T
0.6043489815839023	0.7932185917534821	0.5126204943609219	T	T	T
0.7488683039708902	0.1771603430277610	0.5052568118746360	T	T	T
0.7490068688031539	0.8272077462789309	0.5057480918819055	T	T	T
0.9115009034509018	0.5026699101713115	0.5052095954049659	T	T	T
0.5863108609422949	0.5025946571208869	0.5026569432235989	T	T	T
0.9989653580241356	0.3371843700236895	0.4781716853866831	T	T	T
0.9990575373865723	0.6658934344058597	0.4782190261769753	T	T	T
0.5144046166213232	0.5370932477720590	0.6075928677224970	T	T	T
0.5700158472098157	0.4698948923697611	0.6087004356008435	T	T	T
0.4611123719672082	0.4625703205742995	0.6089503316235773	T	T	T
0.6230875206160605	0.5449995677390052	0.6052850684312171	T	T	T
0.4063510468196488	0.5321925666838762	0.6127187060482135	T	T	T
0.6771368112844335	0.4784526278731652	0.5937916048166111	T	T	T
0.5134534732333803	0.5979813247443513	0.6367140647119423	T	T	T
0.5131285046288531	0.5893043460213861	0.5756853297695430	T	T	T
0.5699484777025715	0.4076651175540036	0.5799749574470624	T	T	T
0.5720123573204088	0.4185330668440839	0.6406820180367243	T	T	T
0.4603431958370165	0.4095296034152512	0.5773640821861948	T	T	T
0.4638613220232928	0.4025881551099423	0.6382259418996464	T	T	T
0.6162650388979574	0.6109081537986987	0.5785845455057005	T	T	T
0.6283951569977156	0.5921323410229139	0.6380393867468861	T	T	T
0.4027423969587669	0.5717880989903189	0.6471193439873023	T	T	T
0.3682933724455943	0.4800352746251585	0.6067900222417085	T	T	T
0.4056746982743472	0.6014117883162010	0.5870514651844944	T	T	T
0.6845227620779430	0.4102513846818636	0.6191924196344297	T	T	T
0.6739211413172010	0.4392248014307773	0.5592773941295505	T	T	T
0.7147922925870603	0.5337605617471898	0.5934763053586479	T	T	T

**C<sub>8</sub>H<sub>18</sub>··· SrTiO<sub>3</sub> (001)**

**Energy: -5379.916436 eV**

1.0000000000000000		
23.3760000000000012	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.6880000000000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.6878999999999991

