

## Supporting Information

### Theoretical Characterization of Zeolite Encapsulated Platinum Clusters in the Presence of Water Molecules

Qianqian Bao<sup>†,‡</sup>, Weiwei Zhang<sup>†,‡,\*</sup>, Donghai Mei<sup>†,‡,§,\*</sup>

<sup>†</sup>*State Key Laboratory of Separation Membranes and Membrane Processes, Tiangong University, Tianjin 300387, China*

<sup>‡</sup>*School of Chemical Engineering and Technology, Tiangong University, Tianjin 300387, China*

<sup>§</sup>*School of Environmental Science and Engineering, Tiangong University, Tianjin 300387, China*

**The Gibbs free energy computational method.** For catalytic reactions in the confinement condition, restrictions and steric hindrance strongly affect the stability of each structure. Therefore, the zero-point energy (ZPE) and entropy corrections should be included. In the present work, the Gibbs free energy change ( $\Delta G$ ) was calculated using standard statistical thermodynamic methods. The room temperature ( $T=298.15\text{K}$ ) is used.

$$\Delta G = \Delta E + \Delta ZPE + T\Delta S \quad (\text{S1})$$

$$\Delta H = \Delta U_{trans} + \Delta U_{rot} + \Delta U_{vib} + \Delta(ZPE) + \Delta E_{elec} \quad (\text{S2})$$

$$\Delta S = \Delta S_{trans} + \Delta S_{rot} + \Delta S_{vib} \quad (\text{S3})$$

where the translational, rotational, and vibrational contributions to the internal energy ( $\Delta U$ ) and ZPE were given below. The electronic term ( $\Delta E_{elec}$ ) was directly derived from DFT calculations. Due to the small change of translational and rotational entropies/internal energies before and after the adsorption, only  $S_{vib}$  and  $U_{vib}$  were calculated in this work.

$$U_{vib} = \sum_i \frac{hv_i}{(e^{hv_i/k_B T} - 1)} \quad (\text{S4})$$

$$S_{vib} = k_B \sum_i \left( \frac{h\nu_i}{k_B T \left( e^{\frac{h\nu_i}{k_B T}} - 1 \right)} - \ln \left( 1 - e^{-\frac{h\nu_i}{k_B T}} \right) \right) \quad (S5)$$

$$ZPE = \sum_i \frac{h\nu_i}{2} \quad (S6)$$

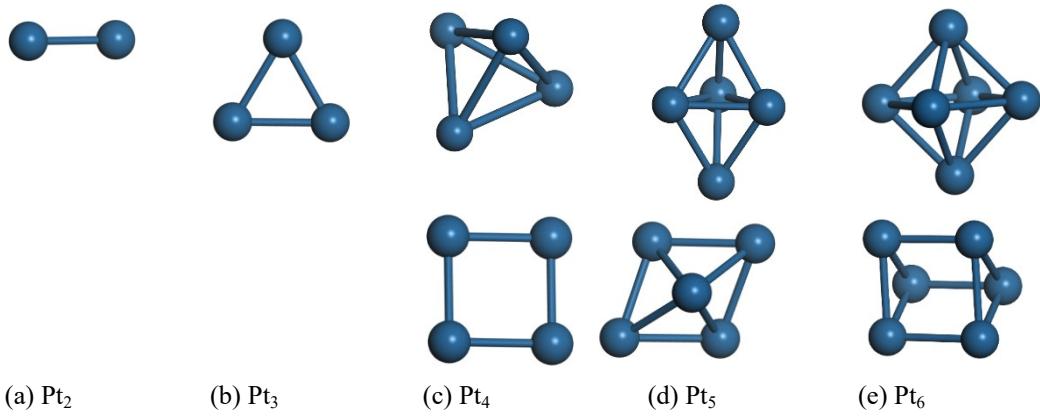
In the above equations,  $k_B$  and  $h$  are Boltzmann and Planck constants, respectively, and  $T$  and  $\nu_i$  temperature and vibrational frequency, respectively. The vibrational frequencies of the molecules were calculated according to the harmonic oscillator approximation with a displacement of 0.01 Å. Only mobile reactants were considered in the vibrational frequency calculations, whereas the atoms on the Silicalite-1 and H-MFI model framework were fixed.

The calculated energy barrier of activation ( $\Delta H^\ddagger$ ) and Gibbs energy of activation ( $\Delta G^\ddagger$ ) were then obtained using the following equations:

$$\Delta H^\ddagger = \Delta U_{vib}^\ddagger + \Delta(ZPE)^\ddagger + (E_{elec}^{TS} - E_{elec}^{IS}) \quad (S11)$$

$$\Delta G^\ddagger = \Delta H^\ddagger - T\Delta S^\ddagger \quad (S12)$$

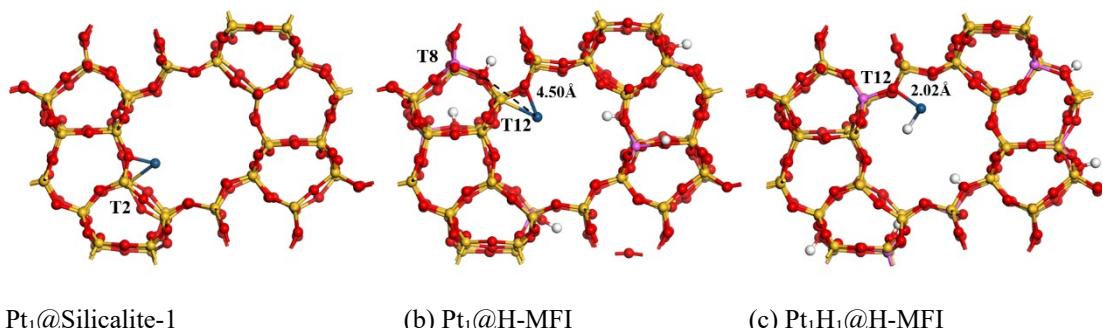
where  $E_{elec}^{TS}$  and  $E_{elec}^{IS}$  are the electronic energy differences between the transition states (TS) and initial states (IS) of each elementary reaction step, respectively.



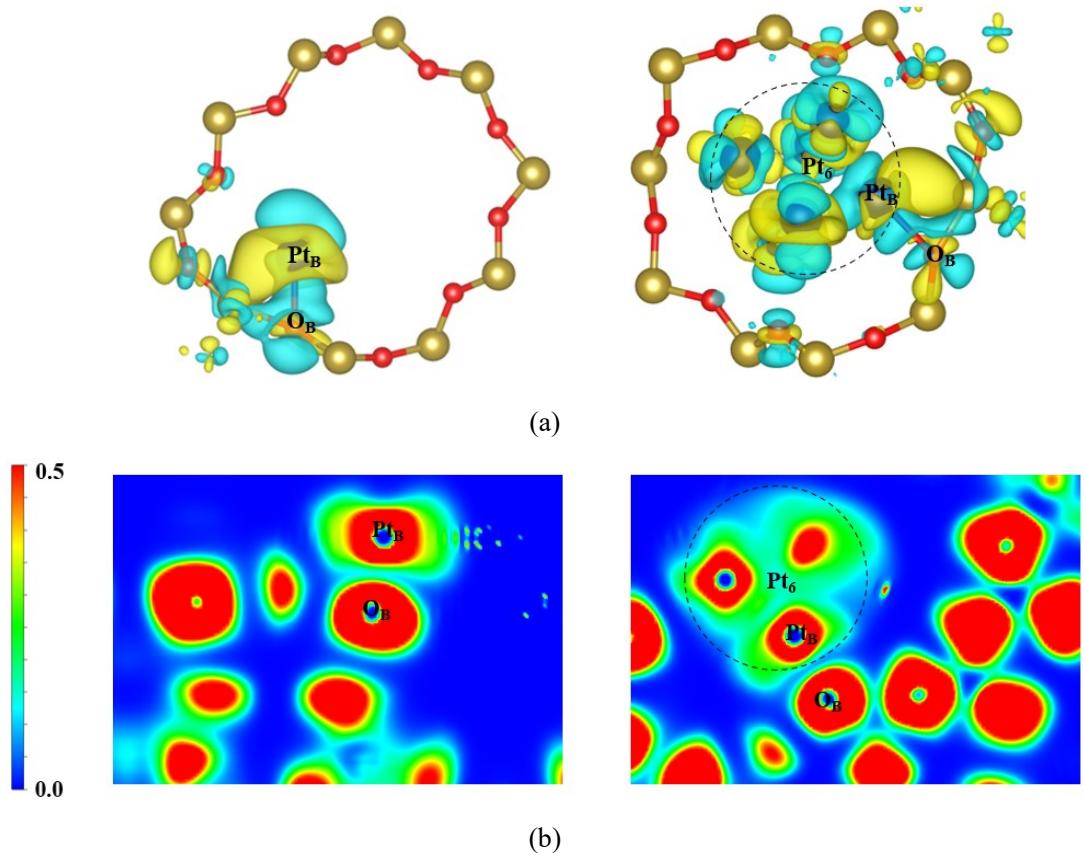
**Figure S1.** Optimized stable configurations of Pt<sub>2</sub>, Pt<sub>3</sub>, Pt<sub>4</sub>, Pt<sub>5</sub>, Pt<sub>6</sub> nanoclusters in vacuum.

**Table S1.** Binding energies (in kJ·mol<sup>-1</sup>) of Pt<sub>2</sub>, Pt<sub>3</sub>, Pt<sub>4</sub>, Pt<sub>5</sub> and Pt<sub>6</sub> nanoclusters shown in Figure S1.

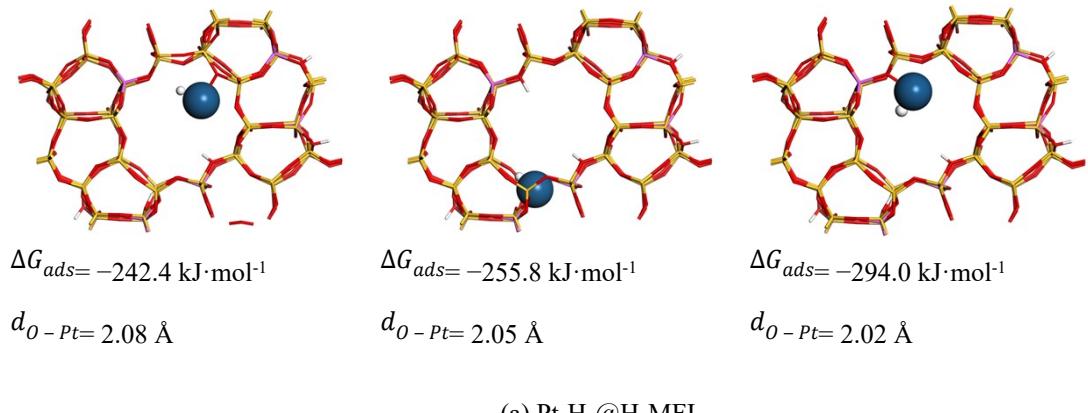
Number of Pt	$\Delta G_b^{Pt_n}$ (Upper)	$\Delta G_b^{Pt_n}$ (Lower)
2	-213.1	
3	-281.2	
4	-309.4	-306.7
5	-332.6	-320.9
6	-351.6	-347.8



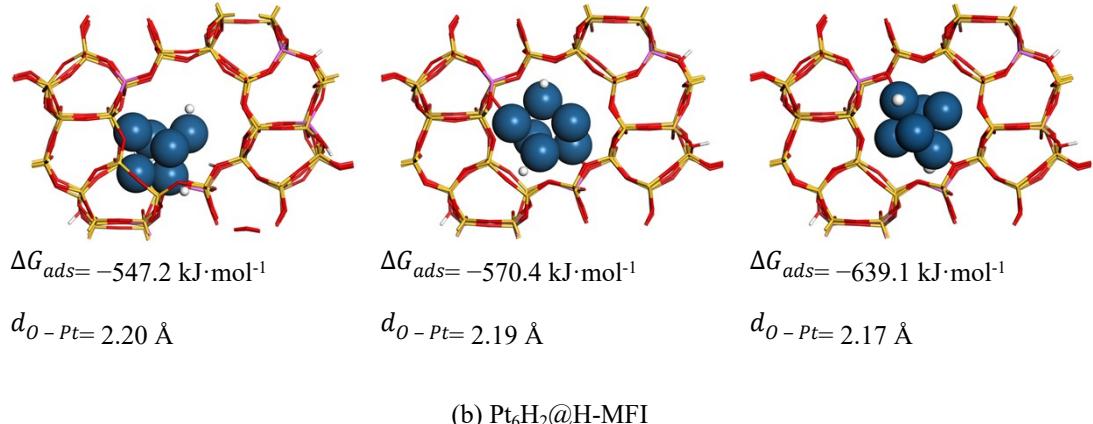
**Figure S2.** The positions of encapsulated Pt<sub>1</sub> atoms in the Silicalite-1 and H-MFI nanopores.



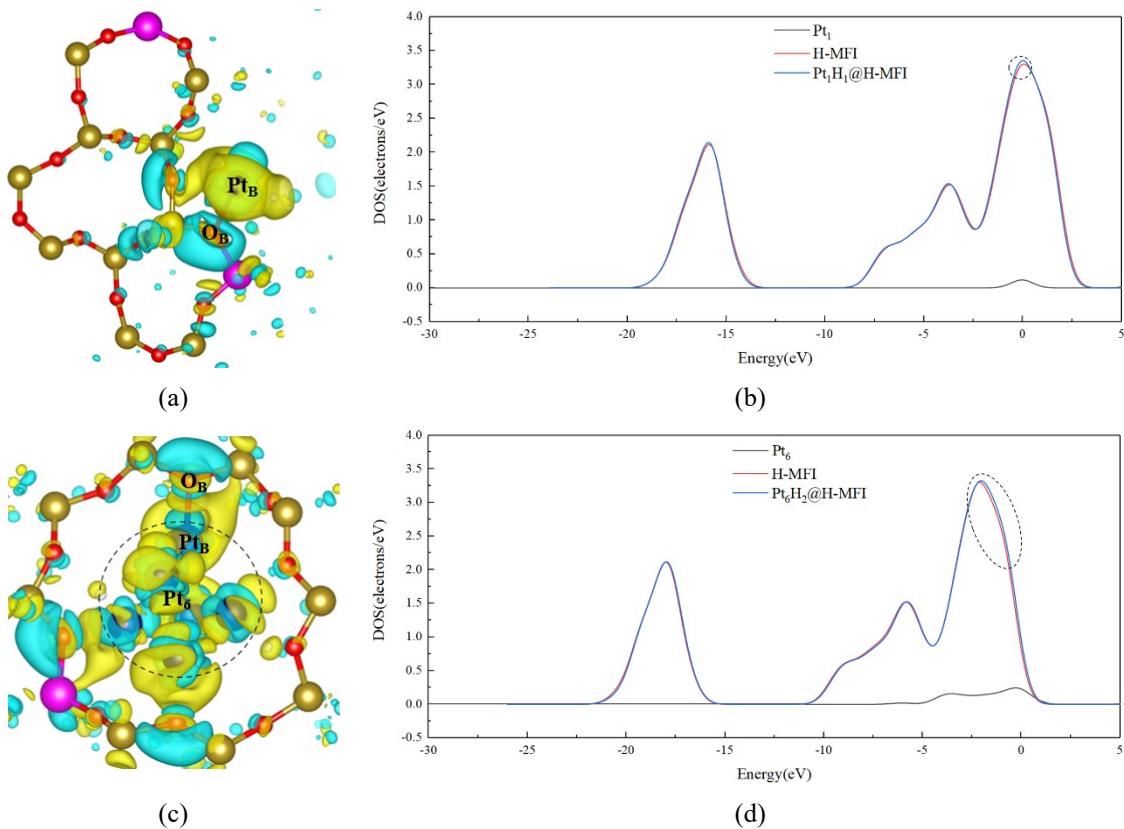
**Figure S3.** Pt<sub>n</sub> (n=1, 6) clusters encapsulated in Silicalite-1 nanopores. (a) Plot of electron density difference of Pt@Silicalite-1 and Pt<sub>6</sub>@Silicalite-1. (b) Electron localization function (ELF) contours between Pt<sub>B</sub> and O<sub>B</sub> of Pt@Silicalite-1 and Pt<sub>6</sub>@Silicalite-1. The color of yellow and cyan mean the gain and loss of electrons, respectively. Si, O, and Pt atoms are represented by gold, red and dark blue. The black line indicates the position of the Pt<sub>6</sub> nanocluster.



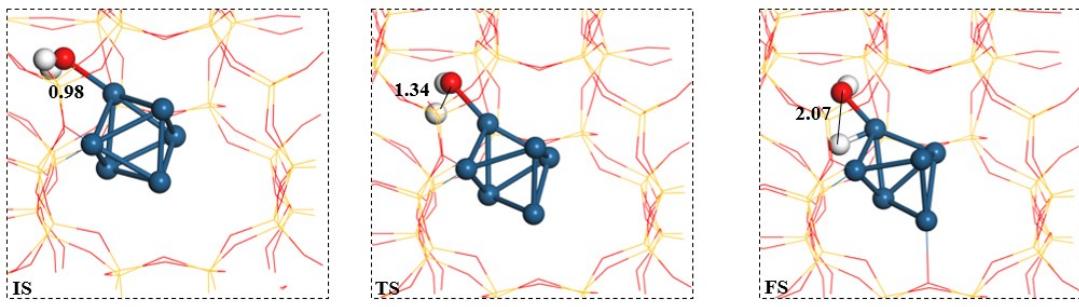
(a) Pt<sub>1</sub>H<sub>1</sub>@H-MFI



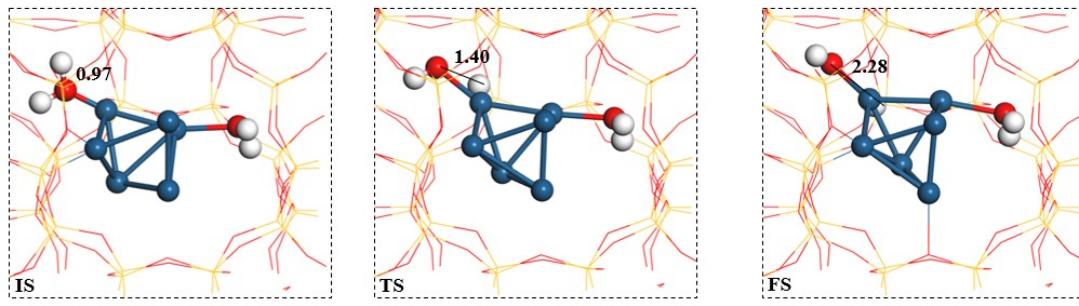
**Figure S4.** The optimized three configurations of  $\text{Pt}_1\text{H}_1@\text{H-MFI}$  and  $\text{Pt}_6\text{H}_2@\text{H-MFI}$ . The configurations in the right panels are the most stable ones while the configurations in the middle and left panels are the less stable structures.



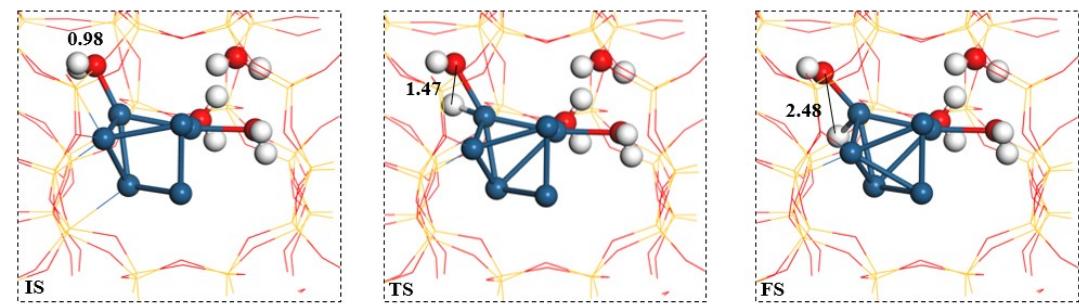
**Figure S5.** The  $\text{Pt}_1$  and  $\text{Pt}_6\text{H}_2$  nanoclusters adsorbed on the H-MFI zeolites. (a) The electron density difference and (b) density of state for  $\text{Pt}_1\text{H}_1@\text{H-MFI}$ . (c) The electron density difference and (d) density of state for  $\text{Pt}_6\text{H}_2@\text{H-MFI}$ . Take the  $\text{O}_p$  orbitals of the H-MFI framework and the  $\text{Pt}_d$  orbitals of the  $\text{Pt}_1$  and  $\text{Pt}_6\text{H}_2$  nanoclusters as examples.



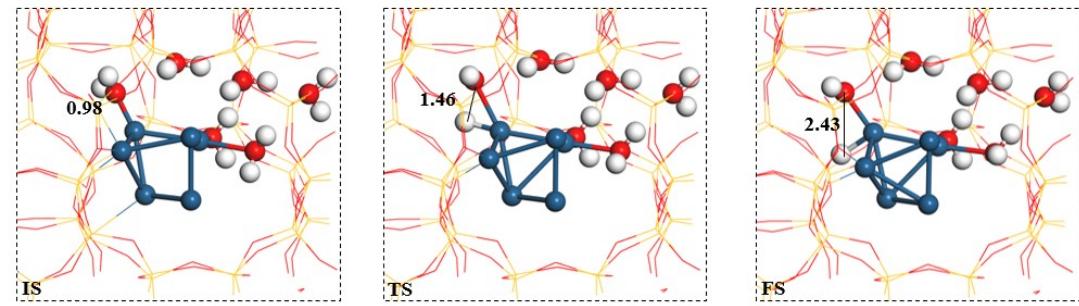
(a)Pt<sub>6</sub>@Silicalite-1-1W



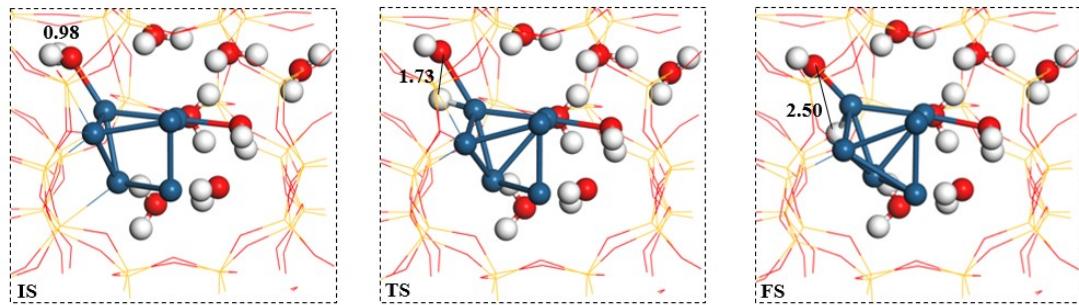
(b)Pt<sub>6</sub>@Silicalite-1-2W



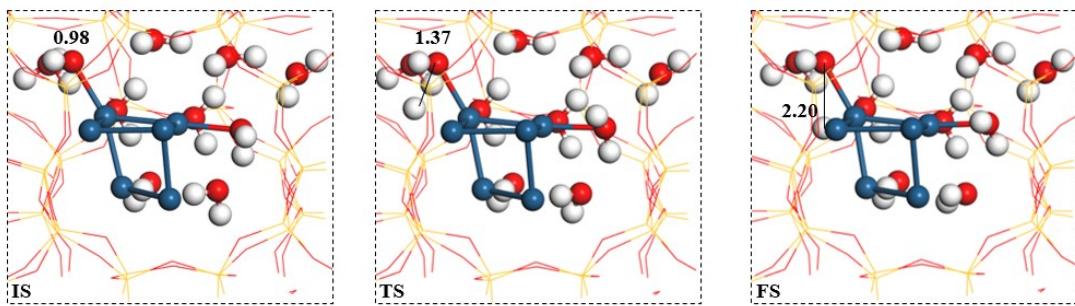
(c)Pt<sub>6</sub>@Silicalite-1-4W



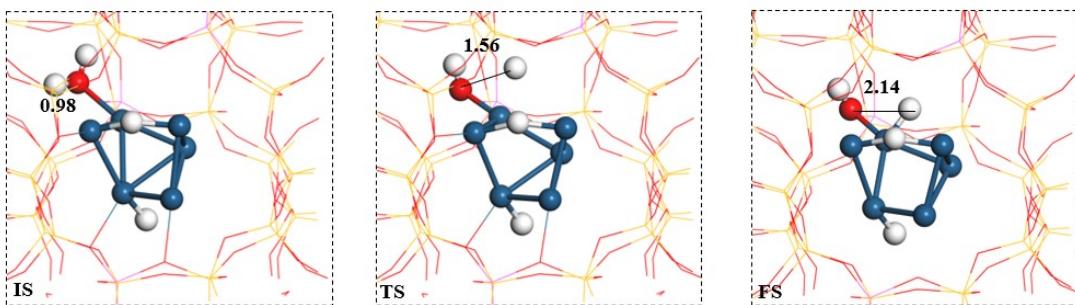
(d)Pt<sub>6</sub>@Silicalite-1-6W



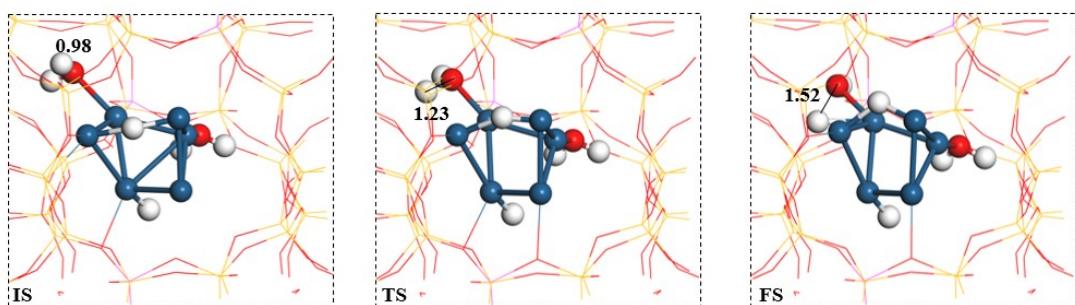
(e) Pt<sub>6</sub>@Silicalite-1-8W



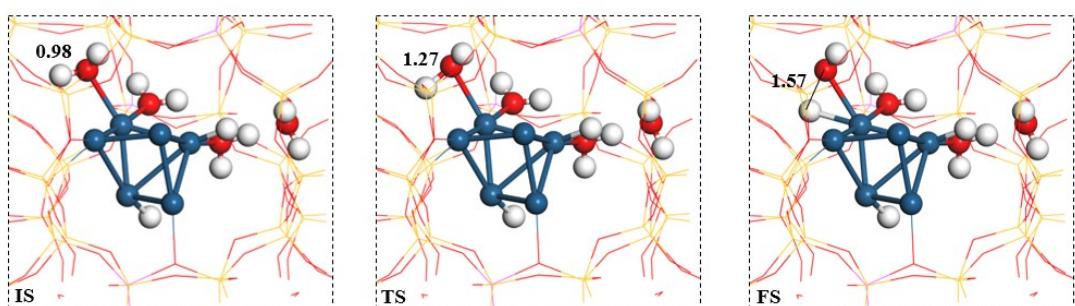
(f) Pt<sub>6</sub>@Silicalite-1-10W



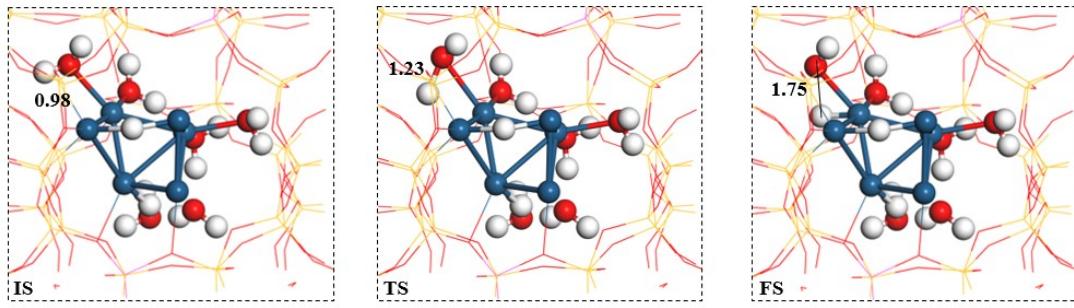
(g) Pt<sub>6</sub>H<sub>2</sub>@H-MFI-1W



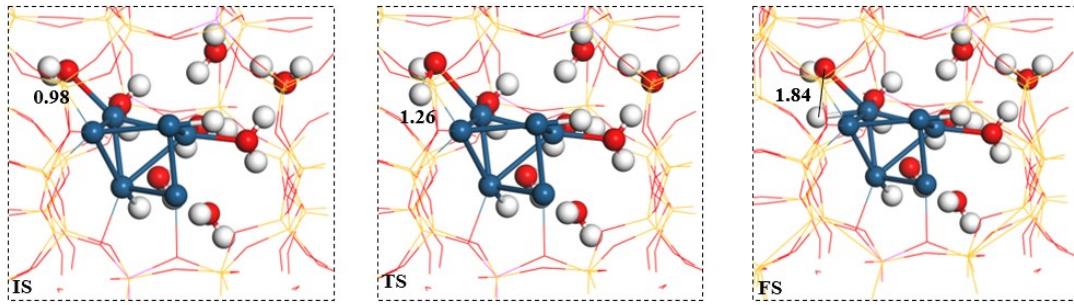
(h) Pt<sub>6</sub>H<sub>2</sub>@H-MFI-2W



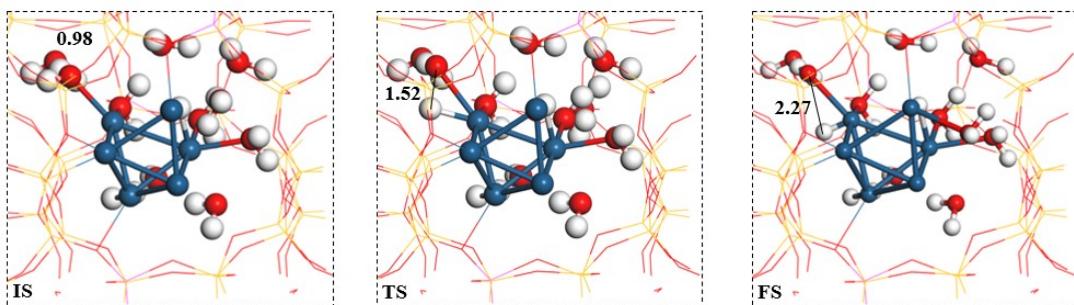
(i) Pt<sub>6</sub>H<sub>2</sub>@H-MFI-4W



(j)  $\text{Pt}_6\text{H}_2@\text{H-MFI-6W}$



(k)  $\text{Pt}_6\text{H}_2@\text{H-MFI-8W}$

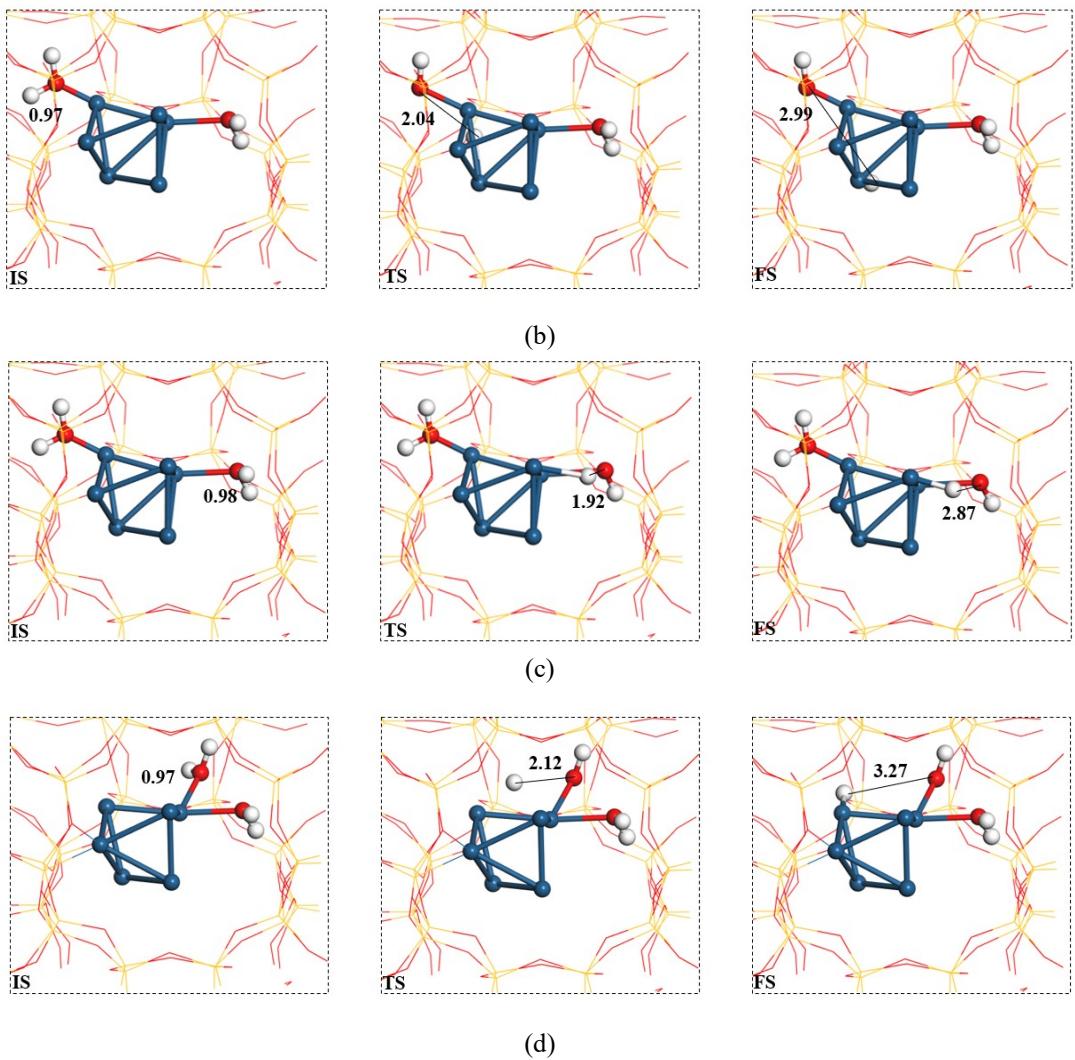


(l)  $\text{Pt}_6\text{H}_2@\text{H-MFI-10W}$

**Figure S6.** The optimized structures for initial structure (IS), transition state (TS) and final state (FS) in the water dissociation process over the encapsulated  $\text{Pt}_6@\text{Silicalite-1-nW}$  and  $\text{Pt}_6\text{H}_2@\text{H-MFI-nW}$  ( $n=1, 2, 4, 6, 8, 10$ ). The marked bond lengths are in angstrom ( $\text{\AA}$ ).



(a)



**Figure S7.** The optimized structures for initial structures, transition states and final states in the water dissociation process over the encapsulated  $\text{Pt}_6@\text{Silicalite-1-2W}$ . The bond lengths are in angstrom ( $\text{\AA}$ ).

**Table S2.** The Gibbs free energy (in  $\text{kJ}\cdot\text{mol}^{-1}$ ) of the water dissociation on the encapsulated  $\text{Pt}_6$  nanocluster in the Silicalite-1 framework in the presence of two water molecules.

Figure S7 configuration	$\Delta G_{\text{IS}}$	$\Delta G_{\text{FS}}$	$\Delta G^\ddagger$
a	-95.2	-96.9	111.7
b	-95.2	-95.4	125.6
c	-95.2	-96.0	113.8
d	-92.9	-93.3	132.4

**Table S3.** The Gibbs free energy (in  $\text{kJ}\cdot\text{mol}^{-1}$ ) of the water dissociation on  $\text{Pt}_6$  nanocluster encapsulated in Silicalite-1 framework under 1, 2, 4, 6, 8 and 10 water molecules environment.

Number of $\text{H}_2\text{O}$	$\Delta G_{\text{IS}}$	$\Delta G_{\text{FS}}$	$\Delta G^\ddagger$
--------------------------------	------------------------	------------------------	---------------------

1	-126.2	-127.7	146.2
2	-95.2	-96.9	111.7
4	-68.0	-75.1	78.3
6	-55.6	-63.1	61.8
8	-54.8	-61.5	52.5
10	-50.1	-59.3	38.4

**Table S4.** The Gibbs free energy (in  $\text{kJ}\cdot\text{mol}^{-1}$ ) of the water dissociation on the  $\text{Pt}_6$  nanocluster encapsulated in H-MFI framework under 1, 2, 4, 6, 8 and 10 water molecules environment.

Number of $\text{H}_2\text{O}$	$\Delta G_{\text{IS}}$	$\Delta G_{\text{FS}}$	$\Delta G^\ddagger$
1	-68.1	-65.0	61.5
2	-65.9	-64.2	69.4
4	-63.8	-61.6	90.6
6	-53.9	-52.9	172.9
8	-49.0	-47.4	215.0
10	-46.7	-45.5	248.4

The content of the CP2K input file is as follows (the details can also refer to <https://github.com/wwzhangxmu/QQbao-PCCP-paper>):

```
&FORCE_EVAL
  METHOD Quickstep
  &DFT
    LSD
    BASIS_SET_FILE_NAME /public/home/*/cp2k/BASIS
    POTENTIAL_FILE_NAME /public/home/*/cp2k/GTH_POTENTIALS
#      WFN_RESTART_FILE_NAME ./SSZ13-RESTART.wfn
#      CHARGE +1
  &MGRID
    CUTOFF 360
  &END MGRID
  &QS
    WF_INTERPOLATION ASPC
    EXTRAPOLATION_ORDER 2
  &END QS
  &SCF
    EPS_SCF 1.E-6
    SCF_GUESS RESTART
    MAX_SCF 1000
  &OT T
    PRECONDITIONER FULL_ALL
#      MINIMIZER CG
    MINIMIZER BROYDEN
    BROYDEN_SIGMA 0.1
    BROYDEN_BETA 0.7
    N_DIIS 4
    LINESEARCH 3PNT
  &END OT
  &END SCF
  &XC
    &XC_FUNCTIONAL PBE
  &END XC_FUNCTIONAL
  &VDW_POTENTIAL
    DISPERSION_FUNCTIONAL PAIR_POTENTIAL
  &PAIR_POTENTIAL
    TYPE DFTD3
    REFERENCE_FUNCTIONAL PBE
    PARAMETER_FILE_NAME /public/home/*/cp2k/dftd3.dat
    R_CUTOFF 4.0
  &END PAIR_POTENTIAL
  &END VDW_POTENTIAL
```

```

&END XC
#
#   &PRINT
#     &MULLIKEN
#       &END MULLIKEN
#     &END PRINT
&END DFT

&SUBSYS
  &CELL
    ABC      10.000   10.000   10.000
    ALPHA_BETA_GAMMA  90.0000   90.0000   90.0000
    PERIODIC XYZ
  &END CELL

  &TOPOLOGY
    CONNECTIVITY OFF
    COORD_FILE ./1.xyz
    COORDINATE XYZ
  &END TOPOLOGY

  &KIND Si
    BASIS_SET DZVP-MOLOPT-SR-GTH-q4
    POTENTIAL GTH-PBE-q4
  &END KIND
  &KIND O
    BASIS_SET DZVP-MOLOPT-SR-GTH-q6
    POTENTIAL GTH-PBE-q6
  &END KIND
  &KIND H
    BASIS_SET DZVP-MOLOPT-SR-GTH-q1
    POTENTIAL GTH-PBE-q1
  &END KIND
  &KIND C
    BASIS_SET DZVP-MOLOPT-SR-GTH-q4
    POTENTIAL GTH-PBE-q4
  &END KIND
  &KIND Pt
    BASIS_SET DZVP-MOLOPT-SR-GTH-q18
    POTENTIAL GTH-PBE-q18
  &END KIND
  &KIND A1
    BASIS_SET DZVP-MOLOPT-SR-GTH-q3
    POTENTIAL GTH-PBE-q3
  &END KIND

```

```

&END SUBSYS
&END FORCE_EVAL
#&EXT_RESTART
#RESTART_FILE_NAME ./SSZ13-1.restart
#RESTART_POS T
#RESTART_VEL T
#&END EXT_RESTART
&GLOBAL
  PROJECT SSZ13
    RUN_TYPE GEO_OPT
#  RUN_TYPE ENERGY
#  RUN_TYPE BAND
    PRINT_LEVEL LOW
&END GLOBAL
&MOTION
  &MD
    ENSEMBLE NVT
    STEPS 40000
    Timestep 0.5
    TEMPERATURE 298.0
#  ANNEALING 0.999
  &THERMOSTAT
    TYPE NOSE
    REGION GLOBAL
    &NOSE
      TIMECON [wavenumber_t] 2000
    &END NOSE
  &END THERMOSTAT
  &END MD
  &GEO_OPT
    MAX_ITER 20000
    OPTIMIZER BFGS
  &END GEO_OPT
  &BAND
    NPROC REP 64
    BAND_TYPE CI-NEB
    NUMBER_OF_REPLICA 7
    K_SPRING 0.10
    &CONVERGENCE_CONTROL
      MAX_DR 0.01
      MAX_FORCE 0.002
      RMS_DR 0.02
      RMS_FORCE 0.001
  &END

```

```

ROTATE_FRAMES F
&CI_NEB
    NSTEPS_IT 5
&END
&OPTIMIZE_BAND
    OPT_TYPE MD
    OPTIMIZE_END_POINTS F
&MD
    Timestep 0.5
    TEMPERATURE 298.0
    MAX_STEPS 1000
    &VEL_CONTROL
        ANNEALING 0.96
        PROJ_VELOCITY_VERLET T
    &END
    &END
&END
&REPLICA
    COORD_FILE_NAME ./1.xyz
&END
&REPLICA
    COORD_FILE_NAME ./2.xyz
&END
&REPLICA
    COORD_FILE_NAME ./3.xyz
&END
&REPLICA
    COORD_FILE_NAME ./4.xyz
&END
&REPLICA
    COORD_FILE_NAME ./5.xyz
&END
&REPLICA
    COORD_FILE_NAME ./6.xyz
&END
&REPLICA
    COORD_FILE_NAME ./7.xyz
&END
&PROGRAM_RUN_INFO
&END
&CONVERGENCE_INFO
&END
&END BAND
&END MOTION

```

Information the coordinates of molecules

(Lattice constants of  $20.022 \times 19.899 \times 13.383 \text{ \AA}^3$ )

	289		
	Pt <sub>1</sub> @Silicalite-1		
Si	8.447481	1.116931	8.746593
Si	6.059258	0.607118	10.774385
Si	5.621977	1.176628	0.312359
Si	2.409247	1.293435	0.185087
Si	1.350684	0.478372	10.821494
Si	3.608164	1.204088	8.983338
Si	8.509550	16.487516	8.987221
Si	6.149157	17.285069	10.926283
Si	5.444983	16.501047	0.488747
Si	2.409447	16.439161	0.420494
Si	1.431573	17.228952	10.948365
Si	3.735705	16.380657	9.061229
Si	1.578334	18.783463	2.061250
Si	3.974567	19.285513	4.079272
Si	4.394228	18.694912	7.038120
Si	7.606358	18.596611	6.890104
Si	8.649103	19.429583	4.135079
Si	6.427662	18.680584	2.255839
Si	1.559514	3.419842	2.285950
Si	3.884869	2.602192	4.284166
Si	4.573825	3.397356	7.205943
Si	7.623977	3.464018	7.065823
Si	8.565812	2.648756	4.202262
Si	6.259077	3.461232	2.372940
Si	11.577321	11.035587	4.661299
Si	13.962742	10.561195	2.631901
Si	14.406830	11.134485	13.102626
Si	17.631372	11.239552	13.217988
Si	18.671915	10.444587	2.616377
Si	16.393814	11.162344	4.426293
Si	11.492828	6.554929	4.385342
Si	13.869039	7.339945	2.456851
Si	14.557996	6.555129	12.904960
Si	17.615755	6.497621	12.967726
Si	18.630070	7.299749	2.435438
Si	16.305117	6.490656	4.318025

Si	18.452074	8.839733	11.302078
Si	16.017799	9.347954	9.325944
Si	15.603946	8.766504	6.379275
Si	12.398222	8.630992	6.542681
Si	11.367890	9.470332	9.268263
Si	13.559299	8.757948	11.161958
Si	18.492119	13.375113	11.109095
Si	16.162760	12.563233	9.152768
Si	15.460187	13.342877	6.231794
Si	12.412438	13.402375	6.275423
Si	11.435765	12.587709	9.123057
Si	13.732489	13.418293	11.025584
Si	11.584128	18.804556	4.649790
Si	13.979360	19.293871	2.621864
Si	14.407631	18.739286	13.062879
Si	17.616756	18.603973	13.188680
Si	18.669514	19.415852	2.559901
Si	16.423044	18.684565	4.418263
Si	11.503839	3.420439	4.393104
Si	13.900272	2.614729	2.456450
Si	14.555393	3.401137	12.907904
Si	17.610350	3.458446	12.969465
Si	18.617256	2.655720	2.431156
Si	16.314726	3.463819	4.307051
Si	18.445868	1.115936	11.323758
Si	16.045429	0.610899	9.315372
Si	15.618361	1.181006	6.359066
Si	12.405030	1.314528	6.500659
Si	11.386311	0.480561	9.250731
Si	13.596740	1.222396	11.142954
Si	18.477303	16.470600	11.098255
Si	16.135729	17.293625	9.150760
Si	15.447973	16.504827	6.217206
Si	12.410636	16.441748	6.270203
Si	11.461394	17.259796	9.119177
Si	13.730287	16.428616	11.031875
Si	8.476913	9.008874	8.469967
Si	6.279700	9.305767	10.667189
Si	5.394727	8.802920	0.446992
Si	2.278303	8.736258	0.204760
Si	1.351485	9.466750	10.789777
Si	3.699865	8.747998	8.988692
Si	8.461497	13.346657	8.981064
Si	6.162371	12.475280	10.988915

Si	5.452190	13.361582	0.478308
Si	2.411650	13.400783	0.410992
Si	1.443386	12.605419	10.929495
Si	3.769141	13.323376	9.067920
Si	1.505454	11.061853	2.082796
Si	3.987381	10.499111	4.033369
Si	4.494339	11.085733	6.967591
Si	7.690650	11.299847	6.714117
Si	8.678936	10.488961	4.025874
Si	6.441277	11.178860	2.235363
Si	1.586143	6.516724	2.269088
Si	3.907694	7.273880	4.304508
Si	4.555405	6.555129	7.194835
Si	7.615568	6.522892	7.006938
Si	8.544989	7.366411	4.150470
Si	6.188400	6.475134	2.468494
O	7.192103	1.164688	9.769857
O	6.333960	1.246473	12.236344
O	4.011007	1.156331	0.243437
O	1.907096	1.407456	12.035199
O	2.085291	0.913762	9.446257
O	4.583035	1.068178	10.282293
O	7.488428	16.744013	10.209757
O	6.185596	16.816645	12.468406
O	3.915703	17.088066	0.424241
O	1.836818	16.413691	12.288271
O	2.267692	16.659243	9.686616
O	4.837716	16.664816	10.213772
O	6.092094	18.896887	10.863918
O	1.669634	18.820871	11.205988
O	8.592241	2.572941	8.028061
O	8.264881	19.897011	7.591507
O	8.088688	17.234524	7.612117
O	3.755727	2.729944	8.440792
O	3.924913	0.163172	7.778467
O	3.919507	17.337601	7.774586
O	19.797752	0.741238	10.522518
O	19.923691	16.922907	10.537374
O	2.827106	18.734510	3.087726
O	3.751522	18.646557	5.548191
O	6.007801	18.738092	7.016841
O	8.099099	18.490946	5.348516
O	7.934918	18.983049	2.753285
O	5.424961	18.824654	3.523342

O	2.589645	3.164140	3.505945
O	3.761533	3.073003	5.833115
O	6.107911	2.821678	7.108113
O	8.173780	3.485310	5.534138
O	7.761127	3.236573	2.926594
O	5.251971	3.155584	3.608325
O	3.918506	0.994552	4.179913
O	8.262078	1.076337	4.510607
O	1.418158	17.331034	1.346731
O	1.752325	0.001592	0.902550
O	1.932123	2.650746	0.915531
O	6.334560	17.168062	1.674080
O	6.085887	19.729660	1.075190
O	6.085887	2.503692	1.092454
O	10.241253	19.232384	3.846542
O	10.106504	2.890131	3.770527
O	12.858728	11.105234	3.677515
O	13.681231	11.200551	1.170210
O	16.018801	11.108218	13.218122
O	18.189384	11.356758	1.353021
O	17.924696	10.858088	3.997770
O	15.446172	11.022852	3.105258
O	12.535975	6.794514	3.177660
O	13.775136	6.869135	0.911249
O	16.097486	7.130807	12.964112
O	18.193991	6.472349	1.102358
O	17.775932	6.722082	3.685009
O	15.186086	6.718300	3.164812
O	13.930507	8.950570	2.519350
O	18.359573	8.890078	2.186916
O	11.422551	12.509109	5.345037
O	11.753115	9.952286	5.859881
O	11.925503	7.291591	5.767538
O	16.274082	12.673873	5.003904
O	16.016998	10.123617	5.609083
O	16.106497	7.453967	5.596369
O	0.198418	10.776702	3.005286
O	0.164581	7.053997	2.841077
O	17.181278	8.785010	10.297014
O	16.265472	8.702230	7.859301
O	13.996979	8.781628	6.451275
O	11.922900	8.477173	8.095912
O	12.016803	9.037529	10.701851
O	14.527762	8.955744	9.865546

O	17.500229	13.099710	9.867688
O	16.258863	13.024095	7.606630
O	13.925502	12.767199	6.276895
O	11.839408	13.430631	7.793725
O	12.264276	13.182093	10.380926
O	14.845111	13.186272	9.863539
O	16.100090	10.953206	9.212857
O	11.765127	11.006932	8.870387
O	18.603239	7.387305	12.032254
O	18.269875	9.950892	12.470146
O	18.094681	12.594674	12.467469
O	13.687639	7.229704	11.705173
O	13.933310	9.768022	12.373253
O	13.931508	12.438666	12.290278
O	9.754518	9.279501	9.463253
O	9.874850	12.760234	9.523745
O	12.834502	18.740679	3.617827
O	13.757317	18.647552	1.159771
O	16.018801	18.742470	13.060069
O	18.107897	18.490351	1.343787
O	17.938311	18.982851	3.938617
O	15.449374	18.830225	3.121049
O	12.610657	3.157374	3.254210
O	13.770731	3.082753	0.913390
O	16.094885	2.820484	12.964247
O	18.190187	3.483320	1.100083
O	17.786943	3.229210	3.692905
O	15.260568	3.229807	3.091205
O	13.932909	1.003109	2.520153
O	18.349762	1.071163	2.174336
O	11.424552	17.336010	5.339951
O	11.758120	-0.015322	5.849576
O	11.853624	2.652935	5.776237
O	16.279488	17.176022	5.002164
O	16.096085	19.729460	5.611358
O	16.106297	2.504488	5.586332
O	0.223045	19.157166	2.858341
O	0.139353	2.895106	2.845627
O	17.196495	1.165484	10.297550
O	16.266073	1.249657	7.845383
O	14.004787	1.167275	6.365356
O	11.928507	1.419396	8.041041
O	12.094890	0.912568	10.638548
O	14.594436	1.071760	9.868625

O	17.456581	16.742821	9.876922
O	16.194193	16.827190	7.611046
O	13.918894	17.083689	6.269668
O	11.843413	16.414684	7.788639
O	12.267879	16.663223	10.383870
O	14.832898	16.661831	9.865546
O	16.097887	18.902857	9.211386
O	11.765327	18.836792	8.865703
O	18.601038	2.569359	12.038277
O	18.274679	19.900593	12.483261
O	18.101290	17.247856	12.463856
O	13.686638	2.738699	11.706779
O	13.935913	0.234012	12.380881
O	13.923298	17.414013	12.289207
O	9.809979	0.741636	9.541009
O	9.914093	17.078318	9.531908
O	7.078377	9.365464	9.192783
O	5.951139	8.454090	12.314635
O	3.832411	9.194333	0.327081
O	1.831012	8.539855	12.043763
O	2.169183	9.040315	9.458168
O	4.753623	8.880725	10.205608
O	7.418952	13.104884	10.189147
O	6.247464	13.115829	12.473358
O	3.923311	12.764014	0.418754
O	1.843626	13.432222	12.271141
O	2.258281	13.099114	9.615953
O	4.761432	12.935943	10.294337
O	6.247064	10.874007	11.133452
O	1.666231	11.017280	11.207192
O	8.579627	7.462722	7.942142
O	8.594043	10.026111	7.199519
O	8.008199	12.609598	7.608102
O	3.760732	7.215178	8.443468
O	4.008204	9.774190	7.771241
O	4.086690	12.430110	7.764683
O	19.791946	9.206073	10.456406
O	19.933702	12.927982	10.540050
O	2.837518	11.021061	3.010372
O	3.749120	11.112995	5.517410
O	6.099902	11.016883	6.769122
O	8.175182	11.529082	5.179221
O	7.998388	10.933904	2.622533
O	5.441579	11.017479	3.512502

O	2.687753	6.646465	3.445454
O	3.674037	6.879084	5.858408
O	6.088890	7.129414	7.026744
O	8.166173	6.486079	5.467625
O	7.742307	6.805657	2.838401
O	5.336263	6.625969	3.850824
O	3.998393	8.875949	4.091451
O	8.255470	8.952560	4.427632
O	1.420761	12.514879	1.348203
O	1.423764	9.927014	0.910847
O	2.011210	7.306117	0.919412
O	6.326752	12.688995	1.669663
O	6.100904	10.107299	1.069436
O	5.590142	7.469289	1.339504
O	10.279895	10.617708	3.774274
O	10.102701	7.132996	3.774407
O	8.594644	14.918281	8.615039
O	3.921309	14.853210	8.540764
O	5.348877	14.930618	0.831218
O	2.418057	14.920271	0.999978
O	1.496845	4.968184	1.838690
O	6.018813	4.981715	1.844980
O	4.661522	4.976143	7.517097
O	7.668626	5.003603	7.606898
O	11.420949	4.986490	4.770504
O	16.179577	4.974750	4.865122
O	14.599641	4.978133	12.562623
O	17.601339	4.977138	12.383825
O	18.442265	14.924051	11.542570
O	13.850218	14.922857	11.623270
O	15.430554	14.923454	5.937636
O	12.429056	14.921863	5.690184
Pt	7.893473	8.170132	-1.528339

290

#### Pt<sub>2</sub>@Silicalite-1

Si	8.447682	1.114145	8.746861
Si	6.059057	0.606124	10.774654
Si	5.621777	1.176230	0.312359
Si	2.408847	1.293236	0.185087
Si	1.350284	0.477775	10.821761
Si	3.607764	1.203491	8.983607
Si	8.509550	16.485128	8.987488
Si	6.149157	17.283674	10.926283
Si	5.445183	16.498857	0.488479

Si	2.409848	16.438364	0.420494
Si	1.431773	17.228355	10.948097
Si	3.735905	16.378269	9.061361
Si	1.578134	18.783064	2.061116
Si	3.974567	19.285116	4.079406
Si	4.393828	18.693916	7.038655
Si	7.605958	18.595018	6.889970
Si	8.648903	19.428787	4.134812
Si	6.427262	18.679789	2.255437
Si	1.559113	3.420041	2.285549
Si	3.884468	2.601794	4.282962
Si	4.571423	3.397555	7.205943
Si	7.621775	3.460635	7.063280
Si	8.566212	2.647960	4.200388
Si	6.258677	3.462028	2.372003
Si	11.580324	11.035587	4.663173
Si	13.962742	10.561593	2.631098
Si	14.405628	11.133093	13.101824
Si	17.630373	11.239752	13.217854
Si	18.670715	10.444985	2.616243
Si	16.393412	11.162344	4.426293
Si	11.495431	6.556323	4.384405
Si	13.869840	7.340940	2.455245
Si	14.556994	6.556522	12.904022
Si	17.615355	6.498019	12.967860
Si	18.629669	7.300147	2.435305
Si	16.304714	6.491651	4.317891
Si	18.450274	8.839931	11.302613
Si	16.016197	9.347555	9.326747
Si	15.603745	8.766902	6.379944
Si	12.398023	8.631390	6.546563
Si	11.364887	9.469735	9.271475
Si	13.555294	8.758147	11.161690
Si	18.492119	13.374516	11.108960
Si	16.162560	12.562836	9.153035
Si	15.460187	13.342279	6.232062
Si	12.412239	13.401977	6.276895
Si	11.436966	12.584327	9.123191
Si	13.731888	13.417100	11.025452
Si	11.584329	18.803759	4.649522
Si	13.979560	19.293871	2.621864
Si	14.408031	18.738291	13.063013
Si	17.616957	18.603575	13.188545
Si	18.669714	19.415653	2.559901

Si	16.423244	18.683968	4.418398
Si	11.504641	3.421235	4.392301
Si	13.900874	2.614729	2.456182
Si	14.555793	3.402132	12.908172
Si	17.610350	3.458844	12.969465
Si	18.617256	2.655720	2.431022
Si	16.314926	3.464615	4.307051
Si	18.445868	1.115936	11.324025
Si	16.046030	0.610302	9.315237
Si	15.619362	1.181006	6.358665
Si	12.405631	1.313931	6.499588
Si	11.388914	0.478173	9.250062
Si	13.597940	1.221799	11.143489
Si	18.477503	16.470005	11.098255
Si	16.135929	17.293028	9.150760
Si	15.447773	16.504230	6.217340
Si	12.411036	16.440754	6.269936
Si	11.461193	17.257607	9.119445
Si	13.730486	16.427422	11.032143
Si	8.474511	9.022406	8.492183
Si	6.245663	9.238111	10.676690
Si	5.388721	8.816252	0.462650
Si	2.275701	8.738049	0.205295
Si	1.348081	9.467546	10.790713
Si	3.682446	8.749192	8.983473
Si	8.460896	13.343872	8.985079
Si	6.168377	12.442248	10.988782
Si	5.454994	13.357801	0.474294
Si	2.412451	13.400186	0.411126
Si	1.443987	12.605419	10.929629
Si	3.773947	13.319993	9.072738
Si	1.503652	11.062650	2.083198
Si	3.984178	10.500106	4.034841
Si	4.493737	11.086131	6.968261
Si	7.689649	11.298255	6.720140
Si	8.685343	10.487170	4.042603
Si	6.442479	11.185427	2.248076
Si	1.585542	6.517321	2.268419
Si	3.907293	7.274477	4.303170
Si	4.551601	6.555129	7.195370
Si	7.606758	6.524484	6.995562
Si	8.546991	7.367605	4.145251
Si	6.188199	6.476528	2.466353
O	7.193103	1.165087	9.770125

O	6.334160	1.246672	12.236077
O	4.011007	1.156530	0.243303
O	1.907096	1.407257	12.035199
O	2.085091	0.913762	9.446391
O	4.583436	1.068576	10.282159
O	7.488828	16.744612	10.209757
O	6.185797	16.817043	12.468674
O	3.916103	17.087669	0.424241
O	1.837018	16.413691	12.288271
O	2.267892	16.659243	9.686348
O	4.837515	16.665014	10.213638
O	6.092494	18.896688	10.863650
O	1.669634	18.820871	11.205854
O	8.592441	2.574732	8.029532
O	8.265081	19.897608	7.589901
O	8.088888	17.234325	7.612518
O	3.755727	2.729745	8.440927
O	3.925113	0.162973	7.778334
O	3.919507	17.336805	7.774854
O	19.797552	0.741238	10.522518
O	19.923691	16.923103	10.537374
O	2.826906	18.734510	3.087726
O	3.751722	18.646557	5.548592
O	6.007801	18.738291	7.016975
O	8.099099	18.490946	5.348516
O	7.934518	18.983049	2.753151
O	5.424961	18.824654	3.523342
O	2.589645	3.164339	3.505677
O	3.761933	3.073202	5.832446
O	6.107111	2.822076	7.108380
O	8.173982	3.485310	5.534004
O	7.760727	3.236771	2.926461
O	5.252171	3.155584	3.608191
O	3.918506	0.994353	4.180046
O	8.262078	1.076337	4.510740
O	1.418158	17.330835	1.346464
O	1.752526	0.001592	0.902683
O	1.932323	2.650746	0.915531
O	6.334360	17.167664	1.673946
O	6.086087	19.729858	1.075324
O	6.086087	2.503692	1.092187
O	10.241453	19.232582	3.846676
O	10.106905	2.890330	3.770794
O	12.859730	11.105433	3.677782