Sr Ti O C H  
54 88 230 8 18

Selective dynamics

Direct

0.0833299999999966	0.1666700000000034	0.0679000000000016	F	F	F
0.0837452354713187	0.1674032330599360	0.2033859970343449	T	T	T
0.0821603869065353	0.1623432460392814	0.3408877143545392	T	T	T
0.2500000000000000	0.1666700000000034	0.0679000000000016	F	F	F
0.2499254225618225	0.1671494826188174	0.2037792620470235	T	T	T
0.2505235048037678	0.1633077239702942	0.3399655184069794	T	T	T
0.4166600000000003	0.1666700000000034	0.0679000000000016	F	F	F
0.4162967641228320	0.1673491129776402	0.2033738115826297	T	T	T
0.4185132756799178	0.1627835670185022	0.3401184427801347	T	T	T
0.0833299999999966	0.5000000000000000	0.0679000000000016	F	F	F
0.0835796756724557	0.5001461317996402	0.2037935150525357	T	T	T
0.0807812848600486	0.4989060909598714	0.3400804950165764	T	T	T
0.2500000000000000	0.5000000000000000	0.0679000000000016	F	F	F
0.2499327645734160	0.5000350284471542	0.2041289206507888	T	T	T
0.2495484545291589	0.5010736732338390	0.3360959660622860	T	T	T
0.4166600000000003	0.5000000000000000	0.0679000000000016	F	F	F
0.4164012179833584	0.5000541166385861	0.2037514055155561	T	T	T
0.4184350502412270	0.4986367360469136	0.3399001463862761	T	T	T
0.0833299999999966	0.8333299999999966	0.0679000000000016	F	F	F
0.0837208416856862	0.8325572617532861	0.2034113978765368	T	T	T
0.0821357985033846	0.8358562828883782	0.3414511984843072	T	T	T
0.2500000000000000	0.8333299999999966	0.0679000000000016	F	F	F
0.2499148474642185	0.8327699334261872	0.2037767086781094	T	T	T
0.2506862634010527	0.8384837291234185	0.3400866177233304	T	T	T
0.4166600000000003	0.8333299999999966	0.0679000000000016	F	F	F
0.4163567909641085	0.8326022187900141	0.2034281719800537	T	T	T
0.4189457199362568	0.8355251674671763	0.3410114464598251	T	T	T
0.5833299999999966	0.1666700000000034	0.0679000000000016	F	F	F
0.5837491841278365	0.1673623328754697	0.2034138230995375	T	T	T
0.5822999029424545	0.1623446526685244	0.3409780780140095	T	T	T
0.7500000000000000	0.1666700000000034	0.0679000000000016	F	F	F
0.7499680131852828	0.1671408089770687	0.2037362368676841	T	T	T
0.7507444668008132	0.1633612620178956	0.3398256884739649	T	T	T
0.9166600000000003	0.1666700000000034	0.0679000000000016	F	F	F
0.9163167481775535	0.1674158717792150	0.2033395403775494	T	T	T
0.9186296117731217	0.1628321769003163	0.3400550229889250	T	T	T
0.5833299999999966	0.5000000000000000	0.0679000000000016	F	F	F
0.5836201543178473	0.5001433256683947	0.2037624656873023	T	T	T
0.5809094444219077	0.4985978878551857	0.3399519304721142	T	T	T
0.7500000000000000	0.5000000000000000	0.0679000000000016	F	F	F
0.7499386404618765	0.5001570695975789	0.2041071299492043	T	T	T
0.7495140572474162	0.5011422876577575	0.3360803816907602	T	T	T
0.9166600000000003	0.5000000000000000	0.0679000000000016	F	F	F
0.9164592919668486	0.5001823757558578	0.2037540564053749	T	T	T
0.9185021751153134	0.4987676965976006	0.3399091070642460	T	T	T
0.5833299999999966	0.8333299999999966	0.0679000000000016	F	F	F
0.5837210324666366	0.8326386712342261	0.2034359069671697	T	T	T
0.5822157619300440	0.8357462227798459	0.3415428393889158	T	T	T
0.7500000000000000	0.8333299999999966	0.0679000000000016	F	F	F
0.7499603682139612	0.8328204742553538	0.2037869691810259	T	T	T
0.7507279146887950	0.8384031052062852	0.3401044416966955	T	T	T
0.9166600000000003	0.8333299999999966	0.0679000000000016	F	F	F
0.9163370985767599	0.8325325491289181	0.2033715283650986	T	T	T
0.9189125839762108	0.8358430897867902	0.3408364672191694	T	T	T
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.0000000000000000	0.1358099999999993	F	F	F
0.0002177954346975	0.9996870626480204	0.2698665281181900	T	T	T
0.0029593343045734	0.9941992145193774	0.4033966270510886	T	T	T
0.1666700000000034	0.0000000000000000	0.0000000000000000	F	F	F
0.1666700000000034	0.0000000000000000	0.1358099999999993	F	F	F
0.1665182608697567	0.9999330196579286	0.2716277318309220	T	T	T
0.1701852981271464	0.0012703665690224	0.4092340248820440	T	T	T
0.3333399999999997	0.0000000000000000	0.0000000000000000	F	F	F
0.3333399999999997	0.0000000000000000	0.1358099999999993	F	F	F
0.3336256502444503	-0.0001226943835138	0.2714980348624828	T	T	T
0.3376902983213327	0.0015150597235420	0.4094089349391406	T	T	T

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0.0000000000000000 0.3333299999999966 0.1358099999999993 F F F  
0.0000613637412155 0.3328742787334074 0.2714951142191595 T T T  
0.4991938841133003 0.3242377656572895 0.4092841469399621 T T T  
0.1666700000000034 0.3333299999999966 0.0000000000000000 F F F  
0.1666700000000034 0.3333299999999966 0.1358099999999993 F F F  
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0.6677579756232918	0.6645251601120831	0.2046002799640262	T	T	T
0.6581035311528766	0.6842000806117328	0.3408418500504515	T	T	T
0.7498260823568060	0.6677356834551277	0.2760587745347994	T	T	T
0.7495039454018656	0.6670970292549891	0.3964495924774367	T	T	T
0.8333399999999997	0.8333299999999966	0.0000000000000000	F	F	F