O	13.681433	11.200748	1.170076
O	16.018400	11.108418	13.218122
O	18.189186	11.356956	1.352754
O	17.924294	10.858088	3.998038
O	15.446372	11.022852	3.105124
O	12.539178	6.793519	3.178596
O	13.775736	6.868339	0.911115
O	16.097286	7.130608	12.964112
O	18.193991	6.472150	1.102358
O	17.775932	6.721882	3.685143
O	15.186487	6.718500	3.164544
O	13.930707	8.950769	2.519484
O	18.359373	8.890078	2.186782
O	11.422951	12.509308	5.345438
O	11.753514	9.951689	5.861085
O	11.925303	7.291392	5.768341
O	16.274082	12.673873	5.003904
O	16.016798	10.123617	5.609083
O	16.106297	7.453967	5.596637
O	0.196616	10.777099	3.005554
O	0.164180	7.053997	2.841077
O	17.180677	8.784812	10.297014
O	16.265472	8.702230	7.859568
O	13.996778	8.781230	6.451275
O	11.923902	8.471999	8.098990
O	12.018206	9.037728	10.700913
O	14.527562	8.955346	9.866081
O	17.500229	13.099910	9.867688
O	16.258863	13.024293	7.606764
O	13.925701	12.767199	6.276895
O	11.839408	13.430830	7.794393
O	12.264276	13.182490	10.380658
O	14.845312	13.186471	9.863673
O	16.100290	10.953007	9.212724
O	11.767329	11.005938	8.869583
O	18.603041	7.387305	12.032521
O	18.269674	9.951092	12.470547
O	18.094681	12.594674	12.467469
O	13.687639	7.228710	11.703835
O	13.934111	9.766827	12.373253
O	13.931707	12.438666	12.290412
O	9.759123	9.288654	9.454287
O	9.876451	12.760632	9.523878
O	12.834702	18.740879	3.617693

O	13.757115	18.647751	1.159771
O	16.019001	18.742670	13.060069
O	18.107897	18.490351	1.343787
O	17.938311	18.982851	3.938617
O	15.449575	18.830225	3.121451
O	12.611056	3.157175	3.254076
O	13.770731	3.082554	0.913122
O	16.094885	2.820484	12.964247
O	18.190187	3.483320	1.100083
O	17.787144	3.229210	3.693039
O	15.260568	3.229807	3.091205
O	13.932709	1.003109	2.520153
O	18.349762	1.071163	2.174336
O	11.424552	17.335810	5.340219
O	11.757919	-0.015322	5.849442
O	11.853423	2.653333	5.776504
O	16.279287	17.175821	5.002432
O	16.096085	19.729460	5.611358
O	16.106096	2.504687	5.586198
O	0.223245	19.157166	2.858341
O	0.139353	2.894907	2.845627
O	17.196495	1.165484	10.297550
O	16.265871	1.249856	7.845383
O	14.005189	1.167474	6.365490
O	11.928507	1.419993	8.040774
O	12.095089	0.913165	10.638281
O	14.594636	1.071959	9.868490
O	17.456781	16.742821	9.877056
O	16.194193	16.827391	7.611046
O	13.918894	17.083889	6.269668
O	11.843413	16.414684	7.788237
O	12.267879	16.663223	10.384272
O	14.832697	16.662029	9.865546
O	16.097887	18.902657	9.211386
O	11.765327	18.835598	8.865569
O	18.601038	2.569359	12.038277
O	18.274479	19.900593	12.483396
O	18.101290	17.247856	12.463722
O	13.686238	2.738898	11.706646
O	13.935913	0.233614	12.381149
O	13.923098	17.414013	12.288940
O	9.812382	0.743427	9.540339
O	9.913692	17.078318	9.531775
O	7.074373	9.371434	9.209913

O	6.011205	8.553585	12.355855
O	3.827606	9.196124	0.331229
O	1.830411	8.540054	12.043630
O	2.157571	9.040712	9.455090
O	4.696560	8.894455	10.226352
O	7.417350	13.100706	10.191690
O	6.248266	13.105880	12.469075
O	3.923711	12.763816	0.418754
O	1.843626	13.432222	12.271676
O	2.259683	13.099114	9.616488
O	4.767438	12.929376	10.297014
O	6.261880	10.836797	11.130775
O	1.666031	11.017280	11.207326
O	8.580829	7.462523	7.940536
O	8.588838	10.020341	7.203132
O	8.008199	12.609598	7.609708
O	3.760132	7.215178	8.443468
O	4.008004	9.772399	7.770036
O	4.086490	12.430110	7.765352
O	19.789143	9.206272	10.456941
O	19.934103	12.928181	10.540050
O	2.836116	11.021061	3.010238
O	3.747718	11.112995	5.518614
O	6.098701	11.016684	6.769389
O	8.175983	11.529680	5.186716
O	7.991581	10.940072	2.656927
O	5.435572	11.020664	3.516517
O	2.687353	6.646067	3.445186
O	3.674037	6.879084	5.857873
O	6.087088	7.130210	7.026610
O	8.166574	6.484686	5.464279
O	7.741306	6.805259	2.838133
O	5.336463	6.626168	3.850156
O	3.998393	8.876148	4.091585
O	8.256071	8.950172	4.430175
O	1.420561	12.515476	1.348337
O	1.421762	9.928407	0.910981
O	2.011010	7.306316	0.919278
O	6.328153	12.690588	1.670332
O	6.099102	10.114662	1.083755
O	5.588941	7.469885	1.336560
O	10.282699	10.616913	3.777218
O	10.104102	7.132598	3.774943
O	8.594243	14.916689	8.615842

O	3.921909	14.851022	8.542235
O	5.349878	14.928429	0.829345
O	2.418257	14.920072	1.000112
O	1.496845	4.968382	1.838557
O	6.018413	4.982312	1.844445
O	4.662523	4.976143	7.516964
O	7.672029	5.005195	7.604890
O	11.420949	4.986888	4.771173
O	16.179379	4.974949	4.865122
O	14.599241	4.978332	12.561954
O	17.601339	4.977337	12.383825
O	18.442265	14.923852	11.542570
O	13.850218	14.922460	11.623270
O	15.430554	14.923255	5.937636
O	12.429056	14.921663	5.690184
Pt	9.103202	6.101431	-3.086254
Pt	7.455792	7.353079	-1.867464

291

#### Pt<sub>3</sub>@Silicalite-1

Si	8.446681	1.101012	8.717285
Si	6.065264	0.608511	10.757658
Si	5.625581	1.176230	0.302188
Si	2.410849	1.293037	0.184284
Si	1.349683	0.477377	10.822164
Si	3.606963	1.201701	8.983874
Si	8.509951	16.489704	8.988960
Si	6.148556	17.285267	10.925881
Si	5.444983	16.498260	0.487944
Si	2.410048	16.437769	0.420494
Si	1.431573	17.227758	10.948097
Si	3.735905	16.377275	9.061496
Si	1.577934	18.782866	2.060179
Si	3.974767	19.284519	4.077666
Si	4.392627	18.692722	7.037852
Si	7.602953	18.588850	6.876721
Si	8.650105	19.427792	4.131064
Si	6.427062	18.680784	2.252225
Si	1.558312	3.420240	2.284077
Si	3.885069	2.601396	4.277073
Si	4.564015	3.398550	7.202731
Si	7.623376	3.430985	7.048425
Si	8.568615	2.645572	4.192492
Si	6.258276	3.462824	2.367051
Si	11.578321	11.035587	4.663440

Si	13.961941	10.561792	2.632035
Si	14.405828	11.134088	13.101824
Si	17.630571	11.239752	13.217854
Si	18.670515	10.445184	2.616510
Si	16.392813	11.162146	4.426695
Si	11.491226	6.557915	4.388152
Si	13.866236	7.340741	2.457788
Si	14.557395	6.556920	12.905227
Si	17.615955	6.498416	12.967860
Si	18.629269	7.300545	2.435706
Si	16.303915	6.492248	4.318293
Si	18.450872	8.840529	11.302211
Si	16.016998	9.347954	9.325944
Si	15.600141	8.766902	6.380345
Si	12.392817	8.632385	6.549908
Si	11.353875	9.481874	9.270002
Si	13.555294	8.760933	11.159682
Si	18.491919	13.374317	11.108693
Si	16.161358	12.563233	9.153035
Si	15.458985	13.342081	6.232329
Si	12.410036	13.401181	6.279170
Si	11.421350	12.588505	9.124530
Si	13.728084	13.416502	11.023578
Si	11.585329	18.803560	4.650057
Si	13.979961	19.293673	2.621730
Si	14.407631	18.738491	13.062478
Si	17.616756	18.603376	13.188545
Si	18.669514	19.415455	2.559901
Si	16.423244	18.683767	4.418665
Si	11.507044	3.422429	4.393238
Si	13.901274	2.614530	2.455914
Si	14.555793	3.401535	12.907770
Si	17.610550	3.459043	12.969465
Si	18.616856	2.655522	2.431022
Si	16.314926	3.464814	4.307319
Si	18.445267	1.115737	11.324160
Si	16.045229	0.610103	9.315505
Si	15.618961	1.180807	6.358932
Si	12.405030	1.313931	6.501194
Si	11.379703	0.478969	9.250999
Si	13.595338	1.221600	11.142552
Si	18.477303	16.469606	11.098255
Si	16.135729	17.292828	9.150760
Si	15.447573	16.503832	6.217340

Si	12.411036	16.439957	6.269936
Si	11.461794	17.258602	9.119310
Si	13.730486	16.426825	11.032143
Si	8.467504	9.049867	8.494057
Si	6.239856	9.225773	10.699307
Si	5.379511	8.823216	0.469074
Si	2.271496	8.738248	0.205429
Si	1.349082	9.467546	10.790177
Si	3.691656	8.750784	9.002610
Si	8.445079	13.352229	8.953361
Si	6.156164	12.439063	10.980083
Si	5.457797	13.356607	0.470412
Si	2.413252	13.399590	0.410590
Si	1.443786	12.605419	10.929361
Si	3.770343	13.319794	9.071934
Si	1.503452	11.063048	2.083733
Si	3.984178	10.501100	4.036179
Si	4.493337	11.084538	6.971740
Si	7.682241	11.342231	6.714385
Si	8.684142	10.483391	4.043674
Si	6.443280	11.187218	2.251021
Si	1.584941	6.517719	2.268151
Si	3.908294	7.274876	4.299824
Si	4.546196	6.562889	7.192159
Si	7.622175	6.590350	7.004797
Si	8.533978	7.359446	4.152611
Si	6.188600	6.477921	2.463543
O	7.171079	1.157923	9.708832
O	6.337563	1.246473	12.222828
O	4.013010	1.156331	0.241429
O	1.907096	1.407456	12.034797
O	2.084691	0.913961	9.446257
O	4.582836	1.069372	10.281490
O	7.488228	16.746202	10.210292
O	6.185196	16.818634	12.468139
O	3.916103	17.087669	0.424375
O	1.837018	16.413889	12.288271
O	2.267892	16.659641	9.686348
O	4.837515	16.665611	10.213505
O	6.093695	18.898678	10.862044
O	1.669634	18.820673	11.205720
O	8.594443	2.574931	8.025785
O	8.270487	19.911139	7.530347
O	8.089087	17.239101	7.613053

O	3.755927	2.730342	8.440659
O	3.925313	0.163172	7.777799
O	3.919306	17.336805	7.774988
O	19.797152	0.741437	10.522518
O	19.923491	16.923304	10.537506
O	2.826706	18.734709	3.087458
O	3.751922	18.646757	5.547254
O	6.007200	18.738291	7.016841
O	8.098899	18.486172	5.339416
O	7.934518	18.983845	2.750608
O	5.425561	18.825052	3.522004
O	2.589045	3.164538	3.505008
O	3.762935	3.075391	5.827761
O	6.103506	2.823071	7.108916
O	8.174181	3.486902	5.530257
O	7.760127	3.236970	2.925390
O	5.253572	3.155185	3.606451
O	3.918706	0.994154	4.180314
O	8.262279	1.076536	4.510339
O	1.418158	17.330835	1.346330
O	1.752926	0.001990	0.902282
O	1.933324	2.650348	0.915130
O	6.334160	17.167664	1.673544
O	6.086087	19.730257	1.071175
O	6.086688	2.500707	1.090179
O	10.242455	19.233179	3.846274
O	10.108507	2.890330	3.771062
O	12.858929	11.105433	3.677916
O	13.681231	11.200551	1.170076
O	16.018200	11.108218	13.217988
O	18.188986	11.356956	1.352754
O	17.923695	10.858088	3.998038
O	15.445971	11.022852	3.104990
O	12.532169	6.794912	3.177660
O	13.774735	6.868737	0.911516
O	16.097086	7.130608	12.963979
O	18.193991	6.472150	1.102491
O	17.775331	6.721882	3.685009
O	15.184685	6.718300	3.164678
O	13.930507	8.950570	2.519350
O	18.359173	8.890277	2.186782
O	11.422751	12.509506	5.345438
O	11.753314	9.952286	5.860683
O	11.926304	7.291790	5.769412

O	16.273680	12.673873	5.004305
O	16.016397	10.123019	5.609217
O	16.105698	7.454563	5.596771
O	0.196216	10.777497	3.005956
O	0.163780	7.053997	2.841211
O	17.180477	8.784812	10.297014
O	16.265072	8.702032	7.859301
O	13.993575	8.780235	6.453015
O	11.920098	8.480755	8.103005
O	12.015002	9.036335	10.699441
O	14.527762	8.955147	9.865948
O	17.499228	13.099910	9.867821
O	16.258663	13.024293	7.606764
O	13.924700	12.767398	6.277430
O	11.836805	13.432222	7.796535
O	12.259470	13.182889	10.380122
O	14.844110	13.186471	9.863807
O	16.100090	10.953206	9.212991
O	11.769131	11.014693	8.870654
O	18.603041	7.387305	12.032254
O	18.269474	9.950892	12.470547
O	18.094481	12.594674	12.467469
O	13.685237	7.229307	11.704237
O	13.933509	9.766827	12.372986
O	13.931107	12.438666	12.289609
O	9.746709	9.357903	9.460979
O	9.853427	12.762025	9.520265
O	12.834903	18.740879	3.617559
O	13.757317	18.647751	1.159503
O	16.018801	18.742868	13.060069
O	18.107897	18.490351	1.343787
O	17.938511	18.982851	3.938617
O	15.449776	18.830425	3.121317
O	12.611457	3.157175	3.253943
O	13.770731	3.082753	0.912988
O	16.094885	2.820484	12.964247
O	18.190187	3.483320	1.100083
O	17.787144	3.229210	3.693039
O	15.260768	3.229807	3.091205
O	13.932709	1.002910	2.520019
O	18.349962	1.071163	2.174336
O	11.424552	17.335810	5.340219
O	11.757919	-0.015123	5.849710
O	11.853224	2.652935	5.776772

O	16.279287	17.175821	5.002566
O	16.095886	19.729460	5.611358
O	16.105896	2.504488	5.586332
O	0.223245	19.157166	2.858073
O	0.139353	2.894907	2.845494
O	17.196295	1.165484	10.297550
O	16.265871	1.249856	7.845650
O	14.004588	1.167673	6.366159
O	11.925903	1.419396	8.042380
O	12.091685	0.913364	10.637076
O	14.593835	1.071760	9.868625
O	17.456781	16.743019	9.877056
O	16.194193	16.827391	7.610912
O	13.918693	17.083889	6.269534
O	11.843614	16.415083	7.788505
O	12.268080	16.663622	10.384137
O	14.832697	16.662029	9.865546
O	16.097887	18.902657	9.211386
O	11.764126	18.837587	8.865970
O	18.601038	2.569359	12.038277
O	18.274479	19.900593	12.483663
O	18.101290	17.247856	12.463722
O	13.686038	2.738699	11.706378
O	13.935311	0.233813	12.380480
O	13.923098	17.413813	12.288940
O	9.794562	0.735666	9.536592
O	9.914494	17.080706	9.532310
O	7.027121	9.287262	9.203356
O	6.013007	8.612088	12.368970
O	3.820398	9.197516	0.334441
O	1.829410	8.539855	12.043630
O	2.158772	9.040514	9.455090
O	4.676138	8.880725	10.277475
O	7.352078	13.100905	10.113533
O	6.251269	13.104487	12.462786
O	3.924913	12.764014	0.418085
O	1.843425	13.432222	12.271542
O	2.256680	13.099710	9.615686
O	4.754624	12.929176	10.300628
O	6.266686	10.837195	11.121407
O	1.665830	11.017280	11.207460
O	8.670127	7.622113	7.698973
O	8.589838	10.124213	7.275802
O	8.006197	12.696358	7.534094

O	3.762134	7.216771	8.446948
O	4.011007	9.769613	7.777799
O	4.085489	12.430110	7.765754
O	19.789545	9.206272	10.456674
O	19.933502	12.927982	10.540184
O	2.836116	11.020862	3.010640
O	3.747518	11.111800	5.520755
O	6.097700	11.021260	6.770862
O	8.175182	11.530077	5.179890
O	7.992182	10.939077	2.656526
O	5.434972	11.021857	3.517855
O	2.686352	6.645669	3.445186
O	3.672235	6.878686	5.855999
O	6.078479	7.134587	7.024603
O	8.090890	6.464787	5.441260
O	7.740505	6.807647	2.831709
O	5.335863	6.625969	3.848415
O	3.998193	8.876347	4.091719
O	8.255871	8.947585	4.432316
O	1.420961	12.515476	1.348337
O	1.419360	9.929602	0.911382
O	2.009808	7.305918	0.919145
O	6.328753	12.691383	1.669395
O	6.097500	10.117448	1.088707
O	5.587940	7.472075	1.334687
O	10.281898	10.616316	3.776549
O	10.096693	7.131006	3.785114
O	8.597046	14.926438	8.617046
O	3.921509	14.851022	8.541834
O	5.350879	14.927632	0.827872
O	2.418257	14.919872	1.000112
O	1.496644	4.968382	1.838423
O	6.017211	4.982511	1.843776
O	4.667128	4.978332	7.521648
O	7.671029	5.005593	7.601812
O	11.420749	4.986888	4.771441
O	16.179379	4.975148	4.865122
O	14.598641	4.978730	12.561686
O	17.601339	4.977337	12.383825
O	18.442064	14.923654	11.542704
O	13.849818	14.921863	11.622869
O	15.430554	14.923056	5.937636
O	12.429056	14.921265	5.690586
Pt	7.321845	5.739269	-3.700132

Pt	9.523664	6.266792	-2.706712
Pt	7.517860	7.391881	-1.780876
292			
<b>Pt<sub>4</sub>@Silicalite-1</b>			
Si	8.445880	1.119518	8.746728
Si	6.059057	0.607118	10.774921
Si	5.621977	1.177225	0.314367
Si	2.408847	1.293236	0.185622
Si	1.352086	0.477775	10.821226
Si	3.608765	1.204885	8.982670
Si	8.508549	16.486719	8.987086
Si	6.148556	17.284472	10.926551
Si	5.445183	16.498659	0.488747
Si	2.410248	16.438166	0.420628
Si	1.432975	17.228355	10.948097
Si	3.736506	16.378269	9.060693
Si	1.579135	18.782665	2.061250
Si	3.974567	19.285713	4.080209
Si	4.394228	18.694315	7.038789
Si	7.606358	18.597010	6.891040
Si	8.648103	19.429981	4.135615
Si	6.427463	18.679588	2.256374
Si	1.560915	3.421036	2.286352
Si	3.884668	2.602391	4.286441
Si	4.575227	3.399545	7.206746
Si	7.623776	3.466207	7.067830
Si	8.565011	2.650348	4.203600
Si	6.258677	3.463620	2.376553
Si	11.575919	11.035986	4.660764
Si	13.961540	10.560598	2.633641
Si	14.409833	11.142245	13.107845
Si	17.634577	11.240149	13.218523
Si	18.674519	10.444387	2.616778
Si	16.394613	11.162743	4.425223
Si	11.487622	6.553935	4.382130
Si	13.864835	7.340343	2.458591
Si	14.559998	6.551746	12.911785
Si	17.617958	6.497421	12.968127
Si	18.632072	7.300346	2.436108
Si	16.304714	6.490258	4.316152
Si	18.457081	8.840927	11.301409
Si	16.025007	9.350939	9.322464
Si	15.604945	8.766305	6.376330
Si	12.400024	8.628206	6.534384

Si	11.358280	9.479685	9.233869
Si	13.583526	8.763321	11.167712
Si	18.495123	13.375510	11.109228
Si	16.164360	12.566418	9.152634
Si	15.459787	13.343274	6.231125
Si	12.412438	13.402972	6.274352
Si	11.432161	12.594476	9.123191
Si	13.732489	13.420682	11.024782
Si	11.583327	18.804953	4.649923
Si	13.979159	19.293472	2.622399
Si	14.408031	18.739487	13.063013
Si	17.617157	18.603775	13.188680
Si	18.670515	19.415653	2.559901
Si	16.423445	18.684565	4.418398
Si	11.502038	3.421036	4.393505
Si	13.899873	2.614729	2.458056
Si	14.556594	3.398351	12.907904
Si	17.612152	3.458048	12.970001
Si	18.618858	2.655323	2.431691
Si	16.315126	3.463620	4.307185
Si	18.446869	1.115339	11.323089
Si	16.046030	0.610700	9.315104
Si	15.617961	1.180807	6.359066
Si	12.404230	1.314926	6.501060
Si	11.383307	0.481556	9.250597
Si	13.595940	1.221600	11.141616
Si	18.478502	16.470800	11.098255
Si	16.136530	17.293625	9.150760
Si	15.447773	16.505226	6.217206
Si	12.410236	16.442345	6.270337
Si	11.459991	17.260792	9.118909
Si	13.729886	16.430008	11.031340
Si	8.466502	8.979026	8.517476
Si	6.285706	9.254030	10.751769
Si	5.389321	8.817247	0.446858
Si	2.277503	8.738248	0.206366
Si	1.357492	9.465954	10.788171
Si	3.710477	8.748198	8.996989
Si	8.456291	13.345861	8.982670
Si	6.164573	12.458963	10.990387
Si	5.454994	13.358199	0.477505
Si	2.413051	13.399787	0.411393
Si	1.446189	12.605021	10.929495
Si	3.772745	13.320192	9.069526

Si	1.507056	11.061853	2.082662
Si	3.985780	10.498315	4.035644
Si	4.493938	11.082747	6.969867
Si	7.692452	11.289300	6.733255
Si	8.681338	10.483391	4.044477
Si	6.442479	11.181049	2.245400
Si	1.589346	6.518116	2.270025
Si	3.913300	7.272686	4.303572
Si	4.556607	6.557915	7.195905
Si	7.617970	6.522494	7.011353
Si	8.543387	7.362033	4.151005
Si	6.197209	6.483293	2.458056
O	7.191502	1.165087	9.771463
O	6.334160	1.248065	12.237950
O	4.011208	1.157127	0.243704
O	1.907296	1.407456	12.035466
O	2.085692	0.913961	9.446123
O	4.583035	1.068775	10.282963
O	7.488228	16.744612	10.210025
O	6.185596	16.817242	12.468807
O	3.916103	17.088066	0.424241
O	1.836818	16.413691	12.288405
O	2.267892	16.659243	9.686214
O	4.837515	16.665215	10.213772
O	6.092094	18.897285	10.864587
O	1.669634	18.820871	11.205988
O	8.592441	2.572742	8.027658
O	8.264681	19.896812	7.593247
O	8.088688	17.234724	7.612117
O	3.755927	2.730342	8.441059
O	3.924913	0.162973	7.778601
O	3.919507	17.337004	7.774854
O	19.798553	0.741238	10.522384
O	19.924091	16.923103	10.537506
O	2.827307	18.734709	3.087993
O	3.751522	18.646557	5.548860
O	6.007801	18.738092	7.016841
O	8.099099	18.491146	5.348917
O	7.934718	18.983250	2.753285
O	5.424961	18.824852	3.523476
O	2.590246	3.163742	3.506212
O	3.761333	3.072804	5.834587
O	6.107911	2.821081	7.108113
O	8.173581	3.485111	5.534540

O	7.761328	3.236373	2.925658
O	5.251971	3.154389	3.608994
O	3.918706	0.994552	4.179645
O	8.262279	1.076735	4.510205
O	1.418158	17.330835	1.346464
O	1.752526	0.001592	0.902817
O	1.932323	2.650945	0.915531
O	6.334560	17.168062	1.673812
O	6.086287	19.730854	1.076261
O	6.086488	2.509264	1.090045
O	10.240851	19.232582	3.846408
O	10.106105	2.889733	3.769456
O	12.858929	11.105433	3.678184
O	13.680832	11.200551	1.171013
O	16.019802	11.108021	13.217854
O	18.189186	11.356758	1.353557
O	17.924696	10.857889	3.997368
O	15.445772	11.022852	3.104990
O	12.535573	6.793320	3.178195
O	13.773334	6.868936	0.910847
O	16.096285	7.130608	12.962641
O	18.193390	6.472548	1.102625
O	17.775732	6.722082	3.684608
O	15.185486	6.718897	3.162938
O	13.930906	8.950372	2.518547
O	18.359373	8.890078	2.186782
O	11.422951	12.509308	5.345304
O	11.753915	9.952683	5.860817
O	11.925903	7.289800	5.765664
O	16.274082	12.673873	5.003770
O	16.017199	10.124213	5.608949
O	16.106697	7.453171	5.595700
O	0.199019	10.777099	3.005822
O	0.164981	7.053599	2.841077
O	17.180677	8.784812	10.298219
O	16.265072	8.701833	7.858632
O	13.998382	8.781827	6.450874
O	11.929708	8.474387	8.092433
O	12.011598	9.033548	10.702251
O	14.526961	8.957535	9.863807
O	17.501429	13.099710	9.868223
O	16.258663	13.024095	7.606362
O	13.925701	12.767199	6.277029
O	11.839809	13.431427	7.793055

O	12.264476	13.182093	10.381327
O	14.845312	13.186072	9.863673
O	16.099289	10.954598	9.213660
O	11.771935	11.011909	8.871724
O	18.602640	7.387504	12.031585
O	18.269274	9.950694	12.469745
O	18.094282	12.594873	12.467201
O	13.683636	7.231098	11.705976
O	13.932909	9.772798	12.374324
O	13.931107	12.439262	12.289475
O	9.767532	9.292037	9.457900
O	9.873649	12.760632	9.524146
O	12.834302	18.740879	3.617960
O	13.757115	18.647949	1.159771
O	16.019001	18.742670	13.060069
O	18.107897	18.490549	1.343787
O	17.938511	18.982851	3.938483
O	15.449374	18.830425	3.121317
O	12.609655	3.157374	3.253407
O	13.769730	3.084345	0.913390
O	16.095284	2.820882	12.964112
O	18.190187	3.483320	1.100484
O	17.786943	3.229210	3.692503
O	15.260366	3.230006	3.090938
O	13.932709	1.003109	2.519484
O	18.349962	1.071163	2.174336
O	11.424552	17.336010	5.339817
O	11.758120	-0.015322	5.849710
O	11.853624	2.652935	5.775836
O	16.279488	17.176022	5.002164
O	16.095886	19.729460	5.611358
O	16.106096	2.504289	5.586332
O	0.223646	19.157166	2.858207
O	0.140354	2.895106	2.845494
O	17.196695	1.165484	10.297684
O	16.266073	1.249856	7.845249
O	14.004588	1.167474	6.365490
O	11.928507	1.419396	8.041577
O	12.094089	0.912767	10.638816
O	14.594636	1.072158	9.868758
O	17.456982	16.742821	9.877056
O	16.194193	16.827190	7.611046
O	13.918894	17.083889	6.269668
O	11.843614	16.414885	7.788773

O	12.267679	16.663424	10.383469
O	14.833298	16.661831	9.865546
O	16.097887	18.902857	9.211386
O	11.765127	18.837786	8.866104
O	18.601038	2.569160	12.038009
O	18.274479	19.900791	12.483128
O	18.101290	17.247856	12.463722
O	13.685637	2.738898	11.707181
O	13.935913	0.234609	12.380881
O	13.923298	17.414412	12.289207
O	9.807576	0.741238	9.542079
O	9.913692	17.078318	9.531908
O	7.085385	9.282087	9.278166
O	5.932719	8.531696	12.316108
O	3.824802	9.197716	0.334441
O	1.830411	8.539457	12.044700
O	2.171386	9.039718	9.457097
O	4.756426	8.877939	10.210694
O	7.418151	13.104089	10.191958
O	6.247665	13.113044	12.472019
O	3.923711	12.764014	0.419156
O	1.843225	13.432222	12.271810
O	2.259082	13.099314	9.615953
O	4.764034	12.933952	10.295944
O	6.257075	10.861869	11.131712
O	1.666031	11.017280	11.207594
O	8.584232	7.458145	7.940536
O	8.584433	10.030888	7.270851
O	8.007399	12.613180	7.608503
O	3.760732	7.215377	8.443736
O	4.007403	9.772598	7.772311
O	4.086690	12.430110	7.764014
O	19.794350	9.206272	10.456139
O	19.934704	12.927784	10.540050
O	2.836917	11.021061	3.010907
O	3.748519	11.112796	5.518882
O	6.099702	11.015291	6.771129
O	8.177986	11.523312	5.195682
O	7.990980	10.941266	2.659604
O	5.435973	11.020465	3.515179
O	2.688354	6.646664	3.446658
O	3.675238	6.878886	5.857605
O	6.089891	7.129215	7.026878
O	8.167374	6.483890	5.470837

O	7.744109	6.804861	2.840810
O	5.339266	6.625770	3.844936
O	3.998193	8.875551	4.091451
O	8.256071	8.948780	4.432048
O	1.420561	12.515277	1.348337
O	1.420361	9.928208	0.911115
O	2.010009	7.305719	0.919011
O	6.328753	12.688995	1.670868
O	6.100503	10.112672	1.079607
O	5.585137	7.474661	1.333482
O	10.280496	10.617112	3.776683
O	10.102099	7.133394	3.775077
O	8.595244	14.918081	8.615842
O	3.921509	14.851619	8.541164
O	5.349077	14.929027	0.830817
O	2.418057	14.920072	1.000112
O	1.496845	4.968581	1.838690
O	6.011405	4.980919	1.846453
O	4.661522	4.976740	7.517365
O	7.667624	5.001812	7.607299
O	11.421550	4.985893	4.770504
O	16.179379	4.974750	4.864587
O	14.597038	4.977934	12.561419
O	17.600538	4.977337	12.383960
O	18.441862	14.924051	11.542704
O	13.850418	14.923654	11.623270
O	15.430554	14.923654	5.937636
O	12.429056	14.922260	5.690050
Pt	10.440472	8.327134	11.152590
Pt	7.939924	8.889281	11.746527
Pt	9.819790	9.270945	13.320501
Pt	9.865640	10.400013	11.641604

293

#### Pt<sub>5</sub>@Silicalite-1

Si	8.447882	1.114543	8.746996
Si	6.059658	0.606124	10.773181
Si	5.621176	1.170658	0.307541
Si	2.407846	1.292639	0.184685
Si	1.350484	0.476979	10.821226
Si	3.607964	1.203491	8.983473
Si	8.508749	16.483137	8.987889
Si	6.148756	17.282681	10.926149
Si	5.444983	16.495476	0.487543
Si	2.410649	16.436972	0.420360

Si	1.432975	17.227360	10.947562
Si	3.736506	16.374092	9.061094
Si	1.578134	18.781672	2.060848
Si	3.974367	19.283524	4.080343
Si	4.393828	18.692524	7.040529
Si	7.605958	18.594620	6.891174
Si	8.649504	19.426798	4.135213
Si	6.427463	18.677202	2.255705
Si	1.557511	3.420837	2.284880
Si	3.880664	2.600998	4.285371
Si	4.573025	3.400142	7.207951
Si	7.622375	3.464814	7.066492
Si	8.574020	2.644975	4.208686
Si	6.271691	3.439144	2.383245
Si	11.577520	11.037378	4.660228
Si	13.962742	10.561593	2.632169
Si	14.408431	11.137271	13.104366
Si	17.633175	11.239752	13.217988
Si	18.674118	10.445184	2.616377
Si	16.395014	11.162942	4.425491
Si	11.492427	6.554731	4.383736
Si	13.868238	7.340741	2.456583
Si	14.558597	6.553338	12.906834
Si	17.616756	6.498217	12.967592
Si	18.630671	7.300943	2.435305
Si	16.305515	6.490855	4.317089
Si	18.455879	8.840728	11.301409
Si	16.021204	9.348948	9.325409
Si	15.606748	8.766902	6.378070
Si	12.402027	8.631191	6.532510
Si	11.380704	9.482670	9.243371
Si	13.570711	8.755958	11.166374
Si	18.495522	13.374516	11.108960
Si	16.164160	12.564627	9.153170
Si	15.460187	13.342877	6.231794
Si	12.412639	13.402972	6.274888
Si	11.429958	12.598057	9.124128
Si	13.732889	13.419089	11.025317
Si	11.584728	18.804157	4.649923
Si	13.979761	19.293472	2.621730
Si	14.407831	18.739286	13.062478
Si	17.616957	18.603376	13.188412
Si	18.669914	19.415257	2.559901
Si	16.423445	18.684166	4.418531

Si	11.507845	3.421036	4.394041
Si	13.901475	2.614331	2.455647
Si	14.554592	3.400341	12.906967
Si	17.610149	3.458645	12.969197
Si	18.616455	2.655323	2.430888
Si	16.314926	3.464018	4.307319
Si	18.445868	1.115737	11.323893
Si	16.045429	0.610501	9.315639
Si	15.619162	1.180807	6.359334
Si	12.405831	1.313931	6.501194
Si	11.387512	0.480163	9.251266
Si	13.596339	1.222794	11.142954
Si	18.478304	16.469805	11.098255
Si	16.136530	17.293226	9.151029
Si	15.447973	16.504627	6.217474
Si	12.410836	16.441549	6.270471
Si	11.460192	17.259199	9.119310
Si	13.730287	16.429012	11.031741
Si	8.458493	9.004497	8.479469
Si	6.301324	9.182592	10.687932
Si	5.370701	8.823416	0.473758
Si	2.268893	8.738845	0.205964
Si	1.356290	9.466352	10.787368
Si	3.703870	8.749192	8.994982
Si	8.449884	13.341682	8.987889
Si	6.171581	12.404839	10.992261
Si	5.457797	13.354219	0.469208
Si	2.414052	13.398992	0.410724
Si	1.447390	12.604823	10.928960
Si	3.780754	13.314221	9.077154
Si	1.505854	11.062650	2.082662
Si	3.985579	10.500902	4.036581
Si	4.494339	11.082351	6.971606
Si	7.690049	11.294673	6.723352
Si	8.682740	10.491947	4.041265
Si	6.441678	11.186422	2.247407
Si	1.586343	6.518713	2.268419
Si	3.908695	7.273682	4.303839
Si	4.551601	6.558711	7.199920
Si	7.611563	6.537020	7.025808
Si	8.551396	7.376758	4.159570
Si	6.205819	6.504386	2.469699
O	7.193103	1.166280	9.769857
O	6.334360	1.247269	12.235140

O	4.011007	1.157326	0.243437
O	1.907096	1.407257	12.034931
O	2.085291	0.913961	9.446391
O	4.583837	1.068974	10.282427
O	7.488828	16.745008	10.209891
O	6.185596	16.818436	12.468807
O	3.916303	17.087669	0.424509
O	1.836818	16.413889	12.288405
O	2.268292	16.659443	9.685812
O	4.837315	16.665611	10.213505
O	6.092494	18.896887	10.863785
O	1.669634	18.820673	11.205988
O	8.592040	2.575130	8.030335
O	8.265081	19.898005	7.589901
O	8.089087	17.234125	7.612786
O	3.755927	2.729546	8.440792
O	3.925113	0.162973	7.778467
O	3.919507	17.335810	7.775390
O	19.797752	0.741437	10.522652
O	19.924091	16.923304	10.537374
O	2.827106	18.735107	3.087993
O	3.751522	18.647154	5.549663
O	6.007801	18.738491	7.016841
O	8.098899	18.490747	5.348917
O	7.934318	18.983446	2.753285
O	5.425161	18.825249	3.523342
O	2.590046	3.164936	3.504740
O	3.763335	3.073600	5.832446
O	6.108111	2.822474	7.108247
O	8.173982	3.486504	5.535477
O	7.768335	3.232394	2.931546
O	5.250770	3.161951	3.605113
O	3.919907	0.994950	4.179244
O	8.262279	1.075342	4.511275
O	1.418358	17.330637	1.346196
O	1.752726	0.001592	0.903353
O	1.933124	2.650746	0.915665
O	6.334160	17.166866	1.673410
O	6.086488	19.730455	1.076662
O	6.082283	2.502498	1.092856
O	10.241653	19.232582	3.846542
O	10.110108	2.889733	3.771062
O	12.859730	11.105433	3.677782
O	13.681231	11.200352	1.170343

O	16.019201	11.108021	13.217854
O	18.188986	11.356758	1.353289
O	17.924696	10.857889	3.997502
O	15.446172	11.022852	3.105124
O	12.535975	6.793320	3.176589
O	13.773133	6.868339	0.910713
O	16.096487	7.130608	12.963979
O	18.193590	6.472349	1.102491
O	17.775932	6.722082	3.684608
O	15.185486	6.718500	3.164143
O	13.930507	8.950570	2.519082
O	18.359173	8.890475	2.186916
O	11.422951	12.509706	5.345438
O	11.754114	9.953281	5.859211
O	11.926105	7.290198	5.766200
O	16.274082	12.674070	5.003904
O	16.017199	10.124213	5.608815
O	16.106697	7.453370	5.596102
O	0.198218	10.777497	3.006491
O	0.164180	7.053599	2.841612
O	17.181078	8.784812	10.298085
O	16.265272	8.702032	7.859435
O	13.999582	8.781827	6.449937
O	11.926704	8.479561	8.086946
O	12.017204	9.038126	10.696630
O	14.526961	8.956341	9.865145
O	17.501230	13.099910	9.868089
O	16.258863	13.024095	7.606764
O	13.925701	12.767199	6.277029
O	11.839609	13.432222	7.793055
O	12.264476	13.182490	10.381461
O	14.845312	13.186072	9.863539
O	16.099489	10.953603	9.213125
O	11.767930	11.015688	8.868379
O	18.602840	7.387504	12.031986
O	18.269474	9.950694	12.470146
O	18.094282	12.594873	12.467201
O	13.686038	7.228113	11.705441
O	13.932509	9.769216	12.373253
O	13.931307	12.438666	12.289877
O	9.766731	9.282884	9.462317
O	9.871647	12.760831	9.524548
O	12.834702	18.740879	3.617559
O	13.757317	18.647751	1.159637

O	16.019001	18.742670	13.060203
O	18.107897	18.490351	1.343787
O	17.938511	18.982851	3.938617
O	15.449575	18.830425	3.121585
O	12.611457	3.157971	3.252872
O	13.769931	3.083947	0.913256
O	16.094284	2.820683	12.964380
O	18.189987	3.483320	1.099949
O	17.786943	3.229210	3.692905
O	15.260568	3.229807	3.091072
O	13.932709	1.003109	2.520019
O	18.349762	1.070964	2.174336
O	11.424552	17.336010	5.340085
O	11.757919	-0.014924	5.849442
O	11.853825	2.652736	5.776772
O	16.279287	17.175821	5.002298
O	16.096085	19.729460	5.611358
O	16.106096	2.504488	5.586332
O	0.223446	19.157166	2.858207
O	0.138953	2.894707	2.845627
O	17.196495	1.165484	10.297684
O	16.266073	1.249856	7.845650
O	14.005189	1.167275	6.365356
O	11.928306	1.419595	8.041176
O	12.094689	0.912568	10.638950
O	14.594436	1.071959	9.868758
O	17.457182	16.742821	9.877190
O	16.194193	16.827391	7.611180
O	13.918894	17.083889	6.269668
O	11.843614	16.414684	7.788639
O	12.267879	16.663223	10.383736
O	14.833098	16.661831	9.865546
O	16.097887	18.902657	9.211386
O	11.765127	18.836792	8.865703
O	18.601038	2.569359	12.038410
O	18.274679	19.900791	12.483797
O	18.101290	17.247856	12.463588
O	13.686238	2.738898	11.706511
O	13.935913	0.234211	12.380881
O	13.923298	17.414211	12.289207
O	9.810780	0.743029	9.540741
O	9.913292	17.078117	9.531507
O	7.081781	9.376409	9.196397
O	5.918303	8.548014	12.370442

O	3.810187	9.201098	0.345415
O	1.829010	8.539258	12.044031
O	2.166981	9.039917	9.455491
O	4.741810	8.879332	10.206278
O	7.413145	13.096725	10.194768
O	6.248666	13.101302	12.465195
O	3.924112	12.763816	0.418888
O	1.842825	13.432222	12.272078
O	2.261685	13.099511	9.616623
O	4.773845	12.924202	10.299825
O	6.266686	10.803764	11.132248
O	1.665630	11.017082	11.207594
O	8.586034	7.464314	7.945889
O	8.598248	10.021933	7.205541
O	8.008599	12.609598	7.609039
O	3.757128	7.214382	8.443468
O	4.006602	9.770608	7.769099
O	4.087090	12.429911	7.764549
O	19.793148	9.206471	10.456139
O	19.935305	12.927982	10.539916
O	2.836517	11.020266	3.010907
O	3.748318	11.112796	5.519417
O	6.099702	11.015887	6.768184
O	8.176384	11.530476	5.188456
O	7.991581	10.942460	2.655723
O	5.436173	11.021061	3.517320
O	2.688754	6.645072	3.444650
O	3.675639	6.878089	5.857070
O	6.085486	7.129215	7.028618
O	8.172780	6.539011	5.499209
O	7.751517	6.808045	2.849508
O	5.336463	6.612637	3.844668
O	4.000196	8.874557	4.091049
O	8.256472	8.956738	4.429238
O	1.420761	12.515676	1.348605
O	1.415555	9.929602	0.911516
O	2.008407	7.304724	0.918877
O	6.327953	12.691582	1.670600
O	6.097300	10.115458	1.087770
O	5.581332	7.472075	1.346598
O	10.282098	10.617708	3.776014
O	10.104102	7.132000	3.775077
O	8.594243	14.915096	8.616511
O	3.922310	14.848435	8.543440

O	5.350479	14.926638	0.828274
O	2.418057	14.919872	1.000245
O	1.497045	4.968382	1.838824
O	6.097900	4.981317	1.827582
O	4.662523	4.976541	7.517097
O	7.671429	5.005593	7.611715
O	11.421350	4.986292	4.770370
O	16.179379	4.974949	4.864855
O	14.598440	4.977934	12.562355
O	17.601139	4.977337	12.383960
O	18.442064	14.923852	11.542704
O	13.850218	14.923255	11.623270
O	15.430554	14.923454	5.937769
O	12.429256	14.922260	5.689916
Pt	7.854830	5.736285	-0.025562
Pt	9.716475	7.012010	-1.728682
Pt	8.516357	5.221298	-2.618919
Pt	7.405937	7.348303	-1.711150
Pt	10.049042	5.515804	-0.538130

294

#### Pt<sub>6</sub>@Silicalite-1

Si	8.447882	1.116732	8.748333
Si	6.059258	0.605328	10.773717
Si	5.621777	1.174638	0.311690
Si	2.408446	1.293236	0.185355
Si	1.351084	0.477178	10.821494
Si	3.608164	1.203691	8.983205
Si	8.508749	16.483337	8.987353
Si	6.148756	17.282681	10.926149
Si	5.444983	16.497267	0.487944
Si	2.410449	16.437569	0.420494
Si	1.432975	17.227560	10.947696
Si	3.736506	16.375484	9.060826
Si	1.578735	18.782269	2.060982
Si	3.974367	19.284519	4.080343
Si	4.394028	18.693121	7.039726
Si	7.606157	18.595417	6.891576
Si	8.648502	19.428389	4.135213
Si	6.427062	18.678396	2.255839
Si	1.560114	3.421434	2.285683
Si	3.883667	2.601197	4.284835
Si	4.572624	3.399147	7.206746
Si	7.622976	3.461630	7.066492
Si	8.566212	2.648358	4.202262

Si	6.260078	3.456656	2.374947
Si	11.577721	11.036184	4.661968
Si	13.963342	10.561593	2.632704
Si	14.409032	11.137868	13.104634
Si	17.634377	11.239552	13.219728
Si	18.683729	10.446378	2.618250
Si	16.397417	11.162344	4.424821
Si	11.498835	6.552342	4.384539
Si	13.868238	7.340940	2.454978
Si	14.557996	6.553537	12.907235
Si	17.617357	6.498615	12.969065
Si	18.636877	7.301142	2.436643
Si	16.306517	6.491253	4.316285
Si	18.456478	8.840927	11.301274
Si	16.021004	9.349346	9.325409
Si	15.605947	8.766902	6.377937
Si	12.400425	8.630992	6.542280
Si	11.356277	9.476899	9.248322
Si	13.572914	8.756157	11.165839
Si	18.495123	13.374516	11.109363
Si	16.164160	12.564825	9.153170
Si	15.460387	13.342479	6.231526
Si	12.412438	13.402574	6.275958
Si	11.432161	12.590694	9.123592
Si	13.732089	13.418891	11.024782
Si	11.583928	18.804157	4.649790
Si	13.979560	19.293472	2.621998
Si	14.408031	18.738888	13.062745
Si	17.617157	18.603376	13.188412
Si	18.670315	19.415455	2.559766
Si	16.423645	18.684166	4.418531
Si	11.503839	3.419046	4.392033
Si	13.900874	2.614331	2.456316
Si	14.555793	3.400540	12.907503
Si	17.611151	3.459043	12.969465
Si	18.618256	2.655323	2.431022
Si	16.315527	3.464217	4.306917
Si	18.446468	1.115538	11.323758
Si	16.046030	0.610302	9.315372
Si	15.618961	1.180807	6.358932
Si	12.405230	1.313931	6.500659
Si	11.386911	0.479765	9.250597
Si	13.596939	1.221799	11.142686
Si	18.478502	16.469805	11.098388

Si	16.136530	17.293028	9.151029
Si	15.447973	16.504431	6.217340
Si	12.410836	16.441549	6.270471
Si	11.459991	17.259001	9.119310
Si	13.730086	16.428616	11.031607
Si	8.466703	9.017033	8.491916
Si	6.319744	9.211645	10.711619
Si	5.377308	8.821425	0.457699
Si	2.273498	8.737651	0.205295
Si	1.357692	9.465755	10.787233
Si	3.713881	8.751183	9.002744
Si	8.453689	13.341682	8.985212
Si	6.168978	12.428716	10.989718
Si	5.455995	13.357203	0.469609
Si	2.413652	13.399787	0.409921
Si	1.446990	12.604225	10.928558
Si	3.777350	13.316610	9.074076
Si	1.516066	11.062053	2.081190
Si	4.004800	10.506871	4.033770
Si	4.494739	11.082151	6.972276
Si	7.690450	11.293081	6.720273
Si	8.679136	10.499111	4.023064
Si	6.449487	11.184831	2.234827
Si	1.599958	6.518912	2.274040
Si	3.924312	7.282039	4.309995
Si	4.551001	6.558312	7.201928
Si	7.608160	6.526076	7.017911
Si	8.554399	7.377355	4.177102
Si	6.169980	6.476328	2.452836
O	7.192703	1.165882	9.771330
O	6.334560	1.248463	12.235809
O	4.011407	1.157127	0.243437
O	1.907296	1.407257	12.035332
O	2.085291	0.913762	9.446257
O	4.583636	1.068974	10.282560
O	7.489029	16.745008	10.209891
O	6.185797	16.818039	12.468807
O	3.916103	17.088066	0.424375
O	1.836818	16.413889	12.288405
O	2.268292	16.659443	9.685946
O	4.837315	16.665413	10.213505
O	6.092494	18.896688	10.864185
O	1.669634	18.820673	11.205854
O	8.592641	2.573736	8.028997

O	8.264681	19.897408	7.592845
O	8.088888	17.234125	7.612518
O	3.755927	2.729745	8.440927
O	3.925113	0.162973	7.778467
O	3.919507	17.336407	7.775256
O	19.798153	0.741238	10.522518
O	19.924091	16.923304	10.537374
O	2.827307	18.734709	3.087993
O	3.751522	18.646757	5.549395
O	6.007801	18.738491	7.016975
O	8.099099	18.491344	5.349185
O	7.934318	18.983250	2.753285
O	5.424961	18.824852	3.523476
O	2.590046	3.163742	3.505811
O	3.762134	3.073202	5.833115
O	6.107511	2.822076	7.108247
O	8.173780	3.486106	5.534406
O	7.761528	3.237567	2.926728
O	5.252171	3.155185	3.608057
O	3.918706	0.994154	4.179779
O	8.262078	1.076735	4.510339
O	1.418358	17.330835	1.346330
O	1.752726	0.001791	0.902951
O	1.932523	2.651144	0.915665
O	6.334160	17.167465	1.673544
O	6.086488	19.730455	1.075993
O	6.086488	2.506080	1.089376
O	10.241053	19.232582	3.846542
O	10.106305	2.891126	3.769991
O	12.858929	11.105035	3.677916
O	13.681032	11.200152	1.170477
O	16.019602	11.108021	13.218255
O	18.190586	11.356160	1.355430
O	17.927698	10.858287	3.997368
O	15.446772	11.022653	3.105392
O	12.534373	6.794713	3.175652
O	13.773533	6.868538	0.910446
O	16.096487	7.130011	12.964380
O	18.194792	6.473145	1.104098
O	17.777134	6.722479	3.684340
O	15.184685	6.718500	3.164410
O	13.930105	8.950570	2.518948
O	18.362175	8.891470	2.189057
O	11.422751	12.509109	5.345304

O	11.753715	9.951291	5.860549
O	11.924702	7.291193	5.767003
O	16.274481	12.673474	5.003636
O	16.017399	10.124014	5.608414
O	16.106497	7.453370	5.595834
O	0.211432	10.775906	3.007829
O	0.171388	7.052803	2.843218
O	17.180878	8.784812	10.298085
O	16.264872	8.701833	7.859435
O	13.998181	8.781230	6.450740
O	11.927906	8.471999	8.097652
O	12.011398	9.036534	10.704928
O	14.525360	8.956938	9.864610
O	17.501230	13.099710	9.868223
O	16.258863	13.024095	7.606630
O	13.925701	12.767199	6.276761
O	11.839609	13.430830	7.793725
O	12.264276	13.182093	10.381060
O	14.845312	13.186072	9.863673
O	16.099289	10.953603	9.213259
O	11.770534	11.009321	8.871457
O	18.602840	7.387504	12.031986
O	18.269474	9.950694	12.470146
O	18.094282	12.594674	12.467737
O	13.690242	7.228909	11.703702
O	13.931908	9.769613	12.373521
O	13.931307	12.438666	12.290010
O	9.762527	9.291838	9.449870
O	9.873849	12.760433	9.523610
O	12.834502	18.741077	3.617827
O	13.757317	18.647751	1.159637
O	16.019001	18.742670	13.060069
O	18.107897	18.490549	1.343787
O	17.938511	18.982851	3.938483
O	15.449374	18.830425	3.121719
O	12.610657	3.157971	3.253140
O	13.769329	3.084345	0.912988
O	16.094484	2.820882	12.964247
O	18.189987	3.483320	1.100216
O	17.787144	3.229210	3.692637
O	15.260366	3.230006	3.091072
O	13.932509	1.003109	2.519751
O	18.349962	1.071163	2.174336
O	11.424753	17.335810	5.340085

O	11.757919	-0.015123	5.849442
O	11.853423	2.653134	5.775969
O	16.279287	17.175821	5.002432
O	16.096085	19.729460	5.611358
O	16.105896	2.504687	5.586064
O	0.223646	19.157166	2.858207
O	0.140154	2.895106	2.845494
O	17.196695	1.165484	10.297684
O	16.265871	1.249856	7.845516
O	14.004988	1.167474	6.365356
O	11.928507	1.419794	8.041176
O	12.094689	0.913364	10.638816
O	14.594636	1.072158	9.868758
O	17.457182	16.742821	9.877190
O	16.194193	16.827391	7.611046
O	13.918894	17.083689	6.269534
O	11.843614	16.414684	7.788505
O	12.267879	16.663424	10.383870
O	14.833098	16.662029	9.865546
O	16.097887	18.902657	9.211386
O	11.765327	18.836592	8.865836
O	18.601038	2.569359	12.038277
O	18.274479	19.900791	12.483529
O	18.101290	17.247856	12.463588
O	13.685237	2.739296	11.707047
O	13.935913	0.234410	12.381149
O	13.923098	17.414211	12.289074
O	9.811380	0.742830	9.541276
O	9.913292	17.078117	9.531507
O	7.077176	9.372031	9.198003
O	5.926512	8.539258	12.357327
O	3.816393	9.200501	0.340999
O	1.829410	8.539059	12.044299
O	2.171386	9.039917	9.456562
O	4.758829	8.877542	10.209757
O	7.415749	13.101701	10.192359
O	6.248666	13.107074	12.467603
O	3.923911	12.764014	0.418888
O	1.843025	13.432422	12.271408
O	2.260283	13.099710	9.615953
O	4.768640	12.930370	10.298085
O	6.263082	10.835205	11.131712
O	1.665830	11.017082	11.207594
O	8.585032	7.460533	7.945086

O	8.593642	10.018749	7.200322
O	8.009200	12.608206	7.607433
O	3.758530	7.215975	8.444807
O	4.006803	9.771007	7.770572
O	4.086690	12.430110	7.764014
O	19.794149	9.206272	10.456139
O	19.935104	12.927982	10.540050
O	2.846728	11.020664	3.011175
O	3.751322	11.113392	5.517543
O	6.099902	11.016684	6.767248
O	8.175383	11.528089	5.181496
O	8.007798	10.935695	2.615172
O	5.475016	11.009918	3.528696
O	2.734004	6.638307	3.427252
O	3.676640	6.878886	5.858007
O	6.087489	7.129215	7.026610
O	8.162970	6.488467	5.475253
O	7.753719	6.803667	2.832512
O	5.352080	6.626168	3.851895
O	4.001797	8.879730	4.091049
O	8.254670	8.955346	4.426026
O	1.421962	12.515476	1.348605
O	1.418959	9.928805	0.911115
O	2.009007	7.305321	0.919546
O	6.326551	12.692577	1.670466
O	6.096098	10.113467	1.084424
O	5.583335	7.476254	1.342984
O	10.281497	10.616117	3.774943
O	10.102099	7.132996	3.777486
O	8.594644	14.915495	8.615708
O	3.921709	14.849828	8.541968
O	5.349478	14.928031	0.829612
O	2.418057	14.920072	1.000112
O	1.497645	4.969775	1.840698
O	6.015009	4.978332	1.844579
O	4.662723	4.976541	7.516830
O	7.671830	5.003206	7.609173
O	11.420348	4.985893	4.770103
O	16.179379	4.975148	4.864319
O	14.597640	4.977735	12.561819
O	17.601139	4.977735	12.384360
O	18.442064	14.923654	11.542704
O	13.850218	14.923056	11.623270
O	15.430554	14.923255	5.937636

O	12.429056	14.922062	5.690050
Pt	7.933317	4.985297	-0.864140
Pt	10.360383	7.808765	-1.176767
Pt	9.270586	6.056858	-2.894475
Pt	9.032324	6.754715	0.771798
Pt	7.710672	7.629078	-1.576651
Pt	10.542985	5.216125	-0.745299
	295		
	Pt <sub>1</sub> @H-MFI		
Si	8.464300	1.025793	8.786342
Si	6.066266	0.535482	10.826847
Si	5.508452	1.156331	0.356657
Si	2.331362	1.356515	0.202351
Si	1.372108	0.527722	10.829256
Si	3.606963	1.186975	8.991636
Si	8.492131	16.645514	9.037941
Si	6.139345	17.195522	10.978878
Si	5.485828	16.456474	0.588451
Si	1.443786	17.343172	10.878238
Si	3.741711	16.413691	9.052396
Si	1.498246	18.832613	2.077711
Si	3.940129	19.278351	4.060135
Si	4.371203	18.721178	6.976692
Si	7.530274	18.572733	6.866550
Si	8.632686	19.332077	4.186203
Si	6.411845	18.698095	2.310709
Si	1.502651	3.490683	2.336538
Si	4.550200	3.475161	7.334553
Si	7.601552	3.487101	7.262151
Si	8.685143	2.508667	4.510339
Si	6.573022	3.505806	2.212477
Si	11.562704	10.929726	4.639217
Si	14.059247	10.642981	2.669775
Si	14.447674	11.151200	13.098344
Si	17.673819	11.337057	13.223877
Si	18.703350	10.504086	2.641670
Si	11.693648	6.626964	4.451320
Si	14.093286	7.464513	2.515335
Si	14.791452	6.759491	13.023801
Si	17.789347	6.583982	13.220531
Si	18.760612	7.427700	2.609283
Si	16.418240	6.489064	4.412509
Si	18.515945	8.881123	11.416770
Si	16.218019	9.502768	9.394197

Si	15.692643	8.775658	6.487410
Si	12.511548	8.634574	6.613879
Si	11.451782	9.426555	9.324739
Si	13.744701	8.859234	11.139742
Si	18.548780	13.518386	11.198761
Si	16.213415	12.670291	9.318851
Si	15.462190	13.439983	6.410323
Si	12.437866	13.336110	6.276761
Si	11.426956	12.496373	9.141660
Si	13.675627	13.395410	11.009124
Si	11.533672	18.836792	4.719783
Si	13.991774	19.416649	2.808289
Si	17.639982	18.647552	13.279416
Si	18.720970	19.367895	2.596570
Si	16.454679	18.663073	4.443558
Si	11.709265	3.445512	4.508197
Si	13.886858	2.700493	2.495528
Si	17.812773	3.517347	13.111593
Si	18.618256	2.536327	2.573149
Si	16.256062	3.461431	4.407022
Si	18.494320	1.118125	11.373543
Si	16.073862	0.623038	9.352843
Si	15.600741	1.112951	6.435751
Si	12.508143	1.296221	6.567841
Si	11.434164	0.552396	9.285527
Si	13.636784	1.443274	11.069882
Si	18.517345	16.597160	11.086344
Si	16.124718	17.288450	9.189035
Si	15.408330	16.550795	6.251467
Si	12.367789	16.434782	6.308746
Si	11.460993	17.375011	9.159459
Si	13.696449	16.438763	11.026656
Si	8.476714	9.005890	8.711396
Si	6.042640	9.552317	10.691010
Si	5.497240	8.799736	0.245846
Si	2.359793	8.629798	0.173979
Si	1.411351	9.429738	10.799010
Si	3.585139	8.955545	8.765329
Si	6.118523	12.716257	10.958938
Si	5.373704	13.333524	0.507350
Si	2.360794	13.363571	0.369906
Si	1.396134	12.563233	10.894030
Si	3.679643	13.334518	9.024960
Si	1.516066	10.974497	1.923405

Si	3.923111	10.472246	3.908104
Si	4.331159	11.147618	6.788795
Si	7.491831	11.341235	6.789999
Si	8.600650	10.456725	4.097340
Si	6.432668	11.064043	2.129905
Si	1.566521	6.547368	2.324226
Si	3.925113	7.306316	4.256196
Si	4.561212	6.595723	7.210092
Si	7.637192	6.570451	7.053778
Si	8.648302	7.371386	4.235051
Si	6.362591	6.628954	2.398903
Al	2.140952	16.395781	0.413401
Al	3.885669	2.660894	4.284567
Al	16.453478	11.133690	4.430710
Al	14.469699	18.877584	12.953808
Al	14.497530	3.554956	12.883145
Al	8.376204	13.308849	8.928736
O	7.255372	1.079720	9.865680
O	6.259478	1.240106	12.291483
O	3.920908	0.999726	0.167421
O	1.829210	1.497997	12.049117
O	2.075881	0.992960	9.451075
O	4.589843	0.909384	10.274130
O	7.498639	16.580246	10.292999
O	6.166375	16.747993	12.540005
O	3.920308	17.166668	0.671559
O	1.839021	16.422644	12.116835
O	2.250072	16.834753	9.536860
O	4.818294	16.586214	10.284568
O	6.178989	18.811718	10.876766
O	1.830411	18.907831	11.203712
O	8.599249	2.511254	8.110634
O	8.261678	19.816021	7.608503
O	7.760127	17.179205	7.697768
O	3.755727	2.731735	8.536881
O	3.851031	0.145263	7.765084
O	4.168380	17.335014	7.784089
O	19.806963	0.739845	10.519975
O	19.860823	17.329044	10.538712
O	2.916605	18.657303	2.921241
O	3.659821	18.581289	5.517142
O	5.972763	18.918974	6.760556
O	8.178386	18.328970	5.386524
O	7.932716	18.992203	2.769612

O	5.426763	18.746649	3.592800
O	2.672336	3.476156	3.410925
O	3.920908	3.161951	5.919034
O	6.099102	2.899881	7.369349
O	8.005796	3.405913	5.664087
O	8.006998	3.074595	3.090402
O	5.589341	3.233388	3.688489
O	3.912299	0.960525	4.083287
O	8.265081	0.954356	4.681374
O	1.185503	17.414211	1.414851
O	1.657621	0.076810	0.923561
O	1.926116	2.745465	0.927977
O	6.344171	17.167465	1.753307
O	6.080481	19.723291	1.096202
O	5.748116	2.484987	1.257601
O	10.207816	19.155375	3.845471
O	10.255268	2.727556	4.354025
O	12.695549	10.855899	3.513974
O	13.765124	11.199356	1.174358
O	16.073061	11.111601	13.055786
O	18.120310	11.389989	1.394107
O	18.096483	11.029021	4.012090
O	15.265973	11.504210	3.264649
O	12.699954	7.040266	3.255281
O	13.859628	7.140159	0.935873
O	16.328941	7.301739	13.301765
O	18.508738	6.483492	1.292798
O	17.922693	6.806254	3.859791
O	15.347063	6.632934	3.175251
O	14.434060	9.043897	2.685165
O	18.281887	8.949774	2.268017
O	11.522460	12.444635	5.277988
O	11.760122	9.868910	5.856802
O	12.191795	7.227317	5.865635
O	16.527359	12.784909	5.271965
O	16.179777	10.044220	5.687775
O	16.015396	7.385713	5.697144
O	0.276704	10.685564	2.911338
O	0.328161	7.378350	3.004751
O	17.198898	8.783021	10.467246
O	16.427250	8.781628	7.955658
O	14.087278	8.941018	6.695248
O	11.923501	8.454687	8.111704
O	12.178782	8.943407	10.698370

O	14.665714	9.367057	9.881740
O	17.332644	13.515401	10.116611
O	16.269276	13.192639	7.770839
O	14.000784	12.761626	6.273416
O	11.846216	13.349046	7.783687
O	12.182185	13.256516	10.382398
O	14.697549	13.008772	9.790334
O	16.598238	11.099463	9.366361
O	11.929107	10.951614	8.954298
O	18.697744	7.464911	12.206768
O	18.435057	10.117049	12.467737
O	18.097084	12.766005	12.561151
O	14.182983	7.374968	11.630764
O	13.867037	9.789909	12.454889
O	13.925502	12.449213	12.288940
O	9.847219	9.284078	9.542480
O	9.858031	12.587709	9.369573
O	12.781043	18.816494	3.679121
O	13.592335	18.820871	1.256664
O	16.094084	18.989019	13.472131
O	18.358171	18.405779	1.339906
O	17.960735	18.828434	3.926840
O	15.431355	18.813908	3.174716
O	12.439868	3.151007	3.098432
O	13.839005	2.896896	0.933464
O	16.251257	2.810336	13.039994
O	18.203802	3.471779	1.293199
O	17.684431	2.908836	3.848817
O	15.102995	3.483519	3.250597
O	14.095488	1.100415	2.846430
O	18.270075	0.988383	2.175942
O	11.418947	17.339193	5.345037
O	11.671624	0.085964	5.849576
O	12.441470	2.720989	5.773962
O	16.261269	17.162689	5.020767
O	16.183582	19.740406	5.610422
O	15.765523	2.487574	5.611091
O	0.266092	19.318745	3.022149
O	0.160977	2.733327	2.928066
O	17.195093	1.175036	10.395246
O	16.365381	1.233340	7.865190
O	14.027613	0.756162	6.687084
O	11.840409	1.501579	8.025785
O	12.089083	1.142402	10.626504

O	14.588630	1.082307	9.777888
O	17.439362	16.653473	9.870364
O	16.190390	16.847090	7.623894
O	13.861430	17.094833	6.286664
O	11.678832	16.490898	7.790914
O	12.183587	16.590591	10.375037
O	14.750607	16.671780	9.790869
O	16.108900	18.897085	9.365825
O	11.936114	18.912607	8.952559
O	18.688534	2.575925	12.125266
O	18.356369	19.919695	12.553388
O	17.855219	17.320488	12.379677
O	13.767527	2.987437	11.451431
O	14.020805	0.490112	12.304330
O	13.853621	17.421972	12.280910
O	9.830201	0.590602	9.540741
O	9.846820	17.414610	9.450674
O	7.252969	8.946989	9.785784
O	5.850629	8.631589	12.042292
O	3.908895	9.031758	0.491290
O	2.078083	8.468418	11.956774
O	2.090497	9.116926	9.363282
O	4.649709	9.532218	9.855643
O	7.261579	13.517192	10.196107
O	6.157766	13.269250	12.482726
O	3.875859	12.691582	0.410457
O	1.836618	13.425258	12.200612
O	2.159173	13.088767	9.548369
O	4.659720	13.009768	10.281624
O	6.352580	11.102249	11.042849
O	1.674640	10.988029	11.210806
O	8.584632	7.550477	7.946424
O	8.336160	10.192864	7.609173
O	7.673431	12.782124	7.453126
O	3.841821	7.382330	8.438785
O	3.662624	9.780358	7.365602
O	3.932321	12.434288	7.694690
O	19.857418	9.120110	10.537506
O	19.837597	12.773368	10.543530
O	2.905793	10.952608	2.756095
O	3.754525	11.357553	5.270493
O	5.930116	10.864058	6.772333
O	8.085685	11.441328	5.272501
O	7.938523	10.859084	2.674994

O	5.432369	10.684967	3.349497
O	2.831111	6.543587	3.343609
O	3.769742	6.788942	5.792029
O	6.101905	7.132000	7.028083
O	8.177385	6.464588	5.513394
O	7.917900	6.878488	2.849107
O	5.424160	6.965048	3.690095
O	3.667029	8.897440	4.193830
O	8.251065	8.919329	4.525060
O	1.340073	12.434687	1.242745
O	1.434176	9.841448	0.746504
O	2.004402	7.220949	0.905360
O	6.247665	12.609001	1.671938
O	6.257075	10.111479	0.824794
O	5.935922	7.464712	1.078135
O	10.187995	10.616913	3.852297
O	10.246659	7.212790	4.009413
O	9.005695	15.081851	8.614637
O	3.835814	14.881666	8.533001
O	5.329656	14.913107	0.926505
O	2.411850	14.824556	1.006000
O	1.085993	5.033651	1.996208
O	6.173383	5.060913	1.998082
O	4.587641	5.054943	7.693485
O	7.687447	5.052953	7.694824
O	11.590536	5.029075	4.759129
O	16.426249	4.961020	4.997881
O	14.855522	5.191649	12.877391
O	17.694641	5.046187	12.625656
O	18.857719	15.076875	11.542169
O	13.921897	14.913704	11.541901
O	15.354470	14.967232	5.948208
O	12.419446	14.903556	5.772891
H	16.225628	1.852199	13.251981
H	6.037835	3.628782	17.846365
H	3.812789	17.727024	14.869986
H	9.875651	15.084437	8.154530
H	17.461586	13.026880	18.819845
H	12.815481	18.228081	14.655322
Pt	8.734797	3.375268	14.594162

296

### Pt<sub>2</sub>@H-MFI

Si	8.445680	1.083501	8.777776
Si	6.060258	0.540059	10.826579

Si	5.527473	1.165683	0.365891
Si	2.329760	1.365867	0.205429
Si	1.357492	0.529910	10.828320
Si	3.602158	1.188766	8.988023
Si	8.509350	16.661831	9.040886
Si	6.140947	17.205471	10.972722
Si	5.488030	16.465031	0.585640
Si	1.443186	17.343967	10.878238
Si	3.742512	16.413094	9.052261
Si	1.507456	18.834005	2.074231
Si	3.946336	19.287903	4.059465
Si	4.378811	18.721178	6.975621
Si	7.553700	18.627056	6.856111
Si	8.666522	19.368692	4.142574
Si	6.417651	18.698095	2.309906
Si	1.513263	3.495060	2.328910
Si	4.541590	3.482325	7.310999
Si	7.587537	3.507398	7.252382
Si	8.684942	2.571150	4.466978
Si	6.661920	3.497448	2.198158
Si	11.561503	10.931517	4.640154
Si	14.053041	10.627856	2.667767
Si	14.447074	11.150604	13.099415
Si	17.672617	11.343425	13.230300
Si	18.683729	10.514433	2.640734
Si	11.691647	6.631939	4.451721
Si	14.090882	7.458145	2.514130
Si	14.790251	6.760287	13.022863
Si	17.788946	6.585176	13.224144
Si	18.757811	7.433670	2.612094
Si	16.415236	6.506973	4.421074
Si	18.516344	8.883312	11.422391
Si	16.217619	9.503165	9.402762
Si	15.693643	8.818242	6.502532
Si	12.510346	8.636763	6.615351
Si	11.444174	9.424564	9.325809
Si	13.741499	8.859035	11.140411
Si	18.549381	13.518983	11.197958
Si	16.214014	12.668500	9.321394
Si	15.457785	13.463066	6.426517
Si	12.439868	13.344070	6.276494
Si	11.426555	12.494781	9.140590
Si	13.675026	13.394813	11.008990
Si	11.565108	18.835400	4.725671

Si	14.013798	19.420628	2.807754
Si	17.639181	18.647949	13.281557
Si	18.735186	19.370483	2.594027
Si	16.480106	18.666456	4.440480
Si	11.712870	3.452676	4.505253
Si	13.887259	2.704274	2.495528
Si	17.812571	3.519735	13.116277
Si	18.624063	2.538516	2.578235
Si	16.256863	3.470585	4.410903
Si	18.470896	1.120513	11.379432
Si	16.032015	0.632788	9.369706
Si	15.602944	1.113548	6.438963
Si	12.510746	1.309155	6.566905
Si	11.418546	0.601945	9.266925
Si	13.592936	1.447055	11.079652
Si	18.516344	16.597755	11.087013
Si	16.123716	17.302380	9.197600
Si	15.403925	16.596363	6.262977
Si	12.383206	16.451696	6.332435
Si	11.485821	17.415804	9.189972
Si	13.715871	16.447319	11.040440
Si	8.456491	9.007879	8.722103
Si	6.009002	9.568832	10.698638
Si	5.496239	8.798343	0.246916
Si	2.358592	8.632585	0.175451
Si	1.409749	9.430335	10.799412
Si	3.578532	8.964898	8.767070
Si	6.118723	12.714068	10.969377
Si	5.374105	13.337305	0.511364
Si	2.360994	13.361780	0.371111
Si	1.396535	12.562836	10.894565
Si	3.681245	13.332727	9.026700
Si	1.499448	10.974497	1.933174
Si	3.926514	10.462695	3.917204
Si	4.332360	11.147618	6.790936
Si	7.492032	11.341833	6.792408
Si	8.599249	10.453741	4.106975
Si	6.434070	11.063844	2.129102
Si	1.564719	6.550950	2.324627
Si	3.951341	7.269901	4.249370
Si	4.561011	6.597911	7.213571
Si	7.635189	6.578013	7.054982
Si	8.646901	7.379942	4.246292
Si	6.387618	6.590947	2.370531

Al	2.143555	16.394787	0.412866
Al	3.936125	2.679002	4.247631
Al	16.456081	11.164534	4.464435
Al	14.469899	18.892906	12.962373
Al	14.491323	3.559334	12.884751
Al	8.374201	13.311038	8.929807
O	7.251167	1.084098	9.865814
O	6.253071	1.238116	12.289342
O	3.927916	1.075740	0.241563
O	1.831613	1.495012	12.048313
O	2.070875	0.993557	9.451476
O	4.586239	0.911175	10.270248
O	7.501041	16.582832	10.287245
O	6.164173	16.810675	12.545627
O	3.919306	17.167265	0.672362
O	1.839221	16.423441	12.116300
O	2.250873	16.834951	9.537127
O	4.822098	16.585617	10.284300
O	6.179190	18.818684	10.870744
O	1.827008	18.910418	11.201973
O	8.598248	2.569757	8.120403
O	8.261678	19.891638	7.589901
O	7.837611	17.249647	7.695091
O	3.755326	2.731735	8.522429
O	3.852433	0.144268	7.764148
O	4.169381	17.335411	7.783955
O	19.785540	0.743029	10.522518
O	19.860222	17.328846	10.538578
O	2.920609	18.659491	2.923383
O	3.664026	18.584473	5.516473
O	5.983975	18.915991	6.767649
O	8.183392	18.409760	5.368323
O	7.941125	18.983646	2.756630
O	5.429766	18.749834	3.591729
O	2.743014	3.479141	3.336114
O	3.929317	3.237965	5.866438
O	6.092294	2.900677	7.364264
O	8.004595	3.404719	5.666094
O	8.093493	3.320745	3.095756
O	5.666026	3.237965	3.675641
O	3.918506	0.973260	4.088908
O	8.259875	1.009874	4.521714
O	1.189907	17.415207	1.414315
O	1.661626	0.078004	0.920081

O	1.915104	2.751435	0.920617
O	6.344171	17.166668	1.755716
O	6.077278	19.719910	1.095532
O	5.827804	2.484589	1.259073
O	10.249262	19.158957	3.839851
O	10.264278	2.730143	4.357772
O	12.693147	10.856297	3.513439
O	13.765325	11.199555	1.176098
O	16.073061	11.111403	13.056188
O	18.110899	11.432174	1.406152
O	18.088875	11.030613	4.018246
O	15.275985	11.447894	3.270136
O	12.697552	7.040067	3.255147
O	13.858627	7.138169	0.934535
O	16.327940	7.301938	13.301899
O	18.505533	6.485681	1.298686
O	17.921692	6.809040	3.862200
O	15.347263	6.632337	3.177392
O	14.431457	9.035339	2.683024
O	18.277884	8.955346	2.264939
O	11.525264	12.448417	5.278790
O	11.759321	9.870302	5.856669
O	12.192397	7.229904	5.866304
O	16.520351	12.853162	5.260992
O	16.178175	10.130979	5.771285
O	16.022005	7.449987	5.680682
O	0.255681	10.688350	2.912007
O	0.326158	7.380340	3.005019
O	17.200098	8.783021	10.472599
O	16.425648	8.776653	7.968238
O	14.084876	8.945198	6.695515
O	11.921899	8.455085	8.112775
O	12.176379	8.944004	10.697835
O	14.663912	9.367852	9.884015
O	17.332844	13.515997	10.117013
O	16.270878	13.189257	7.774720
O	14.004188	12.767796	6.272345
O	11.846216	13.349643	7.783285
O	12.181584	13.256714	10.381327
O	14.697349	13.008971	9.790735
O	16.598238	11.098866	9.368234
O	11.927305	10.950220	8.954700
O	18.697945	7.465110	12.208776
O	18.434256	10.120035	12.474295

O	18.097284	12.767398	12.559678
O	14.182784	7.375564	11.630229
O	13.865636	9.790109	12.455559
O	13.925502	12.449610	12.289342
O	9.838010	9.283281	9.544220
O	9.857431	12.590894	9.369038
O	12.831900	18.808535	3.703879
O	13.594537	18.822863	1.260812
O	16.094284	18.997974	13.474006
O	18.358572	18.406178	1.341913
O	17.998775	18.825848	3.936743
O	15.450376	18.814705	3.172440
O	12.442472	3.152599	3.098298
O	13.841408	2.895703	0.933464
O	16.250656	2.812724	13.041600
O	18.203802	3.472376	1.299088
O	17.684231	2.911025	3.850691
O	15.104596	3.485111	3.252738
O	14.097691	1.104195	2.846163
O	18.272276	0.989378	2.177816
O	11.421949	17.338795	5.356947
O	11.674627	0.090540	5.856535
O	12.445674	2.727158	5.770081
O	16.264671	17.165474	5.017555
O	16.185984	19.741400	5.609217
O	15.766924	2.488569	5.612295
O	0.279507	19.321531	3.021079
O	0.169186	2.736311	2.930074
O	17.122814	1.175434	10.458815
O	16.357573	1.233340	7.878572
O	14.027213	0.757953	6.688690
O	11.841210	1.568041	8.025384
O	12.027616	1.162102	10.644170
O	14.524559	1.074944	9.772668
O	17.437559	16.655464	9.870230
O	16.192791	16.923502	7.620950
O	13.860430	17.158907	6.281980
O	11.761323	16.496071	7.852609
O	12.185589	16.674765	10.448644
O	14.750207	16.669790	9.786319
O	16.105095	18.908030	9.373453
O	11.929908	18.968325	8.950015
O	18.686731	2.577318	12.126604
O	18.357971	19.917505	12.556466

O	17.854618	17.321482	12.380614
O	13.764524	2.987039	11.451699
O	13.945122	0.480362	12.309817
O	13.932509	17.415804	12.290010
O	9.815385	0.669402	9.545692
O	9.866641	17.421972	9.455759
O	7.198709	8.949376	9.770260
O	5.843821	8.629003	12.041354
O	3.907894	9.033151	0.493164
O	2.077483	8.469810	11.957710
O	2.084290	9.115533	9.362614
O	4.602257	9.605645	9.868358
O	7.259977	13.513013	10.198381
O	6.156965	13.277410	12.488079
O	3.877661	12.691185	0.413401
O	1.837018	13.424861	12.201549
O	2.159973	13.088964	9.549172
O	4.662923	13.007579	10.282560
O	6.350177	11.100458	11.112307
O	1.674640	10.988228	11.211206
O	8.580829	7.555451	7.950171
O	8.334758	10.193263	7.612117
O	7.673031	12.784112	7.454198
O	3.844825	7.390091	8.443201
O	3.662224	9.780160	7.363862
O	3.932721	12.434487	7.695359
O	19.856018	9.120507	10.539113
O	19.838198	12.773765	10.543395
O	2.843524	10.947434	2.831174
O	3.756127	11.354768	5.273973
O	5.930917	10.864258	6.773271
O	8.084683	11.445308	5.274642
O	7.938723	10.853512	2.680080
O	5.427964	10.691732	3.344813
O	2.827707	6.545378	3.343609
O	3.771744	6.787748	5.794304
O	6.099902	7.134587	7.027413
O	8.177185	6.463195	5.516339
O	7.922305	6.888039	2.856735
O	5.423159	6.800881	3.680191
O	3.753725	8.872566	4.186337
O	8.254470	8.924900	4.586354
O	1.340873	12.433493	1.244887
O	1.435177	9.846224	0.749582

O	2.003802	7.222342	0.905226
O	6.249467	12.609598	1.672474
O	6.257476	10.110483	0.825062
O	5.931117	7.466105	1.085361
O	10.186193	10.616514	3.853100
O	10.244056	7.215377	4.010350
O	9.004694	15.088616	8.615307
O	3.836215	14.880472	8.534072
O	5.332059	14.919474	0.922490
O	2.411850	14.823561	1.005866
O	1.084391	5.036835	1.999956
O	6.340366	5.043998	1.840966
O	4.587040	5.056734	7.695760
O	7.682642	5.062704	7.694690
O	11.591136	5.035243	4.759932
O	16.425447	4.972760	5.005643
O	14.856724	5.192644	12.875918
O	17.695244	5.047381	12.627263
O	18.857519	15.077870	11.541767
O	13.918293	14.914499	11.540028
O	15.346863	15.004443	6.024224
O	12.423651	14.918878	5.780519
H	16.227230	1.861551	13.280085
H	6.091693	3.669774	17.827227
H	3.813190	17.722647	14.874669
H	9.888265	15.079264	8.183036
H	17.445969	13.146275	18.762030
H	12.802867	18.250566	14.663084
Pt	8.921202	2.975697	14.522295
Pt	9.496234	2.196850	12.353045

297

### Pt<sub>3</sub>@H-MFI

Si	8.467303	1.085889	8.788751
Si	6.071471	0.539064	10.832870
Si	5.581933	1.202497	0.406843
Si	2.365599	1.437106	0.226039
Si	1.400539	0.532895	10.841434
Si	3.618976	1.184587	8.995250
Si	8.516758	16.682924	9.052528
Si	6.139746	17.197115	10.976871
Si	5.490633	16.453487	0.588183
Si	1.444387	17.341978	10.874089
Si	3.742913	16.396179	9.048648
Si	1.545498	18.846144	2.061919

Si	3.950341	19.271784	4.068968
Si	4.395430	18.715010	6.980840
Si	7.565713	18.627653	6.860929
Si	8.660316	19.375856	4.152745
Si	6.403837	18.689341	2.312716
Si	1.488836	3.515158	2.334129
Si	4.532380	3.474565	7.330271
Si	7.591942	3.500831	7.216917
Si	8.669926	2.571548	4.405818
Si	6.575025	3.485708	2.456048
Si	11.555496	10.921765	4.640689
Si	14.050438	10.626663	2.667098
Si	14.443670	11.153588	13.096604
Si	17.670416	11.344221	13.230969
Si	18.684530	10.519607	2.641269
Si	11.636186	6.653430	4.449981
Si	14.079670	7.464513	2.557090
Si	14.766025	6.712331	13.008677
Si	17.756510	6.584181	13.231639
Si	18.718567	7.443619	2.626146
Si	16.407427	6.514733	4.438606
Si	18.514744	8.880725	11.426807
Si	16.219822	9.504359	9.402494
Si	15.686635	8.785807	6.503469
Si	12.505540	8.630992	6.614013
Si	11.442372	9.422575	9.325409
Si	13.742099	8.858239	11.138002
Si	18.549782	13.520575	11.199697
Si	16.211813	12.670291	9.327415
Si	15.454381	13.463265	6.437892
Si	12.436064	13.348846	6.273148
Si	11.423752	12.492393	9.137511
Si	13.664014	13.406553	11.009927
Si	11.551893	18.860472	4.758460
Si	13.994977	19.443710	2.882297
Si	17.653597	18.648548	13.310331
Si	18.771826	19.383417	2.594428
Si	16.485313	18.672028	4.434859
Si	11.687642	3.498642	4.497357
Si	13.927103	2.670645	2.518145
Si	17.767122	3.510582	13.102894
Si	18.620058	2.542495	2.559633
Si	16.272079	3.456854	4.390427
Si	18.501129	1.126880	11.372473

Si	16.087877	0.643136	9.358465
Si	15.627371	1.117926	6.437491
Si	12.527564	1.357510	6.559811
Si	11.438768	0.600751	9.257021
Si	13.666416	1.448448	11.028529
Si	18.513943	16.602135	11.089689
Si	16.120712	17.320290	9.215668
Si	15.400722	16.618252	6.275958
Si	12.363384	16.456871	6.342338
Si	11.481215	17.433115	9.164143
Si	13.704057	16.484133	11.050879
Si	8.455891	9.008277	8.721969
Si	6.011605	9.572016	10.703054
Si	5.500844	8.791180	0.251734
Si	2.361795	8.629997	0.181072
Si	1.408147	9.424366	10.812261
Si	3.577931	8.955147	8.788081
Si	6.122928	12.719242	11.001362
Si	5.353482	13.327157	0.543751
Si	2.349782	13.363770	0.378739
Si	1.387525	12.543534	10.927755
Si	3.678842	13.313028	9.057213
Si	1.501650	10.972905	1.936252
Si	3.911298	10.449960	3.936610
Si	4.326954	11.110009	6.807664
Si	7.490430	11.346411	6.796422
Si	8.586034	10.461502	4.110990
Si	6.416450	11.045537	2.147570
Si	1.539291	6.567466	2.343230
Si	3.888072	7.284228	4.306114
Si	4.555605	6.601493	7.267906
Si	7.621974	6.574232	7.077332
Si	8.589638	7.411383	4.282159
Si	6.339365	6.599901	2.409609
Al	2.164779	16.391205	0.401089
Al	3.829407	2.645572	4.324850
Al	16.454880	11.160355	4.456807
Al	14.531967	18.918377	12.992752
Al	14.388410	3.521327	12.931859
Al	8.368996	13.312829	8.941986
O	7.254571	1.083501	9.865948
O	6.258476	1.235728	12.303125
O	3.992387	1.404073	0.332701
O	1.916306	1.493619	12.048983

O	2.083689	0.990174	9.447997
O	4.592046	0.910379	10.283631
O	7.500641	16.585220	10.289654
O	6.166976	16.746998	12.538400
O	3.925914	17.165075	0.669016
O	1.839621	16.421251	12.111883
O	2.252675	16.832165	9.534451
O	4.819496	16.583826	10.282293
O	6.178789	18.813709	10.877568
O	1.833214	18.905045	11.205318
O	8.592241	2.571747	8.109028
O	8.261878	19.892235	7.598198
O	7.840014	17.245867	7.696831
O	3.759931	2.730143	8.543038
O	3.919306	0.155212	7.772043
O	4.168781	17.330238	7.785427
O	19.835594	0.749396	10.539515
O	19.860022	17.329443	10.539380
O	2.935025	18.655712	2.928334
O	3.664827	18.581686	5.526108
O	5.994987	18.909224	6.765374
O	8.183592	18.403988	5.367921
O	7.930514	18.995584	2.754355
O	5.433570	18.745056	3.602570
O	2.736807	3.475957	3.326345
O	3.834013	3.161553	5.941918
O	6.085687	2.901871	7.288114
O	7.935319	3.404918	5.599447
O	8.073872	3.163941	3.002610
O	5.589942	3.231001	3.846408
O	3.913901	0.956545	4.088774
O	8.266883	1.002114	4.593983
O	1.248772	17.422371	1.413646
O	1.758332	0.094321	0.915665
O	1.834616	2.807152	0.902416
O	6.347374	17.161297	1.755181
O	5.923308	19.655636	1.090045
O	6.175385	2.409968	1.334018
O	10.247459	19.162539	3.839449
O	10.265679	2.723974	4.355096
O	12.686339	10.783667	3.515313
O	13.763923	11.198760	1.175830
O	16.069456	11.111403	13.056456
O	18.109900	11.434960	1.405884

O	18.089876	11.035787	4.018513
O	15.270378	11.450283	3.268530
O	12.687340	7.045838	3.274686
O	13.837004	7.140756	0.944438
O	16.279488	7.294376	13.299758
O	18.427248	6.479314	1.332545
O	17.911480	6.888238	3.927777
O	15.346262	6.636714	3.179533
O	14.435661	9.033548	2.678072
O	18.272276	8.965096	2.260255
O	11.530269	12.444436	5.272367
O	11.757519	9.869904	5.861353
O	12.191195	7.228511	5.861353
O	16.515347	12.851371	5.265006
O	16.179577	10.045812	5.691790
O	16.011993	7.372181	5.756564
O	0.256282	10.687554	2.913212
O	0.282711	7.381932	3.000736
O	17.200298	8.782424	10.473001
O	16.426849	8.784016	7.965428
O	14.082072	8.943805	6.696720
O	11.922099	8.454090	8.114113
O	12.177179	8.943008	10.699709
O	14.665714	9.365664	9.885220
O	17.334045	13.516196	10.118083
O	16.273081	13.183684	7.779270
O	14.002986	12.769189	6.270873
O	11.846016	13.348051	7.781144
O	12.176779	13.253531	10.378517
O	14.695346	13.014344	9.796222
O	16.597437	11.099662	9.369706
O	11.927305	10.948231	8.954967
O	18.686333	7.462125	12.220284
O	18.433054	10.120432	12.475098
O	18.096283	12.767596	12.560615
O	14.179580	7.367804	11.630229
O	13.863633	9.787125	12.456362
O	13.924900	12.454387	12.287601
O	9.837409	9.283281	9.545157
O	9.855629	12.589103	9.367966
O	12.841710	18.738491	3.761426
O	13.583124	18.989616	1.275534
O	16.118309	18.983646	13.627374
O	18.441063	18.406178	1.339237

O	18.000778	18.888927	3.937279
O	15.442367	18.821270	3.171370
O	12.509345	3.311194	3.087592
O	13.851419	2.655124	0.942699
O	16.197197	2.817301	13.040128
O	18.197596	3.469789	1.278478
O	17.698446	2.905254	3.847613
O	15.177677	3.478942	3.171905
O	14.008593	1.132253	3.099503
O	18.277884	0.989577	2.173131
O	11.358080	17.396502	5.450093
O	11.674227	0.157998	5.842751
O	12.510547	2.738898	5.688980
O	16.264671	17.167265	5.015948
O	16.181980	19.738615	5.604533
O	15.772130	2.495932	5.604667
O	0.322554	19.329491	3.016261
O	0.162979	2.737904	2.933955
O	17.202101	1.240703	10.390294
O	16.437862	1.162102	7.849665
O	14.046233	0.826207	6.696318
O	11.845216	1.584358	8.016551
O	12.116914	1.072556	10.632526
O	14.596639	1.163893	9.696920
O	17.436960	16.653872	9.869963
O	16.188787	17.006283	7.621886
O	13.848617	17.159506	6.279438
O	11.758120	16.432396	7.872416
O	12.184188	16.751177	10.452926
O	14.750207	16.666805	9.791806
O	16.107698	18.917183	9.462852
O	11.930308	18.969717	8.862759
O	18.681126	2.580701	12.131289
O	18.347361	19.916512	12.546295
O	17.850014	17.328051	12.384495
O	13.758718	2.985646	11.446614
O	14.184185	0.494291	12.217073
O	13.935913	17.478287	12.285728
O	9.839211	0.667810	9.537529
O	9.859834	17.485052	9.449067
O	7.198309	8.949973	9.771999
O	5.844422	8.627411	12.043363
O	3.910697	9.031559	0.494502
O	2.079485	8.461055	11.962931

O	2.080486	9.121901	9.369573
O	4.603658	9.611018	9.872908
O	7.255773	13.512218	10.209087
O	6.166576	13.263878	12.535723
O	3.857238	12.687802	0.413802
O	1.832614	13.428044	12.211452
O	2.166180	13.088169	9.607522
O	4.672133	13.009171	10.301832
O	6.351178	11.102050	11.117393
O	1.668633	10.970717	11.277586
O	8.584032	7.554854	7.950974
O	8.334758	10.194258	7.612652
O	7.672630	12.789286	7.460353
O	3.846026	7.373972	8.516406
O	3.669031	9.716881	7.355698
O	3.926915	12.355091	7.770304
O	19.854416	9.118518	10.541521
O	19.837196	12.769587	10.547143
O	2.846928	10.947634	2.833984
O	3.758530	11.355762	5.288694
O	5.930516	10.862467	6.774475
O	8.082881	11.456650	5.279192
O	7.931915	10.859282	2.679277
O	5.420556	10.605769	3.350836
O	2.748620	6.547766	3.425647
O	3.761333	6.793320	5.854795
O	6.092895	7.138368	7.109451
O	8.098098	6.466180	5.520086
O	7.842217	6.952711	2.912409
O	5.344272	6.876697	3.679121
O	3.667230	8.881720	4.267170
O	8.178386	8.953754	4.599202
O	1.335868	12.431901	1.249704
O	1.437379	9.844036	0.752392
O	2.004803	7.221546	0.919546
O	6.170780	12.603032	1.750095
O	6.257275	10.110483	0.825463
O	5.929515	7.448992	1.084692
O	10.177382	10.614126	3.854973
O	10.191798	7.293979	4.089310
O	9.013704	15.094386	8.687306
O	3.834814	14.854604	8.534740
O	5.324050	14.913306	0.932795
O	2.411049	14.824556	1.009212

O	1.078785	5.052953	2.005041
O	6.265284	4.995246	1.996476
O	4.586840	5.048376	7.698839
O	7.684443	5.051162	7.691880
O	11.511048	5.061709	4.779203
O	16.429251	4.965994	4.941539
O	14.851918	5.140310	12.965050
O	17.688034	5.049571	12.626995
O	18.856920	15.079861	11.542436
O	13.847216	14.933404	11.542035
O	15.348664	15.015985	6.100641
O	12.421448	14.924648	5.775969
H	16.173971	1.846229	13.179579
H	6.113317	3.385019	18.052328
H	3.817995	17.716677	14.873064
H	9.892069	15.078070	8.242590
H	17.444969	13.126177	18.782640
H	12.657308	18.681379	14.598980
Pt	8.647702	2.476629	14.425135
Pt	8.575222	3.607689	12.221490
Pt	10.090287	1.668929	12.535187

298

#### Pt<sub>4</sub>@H-MFI

Si	8.458694	1.024202	8.781925
Si	6.063262	0.537273	10.828320
Si	5.514259	1.174041	0.356389
Si	2.328558	1.367061	0.202217
Si	1.365901	0.530507	10.828721
Si	3.605561	1.172449	8.984409
Si	8.499539	16.637753	9.053332
Si	6.132739	17.197910	10.981956
Si	5.485427	16.459457	0.593135
Si	1.445388	17.344366	10.876766
Si	3.740710	16.396776	9.050789
Si	1.500449	18.836195	2.076372
Si	3.926114	19.303225	4.061473
Si	4.384818	18.700882	6.970536
Si	7.551697	18.564375	6.857316
Si	8.656912	19.324318	4.175229
Si	6.412446	18.714413	2.310709
Si	1.489637	3.487897	2.338010
Si	4.547596	3.469391	7.330538
Si	7.599550	3.485111	7.262954
Si	8.667323	2.494141	4.513016

Si	6.636892	3.511378	2.176343
Si	11.560903	10.927935	4.639083
Si	14.062852	10.645567	2.672585
Si	14.464493	11.157569	13.103162
Si	17.683630	11.344817	13.230434
Si	18.694740	10.501498	2.628957
Si	11.687441	6.621392	4.451721
Si	14.088280	7.464911	2.510919
Si	14.759617	6.753522	13.003994
Si	17.746300	6.575426	13.187207
Si	18.745996	7.420934	2.575023
Si	16.422646	6.506177	4.398993
Si	18.514343	8.882117	11.418911
Si	16.218420	9.502568	9.391253
Si	15.700251	8.805307	6.475097
Si	12.514952	8.633579	6.612808
Si	11.451982	9.426753	9.323668
Si	13.741899	8.865005	11.138136
Si	18.553988	13.517987	11.196486
Si	16.216217	12.670688	9.318450
Si	15.478607	13.460480	6.404033
Si	12.458088	13.332131	6.267795
Si	11.466999	12.498363	9.136842
Si	13.685037	13.401977	11.015146
Si	11.563705	18.836990	4.721523
Si	14.007992	19.414261	2.785939
Si	17.640182	18.644766	13.280889
Si	18.724173	19.389784	2.577298
Si	16.463890	18.673620	4.440613
Si	11.685039	3.430985	4.568689
Si	13.848617	2.704672	2.510116
Si	17.685432	3.516949	13.085496
Si	18.587624	2.545878	2.527380
Si	16.250854	3.457252	4.371825
Si	18.479704	1.116334	11.378361
Si	16.090279	0.623436	9.329959
Si	15.631576	1.123299	6.436688
Si	12.536574	1.290251	6.578414
Si	11.429358	0.531104	9.274820
Si	13.653401	1.435713	11.007518
Si	18.518948	16.597357	11.086612
Si	16.128922	17.296610	9.191176
Si	15.408530	16.576067	6.252806
Si	12.367390	16.423840	6.311690

Si	11.460993	17.356108	9.149155
Si	13.698652	16.447319	11.012336
Si	8.478716	9.004497	8.709255
Si	6.050448	9.508936	10.717107
Si	5.519464	8.778842	0.233266
Si	2.380415	8.619452	0.143332
Si	1.407747	9.424962	10.799814
Si	3.590145	8.957734	8.773092
Si	6.100103	12.632682	10.990789
Si	5.334861	13.333524	0.512837
Si	2.340572	13.368347	0.371244
Si	1.395734	12.535773	10.909019
Si	3.680043	13.299696	9.033391
Si	1.530281	10.966339	1.910691
Si	3.910096	10.447373	3.919881
Si	4.331960	11.143640	6.786654
Si	7.491431	11.342430	6.790534
Si	8.594844	10.455532	4.102961
Si	6.412646	11.046134	2.131778
Si	1.578735	6.545975	2.287824
Si	3.905892	7.300745	4.286575
Si	4.564615	6.590151	7.235653
Si	7.637992	6.567267	7.065823
Si	8.642296	7.377953	4.250174
Si	6.343971	6.621989	2.428211
Al	2.140552	16.400358	0.412732
Al	3.900886	2.684375	4.268240
Al	16.468294	11.183040	4.433654
Al	14.478108	18.920567	12.931324
Al	14.290702	3.631369	12.796289
Al	8.392822	13.265470	8.940379
O	7.256773	1.079720	9.866616
O	6.260479	1.239310	12.288405
O	3.923711	1.070367	0.165682
O	1.826207	1.497997	12.047913
O	2.073078	0.991965	9.450540
O	4.589643	0.908588	10.270516
O	7.492232	16.579649	10.294337
O	6.165774	16.747993	12.542280
O	3.919507	17.167664	0.672228
O	1.839221	16.423243	12.115764
O	2.251474	16.832365	9.535655
O	4.816292	16.583826	10.283899
O	6.178989	18.812117	10.876097

O	1.828609	18.909025	11.202508
O	8.600650	2.512249	8.115452
O	8.263880	19.815823	7.606496
O	7.829402	17.177214	7.688400
O	3.756127	2.720591	8.533268
O	3.845425	0.098500	7.780208
O	4.169982	17.321085	7.783955
O	19.796152	0.745218	10.526801
O	19.861223	17.329044	10.538176
O	2.917406	18.655712	2.921241
O	3.666228	18.579895	5.513662
O	5.990582	18.906040	6.768319
O	8.182791	18.322403	5.369795
O	7.940725	18.990015	2.765195
O	5.430167	18.822266	3.591194
O	2.662325	3.478942	3.408249
O	3.921909	3.164936	5.913547
O	6.098701	2.898289	7.371624
O	8.007399	3.402331	5.672920
O	8.013605	3.068426	3.105927
O	5.593746	3.233588	3.679121
O	3.835014	0.980225	4.090246
O	8.264481	0.930676	4.682712
O	1.184902	17.416401	1.415118
O	1.663228	0.078601	0.921286
O	1.919309	2.748848	0.930119
O	6.340767	17.175623	1.758928
O	6.078879	19.728466	1.089109
O	5.757526	2.489962	1.261080
O	10.243455	19.155972	3.841590
O	10.261676	2.655720	4.437401
O	12.695549	10.856098	3.513707
O	13.766927	11.198760	1.173957
O	16.086275	11.116179	13.058195
O	18.113503	11.432373	1.407356
O	18.103891	11.028026	4.008476
O	15.267376	11.513362	3.266924
O	12.694749	7.038277	3.255013
O	13.851219	7.131006	0.933330
O	16.286095	7.305520	13.292130
O	18.436657	6.475134	1.272590
O	17.930099	6.811030	3.852431
O	15.342658	6.636316	3.170299
O	14.432657	9.044294	2.683961

O	18.271074	8.950769	2.260121
O	11.525864	12.443840	5.280798
O	11.760122	9.868113	5.856401
O	12.190595	7.225924	5.863628
O	16.585823	12.850377	5.267951
O	16.171768	10.105110	5.700891
O	16.019402	7.402030	5.690452
O	0.275302	10.618106	2.852587
O	0.323355	7.380738	2.926594
O	17.197697	8.784214	10.466577
O	16.428251	8.785409	7.949904
O	14.090483	8.943407	6.692035
O	11.924502	8.454090	8.111034
O	12.176379	8.951565	10.701448
O	14.666115	9.364072	9.879465
O	17.335848	13.515401	10.115674
O	16.270678	13.193832	7.769902
O	14.021606	12.764413	6.264716
O	11.922099	13.347255	7.791851
O	12.190994	13.256117	10.394443
O	14.701153	13.010762	9.792743
O	16.598038	11.100060	9.365959
O	11.935113	10.947434	8.952156
O	18.689535	7.465508	12.207973
O	18.436058	10.119040	12.472154
O	18.099686	12.768990	12.558474
O	14.107500	7.365615	11.631968
O	13.932108	9.782946	12.453150
O	13.927503	12.449213	12.291483
O	9.848021	9.284475	9.542615
O	9.903281	12.592485	9.362078
O	12.832100	18.817291	3.695314
O	13.592735	18.821072	1.243548
O	16.093483	18.987028	13.473470
O	18.357370	18.402397	1.341110
O	17.959734	18.902260	3.926037
O	15.438163	18.817291	3.171102
O	12.445875	3.143644	3.175920
O	13.607351	2.986840	0.926505
O	16.098888	2.828842	13.042269
O	18.111700	3.477549	1.264827
O	17.682829	2.901473	3.838111
O	15.112405	3.477947	3.172842
O	14.098492	1.104792	2.754088

O	18.272276	0.994154	2.102335
O	11.424353	17.339989	5.348917
O	11.682636	0.090142	5.852520
O	12.510145	2.719596	5.784936
O	16.264671	17.170250	5.014476
O	16.183783	19.741598	5.610689
O	15.764522	2.496330	5.597440
O	0.264290	19.321135	3.018134
O	0.126139	2.743077	2.911204
O	17.186283	1.171255	10.392435
O	16.433456	1.234932	7.852208
O	14.061450	0.758749	6.694713
O	11.843413	1.497002	8.028194
O	12.098494	1.069571	10.631857
O	14.585426	1.076337	9.702006
O	17.439562	16.652477	9.869160
O	16.190390	16.916140	7.613455
O	13.855424	17.101002	6.290813
O	11.678632	16.430605	7.799479
O	12.182786	16.586414	10.373163
O	14.757014	16.667801	9.782840
O	16.109501	18.900866	9.369305
O	11.934914	18.897484	8.942655
O	18.599836	2.574931	12.127809
O	18.356569	19.909945	12.550042
O	17.854218	17.318298	12.379542
O	13.769931	2.997187	11.298197
O	14.102295	0.573887	12.299245
O	13.850818	17.496593	12.210917
O	9.828599	0.595975	9.542883
O	9.852225	17.414412	9.453484
O	7.256373	8.948978	9.782840
O	5.923708	8.547217	12.046307
O	3.927916	9.029967	0.415408
O	2.076081	8.456876	11.938573
O	2.091498	9.123095	9.364085
O	4.662523	9.531024	9.865145
O	7.266184	13.361979	10.201593
O	6.090893	13.273031	12.477640
O	3.843623	12.688000	0.414605
O	1.833414	13.426453	12.197267
O	2.162376	13.013746	9.547433
O	4.658518	12.926589	10.277475
O	6.342169	11.028623	11.199564

O	1.668433	10.966339	11.278255
O	8.590038	7.550477	7.947093
O	8.336961	10.194058	7.609842
O	7.678037	12.783516	7.453126
O	3.838217	7.384121	8.449492
O	3.664226	9.779164	7.369750
O	3.934723	12.431105	7.687195
O	19.854614	9.120507	10.536571
O	19.842001	12.769985	10.543395
O	2.910197	10.950818	2.760378
O	3.756728	11.357354	5.269021
O	5.931517	10.863660	6.771932
O	8.084683	11.445308	5.273036
O	7.929112	10.857889	2.677403
O	5.427563	10.602983	3.348828
O	2.829108	6.547567	3.337854
O	3.765738	6.787350	5.827092
O	6.106309	7.133394	7.098477
O	8.173381	6.463394	5.520354
O	7.913495	6.886845	2.856735
O	5.425762	6.967038	3.747642
O	3.594950	8.889679	4.263556
O	8.255470	8.925299	4.584079
O	1.333065	12.432896	1.248099
O	1.499848	9.845030	0.732585
O	2.009208	7.207020	0.852497
O	6.178188	12.592883	1.686124
O	6.259678	10.104115	0.815159
O	5.934320	7.459737	1.096603
O	10.184589	10.616117	3.851494
O	10.240851	7.212591	4.007941
O	9.005695	15.060160	8.687306
O	3.833812	14.853012	8.546919
O	5.328254	14.914499	0.929316
O	2.407645	14.828138	1.006000
O	1.085593	5.032855	1.989115
O	6.175986	5.063102	2.003837
O	4.587641	5.047780	7.697902
O	7.692052	5.049571	7.697768
O	11.579523	5.021711	4.764750
O	16.421644	4.962413	4.935651
O	14.916389	5.191251	12.811546
O	17.684031	5.045789	12.558072
O	18.858320	15.076676	11.541232

O	13.924700	14.924847	11.544845
O	15.353669	14.992305	5.955435
O	12.421849	14.898183	5.765798
H	16.076063	1.847821	13.058597
H	6.050248	3.618036	17.836193
H	3.810587	17.729015	14.870655
H	9.867843	15.056380	8.212880
H	17.517246	13.047576	18.876722
H	12.820086	18.222708	14.637255
Pt	9.761126	5.602961	13.669396
Pt	8.841915	3.340445	14.548392
Pt	9.758322	3.521924	12.189370
Pt	11.703059	3.962289	13.806037

299

### Pt<sub>5</sub>@H-MFI

Si	8.451687	1.061015	8.774162
Si	6.064663	0.540258	10.830997
Si	5.498241	1.162500	0.355319
Si	2.324154	1.357112	0.225905
Si	1.357692	0.535084	10.844379
Si	3.602358	1.189761	8.998060
Si	8.483722	16.647503	9.069927
Si	6.083885	17.201094	10.980484
Si	5.454393	16.456671	0.602770
Si	1.443586	17.345161	10.881048
Si	3.720688	16.399363	9.036336
Si	1.496644	18.827240	2.079451
Si	3.934523	19.309792	4.043272
Si	4.379212	18.729734	6.979770
Si	7.548694	18.573130	6.870297
Si	8.621874	19.348793	4.186604
Si	6.407440	18.702673	2.306962
Si	1.472218	3.467799	2.384181
Si	4.548198	3.472774	7.329602
Si	7.592342	3.508393	7.243683
Si	8.654710	2.528964	4.501640
Si	6.624078	3.488494	2.144894
Si	11.562504	10.933108	4.640020
Si	14.061651	10.647557	2.671916
Si	14.468898	11.158364	13.110522
Si	17.699047	11.344221	13.249973
Si	18.731182	10.498713	2.649299
Si	11.690044	6.631740	4.463097
Si	14.090281	7.469289	2.514264

Si	14.747604	6.736806	13.020589
Si	17.745899	6.576023	13.188813
Si	18.748400	7.422128	2.575425
Si	16.423645	6.507570	4.399260
Si	18.513542	8.883113	11.419312
Si	16.219622	9.503563	9.390450
Si	15.701452	8.804512	6.475766
Si	12.516353	8.640943	6.617358
Si	11.452784	9.424764	9.328486
Si	13.753311	8.860826	11.140277
Si	18.548180	13.514009	11.197690
Si	16.212414	12.672082	9.317379
Si	15.456583	13.467245	6.413803
Si	12.438066	13.344866	6.278100
Si	11.427756	12.486822	9.141392
Si	13.674826	13.399590	11.010997
Si	11.520658	18.835598	4.725403
Si	13.986567	19.400928	2.821672
Si	17.642185	18.642975	13.278747
Si	18.723574	19.387794	2.576897
Si	16.460688	18.673420	4.440480
Si	11.671023	3.438547	4.535097
Si	13.879651	2.662287	2.519751
Si	17.695444	3.518939	13.083220
Si	18.570204	2.541500	2.526711
Si	16.249655	3.458446	4.379587
Si	18.477703	1.115936	11.378093
Si	16.110903	0.590005	9.325274
Si	15.624568	1.120712	6.438294
Si	12.529567	1.286271	6.567039
Si	11.424353	0.609108	9.269200
Si	13.677828	1.408451	10.997079
Si	18.521151	16.585020	11.087682
Si	16.146742	17.259995	9.190641
Si	15.402123	16.579050	6.249460
Si	12.382005	16.451897	6.321728
Si	11.463997	17.424360	9.160262
Si	13.696049	16.454285	11.011399
Si	8.475913	8.996737	8.712467
Si	6.057255	9.520279	10.695694
Si	5.495638	8.793766	0.251600
Si	2.366801	8.579453	0.162336
Si	1.410149	9.410635	10.795130
Si	3.591947	8.955346	8.767203

Si	6.116120	12.653376	10.974328
Si	5.338065	13.331733	0.513104
Si	2.328158	13.330739	0.333772
Si	1.387525	12.529605	10.877301
Si	3.683447	13.301088	9.028841
Si	1.528880	10.922761	1.906141
Si	3.923311	10.461303	3.906096
Si	4.332360	11.142843	6.783308
Si	7.492032	11.341038	6.790802
Si	8.599048	10.457323	4.096135
Si	6.428864	11.066232	2.127763
Si	1.569525	6.515331	2.286887
Si	3.925714	7.286417	4.246426
Si	4.558208	6.593334	7.206880
Si	7.633187	6.574629	7.052172
Si	8.641495	7.368998	4.233846
Si	6.363592	6.599901	2.391676
Al	2.121131	16.367327	0.422100
Al	3.898484	2.684375	4.267437
Al	16.465693	11.179258	4.432048
Al	14.478308	18.896887	12.949257
Al	14.303116	3.561125	12.826267
Al	8.381809	13.278603	8.939844
O	7.254170	1.082108	9.864743
O	6.257676	1.240106	12.292286
O	3.910697	0.995746	0.158053
O	1.753727	1.501181	12.093147
O	2.071276	0.994950	9.463655
O	4.588642	0.910777	10.276404
O	7.436371	16.577858	10.283363
O	6.092294	16.747396	12.537730
O	3.897883	17.166470	0.683068
O	1.838620	16.422644	12.118976
O	2.239260	16.833759	9.532845
O	4.760631	16.589598	10.291527
O	6.175986	18.813709	10.875695
O	1.828009	18.911413	11.203578
O	8.597246	2.558216	8.114648
O	8.266482	19.827364	7.612786
O	7.830204	17.181992	7.692281
O	3.755727	2.731934	8.536881
O	3.852433	0.147452	7.773115
O	4.166978	17.333025	7.779136
O	19.790346	0.743825	10.522920

O	19.858019	17.328247	10.539648
O	2.915003	18.651134	2.920171
O	3.663225	18.653522	5.519952
O	5.987579	18.908827	6.771665
O	8.178987	18.332949	5.382509
O	7.930514	18.992601	2.769210
O	5.422958	18.756599	3.592265
O	2.593450	3.478146	3.501796
O	3.922710	3.157971	5.916357
O	6.100503	2.900478	7.368011
O	8.010402	3.466804	5.652042
O	8.005396	3.073003	3.097897
O	5.588941	3.234185	3.674303
O	3.842021	0.986990	4.007540
O	8.258274	0.966892	4.686727
O	1.181098	17.409039	1.417126
O	1.652816	0.067259	0.927040
O	1.938530	2.728551	0.993822
O	6.340567	17.165873	1.751299
O	6.079480	19.726276	1.093123
O	5.674836	2.488967	1.261883
O	10.200208	19.157364	3.848148
O	10.258872	2.654526	4.435394
O	12.695749	10.856297	3.514911
O	13.761922	11.199157	1.175429
O	16.092682	11.116179	13.135415
O	18.193590	11.433568	1.408695
O	18.103491	11.030414	4.010484
O	15.267376	11.511970	3.264515
O	12.694347	7.038475	3.259028
O	13.846814	7.140955	0.942029
O	16.278687	7.288805	13.294405
O	18.436657	6.475533	1.273125
O	17.930302	6.811229	3.851895
O	15.342458	6.636316	3.171236
O	14.432858	9.046085	2.687173
O	18.277082	8.954550	2.263467
O	11.525064	12.448616	5.279593
O	11.759921	9.869705	5.856535
O	12.194398	7.230500	5.869917
O	16.529562	12.849182	5.261660
O	16.172169	10.102921	5.700623
O	16.019001	7.400637	5.691121
O	0.314746	10.615719	2.921108

O	0.325758	7.375962	2.923249
O	17.197897	8.784613	10.466310
O	16.428852	8.785010	7.949770
O	14.091884	8.944202	6.692437
O	11.924502	8.454687	8.112908
O	12.182786	8.947983	10.704259
O	14.667116	9.365863	9.876788
O	17.330242	13.515003	10.117146
O	16.267473	13.196022	7.768564
O	14.002986	12.768194	6.273416
O	11.844415	13.348846	7.785828
O	12.180183	13.255718	10.381729
O	14.695747	13.010962	9.790869
O	16.597437	11.101254	9.365959
O	11.933912	10.946639	8.953361
O	18.687933	7.465508	12.208776
O	18.433653	10.119040	12.471484
O	18.096684	12.766403	12.560883
O	14.175575	7.370789	11.625679
O	13.935712	9.785334	12.452748
O	13.930507	12.447223	12.289074
O	9.847019	9.282684	9.543685
O	9.854828	12.522242	9.367164
O	12.769031	18.814903	3.680325
O	13.594137	18.829430	1.257868
O	16.094885	18.989616	13.474674
O	18.357170	18.401203	1.340307
O	17.954727	18.903254	3.924565
O	15.430554	18.812714	3.171236
O	12.442270	3.234980	3.093481
O	13.757916	2.734521	0.917940
O	16.114906	2.828643	13.039860
O	18.110100	3.477947	1.264292
O	17.675821	2.901075	3.839315
O	15.110804	3.480733	3.177927
O	14.084275	1.094843	2.932081
O	18.267471	0.990970	2.099659
O	11.417145	17.337801	5.352932
O	11.676029	0.083974	5.856802
O	12.518556	2.662287	5.688846
O	16.266474	17.170649	5.015815
O	16.182180	19.741400	5.611091
O	15.763320	2.495335	5.600919
O	0.261487	19.319540	3.020008

O	0.095705	2.736908	2.923249
O	17.184483	1.172250	10.391499
O	16.430655	1.230156	7.852877
O	14.053041	0.757953	6.697523
O	11.845615	1.571026	8.013875
O	12.098693	1.151754	10.623827
O	14.589631	0.991169	9.701604
O	17.438761	16.578653	9.870899
O	16.193192	16.845898	7.620013
O	13.863232	17.156719	6.280375
O	11.751712	16.497862	7.832401
O	12.184988	16.662428	10.384004
O	14.757814	16.669989	9.783375
O	16.195795	18.868032	9.363817
O	11.927505	18.971109	8.944796
O	18.602840	2.574931	12.126604
O	18.355968	19.910145	12.550712
O	17.853617	17.317104	12.375796
O	13.866635	2.973707	11.276114
O	14.022407	0.508817	12.291216
O	13.854623	17.489630	12.215601
O	9.829200	0.670198	9.539536
O	9.848221	17.419983	9.454020
O	7.251368	8.875551	9.787122
O	5.848826	8.617461	12.049518
O	3.904691	9.023003	0.489952
O	2.081487	8.457274	11.947138
O	2.094101	9.115135	9.360070
O	4.662123	9.534606	9.858186
O	7.260578	13.439785	10.201861
O	6.090492	13.268255	12.473760
O	3.846827	12.683622	0.413669
O	1.842625	13.424861	12.150961
O	2.164178	13.017131	9.533113
O	4.660921	12.924798	10.275200
O	6.421656	11.045139	11.113378
O	1.670636	10.961962	11.215489
O	8.588437	7.548288	7.942543
O	8.332956	10.190080	7.614258
O	7.676235	12.783118	7.452859
O	3.843223	7.382131	8.438651
O	3.663826	9.779364	7.366539
O	3.938928	12.430507	7.684251
O	19.854416	9.117523	10.537239

O	19.831991	12.766999	10.538845
O	2.910197	10.950818	2.752749
O	3.754725	11.353176	5.266746
O	5.931918	10.863063	6.771531
O	8.086485	11.440929	5.273036
O	7.936721	10.860676	2.673790
O	5.433370	10.683972	3.349765
O	2.818697	6.543189	3.331430
O	3.766338	6.788544	5.789620
O	6.099302	7.133791	7.026744
O	8.177785	6.465782	5.513528
O	7.916698	6.880278	2.848036
O	5.418954	6.895800	3.693039
O	3.673036	8.883113	4.187541
O	8.252667	8.919130	4.523989
O	1.329661	12.350513	1.166998
O	1.429771	9.768419	0.753597
O	2.010209	7.140756	0.838177
O	6.237254	12.612384	1.667120
O	6.255473	10.110085	0.824393
O	5.936523	7.463120	1.084023
O	10.188194	10.617311	3.852698
O	10.245658	7.210402	4.008610
O	9.007297	15.071701	8.693998
O	3.833812	14.854803	8.541164
O	5.256576	14.912312	0.927710
O	2.329560	14.774610	1.004394
O	1.079386	5.000021	1.995138
O	6.178188	5.047580	1.983896
O	4.587641	5.053948	7.693218
O	7.684243	5.063301	7.698303
O	11.587933	5.025890	4.781344
O	16.421442	4.963806	4.936855
O	14.777236	5.162000	12.889034
O	17.678225	5.046585	12.557136
O	18.862926	15.068120	11.546719
O	13.911886	14.925445	11.538957
O	15.344661	14.995887	5.950082
O	12.424651	14.917485	5.778646
H	16.104496	1.859363	13.189080
H	6.020014	3.698428	17.800461
H	3.778151	17.725632	14.882833
H	9.874450	15.078666	8.229742
H	17.458984	13.108267	18.808735

H	12.701555	18.431847	14.608882
Pt	11.723481	2.949629	13.309662
Pt	9.498035	5.681164	13.499433
Pt	8.788857	3.305622	14.511054
Pt	9.601749	3.478345	12.103987
Pt	11.127827	4.654376	15.072203
	300		
	Pt <sub>6</sub> @H-MFI		
Si	8.452487	1.056438	8.768676
Si	6.061660	0.536875	10.831129
Si	5.493236	1.162102	0.356122
Si	2.318147	1.357510	0.208507
Si	1.351285	0.529711	10.822966
Si	3.606563	1.189761	8.994045
Si	8.479918	16.641535	9.067785
Si	6.082884	17.199501	10.981421
Si	5.454994	16.456076	0.603841
Si	1.445188	17.343372	10.881048
Si	3.720888	16.397970	9.035532
Si	1.496244	18.829628	2.076372
Si	3.933923	19.307205	4.042335
Si	4.381214	18.727545	6.978030
Si	7.550296	18.569748	6.863739
Si	8.625076	19.350185	4.179913
Si	6.407640	18.703669	2.305757
Si	1.470215	3.469192	2.377089
Si	4.549799	3.473967	7.333349
Si	7.594545	3.501627	7.246894
Si	8.650505	2.531551	4.466175
Si	6.577627	3.502224	2.152789
Si	11.557899	10.927536	4.638949
Si	14.048836	10.626464	2.666161
Si	14.473703	11.158961	13.120560
Si	17.710060	11.345613	13.262152
Si	18.746998	10.494733	2.653180
Si	11.685440	6.629153	4.450249
Si	14.090683	7.455161	2.510785
Si	14.760618	6.732429	13.008410
Si	17.751305	6.578013	13.188813
Si	18.747999	7.420735	2.577967
Si	16.424847	6.493442	4.408895
Si	18.514744	8.885102	11.418911
Si	16.218620	9.502768	9.392859
Si	15.692242	8.774465	6.487677