0.8333399999999999	0.8333299999999999	0.1358099999999999	F	F	F
0.8333399999999999	0.6666700000000003	0.0679000000000001	F	F	F
0.9166600000000003	0.6666700000000003	0.0000000000000000	F	F	F
0.9166600000000003	0.6666700000000003	0.1358099999999999	F	F	F
0.8328743135211272	0.8349954485258831	0.2701721855617168	T	T	T
0.8295300530009515	0.8355958192057011	0.4178981104686024	T	T	T
0.8321157886108341	0.6643889993307340	0.2046267798720348	T	T	T
0.8413846402342590	0.6854023304503593	0.3408359902205265	T	T	T
0.9170527645741213	0.6666619833807352	0.2703759865238697	T	T	T
0.9155877856733862	0.6642886806317205	0.4180169676145340	T	T	T
0.8313428613904734	0.0020296865687283	0.4781798539843641	T	T	T
0.6676206749535019	0.0022969484717245	0.4781013250592936	T	T	T
0.6688360950514853	0.3416205173184095	0.4722754571849745	T	T	T
0.6043818325251031	0.2131593837358768	0.5126749216971419	T	T	T
0.8292829596345943	0.6626417730554459	0.4723443017796862	T	T	T
0.8329211909133111	0.7917848003069244	0.5128486874715877	T	T	T
0.8293160681051532	0.3416954628564010	0.4721185222690266	T	T	T
0.8935384341188892	0.2132517076708756	0.5124128134893973	T	T	T
0.6688392201331150	0.6631557572514024	0.4725940890311697	T	T	T
0.6043178743579781	0.7936720917198380	0.5124368675419982	T	T	T
0.7489719224742034	0.1776815375578679	0.5053773501016940	T	T	T
0.7490386405617486	0.8272592061790230	0.5058255803676699	T	T	T
0.9115065043902726	0.5026686049170498	0.5052499156679651	T	T	T
0.5863018234171740	0.5025367445988101	0.5029022663682138	T	T	T
0.9990115342042989	0.3373972312663033	0.4781665705941204	T	T	T
0.9990754545237430	0.6658979594214600	0.4782106379774591	T	T	T
0.4922289806361776	0.4839698686241537	0.6060160559646612	T	T	T
0.5454541425168761	0.5587505940876666	0.6078711748574909	T	T	T
0.4365311840950224	0.5508579346039600	0.6085105080003830	T	T	T
0.6009687288120498	0.4906919363963085	0.6087009856660228	T	T	T
0.3833941641246622	0.4754367347536049	0.6077739220417530	T	T	T
0.6540931609618433	0.5626131103012327	0.5997919912732993	T	T	T
0.3286462764276908	0.5416508130928130	0.5982753375046806	T	T	T
0.7078261959683837	0.4912061613476785	0.5929691013539157	T	T	T
0.4935577354248589	0.4207673346356639	0.6343161104304478	T	T	T
0.4929576128140457	0.4346495754122441	0.5733787497211119	T	T	T
0.5434911363893073	0.6153863749515752	0.6383290160089177	T	T	T
0.5452721982923925	0.6163084779759583	0.5774597481466586	T	T	T
0.4348934813786773	0.6117453161503746	0.5792656967109271	T	T	T
0.4360896617298060	0.6041808370164415	0.6399941250957395	T	T	T
0.5988598041584438	0.4226026534923860	0.5824200469285786	T	T	T
0.6050700043255154	0.4466617847188449	0.6423313585580644	T	T	T
0.3801669109765128	0.4298945556110340	0.6410959881438683	T	T	T
0.3885120912312580	0.4086344344047504	0.5812280962682768	T	T	T
0.6599480789900685	0.6235096061521418	0.6285116990908350	T	T	T
0.6473383405348632	0.6149048050183905	0.5685168533653061	T	T	T
0.3228281432062938	0.6106009617941983	0.6236064063324416	T	T	T
0.3295419820884053	0.5800835136903392	0.5635037590096689	T	T	T
0.2910306876997176	0.4864185176969729	0.5998130426115991	T	T	T
0.7454060810928286	0.5450508814106875	0.5874052699404898	T	T	T
0.7035441665481731	0.4356928379612672	0.5624343602924514	T	T	T
0.7160772960174393	0.4368375709651124	0.6232914649596053	T	T	T