Si	12.510346	8.633380	6.614013
Si	11.451782	9.423370	9.327282
Si	13.752110	8.863612	11.141214
Si	18.550583	13.515202	11.197824
Si	16.212214	12.671883	9.319118
Si	15.461989	13.437199	6.408316
Si	12.435464	13.333126	6.277832
Si	11.427356	12.483240	9.139117
Si	13.667017	13.395609	11.012469
Si	11.520859	18.833210	4.720586
Si	13.988970	19.402719	2.824081
Si	17.644388	18.645960	13.279283
Si	18.721970	19.387596	2.579439
Si	16.457083	18.670635	4.443692
Si	11.675228	3.448696	4.488257
Si	13.950328	2.660098	2.515603
Si	17.750904	3.520133	13.064485
Si	18.569403	2.542296	2.529387
Si	16.270077	3.466008	4.420405
Si	18.505733	1.116135	11.377691
Si	16.090479	0.620252	9.363282
Si	15.600342	1.112752	6.440836
Si	12.504740	1.289654	6.560213
Si	11.420148	0.553391	9.235475
Si	13.614960	1.378802	11.057704
Si	18.520149	16.595566	11.087280
Si	16.127720	17.284670	9.187430
Si	15.409131	16.550198	6.248389
Si	12.366788	16.430605	6.306204
Si	11.448579	17.393318	9.134032
Si	13.685837	16.458462	11.010997
Si	8.475913	8.996737	8.710995
Si	6.056855	9.497792	10.712958
Si	5.513658	8.780036	0.236076
Si	2.371606	8.577464	0.151094
Si	1.409949	9.418396	10.801687
Si	3.592547	8.956142	8.771486
Si	6.098901	12.630891	10.990923
Si	5.339067	13.330936	0.516851
Si	2.329760	13.330540	0.337921
Si	1.390928	12.525027	10.889078
Si	3.681045	13.299099	9.030179
Si	1.533285	10.920771	1.903598
Si	3.924512	10.466874	3.906364

Si	4.332360	11.142445	6.784244
Si	7.491632	11.340639	6.789598
Si	8.595445	10.449760	4.104299
Si	6.430065	11.060461	2.124551
Si	1.574330	6.519111	2.288627
Si	3.919707	7.299152	4.260345
Si	4.559610	6.594529	7.211296
Si	7.633988	6.572441	7.052172
Si	8.641294	7.373773	4.241207
Si	6.353781	6.619999	2.418977
Al	2.121932	16.367327	0.423170
Al	3.870853	2.676813	4.279214
Al	16.465893	11.121153	4.429371
Al	14.473703	18.906637	12.962774
Al	14.373793	3.558339	12.889034
Al	8.381208	13.265470	8.938238
O	7.256573	1.081511	9.867152
O	6.257676	1.239310	12.291348
O	3.905892	0.994950	0.149488
O	1.752325	1.499987	12.067050
O	2.075480	0.994154	9.454688
O	4.589042	0.910578	10.275467
O	7.434769	16.576067	10.283363
O	6.092294	16.747396	12.538132
O	3.898283	17.166668	0.682801
O	1.839221	16.422844	12.119645
O	2.239861	16.833559	9.532443
O	4.760230	16.589397	10.291260
O	6.176187	18.812714	10.875695
O	1.825606	18.912010	11.201571
O	8.598848	2.554435	8.120537
O	8.265682	19.823980	7.611180
O	7.830204	17.180399	7.690407
O	3.756127	2.732332	8.538622
O	3.856237	0.145462	7.772043
O	4.167179	17.332228	7.779136
O	19.784338	0.741835	10.463633
O	19.860622	17.329044	10.539515
O	2.914002	18.650934	2.918699
O	3.663225	18.652527	5.519818
O	5.989381	18.908030	6.771129
O	8.178586	18.332552	5.375148
O	7.930113	18.991606	2.766400
O	5.422958	18.757395	3.591596

O	2.585641	3.479340	3.499789
O	3.919507	3.156180	5.923851
O	6.099702	2.900080	7.370286
O	8.017209	3.408301	5.666094
O	7.935119	3.074395	3.099235
O	5.527874	3.242542	3.667879
O	3.839419	0.983608	4.008610
O	8.268285	0.967091	4.682177
O	1.180897	17.410034	1.416457
O	1.652015	0.070442	0.923561
O	1.936728	2.727158	0.986461
O	6.340366	17.166071	1.751567
O	6.077477	19.726675	1.091919
O	5.661821	2.486778	1.260143
O	10.202410	19.156569	3.844401
O	10.241453	2.726959	4.278545
O	12.691945	10.855103	3.514644
O	13.754913	11.199555	1.177838
O	16.097286	11.116775	13.212769
O	18.266670	11.436354	1.398925
O	18.106895	11.028424	4.007807
O	15.273182	11.447298	3.264248
O	12.696952	7.034695	3.254076
O	13.852020	7.127225	0.931055
O	16.284693	7.291790	13.295074
O	18.437258	6.474936	1.274329
O	17.928699	6.806851	3.852698
O	15.347063	6.630944	3.174849
O	14.429655	9.032555	2.681150
O	18.278082	8.954351	2.264805
O	11.521459	12.443044	5.277853
O	11.760122	9.868511	5.857204
O	12.190795	7.225924	5.863761
O	16.524956	12.779735	5.269021
O	16.181580	10.042627	5.690318
O	16.016197	7.385315	5.695537
O	0.326759	10.612535	2.926594
O	0.326759	7.375763	2.923918
O	17.198095	8.784214	10.467381
O	16.427450	8.780831	7.955390
O	14.086678	8.939227	6.695248
O	11.923700	8.452896	8.112908
O	12.182586	8.947983	10.704392
O	14.666314	9.366261	9.877458

O	17.331842	13.515997	10.116746
O	16.268074	13.192838	7.770706
O	13.999783	12.761230	6.273817
O	11.844614	13.347652	7.786230
O	12.176779	13.248357	10.381060
O	14.695948	13.013946	9.794617
O	16.597036	11.100657	9.366896
O	11.934713	10.944650	8.952692
O	18.689936	7.467100	12.207705
O	18.430851	10.119836	12.470681
O	18.094082	12.766601	12.559277
O	14.173974	7.372381	11.623671
O	13.940516	9.788517	12.452748
O	13.935311	12.444835	12.290145
O	9.846820	9.282485	9.543418
O	9.856430	12.520849	9.366896
O	12.770432	18.814106	3.680459
O	13.592534	18.828236	1.260679
O	16.096085	18.990015	13.472265
O	18.356970	18.402397	1.341110
O	17.951525	18.903254	3.926572
O	15.431755	18.808535	3.171504
O	12.505341	3.236573	3.082105
O	13.940918	2.733725	0.945643
O	16.181780	2.821081	12.948990
O	18.109299	3.475957	1.260812
O	17.681026	2.903463	3.844401
O	15.122016	3.489091	3.254746
O	14.088881	1.088873	2.942788
O	18.266870	0.991567	2.100596
O	11.417544	17.336805	5.345840
O	11.667821	0.079397	5.855196
O	12.441071	2.661889	5.689114
O	16.264671	17.166866	5.018625
O	16.179379	19.741400	5.615240
O	15.764921	2.487773	5.614704
O	0.261087	19.319939	3.019339
O	0.095705	2.737306	2.921108
O	17.173670	1.168867	10.444227
O	16.365582	1.233937	7.872952
O	14.025810	0.757356	6.691500
O	11.844614	1.566648	8.022708
O	12.099694	0.989577	10.623425
O	14.594636	1.081710	9.786319

O	17.440563	16.653076	9.870499
O	16.190989	16.848484	7.621351
O	13.861231	17.092844	6.284925
O	11.677831	16.483734	7.788907
O	12.180383	16.665413	10.372093
O	14.755013	16.665014	9.786587
O	16.108299	18.896290	9.366093
O	11.922099	18.924746	8.861554
O	18.683529	2.575130	12.126604
O	18.363777	19.913128	12.550846
O	17.854418	17.319096	12.379410
O	13.677428	2.986641	11.374882
O	14.027613	0.564336	12.373521
O	13.854223	17.498583	12.212790
O	9.831002	0.664229	9.536057
O	9.841814	17.417395	9.456294
O	7.251568	8.882117	9.785784
O	5.921906	8.548014	12.048849
O	3.916303	9.027182	0.416077
O	2.076882	8.451105	11.939912
O	2.093300	9.121702	9.364220
O	4.664725	9.530228	9.864075
O	7.262580	13.365760	10.203066
O	6.090092	13.273828	12.477105
O	3.847627	12.683622	0.414472
O	1.843225	13.428640	12.156181
O	2.162176	13.012354	9.537663
O	4.657317	12.925993	10.276136
O	6.345973	11.023648	11.190464
O	1.667632	10.961165	11.277720
O	8.587836	7.547691	7.943078
O	8.333356	10.191273	7.614258
O	7.675834	12.783715	7.449647
O	3.841821	7.382728	8.441327
O	3.663826	9.779164	7.368948
O	3.937126	12.430507	7.685054
O	19.855017	9.119712	10.536571
O	19.836195	12.767199	10.540719
O	2.913201	10.952011	2.751009
O	3.754525	11.354967	5.268085
O	5.931317	10.862864	6.771932
O	8.085685	11.443517	5.273170
O	7.936520	10.854307	2.677671
O	5.434171	10.683574	3.349230

O	2.825905	6.545378	3.333973
O	3.761733	6.789141	5.797917
O	6.099502	7.133394	7.028083
O	8.177586	6.461603	5.515001
O	7.915698	6.885054	2.853791
O	5.434772	6.961466	3.736534
O	3.666629	8.892466	4.191422
O	8.255271	8.920722	4.584480
O	1.330061	12.349718	1.167533
O	1.436579	9.762649	0.754801
O	2.015214	7.143741	0.839382
O	6.240056	12.609399	1.667923
O	6.254472	10.106106	0.819976
O	5.932318	7.461926	1.093659
O	10.183789	10.615122	3.851761
O	10.242053	7.214382	4.008878
O	9.001891	15.063742	8.695471
O	3.832811	14.853210	8.541566
O	5.256576	14.912312	0.929048
O	2.329960	14.775604	1.006000
O	1.080387	5.004599	1.993264
O	6.166375	5.068076	2.002231
O	4.588041	5.054545	7.694021
O	7.684243	5.059320	7.695760
O	11.589535	5.026886	4.765553
O	16.429451	4.965796	5.004038
O	14.851519	5.162199	12.806862
O	17.688236	5.049172	12.553255
O	18.857922	15.074687	11.541499
O	13.848617	14.926837	11.542570
O	15.356273	14.966237	5.947137
O	12.419646	14.899775	5.772624
H	16.150946	1.875680	13.209825
H	5.972363	3.683504	17.799925
H	3.778552	17.725433	14.882967
H	9.854427	15.072298	8.203646
H	17.457783	13.036034	18.803383
H	12.672724	18.497515	14.601121
Pt	10.847719	1.870307	13.497292
Pt	9.758122	5.303283	12.954610
Pt	11.728686	3.893040	12.033995
Pt	8.691550	3.290499	14.453373
Pt	9.101200	2.958385	11.936164
Pt	11.232542	4.211424	14.725851

## Pt1H1@H-MFI

Si	8.453889	1.035743	8.761583
Si	6.013207	0.623834	10.752839
Si	5.688851	1.210257	0.269801
Si	2.506354	1.325472	0.156313
Si	1.405945	0.518966	10.831933
Si	3.617575	1.330049	9.019607
Si	8.508749	16.410505	8.981599
Si	6.096699	17.302977	10.869405
Si	5.349878	16.515574	0.441238
Si	2.338770	16.477964	0.431736
Si	1.422763	17.301783	10.977540
Si	3.623782	16.331110	9.075547
Si	1.535087	18.866043	1.999688
Si	3.899685	19.355358	4.003926
Si	7.737101	18.549450	6.881940
Si	8.658514	19.310188	4.039793
Si	6.376006	18.698494	2.217429
Si	1.658623	3.455063	2.270961
Si	3.887671	2.660297	4.284701
Si	4.531178	3.421036	7.193898
Si	7.606758	3.334276	7.101689
Si	8.626879	2.520010	4.273326
Si	11.550290	11.107423	4.631321
Si	13.960739	10.482594	2.675395
Si	14.398221	10.998973	13.069036
Si	17.598537	11.209903	13.199519
Si	18.659903	10.484385	2.614101
Si	16.400620	11.217265	4.458948
Si	11.564707	6.521101	4.331274
Si	13.958737	7.261344	2.439052
Si	14.631476	6.583783	12.911517
Si	18.801458	7.360441	2.445610
Si	16.396616	6.575426	4.241073
Si	18.509939	8.971863	11.185110
Si	16.031214	9.343575	9.285527
Si	15.547684	8.889679	6.320256
Si	12.334352	8.668005	6.466264
Si	11.420749	9.402476	9.258895
Si	13.569910	8.624624	11.101601
Si	18.461285	13.350239	11.106419
Si	16.091480	12.555672	9.150493
Si	15.445971	13.342678	6.191511

Si	12.430659	13.471026	6.241965
Si	13.835602	13.432222	11.118865
Si	11.569511	18.844551	4.590369
Si	13.975956	19.353371	2.621864
Si	14.412436	18.782070	13.066359
Si	17.606546	18.556215	13.239267
Si	18.623062	19.362921	2.616644
Si	16.403223	18.642179	4.468985
Si	11.634784	3.434767	4.486651
Si	13.887859	2.685370	2.376955
Si	14.524559	3.398152	12.895725
Si	17.554287	3.399943	12.910045
Si	18.681526	2.561598	2.319675
Si	18.491318	1.019426	11.353334
Si	16.067055	0.551003	9.345616
Si	15.635980	1.090465	6.405372
Si	12.437667	1.289057	6.549239
Si	11.323041	0.418476	9.303995
Si	13.604348	1.255229	11.124753
Si	18.492319	16.478163	11.116054
Si	16.165562	17.232534	9.146879
Si	15.442968	16.519156	6.220284
Si	12.426254	16.488111	6.256687
Si	11.447377	17.160698	9.155979
Si	13.810174	16.414684	11.020499
Si	8.537180	8.870577	8.685433
Si	6.078078	9.338799	10.719248
Si	5.521467	8.912563	0.234604
Si	2.361995	8.710191	0.156447
Si	1.390528	9.534408	10.791115
Si	3.639799	8.667408	8.924855
Si	8.437470	13.293327	9.041019
Si	6.035231	12.558856	10.984900
Si	5.357487	13.343673	0.523811
Si	2.339370	13.436999	0.371914
Si	1.401540	12.594276	10.933911
Si	3.704070	13.337106	9.080232
Si	1.523874	11.101054	2.058439
Si	3.900686	10.526969	4.040596
Si	4.465507	11.043149	6.982313
Si	7.660617	11.192192	6.816631
Si	8.658714	10.509060	4.051837
Si	6.369799	11.160752	2.245400
Si	1.651615	6.527071	2.245400

Si	3.908094	7.358849	4.243616
Si	4.543793	6.602887	7.127385
Si	8.648302	7.384718	4.038321
Si	6.253071	6.691039	2.385520
O	7.091592	1.078526	9.622645
O	6.426061	1.238912	12.188970
O	4.078882	0.989975	0.077220
O	1.842625	1.497599	12.058217
O	2.083890	1.002512	9.449737
O	4.526974	1.158719	10.372227
O	7.413145	16.751972	10.127050
O	6.091293	16.749586	12.389580
O	3.835214	17.150551	0.418486
O	1.823003	16.421650	12.275691
O	2.162776	16.585617	9.699864
O	4.755225	16.747993	10.115139
O	6.007601	18.902458	10.793791
O	1.835417	18.864252	11.194880
O	8.595845	2.558216	8.121072
O	8.425858	19.901985	7.514287
O	8.345570	17.238304	7.609574
O	3.759931	2.889335	8.524837
O	4.018215	0.330323	7.852877
O	3.672235	17.324268	7.690675
O	19.840200	0.657662	10.536571
O	19.869032	17.176022	10.629180
O	2.840121	18.738689	2.931680
O	3.677841	18.665262	5.437647
O	6.164774	18.572931	7.098076
O	8.254270	18.421698	5.337676
O	7.927711	18.816893	2.687574
O	5.423159	18.993994	3.505409
O	2.595252	3.403127	3.587313
O	3.690455	2.984054	5.878215
O	6.083885	2.815510	7.114269
O	8.181390	3.323730	5.595031
O	8.007999	3.311393	2.939308
O	5.329056	3.145037	3.776281
O	3.672635	1.067581	4.014499
O	8.186996	0.974852	4.348806
O	1.331863	17.394909	1.321839
O	1.674039	0.094321	0.837910
O	2.331562	2.716611	0.993554
O	6.174785	17.173037	1.670198

O	6.172983	19.733242	0.999978
O	6.083485	2.552246	1.008141
O	10.247059	19.161345	3.693976
O	10.249661	2.649353	3.999644
O	12.854925	11.108218	3.671091
O	13.764123	11.101453	1.174760
O	16.014595	10.938282	13.059132
O	18.101688	11.361334	1.344724
O	17.919489	10.860277	4.011420
O	15.439964	10.942261	3.173779
O	12.776839	6.478916	3.250865
O	13.761520	6.959476	0.860661
O	16.110502	7.222143	12.967994
O	18.595833	6.549756	1.080410
O	17.926897	6.787549	3.695849
O	15.421344	6.728847	2.924721
O	13.844412	8.867790	2.685701
O	18.436657	8.939626	2.182634
O	11.431961	12.595868	5.278657
O	11.605551	9.952286	5.781054
O	12.010797	7.289402	5.682154
O	16.339153	12.772372	4.945420
O	15.941916	10.364792	5.762586
O	16.096687	7.725389	5.354672
O	0.183402	10.861073	2.935160
O	0.342977	7.220353	2.923784
O	17.257162	8.781827	10.213237
O	16.263269	8.777449	7.786364
O	13.939116	8.872368	6.446725
O	11.765727	8.458070	7.963153
O	12.036224	8.718548	10.609373
O	14.599442	8.872766	9.859792
O	17.346659	13.195227	9.944640
O	16.188187	13.010166	7.610109
O	13.925901	12.763218	6.182812
O	11.930510	13.511222	7.758526
O	12.245655	13.350438	10.543530
O	14.680931	13.106476	9.788862
O	16.106096	10.957185	9.363817
O	12.011197	10.881769	9.034195
O	18.775829	7.393474	11.803003
O	18.351963	9.948505	12.463856
O	17.944117	12.609997	12.459038
O	13.772933	7.119663	11.636518

O	13.844011	9.699369	12.297237
O	13.935712	12.360861	12.299513
O	9.821392	9.373026	9.539938
O	9.850022	12.836248	9.622511
O	12.846715	18.742073	3.603507
O	13.763923	18.656904	1.165526
O	16.021004	18.823458	13.139564
O	18.103291	18.408764	1.401468
O	17.940311	18.906437	4.011287
O	15.442167	18.921362	3.180336
O	12.599844	3.310796	3.190373
O	13.603547	3.066038	0.823188
O	16.032415	2.737505	12.962373
O	18.106895	3.399545	1.086700
O	17.956730	3.314377	3.687819
O	15.274983	3.309204	2.862356
O	13.846214	1.064597	2.523499
O	18.192791	1.016839	2.263467
O	11.430360	17.414610	5.355609
O	11.677431	0.152625	5.680816
O	12.182185	2.746858	5.847301
O	16.264271	17.088465	4.936052
O	16.092682	19.560320	5.764728
O	16.090879	2.323805	5.517276
O	0.198618	19.235765	2.851516
O	0.231655	2.725964	2.668838
O	17.259764	1.068576	10.305044
O	16.349564	1.159913	7.872015
O	14.016200	0.992960	6.611470
O	11.761724	1.333432	8.027123
O	12.098693	0.914558	10.632125
O	14.612255	1.071362	9.864208
O	17.498426	16.662029	9.860595
O	16.268475	16.838932	7.587492
O	13.931107	17.160698	6.276628
O	11.846617	16.416676	7.777129
O	12.334553	16.569101	10.384540
O	14.857124	16.503832	9.788058
O	16.018600	18.824057	9.370375
O	11.677831	18.762568	8.954298
O	18.597034	2.480012	12.049518
O	18.356369	19.813633	12.546964
O	17.933905	17.162689	12.473625
O	13.686038	2.802376	11.625946

O	13.931107	0.263662	12.375394
O	13.939316	17.491817	12.209177
O	9.748111	0.668606	9.682066
O	9.937119	16.829977	9.630005
O	7.259376	8.958331	9.699864
O	6.331156	8.710588	12.208776
O	3.916303	9.122498	-0.011777
O	1.665830	8.534880	12.053400
O	2.168182	9.113145	9.454020
O	4.665727	8.716359	10.190619
O	7.332257	13.103492	10.212701
O	6.175786	13.008772	12.542013
O	3.829207	12.766005	0.413802
O	1.826607	13.512218	12.205029
O	2.177793	13.098516	9.597486
O	4.678340	13.258704	10.378383
O	5.913097	10.955195	10.795932
O	1.756330	11.037378	11.290167
O	8.674731	7.376559	8.108358
O	8.417048	9.869308	7.377513
O	8.006798	12.511098	7.683983
O	3.598354	7.143343	8.361297
O	3.929918	9.694196	7.697367
O	4.085689	12.354295	7.866260
O	19.841600	9.371434	10.369283
O	19.844004	12.688000	10.552763
O	2.835315	11.201943	3.010640
O	3.754325	11.196173	5.521290
O	6.065064	10.938282	6.856513
O	8.104706	11.443517	5.271698
O	7.917099	10.947236	2.671649
O	5.421757	10.772324	3.512904
O	2.842523	6.542791	3.334642
O	3.675238	6.878886	5.771018
O	5.999592	7.290794	7.102894
O	8.182991	6.469364	5.275712
O	7.840214	6.979972	2.673923
O	5.429165	7.052404	3.766645
O	3.581135	8.945596	4.097072
O	8.348372	8.954947	4.426829
O	1.336468	12.512690	1.254121
O	1.588946	9.867715	0.994223
O	2.093100	7.274279	0.854505
O	6.093695	12.710685	1.828252

O	6.085287	10.275645	0.915130
O	5.681843	7.630073	1.178507
O	10.233844	10.781079	3.748846
O	10.249062	7.211995	3.678451
O	8.427259	14.854205	8.603395
O	3.823000	14.852813	8.451766
O	5.262182	14.934796	0.752258
O	2.334165	14.944149	0.997301
O	1.332664	4.980919	1.838958
O	6.011405	5.199011	1.915643
O	4.744613	5.004797	7.353022
O	7.755722	4.954055	7.614258
O	11.258570	4.974352	4.772512
O	16.193192	5.142101	4.932305
O	14.682132	4.978929	12.715858
O	17.604744	4.877643	12.310621
O	18.693138	14.911316	11.463343
O	14.012197	14.928827	11.709322
O	15.354872	14.933005	6.019941
O	12.498934	14.994295	5.617247
Al	4.491335	18.872013	6.949658
Al	6.243260	3.572866	2.369059
Al	17.650993	6.441107	13.026209
Al	11.439169	12.505328	9.048916
Al	16.180378	3.538042	4.315349
Al	7.625378	6.728250	6.884081
H	8.264280	5.047183	8.447082
H	19.725874	7.243833	12.012046
H	11.549690	13.746826	11.104545
H	8.937820	4.174213	0.616153
H	18.624264	3.716138	4.278010
H	3.127436	16.967480	6.956350
Pt	9.673429	3.593362	1.824371

296

### Pt2H1@H-MFI

Si	8.431064	1.064000	8.714743
Si	6.007401	0.630798	10.739188
Si	5.680441	1.210655	0.224834
Si	2.515764	1.289455	0.132492
Si	1.373309	0.546228	10.804765
Si	3.610167	1.342387	9.013183
Si	8.508949	16.411303	8.984543
Si	6.095698	17.306160	10.879309
Si	5.356686	16.513582	0.447126

Si	2.325956	16.457666	0.389044
Si	1.418358	17.319891	10.944885
Si	3.626585	16.331905	9.072603
Si	1.534886	18.839777	1.983227
Si	3.832611	19.367300	3.999510
Si	7.734298	18.542685	6.881137
Si	8.666122	19.325113	4.070841
Si	6.359187	18.767145	2.202842
Si	1.675241	3.439542	2.250485
Si	3.849029	2.611744	4.281623
Si	4.533581	3.423424	7.179578
Si	7.607759	3.354175	7.023667
Si	8.652707	2.529561	4.220597
Si	11.546086	11.105831	4.629581
Si	13.957937	10.487967	2.675128
Si	14.398221	10.997780	13.068902
Si	17.598537	11.210898	13.199922
Si	18.659702	10.484584	2.614771
Si	16.399820	11.217863	4.458279
Si	11.496031	6.512545	4.288850
Si	13.882854	7.274676	2.419379
Si	14.638684	6.595523	12.892245
Si	18.770224	7.355864	2.450026
Si	16.341957	6.585773	4.256330
Si	18.511539	8.976439	11.183371
Si	16.031816	9.344570	9.287668
Si	15.538072	8.906395	6.328821
Si	12.326143	8.652881	6.443513
Si	11.422351	9.398297	9.247118
Si	13.568308	8.626415	11.098121
Si	18.461485	13.351830	11.105883
Si	16.091681	12.555871	9.149690
Si	15.446172	13.341882	6.189504
Si	12.429056	13.467245	6.243571
Si	13.834601	13.430035	11.117928
Si	11.568110	18.842363	4.602280
Si	13.953732	19.379637	2.621596
Si	14.418042	18.766945	13.074522
Si	17.609949	18.551041	13.238196
Si	18.630470	19.357548	2.617179
Si	16.389008	18.671431	4.450918
Si	11.607955	3.426807	4.469253
Si	13.915690	2.690146	2.397564
Si	14.584825	3.397157	12.905896

Si	17.600739	3.415863	12.923161
Si	18.716764	2.542893	2.323824
Si	18.458281	1.022411	11.360963
Si	16.041225	0.537074	9.339862
Si	15.634579	1.092654	6.404970
Si	12.434663	1.299803	6.544154
Si	11.314032	0.473198	9.289809
Si	13.622168	1.230753	11.117258
Si	18.481506	16.480154	11.090894
Si	16.167164	17.224375	9.105927
Si	15.428152	16.522936	6.179333
Si	12.420047	16.486521	6.256285
Si	11.448980	17.189156	9.154240
Si	13.815580	16.412895	11.012336
Si	8.537781	8.870775	8.686102
Si	6.078679	9.337407	10.720319
Si	5.520866	8.901420	0.236611
Si	2.361995	8.706808	0.167555
Si	1.393731	9.531223	10.795665
Si	3.640400	8.667009	8.925390
Si	8.437271	13.291935	9.041421
Si	6.035231	12.556667	10.984632
Si	5.368298	13.340091	0.527290
Si	2.339971	13.430830	0.369772
Si	1.402140	12.592883	10.932038
Si	3.704871	13.336509	9.080098
Si	1.522673	11.101254	2.059376
Si	3.888873	10.522989	4.041265
Si	4.465707	11.042751	6.982045
Si	7.660617	11.191795	6.816230
Si	8.654309	10.507867	4.051971
Si	6.365594	11.148017	2.248210
Si	1.638200	6.515331	2.264538
Si	3.886070	7.376360	4.248701
Si	4.543793	6.604876	7.127519
Si	8.591040	7.384320	4.034707
Si	6.201814	6.660992	2.395022
O	7.094595	1.078526	9.614749
O	6.424659	1.321095	12.140388
O	4.081285	0.910976	0.001472
O	1.833214	1.493221	12.048983
O	2.066070	1.079521	9.447328
O	4.517964	1.155336	10.365268
O	7.410743	16.756948	10.128120

O	6.094296	16.747198	12.394398
O	3.829007	17.085680	0.410858
O	1.830611	16.419460	12.223096
O	2.160974	16.586016	9.683270
O	4.757027	16.752172	10.115139
O	6.009203	18.911213	10.869405
O	1.832013	18.888927	11.120337
O	8.593442	2.559807	8.038900
O	8.425458	19.894623	7.509603
O	8.345570	17.236116	7.612250
O	3.766739	2.894707	8.515871
O	4.011407	0.328930	7.856491
O	3.674037	17.324865	7.688534
O	19.793348	0.656667	10.525061
O	19.862024	17.183582	10.624095
O	2.829509	18.658298	2.927397
O	3.684248	18.657501	5.433498
O	6.162571	18.573130	7.100351
O	8.256672	18.409958	5.346509
O	7.892272	18.822266	2.747664
O	5.355484	19.164728	3.424977
O	2.673738	3.477549	3.519060
O	3.682446	2.989029	5.869115
O	6.087689	2.817897	7.106507
O	8.175783	3.399545	5.514331
O	8.010001	3.151206	2.842014
O	5.335863	2.906050	3.772534
O	3.425964	1.044698	4.086901
O	8.254870	0.975250	4.434859
O	1.320251	17.398094	1.250775
O	1.674840	0.083974	0.838043
O	2.339170	2.658705	0.994223
O	6.103306	17.244473	1.679165
O	6.256674	19.744186	0.917672
O	5.994987	2.554435	0.995963
O	10.251864	19.159950	3.698392
O	10.273088	2.580303	4.002722
O	12.853123	11.110607	3.672162
O	13.764123	11.103841	1.173555
O	16.014595	10.938878	13.058730
O	18.101688	11.361732	1.344724
O	17.918488	10.860476	4.011688
O	15.438963	10.942859	3.173779
O	12.609856	6.540602	3.107666

O	13.769529	6.964053	0.839114
O	16.106096	7.279850	12.894119
O	18.521751	6.551149	1.087369
O	17.859022	6.795110	3.680459
O	15.285796	6.714520	3.007963
O	13.841008	8.876944	2.682355
O	18.436457	8.941217	2.182500
O	11.431160	12.595073	5.278790
O	11.603750	9.952683	5.779716
O	12.015202	7.295570	5.610422
O	16.339954	12.773565	4.944082
O	15.940114	10.373747	5.765664
O	16.100491	7.769963	5.347579
O	0.182601	10.861670	2.935829
O	0.320953	7.212790	2.923918
O	17.259365	8.782822	10.212032
O	16.262268	8.779439	7.788237
O	13.932308	8.870975	6.447394
O	11.764927	8.453493	7.949235
O	12.039028	8.720538	10.599737
O	14.600442	8.873561	9.859122
O	17.346260	13.195823	9.944238
O	16.187786	13.011359	7.609574
O	13.926102	12.763417	6.183214
O	11.930709	13.511421	7.760534
O	12.245054	13.349842	10.543262
O	14.680931	13.107272	9.788461
O	16.106297	10.958380	9.364085
O	12.011798	10.879580	9.031919
O	18.778633	7.398050	11.802334
O	18.352165	9.949500	12.463990
O	17.944517	12.611190	12.458637
O	13.766326	7.120061	11.627419
O	13.843410	9.699170	12.296569
O	13.935712	12.361259	12.299646
O	9.824395	9.372628	9.537930
O	9.850224	12.835452	9.622779
O	12.846315	18.741077	3.609663
O	13.763923	18.656706	1.169407
O	16.022404	18.823061	13.139564
O	18.103491	18.405779	1.400665
O	17.938711	18.904249	4.010885
O	15.447573	19.067619	3.179667
O	12.680733	3.323730	3.262508

O	13.676227	3.065242	0.830950
O	16.092482	2.739296	12.966923
O	18.187183	3.401933	1.084692
O	18.016796	3.315372	3.692503
O	15.351267	3.230603	2.854460
O	13.760319	1.073949	2.513729
O	18.193590	1.010471	2.263199
O	11.427356	17.407446	5.354003
O	11.681234	0.089744	5.761783
O	12.177780	2.747654	5.843152
O	16.185385	17.103390	4.858163
O	16.095886	19.559921	5.770884
O	16.096687	2.323805	5.520220
O	0.208229	19.228802	2.848170
O	0.270097	2.660496	2.670845
O	17.168465	1.070168	10.374904
O	16.347963	1.160709	7.879509
O	14.015600	0.994154	6.612005
O	11.772335	1.404471	8.039704
O	12.027015	0.992562	10.705998
O	14.523759	0.989577	9.793011
O	17.514645	16.658648	9.801041
O	16.269876	16.847885	7.536770
O	13.922897	17.161297	6.277430
O	11.845416	16.427818	7.781814
O	12.338958	16.581041	10.377446
O	14.866135	16.504431	9.781903
O	16.021204	18.814505	9.366629
O	11.678632	18.813908	8.968752
O	18.605844	2.481604	12.044165
O	18.355568	19.812439	12.550310
O	17.931704	17.161297	12.461848
O	13.767727	2.757006	11.629292
O	13.928304	0.250329	12.372583
O	13.939517	17.489033	12.207036
O	9.745708	0.745815	9.630005
O	9.941524	16.838137	9.629604
O	7.259777	8.958729	9.700267
O	6.330956	8.709394	12.209311
O	3.915502	9.120707	-0.010706
O	1.665830	8.531497	12.060760
O	2.168383	9.112549	9.455625
O	4.665927	8.716160	10.191021
O	7.331856	13.103492	10.212568

O	6.176786	13.005190	12.540406
O	3.834213	12.771178	0.414472
O	1.826607	13.510626	12.203557
O	2.177593	13.098119	9.595477
O	4.678541	13.258505	10.378517
O	5.913297	10.954001	10.795130
O	1.756530	11.036582	11.290435
O	8.675733	7.377554	8.109964
O	8.417048	9.870103	7.378583
O	8.006998	12.511695	7.684117
O	3.597553	7.143343	8.361966
O	3.929718	9.694196	7.697634
O	4.085689	12.354095	7.865992
O	19.844404	9.371434	10.369818
O	19.843803	12.688598	10.552897
O	2.834314	11.209703	3.009034
O	3.754325	11.196173	5.521692
O	6.064864	10.938480	6.856914
O	8.104706	11.444711	5.272367
O	7.914897	10.946639	2.671515
O	5.414350	10.760782	3.515179
O	2.838319	6.538414	3.340531
O	3.673836	6.880079	5.772490
O	5.998591	7.292585	7.104366
O	8.172179	6.468170	5.282939
O	7.779748	6.974599	2.676600
O	5.417152	7.130011	3.767850
O	3.504050	8.952361	4.098812
O	8.340565	8.958529	4.428703
O	1.335868	12.511695	1.253452
O	1.588145	9.870502	0.994089
O	2.094501	7.288805	0.900542
O	6.092094	12.697353	1.832267
O	6.083485	10.267686	0.914996
O	5.677238	7.612761	1.173288
O	10.228639	10.782075	3.748043
O	10.176181	7.212393	3.674570
O	8.428261	14.855201	8.606474
O	3.825203	14.852613	8.451900
O	5.340068	14.932409	0.758415
O	2.328158	14.939175	0.989941
O	1.327058	4.970969	1.835211
O	5.929915	5.142101	2.014275
O	4.744413	5.006986	7.349409

O	7.752318	4.954453	7.605158
O	11.188694	4.968979	4.759798
O	16.190790	5.139315	4.935249
O	14.689540	4.982112	12.712780
O	17.607946	4.887195	12.311691
O	18.689535	14.916290	11.459060
O	14.011995	14.929822	11.706913
O	15.355672	14.933205	6.015792
O	12.495930	14.992305	5.621931
Al	4.489333	18.874401	6.946580
Al	6.243660	3.496254	2.411884
Al	17.630972	6.464588	13.003325
Al	11.437967	12.501547	9.047578
Al	16.221624	3.534261	4.315482
Al	7.624177	6.727653	6.891710
H	8.249264	5.016538	8.446547
H	19.727877	7.246818	12.012982
H	11.545285	13.726131	11.113511
H	8.405035	2.604381	0.030246
H	18.692938	3.691264	4.288850
H	3.137848	16.961708	6.950996
Pt	10.729189	1.775986	-0.634756
Pt	9.380507	2.584283	1.207682

297

#### Pt3H1@H-MFI

Si	8.448283	1.050866	8.746058
Si	6.000793	0.616272	10.728750
Si	5.690853	1.220008	0.246649
Si	2.499747	1.319901	0.137979
Si	1.384922	0.550008	10.799948
Si	3.621579	1.347958	9.012113
Si	8.508148	16.407919	8.979190
Si	6.095497	17.299196	10.863115
Si	5.358888	16.512390	0.430799
Si	2.342574	16.493484	0.432940
Si	1.421962	17.327850	10.958403
Si	3.621979	16.330513	9.072336
Si	1.535687	18.869226	2.003034
Si	3.922710	19.347200	3.985190
Si	7.742707	18.546864	6.875784
Si	8.667124	19.315561	4.042335
Si	6.402635	18.707050	2.161087
Si	1.674640	3.454467	2.243526
Si	3.913700	2.638806	4.268508

Si	4.568419	3.432180	7.179043
Si	7.635590	3.340843	7.071444
Si	8.638492	2.524586	4.231705
Si	11.546686	11.107025	4.630250
Si	13.959138	10.489559	2.675395
Si	14.398221	10.997979	13.068902
Si	17.598135	11.211096	13.200590
Si	18.661304	10.485977	2.614904
Si	16.400620	11.217067	4.459082
Si	11.516654	6.523688	4.295809
Si	13.917091	7.276865	2.420316
Si	14.645492	6.613035	12.904960
Si	18.777231	7.359446	2.449624
Si	16.354370	6.578211	4.235987
Si	18.511740	8.980220	11.181898
Si	16.031414	9.344570	9.284189
Si	15.541677	8.891869	6.320925
Si	12.328145	8.658054	6.448866
Si	11.420548	9.398099	9.250062
Si	13.567708	8.626216	11.097987
Si	18.461885	13.349842	11.106284
Si	16.091681	12.555871	9.150359
Si	15.445571	13.341483	6.191511
Si	12.429457	13.468240	6.243571
Si	13.834200	13.427845	11.118061
Si	11.565308	18.827240	4.578860
Si	13.985366	19.332077	2.622399
Si	14.415439	18.764757	13.070507
Si	17.608347	18.553032	13.243282
Si	18.621662	19.370283	2.618786
Si	16.406027	18.639393	4.472733
Si	11.625574	3.428996	4.475543
Si	13.989171	2.655720	2.466621
Si	14.624269	3.428598	12.940558
Si	17.627369	3.420041	12.926774
Si	18.710558	2.564185	2.347914
Si	18.473497	1.016441	11.360963
Si	16.049435	0.560356	9.355252
Si	15.629173	1.088276	6.409520
Si	12.418245	1.278909	6.535990
Si	11.325644	0.438176	9.313766
Si	13.606351	1.239111	11.144560
Si	18.493519	16.478163	11.115787
Si	16.163361	17.235718	9.148351

Si	15.442167	16.517761	6.221757
Si	12.425853	16.486122	6.257088
Si	11.449380	17.150152	9.170567
Si	13.809974	16.400955	11.020499
Si	8.536981	8.869781	8.685701
Si	6.079279	9.337605	10.720719
Si	5.521667	8.906395	0.236076
Si	2.363597	8.709593	0.165682
Si	1.394532	9.532218	10.795397
Si	3.640800	8.668005	8.925792
Si	8.436871	13.290741	9.041019
Si	6.035431	12.557463	10.985436
Si	5.358088	13.342279	0.524881
Si	2.339571	13.442769	0.372583
Si	1.402741	12.594077	10.934313
Si	3.704670	13.335713	9.080098
Si	1.525076	11.103244	2.058172
Si	3.901487	10.525974	4.040462
Si	4.465907	11.042552	6.981644
Si	7.661017	11.191197	6.815828
Si	8.655910	10.510453	4.051837
Si	6.369598	11.156374	2.244463
Si	1.642805	6.524683	2.264671
Si	3.907894	7.358451	4.245489
Si	4.545394	6.611443	7.126448
Si	8.601651	7.392478	4.036714
Si	6.228444	6.661986	2.374412
O	7.094395	1.078725	9.620102
O	6.432268	1.251050	12.150559
O	4.076279	0.992960	0.072937
O	1.835617	1.493221	12.044968
O	2.075280	1.085092	9.442778
O	4.516963	1.155535	10.371692
O	7.414546	16.752371	10.125176
O	6.091093	16.746799	12.378874
O	3.844424	17.151745	0.422635
O	1.825606	16.492092	12.279170
O	2.162176	16.584026	9.698393
O	4.753222	16.747795	10.112463
O	6.007601	18.900667	10.792319
O	1.835016	18.895494	11.117793
O	8.597647	2.564583	8.119867
O	8.431464	19.899000	7.521380
O	8.347372	17.237509	7.609574

O	3.832211	2.894907	8.524837
O	4.011208	0.328930	7.857828
O	3.673236	17.325064	7.689069
O	19.806763	0.656070	10.522652
O	19.866629	17.179205	10.627173
O	2.837718	18.735905	2.934357
O	3.751722	18.659889	5.426673
O	6.172182	18.573925	7.104500
O	8.255271	18.414137	5.334866
O	7.932516	18.826843	2.687306
O	5.421757	18.993793	3.426717
O	2.667731	3.401734	3.513171
O	3.745115	2.984054	5.861486
O	6.110314	2.818295	7.106507
O	8.264881	3.324725	5.593826
O	8.000590	3.231598	2.927799
O	5.354484	3.074196	3.768118
O	3.666228	1.050468	4.016774
O	8.262478	0.963908	4.430308
O	1.331263	17.398094	1.328263
O	1.675040	0.092928	0.836705
O	2.257881	2.727755	0.920081
O	6.250067	17.178608	1.602614
O	6.181191	19.721701	0.925702
O	6.080281	2.545679	0.999309
O	10.252866	19.153584	3.686481
O	10.270885	2.658108	3.899806
O	12.853924	11.110009	3.672028
O	13.764123	11.103443	1.173555
O	16.014395	10.938282	13.058998
O	18.101688	11.361932	1.344992
O	17.919489	10.860676	4.011822
O	15.439964	10.943057	3.173912
O	12.686940	6.541398	3.174983
O	13.762722	6.961068	0.842460
O	16.112103	7.286815	12.961703
O	18.525755	6.550950	1.091384
O	17.876442	6.792126	3.684875
O	15.354872	6.718300	2.936096
O	13.845213	8.876745	2.682087
O	18.436457	8.942411	2.182767
O	11.431360	12.595868	5.278790
O	11.604551	9.954276	5.780519
O	12.013399	7.300147	5.623938

O	16.339153	12.772572	4.945554
O	15.941515	10.365191	5.762988
O	16.091881	7.727578	5.356144
O	0.184202	10.862267	2.935293
O	0.324356	7.216173	2.925122
O	17.258162	8.782622	10.212166
O	16.262669	8.777847	7.785560
O	13.934912	8.870975	6.446725
O	11.765527	8.454687	7.952313
O	12.037626	8.717951	10.603084
O	14.600642	8.872766	9.859390
O	17.346859	13.195424	9.944640
O	16.188187	13.010364	7.610109
O	13.925901	12.762821	6.183080
O	11.930510	13.511023	7.760534
O	12.245655	13.349643	10.543128
O	14.681131	13.106476	9.788461
O	16.106297	10.957583	9.363952
O	12.011798	10.878783	9.032990
O	18.777832	7.403423	11.803270
O	18.351963	9.950296	12.463990
O	17.944117	12.610394	12.458904
O	13.774135	7.117872	11.631299
O	13.843810	9.697778	12.296836
O	13.935512	12.359269	12.299379
O	9.823193	9.372628	9.538332
O	9.850224	12.836049	9.622511
O	12.849719	18.741474	3.601232
O	13.763122	18.651731	1.164053
O	16.022005	18.821867	13.139965
O	18.102291	18.411350	1.405750
O	17.940912	18.907631	4.012357
O	15.448975	18.909224	3.181808
O	12.767229	3.246920	3.349765
O	13.685837	3.145037	0.906832
O	16.101292	2.741286	12.969065
O	18.184580	3.404719	1.093123
O	18.029409	3.310796	3.751255
O	15.428351	3.231399	2.847769
O	13.925301	1.043305	2.514532
O	18.193991	1.030768	2.270292
O	11.429759	17.405855	5.354137
O	11.684238	0.101286	5.696073
O	12.097893	2.733327	5.862958

O	16.265072	17.086874	4.938327
O	16.091881	19.560717	5.766333
O	16.091881	2.320024	5.524503
O	0.195615	19.238354	2.851248
O	0.256282	2.726163	2.679143
O	17.190489	1.072158	10.376376
O	16.346560	1.158719	7.880178
O	14.007992	0.997736	6.609730
O	11.761122	1.326268	8.026454
O	12.097692	0.987985	10.626236
O	14.607450	1.143596	9.870766
O	17.495422	16.664419	9.861933
O	16.267673	16.840324	7.589767
O	13.931107	17.160500	6.277163
O	11.846416	16.424238	7.779806
O	12.331750	16.501245	10.378918
O	14.855723	16.505823	9.788461
O	16.012394	18.831419	9.372383
O	11.677231	18.766945	9.037406
O	18.610849	2.477426	12.045102
O	18.357170	19.811245	12.551515
O	17.933905	17.162092	12.474027
O	13.674425	2.751037	11.782795
O	13.935712	0.244758	12.373788
O	13.936713	17.486444	12.203958
O	9.749912	0.742034	9.700399
O	9.935316	16.830177	9.631478
O	7.259576	8.958928	9.699999
O	6.330956	8.710390	12.209177
O	3.915703	9.122697	-0.012446
O	1.665630	8.532094	12.059823
O	2.168182	9.112947	9.455491
O	4.665927	8.716757	10.191154
O	7.331856	13.103691	10.212969
O	6.175385	13.008971	12.542147
O	3.828006	12.767796	0.414204
O	1.826207	13.514605	12.204627
O	2.177793	13.098516	9.597351
O	4.678541	13.258904	10.378517
O	5.913097	10.954798	10.795799
O	1.756530	11.037180	11.290970
O	8.675132	7.376957	8.108625
O	8.417048	9.869904	7.378583
O	8.006598	12.510700	7.683850

O	3.597953	7.145134	8.361699
O	3.929518	9.694594	7.697634
O	4.085689	12.354095	7.865992
O	19.844805	9.372231	10.369015
O	19.844404	12.688000	10.553031
O	2.835515	11.202342	3.010907
O	3.754125	11.196173	5.521157
O	6.065064	10.938480	6.856647
O	8.104905	11.446103	5.272367
O	7.916899	10.948231	2.670979
O	5.421757	10.772324	3.513171
O	2.838319	6.541597	3.342672
O	3.673836	6.880477	5.772490
O	6.001194	7.295172	7.103830
O	8.174782	6.467971	5.277720
O	7.788758	7.045639	2.669240
O	5.422758	7.048027	3.764638
O	3.580334	8.945596	4.097340
O	8.344169	8.962908	4.433520
O	1.336869	12.515875	1.254121
O	1.587945	9.871496	0.993688
O	2.095703	7.291392	0.897732
O	6.092895	12.707104	1.828118
O	6.084085	10.272860	0.914460
O	5.673834	7.622312	1.174626
O	10.231042	10.782272	3.747508
O	10.188994	7.207617	3.675106
O	8.427460	14.852613	8.603395
O	3.822800	14.852215	8.450964
O	5.261782	14.934597	0.752660
O	2.332162	14.956287	0.988736
O	1.330262	4.983704	1.839627
O	6.011205	5.157821	1.925546
O	4.748417	5.016737	7.351416
O	7.756923	4.956045	7.611849
O	11.261173	4.973357	4.762207
O	16.188387	5.142300	4.932974
O	14.764422	4.995644	12.714787
O	17.674820	4.889184	12.313431
O	18.692938	14.911913	11.462808
O	14.015800	14.923056	11.711999
O	15.355072	14.932608	6.020477
O	12.498733	14.992305	5.620593
Al	4.503748	18.876192	6.958089

Al	6.303526	3.532072	2.388063
Al	17.640383	6.468369	13.009480
Al	11.437967	12.501348	9.048782
Al	16.249655	3.536251	4.340508
Al	7.624978	6.725862	6.887427
H	8.249664	5.042208	8.454844
H	19.728277	7.245425	12.004149
H	11.551291	13.763541	11.093437
H	8.988677	3.382830	0.091807
H	18.711760	3.759120	4.288047
H	3.169883	16.946386	6.936409
Pt	9.419550	2.050592	-0.838177
Pt	11.685240	2.648159	0.026900
Pt	9.726888	2.782875	1.567551

298

#### Pt4H1@H-MFI

Si	8.454690	1.032957	8.780453
Si	6.014608	0.626620	10.766356
Si	5.715079	1.174240	0.300984
Si	2.516965	1.317314	0.158455
Si	1.423364	0.519563	10.828185
Si	3.631590	1.332238	9.022150
Si	8.506146	16.415878	8.977183
Si	6.097500	17.305563	10.871012
Si	5.352281	16.516369	0.442174
Si	2.340572	16.479954	0.432672
Si	1.424365	17.299196	10.977004
Si	3.625183	16.334095	9.074210
Si	1.539892	18.866640	2.002498
Si	3.917304	19.366104	3.998840
Si	7.742908	18.563578	6.880335
Si	8.659715	19.351580	4.020655
Si	6.393625	18.692524	2.187585
Si	1.672638	3.452874	2.247809
Si	3.900285	2.660496	4.319631
Si	4.570221	3.418847	7.194969
Si	7.660617	3.296269	7.068901
Si	8.728992	2.542296	4.216850
Si	11.541882	11.110607	4.631187
Si	13.959938	10.502095	2.676868
Si	14.399622	11.002555	13.065689
Si	17.599937	11.212291	13.199519
Si	18.662907	10.485977	2.614369
Si	16.403624	11.222837	4.460153

Si	11.484018	6.501998	4.311601
Si	13.937314	7.293581	2.432628
Si	14.643089	6.595125	12.889302
Si	18.779234	7.358849	2.448955
Si	16.370789	6.588360	4.274396
Si	18.513742	8.977036	11.183638
Si	16.032616	9.348152	9.290212
Si	15.539274	8.912563	6.333237
Si	12.326344	8.659050	6.447662
Si	11.415743	9.399691	9.249260
Si	13.564704	8.631390	11.096916
Si	18.463686	13.352229	11.106016
Si	16.091881	12.559651	9.150760
Si	15.444570	13.345464	6.192047
Si	12.430258	13.475204	6.242099
Si	13.833600	13.435605	11.117526
Si	11.564507	18.858480	4.592912
Si	13.984165	19.337252	2.625611
Si	14.411634	18.782070	13.067563
Si	17.606546	18.556614	13.240337
Si	18.624664	19.367895	2.617179
Si	16.406227	18.640188	4.471528
Si	11.641392	3.393576	4.511945
Si	14.002385	2.664874	2.445877
Si	14.566204	3.399744	12.866952
Si	17.583118	3.407107	12.918878
Si	18.697744	2.567767	2.336672
Si	18.497524	1.017237	11.351728
Si	16.067453	0.551202	9.346286
Si	15.628372	1.088077	6.407915
Si	12.431259	1.316319	6.554057
Si	11.320238	0.417083	9.304933
Si	13.599142	1.249060	11.124485
Si	18.493120	16.479755	11.116188
Si	16.165361	17.232733	9.147682
Si	15.441767	16.521145	6.221355
Si	12.423250	16.493685	6.255348
Si	11.444775	17.161694	9.155043
Si	13.807971	16.417074	11.019429
Si	8.531775	8.867592	8.681151
Si	6.077678	9.339198	10.720587
Si	5.522468	8.904604	0.236879
Si	2.363197	8.709195	0.166217
Si	1.396134	9.532417	10.795264

Si	3.641201	8.666015	8.924186
Si	8.436469	13.297109	9.040484
Si	6.035431	12.559651	10.985034
Si	5.357487	13.344866	0.523543
Si	2.340772	13.438990	0.372315
Si	1.403542	12.594873	10.933778
Si	3.704871	13.339096	9.079697
Si	1.525676	11.103443	2.058038
Si	3.901487	10.526174	4.041265
Si	4.465106	11.043547	6.982848
Si	7.659616	11.192988	6.817568
Si	8.651306	10.509657	4.051569
Si	6.367797	11.158762	2.243526
Si	1.643606	6.522494	2.265608
Si	3.908695	7.357655	4.247363
Si	4.547397	6.600300	7.128856
Si	8.590038	7.384320	4.044610
Si	6.229445	6.649848	2.373877
O	7.087388	1.075342	9.630407
O	6.419654	1.248662	12.202486
O	4.089093	0.995547	0.160195
O	1.913703	1.489241	12.040686
O	2.089095	1.008680	9.443046
O	4.527775	1.154142	10.379855
O	7.412745	16.751972	10.126246
O	6.091293	16.747993	12.389313
O	3.835814	17.149954	0.418353
O	1.822202	16.421053	12.277029
O	2.162977	16.584623	9.699329
O	4.755425	16.748194	10.115541
O	6.007601	18.903454	10.795932
O	1.835817	18.860472	11.192739
O	8.593843	2.565379	8.184106
O	8.427660	19.909546	7.524057
O	8.346371	17.242086	7.604622
O	3.830809	2.885753	8.537952
O	4.016213	0.329129	7.853814
O	3.673236	17.325462	7.690274
O	19.850811	0.660647	10.540719
O	19.869232	17.175623	10.629046
O	2.841722	18.742868	2.938104
O	3.751122	18.655313	5.428279
O	6.172182	18.571537	7.104901
O	8.254870	18.487963	5.338345

O	7.930714	18.812515	2.682489
O	5.422758	19.071999	3.431669
O	2.667131	3.401535	3.515313
O	3.675238	2.986243	5.914885
O	6.115920	2.812525	7.098343
O	8.333356	3.311592	5.611091
O	8.075473	3.405714	2.995651
O	5.343271	3.150012	3.854170
O	3.666429	1.067979	4.090916
O	8.184593	1.007287	4.267705
O	1.332865	17.395706	1.323846
O	1.672838	0.092928	0.836973
O	2.254477	2.731337	0.922223
O	6.175185	17.159903	1.675552
O	6.179190	19.638920	0.907769
O	6.167977	2.408575	1.171146
O	10.249661	19.159950	3.690362
O	10.348970	2.499314	4.089444
O	12.851721	11.109612	3.673098
O	13.763923	11.102249	1.172619
O	16.014797	10.937685	13.059533
O	18.101488	11.361533	1.345125
O	17.919289	10.860277	4.011554
O	15.440966	10.943057	3.174716
O	12.606051	6.548164	3.086254
O	13.765325	6.964451	0.850624
O	16.103292	7.279850	12.964647
O	18.524153	6.550751	1.090179
O	17.872839	6.795310	3.683403
O	15.330244	6.718897	3.002208
O	13.842010	8.881521	2.685701
O	18.436058	8.941815	2.182901
O	11.431560	12.597062	5.278924
O	11.603750	9.952883	5.778780
O	12.021408	7.297759	5.608949
O	16.339153	12.775556	4.945152
O	15.940516	10.375339	5.765263
O	16.100691	7.777524	5.347579
O	0.184603	10.861670	2.935695
O	0.324557	7.216173	2.925122
O	17.258162	8.781827	10.214308
O	16.261868	8.779240	7.790646
O	13.932709	8.870577	6.446591
O	11.764727	8.453294	7.950706

O	12.032620	8.715762	10.603485
O	14.599841	8.872766	9.860327
O	17.347261	13.195027	9.945310
O	16.187986	13.009967	7.609708
O	13.925502	12.763218	6.182411
O	11.930709	13.510028	7.758794
O	12.244854	13.350039	10.542994
O	14.680530	13.106079	9.789129
O	16.105896	10.959374	9.364220
O	12.010997	10.877988	9.033123
O	18.774828	7.395862	11.802602
O	18.351765	9.948903	12.464257
O	17.944117	12.610394	12.458368
O	13.768728	7.122051	11.630764
O	13.843210	9.698574	12.297907
O	13.935512	12.361657	12.298175
O	9.819189	9.370240	9.537395
O	9.849422	12.836447	9.621976
O	12.847116	18.746252	3.604711
O	13.763122	18.655712	1.165258
O	16.020803	18.823658	13.139162
O	18.103092	18.411949	1.402672
O	17.941713	18.907631	4.011153
O	15.448574	18.909622	3.181541
O	12.774237	3.243537	3.350033
O	13.680431	3.055889	0.851293
O	16.062048	2.739694	12.960633
O	18.112701	3.402132	1.099949
O	18.026608	3.310796	3.749649
O	15.415338	3.298657	2.841612
O	13.931908	1.052458	2.518145
O	18.195593	1.027584	2.267482
O	11.431160	17.420181	5.354940
O	11.682636	0.164366	5.684430
O	12.189193	2.811728	5.935093
O	16.265673	17.086874	4.937658
O	16.093082	19.560717	5.764728
O	16.092682	2.321417	5.520622
O	0.199419	19.236761	2.851382
O	0.247472	2.728352	2.674459
O	17.262568	1.069372	10.305981
O	16.349163	1.159913	7.872818
O	14.012997	0.993955	6.611068
O	11.761122	1.331243	8.034350

O	12.098894	0.914956	10.632928
O	14.613056	1.072954	9.867019
O	17.498026	16.662029	9.861130
O	16.268475	16.838335	7.588697
O	13.931307	17.160898	6.276761
O	11.846817	16.416277	7.776995
O	12.333152	16.567509	10.384540
O	14.856925	16.503832	9.788461
O	16.018600	18.824453	9.370911
O	11.678832	18.761175	8.955503
O	18.602840	2.481206	12.048716
O	18.356369	19.814629	12.546697
O	17.933704	17.163088	12.474160
O	13.693846	2.802575	11.630630
O	13.932108	0.265652	12.377401
O	13.939517	17.492613	12.209044
O	9.751114	0.663632	9.694244
O	9.935917	16.829380	9.629336
O	7.259176	8.958132	9.700534
O	6.331357	8.709593	12.209311
O	3.916703	9.120906	-0.010840
O	1.665830	8.532094	12.060225
O	2.168583	9.112150	9.455224
O	4.665727	8.716359	10.191021
O	7.332257	13.103292	10.212568
O	6.175786	13.008176	12.542013
O	3.829007	12.765607	0.413802
O	1.826407	13.512218	12.205162
O	2.177793	13.098119	9.596816
O	4.678340	13.258505	10.378383
O	5.913297	10.955195	10.795932
O	1.756330	11.036981	11.290702
O	8.674531	7.373177	8.109563
O	8.417449	9.869705	7.376977
O	8.006998	12.511297	7.684518
O	3.598554	7.143144	8.361163
O	3.929518	9.694395	7.697500
O	4.085289	12.354493	7.866394
O	19.844805	9.371037	10.369550
O	19.844604	12.687603	10.552897
O	2.835716	11.201744	3.011309
O	3.754125	11.196173	5.521290
O	6.064464	10.938282	6.856513
O	8.104706	11.444711	5.272635

O	7.915897	10.947434	2.670042
O	5.421957	10.771925	3.513171
O	2.839720	6.541995	3.342940
O	3.676039	6.879482	5.773427
O	6.002796	7.289999	7.104901
O	8.173982	6.465782	5.287356
O	7.812784	6.975595	2.669240
O	5.426162	7.047032	3.761426
O	3.581535	8.944799	4.097340
O	8.340764	8.958529	4.428435
O	1.336268	12.513885	1.254121
O	1.587945	9.871099	0.993955
O	2.095502	7.291591	0.899204
O	6.092895	12.707701	1.827181
O	6.084485	10.270869	0.915130
O	5.679240	7.618531	1.177570
O	10.228038	10.780880	3.748311
O	10.181787	7.216969	3.685410
O	8.427460	14.856593	8.602459
O	3.822800	14.853609	8.451499
O	5.260981	14.933802	0.751455
O	2.333764	14.944944	0.997569
O	1.330462	4.983506	1.840163
O	6.015610	5.139514	1.923137
O	4.750620	5.006788	7.354227
O	7.757924	4.913660	7.613589
O	11.262375	4.958433	4.758058
O	16.190989	5.147274	4.943948
O	14.686937	4.986292	12.717999
O	17.602942	4.884408	12.312093
O	18.692739	14.912112	11.463611
O	14.012397	14.929822	11.709188
O	15.354872	14.933802	6.020209
O	12.499134	14.996483	5.617515
Al	4.506552	18.875992	6.957688
Al	6.322146	3.523715	2.471439
Al	17.634777	6.458419	13.010551
Al	11.436767	12.503736	9.047978
Al	16.247051	3.541624	4.341311
Al	7.621574	6.689845	6.904424
H	8.209020	4.983903	8.479068
H	19.725073	7.239058	12.006961
H	11.550290	13.770107	11.088753
H	11.072165	1.834688	0.265117

H	18.724974	3.611669	4.362456
H	3.160272	16.953550	6.940959
Pt	10.227838	4.990470	-0.878192
Pt	11.417746	3.298458	0.705016
Pt	11.315233	5.894880	1.195503
Pt	9.194902	4.316491	1.345661
	299		
Pt5H1@H-MFI			
Si	8.445279	1.051264	8.766668
Si	6.025620	0.615675	10.818015
Si	5.556305	1.165285	0.391051
Si	2.450693	1.293037	0.147347
Si	1.377514	0.552794	10.787368
Si	3.639599	1.338606	9.023890
Si	8.505746	16.411104	8.981733
Si	6.097900	17.297205	10.891889
Si	5.345073	16.503036	0.445386
Si	2.336767	16.497066	0.432137
Si	1.419760	17.325462	10.948499
Si	3.627786	16.330313	9.075950
Si	1.513263	18.869823	2.023376
Si	3.904691	19.363518	4.008208
Si	7.732897	18.558006	6.892379
Si	8.646100	19.357349	4.060536
Si	6.387218	18.663670	2.215422
Si	1.683249	3.439741	2.230545
Si	3.884468	2.678803	4.359379
Si	4.551601	3.425613	7.189214
Si	7.643398	3.309204	7.027547
Si	8.727189	2.554435	4.169875
Si	11.545886	11.105035	4.629581
Si	13.958937	10.488166	2.675395
Si	14.397619	10.997581	13.068768
Si	17.598135	11.209504	13.200590
Si	18.660704	10.484584	2.614904
Si	16.400219	11.215474	4.459082
Si	11.520859	6.513341	4.298218
Si	13.917493	7.275472	2.419647
Si	14.630075	6.594728	12.893986
Si	18.775629	7.356859	2.449357
Si	16.353567	6.574629	4.235987
Si	18.510738	8.976638	11.182301
Si	16.030815	9.342779	9.284055
Si	15.541276	8.889679	6.320390

Si	12.327945	8.656861	6.447929
Si	11.418146	9.397701	9.248724
Si	13.565705	8.627212	11.096783
Si	18.461685	13.347453	11.106284
Si	16.091480	12.554478	9.150493
Si	15.446172	13.339495	6.191244
Si	12.428857	13.467046	6.241965
Si	13.834601	13.431029	11.118597
Si	11.592537	18.856094	4.610310
Si	13.986167	19.354166	2.625209
Si	14.421245	18.790228	13.065824
Si	17.611551	18.552832	13.246226
Si	18.625265	19.361130	2.628555
Si	16.401421	18.639194	4.470725
Si	11.675629	3.447900	4.489060
Si	13.976957	2.679600	2.434234
Si	14.602645	3.404321	12.867755
Si	17.597336	3.415066	12.916737
Si	18.700348	2.547868	2.311244
Si	18.468092	1.020819	11.363907
Si	16.084272	0.530905	9.325409
Si	15.636181	1.091659	6.400018
Si	12.452282	1.341193	6.527023
Si	11.335855	0.424446	9.229051
Si	13.693246	1.262393	11.090359
Si	18.493320	16.474581	11.117928
Si	16.168566	17.221392	9.144337
Si	15.442367	16.515772	6.218009
Si	12.427254	16.484928	6.257088
Si	11.445577	17.158310	9.155979
Si	13.809974	16.415680	11.022105
Si	8.535979	8.865005	8.683024
Si	6.079480	9.336213	10.719649
Si	5.521667	8.904205	0.235808
Si	2.363397	8.708400	0.167020
Si	1.394332	9.531024	10.795264
Si	3.641001	8.665815	8.924855
Si	8.436270	13.290343	9.040351
Si	6.035431	12.555672	10.985436
Si	5.357286	13.334917	0.526086
Si	2.338169	13.443565	0.372583
Si	1.402741	12.592883	10.934179
Si	3.705071	13.334319	9.080366
Si	1.523874	11.103642	2.058038

Si	3.889273	10.521596	4.040863
Si	4.466107	11.041557	6.981376
Si	7.661618	11.189009	6.815427
Si	8.654710	10.501100	4.052238
Si	6.366796	11.150006	2.248076
Si	1.643005	6.519907	2.265876
Si	3.891276	7.375366	4.249638
Si	4.547596	6.605474	7.126581
Si	8.597246	7.368003	4.036848
Si	6.205018	6.666762	2.391274
O	7.176686	1.076735	9.776014
O	6.343170	1.319304	12.288137
O	3.998393	0.827599	0.075882
O	1.830411	1.490435	12.042292
O	2.085091	1.091062	9.443982
O	4.556006	1.096833	10.370354
O	7.407740	16.761326	10.126782
O	6.094497	16.735060	12.402561
O	3.838417	17.152939	0.420762
O	1.823604	16.498461	12.276628
O	2.164979	16.579050	9.696385
O	4.760431	16.756948	10.115808
O	6.013207	18.904648	10.955056
O	1.836218	18.894102	11.048336
O	8.583832	2.553241	8.125221
O	8.412443	19.906761	7.529543
O	8.344569	17.240494	7.609039
O	3.839619	2.887743	8.547990
O	4.012809	0.327538	7.857026
O	3.672836	17.323870	7.690809
O	19.798353	0.658060	10.520644
O	19.864626	17.176817	10.626771
O	2.838519	18.755007	2.931814
O	3.681045	18.658895	5.434435
O	6.160169	18.571936	7.100886
O	8.259074	18.477814	5.355341
O	7.917099	18.736500	2.755694
O	5.407942	19.006729	3.451743
O	2.663727	3.395167	3.513707
O	3.595751	2.984452	5.946201
O	6.098901	2.813519	7.096737
O	8.331755	3.312188	5.587938
O	7.935920	3.396163	3.006223
O	5.336864	3.232991	4.014900

O	3.746517	1.074745	4.090648
O	8.247663	0.997736	4.358575
O	1.330061	17.402273	1.333348
O	1.587344	0.094520	0.843664
O	2.333965	2.721785	0.922089
O	6.177788	17.153137	1.670466
O	6.176987	19.645090	0.931591
O	5.757726	2.403799	1.333348
O	10.253867	19.152987	3.686481
O	10.359783	2.578114	4.104700
O	12.853522	11.110408	3.671760
O	13.764123	11.103841	1.173555
O	16.014196	10.938480	13.058865
O	18.101688	11.361732	1.344992
O	17.919489	10.860476	4.011688
O	15.439764	10.943455	3.173779
O	12.687540	6.544384	3.173912
O	13.765925	6.964053	0.840720
O	16.108900	7.229904	12.893584
O	18.524553	6.550551	1.088306
O	17.875441	6.793121	3.684206
O	15.355873	6.718897	2.935695
O	13.845413	8.876944	2.681819
O	18.436857	8.941217	2.182366
O	11.431160	12.595868	5.277586
O	11.604751	9.955072	5.781188
O	12.012799	7.303530	5.620325
O	16.339354	12.771974	4.945286
O	15.941317	10.364792	5.763256
O	16.092281	7.726185	5.355877
O	0.183602	10.862267	2.935026
O	0.324557	7.214184	2.923784
O	17.258564	8.782622	10.211764
O	16.262869	8.778047	7.785159
O	13.934912	8.871372	6.446859
O	11.765327	8.454886	7.951911
O	12.035224	8.720936	10.602682
O	14.600042	8.873362	9.859122
O	17.346460	13.195623	9.944507
O	16.187986	13.010563	7.610510
O	13.925502	12.763218	6.182946
O	11.930709	13.511620	7.759196
O	12.245455	13.350239	10.542860
O	14.681131	13.107671	9.788996

O	16.106096	10.957185	9.364085
O	12.011197	10.878983	9.032588
O	18.780436	7.398050	11.802602
O	18.351963	9.949102	12.463856
O	17.943916	12.609598	12.459172
O	13.765526	7.120459	11.627285
O	13.843810	9.698574	12.296434
O	13.935712	12.361458	12.299513
O	9.820590	9.372429	9.537395
O	9.850224	12.837840	9.622377
O	12.846115	18.742271	3.599759
O	13.764524	18.666855	1.162180
O	16.026209	18.820475	13.143712
O	18.108097	18.408367	1.408293
O	17.937107	18.905045	4.015971
O	15.444570	18.906239	3.179935
O	12.837105	3.399943	3.347490
O	13.684035	3.059073	0.831620
O	16.091080	2.735914	12.965718
O	18.118109	3.402729	1.093525
O	18.031212	3.314775	3.697857
O	15.426750	3.231797	2.831709
O	13.932909	1.064597	2.601120
O	18.191790	1.009675	2.262262
O	11.430960	17.419983	5.356546
O	11.681636	0.167749	5.688177
O	12.270482	2.810336	5.866706
O	16.264471	17.086079	4.936855
O	16.092281	19.558926	5.764728
O	16.097086	2.324203	5.518748
O	0.196816	19.230194	2.916424
O	0.265492	2.657114	2.594830
O	17.186083	1.072556	10.374502
O	16.359776	1.159913	7.867331
O	14.020605	0.987388	6.614146
O	11.771734	1.399696	8.015212
O	12.162764	0.913165	10.578191
O	14.595838	0.998532	9.786319
O	17.500229	16.659046	9.861264
O	16.268875	16.837341	7.584146
O	13.930707	17.160698	6.276360
O	11.846216	16.417273	7.776995
O	12.335354	16.574076	10.384540
O	14.856323	16.504032	9.788728

O	16.026810	18.813112	9.368234
O	11.684038	18.763762	8.947071
O	18.608446	2.481007	12.047243
O	18.357370	19.811644	12.551247
O	17.934505	17.162291	12.474428
O	13.834802	2.808943	11.553812
O	14.017801	0.315200	12.372583
O	13.938315	17.501966	12.208241
O	9.776543	0.667412	9.616756
O	9.936117	16.832165	9.629738
O	7.259576	8.958928	9.699731
O	6.330956	8.710191	12.208910
O	3.915502	9.122100	-0.011777
O	1.665430	8.531696	12.060760
O	2.168583	9.112549	9.455491
O	4.665526	8.716757	10.191021
O	7.331656	13.104089	10.213103
O	6.175585	13.008573	12.542280
O	3.825804	12.766999	0.413802
O	1.826006	13.515003	12.204226
O	2.177993	13.098716	9.597618
O	4.678741	13.258904	10.378918
O	5.913097	10.954201	10.795665
O	1.756530	11.036781	11.290836
O	8.674531	7.373177	8.109429
O	8.417449	9.869705	7.378985
O	8.006598	12.511098	7.683047
O	3.598154	7.143144	8.361163
O	3.929317	9.694395	7.697768
O	4.085689	12.354095	7.865725
O	19.844404	9.371633	10.369818
O	19.844604	12.687802	10.552496
O	2.834514	11.210102	3.008900
O	3.754525	11.196173	5.521290
O	6.065064	10.939077	6.856914
O	8.105105	11.442920	5.271297
O	7.915297	10.947037	2.672318
O	5.414350	10.763369	3.514644
O	2.840321	6.536822	3.342271
O	3.674037	6.880477	5.773025
O	6.002595	7.290596	7.105436
O	8.171178	6.465185	5.289765
O	7.780549	6.978181	2.676734
O	5.418754	7.131006	3.767047

O	3.504050	8.951764	4.098678
O	8.346170	8.951167	4.426293
O	1.336068	12.516670	1.253719
O	1.588145	9.871496	0.993822
O	2.095102	7.289601	0.899204
O	6.091693	12.701731	1.830259
O	6.083684	10.271465	0.914327
O	5.676638	7.619725	1.172886
O	10.229039	10.781676	3.747775
O	10.177783	7.147323	3.668414
O	8.426458	14.855400	8.605671
O	3.826004	14.852613	8.452837
O	5.259179	14.926837	0.754132
O	2.330360	14.960069	0.986193
O	1.330862	4.974153	1.840430
O	5.919504	5.159015	1.990454
O	4.746615	5.009573	7.351014
O	7.754721	4.911273	7.609708
O	11.260372	4.977735	4.767694
O	16.189789	5.138718	4.931502
O	14.685336	4.982908	12.716928
O	17.609949	4.883016	12.304999
O	18.693541	14.909525	11.464280
O	14.011795	14.930618	11.709456
O	15.354071	14.931015	6.020075
O	12.497131	14.993896	5.617515
Al	4.486330	18.873405	6.949122
Al	6.206619	3.565702	2.547186
Al	17.642984	6.454041	13.003458
Al	11.437568	12.500552	9.046507
Al	16.240644	3.535455	4.320166
Al	7.624177	6.693028	6.903086
H	8.243458	4.970372	8.456049
H	19.731279	7.253185	12.012314
H	11.544685	13.722151	11.114984
H	9.547091	1.207869	-1.365735
H	18.717966	3.667983	4.295943
H	3.141051	16.954943	6.952736
Pt	11.582326	2.163220	0.819307
Pt	8.412243	0.617864	-0.335646
Pt	10.300919	-0.052135	1.392769
Pt	9.155860	2.313060	1.533558
Pt	11.025114	0.359774	-0.984186

Pt6H2@H-MFI			
Si	8.443878	1.075939	8.766802
Si	6.062661	0.637763	10.822966
Si	5.606761	1.176031	0.343140
Si	2.445888	1.276123	0.177994
Si	1.416757	0.541054	10.820557
Si	3.665828	1.321095	9.043696
Si	8.605656	16.472391	9.053733
Si	6.157566	17.308748	10.917986
Si	5.423960	16.502041	0.482189
Si	2.381617	16.475973	0.441371
Si	1.399137	17.354713	11.015949
Si	3.630789	16.381056	9.129348
Si	1.538290	18.837986	2.052149
Si	3.941531	19.374462	4.056119
Si	7.700661	18.525372	6.931457
Si	8.636290	19.367300	4.146589
Si	6.418252	18.716999	2.209667
Si	1.626387	3.408102	2.322486
Si	3.918305	2.693529	4.343185
Si	4.530578	3.373677	7.251578
Si	7.568116	3.373080	7.184530
Si	8.645499	2.591646	4.355096
Si	11.600546	10.933904	4.618072
Si	14.145342	10.467471	2.709924
Si	14.448276	11.089712	13.130196
Si	17.661806	11.237164	13.244219
Si	18.730181	10.534531	2.679678
Si	16.465893	11.333475	4.515558
Si	11.734694	6.552542	4.477015
Si	14.192994	7.302734	2.551871
Si	14.853320	6.632934	13.073050
Si	18.915182	7.402030	2.708853
Si	16.499529	6.529061	4.439275
Si	18.545376	8.949376	11.321884
Si	16.179577	9.484859	9.352978
Si	15.618361	8.918732	6.419959
Si	12.452682	8.653080	6.604912
Si	11.460192	9.397502	9.388576
Si	13.782543	8.725513	11.169854
Si	18.483709	13.466052	11.134389
Si	16.145540	12.667704	9.246984
Si	15.474202	13.420483	6.279170
Si	12.450480	13.377899	6.230456

Si	13.791153	13.449138	11.148173
Si	11.536275	18.796198	4.640020
Si	13.952129	19.300837	2.645551
Si	14.388410	18.872610	13.090047
Si	17.529261	18.617306	13.227356
Si	18.614452	19.344416	2.558161
Si	16.397617	18.626459	4.410368
Si	11.724883	3.378651	4.547544
Si	13.936713	2.628658	2.460866
Si	14.641287	3.443522	12.964782
Si	17.694641	3.418250	12.995161
Si	18.681126	2.512249	2.408271
Si	18.524153	1.035345	11.382509
Si	16.069656	0.550804	9.424442
Si	15.552089	0.988781	6.482993
Si	12.459691	1.198716	6.572258
Si	11.354275	0.462254	9.330359
Si	13.603747	1.363081	11.159281
Si	18.453676	16.554178	11.114984
Si	16.162157	17.271338	9.154106
Si	15.422145	16.594374	6.231928
Si	12.394018	16.444534	6.308479
Si	11.505442	17.212236	9.241632
Si	13.864033	16.438763	11.035489
Si	8.532375	9.031758	8.797716
Si	5.948536	9.474710	10.674950
Si	5.471012	8.873760	0.281444
Si	2.271896	8.675566	0.172641
Si	1.423164	9.571817	10.752839
Si	3.536686	8.756556	8.706043
Si	8.355982	13.329544	8.932618
Si	5.991183	12.644820	10.986373
Si	5.378310	13.359990	0.487810
Si	2.361795	13.434810	0.258560
Si	1.368103	12.644621	10.810922
Si	3.709075	13.380883	9.009972
Si	1.542295	11.092300	1.997814
Si	3.957949	10.471451	3.957219
Si	4.456296	11.106826	6.856781
Si	7.612164	11.236766	6.797494
Si	8.651505	10.475630	4.040997
Si	6.398831	11.108418	2.153191
Si	1.667432	6.513341	2.234693
Si	4.039639	7.289203	4.123302

Si	4.498142	6.559706	7.051369
Si	8.724386	7.370390	4.215645
Si	6.473713	6.616616	2.357951
O	7.181491	1.161704	9.783508
O	6.347174	1.332238	12.263646
O	4.007003	0.908389	0.149890
O	1.841023	1.499390	12.061429
O	2.112321	0.997139	9.440101
O	4.571623	1.085689	10.382398
O	7.483623	16.745804	10.193563
O	6.167977	16.742222	12.436421
O	3.896281	17.090456	0.416077
O	1.753727	16.493484	12.328018
O	2.166180	16.582832	9.784312
O	4.829707	16.752571	10.118887
O	6.094497	18.910816	10.879442
O	1.847230	18.899473	11.199296
O	8.656111	2.562394	8.115049
O	8.182390	19.973225	7.522317
O	8.510951	17.330238	7.692816
O	3.756928	2.894907	8.610622
O	4.170382	0.395393	7.853011
O	3.588343	17.413017	7.779940
O	19.848209	0.663433	10.532421
O	19.830790	17.322081	10.710281
O	2.760233	18.818285	3.086120
O	3.759731	18.672625	5.488369
O	6.146153	18.316433	7.197110
O	8.099299	18.409163	5.354940
O	7.918100	18.978472	2.748199
O	5.403137	18.987427	3.437825
O	2.589045	3.323332	3.601499
O	3.678442	2.908239	5.949279
O	6.059057	2.737705	7.270717
O	8.092692	3.407505	5.668638
O	8.002593	3.151604	3.010506
O	5.258378	3.397157	3.846943
O	3.841421	1.086883	4.088908
O	8.339964	0.996343	4.599470
O	1.415355	17.331034	1.423817
O	1.664429	0.004776	0.832958
O	2.176391	2.654526	0.998104
O	6.265084	17.173832	1.683983
O	6.173182	19.658819	0.919145

O	5.852631	2.495733	1.176499
O	10.199006	19.070604	3.771195
O	10.267882	2.736511	4.342382
O	12.840109	10.696509	3.609529
O	13.847415	11.109413	1.242612
O	16.065052	11.029817	13.053110
O	18.107496	11.365711	1.408293
O	17.965340	11.017678	4.018112
O	15.435359	11.276565	3.262909
O	12.850320	6.878886	3.340798
O	13.920896	6.964451	0.988201
O	16.334949	7.218562	13.292531
O	18.683529	6.474139	1.419803
O	18.025206	6.963058	4.010082
O	15.525058	6.545577	3.103652
O	14.516950	8.894853	2.679143
O	18.526155	8.959126	2.346709
O	11.593940	12.451202	5.188991
O	11.670223	9.870700	5.859746
O	12.257068	7.230700	5.868044
O	16.436459	12.846795	5.105748
O	16.096285	10.284202	5.692325
O	15.936710	7.623307	5.523031
O	0.259886	10.941863	2.990030
O	0.500350	7.289601	3.094016
O	17.257961	8.784812	10.370354
O	16.412834	8.871571	7.867733
O	14.024610	9.040514	6.698727
O	11.842812	8.467621	8.111437
O	12.171374	8.620445	10.715902
O	14.657305	9.190353	9.876521
O	17.271976	13.510427	10.048091
O	16.188988	13.093741	7.703791
O	13.989371	12.765607	6.193385
O	11.849219	13.337504	7.709010
O	12.180784	13.437396	10.544466
O	14.670320	13.017926	9.868758
O	16.441465	11.087126	9.450005
O	12.025213	10.887539	9.356858
O	18.852915	7.391284	11.967748
O	18.355968	9.874084	12.626727
O	18.100889	12.597659	12.463856
O	14.181783	7.274080	11.712133
O	13.845413	9.789512	12.379542

O	13.923499	12.436676	12.379810
O	9.857030	9.369444	9.691166
O	9.685843	12.603231	9.450941
O	12.845314	18.736500	3.680058
O	13.678629	18.660885	1.160841
O	15.982760	19.065233	13.299223
O	18.111900	18.390856	1.341378
O	17.928499	18.899076	3.946647
O	15.440765	18.821470	3.105793
O	12.585629	3.160956	3.187161
O	13.775736	2.988233	0.878059
O	16.166162	2.817499	12.962774
O	18.185781	3.407505	1.182790
O	17.947319	3.133893	3.840519
O	15.274783	3.315173	3.016127
O	13.935712	1.009675	2.666964
O	18.186983	0.992363	2.185042
O	11.421550	17.334816	5.362568
O	11.602348	0.077606	5.764058
O	12.435063	2.655323	5.843955
O	16.260466	17.088066	4.932706
O	16.099089	19.572060	5.686169
O	15.777135	2.335745	5.678139
O	0.175393	19.229200	2.845895
O	0.224647	2.656317	2.765463
O	17.266771	1.078725	10.372763
O	16.351166	1.064597	7.917651
O	13.978559	0.667213	6.777553
O	11.758120	1.339800	8.031005
O	12.094689	1.087878	10.631455
O	14.662311	1.159316	9.946112
O	17.522654	16.658447	9.789397
O	16.260666	17.012054	7.563670
O	13.883855	17.155127	6.282784
O	11.847818	16.423243	7.858097
O	12.349169	16.497862	10.458681
O	14.867736	16.488510	9.768787
O	15.945320	18.826445	9.537930
O	11.841812	18.803759	9.117704
O	18.689335	2.473247	12.120448
O	18.366381	19.814032	12.546027
O	17.686434	17.238703	12.379007
O	13.765526	2.891723	11.698883
O	13.847816	0.325946	12.388778

O	14.103296	17.576986	12.140388
O	9.754718	0.581250	9.614615
O	10.004793	16.908777	9.777486
O	7.269388	9.283083	9.784312
O	6.092094	8.625023	12.117771
O	3.855236	9.028973	0.322932
O	1.912501	8.612487	11.965205
O	2.089696	9.121304	9.361409
O	4.659720	8.946989	9.876253
O	7.238554	13.173536	10.118752
O	6.252069	13.110257	12.520064
O	3.859241	12.774163	0.247184
O	1.754528	13.524356	12.123259
O	2.162776	13.097919	9.456027
O	4.598453	13.265271	10.373565
O	5.759128	11.032006	11.037897
O	1.749722	11.101851	11.197155
O	8.589237	7.463518	8.284880
O	8.497537	10.042429	7.519373
O	7.766133	12.675861	7.543194
O	3.504651	7.221944	8.194143
O	3.745115	9.778966	7.456874
O	4.170983	12.429314	7.781411
O	19.841402	9.366858	10.459216
O	19.798153	12.772770	10.456539
O	2.925815	11.102845	2.853122
O	3.844624	11.342231	5.352129
O	6.048646	10.782870	6.853434
O	8.101501	11.437547	5.258582
O	7.936520	10.865451	2.612629
O	5.492635	10.613530	3.415074
O	3.084790	6.560502	3.019606
O	3.749920	6.713127	5.603328
O	5.933519	7.289402	7.108113
O	8.265282	6.545179	5.510584
O	8.016007	6.965844	2.780051
O	5.577328	6.972610	3.689292
O	3.668631	8.887888	4.174425
O	8.348974	8.951963	4.507796
O	1.407547	12.497169	1.177704
O	1.431573	9.861347	0.916735
O	1.843225	7.222939	0.757478
O	6.094897	12.663127	1.771106
O	6.099102	10.283604	0.766712

O	5.931717	7.627685	1.168604
O	10.243256	10.697504	3.764370
O	10.343966	7.208413	3.939018
O	8.591841	14.911117	8.619857
O	3.827005	14.920868	8.451900
O	5.338866	14.927832	0.834832
O	2.410048	14.919474	0.918877
O	1.319650	4.957239	1.925948
O	6.339365	5.136131	1.765619
O	4.593447	4.980321	7.365201
O	7.442378	4.916844	7.755047
O	11.668820	4.977337	4.847858
O	16.510542	5.065291	5.097451
O	14.769629	5.043202	12.799100
O	17.852816	4.915650	12.462786
O	18.772026	15.009816	11.544712
O	14.019004	14.943751	11.714675
O	15.350667	15.000663	6.107600
O	12.431259	14.930020	5.696340
Al	4.544393	18.865446	7.006670
Al	6.370600	3.518342	2.496331
Al	17.860224	6.422203	13.301765
Al	11.364286	12.470305	9.101779
Al	16.170166	3.488295	4.475945
Al	7.529073	6.582987	7.069303
H	10.155158	5.420687	9.088262
H	19.305613	6.771232	11.361096
H	11.728086	14.292258	10.725404
H	18.613050	3.560926	4.415721
H	2.954246	17.122293	7.091117
H	6.810283	6.244505	12.685746
Pt	7.126230	4.806802	-3.510227
Pt	10.706764	7.328006	-1.602481
Pt	9.185493	6.212269	-3.372382
Pt	7.123627	4.658157	-0.965985
Pt	8.109110	7.314674	-1.147592
Pt	9.680237	5.051362	-1.203266

297

#### Pt6@Silicalite-1-W\_IS

Si	8.459094	1.062209	8.784334
Si	6.071871	0.545830	10.827249
Si	5.610765	1.207869	0.396940
Si	2.397434	1.361092	0.274887
Si	1.400138	0.539860	10.909420

Si	3.606563	1.206277	9.006492
Si	8.501341	16.476372	9.011978
Si	6.177788	17.207064	10.979145
Si	5.439977	16.500648	0.527156
Si	2.402840	16.442345	0.412196
Si	1.434977	17.327055	10.978878
Si	3.735504	16.389015	9.107533
Si	1.559113	18.803959	2.059108
Si	3.942532	19.293076	4.110722
Si	4.381014	18.732122	7.032901
Si	7.556703	18.564573	6.910446
Si	8.639092	19.371279	4.208686
Si	6.398831	18.690733	2.313385
Si	1.448992	3.411286	2.390873
Si	3.857038	2.628459	4.295408
Si	4.549399	3.427205	7.232441
Si	7.621775	3.493469	7.197378
Si	8.591841	2.566772	4.409698
Si	6.331758	3.476156	2.475454
Si	11.577121	10.977283	4.611514
Si	14.082273	10.568358	2.661611
Si	14.463893	11.143440	13.067429
Si	17.668013	11.321735	13.168738
Si	18.649090	10.497519	2.590547
Si	16.461687	11.237562	4.489461
Si	11.664216	6.558312	4.461357
Si	14.058046	7.368003	2.514532
Si	14.725580	6.674921	12.982448
Si	17.765520	6.550950	13.173958
Si	18.741993	7.395264	2.589209
Si	16.419241	6.468170	4.410234
Si	18.557390	8.877143	11.382376
Si	16.237841	9.522666	9.366629
Si	15.689839	8.792374	6.425312
Si	12.508344	8.645917	6.541878
Si	11.457189	9.493017	9.261304
Si	13.732288	8.858239	11.118196
Si	18.532763	13.486547	11.156337
Si	16.209810	12.687404	9.242434
Si	15.475803	13.377899	6.301787
Si	12.431059	13.387848	6.261237
Si	11.445376	12.579749	9.111682
Si	13.689442	13.408145	11.001897
Si	11.561703	18.817888	4.655678

Si	13.991974	19.372869	2.669106
Si	14.356174	18.800774	13.070107
Si	17.554689	18.615713	13.210092
Si	18.638680	19.337051	2.547588
Si	16.431454	18.658298	4.433520
Si	11.643193	3.383029	4.454398
Si	13.893866	2.684773	2.499409
Si	14.608451	3.481330	12.939354
Si	17.647991	3.497846	13.074389
Si	18.535166	2.529959	2.515201
Si	16.248053	3.444119	4.409431
Si	18.490717	1.119916	11.414897
Si	16.112303	0.623834	9.360338
Si	15.591331	1.098425	6.432807
Si	12.486520	1.245876	6.542146
Si	11.423952	0.551600	9.279103
Si	13.629976	1.326467	11.120605
Si	18.496923	16.539850	11.094775
Si	16.127319	17.287058	9.170835
Si	15.424548	16.512589	6.232463
Si	12.392616	16.452892	6.274486
Si	11.458990	17.337202	9.156917
Si	13.705460	16.450304	11.020634
Si	8.500740	9.134039	8.495796
Si	6.213427	9.392925	10.616467
Si	5.298421	8.802322	0.479647
Si	2.285511	8.676761	0.278634
Si	1.465811	9.453218	10.846654
Si	3.678442	8.903608	8.869315
Si	8.473110	13.382874	8.958848
Si	6.219433	12.528211	10.991324
Si	5.443181	13.366755	0.472688
Si	2.404042	13.402574	0.404167
Si	1.400739	12.572188	10.958670
Si	3.743113	13.306461	9.072068
Si	1.486834	11.019270	2.003703
Si	3.948739	10.471848	3.974483
Si	4.381214	11.095683	6.875650
Si	7.585535	11.391978	6.756274
Si	8.595644	10.499309	4.125310
Si	6.413047	11.096080	2.168314
Si	1.581738	6.525479	2.338947
Si	3.951141	7.254777	4.325787
Si	4.554804	6.592340	7.238195

Si	7.628982	6.588758	7.052707
Si	8.650305	7.410985	4.280419
Si	6.313937	6.569257	2.550934
O	7.253370	1.087480	9.862736
O	6.255673	1.240902	12.289877
O	3.996391	1.165882	0.410457
O	1.920110	1.495410	12.118441
O	2.090096	0.995746	9.522407
O	4.600655	0.985000	10.280821
O	7.503445	16.580046	10.285907
O	6.255673	16.822615	12.546831
O	3.913100	17.086874	0.418486
O	1.829410	16.422644	12.274220
O	2.255678	16.745804	9.698125
O	4.838316	16.585020	10.295542
O	6.170179	18.826244	10.866863
O	1.767142	18.895693	11.290970
O	8.586234	2.560205	8.120002
O	8.262279	19.841293	7.620682
O	7.832806	17.169853	7.696430
O	3.754725	2.727954	8.456182
O	3.848028	0.168943	7.781948
O	4.014211	17.397696	7.863985
O	19.845406	0.751983	10.616065
O	19.871834	17.253229	10.619411
O	2.820699	18.744461	3.081436
O	3.660222	18.652925	5.577633
O	5.978369	18.893902	6.793345
O	8.183592	18.393839	5.424799
O	7.909891	18.982054	2.819530
O	5.416151	18.831221	3.601767
O	2.507355	3.164737	3.591194
O	3.767339	3.071212	5.852787
O	6.100103	2.897295	7.195638
O	8.172580	3.485708	5.676801
O	7.776745	3.077778	3.095890
O	5.171482	3.313979	3.601499
O	3.924913	1.015446	4.175496
O	8.260076	0.995746	4.681374
O	1.420361	17.344765	1.343118
O	1.674440	0.066264	0.923427
O	1.928919	2.731337	1.000112
O	6.259478	17.172041	1.757456
O	6.091693	19.730057	1.100618

O	6.088089	2.560205	1.165392
O	10.206614	19.163931	3.840519
O	10.182187	2.736311	4.180180
O	12.763224	10.941266	3.515313
O	13.852020	11.194979	1.183057
O	16.079268	11.037777	12.973480
O	18.100288	11.370687	1.339638
O	17.948120	11.022653	3.938617
O	15.411533	11.272983	3.255415
O	12.692145	6.886447	3.249259
O	13.848617	7.043848	0.927710
O	16.257063	7.198264	13.281424
O	18.439060	6.476328	1.270984
O	17.915686	6.805060	3.860327
O	15.352068	6.624576	3.174314
O	14.339356	8.961714	2.679410
O	18.285292	8.933258	2.267348
O	11.511648	12.458365	5.283876
O	11.764527	9.864332	5.774899
O	12.188191	7.215178	5.852252
O	16.425848	12.688199	5.190731
O	16.179977	10.035265	5.525841
O	16.020203	7.386310	5.690050
O	0.182601	10.778692	2.932617
O	0.299729	7.296566	3.005956
O	17.270576	8.783220	10.380122
O	16.424847	8.869979	7.880178
O	14.091484	8.953157	6.609195
O	11.923301	8.533288	8.042781
O	12.177780	8.951366	10.622622
O	14.685536	9.356709	9.880267
O	17.346859	13.513809	10.045147
O	16.260466	13.179307	7.704192
O	13.950930	12.761230	6.279304
O	11.843213	13.425060	7.779003
O	12.181184	13.263281	10.396317
O	14.705957	13.009768	9.788461
O	16.596436	11.110806	9.366226
O	11.927106	11.024842	8.949747
O	18.685732	7.470881	12.204226
O	18.442663	10.100733	12.449670
O	18.088076	12.759636	12.542682
O	14.104096	7.357854	11.630095
O	13.847415	9.781552	12.447127

O	13.925100	12.449014	12.287736
O	9.834005	9.359694	9.457900
O	9.844817	12.600246	9.368234
O	12.846115	18.827240	3.674838
O	13.678629	18.819281	1.172083
O	15.962539	18.907433	13.214910
O	18.106895	18.395830	1.335222
O	17.950924	18.842165	3.927777
O	15.433158	18.820274	3.164946
O	12.451682	3.151206	3.073272
O	13.849017	3.068028	0.927576
O	16.129923	2.893713	12.964915
O	18.106895	3.478345	1.258537
O	17.675220	2.904060	3.843865
O	15.104396	3.483718	3.244307
O	14.095888	1.093052	2.753552
O	18.269274	0.975051	2.105681
O	11.431560	17.322477	5.286018
O	11.674627	0.013332	5.856267
O	12.418044	2.640995	5.691255
O	16.269276	17.160101	5.017688
O	16.185585	19.739212	5.610823
O	15.762719	2.484987	5.617247
O	0.195214	19.149008	2.858475
O	0.071278	2.737108	2.923918
O	17.260965	1.162102	10.365936
O	16.356571	1.235330	7.867733
O	14.023008	0.755167	6.691901
O	11.845015	1.494216	8.015748
O	12.098693	1.159913	10.620347
O	14.662711	1.155137	9.873443
O	17.441364	16.653673	9.869293
O	16.191792	16.839727	7.618139
O	13.899272	17.093639	6.271408
O	11.839008	16.503435	7.805635
O	12.189993	16.663820	10.452793
O	14.756615	16.672775	9.793680
O	16.104294	18.898678	9.366361
O	11.923501	18.906040	9.028440
O	18.609648	2.578712	12.135437
O	18.336748	19.882881	12.561151
O	17.846209	17.251240	12.393461
O	13.769529	2.830832	11.712668
O	13.854823	0.237196	12.298442

O	13.937314	17.429533	12.297773
O	9.832403	0.665423	9.545024
O	9.860435	17.257010	9.443581
O	7.104006	9.466153	9.188232
O	5.346475	8.532890	12.281579
O	3.745716	9.123294	0.831352
O	2.086092	8.538462	12.052998
O	2.170785	9.114339	9.437960
O	4.684947	9.521074	9.959228
O	7.438974	13.263679	10.194099
O	6.242859	13.255521	12.453953
O	3.917304	12.765607	0.412598
O	1.824004	13.437994	12.270873
O	2.253676	13.100307	9.690899
O	4.838316	12.932559	10.211364
O	6.425660	10.942659	11.214151
O	1.672838	11.009719	11.292041
O	8.595644	7.619526	7.862781
O	8.599249	10.209579	7.268442
O	7.838413	12.763218	7.594718
O	3.909896	7.314276	8.536614
O	3.763735	9.700961	7.441885
O	3.919907	12.361060	7.771776
O	19.921089	9.116528	10.542325
O	19.854614	12.767796	10.542325
O	2.821500	10.943256	2.920305
O	3.757328	11.276365	5.371936
O	6.010203	11.017280	6.850892
O	8.012403	11.598132	5.184039
O	7.933918	10.780085	2.663619
O	5.428565	10.854109	3.427386
O	2.842323	6.557915	3.361007
O	3.680444	6.874110	5.882766
O	6.096498	7.132200	7.092722
O	8.175383	6.466180	5.521826
O	7.847222	6.962063	2.928736
O	5.421357	6.633332	3.922959
O	3.916904	8.864010	4.178976
O	8.262078	8.963902	4.602816
O	1.420961	12.507119	1.338969
O	1.331263	9.873685	0.839248
O	1.919509	7.218362	0.910446
O	6.265484	12.624921	1.665247
O	6.176587	10.102723	0.911115

O	5.683044	7.529981	1.426762
O	10.189996	10.633628	3.846007
O	10.242854	7.211597	4.015569
O	8.838111	14.934796	8.626013
O	3.841821	14.858186	8.548793
O	5.345874	14.929623	0.849553
O	2.415654	14.923255	0.996900
O	1.243566	4.973357	2.019763
O	6.333960	5.035641	1.924877
O	4.582635	5.004599	7.531417
O	7.680439	5.063500	7.709144
O	11.580725	4.970770	4.770638
O	16.423445	4.950871	5.000290
O	14.677728	5.078424	12.716259
O	17.691839	5.044993	12.552183
O	18.852915	15.022949	11.540429
O	13.926102	14.923255	11.544578
O	15.353669	14.934200	5.937769
O	12.420848	14.921863	5.701694
O	9.680036	8.548411	14.635650
Pt	7.477616	5.205778	-3.059621
Pt	9.160666	6.798295	0.017532
Pt	9.468204	7.030715	-2.580510
Pt	7.114417	5.100910	-0.515647
Pt	7.100602	7.560426	-1.741262
Pt	9.508247	4.682036	-1.460621
H	8.966051	9.219406	14.604332
H	10.473707	9.001711	14.295721

297

#### Pt6@Silicalite-1-1W\_FS

Si	8.461898	1.021814	8.794505
Si	6.070069	0.543641	10.830594
Si	5.612566	1.210257	0.402427
Si	2.397835	1.360495	0.275690
Si	1.398937	0.539263	10.910357
Si	3.605762	1.204486	9.006893
Si	8.503544	16.476969	9.012246
Si	6.178188	17.205471	10.979145
Si	5.440378	16.498461	0.527290
Si	2.403241	16.442345	0.412196
Si	1.433175	17.326458	10.979413
Si	3.734503	16.392797	9.107131
Si	1.557912	18.803560	2.059108
Si	3.942532	19.293472	4.108447

Si	4.378811	18.732521	7.029956
Si	7.552498	18.553230	6.903353
Si	8.639893	19.369091	4.206679
Si	6.399031	18.689539	2.312716
Si	1.449192	3.411485	2.391944
Si	3.864046	2.629056	4.289519
Si	4.545794	3.422827	7.229497
Si	7.627581	3.453670	7.199118
Si	8.598448	2.563389	4.415721
Si	6.353981	3.481927	2.476257
Si	11.581526	10.976686	4.609239
Si	14.087278	10.589252	2.665626
Si	14.440066	11.152593	13.090047
Si	17.645988	11.317358	13.183862
Si	18.673519	10.491549	2.592555
Si	16.490520	11.235373	4.485446
Si	11.666218	6.571247	4.464168
Si	14.064854	7.389493	2.512926
Si	14.722576	6.678104	12.981377
Si	17.762516	6.551547	13.170612
Si	18.714363	7.393474	2.588942
Si	16.394413	6.462797	4.417862
Si	18.555187	8.881919	11.383982
Si	16.234037	9.523264	9.368502
Si	15.689239	8.796949	6.426249
Si	12.506541	8.650494	6.547231
Si	11.445976	9.481476	9.276961
Si	13.728284	8.865801	11.127698
Si	18.519949	13.481174	11.164100
Si	16.208410	12.687603	9.241096
Si	15.477806	13.374516	6.298575
Si	12.431659	13.385262	6.259631
Si	11.451782	12.573382	9.109808
Si	13.688641	13.407747	11.001763
Si	11.562704	18.817688	4.656883
Si	13.991974	19.372274	2.668972
Si	14.355574	18.800177	13.069704
Si	17.553888	18.614918	13.209825
Si	18.637478	19.337051	2.547454
Si	16.430855	18.657303	4.433922
Si	11.653404	3.388999	4.465773
Si	13.890462	2.684176	2.499543
Si	14.607050	3.483320	12.939354
Si	17.646790	3.498045	13.074255

Si	18.534966	2.530158	2.514800
Si	16.245649	3.439542	4.408494
Si	18.489515	1.119717	11.415432
Si	16.111504	0.623038	9.360606
Si	15.590731	1.096833	6.433744
Si	12.486320	1.245479	6.545224
Si	11.426354	0.541850	9.280844
Si	13.628975	1.326666	11.120872
Si	18.495722	16.535870	11.095578
Si	16.126919	17.286062	9.170835
Si	15.424747	16.510399	6.232463
Si	12.393817	16.450901	6.273282
Si	11.460793	17.334219	9.156114
Si	13.705258	16.448713	11.020901
Si	8.517559	9.077924	8.535945
Si	6.189601	9.389144	10.633061
Si	5.349878	8.797945	0.431200
Si	2.295923	8.654672	0.256151
Si	1.470616	9.448045	10.816141
Si	3.679243	8.889281	8.841211
Si	8.492131	13.384864	8.948677
Si	6.233449	12.555274	10.972186
Si	5.443982	13.361979	0.472955
Si	2.403040	13.401977	0.404167
Si	1.398737	12.568009	10.957733
Si	3.742312	13.316809	9.065779
Si	1.511461	11.015092	1.999956
Si	3.961753	10.455133	3.962171
Si	4.430668	11.105035	6.871502
Si	7.630985	11.377253	6.765374
Si	8.619671	10.482395	4.089310
Si	6.436472	11.074590	2.131109
Si	1.560915	6.527469	2.343230
Si	3.940930	7.261145	4.303438
Si	4.554804	6.585574	7.215445
Si	7.626180	6.588957	7.025406
Si	8.648703	7.412576	4.257936
Si	6.335561	6.561695	2.492316
O	7.253170	1.084296	9.865680
O	6.255673	1.242096	12.291348
O	3.996992	1.166678	0.410055
O	1.920510	1.495410	12.118575
O	2.089896	0.995746	9.523075
O	4.600855	0.985995	10.281222

O	7.503644	16.580046	10.285504
O	6.255473	16.822216	12.546831
O	3.913500	17.086079	0.418620
O	1.829410	16.422447	12.274352
O	2.255078	16.746403	9.698526
O	4.838316	16.585220	10.294740
O	6.169779	18.825249	10.867264
O	1.766941	18.895294	11.290970
O	8.588838	2.508070	8.110499
O	8.260076	19.823980	7.616801
O	7.831405	17.166071	7.696296
O	3.754525	2.727755	8.456985
O	3.848228	0.169340	7.781545
O	4.013210	17.400084	7.863717
O	19.845005	0.752182	10.616199
O	19.870632	17.251837	10.619946
O	2.820299	18.744261	3.080499
O	3.658820	18.652725	5.574956
O	5.975966	18.892906	6.790668
O	8.183392	18.388468	5.419713
O	7.910292	18.982254	2.816988
O	5.416351	18.831020	3.601366
O	2.509758	3.165334	3.590793
O	3.767339	3.070814	5.850245
O	6.097700	2.893912	7.197110
O	8.168375	3.485509	5.679879
O	7.819191	3.083350	3.086254
O	5.181093	3.309602	3.601633
O	3.924512	1.015048	4.175630
O	8.258875	0.994154	4.681374
O	1.420361	17.344366	1.343118
O	1.674440	0.065866	0.923427
O	1.929320	2.731735	0.999978
O	6.259278	17.171045	1.757322
O	6.091493	19.729063	1.100350
O	6.092494	2.560603	1.167131
O	10.207816	19.164728	3.840519
O	10.191197	2.733526	4.249237
O	12.770831	10.942859	3.521870
O	13.850619	11.262634	1.209020
O	16.055841	11.031807	13.048426
O	18.111101	11.371084	1.347936
O	17.996374	11.025042	3.954141
O	15.430354	11.273181	3.258493

O	12.682735	6.959476	3.252470
O	13.847615	7.044246	0.931189
O	16.255461	7.198662	13.281557
O	18.436657	6.474538	1.266969
O	17.873037	6.808641	3.850156
O	15.341456	6.623183	3.173645
O	14.344161	8.979424	2.673254
O	18.278484	8.935447	2.265207
O	11.512049	12.457769	5.284813
O	11.764927	9.864730	5.776906
O	12.189993	7.216372	5.856936
O	16.431053	12.686408	5.189259
O	16.183981	10.035862	5.523298
O	16.016998	7.387106	5.694065
O	0.224447	10.706260	2.929137
O	0.269496	7.290794	3.006759
O	17.270977	8.783816	10.380257
O	16.424246	8.870577	7.881516
O	14.091283	8.953953	6.609864
O	11.918695	8.533288	8.046930
O	12.181184	8.949178	10.626504
O	14.685135	9.356709	9.885085
O	17.346859	13.514605	10.041265
O	16.260666	13.178908	7.702987
O	13.952930	12.760831	6.279036
O	11.844415	13.423865	7.778334
O	12.182786	13.263878	10.391766
O	14.705758	13.010166	9.787925
O	16.596636	11.111005	9.366629
O	11.920498	11.015291	8.951354
O	18.685532	7.473070	12.203824
O	18.437658	10.107897	12.451811
O	18.018999	12.762223	12.538533
O	14.104498	7.361436	11.631032
O	13.848617	9.785334	12.457700
O	13.925701	12.450605	12.285192
O	9.832603	9.286067	9.517990
O	9.851825	12.597659	9.366494
O	12.846115	18.827438	3.674972
O	13.678829	18.819281	1.171949
O	15.962139	18.907433	13.214910
O	18.106895	18.395830	1.334954
O	17.950323	18.842564	3.927911
O	15.433158	18.820475	3.164946

O	12.446675	3.150012	3.076484
O	13.848215	3.068227	0.928111
O	16.128521	2.894508	12.965050
O	18.106895	3.478345	1.258404
O	17.674820	2.904060	3.843598
O	15.102594	3.482723	3.243638
O	14.095287	1.093052	2.753552
O	18.269073	0.975250	2.105547
O	11.431761	17.322678	5.286419
O	11.674427	0.014526	5.856401
O	12.426254	2.642388	5.696742
O	16.269476	17.159704	5.017822
O	16.185585	19.739012	5.610823
O	15.762119	2.483196	5.617916
O	0.194213	19.149008	2.857940
O	0.071278	2.736908	2.924186
O	17.260765	1.162102	10.365803
O	16.356571	1.235131	7.868134
O	14.022608	0.754172	6.692972
O	11.842212	1.492624	8.019495
O	12.097492	1.159515	10.619411
O	14.662109	1.154938	9.873443
O	17.441563	16.653275	9.869428
O	16.191990	16.839727	7.618006
O	13.900072	17.093241	6.271274
O	11.838808	16.502640	7.803895
O	12.189795	16.663223	10.453060
O	14.756413	16.673174	9.793813
O	16.104496	18.898279	9.366361
O	11.928306	18.901463	9.027369
O	18.609247	2.578712	12.135571
O	18.336748	19.882484	12.561284
O	17.846409	17.250643	12.393461
O	13.769931	2.830832	11.712668
O	13.854823	0.237196	12.298308
O	13.937314	17.429533	12.297639
O	9.829600	0.597368	9.547566
O	9.861635	17.258005	9.443046
O	7.083783	9.296017	9.209512
O	5.432369	8.618257	12.200747
O	3.783557	9.044494	0.755470
O	2.086092	8.534482	12.033191
O	2.162776	9.119314	9.383625
O	4.678140	9.449637	9.962841

O	7.488628	13.262286	10.205876
O	6.242659	13.245371	12.451544
O	3.915502	12.765208	0.411126
O	1.823403	13.434611	12.269802
O	2.255478	13.098318	9.690363
O	4.849929	13.003399	10.213103
O	6.424860	10.955195	11.130239
O	1.675841	11.000963	11.284278
O	8.607858	7.567192	7.870409
O	8.603453	10.200624	7.354762
O	7.843218	12.763816	7.593514
O	3.914101	7.300745	8.524302
O	3.838017	9.699170	7.436666
O	3.924913	12.356483	7.772713
O	19.921089	9.116130	10.540451
O	19.850210	12.766403	10.550220
O	2.834114	10.951016	2.922714
O	3.837617	11.279947	5.357482
O	6.054252	11.014296	6.853970
O	8.085284	11.543610	5.207593
O	7.941726	10.852915	2.667634
O	5.436373	10.699493	3.348293
O	2.831712	6.552144	3.352843
O	3.682646	6.867941	5.863360
O	6.093495	7.127424	7.024335
O	8.178987	6.463394	5.509514
O	7.849625	6.959874	2.916825
O	5.416952	6.716709	3.843865
O	3.828807	8.862417	4.184730
O	8.262879	8.960520	4.598265
O	1.419560	12.504532	1.340307
O	1.400539	9.879456	0.829880
O	1.913903	7.214980	0.911382
O	6.255273	12.615170	1.667656
O	6.184395	10.116652	0.842460
O	5.763332	7.458145	1.265363
O	10.210419	10.625270	3.838244
O	10.243054	7.209208	4.019450
O	8.840914	14.938179	8.622667
O	3.837617	14.865349	8.541164
O	5.346274	14.926837	0.847144
O	2.415254	14.922658	0.996498
O	1.240763	4.972561	2.018826
O	6.331758	5.022110	1.938394

O	4.585839	5.000818	7.530079
O	7.686445	5.049371	7.702318
O	11.588933	4.978730	4.766623
O	16.416037	4.945101	5.001629
O	14.677327	5.080414	12.717063
O	17.691839	5.044795	12.550979
O	18.852514	15.018572	11.541767
O	13.926302	14.923255	11.544444
O	15.354271	14.932806	5.937502
O	12.421448	14.921066	5.701426
O	10.262276	8.196597	14.629359
Pt	7.409542	5.114043	-3.408249
Pt	9.614764	6.974599	-0.085517
Pt	9.396324	6.675915	-2.603261
Pt	6.239056	5.297910	-1.185332
Pt	7.308831	7.703897	-1.585216
Pt	8.696355	4.804614	-0.951665
H	9.421151	8.288730	12.743427
H	11.183488	7.974923	14.867845

300

#### Pt6@Silicalite-1-2W\_IS

Si	8.460496	1.024997	8.789286
Si	6.056455	0.534288	10.820424
Si	5.601955	1.208466	0.405906
Si	2.391628	1.363281	0.274887
Si	1.397535	0.538865	10.910089
Si	3.600956	1.206874	9.002610
Si	8.499939	16.463240	9.008767
Si	6.175585	17.196318	10.982491
Si	5.437775	16.486919	0.537461
Si	2.402240	16.440155	0.412598
Si	1.433575	17.325861	10.979012
Si	3.733302	16.387821	9.104723
Si	1.558913	18.803360	2.059510
Si	3.944334	19.294270	4.108715
Si	4.383616	18.731726	7.030090
Si	7.559506	18.548853	6.890505
Si	8.636290	19.370085	4.182054
Si	6.397429	18.689739	2.306426
Si	1.449793	3.414270	2.393148
Si	3.863245	2.630051	4.292865
Si	4.556807	3.413872	7.231638
Si	7.614166	3.453471	7.208218
Si	8.598047	2.562991	4.422814

Si	6.358587	3.467998	2.482680
Si	11.571314	10.975891	4.612853
Si	14.082072	10.585273	2.664555
Si	14.446672	11.148813	13.087103
Si	17.649593	11.316959	13.178909
Si	18.650692	10.498315	2.591350
Si	16.464891	11.237363	4.491602
Si	11.664415	6.572441	4.459484
Si	14.062852	7.385514	2.512524
Si	14.724979	6.679100	12.982046
Si	17.765921	6.553338	13.173155
Si	18.737389	7.396657	2.588005
Si	16.416437	6.470359	4.410903
Si	18.560392	8.880924	11.382376
Si	16.236040	9.522268	9.369170
Si	15.688638	8.793368	6.427454
Si	12.505941	8.647906	6.547499
Si	11.461594	9.503762	9.267461
Si	13.726683	8.862816	11.122879
Si	18.521351	13.480378	11.162761
Si	16.206005	12.687404	9.243103
Si	15.474803	13.376307	6.302055
Si	12.428255	13.384266	6.267527
Si	11.451583	12.582536	9.128945
Si	13.690442	13.407150	11.008856
Si	11.562104	18.817888	4.655277
Si	13.992575	19.373667	2.669373
Si	14.358377	18.799780	13.071444
Si	17.556490	18.614717	13.209958
Si	18.638880	19.338047	2.547588
Si	16.431854	18.657900	4.433654
Si	11.651602	3.390590	4.465372
Si	13.890662	2.685967	2.500747
Si	14.608851	3.485509	12.941228
Si	17.647791	3.500035	13.074522
Si	18.535967	2.531153	2.515335
Si	16.248053	3.445512	4.409297
Si	18.489716	1.120911	11.415699
Si	16.112904	0.623038	9.359802
Si	15.591731	1.098823	6.432271
Si	12.486920	1.245876	6.542012
Si	11.424152	0.546626	9.283385
Si	13.635582	1.328059	11.123682
Si	18.496723	16.535074	11.095712

Si	16.128120	17.285864	9.170835
Si	15.424747	16.511196	6.232196
Si	12.393618	16.450304	6.272077
Si	11.456989	17.330437	9.156515
Si	13.707061	16.449110	11.021169
Si	8.528770	9.140207	8.522696
Si	6.195407	9.447846	10.566147
Si	5.277599	8.748993	0.413267
Si	2.292919	8.669198	0.283318
Si	1.477023	9.447846	10.830594
Si	3.664426	8.924105	8.814044
Si	8.467704	13.358199	8.951889
Si	6.205619	12.542738	11.001763
Si	5.442980	13.368745	0.485268
Si	2.402440	13.400385	0.402427
Si	1.399738	12.568009	10.957064
Si	3.740910	13.311038	9.067518
Si	1.487835	11.017878	2.002364
Si	3.955346	10.477221	3.961636
Si	4.397232	11.100857	6.857985
Si	7.592342	11.320939	6.747307
Si	8.586434	10.482594	4.085161
Si	6.412846	11.042751	2.096179
Si	1.577734	6.527469	2.338679
Si	3.953744	7.271891	4.301965
Si	4.554404	6.586768	7.248233
Si	7.620573	6.576222	7.060470
Si	8.639293	7.404219	4.269311
Si	6.331557	6.553935	2.485223
O	7.254571	1.081909	9.871434
O	6.261480	1.241300	12.288003
O	3.993188	1.166081	0.406174
O	1.919909	1.495211	12.117371
O	2.088695	0.994950	9.522808
O	4.596250	0.985597	10.280954
O	7.503845	16.580046	10.285237
O	6.252069	16.812466	12.551247
O	3.914701	17.083689	0.418085
O	1.829610	16.423042	12.274352
O	2.255478	16.746403	9.698125
O	4.836915	16.585020	10.294205
O	6.170380	18.821270	10.869673
O	1.766941	18.895294	11.290836
O	8.589838	2.505085	8.110232

O	8.268085	19.819405	7.621217
O	7.834008	17.165674	7.694021
O	3.753524	2.727158	8.457253
O	3.850431	0.168147	7.781814
O	4.015212	17.400084	7.863851
O	19.844204	0.752182	10.615932
O	19.870832	17.252234	10.619946
O	2.822301	18.744062	3.080633
O	3.662224	18.652925	5.575492
O	5.983574	18.894499	6.789598
O	8.180188	18.386278	5.398435
O	7.921304	18.987825	2.774965
O	5.420155	18.832214	3.599626
O	2.510158	3.163742	3.591194
O	3.769742	3.070615	5.851985
O	6.097500	2.832026	7.196173
O	8.165772	3.483121	5.685099
O	7.823596	3.078972	3.088930
O	5.181694	3.307811	3.602168
O	3.925313	1.015048	4.175229
O	8.258875	0.989975	4.678831
O	1.420761	17.344765	1.342984
O	1.674640	0.065667	0.923427
O	1.928319	2.731934	1.000915
O	6.260078	17.172239	1.757456
O	6.089291	19.729261	1.094328
O	6.095297	2.549062	1.169942
O	10.208817	19.164927	3.836772
O	10.190598	2.732730	4.252181
O	12.760420	10.941465	3.518792
O	13.844612	11.254676	1.203801
O	16.058443	11.030613	13.046819
O	18.104492	11.373473	1.342047
O	17.950323	11.022256	3.940491
O	15.417340	11.275570	3.257288
O	12.684338	6.958681	3.255415
O	13.849017	7.044047	0.929985
O	16.257263	7.198862	13.282360
O	18.438059	6.475930	1.270314
O	17.911079	6.805856	3.859524
O	15.348264	6.626765	3.174448
O	14.342359	8.978230	2.673120
O	18.283089	8.934851	2.266545
O	11.509846	12.457968	5.285883

O	11.764126	9.864133	5.775032
O	12.186991	7.215975	5.855865
O	16.426249	12.688797	5.191534
O	16.179977	10.034866	5.526644
O	16.019602	7.386907	5.690987
O	0.183802	10.777896	2.932081
O	0.291921	7.294973	3.006357
O	17.271976	8.783816	10.380792
O	16.424046	8.869979	7.881918
O	14.090483	8.953356	6.609462
O	11.921499	8.534284	8.047868
O	12.178982	8.952361	10.623425
O	14.685536	9.357107	9.884417
O	17.345259	13.514804	10.041666
O	16.259066	13.179307	7.704727
O	13.949928	12.761230	6.279572
O	11.844415	13.425856	7.786899
O	12.170373	13.258306	10.438473
O	14.699552	13.011160	9.787925
O	16.595634	11.111204	9.366761
O	11.936915	11.033000	8.950150
O	18.685732	7.472870	12.203824
O	18.437458	10.106901	12.449938
O	18.018398	12.763218	12.537061
O	14.105098	7.361835	11.631433
O	13.846614	9.784338	12.456362
O	13.928304	12.448616	12.289475
O	9.847219	9.447249	9.448934
O	9.848221	12.601241	9.370108
O	12.846315	18.827438	3.674838
O	13.678829	18.819479	1.172083
O	15.964141	18.907831	13.214776
O	18.107296	18.396029	1.335490
O	17.950924	18.842960	3.927911
O	15.433158	18.820475	3.165080
O	12.446675	3.149813	3.077555
O	13.848415	3.068028	0.928379
O	16.129522	2.894310	12.964782
O	18.106895	3.478146	1.258537
O	17.674820	2.904060	3.843731
O	15.102594	3.483320	3.245244
O	14.095287	1.093848	2.753418
O	18.269474	0.975648	2.105681
O	11.431360	17.322876	5.286151

O	11.674027	0.013929	5.856535
O	12.426053	2.642786	5.696876
O	16.269276	17.160101	5.017688
O	16.185385	19.739212	5.610823
O	15.762519	2.484987	5.616979
O	0.195615	19.149008	2.858743
O	0.072079	2.736709	2.924186
O	17.260365	1.162102	10.365936
O	16.356173	1.235529	7.867733
O	14.022608	0.754769	6.693374
O	11.839008	1.490435	8.019361
O	12.098494	1.161306	10.622622
O	14.661309	1.154341	9.872773
O	17.441563	16.653473	9.869695
O	16.191591	16.839928	7.618006
O	13.899073	17.093439	6.271274
O	11.838608	16.503832	7.803761
O	12.189993	16.664021	10.453060
O	14.756413	16.673571	9.793412
O	16.104094	18.898479	9.366361
O	11.918896	18.904648	9.028306
O	18.609247	2.578911	12.135704
O	18.337149	19.882881	12.561016
O	17.846409	17.250841	12.393060
O	13.769931	2.831429	11.713605
O	13.854623	0.236400	12.298575
O	13.937113	17.430729	12.297505
O	9.826597	0.669999	9.612473
O	9.857030	17.253428	9.442376
O	7.167476	9.625345	9.198939
O	5.172684	8.530901	12.212657
O	3.748519	9.045290	0.907635
O	2.088295	8.541248	12.051927
O	2.159973	9.122498	9.397811
O	4.685148	9.597884	9.861130
O	7.436371	13.256913	10.194634
O	6.242459	13.270246	12.463990
O	3.916904	12.767596	0.411795
O	1.824004	13.437396	12.267796
O	2.252475	13.099314	9.688490
O	4.841920	13.004395	10.217252
O	6.344371	10.955394	11.282538
O	1.674840	11.005540	11.288159
O	8.595244	7.557441	7.954855

O	8.601851	10.112274	7.197244
O	7.843218	12.687006	7.603551
O	3.850231	7.315668	8.518146
O	3.752723	9.695190	7.367074
O	3.925513	12.355289	7.773382
O	19.925093	9.116528	10.542459
O	19.849810	12.766999	10.549284
O	2.818097	10.951614	2.920438
O	3.835014	11.343425	5.341289
O	6.016811	10.944251	6.852765
O	8.004995	11.542813	5.174403
O	7.946331	10.768146	2.603663
O	5.430167	10.768742	3.350301
O	2.838118	6.554133	3.359802
O	3.747317	6.870130	5.861486
O	6.098300	7.132598	7.104500
O	8.175383	6.470956	5.532934
O	7.849425	6.955496	2.919502
O	5.423159	6.713724	3.841055
O	3.834814	8.876347	4.185667
O	8.260276	8.956938	4.593581
O	1.419560	12.507119	1.337497
O	1.336468	9.872293	0.837374
O	1.910499	7.211995	0.907100
O	6.262481	12.599450	1.661901
O	6.181792	10.041433	0.840319
O	5.766536	7.448394	1.274062
O	10.187995	10.628852	3.839717
O	10.235646	7.209806	4.016372
O	8.832105	14.921464	8.622131
O	3.837817	14.862165	8.540629
O	5.346875	14.925046	0.918341
O	2.415254	14.922260	0.996097
O	1.241965	4.972959	2.020699
O	6.335161	5.003006	1.928490
O	4.589643	4.992460	7.530347
O	7.676635	5.038626	7.703523
O	11.587732	4.979526	4.766623
O	16.422045	4.951667	4.999354
O	14.677728	5.080812	12.716660
O	17.691639	5.045789	12.551782
O	18.852314	15.018572	11.541634
O	13.927503	14.924449	11.545381
O	15.353470	14.933802	5.937769

O	12.419646	14.919673	5.703701
O	9.011501	2.564384	12.297371
O	9.088185	8.591393	13.564607
Pt	7.129834	5.011563	-3.320055
Pt	9.260776	7.169808	-0.518859
Pt	9.030522	6.781778	-3.028172
Pt	6.483123	5.000619	-0.914193
Pt	6.888969	7.529782	-1.861709
Pt	9.009099	4.761632	-1.180782
H	8.082281	2.265700	12.191111
H	9.513653	2.150485	11.568533
H	8.974661	9.466153	13.135950
H	8.942626	8.736656	14.516809

300

#### Pt6@Silicalite-1-2W\_FS

Si	8.465302	1.051861	8.786609
Si	6.059258	0.534288	10.815740
Si	5.595748	1.188567	0.402828
Si	2.387023	1.362087	0.275021
Si	1.395734	0.537671	10.909956
Si	3.600156	1.205481	9.002209
Si	8.502542	16.465427	9.010239
Si	6.176587	17.196318	10.982358
Si	5.438175	16.485525	0.536926
Si	2.402440	16.439758	0.412598
Si	1.432574	17.324865	10.978745
Si	3.733502	16.383642	9.106061
Si	1.556911	18.801968	2.060580
Si	3.943333	19.291882	4.109786
Si	4.384017	18.729137	7.031963
Si	7.560907	18.557211	6.901881
Si	8.636690	19.369091	4.188478
Si	6.399031	18.684166	2.310174
Si	1.447190	3.414668	2.393014
Si	3.861042	2.627464	4.290456
Si	4.544794	3.424220	7.227757
Si	7.621574	3.487698	7.198314
Si	8.602653	2.562195	4.420137
Si	6.356585	3.455063	2.482011
Si	11.569712	11.000566	4.615530
Si	14.071261	10.585073	2.664689
Si	14.434260	11.148215	13.092321
Si	17.638380	11.316562	13.179847
Si	18.645687	10.500106	2.591618

Si	16.459486	11.236567	4.488658
Si	11.663815	6.578211	4.456807
Si	14.050638	7.393474	2.507439
Si	14.721775	6.683079	12.982046
Si	17.762716	6.553537	13.171683
Si	18.712761	7.395264	2.589744
Si	16.387606	6.467772	4.412375
Si	18.551382	8.882117	11.385052
Si	16.231033	9.522468	9.368903
Si	15.685835	8.795358	6.427721
Si	12.503939	8.653479	6.540540
Si	11.473407	9.508141	9.259296
Si	13.721076	8.865204	11.126225
Si	18.517546	13.479583	11.163563
Si	16.203403	12.686408	9.243237
Si	15.476604	13.375113	6.301653
Si	12.434463	13.393420	6.271140
Si	11.463797	12.572784	9.126671
Si	13.688040	13.404962	11.010462
Si	11.562304	18.817490	4.655678
Si	13.992373	19.373468	2.669240
Si	14.357575	18.798586	13.071177
Si	17.555490	18.614321	13.209690
Si	18.636877	19.338245	2.547588
Si	16.431053	18.657303	4.434055
Si	11.654406	3.395366	4.465640
Si	13.890862	2.685967	2.499811
Si	14.610053	3.488096	12.940960
Si	17.647390	3.500632	13.074255
Si	18.533964	2.531551	2.515603
Si	16.246050	3.444517	4.409029
Si	18.488314	1.120712	11.416234
Si	16.112904	0.622242	9.359267
Si	15.591532	1.098226	6.432271
Si	12.487521	1.246274	6.541610
Si	11.422551	0.547222	9.283653
Si	13.636583	1.327462	11.123549
Si	18.495722	16.533682	11.095712
Si	16.127319	17.285069	9.170701
Si	15.425749	16.509804	6.232329
Si	12.396421	16.453688	6.273416
Si	11.458390	17.330637	9.157318
Si	13.706861	16.446722	11.021704
Si	8.553598	9.223783	8.441729

Si	6.261480	9.399094	10.578727
Si	5.309033	8.731880	0.422234
Si	2.280305	8.664224	0.278768
Si	1.460805	9.454811	10.849598
Si	3.667830	8.890277	8.849108
Si	8.478716	13.354816	8.912945
Si	6.215229	12.508711	10.992529
Si	5.446985	13.366358	0.476167
Si	2.403641	13.400385	0.403096
Si	1.396735	12.573382	10.958135
Si	3.743913	13.299099	9.069392
Si	1.485632	11.019270	2.005309
Si	3.959551	10.464288	3.954007
Si	4.403238	11.085335	6.873509
Si	7.583733	11.400734	6.691768
Si	8.581830	10.509259	4.070707
Si	6.418252	11.044541	2.093637
Si	1.561916	6.529857	2.346709
Si	3.951742	7.265523	4.299423
Si	4.551201	6.590947	7.242879
Si	7.631385	6.637510	7.037317
Si	8.645299	7.419143	4.268106
Si	6.338765	6.532444	2.505565
O	7.255372	1.086883	9.869293
O	6.260879	1.240106	12.287201
O	3.989583	1.165285	0.403497
O	1.919509	1.495211	12.116567
O	2.088695	0.995348	9.523075
O	4.596851	0.986592	10.280554
O	7.503644	16.580046	10.285639
O	6.252069	16.814257	12.551247
O	3.914901	17.083292	0.418353
O	1.829811	16.423042	12.274352
O	2.255879	16.746004	9.697858
O	4.837315	16.584822	10.294872
O	6.170380	18.822065	10.869138
O	1.767342	18.894897	11.290435
O	8.589437	2.552843	8.122009
O	8.268085	19.834528	7.624965
O	7.834008	17.168657	7.696028
O	3.755126	2.727357	8.456718
O	3.850431	0.167749	7.781814
O	4.015412	17.397099	7.864654
O	19.843603	0.752381	10.615797

O	19.870432	17.252035	10.620080
O	2.821500	18.744062	3.080901
O	3.662224	18.652527	5.577633
O	5.983174	18.895494	6.793211
O	8.182190	18.393839	5.412353
O	7.920302	18.987228	2.780988
O	5.419555	18.831818	3.600429
O	2.509357	3.163742	3.590525
O	3.766739	3.069819	5.850379
O	6.099502	2.896697	7.196441
O	8.168776	3.485907	5.681084
O	7.825398	3.077380	3.087726
O	5.180892	3.304428	3.602971
O	3.924712	1.013058	4.175898
O	8.258875	0.991567	4.679634
O	1.420761	17.344168	1.342984
O	1.674240	0.064075	0.923695
O	1.928319	2.732133	1.001048
O	6.260078	17.169455	1.758125
O	6.088890	19.719313	1.094729
O	6.101104	2.512249	1.180247
O	10.207415	19.164728	3.838244
O	10.193399	2.732730	4.250441
O	12.760020	10.944650	3.526153
O	13.846214	11.263630	1.209556
O	16.049034	11.031209	13.047087
O	18.104092	11.374666	1.340709
O	17.948523	11.023051	3.940892
O	15.412535	11.274774	3.257288
O	12.683936	6.955496	3.256485
O	13.849017	7.042655	0.927977
O	16.256662	7.199060	13.280219
O	18.436857	6.474936	1.267638
O	17.870235	6.808641	3.849219
O	15.335851	6.625372	3.170433
O	14.344361	8.980418	2.673923
O	18.279884	8.937635	2.264805
O	11.510448	12.495378	5.277988
O	11.761523	9.871894	5.770884
O	12.186991	7.217367	5.854928
O	16.427050	12.688199	5.191132
O	16.180779	10.034866	5.526778
O	16.016798	7.387106	5.694199
O	0.181600	10.777896	2.931814

O	0.268295	7.291193	3.008365
O	17.269976	8.783816	10.379587
O	16.423445	8.870178	7.882186
O	14.089682	8.954550	6.608659
O	11.926304	8.534880	8.041577
O	12.176179	8.950969	10.621151
O	14.684134	9.356112	9.886022
O	17.344458	13.514804	10.041265
O	16.259665	13.179506	7.705128
O	13.951929	12.762025	6.280910
O	11.845416	13.426652	7.787702
O	12.168771	13.259500	10.438071
O	14.698550	13.011957	9.788058
O	16.595634	11.111204	9.367029
O	11.999986	11.033598	8.953495
O	18.685732	7.473070	12.203824
O	18.435856	10.108493	12.451677
O	18.017597	12.762223	12.537462
O	14.104498	7.361635	11.629694
O	13.847415	9.783940	12.456227
O	13.928104	12.449809	12.289609
O	9.856030	9.443469	9.399149
O	9.852426	12.596864	9.360740
O	12.846115	18.827837	3.674838
O	13.678829	18.819479	1.172083
O	15.963540	18.907831	13.214776
O	18.107296	18.396029	1.335222
O	17.950523	18.843956	3.928178
O	15.433158	18.820475	3.164946
O	12.446075	3.149614	3.076082
O	13.847816	3.067829	0.927308
O	16.129522	2.894110	12.964647
O	18.107096	3.478146	1.258270
O	17.674221	2.904060	3.843999
O	15.102795	3.482524	3.243370
O	14.094887	1.093848	2.753285
O	18.269474	0.975847	2.105280
O	11.431360	17.323870	5.287222
O	11.673827	0.014725	5.856401
O	12.426053	2.643184	5.696608
O	16.269676	17.159903	5.017688
O	16.185385	19.739012	5.610957
O	15.762319	2.483992	5.617113
O	0.194213	19.149008	2.858743

O	0.071078	2.736311	2.924320
O	17.260164	1.162102	10.365803
O	16.356173	1.235330	7.867733
O	14.022608	0.754570	6.693508
O	11.839008	1.491032	8.019228
O	12.098293	1.161903	10.623158
O	14.661710	1.154540	9.872640
O	17.441563	16.653673	9.869561
O	16.192392	16.840126	7.618006
O	13.902075	17.096624	6.271809
O	11.839008	16.505026	7.804698
O	12.190194	16.664419	10.453462
O	14.756013	16.673969	9.793680
O	16.104294	18.898081	9.366494
O	11.918495	18.905842	9.028841
O	18.609247	2.578911	12.135839
O	18.337149	19.882484	12.561151
O	17.846609	17.250643	12.393060
O	13.769329	2.831628	11.714006
O	13.854423	0.236201	12.298710
O	13.936913	17.430529	12.297237
O	9.824995	0.675372	9.607254
O	9.858232	17.255617	9.443046
O	7.196106	9.616192	9.199073
O	5.345874	8.456677	12.209980
O	3.761533	9.044891	0.822385
O	2.085491	8.538263	12.051927
O	2.175390	9.119314	9.444116
O	4.756627	9.450035	9.880267
O	7.426360	13.179903	10.127585
O	6.243059	13.264076	12.447796
O	3.918105	12.767796	0.410055
O	1.824004	13.439187	12.269267
O	2.252875	13.099314	9.689292
O	4.836314	12.930967	10.212434
O	6.349977	10.919179	11.286152
O	1.673239	11.011311	11.292174
O	8.589838	7.707679	7.787969
O	8.668725	10.279426	7.193095
O	7.842617	12.775356	7.525663
O	3.839619	7.295172	8.519485
O	3.757128	9.701360	7.434659
O	3.926114	12.355091	7.766691
O	19.918285	9.117523	10.544065

O	19.848608	12.767796	10.549417
O	2.819698	10.949027	2.918966
O	3.834213	11.279748	5.354672
O	6.028023	10.946837	6.856111
O	7.929513	11.601316	5.103340
O	7.940525	10.768146	2.594428
O	5.428765	10.769538	3.345884
O	2.832913	6.553736	3.358196
O	3.742913	6.869931	5.860014
O	6.090492	7.136179	7.103429
O	8.173181	6.467175	5.516205
O	7.849825	6.956292	2.923918
O	5.421357	6.708351	3.848415
O	3.834814	8.867990	4.181117
O	8.265081	8.975444	4.592778
O	1.420160	12.506920	1.337631
O	1.338471	9.871894	0.838980
O	1.910299	7.212790	0.914460
O	6.261480	12.599649	1.655879
O	6.179190	10.041433	0.836973
O	5.759929	7.457150	1.326925
O	10.176982	10.699892	3.848951
O	10.235447	7.211398	4.016774
O	8.834707	14.925643	8.626414
O	3.841421	14.854604	8.547455
O	5.348476	14.922658	0.914594
O	2.415454	14.922460	0.996632
O	1.240563	4.973357	2.021235
O	6.333759	4.989675	1.934914
O	4.584437	4.998828	7.533558
O	7.681440	5.079419	7.694556
O	11.586931	4.981516	4.766356
O	16.415037	4.948682	5.000290
O	14.677527	5.082006	12.716125
O	17.692039	5.045392	12.551113
O	18.852314	15.017975	11.541634
O	13.927703	14.924051	11.545247
O	15.353870	14.933602	5.937903
O	12.423050	14.926041	5.705307
O	9.006096	2.414346	12.642920
O	9.686844	8.464040	14.387260
Pt	7.015909	5.072852	-3.516785
Pt	9.073569	7.144736	-0.237682
Pt	9.164870	6.040143	-2.531796

Pt	6.445082	4.857147	-1.096603
Pt	6.986877	7.385116	-1.872014
Pt	8.848522	4.648407	-0.308880
H	8.115316	2.127203	12.343810
H	9.601350	2.272665	11.882096
H	8.917999	8.998129	14.679947
H	10.563406	6.954700	12.925436

306

#### Pt6@Silicalite-1-4W\_IS

Si	8.448883	1.058428	8.775233
Si	6.053051	0.531303	10.818416
Si	5.598952	1.216028	0.411527
Si	2.389426	1.363479	0.275957
Si	1.398136	0.537870	10.910491
Si	3.599154	1.207272	9.001272
Si	8.494934	16.460253	9.008767
Si	6.173783	17.194328	10.983696
Si	5.436773	16.483934	0.538398
Si	2.402840	16.437370	0.413267
Si	1.434176	17.324865	10.979682
Si	3.732101	16.387424	9.104188
Si	1.558312	18.801769	2.059108
Si	3.943133	19.293472	4.108983
Si	4.382616	18.731525	7.030492
Si	7.558505	18.554823	6.899606
Si	8.633687	19.372074	4.188344
Si	6.396428	18.690136	2.306828
Si	1.450193	3.419245	2.391810
Si	3.855036	2.627862	4.295542
Si	4.553403	3.415863	7.229898
Si	7.606157	3.470187	7.197913
Si	8.595644	2.569359	4.413178
Si	6.329354	3.492673	2.486026
Si	11.577321	10.973901	4.610310
Si	14.092084	10.577313	2.666295
Si	14.466295	11.141450	13.069437
Si	17.672218	11.319347	13.173824
Si	18.683329	10.489161	2.589075
Si	16.494724	11.233782	4.483171
Si	11.666018	6.571446	4.461357
Si	14.061049	7.383325	2.511588
Si	14.724979	6.678502	12.982581
Si	17.768124	6.555726	13.175162
Si	18.753605	7.396657	2.587336

Si	16.422443	6.481503	4.397922
Si	18.563597	8.878535	11.379832
Si	16.238642	9.520876	9.367164
Si	15.689439	8.794165	6.423439
Si	12.503539	8.648503	6.552719
Si	11.455988	9.500778	9.278033
Si	13.731288	8.857841	11.118731
Si	18.534365	13.481772	11.156872
Si	16.212214	12.685613	9.241764
Si	15.479008	13.372725	6.298575
Si	12.430858	13.383073	6.261103
Si	11.451182	12.574775	9.110477
Si	13.690242	13.403171	11.001629
Si	11.560502	18.817688	4.656347
Si	13.993977	19.370682	2.670712
Si	14.360979	18.794607	13.072648
Si	17.558693	18.613922	13.210627
Si	18.639881	19.350185	2.542101
Si	16.432455	18.665262	4.434859
Si	11.657408	3.389596	4.452926
Si	13.926302	2.682982	2.492985
Si	14.624069	3.485111	12.943101
Si	17.657000	3.503617	13.075057
Si	18.540972	2.534337	2.514130
Si	16.260267	3.441532	4.392033
Si	18.491518	1.120712	11.416101
Si	16.119513	0.621446	9.355654
Si	15.589929	1.104395	6.428658
Si	12.485919	1.249259	6.538533
Si	11.405932	0.562346	9.283520
Si	13.643191	1.318110	11.119534
Si	18.497925	16.535671	11.095042
Si	16.128521	17.284271	9.169765
Si	15.427551	16.509804	6.229787
Si	12.395619	16.449509	6.272077
Si	11.444375	17.323473	9.157586
Si	13.706460	16.445131	11.019830
Si	8.502743	9.079913	8.652244
Si	6.109713	9.470134	10.662103
Si	5.411146	8.741431	0.305668
Si	2.354387	8.663030	0.258158
Si	1.478024	9.442871	10.823903
Si	3.650611	8.921517	8.794772
Si	8.481318	13.361979	8.945599

Si	6.215630	12.594476	10.988112
Si	5.444782	13.364567	0.490353
Si	2.402039	13.395808	0.403364
Si	1.404143	12.562836	10.956797
Si	3.739108	13.312829	9.062031
Si	1.523274	11.005141	1.994335
Si	3.970162	10.475630	3.970870
Si	4.401836	11.098667	6.859323
Si	7.608360	11.292483	6.806862
Si	8.600650	10.484584	4.120358
Si	6.414047	11.047924	2.120001
Si	1.592750	6.533041	2.329445
Si	3.939929	7.273283	4.323914
Si	4.537986	6.588957	7.242879
Si	7.609561	6.584380	7.052172
Si	8.643698	7.406806	4.273459
Si	6.308932	6.589554	2.545313
O	7.250968	1.084893	9.870097
O	6.258076	1.241698	12.288405
O	3.991986	1.166479	0.406576
O	1.919909	1.495012	12.117371
O	2.088094	0.994950	9.522942
O	4.594648	0.985995	10.280821
O	7.501643	16.579449	10.285907
O	6.251869	16.813858	12.552183
O	3.914301	17.083689	0.418219
O	1.829410	16.423042	12.274888
O	2.255078	16.746998	9.698258
O	4.836114	16.585220	10.294070
O	6.170580	18.820871	10.869673
O	1.767342	18.895096	11.290970
O	8.588437	2.549460	8.116254
O	8.271088	19.828756	7.627374
O	7.833007	17.168261	7.695091
O	3.754125	2.727556	8.458056
O	3.850030	0.168545	7.781814
O	4.015011	17.401079	7.864252
O	19.844604	0.751784	10.615664
O	19.871235	17.253428	10.619678
O	2.821500	18.743864	3.080633
O	3.662224	18.652527	5.576027
O	5.982974	18.896688	6.792140
O	8.182190	18.393839	5.410881
O	7.920903	18.988621	2.777910

O	5.419755	18.832613	3.599893
O	2.506754	3.162946	3.591328
O	3.765538	3.069421	5.853456
O	6.095898	2.833817	7.195771
O	8.165172	3.485111	5.681218
O	7.775544	3.072605	3.099503
O	5.168479	3.307811	3.606183
O	3.924312	1.013456	4.175898
O	8.259875	0.993358	4.677493
O	1.420761	17.343967	1.342716
O	1.674440	0.065070	0.923427
O	1.928519	2.732531	1.000781
O	6.260278	17.173832	1.756920
O	6.090292	19.733242	1.094596
O	6.092695	2.562991	1.169139
O	10.206014	19.163931	3.837442
O	10.191598	2.732929	4.256865
O	12.766828	10.942062	3.515580
O	13.854022	11.197166	1.185199
O	16.082672	11.038572	12.975756
O	18.106695	11.367502	1.346464
O	17.997974	11.025439	3.948119
O	15.428351	11.273779	3.257556
O	12.684136	6.956890	3.255147
O	13.848215	7.042853	0.928513
O	16.256863	7.197071	13.282360
O	18.439661	6.475732	1.271519
O	17.921692	6.808244	3.857382
O	15.347864	6.627959	3.170165
O	14.345162	8.971265	2.677403
O	18.285292	8.931666	2.266946
O	11.512449	12.456574	5.282136
O	11.764927	9.864133	5.775702
O	12.187591	7.216571	5.857070
O	16.431053	12.685613	5.188188
O	16.183582	10.036061	5.522094
O	16.020603	7.385116	5.688311
O	0.231254	10.706060	2.926996
O	0.308939	7.296167	3.005153
O	17.271976	8.783220	10.380658
O	16.425047	8.870178	7.878706
O	14.090483	8.952760	6.609730
O	11.914692	8.535477	8.053086
O	12.183786	8.950172	10.626771

O	14.687537	9.355714	9.881338
O	17.347860	13.514009	10.045414
O	16.260866	13.179705	7.703523
O	13.952930	12.761230	6.278501
O	11.844415	13.426652	7.778200
O	12.183187	13.265072	10.395647
O	14.709562	13.010563	9.789263
O	16.596836	11.110209	9.366093
O	11.935715	11.027230	8.948142
O	18.685732	7.471279	12.203156
O	18.443665	10.100136	12.449938
O	18.088274	12.758841	12.544288
O	14.105699	7.355268	11.629961
O	13.849818	9.780955	12.449268
O	13.926302	12.447819	12.288806
O	9.850423	9.444861	9.531239
O	9.853827	12.599848	9.368100
O	12.845114	18.827837	3.674570
O	13.678430	18.819479	1.171682
O	15.965542	18.908030	13.214643
O	18.106895	18.397421	1.337631
O	17.944317	18.904846	3.932193
O	15.433358	18.818285	3.165213
O	12.509144	3.155982	3.098298
O	13.847216	3.065839	0.920215
O	16.139334	2.891126	12.962641
O	18.107695	3.480136	1.258671
O	17.687634	2.899284	3.846140
O	15.176476	3.476156	3.170968
O	14.098290	1.089669	2.752214
O	18.270676	0.983409	2.096313
O	11.431761	17.322876	5.287088
O	11.674227	0.013929	5.856802
O	12.424452	2.643582	5.695939
O	16.272280	17.163683	5.015815
O	16.182381	19.740803	5.614838
O	15.761719	2.489962	5.607879
O	0.193813	19.148609	2.857137
O	0.075082	2.737108	2.923383
O	17.261166	1.162102	10.366204
O	16.355772	1.237718	7.865457
O	14.022206	0.756759	6.693641
O	11.840610	1.492226	8.018960
O	12.100896	1.163694	10.623693

O	14.666716	1.155137	9.871837
O	17.441765	16.654070	9.869695
O	16.191990	16.839928	7.617068
O	13.901875	17.092844	6.271007
O	11.839209	16.505226	7.804564
O	12.189795	16.666407	10.451856
O	14.756213	16.674168	9.793412
O	16.103895	18.898081	9.366093
O	11.847818	18.910019	9.028975
O	18.611248	2.578712	12.134902
O	18.337149	19.882881	12.561151
O	17.846409	17.250841	12.393060
O	13.766726	2.829837	11.714140
O	13.854823	0.234808	12.299646
O	13.936513	17.429136	12.296702
O	9.815585	0.747406	9.616087
O	9.849222	17.249249	9.446257
O	7.091392	9.456005	9.284724
O	5.080983	8.708001	12.049652
O	3.834213	9.040115	0.755470
O	2.084490	8.534880	12.038009
O	2.150763	9.121901	9.384830
O	4.683546	9.613207	9.796758
O	7.483022	13.266863	10.208151
O	6.242459	13.280593	12.466533
O	3.917104	12.768194	0.412063
O	1.823604	13.435804	12.268196
O	2.254077	13.099710	9.688087
O	4.842721	13.018723	10.210694
O	6.344171	11.016286	11.214285
O	1.675241	11.000764	11.286286
O	8.598047	7.542716	7.952580
O	8.591640	10.111479	7.357304
O	7.840815	12.692577	7.611046
O	3.845425	7.310494	8.521626
O	3.747718	9.693996	7.354896
O	3.926314	12.354692	7.772579
O	19.923891	9.116329	10.539380
O	19.856218	12.767199	10.542191
O	2.839520	10.952210	2.924052
O	3.835614	11.347007	5.345572
O	6.022617	10.941465	6.855709
O	8.087086	11.527291	5.255906
O	7.936120	10.777298	2.661879

O	5.462402	10.760982	3.400754
O	2.843925	6.552741	3.360204
O	3.680644	6.868140	5.879554
O	6.086688	7.133194	7.098343
O	8.175583	6.469961	5.532131
O	7.851427	6.960472	2.924721
O	5.426563	6.710540	3.925368
O	3.833412	8.875153	4.187675
O	8.262279	8.955346	4.602548
O	1.420160	12.500552	1.340307
O	1.414554	9.870502	0.831218
O	1.920710	7.219357	0.901747
O	6.261079	12.603629	1.671001
O	6.183794	10.105309	0.827872
O	5.682243	7.533562	1.418464
O	10.196604	10.626265	3.837174
O	10.238449	7.209806	4.015703
O	8.835908	14.925046	8.617448
O	3.836415	14.865150	8.537952
O	5.346475	14.924847	0.919546
O	2.414253	14.920669	0.995963
O	1.243967	4.975944	2.018157
O	6.329555	5.041411	1.988848
O	4.589643	4.992858	7.528874
O	7.673231	5.048973	7.701114
O	11.587532	4.977934	4.764348
O	16.424646	4.953657	4.946892
O	14.678928	5.077429	12.715055
O	17.691839	5.046984	12.551648
O	18.852915	15.020959	11.540696
O	13.926102	14.922062	11.544578
O	15.354872	14.932608	5.937100
O	12.421247	14.920469	5.701426
O	10.184991	3.153594	14.716885
O	8.844718	2.485783	12.212523
O	9.619970	8.037804	14.435038
O	11.187093	4.393699	12.545492
Pt	7.125229	5.073449	-3.378003
Pt	9.346869	7.187917	-0.649477
Pt	8.942426	6.874706	-3.099369
Pt	6.531577	5.040417	-0.989807
Pt	6.939425	7.734144	-1.476413
Pt	9.016507	4.730390	-1.112663
H	9.482419	3.803495	14.465818

H	9.835808	2.327387	14.338011
H	7.880859	2.296146	12.146679
H	9.239752	2.121830	11.395624
H	8.848322	8.636564	14.520555
H	10.400428	8.616864	14.357818
H	11.641191	3.884285	11.848372
H	11.140841	3.814638	13.362792

306

Pt6@Silicalite-1-4W\_FS

Si	8.449684	1.060617	8.774697
Si	6.052050	0.529910	10.814937
Si	5.596950	1.207670	0.408583
Si	2.387824	1.361888	0.275021
Si	1.396735	0.537273	10.909956
Si	3.598154	1.206675	9.001139
Si	8.495735	16.457069	9.008901
Si	6.174584	17.193134	10.982759
Si	5.437174	16.485128	0.537327
Si	2.402640	16.438564	0.412598
Si	1.433175	17.324667	10.978878
Si	3.732501	16.385433	9.104321
Si	1.556911	18.801172	2.060045
Si	3.942932	19.293076	4.109250
Si	4.383417	18.730532	7.031295
Si	7.559706	18.554623	6.900543
Si	8.635889	19.371279	4.188612
Si	6.397630	18.688145	2.308300
Si	1.448992	3.414469	2.392077
Si	3.855636	2.628260	4.295809
Si	4.555005	3.413475	7.232040
Si	7.605156	3.474167	7.194166
Si	8.599048	2.567966	4.413178
Si	6.330356	3.481529	2.480004
Si	11.567511	10.971712	4.605492
Si	14.057446	10.565374	2.652511
Si	14.456484	11.139858	13.066760
Si	17.662807	11.319745	13.169006
Si	18.658300	10.507269	2.592689
Si	16.445068	11.236766	4.478487
Si	11.666218	6.574232	4.457075
Si	14.053241	7.384121	2.506904
Si	14.720574	6.680890	12.982046
Si	17.765520	6.556522	13.175832
Si	18.759012	7.394667	2.589744

Si	16.417639	6.484288	4.394844
Si	18.558792	8.879133	11.380368
Si	16.234438	9.520876	9.366629
Si	15.687636	8.793965	6.423707
Si	12.504940	8.649100	6.544822
Si	11.458190	9.500380	9.265587
Si	13.725281	8.858040	11.119266
Si	18.531160	13.481772	11.156337
Si	16.209009	12.685016	9.241632
Si	15.475803	13.373522	6.300181
Si	12.427855	13.380088	6.260032
Si	11.447577	12.574974	9.110344
Si	13.687039	13.401977	11.001629
Si	11.561904	18.816692	4.656749
Si	13.993977	19.371078	2.670444
Si	14.360179	18.793810	13.072648
Si	17.557491	18.613724	13.210494
Si	18.638279	19.349789	2.542235
Si	16.431654	18.664665	4.435126
Si	11.659410	3.392381	4.453193
Si	13.926102	2.683380	2.492584
Si	14.622466	3.487698	12.943101
Si	17.654598	3.503816	13.074656
Si	18.538568	2.534138	2.514130
Si	16.259665	3.443522	4.392301
Si	18.490116	1.120911	11.416502
Si	16.118912	0.621048	9.355387
Si	15.590130	1.104792	6.428391
Si	12.486520	1.249060	6.537730
Si	11.407535	0.561749	9.282985
Si	13.643591	1.318110	11.120202
Si	18.496723	16.535074	11.094775
Si	16.127522	17.283873	9.169497
Si	15.426351	16.509804	6.229921
Si	12.395420	16.447319	6.271408
Si	11.444775	17.322081	9.157318
Si	13.706059	16.443539	11.020232
Si	8.532375	9.148765	8.513194
Si	6.209022	9.417003	10.567618
Si	5.321847	8.774663	0.408717
Si	2.289315	8.668005	0.270470
Si	1.474420	9.447647	10.821629
Si	3.661423	8.911170	8.807085
Si	8.467504	13.354418	8.950685

Si	6.207821	12.541544	10.993600
Si	5.444582	13.366954	0.483795
Si	2.402640	13.399390	0.398546
Si	1.401740	12.566019	10.953049
Si	3.742312	13.309048	9.064841
Si	1.490838	11.019469	2.001428
Si	3.957148	10.479809	3.960565
Si	4.400836	11.100458	6.849152
Si	7.596947	11.331883	6.725493
Si	8.589638	10.496722	4.079674
Si	6.424059	11.063048	2.109830
Si	1.588145	6.524882	2.335334
Si	3.954345	7.274676	4.302501
Si	4.554804	6.584579	7.245557
Si	7.621574	6.590947	7.050566
Si	8.649103	7.418745	4.268642
Si	6.344371	6.569456	2.490844
O	7.250968	1.084893	9.869428
O	6.257275	1.240305	12.286665
O	3.990985	1.166081	0.405639
O	1.919709	1.495012	12.116835
O	2.087694	0.994950	9.522942
O	4.594048	0.985995	10.280687
O	7.501843	16.579649	10.285772
O	6.252069	16.815054	12.551782
O	3.914501	17.084087	0.418219
O	1.829610	16.423243	12.274352
O	2.255478	16.746599	9.697991
O	4.836114	16.585020	10.294070
O	6.170380	18.820673	10.869539
O	1.767542	18.894897	11.290702
O	8.586635	2.555231	8.117994
O	8.271088	19.830547	7.627374
O	7.833407	17.167862	7.695493
O	3.753524	2.726760	8.458056
O	3.850231	0.168147	7.781814
O	4.015212	17.399687	7.864252
O	19.844004	0.751983	10.615797
O	19.870832	17.253229	10.619678
O	2.821300	18.744261	3.080767
O	3.662424	18.652925	5.576562
O	5.983574	18.896488	6.792943
O	8.182190	18.394438	5.411550
O	7.920903	18.988621	2.778712

O	5.419555	18.832613	3.599893
O	2.507555	3.163344	3.591194
O	3.767339	3.069819	5.853189
O	6.096899	2.832623	7.194701
O	8.165172	3.485111	5.679344
O	7.775544	3.074395	3.099637
O	5.169880	3.311194	3.602971
O	3.925113	1.014252	4.175362
O	8.259675	0.993358	4.677091
O	1.420761	17.343769	1.342984
O	1.674440	0.064075	0.923561
O	1.929320	2.731735	1.000379
O	6.260078	17.172836	1.757054
O	6.090492	19.730455	1.094997
O	6.092695	2.553639	1.166328
O	10.207215	19.164129	3.837575
O	10.193000	2.733128	4.256597
O	12.757617	10.942261	3.518792
O	13.851419	11.198561	1.179310
O	16.076263	11.039169	12.973883
O	18.100288	11.370886	1.339371
O	17.939512	11.023051	3.934468
O	15.371289	11.280146	3.266389
O	12.685939	6.952312	3.256753
O	13.849216	7.040664	0.926907
O	16.256262	7.196871	13.280754
O	18.440462	6.476925	1.272456
O	17.920691	6.811627	3.856178
O	15.346062	6.628556	3.168024
O	14.346364	8.968081	2.677135
O	18.350363	8.938233	2.261593
O	11.510448	12.455182	5.282805
O	11.764126	9.864929	5.775166
O	12.187191	7.214980	5.856133
O	16.426249	12.686807	5.189125
O	16.180578	10.035464	5.524235
O	16.021004	7.384718	5.688311
O	0.191010	10.784861	2.935293
O	0.315146	7.293780	3.009703
O	17.271578	8.783220	10.379454
O	16.425047	8.869781	7.878706
O	14.090683	8.952560	6.609596
O	11.921499	8.532890	8.046127
O	12.178782	8.951366	10.620347

O	14.685736	9.354520	9.881071
O	17.347061	13.514009	10.044477
O	16.260466	13.179903	7.703791
O	13.950930	12.761626	6.279438
O	11.843012	13.426652	7.778334
O	12.181584	13.266664	10.392168
O	14.707160	13.011160	9.788461
O	16.596636	11.110009	9.366226
O	11.936315	11.029021	8.947874
O	18.686333	7.471676	12.203557
O	18.442863	10.101528	12.449000
O	18.088076	12.758841	12.543218
O	14.104698	7.354671	11.627016
O	13.851419	9.779762	12.443915
O	13.926102	12.450008	12.287201
O	9.844216	9.449240	9.445187
O	9.847420	12.600445	9.368368
O	12.845513	18.827837	3.674570
O	13.678229	18.819281	1.171816
O	15.964742	18.908030	13.214643
O	18.106895	18.397223	1.337363
O	17.943916	18.904648	3.932461
O	15.433358	18.818483	3.165080
O	12.509144	3.155782	3.098165
O	13.847014	3.065839	0.919948
O	16.137531	2.891126	12.962641
O	18.107897	3.480136	1.258404
O	17.687435	2.899483	3.846542
O	15.176476	3.476156	3.170968
O	14.098290	1.089868	2.752214
O	18.270876	0.983210	2.096179
O	11.431560	17.322876	5.287356
O	11.674027	0.013929	5.856936
O	12.424252	2.643582	5.696073
O	16.272079	17.163683	5.016082
O	16.182381	19.741003	5.614838
O	15.761919	2.490360	5.607745
O	0.193012	19.148808	2.857270
O	0.074282	2.736511	2.923650
O	17.260765	1.162102	10.365936
O	16.355972	1.237718	7.865457
O	14.022407	0.756759	6.693641
O	11.840409	1.492425	8.018559
O	12.100696	1.163893	10.623693

O	14.666314	1.154938	9.871837
O	17.441563	16.654268	9.869561
O	16.191990	16.840324	7.616934
O	13.900874	17.093639	6.271007
O	11.839008	16.505226	7.804163
O	12.189593	16.666607	10.451989
O	14.755814	16.674566	9.793546
O	16.104094	18.898081	9.366093
O	11.847217	18.909821	9.028841
O	18.610849	2.578911	12.135169
O	18.337149	19.882683	12.561284
O	17.846609	17.250841	12.393060
O	13.766326	2.829837	11.714006
O	13.854623	0.234609	12.299780
O	13.936513	17.429136	12.296434
O	9.815986	0.748003	9.615686
O	9.848822	17.248453	9.445856
O	7.168476	9.621166	9.193050
O	5.332459	8.538263	12.202753
O	3.766739	9.041509	0.831753
O	2.086693	8.539855	12.043363
O	2.157971	9.123493	9.387907
O	4.691355	9.526447	9.871302
O	7.437372	13.261091	10.193698
O	6.240857	13.264873	12.460242
O	3.916904	12.767796	0.410992
O	1.825205	13.437595	12.262710
O	2.253676	13.098716	9.684340
O	4.840719	13.007180	10.216047
O	6.344171	10.951614	11.217630
O	1.675841	11.002954	11.286553
O	8.595445	7.563013	7.948164
O	8.599249	10.118840	7.189750
O	7.839814	12.686210	7.603551
O	3.843823	7.304525	8.514131
O	3.756527	9.695987	7.368279
O	3.929718	12.352504	7.771375
O	19.924091	9.115533	10.540318
O	19.855217	12.767199	10.541789
O	2.821300	10.949624	2.916691
O	3.827405	11.343425	5.338211
O	6.018413	10.944650	6.780631
O	8.014806	11.588580	5.160217
O	7.941325	10.774712	2.609685

O	5.428965	10.769339	3.350836
O	2.843724	6.552342	3.358865
O	3.747317	6.868936	5.859881
O	6.095497	7.134190	7.103429
O	8.175783	6.473145	5.527581
O	7.859235	6.952312	2.923383
O	5.423159	6.715515	3.837174
O	3.834814	8.876745	4.184195
O	8.258875	8.966091	4.594786
O	1.420160	12.507715	1.335757
O	1.340473	9.870700	0.837508
O	1.914704	7.213189	0.904691
O	6.261480	12.611389	1.666050
O	6.173383	10.099141	0.831218
O	5.836012	7.469289	1.258002
O	10.185992	10.630245	3.843999
O	10.238650	7.210004	4.017845
O	8.831103	14.919673	8.620660
O	3.837617	14.861568	8.539157
O	5.346675	14.925046	0.916468
O	2.414853	14.921663	0.995160
O	1.244367	4.972362	2.017621
O	6.333759	5.017931	1.923806
O	4.589643	4.990470	7.528874
O	7.670428	5.051560	7.702051
O	11.586731	4.978730	4.764750
O	16.425848	4.955647	4.945420
O	14.679330	5.078225	12.714252
O	17.692440	5.047183	12.552051
O	18.853115	15.020760	11.540429
O	13.925901	14.921663	11.544310
O	15.354470	14.933602	5.937368
O	12.420848	14.919673	5.701560
O	10.184589	3.150808	14.717151
O	8.850525	2.403401	12.217743
O	9.674830	8.454886	14.226531
O	11.186491	4.392107	12.544823
Pt	7.046742	5.010369	-3.346018
Pt	9.343667	7.191499	-0.582963
Pt	9.115616	6.655818	-3.100574
Pt	6.520364	4.976740	-0.931724
Pt	6.982872	7.467498	-1.939732
Pt	9.005095	4.700940	-1.117079
H	9.487225	3.822797	14.528988

H	9.817787	2.359623	14.281535
H	7.892472	2.195059	12.146813
H	9.265982	2.025718	11.418108
H	8.866342	8.976837	14.400912
H	10.665919	7.917812	12.018068
H	11.631380	3.849064	11.867242
H	11.136637	3.839313	13.380056

312

Pt6@Silicalite-1-6W\_IS

Si	8.461297	1.060020	8.786877
Si	6.056455	0.533293	10.821761
Si	5.595148	1.209859	0.409921
Si	2.387023	1.363479	0.276493
Si	1.397335	0.538069	10.910357
Si	3.600156	1.207670	9.003815
Si	8.497136	16.458662	9.010239
Si	6.173584	17.196716	10.979012
Si	5.435773	16.489704	0.527692
Si	2.401839	16.436176	0.412866
Si	1.433575	17.325064	10.979280
Si	3.731100	16.384439	9.104188
Si	1.558112	18.801172	2.059108
Si	3.936726	19.297653	4.113667
Si	4.379612	18.731525	7.034640
Si	7.554101	18.559200	6.917673
Si	8.636690	19.375656	4.224076
Si	6.382813	18.686554	2.315125
Si	1.446589	3.419643	2.392211
Si	3.856437	2.633434	4.293400
Si	4.552402	3.416459	7.230433
Si	7.603554	3.474167	7.202463
Si	8.591040	2.577915	4.416524
Si	6.329555	3.495856	2.474249
Si	11.584329	10.960567	4.619143
Si	14.118112	10.623281	2.674592
Si	14.479911	11.146823	13.071311
Si	17.678625	11.318551	13.189348
Si	18.681726	10.497320	2.626414
Si	16.495525	11.244726	4.497223
Si	11.655005	6.588758	4.490799
Si	14.087278	7.440037	2.569536
Si	14.719373	6.665767	13.053243
Si	17.771727	6.556124	13.207148
Si	18.747799	7.395662	2.639529

Si	16.421043	6.471155	4.426159
Si	18.553185	8.873960	11.391744
Si	16.217619	9.492420	9.371982
Si	15.681030	8.797348	6.426919
Si	12.496531	8.636166	6.586577
Si	11.464797	9.494012	9.323535
Si	13.730887	8.811675	11.159682
Si	18.530962	13.477592	11.158746
Si	16.194193	12.684420	9.246315
Si	15.477206	13.374715	6.304464
Si	12.428255	13.377301	6.266590
Si	11.457789	12.577561	9.130954
Si	13.688841	13.409738	11.013540
Si	11.563906	18.817888	4.659961
Si	13.995378	19.376253	2.672585
Si	14.374794	18.814903	13.077199
Si	17.570105	18.614519	13.209290
Si	18.640081	19.338644	2.549328
Si	16.432856	18.656904	4.435662
Si	11.646996	3.403127	4.468316
Si	13.891263	2.689748	2.506636
Si	14.612856	3.485509	12.948320
Si	17.648991	3.504015	13.075727
Si	18.535166	2.531750	2.516673
Si	16.248653	3.447701	4.410903
Si	18.491718	1.124293	11.415432
Si	16.118912	0.621645	9.356993
Si	15.590930	1.099619	6.431067
Si	12.487521	1.251050	6.541075
Si	11.405332	0.565132	9.285929
Si	13.643991	1.325870	11.118463
Si	18.497925	16.533283	11.093704
Si	16.128120	17.284868	9.170032
Si	15.422345	16.509205	6.232196
Si	12.391816	16.446125	6.275021
Si	11.446377	17.327055	9.159192
Si	13.708862	16.457468	11.025317
Si	8.501141	9.066382	8.638191
Si	6.099702	9.463169	10.664110
Si	5.417753	8.740636	0.304865
Si	2.355588	8.662632	0.257355
Si	1.458402	9.443667	10.829658
Si	3.616374	8.922911	8.802669
Si	8.484323	13.359791	8.941986

Si	6.217832	12.590694	10.981554
Si	5.446785	13.355412	0.480048
Si	2.401839	13.394017	0.403765
Si	1.402541	12.562836	10.956930
Si	3.738708	13.308651	9.059220
Si	1.529681	11.001560	1.998350
Si	4.002798	10.461700	3.955078
Si	4.404840	11.085733	6.862669
Si	7.612164	11.295070	6.789063
Si	8.598648	10.476823	4.098410
Si	6.443280	11.050114	2.112774
Si	1.591549	6.533837	2.329177
Si	3.957348	7.254777	4.315482
Si	4.495339	6.589753	7.251712
Si	7.556903	6.583783	7.072782
Si	8.585835	7.408597	4.311468
Si	6.310934	6.574232	2.535275
O	7.247363	1.087679	9.866884
O	6.254472	1.237320	12.292955
O	3.990184	1.164888	0.408717
O	1.919909	1.495012	12.117638
O	2.088495	0.994950	9.523343
O	4.596050	0.985995	10.282025
O	7.502244	16.579250	10.286174
O	6.255673	16.823212	12.548838
O	3.913300	17.085878	0.418888
O	1.829610	16.423042	12.274487
O	2.255078	16.746599	9.698258
O	4.836114	16.584822	10.293668
O	6.170980	18.822065	10.868200
O	1.767142	18.895096	11.290836
O	8.586835	2.552644	8.120135
O	8.269887	19.833334	7.632192
O	7.832406	17.166866	7.697768
O	3.753725	2.727158	8.458458
O	3.849029	0.169142	7.782750
O	4.014611	17.399288	7.864788
O	19.844604	0.752580	10.615129
O	19.871035	17.253031	10.619678
O	2.822501	18.744062	3.080901
O	3.661023	18.653124	5.578971
O	5.979570	18.895693	6.795486
O	8.180388	18.393839	5.428279
O	7.913095	18.984442	2.812839

O	5.415751	18.833012	3.605514
O	2.506154	3.163344	3.590525
O	3.766739	3.069620	5.852386
O	6.094697	2.834414	7.196039
O	8.163169	3.487300	5.684697
O	7.773341	3.074595	3.098165
O	5.171482	3.311790	3.600696
O	3.925313	1.017038	4.175095
O	8.258474	0.997935	4.679634
O	1.420961	17.343372	1.342984
O	1.674440	0.063677	0.923427
O	1.928118	2.732332	1.001450
O	6.260679	17.172239	1.755983
O	6.092294	19.729261	1.101019
O	6.094096	2.555629	1.166864
O	10.200208	19.160946	3.841055
O	10.185591	2.733924	4.257802
O	12.769230	10.940072	3.513573
O	13.916090	11.267809	1.198448
O	16.093283	11.036184	12.971206
O	18.107096	11.364319	1.367609
O	18.012991	11.027031	4.001785
O	15.435961	11.351584	3.266924
O	12.759620	7.131006	3.427654
O	13.852221	7.043052	1.002922
O	16.259066	7.198065	13.296144
O	18.430250	6.477125	1.320099
O	17.934305	6.804463	3.924431
O	15.365283	6.626566	3.180470
O	14.430656	9.030365	2.671916
O	18.279284	8.934651	2.342025
O	11.513050	12.450605	5.283474
O	11.767130	9.855776	5.787211
O	12.172574	7.197071	5.929204
O	16.433456	12.694169	5.198627
O	16.178976	10.036857	5.521023
O	16.016598	7.389493	5.696742
O	0.237261	10.707253	2.930877
O	0.314546	7.297163	3.011309
O	17.272579	8.784413	10.383067
O	16.427250	8.870975	7.876297
O	14.085076	8.955147	6.613210
O	11.930308	8.535875	8.104477
O	12.175178	8.953754	10.692616

O	14.683734	9.208262	9.883346
O	17.342655	13.506048	10.046618
O	16.259066	13.180102	7.709277
O	13.951730	12.761427	6.279973
O	11.845615	13.423269	7.787702
O	12.169971	13.259898	10.441015
O	14.691342	13.017926	9.788461
O	16.514345	11.097871	9.370509
O	11.931310	11.023449	8.958580
O	18.683128	7.466901	12.214530
O	18.444866	10.101528	12.456495
O	18.090677	12.757050	12.548838
O	14.089080	7.316464	11.699285
O	13.856224	9.784537	12.457833
O	13.929706	12.447819	12.289475
O	9.850423	9.373026	9.535387
O	9.855228	12.599450	9.369170
O	12.843513	18.828035	3.672831
O	13.680031	18.821470	1.172619
O	15.979157	18.911810	13.215981
O	18.109900	18.395233	1.336828
O	17.951124	18.841169	3.928044
O	15.433558	18.820076	3.166016
O	12.450881	3.148221	3.085718
O	13.845213	3.064048	0.930119
O	16.131325	2.891325	12.964247
O	18.106895	3.477151	1.259474
O	17.674620	2.903463	3.844267
O	15.105797	3.483519	3.243772
O	14.094887	1.094644	2.753017
O	18.269674	0.974852	2.106618
O	11.430759	17.322477	5.286954
O	11.673225	0.015720	5.856401
O	12.424452	2.643383	5.694868
O	16.268276	17.159903	5.018358
O	16.185183	19.739012	5.610957
O	15.762119	2.484191	5.616444
O	0.197217	19.148808	2.860349
O	0.071679	2.736709	2.923784
O	17.261366	1.162102	10.366339
O	16.356771	1.235529	7.866528
O	14.022007	0.754371	6.693106
O	11.841812	1.493022	8.018960
O	12.103499	1.162898	10.624630

O	14.667315	1.155137	9.871569
O	17.441563	16.653673	9.869293
O	16.190790	16.840126	7.617470
O	13.895667	17.093241	6.271274
O	11.838207	16.504627	7.807910
O	12.189993	16.667006	10.453730
O	14.756213	16.674566	9.794350
O	16.104294	18.898081	9.366361
O	11.849219	18.910618	9.029243
O	18.609247	2.580701	12.135839
O	18.342354	19.885071	12.559946
O	17.847811	17.250244	12.391855
O	13.768128	2.831429	11.714809
O	13.854823	0.243166	12.301520
O	13.933310	17.470528	12.283720
O	9.822793	0.737656	9.609931
O	9.849823	17.249050	9.447596
O	7.084584	9.386159	9.287401
O	5.078780	8.708797	12.044165
O	3.836816	9.038921	0.753463
O	2.083289	8.535875	12.036536
O	2.105113	9.124487	9.377736
O	4.674336	9.608033	9.792608
O	7.486026	13.265669	10.205742
O	6.248466	13.271837	12.461046
O	3.917304	12.766403	0.412196
O	1.823604	13.435605	12.268598
O	2.254277	13.098915	9.688222
O	4.842721	13.018125	10.209490
O	6.345372	11.011311	11.207594
O	1.673839	11.000963	11.287491
O	8.589638	7.532766	7.940134
O	8.591240	10.114463	7.359045
O	7.842016	12.690389	7.607299
O	3.773746	7.306714	8.518815
O	3.744314	9.688425	7.361721
O	3.927716	12.351708	7.768297
O	19.907473	9.115732	10.543663
O	19.855217	12.767199	10.542191
O	2.852134	10.946441	2.925658
O	3.836015	11.286513	5.347311
O	6.027223	10.941266	6.855843
O	8.082080	11.528286	5.230076
O	7.994184	10.778094	2.602191

O	5.506650	10.773716	3.413602
O	2.844325	6.554731	3.357527
O	3.672035	6.867941	5.870186
O	6.036232	7.140159	7.114002
O	8.021614	6.471155	5.524101
O	7.852628	6.955099	2.923516
O	5.424761	6.632138	3.918944
O	3.914701	8.861423	4.180582
O	8.186395	8.965693	4.596392
O	1.422563	12.496771	1.341780
O	1.415555	9.869904	0.832289
O	1.920710	7.219158	0.901077
O	6.262881	12.606614	1.669663
O	6.181191	10.108692	0.828809
O	5.679641	7.534757	1.425959
O	10.199607	10.616117	3.842527
O	10.184589	7.221546	4.178307
O	8.836308	14.924449	8.617046
O	3.836415	14.862564	8.537417
O	5.347876	14.925245	0.858921
O	2.414853	14.919872	0.996097
O	1.243767	4.976143	2.018023
O	6.332558	5.036238	1.924609
O	4.584638	4.993057	7.530347
O	7.665422	5.048575	7.710482
O	11.593940	4.984899	4.772378
O	16.422045	4.948085	5.005108
O	14.679930	5.075638	12.731649
O	17.695044	5.050963	12.562756
O	18.851913	15.018572	11.539626
O	13.926102	14.930817	11.548325
O	15.352869	14.933404	5.938439
O	12.417044	14.917286	5.706511
O	11.006694	5.718177	15.310286
O	10.183188	3.143246	14.634311
O	8.685544	2.653532	11.948878
O	9.343065	0.582245	14.131378
O	9.699858	8.001786	14.170857
O	11.102999	4.313108	12.449938
Pt	7.069968	5.107476	-3.311757
Pt	9.371497	7.261145	-0.677581
Pt	8.944828	6.856797	-3.106596
Pt	6.474514	5.107079	-0.911918
Pt	6.957244	7.762202	-1.431579

Pt	8.958042	4.800435	-1.037584
H	10.112311	6.023228	15.070596
H	10.957039	4.748498	15.194255
H	9.385913	3.603311	14.257980
H	9.960945	2.179139	14.599514
H	8.024617	2.234459	12.536927
H	8.165973	2.846154	11.132648
H	9.880456	0.135711	13.457143
H	9.045339	-0.115215	14.747664
H	8.998688	8.281367	14.797182
H	10.483719	8.545426	14.370799
H	11.365488	3.777825	11.678006
H	11.050342	3.683902	13.229765

312

#### Pt6@Silicalite-1-6W\_FS

Si	8.441675	1.088276	8.821136
Si	6.041638	0.535084	10.813465
Si	5.589341	1.192547	0.399750
Si	2.382618	1.361888	0.274887
Si	1.396334	0.538268	10.907948
Si	3.596351	1.210058	9.000202
Si	8.497537	16.455677	9.009034
Si	6.175185	17.196915	10.976469
Si	5.434371	16.487913	0.523275
Si	2.400437	16.436375	0.409520
Si	1.432374	17.326260	10.976604
Si	3.732301	16.383842	9.103652
Si	1.557111	18.799381	2.060045
Si	3.935724	19.296259	4.115942
Si	4.385018	18.732122	7.035845
Si	7.561108	18.568752	6.930387
Si	8.639092	19.370283	4.213638
Si	6.377007	18.677797	2.313653
Si	1.446189	3.416061	2.393282
Si	3.858640	2.632041	4.295140
Si	4.545794	3.432776	7.232307
Si	7.613165	3.491678	7.201527
Si	8.606256	2.572941	4.426561
Si	6.351178	3.456854	2.483350
Si	11.589934	10.958579	4.635603
Si	14.107100	10.622484	2.673790
Si	14.471500	11.142245	13.072381
Si	17.671217	11.317358	13.182256
Si	18.669714	10.510652	2.625076

Si	16.486115	11.244527	4.496153
Si	11.641791	6.579007	4.455335
Si	14.082474	7.446405	2.564718
Si	14.712966	6.671537	13.049764
Si	17.767723	6.558711	13.204605
Si	18.737787	7.399444	2.638994
Si	16.414434	6.473343	4.423215
Si	18.553585	8.875153	11.387729
Si	16.215616	9.492818	9.369840
Si	15.679228	8.796552	6.425580
Si	12.503138	8.587613	6.549105
Si	11.478211	9.505156	9.270002
Si	13.720476	8.815854	11.150314
Si	18.529160	13.477394	11.157140
Si	16.191591	12.683822	9.246851
Si	15.480409	13.374317	6.306070
Si	12.433661	13.371928	6.313832
Si	11.461394	12.564030	9.153438
Si	13.688641	13.407150	11.017689
Si	11.567511	18.822065	4.683783
Si	13.993776	19.375458	2.677938
Si	14.376797	18.814903	13.078671
Si	17.571306	18.614122	13.209155
Si	18.639280	19.338446	2.549729
Si	16.432655	18.656307	4.436866
Si	11.654805	3.406709	4.467380
Si	13.891064	2.691937	2.506101
Si	14.616060	3.489091	12.949123
Si	17.649792	3.505408	13.075459
Si	18.533363	2.531949	2.517209
Si	16.247852	3.450288	4.410903
Si	18.490917	1.124691	11.415565
Si	16.119310	0.620849	9.356457
Si	15.591731	1.100614	6.430799
Si	12.493126	1.268561	6.548971
Si	11.393118	0.570106	9.289809
Si	13.643991	1.323880	11.117258
Si	18.496923	16.532288	11.093437
Si	16.127119	17.284073	9.170567
Si	15.425550	16.507017	6.233668
Si	12.398422	16.448513	6.321862
Si	11.442372	17.336407	9.183281
Si	13.710464	16.455479	11.028797
Si	8.565412	9.188164	8.471841

Si	6.272091	9.419191	10.537506
Si	5.336463	8.762724	0.408984
Si	2.284510	8.664025	0.266456
Si	1.460605	9.454413	10.843978
Si	3.668030	8.893261	8.846564
Si	8.474711	13.351632	8.946001
Si	6.212226	12.539753	10.985837
Si	5.445183	13.354020	0.472018
Si	2.399036	13.397002	0.373252
Si	1.409148	12.570198	10.915309
Si	3.759931	13.302681	9.045837
Si	1.510460	11.019071	1.998082
Si	3.999995	10.466676	3.947584
Si	4.446686	11.065435	6.857182
Si	7.623776	11.348798	6.699129
Si	8.605856	10.518015	4.069503
Si	6.464303	11.061457	2.103138
Si	1.579335	6.528066	2.339348
Si	3.961153	7.255176	4.303839
Si	4.529977	6.596519	7.237125
Si	7.600952	6.611244	7.051102
Si	8.602653	7.452374	4.301296
Si	6.340166	6.539011	2.507305
O	7.187898	1.158520	9.855911
O	6.251669	1.235131	12.287201
O	3.986780	1.163694	0.406709
O	1.919309	1.495012	12.116300
O	2.085892	0.995547	9.520666
O	4.583035	0.985000	10.283230
O	7.502043	16.579250	10.285772
O	6.255673	16.825201	12.547768
O	3.912899	17.086277	0.418888
O	1.829610	16.424238	12.271676
O	2.255879	16.746403	9.697322
O	4.835914	16.585617	10.294070
O	6.172983	18.825249	10.866059
O	1.767142	18.895693	11.290300
O	8.586635	2.561996	8.117326
O	8.260877	19.822786	7.694690
O	7.833608	17.165674	7.696430
O	3.753925	2.729148	8.456182
O	3.849630	0.169340	7.782215
O	4.015612	17.399687	7.864654
O	19.844004	0.752779	10.614994

O	19.870432	17.253031	10.619411
O	2.823302	18.743664	3.080901
O	3.662424	18.652925	5.580845
O	5.983975	18.897881	6.792408
O	8.179387	18.401798	5.430554
O	7.920103	18.991207	2.779248
O	5.417552	18.833408	3.605648
O	2.508757	3.163543	3.590257
O	3.766739	3.070416	5.852787
O	6.095497	2.895305	7.194166
O	8.165973	3.488096	5.682957
O	7.818191	3.074395	3.091072
O	5.178290	3.306816	3.602034
O	3.925714	1.015645	4.175229
O	8.258675	0.994154	4.677091
O	1.421161	17.342178	1.342984
O	1.674440	0.061488	0.923427
O	1.928319	2.731735	1.001316
O	6.259077	17.166866	1.755582
O	6.093896	19.720308	1.096871
O	6.106109	2.505284	1.184797
O	10.206614	19.155375	3.843062
O	10.194802	2.729148	4.256062
O	12.770031	10.945843	3.523209
O	13.919694	11.270197	1.199117
O	16.089277	11.034990	12.969065
O	18.104492	11.364916	1.357304
O	18.005983	11.027629	4.003524
O	15.432557	11.350788	3.265452
O	12.766427	7.134587	3.428457
O	13.853022	7.041460	1.000781
O	16.257263	7.198264	13.294271
O	18.429850	6.480308	1.317423
O	17.932302	6.804463	3.924164
O	15.363481	6.628158	3.178061
O	14.433259	9.032355	2.672318
O	18.283089	8.941815	2.342293
O	11.514051	12.433293	5.354271
O	11.760922	9.799462	5.760445
O	12.177581	7.133593	5.925189
O	16.433657	12.694568	5.198894
O	16.178776	10.036657	5.521960
O	16.017799	7.388698	5.696876
O	0.216438	10.778294	2.935293

O	0.306737	7.298356	3.012513
O	17.274780	8.784613	10.380792
O	16.427851	8.870975	7.874959
O	14.084075	8.950372	6.609998
O	11.923501	8.529905	8.059645
O	12.180784	8.947784	10.630384
O	14.686136	9.207864	9.881205
O	17.342054	13.506048	10.046217
O	16.261269	13.181098	7.710884
O	13.958337	12.759835	6.287869
O	11.852424	13.429636	7.833204
O	12.168970	13.260893	10.453060
O	14.690541	13.018723	9.789129
O	16.515347	11.098070	9.370643
O	11.999584	11.030613	8.958045
O	18.684330	7.467896	12.213326
O	18.446068	10.100932	12.453685
O	18.091478	12.756652	12.546964
O	14.084275	7.320444	11.694200
O	13.854223	9.782746	12.450071
O	13.931508	12.447422	12.290680
O	9.855028	9.452423	9.445455
O	9.852025	12.594476	9.370509
O	12.839108	18.825647	3.677782
O	13.678629	18.822464	1.174224
O	15.980959	18.912607	13.216649
O	18.110498	18.395033	1.336962
O	17.950924	18.841169	3.928312
O	15.433358	18.819878	3.166819
O	12.451482	3.143843	3.084648
O	13.845813	3.063053	0.928111
O	16.132927	2.891325	12.963711
O	18.107296	3.477350	1.259474
O	17.674419	2.903463	3.844668
O	15.107200	3.483121	3.242032
O	14.094087	1.094047	2.752348
O	18.270075	0.974852	2.106484
O	11.429358	17.339790	5.353200
O	11.663014	0.063677	5.842884
O	12.428857	2.651343	5.696742
O	16.268675	17.159506	5.018491
O	16.185183	19.739212	5.611091
O	15.762519	2.484390	5.615908
O	0.197217	19.149008	2.860884

O	0.071278	2.735914	2.924186
O	17.261166	1.162102	10.366339
O	16.357172	1.235728	7.866528
O	14.022407	0.754968	6.694176
O	11.841210	1.495410	8.024313
O	12.102498	1.163893	10.626369
O	14.667716	1.155137	9.871434
O	17.441364	16.653872	9.869561
O	16.192791	16.840525	7.618407
O	13.901675	17.096027	6.276226
O	11.847017	16.499653	7.853680
O	12.190795	16.668797	10.464972
O	14.755412	16.675362	9.795285
O	16.104496	18.897881	9.366494
O	11.847017	18.916388	9.031651
O	18.609848	2.580900	12.136106
O	18.342955	19.885071	12.559946
O	17.848211	17.250046	12.391722
O	13.767727	2.831230	11.715344
O	13.854623	0.243166	12.302457
O	13.934310	17.472715	12.285327
O	9.811180	0.739646	9.616623
O	9.845819	17.250046	9.450540
O	7.173882	9.624351	9.124797
O	5.415350	8.527915	12.207571
O	3.772345	9.050464	0.760957
O	2.082288	8.537268	12.044834
O	2.174389	9.119911	9.439967
O	4.751220	9.453418	9.876387
O	7.440976	13.260694	10.188345
O	6.245663	13.258107	12.453418
O	3.914701	12.765805	0.407780
O	1.836418	13.441774	12.225103
O	2.249071	13.088767	9.622244
O	4.837716	13.006782	10.219794
O	6.350378	10.948430	11.209333
O	1.674039	11.013500	11.286955
O	8.596045	7.624501	7.868535
O	8.683141	10.196446	7.185065
O	7.836410	12.693771	7.598600
O	3.835414	7.296963	8.520823
O	3.760332	9.704344	7.431179
O	4.015612	12.351708	7.761069
O	19.917685	9.115932	10.543262

O	19.854815	12.768194	10.537909
O	2.839520	10.943852	2.921643
O	3.838618	11.277162	5.351460
O	6.068267	10.871023	6.777151
O	8.007197	11.612659	5.125556
O	7.994584	10.782075	2.583990
O	5.484025	10.769339	3.359133
O	2.840121	6.554929	3.356323
O	3.686851	6.870528	5.862825
O	6.074474	7.139761	7.105169
O	8.093293	6.473543	5.516205
O	7.853829	6.958282	2.929003
O	5.414549	6.635123	3.852431
O	3.915903	8.862816	4.178039
O	8.187997	9.010267	4.589432
O	1.425166	12.506721	1.327727
O	1.342875	9.869705	0.837642
O	1.914904	7.213786	0.908973
O	6.262881	12.610991	1.662704
O	6.179990	10.091778	0.836036
O	5.761731	7.469090	1.327995
O	10.197003	10.694718	3.850824
O	10.201609	7.300745	4.181653
O	8.833305	14.919275	8.620927
O	3.840019	14.861768	8.537149
O	5.346475	14.923654	0.850222
O	2.412851	14.917286	0.985658
O	1.242966	4.973158	2.018826
O	6.340968	4.990271	1.920461
O	4.580833	5.006390	7.528473
O	7.674032	5.068872	7.706066
O	11.587732	4.980521	4.773850
O	16.422443	4.949279	5.004439
O	14.680130	5.077628	12.728705
O	17.695642	5.051560	12.562355
O	18.852514	15.018173	11.539492
O	13.927503	14.930618	11.548994
O	15.353870	14.933205	5.938439
O	12.420447	14.918081	5.772624
O	11.012100	5.717978	15.477976
O	10.182589	3.161354	14.636989
O	8.764230	2.484788	11.965072
O	9.351074	0.579061	14.131646
O	9.681838	8.286142	14.310978

O	11.186892	4.310123	12.450071
Pt	7.053550	5.053351	-3.369973
Pt	9.404133	7.162446	-0.632213
Pt	9.166672	6.642286	-3.146477
Pt	6.537183	5.002608	-0.947516
Pt	7.057555	7.484213	-1.953249
Pt	9.015706	4.679648	-1.135949
H	10.425655	6.404095	15.101645
H	10.583229	4.855555	15.317647
H	9.395524	3.567692	14.178754
H	9.953736	2.213366	14.755294
H	9.002692	1.873093	12.699932
H	7.789559	2.403600	11.900700
H	10.100098	-0.004577	13.918186
H	8.779246	0.038604	14.719160
H	8.859735	8.773668	14.513195
H	10.145348	8.405537	11.924521
H	11.535475	3.743201	11.736222
H	11.178482	3.751359	13.276339

318

#### Pt6@Silicalite-1-8W\_IS

Si	8.462699	1.011267	8.776304
Si	6.056855	0.528517	10.817747
Si	5.594947	1.220207	0.406977
Si	2.385821	1.363281	0.275957
Si	1.394933	0.537870	10.910224
Si	3.599555	1.205680	9.002209
Si	8.505946	16.471397	9.010105
Si	6.176386	17.193134	10.981153
Si	5.434972	16.482342	0.534918
Si	2.400838	16.437569	0.412330
Si	1.431373	17.325661	10.979145
Si	3.731500	16.389414	9.104990
Si	1.555109	18.801571	2.059644
Si	3.937126	19.295065	4.111793
Si	4.385218	18.730928	7.030358
Si	7.559706	18.537710	6.876988
Si	8.635288	19.361927	4.194901
Si	6.380811	18.687151	2.308300
Si	1.444587	3.418250	2.392077
Si	3.852433	2.629255	4.294872
Si	4.552602	3.413674	7.229898
Si	7.612364	3.442726	7.202062
Si	8.593442	2.565578	4.415587

Si	6.328353	3.494065	2.486562
Si	11.574918	10.966737	4.615530
Si	14.106501	10.624474	2.671782
Si	14.453280	11.151797	13.088976
Si	17.657000	11.316163	13.184932
Si	18.679525	10.486973	2.592020
Si	16.492121	11.244328	4.485045
Si	11.659410	6.590151	4.480896
Si	14.088881	7.440833	2.555886
Si	14.721775	6.691039	13.024202
Si	17.765120	6.554731	13.177571
Si	18.748199	7.393275	2.589878
Si	16.424246	6.472946	4.412375
Si	18.559193	8.879133	11.383714
Si	16.238041	9.521473	9.366226
Si	15.686235	8.797547	6.422770
Si	12.499734	8.641340	6.569314
Si	11.459991	9.515701	9.298107
Si	13.747106	8.859035	11.130106
Si	18.521151	13.479185	11.163697
Si	16.206207	12.687006	9.243371
Si	15.478208	13.375113	6.300850
Si	12.430058	13.382277	6.264181
Si	11.457789	12.588108	9.129749
Si	13.694047	13.411926	11.011265
Si	11.564507	18.818285	4.656883
Si	13.993175	19.376055	2.669641
Si	14.361980	18.816692	13.074924
Si	17.559093	18.615515	13.209557
Si	18.636076	19.338446	2.548257
Si	16.430655	18.657900	4.434859
Si	11.648999	3.399943	4.466577
Si	13.894467	2.688753	2.501684
Si	14.602645	3.501229	12.940692
Si	17.641384	3.502025	13.073586
Si	18.532763	2.532347	2.514800
Si	16.248653	3.448895	4.410769
Si	18.487713	1.122702	11.415967
Si	16.111704	0.623635	9.359402
Si	15.590731	1.100017	6.432137
Si	12.486720	1.249259	6.542681
Si	11.423351	0.548217	9.281780
Si	13.633180	1.331044	11.121273
Si	18.495123	16.533880	11.095444

Si	16.126720	17.286461	9.170835
Si	15.424148	16.510201	6.232463
Si	12.393017	16.449509	6.274084
Si	11.461994	17.336805	9.157720
Si	13.707461	16.459259	11.025584
Si	8.494934	9.072750	8.645686
Si	6.093095	9.474312	10.667590
Si	5.408143	8.742029	0.304062
Si	2.350783	8.662632	0.259095
Si	1.473419	9.443667	10.825108
Si	3.644805	8.922911	8.791561
Si	8.488527	13.376904	8.950685
Si	6.215829	12.598455	10.986641
Si	5.443381	13.363571	0.490755
Si	2.400638	13.396604	0.403899
Si	1.399137	12.563831	10.958670
Si	3.735304	13.315814	9.063235
Si	1.515665	11.007331	1.993398
Si	3.952543	10.462297	3.961903
Si	4.392025	11.109015	6.854773
Si	7.599350	11.335665	6.806594
Si	8.583832	10.482196	4.122901
Si	6.408842	11.033399	2.092298
Si	1.587544	6.532245	2.330248
Si	3.929317	7.272686	4.323646
Si	4.533381	6.586569	7.244619
Si	7.595545	6.571048	7.065689
Si	8.610661	7.420735	4.305579
Si	6.313137	6.593334	2.551335
O	7.256573	1.082904	9.870230
O	6.255273	1.238514	12.288137
O	3.990184	1.166479	0.407914
O	1.920110	1.495012	12.117103
O	2.088695	0.994751	9.523478
O	4.597451	0.985796	10.280286
O	7.504446	16.580246	10.284969
O	6.252470	16.814058	12.551782
O	3.914301	17.083689	0.418353
O	1.829811	16.423042	12.274085
O	2.255078	16.747198	9.698526
O	4.836714	16.585020	10.294472
O	6.170780	18.819281	10.870209
O	1.767142	18.895294	11.290702
O	8.583031	2.497524	8.106351

O	8.259475	19.813036	7.605024
O	7.833608	17.164879	7.693753
O	3.753925	2.726959	8.458725
O	3.851832	0.168147	7.781545
O	4.015612	17.401278	7.864252
O	19.843403	0.752978	10.615797
O	19.869831	17.252035	10.620080
O	2.821700	18.743864	3.079562
O	3.660822	18.652327	5.576964
O	5.984375	18.893503	6.784379
O	8.172179	18.336531	5.373810
O	7.919301	18.988621	2.769344
O	5.417953	18.834204	3.602838
O	2.505152	3.163145	3.590525
O	3.765337	3.069421	5.853055
O	6.093896	2.831230	7.196709
O	8.164371	3.482922	5.683091
O	7.774943	3.071212	3.100306
O	5.168078	3.307413	3.606317
O	3.924512	1.014252	4.175764
O	8.258474	0.985199	4.677225
O	1.420761	17.343769	1.343118
O	1.674840	0.063478	0.923427
O	1.928319	2.732531	1.001450
O	6.259678	17.173235	1.755850
O	6.092094	19.734434	1.094328
O	6.092294	2.564583	1.168470
O	10.203211	19.162140	3.838111
O	10.186193	2.733526	4.260478
O	12.763424	10.938679	3.517721
O	13.846214	11.267013	1.202596
O	16.066053	11.031209	13.048693
O	18.112301	11.370090	1.350077
O	17.993370	11.023648	3.949591
O	15.426550	11.351981	3.260902
O	12.764425	7.132598	3.423907
O	13.852820	7.047032	0.987532
O	16.261667	7.203637	13.295208
O	18.441463	6.474538	1.272723
O	17.921291	6.804065	3.861799
O	15.358676	6.627163	3.177124
O	14.429655	9.032156	2.670176
O	18.284891	8.929875	2.268151
O	11.511449	12.452396	5.284813

O	11.764527	9.858164	5.782928
O	12.174978	7.190902	5.932015
O	16.434458	12.690786	5.195281
O	16.180779	10.039245	5.518480
O	16.020803	7.389096	5.691523
O	0.227850	10.706060	2.927933
O	0.305936	7.296167	3.005554
O	17.271378	8.784214	10.380390
O	16.424446	8.871969	7.877903
O	14.087079	8.954152	6.612273
O	11.924302	8.534482	8.090292
O	12.188793	8.945993	10.638682
O	14.685736	9.359494	9.881071
O	17.345259	13.514804	10.042470
O	16.258863	13.179506	7.705664
O	13.951730	12.761030	6.279036
O	11.845615	13.425856	7.785025
O	12.172574	13.259898	10.441015
O	14.699552	13.011957	9.788326
O	16.595634	11.111403	9.366761
O	11.935514	11.033996	8.952024
O	18.685129	7.471876	12.204627
O	18.439060	10.106503	12.451009
O	18.019400	12.763218	12.538935
O	14.168968	7.372181	11.640132
O	13.847816	9.787920	12.459038
O	13.929706	12.449412	12.288806
O	9.846219	9.445658	9.528428
O	9.854828	12.600643	9.368770
O	12.845314	18.828035	3.674035
O	13.679431	18.820871	1.173421
O	15.968745	18.910418	13.215981
O	18.108297	18.395630	1.335490
O	17.950323	18.841368	3.928178
O	15.432957	18.820673	3.165615
O	12.456687	3.150410	3.087458
O	13.845813	3.068426	0.927843
O	16.120712	2.898687	12.964380
O	18.105894	3.477947	1.257333
O	17.674820	2.904060	3.844267
O	15.106598	3.484315	3.243772
O	14.095488	1.095241	2.752883
O	18.269474	0.975648	2.105815
O	11.430960	17.323074	5.286018

O	11.673026	0.015521	5.855330
O	12.424051	2.644776	5.696207
O	16.268875	17.159903	5.018090
O	16.185385	19.739609	5.611091
O	15.762719	2.485385	5.616444
O	0.194213	19.149008	2.859010
O	0.070277	2.736709	2.923383
O	17.260164	1.161903	10.365669
O	16.356173	1.235529	7.867331
O	14.022206	0.754769	6.692304
O	11.841611	1.492027	8.018425
O	12.099295	1.157923	10.622087
O	14.662109	1.155734	9.873308
O	17.441364	16.653673	9.869293
O	16.191391	16.839928	7.618006
O	13.898071	17.093241	6.270873
O	11.838007	16.503832	7.805099
O	12.190394	16.663622	10.453595
O	14.756413	16.673571	9.794350
O	16.104294	18.898876	9.366361
O	11.925903	18.905045	9.028172
O	18.607244	2.579706	12.136776
O	18.339750	19.883280	12.560615
O	17.846809	17.250841	12.393193
O	13.766726	2.836403	11.713605
O	13.855023	0.245554	12.299914
O	13.934111	17.465551	12.285059
O	9.820189	0.589607	9.551447
O	9.860635	17.257210	9.442911
O	7.077977	9.382578	9.296903
O	5.079181	8.707206	12.041221
O	3.834613	9.039320	0.753998
O	2.084891	8.535278	12.037875
O	2.147359	9.122498	9.385097
O	4.678941	9.615396	9.794350
O	7.486026	13.265669	10.209087
O	6.242659	13.279201	12.467068
O	3.916503	12.768194	0.411795
O	1.823604	13.436004	12.268732
O	2.251874	13.099910	9.690631
O	4.842320	13.018723	10.210025
O	6.345773	11.017082	11.209601
O	1.675040	11.001560	11.286152
O	8.600049	7.538537	7.943212

O	8.526168	10.114264	7.362122
O	7.842818	12.744116	7.600340
O	3.843223	7.311688	8.522964
O	3.751122	9.697181	7.353022
O	3.919907	12.357876	7.774319
O	19.920889	9.116727	10.541121
O	19.850010	12.766800	10.549685
O	2.833313	10.959573	2.919100
O	3.838818	11.342629	5.334330
O	6.013608	11.015092	6.856647
O	8.086285	11.535251	5.254300
O	7.931715	10.775308	2.653046
O	5.434571	10.692329	3.343743
O	2.842123	6.547766	3.357126
O	3.680043	6.866747	5.880892
O	6.080281	7.132598	7.106239
O	8.097898	6.465583	5.528250
O	7.862238	6.957885	2.928736
O	5.422758	6.716709	3.926439
O	3.756728	8.870775	4.189816
O	8.183191	8.965296	4.602280
O	1.418158	12.502741	1.339638
O	1.413954	9.871099	0.830817
O	1.921111	7.219158	0.902683
O	6.259678	12.599848	1.672206
O	6.190802	10.117448	0.771530
O	5.684246	7.536348	1.420739
O	10.185792	10.617112	3.843330
O	10.218428	7.294775	4.173489
O	8.839713	14.933602	8.621061
O	3.836215	14.866941	8.538488
O	5.346875	14.924051	0.919278
O	2.414853	14.921066	0.996097
O	1.243366	4.975148	2.017354
O	6.329955	5.045392	1.995405
O	4.589443	4.991067	7.529945
O	7.678037	5.030268	7.709277
O	11.590536	4.988082	4.771575
O	16.425047	4.953657	5.002298
O	14.673323	5.097925	12.726296
O	17.691238	5.047183	12.552451
O	18.852314	15.018173	11.541634
O	13.927503	14.930220	11.547121
O	15.353270	14.933205	5.937903

O	12.418845	14.919077	5.703433
O	11.006292	5.720963	15.315506
O	10.186592	3.147624	14.715813
O	8.678936	2.723775	12.206367
O	10.440472	3.494065	10.111124
O	9.352476	0.661841	14.135794
O	9.682839	8.548411	14.552942
O	11.018507	4.475484	12.542548
O	12.094489	5.636193	9.532176
Pt	7.144650	5.125585	-3.371312
Pt	9.376102	7.376360	-0.663663
Pt	8.975462	6.923260	-3.096559
Pt	6.403636	5.132947	-1.005063
Pt	6.960848	7.771554	-1.427966
Pt	8.895374	4.925600	-0.924765
H	10.118918	6.020244	15.043830
H	10.959442	4.747901	15.218479
H	9.334256	3.558339	14.450294
H	10.001589	2.170981	14.658802
H	7.762929	2.678206	11.852922
H	9.277994	2.535331	11.447417
H	9.656210	4.089046	10.018782
H	11.151052	4.028154	9.668682
H	8.771438	0.954356	13.412711
H	8.860736	0.002189	14.658266
H	9.004894	9.250051	14.655189
H	10.548190	8.975444	14.692126
H	11.081175	3.967463	11.684832
H	11.010899	3.813246	13.292665
H	11.558901	6.176848	10.151006
H	12.061852	6.139239	8.698950

318

#### Pt6@Silicalite-1-8W\_FS

Si	8.460496	1.014451	8.772958
Si	6.054052	0.525931	10.814267
Si	5.595348	1.216625	0.406308
Si	2.385821	1.362684	0.275556
Si	1.394732	0.537472	10.909956
Si	3.598554	1.205680	9.001139
Si	8.505746	16.462442	9.009302
Si	6.176587	17.190746	10.980484
Si	5.434972	16.482740	0.534785
Si	2.400838	16.438963	0.412063
Si	1.431373	17.325264	10.978477

Si	3.731900	16.386030	9.104589
Si	1.554909	18.801769	2.060313
Si	3.937927	19.296658	4.111258
Si	4.385218	18.729734	7.030224
Si	7.559906	18.536118	6.878193
Si	8.635689	19.362522	4.195303
Si	6.383214	18.687151	2.308166
Si	1.445588	3.416061	2.392211
Si	3.856437	2.632240	4.292731
Si	4.553603	3.413872	7.230300
Si	7.611563	3.458446	7.199920
Si	8.603052	2.567767	4.415319
Si	6.332158	3.501229	2.476792
Si	11.564507	10.959573	4.609641
Si	14.070860	10.613530	2.657730
Si	14.441268	11.155181	13.086968
Si	17.643785	11.316761	13.179312
Si	18.645086	10.498713	2.592421
Si	16.443668	11.247711	4.479023
Si	11.657809	6.571645	4.455736
Si	14.081873	7.444614	2.553744
Si	14.707760	6.697009	13.024469
Si	17.759714	6.555726	13.175029
Si	18.733383	7.396259	2.589477
Si	16.415636	6.472747	4.410635
Si	18.554186	8.881123	11.384250
Si	16.235640	9.522468	9.364620
Si	15.683433	8.796751	6.420093
Si	12.504139	8.611292	6.525551
Si	11.500436	9.538586	9.246716
Si	13.727283	8.873760	11.132248
Si	18.518547	13.479782	11.162895
Si	16.203604	12.688000	9.242300
Si	15.474803	13.375909	6.301385
Si	12.426854	13.377700	6.260835
Si	11.464396	12.589899	9.127474
Si	13.691043	13.413916	11.010060
Si	11.565308	18.817091	4.657016
Si	13.993175	19.382622	2.670042
Si	14.361580	18.817688	13.076128
Si	17.558693	18.615116	13.209690
Si	18.635677	19.338047	2.548391
Si	16.430052	18.657900	4.434725
Si	11.663216	3.404520	4.462294

Si	13.922698	2.702682	2.495528
Si	14.605247	3.503617	12.939622
Si	17.643187	3.502025	13.074656
Si	18.534966	2.531352	2.514800
Si	16.260267	3.449094	4.403275
Si	18.487312	1.122105	11.415833
Si	16.112103	0.623237	9.357929
Si	15.590731	1.102007	6.429193
Si	12.486920	1.247866	6.542012
Si	11.422751	0.546427	9.280977
Si	13.633380	1.331243	11.121273
Si	18.494520	16.533880	11.095177
Si	16.126118	17.286062	9.170300
Si	15.422345	16.510399	6.232329
Si	12.392616	16.446325	6.272612
Si	11.460993	17.334019	9.157051
Si	13.707061	16.459658	11.026388
Si	8.587635	9.204880	8.399439
Si	6.303126	9.465954	10.473670
Si	5.311436	8.758744	0.392390
Si	2.290517	8.666214	0.279571
Si	1.464409	9.453815	10.850937
Si	3.674638	8.902017	8.850178
Si	8.474511	13.356607	8.950952
Si	6.201014	12.550499	10.989317
Si	5.429365	13.362975	0.496777
Si	2.395832	13.399787	0.401624
Si	1.397335	12.572587	10.954923
Si	3.738107	13.309048	9.058685
Si	1.484631	11.017878	2.003970
Si	3.950941	10.451950	3.951063
Si	4.411848	11.084141	6.867888
Si	7.604755	11.370289	6.687084
Si	8.575222	10.494135	4.064551
Si	6.410844	11.033796	2.077711
Si	1.574530	6.528265	2.341490
Si	3.949940	7.267314	4.299824
Si	4.548198	6.585773	7.248902
Si	7.614566	6.607861	7.058596
Si	8.632484	7.437252	4.308523
Si	6.377007	6.588360	2.514264
O	7.255972	1.083103	9.869695
O	6.253071	1.237718	12.285460
O	3.990385	1.166479	0.407512

O	1.920310	1.495012	12.116701
O	2.088295	0.994751	9.523210
O	4.596050	0.985796	10.279750
O	7.504846	16.579847	10.284568
O	6.252470	16.814655	12.551782
O	3.914301	17.083889	0.418353
O	1.829811	16.423441	12.273817
O	2.255478	16.746799	9.698125
O	4.836314	16.584822	10.293936
O	6.170780	18.818285	10.869940
O	1.767142	18.895096	11.290568
O	8.579627	2.506478	8.107823
O	8.259275	19.814032	7.604622
O	7.834208	17.163485	7.694423
O	3.753925	2.726561	8.457923
O	3.852032	0.167550	7.781278
O	4.015612	17.400084	7.864252
O	19.843203	0.752978	10.615797
O	19.869831	17.252035	10.619946
O	2.822101	18.744461	3.079830
O	3.661223	18.652925	5.576295
O	5.984375	18.892708	6.784780
O	8.171979	18.337923	5.374479
O	7.920703	18.989416	2.769478
O	5.418554	18.834602	3.602302
O	2.506955	3.163742	3.590391
O	3.767540	3.069620	5.851985
O	6.096498	2.835608	7.195905
O	8.167173	3.483718	5.682288
O	7.779147	3.075191	3.097763
O	5.172483	3.312388	3.600964
O	3.925914	1.016640	4.174827
O	8.259475	0.987786	4.676288
O	1.420761	17.344366	1.343118
O	1.674840	0.063677	0.923561
O	1.929120	2.732531	1.000915
O	6.259878	17.173235	1.755850
O	6.092695	19.733639	1.094060
O	6.093095	2.561399	1.166864
O	10.203812	19.162338	3.838244
O	10.197405	2.731735	4.253787
O	12.754615	10.939277	3.520934
O	13.841809	11.269998	1.194299
O	16.054039	11.031012	13.045482

O	18.104092	11.373672	1.340575
O	17.936909	11.023449	3.935807
O	15.367685	11.358549	3.270538
O	12.771832	7.134587	3.427386
O	13.852421	7.045241	0.986862
O	16.252857	7.204035	13.285304
O	18.437658	6.475930	1.269779
O	17.915285	6.804463	3.862869
O	15.356473	6.628158	3.174582
O	14.431658	9.031161	2.668035
O	18.283089	8.934651	2.265876
O	11.509846	12.447422	5.285214
O	11.766329	9.850005	5.777174
O	12.180784	7.142149	5.928936
O	16.430052	12.691980	5.195816
O	16.177776	10.038847	5.520354
O	16.021204	7.387702	5.692325
O	0.180198	10.778094	2.932349
O	0.289518	7.294775	3.006223
O	17.270176	8.784016	10.379186
O	16.422045	8.871372	7.877903
O	14.086278	8.950570	6.608927
O	11.930510	8.529308	8.048804
O	12.178782	8.952163	10.615664
O	14.685536	9.350939	9.886826
O	17.344458	13.514804	10.041533
O	16.258663	13.180102	7.705396
O	13.950528	12.761427	6.279839
O	11.844415	13.428840	7.782884
O	12.170773	13.263679	10.441551
O	14.698550	13.012951	9.788326
O	16.594633	11.111403	9.367164
O	12.013200	11.053696	8.950819
O	18.683929	7.472672	12.204360
O	18.436657	10.107697	12.450473
O	18.018198	12.762821	12.537329
O	14.096087	7.360441	11.640667
O	13.848817	9.786527	12.458101
O	13.928704	12.453192	12.285862
O	9.875251	9.531223	9.363015
O	9.856430	12.598256	9.367833
O	12.845714	18.829826	3.673366
O	13.679831	18.822464	1.174492
O	15.968546	18.911015	13.215981

O	18.108297	18.395432	1.335490
O	17.949923	18.841568	3.928178
O	15.431955	18.822464	3.165481
O	12.516152	3.223638	3.098298
O	13.845813	3.068028	0.920750
O	16.121714	2.900080	12.963443
O	18.106695	3.477748	1.257601
O	17.686033	2.902269	3.847747
O	15.182082	3.480335	3.175652
O	14.092284	1.104594	2.753418
O	18.269674	0.975250	2.104878
O	11.430759	17.322678	5.285348
O	11.673026	0.014128	5.855732
O	12.424851	2.640796	5.694735
O	16.268475	17.160301	5.018223
O	16.185385	19.740206	5.611091
O	15.761118	2.487375	5.609217
O	0.194013	19.149206	2.859278
O	0.072279	2.735516	2.923115
O	17.259964	1.162102	10.365268
O	16.355772	1.236723	7.865992
O	14.022808	0.755167	6.692437
O	11.841611	1.491828	8.018693
O	12.098894	1.158321	10.621686
O	14.662311	1.156530	9.873308
O	17.441164	16.654070	9.869293
O	16.191191	16.840324	7.617603
O	13.896269	17.093838	6.270739
O	11.837606	16.503832	7.803761
O	12.189993	16.664021	10.453595
O	14.756013	16.674168	9.794617
O	16.104294	18.899076	9.366226
O	11.924903	18.904249	9.028440
O	18.607244	2.579706	12.136508
O	18.339552	19.883280	12.560615
O	17.846809	17.250841	12.393060
O	13.766525	2.840781	11.710794
O	13.855223	0.247146	12.300048
O	13.933509	17.469133	12.284122
O	9.817987	0.593388	9.551046
O	9.859033	17.253428	9.442108
O	7.247563	9.698972	9.119980
O	5.250569	8.376882	12.220017
O	3.764136	9.047279	0.834564

O	2.085091	8.538462	12.053132
O	2.178994	9.119115	9.444785
O	4.757427	9.522666	9.863539
O	7.439974	13.260893	10.194634
O	6.179190	13.265669	12.454086
O	3.907293	12.766005	0.415275
O	1.823403	13.441177	12.264851
O	2.251874	13.098716	9.684742
O	4.837716	13.007380	10.208955
O	6.353181	10.956389	11.212813
O	1.673038	11.011909	11.291906
O	8.595044	7.634450	7.864252
O	8.677135	10.197640	7.107043
O	7.842217	12.698348	7.600206
O	3.841621	7.300745	8.524035
O	3.758930	9.701957	7.427833
O	3.929918	12.353300	7.765754
O	19.920488	9.117324	10.543530
O	19.848608	12.767796	10.548615
O	2.819298	10.955394	2.916825
O	3.838017	11.278953	5.349586
O	6.038435	10.946042	6.843665
O	7.996787	11.612459	5.111503
O	7.934518	10.770134	2.590414
O	5.432970	10.691932	3.334508
O	2.838319	6.547169	3.356992
O	3.746316	6.867742	5.861486
O	6.086488	7.135981	7.111057
O	8.097898	6.468170	5.518882
O	7.915497	6.946741	2.925122
O	5.426563	6.718500	3.845203
O	3.757529	8.863612	4.183660
O	8.181390	8.982011	4.591172
O	1.416356	12.506721	1.337631
O	1.338671	9.870899	0.838579
O	1.912902	7.212591	0.910579
O	6.256474	12.601440	1.669395
O	6.170380	10.109289	0.758415
O	5.843621	7.539731	1.341244
O	10.177783	10.621091	3.846542
O	10.233844	7.308107	4.184195
O	8.833906	14.921464	8.622399
O	3.837016	14.862564	8.538354
O	5.346675	14.924449	0.919680

O	2.414653	14.922460	0.996097
O	1.241764	4.973158	2.018826
O	6.336162	5.042407	1.931836
O	4.588842	4.990072	7.530213
O	7.675633	5.051958	7.706467
O	11.585931	4.980720	4.781344
O	16.422443	4.951866	5.000558
O	14.670719	5.102900	12.717865
O	17.690437	5.047381	12.552051
O	18.852514	15.018373	11.541499
O	13.927904	14.931613	11.547254
O	15.353069	14.934398	5.938171
O	12.418645	14.917684	5.702363
O	11.013701	5.708824	15.482123
O	10.268282	3.062058	14.723174
O	8.688947	2.564782	12.209044
O	10.437868	3.485708	10.120626
O	9.516657	0.577270	14.135660
O	9.755919	8.543835	14.307632
O	11.013301	4.471504	12.630742
O	12.093088	5.639177	9.534852
Pt	7.006699	5.083200	-3.419758
Pt	9.206315	7.277661	-0.415007
Pt	9.154859	6.481701	-2.795441
Pt	6.366195	5.044795	-1.005866
Pt	6.962250	7.523414	-1.919390
Pt	8.831304	4.793072	-0.731381
H	10.328549	6.234953	15.027235
H	10.817486	4.772775	15.286599
H	9.358684	3.392779	14.564051
H	10.148952	2.072282	14.674460
H	7.774342	2.488569	11.863495
H	9.292410	2.449567	11.441127
H	9.648201	4.060391	9.983584
H	11.156259	4.000296	9.682199
H	8.954439	0.902022	13.408027
H	8.988876	-0.059498	14.651040
H	9.004093	9.109962	14.578369
H	10.342364	7.733747	12.013385
H	11.055147	3.992137	11.760579
H	11.053546	3.782004	13.356502
H	12.571012	6.016065	10.295944
H	12.065256	6.348776	8.866906

Pt6@Silicalite-1-10W\_IS

Si	8.459495	1.010471	8.775233
Si	6.054252	0.527920	10.811992
Si	5.592745	1.219013	0.412866
Si	2.384820	1.363678	0.276359
Si	1.396334	0.537671	10.910089
Si	3.598754	1.206874	9.000737
Si	8.504544	16.469009	9.008499
Si	6.176386	17.194328	10.977808
Si	5.434171	16.491495	0.524881
Si	2.401238	16.435579	0.412866
Si	1.432975	17.325264	10.979682
Si	3.731500	16.389215	9.104455
Si	1.556710	18.800377	2.059108
Si	3.937126	19.295862	4.111927
Si	4.384818	18.731127	7.029956
Si	7.559105	18.536915	6.875248
Si	8.633886	19.362125	4.192091
Si	6.381011	18.684366	2.309103
Si	1.447190	3.419643	2.392747
Si	3.854635	2.630250	4.295676
Si	4.550200	3.414469	7.231236
Si	7.601552	3.439343	7.204337
Si	8.589237	2.566772	4.418130
Si	6.328353	3.498244	2.483751
Si	11.572116	10.960767	4.608838
Si	14.082474	10.605371	2.656392
Si	14.498529	11.164534	13.052306
Si	17.681828	11.318750	13.162448
Si	18.645487	10.470057	2.588540
Si	16.450274	11.246716	4.479290
Si	11.662814	6.593334	4.493610
Si	14.114508	7.440833	2.578770
Si	14.778438	6.696013	13.027548
Si	17.806767	6.545577	13.194434
Si	18.763216	7.377355	2.618518
Si	16.439062	6.470160	4.432316
Si	18.557390	8.871571	11.382911
Si	16.245850	9.523662	9.362479
Si	15.681430	8.800731	6.423974
Si	12.494127	8.644524	6.580153
Si	11.453985	9.506946	9.308278
Si	13.771932	8.864408	11.127563
Si	18.535166	13.484557	11.155802

Si	16.213816	12.687006	9.240694
Si	15.476805	13.375313	6.300717
Si	12.428657	13.378297	6.256151
Si	11.451383	12.576765	9.108068
Si	13.690844	13.415110	10.994268
Si	11.562905	18.817091	4.655812
Si	13.993175	19.375656	2.669909
Si	14.362380	18.816296	13.075325
Si	17.559494	18.615116	13.210092
Si	18.638079	19.337849	2.548391
Si	16.431454	18.657104	4.434323
Si	11.647798	3.400739	4.467513
Si	13.893666	2.688753	2.502219
Si	14.605247	3.505010	12.940826
Si	17.644987	3.499040	13.075191
Si	18.535366	2.531153	2.515870
Si	16.249054	3.446308	4.410635
Si	18.489115	1.120911	11.415298
Si	16.112303	0.622839	9.359802
Si	15.591731	1.098624	6.432004
Si	12.486920	1.247468	6.540406
Si	11.427356	0.527920	9.283118
Si	13.634381	1.333233	11.122746
Si	18.496323	16.537264	11.094374
Si	16.126919	17.286062	9.170300
Si	15.423747	16.509804	6.232196
Si	12.394218	16.446524	6.270070
Si	11.460192	17.326059	9.155712
Si	13.707862	16.458462	11.025584
Si	8.492931	9.007879	8.700689
Si	6.026622	9.454612	10.720587
Si	5.434772	8.742029	0.321192
Si	2.357590	8.664821	0.259363
Si	1.460805	9.445458	10.830193
Si	3.608164	8.924702	8.790089
Si	8.487326	13.373719	8.946937
Si	6.218032	12.590495	10.982759
Si	5.442180	13.360388	0.476836
Si	2.399236	13.392226	0.408182
Si	1.402541	12.564825	10.960008
Si	3.736506	13.315814	9.063370
Si	1.498647	11.000566	2.003837
Si	3.957348	10.486973	3.974751
Si	4.381014	11.109810	6.852364

Si	7.599150	11.320342	6.825196
Si	8.586034	10.487967	4.124239
Si	6.404237	11.077375	2.135258
Si	1.598757	6.533041	2.328910
Si	3.948939	7.275074	4.322174
Si	4.491135	6.585773	7.251846
Si	7.547693	6.584579	7.061808
Si	8.586234	7.412179	4.312270
Si	6.311735	6.583385	2.556019
O	7.257174	1.081113	9.869963
O	6.253071	1.239907	12.287333
O	3.989183	1.165683	0.407512
O	1.919909	1.495012	12.117103
O	2.088295	0.994353	9.523210
O	4.595650	0.985995	10.280286
O	7.504846	16.580444	10.284033
O	6.255874	16.823809	12.547901
O	3.911898	17.087271	0.418486
O	1.829610	16.422844	12.274352
O	2.255078	16.747198	9.698526
O	4.836714	16.585220	10.293936
O	6.170580	18.820673	10.869272
O	1.767542	18.895294	11.290970
O	8.585032	2.491355	8.095243
O	8.259675	19.811245	7.605024
O	7.833608	17.164879	7.693218
O	3.752123	2.726362	8.459260
O	3.851632	0.167749	7.781679
O	4.015612	17.401478	7.864119
O	19.843803	0.752381	10.615530
O	19.871035	17.253826	10.619411
O	2.822301	18.743664	3.079696
O	3.660622	18.652130	5.576696
O	5.984175	18.893305	6.784244
O	8.172179	18.336531	5.372338
O	7.919101	18.988621	2.767471
O	5.417953	18.833609	3.602838
O	2.505553	3.162349	3.590927
O	3.764136	3.068824	5.853323
O	6.088490	2.825260	7.193229
O	8.163970	3.481529	5.685366
O	7.775544	3.069819	3.099637
O	5.168679	3.305622	3.605380
O	3.924312	1.014252	4.175630

O	8.258675	0.984603	4.676957
O	1.420561	17.342974	1.342984
O	1.674640	0.063279	0.923293
O	1.927718	2.732531	1.001450
O	6.258076	17.170649	1.754511
O	6.092294	19.732643	1.094194
O	6.093495	2.563588	1.166328
O	10.203611	19.162737	3.837843
O	10.185391	2.733725	4.260077
O	12.760420	10.943256	3.513573
O	13.928504	11.275768	1.177972
O	16.099089	11.038174	12.896528
O	18.099087	11.361732	1.339638
O	17.941513	11.020066	3.930186
O	15.371890	11.358150	3.273750
O	12.770231	7.124240	3.422167
O	13.933709	7.043251	1.002521
O	16.307919	7.200254	13.302435
O	18.508938	6.467772	1.279683
O	17.944717	6.806055	3.913189
O	15.407729	6.631740	3.173912
O	14.442069	9.028176	2.677805
O	18.279884	8.901221	2.271229
O	11.511848	12.448814	5.280263
O	11.764927	9.858761	5.783731
O	12.175978	7.198662	5.931613
O	16.431854	12.691383	5.195281
O	16.177975	10.038847	5.520488
O	16.018801	7.389693	5.697946
O	0.190209	10.708249	2.923383
O	0.323155	7.297759	3.013584
O	17.270176	8.782424	10.380658
O	16.425648	8.871173	7.876966
O	14.084675	8.953555	6.614414
O	11.928707	8.533288	8.100730
O	12.211617	8.945794	10.646311
O	14.690941	9.363076	9.873443
O	17.348263	13.514605	10.046083
O	16.260866	13.180501	7.704459
O	13.951929	12.761230	6.279438
O	11.844214	13.425856	7.776326
O	12.182786	13.266863	10.393640
O	14.711364	13.011758	9.788594
O	16.598238	11.112000	9.365959

O	11.935314	11.027430	8.952960
O	18.692739	7.468094	12.202753
O	18.449871	10.094563	12.450473
O	18.094282	12.762025	12.544823
O	14.256865	7.387504	11.631968
O	13.853222	9.796278	12.456227
O	13.921296	12.455978	12.280375
O	9.849022	9.450035	9.536057
O	9.853427	12.600246	9.368100
O	12.845314	18.828434	3.674437
O	13.679630	18.820871	1.173288
O	15.968745	18.910816	13.215847
O	18.108097	18.395630	1.335891
O	17.950724	18.842165	3.928178
O	15.432957	18.820673	3.165615
O	12.454684	3.149216	3.086923
O	13.846013	3.070416	0.927174
O	16.121714	2.900279	12.964247
O	18.106094	3.477151	1.258671
O	17.675020	2.903662	3.844133
O	15.105998	3.484315	3.244173
O	14.095287	1.095440	2.752482
O	18.269474	0.975250	2.106083
O	11.430960	17.323074	5.285482
O	11.672826	0.014725	5.856535
O	12.423050	2.643980	5.698348
O	16.268875	17.159903	5.018090
O	16.185183	19.739212	5.610957
O	15.761919	2.484191	5.616979
O	0.195615	19.148808	2.859278
O	0.071479	2.737108	2.923383
O	17.259964	1.162102	10.365803
O	16.355772	1.235529	7.867733
O	14.021606	0.754769	6.693641
O	11.839809	1.493420	8.023510
O	12.097692	1.160112	10.619010
O	14.661109	1.156132	9.873175
O	17.441164	16.654469	9.869160
O	16.191391	16.840324	7.617738
O	13.897870	17.093838	6.270605
O	11.838207	16.502439	7.800951
O	12.190194	16.663223	10.454130
O	14.756213	16.673969	9.794350
O	16.104094	18.898876	9.366494

O	11.928707	18.897085	9.026567
O	18.607645	2.578314	12.135972
O	18.339352	19.883280	12.560749
O	17.846609	17.251240	12.392926
O	13.767727	2.838990	11.714140
O	13.854223	0.245753	12.299379
O	13.933910	17.466148	12.284524
O	9.825796	0.589607	9.544354
O	9.860234	17.256413	9.442242
O	7.088589	9.210650	9.445455
O	5.083786	8.716558	12.023020
O	3.842822	9.037330	0.747173
O	2.084090	8.536671	12.036939
O	2.102510	9.125085	9.375594
O	4.665727	9.612610	9.783776
O	7.486826	13.262882	10.208419
O	6.248065	13.270445	12.459842
O	3.915302	12.766204	0.411260
O	1.823003	13.435408	12.272078
O	2.253676	13.100507	9.691701
O	4.843522	13.016533	10.210426
O	6.346573	11.003350	11.207192
O	1.674640	11.002157	11.287623
O	8.597246	7.547890	7.865992
O	8.499539	10.115458	7.451386
O	7.839814	12.744713	7.599403
O	3.770743	7.308903	8.518280
O	3.747718	9.695588	7.355163
O	3.919707	12.359070	7.776059
O	19.912279	9.116528	10.539782
O	19.856218	12.767596	10.541924
O	2.826506	10.946837	2.922312
O	3.764937	11.342829	5.353200
O	6.005198	11.014693	6.855576
O	8.090690	11.526098	5.273571
O	7.931515	10.849133	2.674325
O	5.436373	10.848736	3.417483
O	2.848130	6.557517	3.360605
O	3.667029	6.869931	5.872327
O	6.027223	7.139164	7.109318
O	8.019412	6.466180	5.517008
O	7.856833	6.954303	2.927799
O	5.428565	6.704769	3.930453
O	3.907093	8.880924	4.186337

O	8.185794	8.967087	4.599737
O	1.417157	12.495975	1.342716
O	1.413954	9.869308	0.833627
O	1.922312	7.219954	0.899873
O	6.261480	12.624323	1.664578
O	6.177187	10.122422	0.847010
O	5.671431	7.525205	1.436264
O	10.184391	10.617112	3.845070
O	10.189196	7.217766	4.176969
O	8.839713	14.932409	8.621329
O	3.836616	14.867140	8.538890
O	5.344472	14.928229	0.851694
O	2.414653	14.919673	0.996766
O	1.245168	4.976541	2.018692
O	6.333158	5.042208	1.998751
O	4.581634	4.990670	7.527938
O	7.671229	5.030069	7.687463
O	11.593940	4.985893	4.770504
O	16.425648	4.947091	5.008052
O	14.672521	5.105487	12.723620
O	17.696043	5.044795	12.556601
O	18.853315	15.022949	11.540295
O	13.926102	14.929225	11.545649
O	15.353270	14.934001	5.938037
O	12.420246	14.918281	5.699820
O	11.006093	5.713799	15.297706
O	10.178985	3.153196	14.719561
O	8.596445	2.656516	12.200880
O	10.187794	3.479340	10.120225
O	9.354078	0.734273	14.140746
O	9.508448	8.469213	14.558562
O	11.326646	4.291419	12.616958
O	12.083477	5.804936	10.376108
O	11.674427	6.965446	12.881941
O	11.918495	9.280496	14.472644
Pt	7.046142	5.122599	-3.558406
Pt	9.434166	7.333379	-0.720273
Pt	9.020111	6.757900	-3.152767
Pt	6.362190	5.341488	-1.170477
Pt	7.091992	7.860702	-1.194700
Pt	8.820091	4.868887	-0.967323
H	10.105904	6.081334	15.197600
H	10.877552	4.739942	15.226107
H	9.329251	3.564707	14.435707

H	9.971156	2.176155	14.721702
H	7.650005	2.512050	11.981265
H	9.087185	2.600600	11.338881
H	9.614964	4.286842	9.999243
H	10.699156	3.385019	9.297571
H	8.866543	1.055642	13.359982
H	8.816087	0.056513	14.586667
H	8.791460	9.130259	14.594964
H	10.399426	8.950969	14.641404
H	11.479613	3.874932	11.729530
H	11.293008	3.596346	13.340576
H	11.136637	6.062429	10.144715
H	12.629277	6.329275	9.768252
H	11.898874	6.479910	12.033459
H	11.656608	6.300024	13.619345
H	12.025012	10.108692	13.976805
H	12.132331	8.570698	13.821962

324

#### Pt6@Silicalite-1-10W\_FS

Si	8.459495	1.007088	8.790490
Si	6.072072	0.546228	10.834877
Si	5.607562	1.203691	0.406709
Si	2.397434	1.361291	0.274485
Si	1.399738	0.539661	10.909956
Si	3.607564	1.202895	9.009302
Si	8.503343	16.476770	9.010372
Si	6.178589	17.208057	10.978745
Si	5.437374	16.496868	0.524614
Si	2.402440	16.438963	0.412330
Si	1.434176	17.327253	10.979815
Si	3.734904	16.397175	9.107399
Si	1.557912	18.802366	2.056967
Si	3.936926	19.294270	4.111258
Si	4.387220	18.734114	7.030492
Si	7.562109	18.542685	6.877256
Si	8.635489	19.363916	4.187809
Si	6.382613	18.682575	2.310174
Si	1.484631	3.430588	2.391542
Si	3.908895	2.628857	4.299155
Si	4.548798	3.408301	7.229631
Si	7.617370	3.408301	7.186136
Si	8.646701	2.565379	4.414516
Si	6.401233	3.441532	2.531796
Si	11.576921	10.963553	4.607633

Si	14.103896	10.615122	2.666161
Si	14.499531	11.165926	13.055920
Si	17.683229	11.319745	13.162716
Si	18.649290	10.469262	2.587871
Si	16.467695	11.247711	4.488123
Si	11.671624	6.599702	4.478621
Si	14.126522	7.441629	2.575425
Si	14.786246	6.688850	13.029689
Si	17.812370	6.541398	13.195504
Si	18.764017	7.376957	2.620525
Si	16.442867	6.463394	4.433922
Si	18.560192	8.870975	11.383847
Si	16.253658	9.525652	9.360338
Si	15.684233	8.798144	6.422636
Si	12.497531	8.643529	6.571187
Si	11.472205	9.502370	9.302791
Si	13.793156	8.865602	11.132381
Si	18.536167	13.487741	11.156069
Si	16.213816	12.689195	9.241096
Si	15.476405	13.379491	6.301653
Si	12.429857	13.383271	6.254947
Si	11.450181	12.582138	9.108470
Si	13.691443	13.414514	10.994938
Si	11.562304	18.819080	4.655544
Si	13.992174	19.371677	2.668303
Si	14.354172	18.800974	13.070775
Si	17.552887	18.615515	13.211029
Si	18.640081	19.350185	2.541967
Si	16.431253	18.665859	4.433520
Si	11.691446	3.407505	4.469655
Si	13.933910	2.683977	2.490175
Si	14.608651	3.496851	12.936008
Si	17.650595	3.495657	13.078805
Si	18.558792	2.536725	2.518413
Si	16.264071	3.438547	4.400598
Si	18.490517	1.118921	11.415164
Si	16.113104	0.623834	9.359000
Si	15.589128	1.100216	6.431736
Si	12.486320	1.245876	6.546027
Si	11.420148	0.552993	9.283253
Si	13.632379	1.324278	11.121273
Si	18.496323	16.540646	11.094909
Si	16.127119	17.287058	9.170032
Si	15.425949	16.514380	6.230188

Si	12.393017	16.451897	6.274218
Si	11.459991	17.341183	9.156247
Si	13.704257	16.453091	11.019696
Si	8.479717	9.026385	8.675529
Si	6.019214	9.485456	10.692616
Si	5.427563	8.736457	0.349296
Si	2.352985	8.663229	0.260567
Si	1.463408	9.445458	10.828855
Si	3.610567	8.920722	8.782193
Si	8.488927	13.383073	8.947206
Si	6.218032	12.604823	10.982224
Si	5.440578	13.366158	0.478175
Si	2.400437	13.396008	0.408182
Si	1.402741	12.566418	10.959607
Si	3.735504	13.324370	9.062299
Si	1.499848	11.003749	2.002364
Si	3.954145	10.487370	3.977829
Si	4.379212	11.113791	6.852899
Si	7.595946	11.331087	6.821851
Si	8.591240	10.489360	4.125443
Si	6.407640	11.090111	2.158678
Si	1.598156	6.532245	2.329445
Si	3.951542	7.273085	4.320166
Si	4.527575	6.583783	7.240604
Si	7.586135	6.556522	7.041734
Si	8.619671	7.420934	4.289519
Si	6.314138	6.534235	2.555618
O	7.253370	1.081511	9.864075
O	6.245462	1.234136	12.297639
O	3.994990	1.165882	0.410858
O	1.919909	1.495410	12.117906
O	2.090297	0.994950	9.522407
O	4.602657	0.985399	10.281356
O	7.503445	16.579649	10.284300
O	6.255673	16.822615	12.546831
O	3.912098	17.087072	0.418353
O	1.829410	16.422447	12.274220
O	2.254878	16.747198	9.698660
O	4.838717	16.585617	10.295408
O	6.170380	18.825848	10.867264
O	1.767142	18.895693	11.291237
O	8.586635	2.491952	8.107288
O	8.261077	19.815025	7.606362
O	7.833407	17.165674	7.692147

O	3.753925	2.726362	8.460332
O	3.851031	0.169340	7.781545
O	4.015212	17.402870	7.863182
O	19.845205	0.751983	10.616065
O	19.871433	17.253628	10.619411
O	2.820499	18.742470	3.079696
O	3.660822	18.652925	5.577767
O	5.985376	18.893703	6.783575
O	8.172980	18.342300	5.373542
O	7.916698	18.987427	2.771619
O	5.416752	18.833807	3.604310
O	2.663727	3.307413	3.509692
O	3.758530	3.069421	5.854527
O	6.091693	2.828046	7.195504
O	8.173181	3.477947	5.675864
O	7.911893	3.148221	3.086387
O	5.348476	3.163543	3.752192
O	3.905091	1.014252	4.173087
O	8.263280	0.993159	4.672139
O	1.420160	17.342974	1.342850
O	1.674440	0.065468	0.923159
O	1.927918	2.729546	0.999175
O	6.258076	17.167067	1.757322
O	6.091493	19.717720	1.095532
O	6.096699	2.491753	1.254924
O	10.205214	19.162937	3.837709
O	10.243256	2.723576	4.262619
O	12.768029	10.944052	3.512904
O	13.927503	11.273779	1.182388
O	16.099289	11.037975	12.898001
O	18.099686	11.361334	1.340174
O	17.952726	11.018475	3.933532
O	15.414938	11.353573	3.261571
O	12.784648	7.122648	3.416680
O	13.935913	7.044445	1.000379
O	16.313925	7.199657	13.301899
O	18.509336	6.467772	1.282627
O	17.946720	6.805856	3.915866
O	15.417140	6.632934	3.172306
O	14.441467	9.031758	2.676466
O	18.280487	8.901022	2.272032
O	11.512650	12.449412	5.280664
O	11.765527	9.859756	5.782794
O	12.172976	7.198065	5.926929

O	16.432455	12.692577	5.197422
O	16.178577	10.038448	5.521023
O	16.019001	7.387504	5.697010
O	0.193813	10.708249	2.922714
O	0.323956	7.298954	3.014387
O	17.272379	8.782025	10.381060
O	16.427050	8.870577	7.875762
O	14.086678	8.953157	6.613477
O	11.930510	8.530303	8.092165
O	12.242051	8.945396	10.632660
O	14.699151	9.363076	9.873041
O	17.348461	13.514605	10.046484
O	16.260666	13.180501	7.704593
O	13.952129	12.761626	6.279036
O	11.844415	13.425060	7.775925
O	12.182385	13.264673	10.395246
O	14.710163	13.009768	9.788058
O	16.599239	11.113194	9.365558
O	11.930108	11.026434	8.952826
O	18.694139	7.467896	12.202888
O	18.450073	10.094365	12.450205
O	18.094282	12.762025	12.544555
O	14.259667	7.383922	11.632905
O	13.853422	9.795084	12.460912
O	13.920896	12.453391	12.281044
O	9.858232	9.371832	9.538198
O	9.852225	12.599051	9.367431
O	12.846115	18.828035	3.674570
O	13.678629	18.818882	1.172217
O	15.961138	18.907234	13.215178
O	18.106495	18.398615	1.337363
O	17.944317	18.904846	3.931926
O	15.432756	18.818882	3.164678
O	12.515752	3.159165	3.099637
O	13.847216	3.069222	0.920750
O	16.127319	2.899881	12.964514
O	18.110899	3.478146	1.262017
O	17.692039	2.902070	3.845739
O	15.181280	3.479738	3.175920
O	14.099292	1.091460	2.752482
O	18.274879	0.986791	2.098856
O	11.431560	17.323273	5.285616
O	11.674027	0.015322	5.854795
O	12.434261	2.646169	5.707181

O	16.272280	17.163883	5.015681
O	16.183382	19.740007	5.614570
O	15.761317	2.485783	5.609485
O	0.194414	19.148609	2.857270
O	0.101512	2.741883	2.928736
O	17.261166	1.162102	10.365669
O	16.356173	1.237320	7.866661
O	14.023208	0.754371	6.692972
O	11.843813	1.490833	8.017889
O	12.102097	1.155933	10.623425
O	14.664514	1.156530	9.873710
O	17.441164	16.654070	9.869293
O	16.191990	16.839928	7.617470
O	13.900072	17.093639	6.270471
O	11.839008	16.503832	7.805099
O	12.189393	16.663622	10.452124
O	14.756815	16.672974	9.793412
O	16.104294	18.898876	9.366226
O	11.926504	18.906836	9.028440
O	18.608847	2.577518	12.135704
O	18.336147	19.881887	12.561551
O	17.846008	17.251438	12.394398
O	13.770330	2.833817	11.711597
O	13.856025	0.238390	12.299646
O	13.937514	17.430132	12.297773
O	9.822993	0.587816	9.551715
O	9.861034	17.256413	9.442911
O	7.072371	9.289450	9.388041
O	5.096600	8.790383	12.041890
O	3.839619	9.033350	0.753597
O	2.085692	8.536671	12.036939
O	2.107716	9.119314	9.373721
O	4.655515	9.615993	9.782438
O	7.490430	13.264474	10.208419
O	6.248466	13.271439	12.461848
O	3.915703	12.765805	0.411527
O	1.823203	13.434412	12.272211
O	2.253876	13.100307	9.691031
O	4.842721	13.017131	10.209087
O	6.348976	11.016087	11.206656
O	1.675441	11.001362	11.285884
O	8.602052	7.544507	7.869204
O	8.508749	10.123418	7.440814
O	7.840214	12.748096	7.600741

O	3.840219	7.312285	8.522696
O	3.747918	9.695987	7.352487
O	3.919707	12.360264	7.777531
O	19.915281	9.116130	10.539515
O	19.856218	12.767199	10.542191
O	2.827106	10.946441	2.922178
O	3.762334	11.344420	5.354940
O	6.005198	11.014495	6.855308
O	8.090890	11.526894	5.272635
O	7.936320	10.852516	2.679009
O	5.433170	10.854706	3.428323
O	2.848330	6.559905	3.361676
O	3.677240	6.871722	5.876609
O	6.076677	7.129414	7.103964
O	8.103304	6.462797	5.513662
O	7.856031	6.946343	2.926193
O	5.431568	6.698600	3.929383
O	3.909496	8.879730	4.186203
O	8.188197	8.965494	4.597596
O	1.417758	12.497965	1.342315
O	1.414354	9.870302	0.833092
O	1.921912	7.219755	0.900007
O	6.261880	12.625717	1.664176
O	6.175986	10.099339	0.907367
O	5.670831	7.462523	1.416323
O	10.188395	10.617908	3.844936
O	10.232243	7.289003	4.104566
O	8.840313	14.936189	8.621195
O	3.836415	14.872712	8.539157
O	5.343872	14.930220	0.852229
O	2.414653	14.920669	0.996632
O	1.240563	4.981317	2.015480
O	6.327552	4.983704	2.012268
O	4.589443	4.989873	7.529811
O	7.680839	5.006390	7.691344
O	11.592537	4.996241	4.767560
O	16.423847	4.939728	5.006313
O	14.673323	5.101109	12.721478
O	17.697845	5.043202	12.557671
O	18.853115	15.024143	11.540429
O	13.926501	14.925445	11.544310
O	15.354071	14.935991	5.937502
O	12.420447	14.920669	5.700891
O	11.003690	5.708625	15.291417

O	10.269884	3.150609	14.720899
O	8.667924	2.731536	12.375929
O	10.606255	3.481728	9.948655
O	9.352676	0.750590	14.132180
O	9.505044	8.374495	14.472912
O	11.190095	4.279877	12.425849
O	12.083277	5.807921	10.360450
O	11.673827	6.954900	12.888766
O	11.843614	9.285072	14.471039
Pt	7.208520	5.126779	-3.527491
Pt	9.415345	7.292585	-0.798965
Pt	9.025917	6.895401	-3.217273
Pt	6.431467	5.327957	-1.189615
Pt	7.085785	7.936716	-1.214507
Pt	8.915195	4.753473	-1.071844
H	10.106504	6.089094	15.234002
H	10.855728	4.733176	15.204160
H	9.406735	3.415464	14.330918
H	10.150953	2.162822	14.789954
H	8.407638	4.456381	13.718246
H	9.213123	2.397630	11.640400
H	9.773138	4.004475	9.903822
H	11.298615	4.117501	9.670021
H	8.883161	1.329651	13.474674
H	8.709769	0.146059	14.535143
H	8.758424	9.001909	14.516273
H	10.386011	8.892067	14.556020
H	11.258370	3.787178	11.553946
H	11.142643	3.622215	13.185869
H	11.178883	6.191972	10.148730
H	12.702356	6.315346	9.809204
H	11.923100	6.414443	12.091808
H	11.636987	6.332061	13.667523
H	11.974358	10.154062	14.056031
H	12.133131	8.629003	13.795867

303

#### Pt6H2@H-MFI-1W\_IS

Si	8.444679	1.076735	8.762385
Si	6.062862	0.637763	10.822966
Si	5.604758	1.170857	0.343809
Si	2.443485	1.275924	0.178262
Si	1.415555	0.541054	10.820022
Si	3.667029	1.323085	9.043028
Si	8.607657	16.474382	9.054670

Si	6.158367	17.308548	10.917583
Si	5.423159	16.502241	0.481788
Si	2.380616	16.475777	0.440702
Si	1.397135	17.354914	11.015414
Si	3.630389	16.381653	9.130150
Si	1.537089	18.837587	2.052685
Si	3.940329	19.374065	4.057458
Si	7.700661	18.524775	6.931190
Si	8.637891	19.367498	4.147392
Si	6.418653	18.715010	2.212344
Si	1.623984	3.407306	2.323690
Si	3.917304	2.693728	4.345995
Si	4.536584	3.386611	7.254389
Si	7.605958	3.422230	7.194166
Si	8.647101	2.591845	4.357772
Si	11.606153	10.934501	4.623960
Si	14.147944	10.471053	2.706310
Si	14.444871	11.079564	13.121363
Si	17.658001	11.236965	13.243549
Si	18.727777	10.536122	2.679410
Si	16.464891	11.333277	4.517833
Si	11.744305	6.551746	4.490532
Si	14.202605	7.303729	2.549595
Si	14.851519	6.654425	13.060604
Si	18.913982	7.403423	2.709656
Si	16.501131	6.530454	4.444628
Si	18.542574	8.953754	11.319877
Si	16.173571	9.481874	9.356858
Si	15.618961	8.919528	6.425982
Si	12.450881	8.658652	6.621507
Si	11.485620	9.377802	9.411461
Si	13.738296	8.722926	11.152590
Si	18.480106	13.465256	11.134254
Si	16.144739	12.663127	9.247519
Si	15.474604	13.419488	6.280776
Si	12.451682	13.379292	6.230456
Si	13.788951	13.445356	11.146835
Si	11.537477	18.795799	4.640422
Si	13.952331	19.301434	2.644882
Si	14.388009	18.871813	13.089109
Si	17.529261	18.618500	13.226553
Si	18.613251	19.345211	2.557893
Si	16.397217	18.626060	4.410635
Si	11.727085	3.375468	4.546607

Si	13.937715	2.629056	2.454844
Si	14.645692	3.453074	12.961168
Si	17.696043	3.442527	12.989540
Si	18.678324	2.514438	2.404658
Si	18.522753	1.041315	11.385186
Si	16.069256	0.550605	9.425513
Si	15.553490	0.988980	6.483662
Si	12.460892	1.197920	6.572927
Si	11.355276	0.462055	9.330762
Si	13.604348	1.365071	11.160887
Si	18.452074	16.552982	11.115117
Si	16.161358	17.270741	9.154374
Si	15.422145	16.593378	6.232329
Si	12.394818	16.443737	6.308211
Si	11.507243	17.211441	9.241899
Si	13.864033	16.435579	11.036291
Si	8.546791	9.086878	8.799725
Si	5.939326	9.487844	10.656214
Si	5.453592	8.875153	0.288671
Si	2.262686	8.675963	0.172641
Si	1.420361	9.572215	10.752571
Si	3.530879	8.759340	8.700824
Si	8.360186	13.334718	8.934893
Si	5.991783	12.649993	10.985436
Si	5.376508	13.360586	0.487275
Si	2.360193	13.434810	0.258024
Si	1.364499	12.644223	10.811323
Si	3.705672	13.383471	9.012246
Si	1.538891	11.093096	1.998751
Si	3.955346	10.472246	3.956550
Si	4.446085	11.117373	6.855041
Si	7.607358	11.270396	6.793211
Si	8.652307	10.481600	4.044477
Si	6.396628	11.108218	2.152789
Si	1.665830	6.513341	2.234827
Si	4.040440	7.288805	4.121429
Si	4.504349	6.567665	7.048693
Si	8.717778	7.370390	4.222069
Si	6.472512	6.616020	2.350992
O	7.183093	1.163296	9.783776
O	6.346573	1.326865	12.267260
O	4.006002	0.909185	0.151763
O	1.841423	1.499589	12.061296
O	2.114323	0.997537	9.440502

O	4.572624	1.086286	10.382131
O	7.484824	16.746599	10.194500
O	6.167777	16.742620	12.436554
O	3.895680	17.090654	0.415944
O	1.753927	16.493685	12.327082
O	2.165980	16.583031	9.784445
O	4.829907	16.752769	10.118887
O	6.094697	18.911213	10.879309
O	1.847029	18.899872	11.199028
O	8.665121	2.562991	8.116254
O	8.181991	19.973225	7.521514
O	8.510951	17.331034	7.692816
O	3.759731	2.896101	8.608748
O	4.172184	0.397781	7.852208
O	3.588343	17.413416	7.780208
O	19.847208	0.664826	10.533760
O	19.829588	17.322279	10.710281
O	2.760033	18.818483	3.086254
O	3.759130	18.673420	5.489974
O	6.145953	18.316433	7.197244
O	8.099099	18.409163	5.354672
O	7.918301	18.978870	2.748868
O	5.401936	18.987427	3.438361
O	2.589045	3.323133	3.602034
O	3.684649	2.910030	5.953695
O	6.083885	2.814117	7.277006
O	8.095695	3.412281	5.665426
O	8.003594	3.151007	3.011844
O	5.257576	3.396958	3.847211
O	3.841621	1.087281	4.089577
O	8.339964	0.996542	4.599470
O	1.415355	17.331034	1.423817
O	1.664229	0.004378	0.833226
O	2.176792	2.654925	0.998640
O	6.264884	17.173632	1.683849
O	6.173182	19.658421	0.921420
O	5.851229	2.498518	1.174626
O	10.199807	19.070604	3.771463
O	10.269083	2.736511	4.341980
O	12.838907	10.695115	3.606050
O	13.846814	11.109015	1.240470
O	16.063650	11.031209	13.054582
O	18.107695	11.366110	1.407624
O	17.963737	11.017878	4.018112

O	15.435760	11.276962	3.263311
O	12.843912	6.881074	3.332367
O	13.922498	6.960869	0.991546
O	16.324537	7.272885	13.291996
O	18.681526	6.476328	1.420070
O	18.025606	6.962859	4.010752
O	15.526259	6.544384	3.106730
O	14.515750	8.895649	2.680213
O	18.526356	8.959923	2.347111
O	11.593739	12.452396	5.187519
O	11.670223	9.869108	5.857204
O	12.257668	7.237067	5.868178
O	16.436459	12.847192	5.105882
O	16.096285	10.283604	5.692192
O	15.936510	7.624501	5.523566
O	0.258884	10.942062	2.992171
O	0.500350	7.289601	3.094283
O	17.260965	8.784413	10.368880
O	16.418640	8.872169	7.867733
O	14.025210	9.040514	6.696988
O	11.838207	8.456279	8.108625
O	12.179783	8.634972	10.699173
O	14.665915	9.190553	9.880000
O	17.271177	13.510824	10.047153
O	16.189188	13.093941	7.704326
O	13.989572	12.765805	6.192180
O	11.847417	13.346856	7.704058
O	12.179983	13.431029	10.540719
O	14.670719	13.018324	9.868358
O	16.444468	11.085932	9.449067
O	12.020608	10.875201	9.213259
O	18.853115	7.399244	11.971094
O	18.356770	9.875874	12.627129
O	18.100889	12.597858	12.464257
O	14.180982	7.280447	11.709322
O	13.845813	9.785931	12.377669
O	13.923298	12.436676	12.380614
O	9.868443	9.367852	9.703211
O	9.686243	12.604624	9.452547
O	12.845513	18.736898	3.679924
O	13.678629	18.661083	1.160574
O	15.982361	19.065430	13.299089
O	18.111900	18.391651	1.340843
O	17.928499	18.899275	3.946513

O	15.440765	18.821867	3.105927
O	12.586830	3.161752	3.185823
O	13.776938	2.988631	0.871233
O	16.170769	2.823668	12.961302
O	18.185982	3.410887	1.179578
O	17.946520	3.133893	3.839449
O	15.274183	3.315372	3.015324
O	13.935512	1.010471	2.666028
O	18.186983	0.993159	2.184507
O	11.421550	17.335014	5.362836
O	11.602348	0.078004	5.764058
O	12.435263	2.655124	5.844223
O	16.260466	17.088066	4.932840
O	16.099489	19.572258	5.686169
O	15.777135	2.335745	5.678006
O	0.174792	19.229597	2.845895
O	0.222645	2.656516	2.765062
O	17.266972	1.079123	10.373163
O	16.351166	1.064995	7.918855
O	13.979560	0.667412	6.777687
O	11.757919	1.339601	8.031138
O	12.094089	1.089470	10.632125
O	14.661309	1.159316	9.946112
O	17.522253	16.658648	9.789263
O	16.260666	17.012451	7.563804
O	13.884255	17.155325	6.282784
O	11.847618	16.423840	7.857695
O	12.349369	16.498260	10.458948
O	14.867336	16.488909	9.769055
O	15.945320	18.826643	9.538065
O	11.841611	18.804157	9.117838
O	18.687534	2.482002	12.121117
O	18.366581	19.816021	12.545894
O	17.686434	17.239498	12.379007
O	13.766525	2.893713	11.698883
O	13.847615	0.325946	12.388643
O	14.103296	17.576389	12.139987
O	9.754118	0.582245	9.614882
O	10.005795	16.910170	9.778155
O	7.264582	9.293429	9.782572
O	6.019614	8.622635	12.102783
O	3.844624	9.032753	0.329891
O	1.912501	8.612885	11.964670
O	2.088094	9.122100	9.360606

O	4.652312	8.947784	9.871034
O	7.240155	13.174531	10.119422
O	6.252670	13.110058	12.521403
O	3.858640	12.774163	0.247452
O	1.754528	13.524555	12.123125
O	2.161175	13.098119	9.456964
O	4.597852	13.266067	10.373699
O	5.757726	11.037180	11.039235
O	1.750123	11.102050	11.196887
O	8.587635	7.538935	8.280865
O	8.503943	10.111279	7.529945
O	7.765532	12.697154	7.542926
O	3.505852	7.224133	8.191734
O	3.747918	9.781155	7.452859
O	4.166378	12.433493	7.783687
O	19.841801	9.368051	10.458815
O	19.796152	12.772770	10.456539
O	2.925214	11.102648	2.851918
O	3.840620	11.344620	5.348917
O	6.041238	10.840179	6.847680
O	8.100301	11.442920	5.252560
O	7.938122	10.862664	2.609283
O	5.492435	10.613132	3.414940
O	3.085190	6.560103	3.018937
O	3.751722	6.713923	5.602258
O	5.943531	7.286218	7.109451
O	8.265882	6.546572	5.512056
O	8.018810	6.967038	2.777776
O	5.580131	6.970819	3.686481
O	3.669632	8.887690	4.173890
O	8.350575	8.953555	4.504986
O	1.407547	12.497766	1.178239
O	1.427769	9.862541	0.917405
O	1.842625	7.221745	0.757612
O	6.095097	12.662131	1.770303
O	6.099102	10.281217	0.765106
O	5.927113	7.629476	1.169808
O	10.245858	10.695115	3.762095
O	10.346768	7.209408	3.928312
O	8.592641	14.915296	8.620793
O	3.826805	14.922062	8.452168
O	5.338666	14.927832	0.834965
O	2.410248	14.919474	0.918877
O	1.320451	4.956841	1.926215

O	6.335361	5.131952	1.761738
O	4.596050	4.990868	7.370687
O	7.587337	4.962015	7.785293
O	11.668020	4.976939	4.846787
O	16.510742	5.064494	5.097852
O	14.772231	5.053351	12.801107
O	17.848812	4.950473	12.466801
O	18.772026	15.009617	11.544712
O	14.018203	14.941562	11.714140
O	15.350667	15.000264	6.107600
O	12.431859	14.930817	5.694199
O	11.011899	7.954227	13.970380
Al	4.544193	18.865047	7.008142
Al	6.374404	3.514562	2.504762
Al	17.843807	6.458021	13.307118
Al	11.361684	12.457968	9.080767
Al	16.169567	3.488096	4.475410
Al	7.565113	6.622188	7.093392
H	10.132333	5.591818	9.244174
H	19.276581	6.763869	11.359625
H	11.721679	14.282309	10.719917
H	18.612249	3.563115	4.413044
H	2.949241	17.125875	7.094596
H	7.088389	6.097253	12.601031
H	10.916395	7.653952	14.902639
H	10.426056	8.733473	13.889681
Pt	7.206118	4.719844	-3.420829
Pt	10.180586	6.426581	-0.732050
Pt	9.156461	6.386186	-3.216470
Pt	6.821696	4.454192	-0.905761
Pt	7.951737	7.513863	-1.085094
Pt	9.221732	4.270525	-1.659492

303

#### Pt6H2@H-MFI-1W\_FS

Si	8.445680	1.071561	8.756899
Si	6.037033	0.627415	10.786564
Si	5.608362	1.212048	0.315705
Si	2.439480	1.278113	0.178663
Si	1.408948	0.538865	10.820825
Si	3.645806	1.323085	9.032990
Si	8.610460	16.472195	9.054537
Si	6.158166	17.302380	10.916112
Si	5.422558	16.513186	0.485268
Si	2.378213	16.474182	0.439498

Si	1.394132	17.354317	11.014477
Si	3.628787	16.379265	9.130150
Si	1.534686	18.836195	2.053220
Si	3.936325	19.374462	4.058529
Si	7.700861	18.520796	6.929049
Si	8.642096	19.368692	4.148730
Si	6.418052	18.757395	2.209935
Si	1.619780	3.409893	2.324761
Si	3.914501	2.693330	4.345594
Si	4.535784	3.389795	7.254121
Si	7.607759	3.420439	7.189750
Si	8.652507	2.591447	4.355631
Si	11.606552	10.931517	4.621284
Si	14.145743	10.467471	2.705374
Si	14.439065	11.077375	13.123236
Si	17.652796	11.235771	13.243817
Si	18.724773	10.536521	2.679812
Si	16.461487	11.332282	4.516763
Si	11.743303	6.555924	4.479290
Si	14.194797	7.304127	2.547454
Si	14.843710	6.656415	13.063548
Si	18.911379	7.403423	2.709924
Si	16.496325	6.532046	4.441149
Si	18.539570	8.953356	11.320412
Si	16.168165	9.479287	9.358063
Si	15.616960	8.919130	6.425714
Si	12.450279	8.654274	6.616154
Si	11.492828	9.377205	9.410391
Si	13.733290	8.718747	11.158076
Si	18.477503	13.463465	11.134789
Si	16.143738	12.660739	9.247519
Si	15.474803	13.417896	6.280642
Si	12.451080	13.376307	6.229117
Si	13.788951	13.443168	11.147905
Si	11.540280	18.795004	4.641626
Si	13.952930	19.303024	2.644347
Si	14.387008	18.871017	13.089109
Si	17.527658	18.618299	13.226686
Si	18.611248	19.345610	2.558294
Si	16.396416	18.625862	4.411170
Si	11.729288	3.382034	4.545269
Si	13.936913	2.631245	2.452167
Si	14.644892	3.456854	12.960767
Si	17.693840	3.444716	12.989005

Si	18.674719	2.516229	2.405862
Si	18.518547	1.042509	11.386926
Si	16.067253	0.550605	9.425112
Si	15.553289	0.989776	6.483127
Si	12.461492	1.199512	6.571187
Si	11.358480	0.460662	9.330092
Si	13.604948	1.366066	11.162226
Si	18.449871	16.551191	11.115117
Si	16.160557	17.270542	9.153438
Si	15.422145	16.591787	6.231928
Si	12.396020	16.441549	6.307408
Si	11.509246	17.209053	9.241899
Si	13.864433	16.433590	11.036826
Si	8.544389	9.090261	8.796379
Si	5.940327	9.485256	10.660764
Si	5.449788	8.879730	0.299378
Si	2.260083	8.676561	0.172908
Si	1.417357	9.572016	10.753241
Si	3.530279	8.761131	8.701894
Si	8.360786	13.332727	8.934625
Si	5.992384	12.649397	10.986641
Si	5.378310	13.365959	0.488747
Si	2.360594	13.433816	0.257623
Si	1.362697	12.643625	10.811591
Si	3.705271	13.381680	9.012916
Si	1.536088	11.093892	1.999286
Si	3.954946	10.483588	3.955212
Si	4.447086	11.117770	6.854639
Si	7.607759	11.272187	6.787189
Si	8.656712	10.478813	4.040462
Si	6.400032	11.112000	2.153726
Si	1.666231	6.516524	2.236567
Si	4.032431	7.309500	4.123704
Si	4.499144	6.570650	7.046953
Si	8.730793	7.375763	4.217519
Si	6.471511	6.635919	2.378694
O	7.179889	1.162898	9.778021
O	6.339365	1.332636	12.222426
O	4.011007	0.920528	0.156046
O	1.842424	1.498793	12.060091
O	2.098105	0.997935	9.436219
O	4.534182	1.080715	10.385476
O	7.486626	16.747198	10.194634
O	6.167377	16.743814	12.436554

O	3.891876	17.092644	0.415542
O	1.753727	16.493484	12.325074
O	2.165379	16.583429	9.784178
O	4.829106	16.752571	10.118351
O	6.092294	18.908627	10.877033
O	1.846829	18.899672	11.198627
O	8.664520	2.562394	8.116254
O	8.181789	19.971235	7.518837
O	8.510751	17.330637	7.693218
O	3.758730	2.896101	8.607678
O	4.171584	0.397184	7.852074
O	3.587942	17.413017	7.780475
O	19.843603	0.664826	10.534562
O	19.827385	17.322477	10.710281
O	2.759232	18.818483	3.085718
O	3.758129	18.672625	5.490376
O	6.145552	18.317429	7.197913
O	8.098899	18.409163	5.353601
O	7.920103	18.983646	2.749939
O	5.398732	18.992601	3.439431
O	2.588444	3.322934	3.601633
O	3.685650	2.910428	5.953695
O	6.084686	2.816106	7.278211
O	8.095295	3.413475	5.663686
O	8.004795	3.147027	3.011443
O	5.257576	3.387407	3.841724
O	3.840219	1.087281	4.089711
O	8.339964	0.997139	4.600540
O	1.414755	17.330835	1.423416
O	1.666431	0.004378	0.832958
O	2.176992	2.655720	0.999576
O	6.258677	17.228952	1.667923
O	6.181792	19.730455	0.935338
O	5.925911	2.580104	1.078135
O	10.201810	19.070604	3.771865
O	10.271086	2.736113	4.342382
O	12.840709	10.696509	3.607923
O	13.847415	11.110408	1.241942
O	16.059647	11.031807	13.054447
O	18.107695	11.366309	1.406821
O	17.961935	11.018275	4.018112
O	15.434759	11.276763	3.262642
O	12.850920	6.879084	3.339594
O	13.926501	6.961665	0.992617

O	16.320932	7.271891	13.289855
O	18.681726	6.476130	1.419669
O	18.025206	6.962262	4.011153
O	15.525459	6.545378	3.105258
O	14.517551	8.895451	2.680883
O	18.526756	8.960122	2.346977
O	11.593739	12.451004	5.187652
O	11.670223	9.869108	5.857873
O	12.257268	7.232491	5.867375
O	16.436459	12.846993	5.105748
O	16.096085	10.283604	5.692727
O	15.936710	7.624302	5.524101
O	0.257483	10.942261	2.992573
O	0.499749	7.289800	3.094551
O	17.260164	8.784214	10.368213
O	16.416838	8.872169	7.868268
O	14.024209	9.040514	6.697255
O	11.837207	8.455881	8.106484
O	12.178581	8.632783	10.695827
O	14.661910	9.188960	9.882141
O	17.270576	13.510626	10.046618
O	16.189188	13.093941	7.704727
O	13.989771	12.765805	6.192582
O	11.847417	13.347255	7.703791
O	12.180183	13.430234	10.540719
O	14.670118	13.018523	9.868223
O	16.444069	11.084141	9.449202
O	12.019006	10.875998	9.211786
O	18.852915	7.399244	11.971361
O	18.356569	9.876272	12.627129
O	18.100687	12.597062	12.464659
O	14.182182	7.277064	11.706511
O	13.846214	9.785532	12.376866
O	13.923699	12.436875	12.381015
O	9.867843	9.358897	9.701872
O	9.686443	12.604424	9.452414
O	12.846115	18.736898	3.679522
O	13.678430	18.661083	1.160708
O	15.981359	19.065430	13.299089
O	18.111900	18.391850	1.340843
O	17.928299	18.899076	3.947048
O	15.440966	18.822065	3.105793
O	12.586830	3.160160	3.185288
O	13.775736	2.986442	0.867888

O	16.170166	2.823668	12.960901
O	18.185982	3.410887	1.179042
O	17.945318	3.134888	3.839984
O	15.273782	3.314775	3.014655
O	13.935512	1.011267	2.665358
O	18.186783	0.993557	2.184909
O	11.421750	17.334816	5.363237
O	11.602147	0.078004	5.764460
O	12.434863	2.655522	5.843687
O	16.260466	17.088066	4.932840
O	16.099289	19.572458	5.686303
O	15.776936	2.336143	5.677738
O	0.174191	19.229996	2.845627
O	0.220642	2.656915	2.764794
O	17.265572	1.079322	10.372896
O	16.350765	1.064995	7.918855
O	13.979159	0.667213	6.777821
O	11.757318	1.339601	8.031005
O	12.092687	1.090465	10.632393
O	14.658306	1.158321	9.944907
O	17.521852	16.658846	9.788862
O	16.260666	17.013048	7.563001
O	13.884255	17.155325	6.282784
O	11.847618	16.423840	7.857160
O	12.349569	16.498857	10.459484
O	14.866935	16.489305	9.768921
O	15.945320	18.826445	9.538065
O	11.841011	18.803360	9.117838
O	18.687132	2.482599	12.121653
O	18.366180	19.815622	12.546295
O	17.686234	17.239498	12.379275
O	13.766126	2.893713	11.698081
O	13.847216	0.325548	12.388510
O	14.102896	17.576191	12.139720
O	9.753316	0.583837	9.615017
O	10.006194	16.910568	9.778155
O	7.265783	9.290246	9.785784
O	6.016211	8.616665	12.110947
O	3.842422	9.033350	0.331095
O	1.912902	8.613083	11.964670
O	2.088295	9.122298	9.361409
O	4.654715	8.946989	9.871034
O	7.239354	13.174333	10.118887
O	6.252069	13.112048	12.521804

O	3.861243	12.777147	0.247452
O	1.754928	13.524555	12.122857
O	2.160974	13.098119	9.457365
O	4.598453	13.265669	10.374101
O	5.757927	11.035190	11.040574
O	1.750123	11.102050	11.196754
O	8.576424	7.534557	8.271497
O	8.503143	10.111080	7.529276
O	7.765332	12.696358	7.542525
O	3.505251	7.224929	8.192805
O	3.748318	9.781354	7.452993
O	4.166578	12.433493	7.783955
O	19.840599	9.367852	10.459216
O	19.795351	12.772969	10.456539
O	2.923812	11.106030	2.849776
O	3.840620	11.349395	5.350256
O	6.042039	10.839383	6.848081
O	8.100701	11.443318	5.249750
O	7.936921	10.864058	2.610354
O	5.490833	10.615520	3.412799
O	3.086391	6.563685	3.021881
O	3.750521	6.714719	5.600251
O	5.938525	7.287611	7.109451
O	8.265482	6.545975	5.504830
O	8.022614	6.973207	2.780051
O	5.579531	7.051012	3.693440
O	3.660021	8.904205	4.176299
O	8.349174	8.954947	4.508063
O	1.407346	12.498562	1.177704
O	1.426968	9.863138	0.917672
O	1.843025	7.221745	0.757746
O	6.095297	12.666510	1.770705
O	6.098300	10.284002	0.765775
O	5.931517	7.627486	1.166195
O	10.246058	10.696906	3.763434
O	10.346368	7.209208	3.935539
O	8.592241	14.914499	8.620660
O	3.826805	14.921265	8.452168
O	5.341469	14.936189	0.836839
O	2.410248	14.919474	0.918609
O	1.322053	4.958632	1.926483
O	6.327353	5.149463	1.841099
O	4.596851	4.992659	7.370553
O	7.593944	4.968780	7.782081

O	11.667419	4.978332	4.847055
O	16.511343	5.065689	5.097451
O	14.773433	5.053351	12.800439
O	17.849813	4.951866	12.466666
O	18.772226	15.009020	11.544444
O	14.018203	14.940966	11.714274
O	15.350667	14.999668	6.107734
O	12.431659	14.930020	5.694065
O	11.011498	7.288407	13.553098
Al	4.542791	18.862263	7.008008
Al	6.383615	3.534460	2.507171
Al	17.838600	6.460210	13.308591
Al	11.363285	12.459361	9.081303
Al	16.165361	3.491678	4.475811
Al	7.558105	6.631143	7.071578
H	10.225837	5.766332	9.283921
H	19.258760	6.759292	11.352933
H	11.708665	14.268180	10.743471
H	18.605242	3.584606	4.404078
H	2.949241	17.124084	7.094863
H	6.985675	5.771307	12.541745
H	9.827799	5.251347	13.559120
H	10.440272	7.698127	14.236701
Pt	7.243158	4.741136	-3.477573
Pt	10.002790	6.075364	-0.909776
Pt	9.150455	6.487870	-3.223162
Pt	6.765033	4.125063	-1.073852
Pt	7.770739	7.260747	-1.090045
Pt	9.169275	3.850854	-1.781277

306

#### Pt6H2@H-MFI-2W\_IS

Si	8.421453	1.068178	8.780319
Si	6.035832	0.643136	10.843575
Si	5.599953	1.219212	0.357594
Si	2.444686	1.276720	0.178663
Si	1.415355	0.540656	10.821761
Si	3.661623	1.323483	9.060961
Si	8.606256	16.476372	9.054402
Si	6.159768	17.313522	10.915844
Si	5.426963	16.518559	0.477639
Si	2.382017	16.473986	0.442977
Si	1.396935	17.354713	11.018893
Si	3.629188	16.381454	9.143400
Si	1.541894	18.837191	2.053755

Si	3.934723	19.373865	4.078068
Si	7.699861	18.525969	6.932528
Si	8.639693	19.370283	4.151407
Si	6.407440	18.748241	2.248612
Si	1.625987	3.406709	2.324359
Si	3.915102	2.694126	4.351349
Si	4.534182	3.386412	7.259207
Si	7.593143	3.441333	7.225081
Si	8.641695	2.598611	4.372226
Si	11.609756	10.930521	4.624094
Si	14.165365	10.492146	2.713671
Si	14.454282	11.080957	13.122031
Si	17.664808	11.243134	13.246360
Si	18.728378	10.532939	2.682890
Si	16.462889	11.343425	4.518770
Si	11.744905	6.554731	4.487721
Si	14.204206	7.328205	2.557893
Si	14.856524	6.662185	13.068233
Si	18.914984	7.395066	2.712199
Si	16.498327	6.523290	4.442085
Si	18.552586	8.978031	11.310107
Si	16.178577	9.483465	9.354449
Si	15.620363	8.919726	6.422636
Si	12.455086	8.652881	6.613477
Si	11.475410	9.365863	9.395134
Si	13.739296	8.726906	11.147103
Si	18.484711	13.465256	11.133184
Si	16.147141	12.665117	9.247519
Si	15.473201	13.421080	6.282784
Si	12.449079	13.377301	6.231928
Si	13.789752	13.437595	11.144827
Si	11.536877	18.794607	4.640957
Si	13.952731	19.301035	2.646488
Si	14.391813	18.864252	13.090716
Si	17.532063	18.617306	13.226821
Si	18.616655	19.345610	2.558161
Si	16.398819	18.624866	4.409565
Si	11.723681	3.379248	4.546072
Si	13.935712	2.629653	2.458725
Si	14.658306	3.454865	12.974015
Si	17.704453	3.449293	12.990210
Si	18.680725	2.514438	2.405996
Si	18.525354	1.041514	11.385721
Si	16.081268	0.545432	9.417350

Si	15.550486	0.987587	6.478175
Si	12.458889	1.198716	6.569983
Si	11.350672	0.470014	9.332100
Si	13.625371	1.354923	11.155534
Si	18.454077	16.552387	11.115252
Si	16.162157	17.267357	9.153838
Si	15.420744	16.593775	6.231794
Si	12.393618	16.442743	6.309014
Si	11.506442	17.211840	9.244709
Si	13.860629	16.430405	11.034285
Si	8.537380	9.124487	8.640868
Si	6.070870	9.444264	10.596392
Si	5.350079	8.912364	0.369371
Si	2.215434	8.687108	0.207838
Si	1.450394	9.568235	10.748825
Si	3.595951	8.750784	8.697210
Si	8.350976	13.350637	8.962060
Si	6.001995	12.602833	10.990387
Si	5.388921	13.347852	0.494502
Si	2.366400	13.432422	0.258693
Si	1.368904	12.642233	10.811858
Si	3.712479	13.357203	9.027369
Si	1.528079	11.093693	2.001160
Si	3.949940	10.481600	3.962840
Si	4.481324	11.112995	6.857985
Si	7.659816	11.288504	6.750520
Si	8.656912	10.485579	4.046885
Si	6.397029	11.127521	2.187719
Si	1.666031	6.510555	2.236299
Si	4.028626	7.305122	4.122633
Si	4.492336	6.564083	7.034908
Si	8.706766	7.358053	4.225147
Si	6.455493	6.649052	2.356613
O	7.161469	1.156729	9.795821
O	6.344972	1.326268	12.282383
O	4.007403	0.913364	0.156447
O	1.839621	1.499390	12.062634
O	2.102310	0.997935	9.438228
O	4.518965	1.082904	10.441952
O	7.487026	16.749985	10.195704
O	6.171381	16.748989	12.432808
O	3.893878	17.093838	0.417148
O	1.751925	16.494480	12.331364
O	2.161975	16.585817	9.786587

O	4.831909	16.757147	10.122099
O	6.092294	18.915194	10.879175
O	1.845828	18.900070	11.200501
O	8.601851	2.572344	8.188255
O	8.182390	19.975611	7.524725
O	8.511553	17.333223	7.692415
O	3.759331	2.893315	8.613834
O	4.173786	0.402159	7.864922
O	3.589144	17.408640	7.785293
O	19.846207	0.664428	10.534027
O	19.828787	17.323074	10.711084
O	2.766039	18.818684	3.088127
O	3.750120	18.672625	5.509112
O	6.145753	18.317429	7.198047
O	8.100701	18.410355	5.356546
O	7.922104	18.979467	2.755158
O	5.416151	18.984243	3.507550
O	2.589645	3.322934	3.602838
O	3.682246	2.909035	5.956506
O	6.078078	2.814714	7.276337
O	8.095494	3.407704	5.689916
O	8.000791	3.155584	3.017733
O	5.256175	3.397754	3.850557
O	3.840620	1.087878	4.090113
O	8.339964	0.999527	4.600272
O	1.415756	17.331432	1.425022
O	1.664829	0.004378	0.833895
O	2.175991	2.655124	0.998773
O	6.254673	17.225967	1.673544
O	6.171581	19.739807	1.001182
O	5.842820	2.563389	1.163518
O	10.201609	19.071600	3.771865
O	10.266480	2.737108	4.342917
O	12.843311	10.693324	3.602838
O	13.845413	11.107224	1.238463
O	16.070057	11.030215	13.054715
O	18.107695	11.364916	1.411103
O	17.955128	11.015887	4.016238
O	15.428753	11.345813	3.262775
O	12.851721	6.887641	3.337453
O	13.923298	6.969625	0.995026
O	16.329142	7.277462	13.290792
O	18.682127	6.475930	1.416724
O	18.035015	6.900973	4.002989

O	15.524458	6.547368	3.104990
O	14.579419	8.923109	2.681418
O	18.524754	8.954749	2.352999
O	11.594740	12.450008	5.186850
O	11.674027	9.867715	5.856802
O	12.266078	7.229904	5.870587
O	16.438862	12.852166	5.111369
O	16.094484	10.285196	5.687909
O	15.939514	7.623506	5.521290
O	0.254079	10.945445	3.003413
O	0.500550	7.288805	3.095622
O	17.263968	8.787598	10.368880
O	16.419641	8.872566	7.865992
O	14.028214	9.041111	6.696720
O	11.845216	8.449314	8.101266
O	12.177179	8.636763	10.695962
O	14.668517	9.190950	9.879063
O	17.271976	13.511222	10.048224
O	16.188988	13.094537	7.704861
O	13.988570	12.766204	6.192983
O	11.845015	13.343473	7.706467
O	12.181384	13.365760	10.549953
O	14.671321	13.017926	9.867019
O	16.444069	11.087523	9.449202
O	12.007593	10.867840	9.210047
O	18.859121	7.439440	11.980997
O	18.358572	9.887415	12.623114
O	18.100889	12.601241	12.464257
O	14.177578	7.279651	11.710125
O	13.844412	9.785731	12.378874
O	13.926702	12.435084	12.383692
O	9.847420	9.293032	9.622912
O	9.690248	12.676260	9.534183
O	12.845714	18.736898	3.680058
O	13.678430	18.661680	1.160038
O	15.983762	19.066227	13.298420
O	18.111900	18.392248	1.341512
O	17.929100	18.899473	3.945977
O	15.440966	18.821669	3.105392
O	12.585629	3.160160	3.185556
O	13.776938	2.986243	0.869494
O	16.175173	2.824663	12.960767
O	18.186182	3.410887	1.180247
O	17.946520	3.134689	3.839449

O	15.273782	3.314975	3.014119
O	13.935512	1.010272	2.664555
O	18.186783	0.993358	2.184909
O	11.421750	17.334417	5.362568
O	11.602147	0.077407	5.764594
O	12.434863	2.655323	5.843286
O	16.260267	17.087870	4.932706
O	16.098888	19.571264	5.685099
O	15.775734	2.335347	5.677069
O	0.176994	19.229200	2.846163
O	0.223446	2.655920	2.765329
O	17.267172	1.079720	10.373298
O	16.352367	1.063403	7.911494
O	13.977158	0.667412	6.778356
O	11.758320	1.342785	8.031406
O	12.092087	1.162898	10.625834
O	14.670118	1.158122	9.942231
O	17.522654	16.658447	9.789531
O	16.260067	17.013447	7.563001
O	13.882854	17.155724	6.282382
O	11.848019	16.427221	7.858498
O	12.349770	16.501644	10.459216
O	14.867736	16.488111	9.769992
O	15.945120	18.825249	9.537529
O	11.843413	18.812914	9.124663
O	18.687334	2.482997	12.120850
O	18.365580	19.816816	12.546027
O	17.686033	17.239498	12.378874
O	13.770330	2.892320	11.700624
O	13.845813	0.323160	12.386234
O	14.102896	17.574598	12.138783
O	9.752316	0.583240	9.617693
O	10.005994	16.912758	9.778557
O	7.184294	9.614799	9.384830
O	5.591944	8.700241	12.123125
O	3.757128	9.041906	0.582294
O	1.921712	8.617262	11.984477
O	2.158572	9.126080	9.376398
O	4.765837	8.875551	9.796491
O	7.185094	13.252138	10.107244
O	6.258476	13.036830	12.540273
O	3.864646	12.773169	0.252270
O	1.755129	13.523957	12.124865
O	2.157971	13.095929	9.456696

O	4.590844	13.185077	10.384137
O	5.844422	11.000366	11.036559
O	1.750523	11.101851	11.199965
O	8.510951	7.549084	8.202173
O	8.664721	10.123617	7.350880
O	7.845220	12.688995	7.546005
O	3.505051	7.218760	8.180760
O	3.756928	9.785532	7.446569
O	4.170182	12.432497	7.779806
O	19.860022	9.368250	10.454533
O	19.797953	12.772372	10.457209
O	2.920409	11.103045	2.849508
O	3.847227	11.347206	5.355743
O	6.089090	10.856695	6.846208
O	8.093893	11.516149	5.187920
O	7.950336	10.855700	2.600986
O	5.492635	10.613729	3.430732
O	3.086591	6.560502	3.017599
O	3.739108	6.708749	5.590614
O	5.929315	7.282039	7.032231
O	8.182991	6.472349	5.445141
O	8.013405	6.968033	2.764660
O	5.580131	7.040465	3.685812
O	3.662224	8.899430	4.175362
O	8.348773	8.954152	4.504852
O	1.408548	12.498363	1.178239
O	1.342075	9.866720	0.918743
O	1.830011	7.212790	0.757746
O	6.088290	12.684021	1.822898
O	6.090692	10.278232	0.826400
O	5.922507	7.639425	1.166195
O	10.250663	10.693723	3.760355
O	10.334955	7.210801	4.008208
O	8.592842	14.922658	8.617046
O	3.830609	14.911117	8.515470
O	5.344272	14.931214	0.766846
O	2.411249	14.918678	0.919546
O	1.319250	4.954254	1.927554
O	6.266886	5.151055	1.752236
O	4.593848	4.989077	7.368145
O	7.588938	4.961418	7.859167
O	11.671425	4.976939	4.846252
O	16.505537	5.060714	5.100395
O	14.768026	5.055938	12.799234

O	17.849213	4.957438	12.466666
O	18.772026	15.010015	11.544845
O	14.014599	14.935593	11.712400
O	15.349866	15.001260	6.108001
O	12.431459	14.930020	5.695270
O	10.185992	8.537666	14.294517
O	11.261374	4.149737	12.120448
Al	4.542391	18.865446	7.023398
Al	6.371000	3.522322	2.515201
Al	17.855419	6.471354	13.299223
Al	11.339860	12.451799	9.076886
Al	16.169966	3.487101	4.474473
Al	7.525469	6.572042	7.054180
H	10.167772	5.899457	9.546094
H	19.378893	6.831923	11.417706
H	11.637587	14.128289	10.842238
H	18.606243	3.591571	4.398591
H	2.947438	17.126074	7.100485
H	6.834509	6.457225	12.364420
H	9.338861	8.926890	14.594296
H	10.746608	9.284475	14.009859
H	11.815582	4.790287	11.633307
H	11.504841	3.272789	11.756564
Pt	7.267585	4.785709	-3.187964
Pt	9.789156	7.040465	-0.637432
Pt	9.028721	6.674921	-3.121451
Pt	6.730395	4.864908	-0.679321
Pt	7.572921	8.029446	-1.278612
Pt	9.144447	4.611394	-1.253318

306

#### Pt6H2@H-MFI-2W\_FS

Si	8.417850	1.069770	8.778178
Si	6.033830	0.642539	10.843308
Si	5.600353	1.221998	0.361073
Si	2.444886	1.276720	0.178529
Si	1.411351	0.541253	10.821896
Si	3.660021	1.324080	9.060826
Si	8.604855	16.476770	9.055340
Si	6.158166	17.311731	10.923338
Si	5.423960	16.523335	0.490487
Si	2.380015	16.474979	0.442041
Si	1.395133	17.355907	11.018358
Si	3.628587	16.384638	9.143534
Si	1.541694	18.837587	2.054023

Si	3.934323	19.374861	4.077934
Si	7.699259	18.524975	6.931190
Si	8.640894	19.372473	4.151540
Si	6.408642	18.754608	2.250753
Si	1.626988	3.408102	2.324092
Si	3.917104	2.695121	4.350412
Si	4.533782	3.387208	7.259876
Si	7.592342	3.439940	7.225616
Si	8.641895	2.600800	4.370620
Si	11.603550	10.929526	4.620481
Si	14.147144	10.471848	2.711262
Si	14.428654	11.079365	13.126582
Si	17.633974	11.265023	13.250241
Si	18.726976	10.532740	2.667232
Si	16.483311	11.329495	4.513417
Si	11.740900	6.555129	4.491201
Si	14.192994	7.307112	2.559901
Si	14.859126	6.659797	13.057392
Si	18.912781	7.394269	2.712332
Si	16.496325	6.524882	4.443156
Si	18.532963	8.986787	11.331387
Si	16.175573	9.480480	9.356858
Si	15.617961	8.920523	6.424777
Si	12.449679	8.655070	6.618563
Si	11.478412	9.375016	9.409185
Si	13.734090	8.728498	11.147771
Si	18.479704	13.466249	11.133184
Si	16.144939	12.662331	9.246181
Si	15.474604	13.414514	6.278100
Si	12.448678	13.373719	6.229921
Si	13.788351	13.436004	11.145630
Si	11.537276	18.793411	4.639886
Si	13.952331	19.304020	2.644749
Si	14.392413	18.862860	13.089912
Si	17.532263	18.617107	13.225616
Si	18.616455	19.346006	2.557893
Si	16.398417	18.623276	4.407423
Si	11.723681	3.382034	4.540986
Si	13.933109	2.633434	2.440926
Si	14.664112	3.452278	12.951264
Si	17.706255	3.447900	12.991146
Si	18.681526	2.514637	2.406799
Si	18.517948	1.042907	11.382108
Si	16.083471	0.539661	9.396606

Si	15.546882	0.988980	6.465729
Si	12.459691	1.200507	6.563023
Si	11.349070	0.454095	9.312695
Si	13.648597	1.342983	11.135861
Si	18.454277	16.550198	11.115652
Si	16.173771	17.259398	9.147549
Si	15.420342	16.588602	6.227645
Si	12.395019	16.439957	6.306471
Si	11.507044	17.201094	9.244709
Si	13.863232	16.428217	11.032544
Si	8.557603	9.061010	8.756229
Si	5.948936	9.494211	10.612720
Si	5.467007	8.876546	0.250396
Si	2.273898	8.656861	0.148016
Si	1.409549	9.560275	10.751769
Si	3.518266	8.770086	8.689716
Si	8.370398	13.344270	8.931681
Si	5.997390	12.645416	10.968841
Si	5.399333	13.383073	0.468940
Si	2.380215	13.435408	0.251333
Si	1.363698	12.634672	10.814535
Si	3.699465	13.362776	9.019875
Si	1.555109	11.098866	1.976000
Si	3.944534	10.481002	3.951598
Si	4.466107	11.119363	6.851025
Si	7.638192	11.274972	6.762296
Si	8.659314	10.468068	4.008342
Si	6.396628	11.112597	2.128566
Si	1.668033	6.513341	2.238842
Si	4.031229	7.306912	4.126246
Si	4.504349	6.569257	7.048291
Si	8.710972	7.351089	4.202530
Si	6.457695	6.644674	2.361698
O	7.163270	1.155137	9.798230
O	6.344571	1.328656	12.281312
O	4.007603	0.913364	0.155109
O	1.839221	1.499191	12.062232
O	2.101109	0.997935	9.438628
O	4.518364	1.082506	10.441684
O	7.483623	16.748789	10.196508
O	6.169579	16.746202	12.442176
O	3.890875	17.096027	0.415810
O	1.752325	16.493883	12.329089
O	2.161575	16.586214	9.786453

O	4.832309	16.756351	10.122901
O	6.092294	18.914000	10.880380
O	1.845227	18.900866	11.200233
O	8.601651	2.573339	8.188925
O	8.182991	19.975212	7.525127
O	8.511151	17.333422	7.693084
O	3.758730	2.893713	8.613834
O	4.173586	0.402557	7.865324
O	3.589344	17.409636	7.785159
O	19.841801	0.664627	10.532956
O	19.827785	17.323671	10.711084
O	2.766039	18.818684	3.088127
O	3.749920	18.672625	5.508844
O	6.145352	18.317825	7.198314
O	8.101101	18.410753	5.356412
O	7.923306	18.980860	2.755961
O	5.415951	18.985237	3.508621
O	2.589645	3.323531	3.602971
O	3.682847	2.910030	5.957041
O	6.077878	2.815907	7.276204
O	8.095896	3.409097	5.692192
O	7.999990	3.155185	3.018402
O	5.257176	3.397356	3.850557
O	3.840019	1.088276	4.090782
O	8.340164	1.000522	4.601209
O	1.415155	17.331631	1.425022
O	1.665029	0.004378	0.833761
O	2.175991	2.655522	0.998506
O	6.256474	17.234724	1.675953
O	6.171581	19.741003	1.000245
O	5.841419	2.563787	1.164723
O	10.202209	19.071600	3.771865
O	10.266881	2.736709	4.343453
O	12.842911	10.697105	3.610600
O	13.845813	11.110009	1.246091
O	16.045630	11.033796	13.055786
O	18.098886	11.370488	1.409364
O	17.996973	11.020862	4.024804
O	15.442768	11.274972	3.264381
O	12.847716	6.878089	3.339995
O	13.918693	6.964252	0.987264
O	16.328140	7.276865	13.292130
O	18.682728	6.472349	1.419669
O	18.034016	6.902764	4.003658

O	15.524858	6.545577	3.102849
O	14.517752	8.896047	2.678741
O	18.523352	8.953157	2.349921
O	11.593739	12.449809	5.187385
O	11.671225	9.868711	5.858141
O	12.266078	7.230899	5.873397
O	16.439062	12.844805	5.104544
O	16.099489	10.283604	5.689649
O	15.939113	7.623904	5.521424
O	0.256882	10.941068	2.930342
O	0.500750	7.289800	3.094551
O	17.260365	8.784613	10.374101
O	16.419441	8.872169	7.867331
O	14.026212	9.040912	6.697255
O	11.838808	8.455085	8.107823
O	12.179983	8.633978	10.694757
O	14.667516	9.189955	9.879465
O	17.270777	13.511023	10.046217
O	16.189188	13.094138	7.703523
O	13.988770	12.765607	6.192716
O	11.845416	13.344866	7.705262
O	12.182385	13.362576	10.549417
O	14.669918	13.018723	9.866484
O	16.444670	11.085534	9.449202
O	12.015402	10.871222	9.206969
O	18.858721	7.463717	12.043095
O	18.358772	9.940347	12.615084
O	18.096884	12.609598	12.465462
O	14.178579	7.281442	11.709991
O	13.845213	9.783343	12.377669
O	13.924299	12.438069	12.384629
O	9.857832	9.369246	9.692905
O	9.697455	12.677852	9.530704
O	12.846515	18.737696	3.679388
O	13.677828	18.663073	1.158165
O	15.983162	19.066626	13.298018
O	18.111700	18.392845	1.340709
O	17.928900	18.899275	3.945309
O	15.439964	18.822266	3.104053
O	12.587430	3.159961	3.181407
O	13.772733	2.984054	0.844200
O	16.179777	2.822275	12.962774
O	18.187384	3.410689	1.181184
O	17.945719	3.134689	3.839047

O	15.270178	3.314975	3.008499
O	13.936112	1.013655	2.658533
O	18.187183	0.993756	2.185176
O	11.422150	17.334417	5.362836
O	11.601347	0.076810	5.764594
O	12.434663	2.656317	5.840609
O	16.260466	17.087271	4.930966
O	16.098288	19.570269	5.682422
O	15.774532	2.338928	5.671715
O	0.176794	19.229200	2.846163
O	0.225047	2.656516	2.765195
O	17.252357	1.086684	10.372896
O	16.355772	1.064597	7.892624
O	13.975556	0.667611	6.776081
O	11.758921	1.342983	8.029265
O	12.089083	1.156530	10.622355
O	14.609853	1.073949	9.867286
O	17.526857	16.646309	9.789129
O	16.262268	17.010462	7.555641
O	13.883655	17.154928	6.282248
O	11.848019	16.426226	7.856758
O	12.351372	16.502838	10.459885
O	14.871140	16.494480	9.767984
O	16.020803	18.820673	9.536057
O	11.844013	18.806347	9.123995
O	18.687733	2.481803	12.119780
O	18.363977	19.817614	12.544154
O	17.686033	17.239300	12.378472
O	13.849017	2.888937	11.628088
O	13.847216	0.326145	12.382219
O	14.102896	17.575195	12.137177
O	9.754518	0.585429	9.618095
O	10.004993	16.913155	9.778690
O	7.250767	9.282287	9.708162
O	6.020616	8.611491	12.052328
O	3.855236	9.023003	0.241028
O	1.834215	8.547019	11.958648
O	2.078684	9.121104	9.357929
O	4.600054	9.028973	9.879599
O	7.178888	13.182490	10.035377
O	6.255073	13.185276	12.475365
O	3.885269	12.781526	0.240493
O	1.756930	13.521769	12.121653
O	2.151764	13.092546	9.457499

O	4.579832	13.189854	10.375037
O	5.841819	11.032802	11.047533
O	1.749722	11.088519	11.199697
O	8.596445	7.534557	8.195884
O	8.512153	10.115059	7.516160
O	7.846821	12.690588	7.525394
O	3.508054	7.230103	8.193742
O	3.751522	9.785532	7.444695
O	4.166578	12.433293	7.779672
O	19.831190	9.369046	10.456406
O	19.795151	12.770382	10.458548
O	2.918407	11.109810	2.852453
O	3.847027	11.346411	5.348248
O	6.066866	10.855502	6.851025
O	8.095095	11.440732	5.205987
O	7.928912	10.866246	2.594562
O	5.446584	10.612932	3.347624
O	3.087192	6.562491	3.021881
O	3.750921	6.714122	5.601321
O	5.942729	7.283631	7.109719
O	8.182590	6.478119	5.440457
O	8.009000	6.956292	2.760244
O	5.577929	7.044843	3.685946
O	3.659221	8.900026	4.177504
O	8.344769	8.942014	4.440881
O	1.416156	12.507715	1.170477
O	1.498046	9.862343	0.909375
O	1.844827	7.217367	0.759084
O	6.100103	12.671683	1.754511
O	6.097099	10.279226	0.747307
O	5.924911	7.636440	1.153882
O	10.249462	10.697105	3.760623
O	10.337558	7.208612	4.010350
O	8.592441	14.923255	8.616913
O	3.828206	14.913903	8.511856
O	5.343071	14.945741	0.839248
O	2.413051	14.919474	0.917806
O	1.321252	4.957438	1.926751
O	6.259077	5.152846	1.764950
O	4.593447	4.992062	7.370955
O	7.586736	4.970173	7.854216
O	11.672025	4.975546	4.847992
O	16.505335	5.060913	5.099459
O	14.769428	5.054346	12.798698

O	17.848612	4.954652	12.468139
O	18.773228	15.009418	11.545247
O	14.015600	14.935991	11.711731
O	15.350667	14.997279	6.106797
O	12.431659	14.929027	5.694601
O	10.929209	7.539333	13.799212
O	11.004891	3.321939	11.711329
Al	4.542191	18.866838	7.022194
Al	6.372802	3.530481	2.511320
Al	17.848410	6.462201	13.306851
Al	11.349871	12.450605	9.077021
Al	16.166763	3.490285	4.467915
Al	7.560507	6.599105	7.057124
H	10.436467	5.746433	9.281646
H	19.577110	6.952909	11.620192
H	11.598945	14.059440	10.915174
H	18.602840	3.593362	4.399929
H	2.946037	17.128462	7.101154
H	7.482021	6.101830	13.222538
H	10.019009	8.222665	12.564764
H	11.903479	7.415164	13.808981
H	11.624372	3.916322	11.248278
H	11.166268	2.422902	11.320546
Pt	7.218531	4.958632	-3.312962
Pt	10.137739	6.280324	-0.825463
Pt	9.366091	6.477523	-3.250329
Pt	6.714377	4.846799	-0.798028
Pt	7.935920	7.460732	-1.169407
Pt	9.014304	4.079693	-1.560859

312

#### Pt6H2@H-MFI-4W\_IS

Si	8.461698	1.080118	8.740572
Si	6.057456	0.643534	10.791783
Si	5.601955	1.251050	0.287868
Si	2.462906	1.276919	0.158187
Si	1.408948	0.541651	10.818952
Si	3.659421	1.339004	9.044901
Si	8.589638	16.468613	9.040886
Si	6.119724	17.317900	10.890684
Si	5.427563	16.518160	0.466665
Si	2.378213	16.476173	0.432405
Si	1.364099	17.360683	11.014477
Si	3.577731	16.384836	9.141526
Si	1.539692	18.839378	2.049607

Si	3.932521	19.369289	4.068298
Si	7.743909	18.544674	6.927309
Si	8.638291	19.376055	4.143109
Si	6.407640	18.771124	2.215690
Si	1.634396	3.399943	2.314456
Si	3.916103	2.683579	4.342516
Si	4.522769	3.393177	7.249839
Si	7.576725	3.431782	7.178240
Si	8.633687	2.611545	4.339839
Si	11.589734	10.937685	4.626369
Si	14.143741	10.515627	2.713805
Si	14.435061	11.074590	13.117348
Si	17.644987	11.256865	13.237528
Si	18.720770	10.536122	2.679009
Si	16.457483	11.344221	4.519707
Si	11.731091	6.574232	4.470056
Si	14.177177	7.354073	2.566458
Si	14.854722	6.651440	13.038255
Si	18.907175	7.394468	2.709388
Si	16.488916	6.522295	4.458413
Si	18.558191	8.960320	11.303415
Si	16.179577	9.432723	9.370375
Si	15.619362	8.922314	6.429060
Si	12.452082	8.653279	6.613210
Si	11.479213	9.376011	9.393394
Si	13.719675	8.695067	11.154463
Si	18.479704	13.463265	11.131444
Si	16.147743	12.630891	9.249795
Si	15.452378	13.410334	6.287601
Si	12.418645	13.377501	6.227511
Si	13.789952	13.435009	11.142552
Si	11.535274	18.796795	4.642161
Si	13.952930	19.298250	2.649031
Si	14.390011	18.859278	13.100485
Si	17.530260	18.617504	13.227490
Si	18.613852	19.345211	2.559633
Si	16.397017	18.626060	4.414516
Si	11.720677	3.379447	4.530815
Si	13.941518	2.624280	2.453104
Si	14.658505	3.448895	12.962106
Si	17.702650	3.444318	12.991280
Si	18.686333	2.512647	2.404925
Si	18.518747	1.041713	11.383714
Si	16.058846	0.540457	9.430465

Si	15.532065	0.985995	6.489149
Si	12.432860	1.215033	6.574399
Si	11.346467	0.502052	9.330895
Si	13.610954	1.349351	11.190330
Si	18.434055	16.545422	11.117928
Si	16.158154	17.263577	9.149155
Si	15.417541	16.587408	6.229787
Si	12.390413	16.443140	6.309415
Si	11.485821	17.209253	9.246047
Si	13.856826	16.430206	11.032946
Si	8.565011	9.164683	8.633909
Si	6.088690	9.402476	10.614459
Si	5.346074	8.922513	0.309549
Si	2.220840	8.691286	0.237950
Si	1.447591	9.572613	10.775055
Si	3.601157	8.753769	8.697880
Si	8.342967	13.348647	8.979725
Si	6.016211	12.567413	11.004439
Si	5.379110	13.370337	0.483662
Si	2.361395	13.436004	0.256820
Si	1.365300	12.644820	10.811591
Si	3.715482	13.344866	9.030849
Si	1.515265	11.102845	2.000357
Si	3.914101	10.488365	3.953472
Si	4.476519	11.112597	6.847814
Si	7.644199	11.317159	6.744497
Si	8.643897	10.501299	4.036982
Si	6.380411	11.112796	2.136596
Si	1.648411	6.494039	2.238441
Si	3.961153	7.344721	4.134544
Si	4.470111	6.571247	7.024469
Si	8.695955	7.387305	4.248433
Si	6.412646	6.706361	2.386992
O	7.171479	1.077929	9.706155
O	6.419253	1.319503	12.226576
O	4.023821	0.914757	0.002141
O	1.831012	1.502972	12.056746
O	2.110919	0.997537	9.441974
O	4.581834	1.156530	10.382933
O	7.415548	16.748789	10.121296
O	6.160569	16.737646	12.402161
O	3.892677	17.093639	0.411661
O	1.752125	16.495077	12.315706
O	2.097304	16.582434	9.766378

O	4.751421	16.833160	10.125578
O	6.091093	18.920168	10.882654
O	1.841023	18.899473	11.198627
O	8.601050	2.570553	8.117326
O	8.424056	19.910938	7.527938
O	8.506146	17.320290	7.679968
O	3.753124	2.904458	8.604734
O	4.165977	0.407333	7.861175
O	3.588343	17.408838	7.778869
O	19.841202	0.664229	10.530949
O	19.793949	17.332626	10.714163
O	2.758631	18.816893	3.087592
O	3.755927	18.666256	5.502554
O	6.179590	18.476818	7.202062
O	8.102303	18.411350	5.346642
O	7.918900	18.982054	2.747798
O	5.392725	18.984243	3.451476
O	2.590647	3.326317	3.600830
O	3.679443	2.910229	5.948074
O	6.067267	2.814316	7.272322
O	8.093092	3.414867	5.661277
O	7.999189	3.221648	3.007829
O	5.274996	3.328904	3.834631
O	3.834613	1.079521	4.092923
O	8.337961	1.008282	4.591708
O	1.415756	17.332626	1.421007
O	1.675040	0.013730	0.832824
O	2.251474	2.654726	1.004929
O	6.257676	17.242285	1.654139
O	6.178789	19.803684	0.997435
O	5.845022	2.583288	1.097005
O	10.200607	19.073193	3.770259
O	10.263677	2.736511	4.339170
O	12.834101	10.705662	3.616890
O	13.841208	11.113392	1.235920
O	16.051237	11.032006	13.057259
O	18.105894	11.362727	1.401735
O	17.949722	11.017479	4.014365
O	15.425149	11.344022	3.262240
O	12.765626	6.960472	3.263445
O	13.932308	6.965446	0.995428
O	16.330744	7.279850	13.215714
O	18.675520	6.478319	1.410702
O	18.021801	6.898187	3.996699

O	15.447573	6.547567	3.173243
O	14.522157	8.940820	2.678875
O	18.523352	8.955346	2.351661
O	11.531870	12.459759	5.193809
O	11.672424	9.868711	5.855330
O	12.266078	7.227118	5.858944
O	16.431654	12.851371	5.116455
O	16.093884	10.284599	5.688712
O	15.940715	7.626889	5.528116
O	0.246871	10.946241	3.003814
O	0.493943	7.288009	3.095354
O	17.269375	8.708001	10.372495
O	16.423044	8.868387	7.865457
O	14.026212	9.040115	6.695916
O	11.843614	8.450509	8.099392
O	12.167569	8.643131	10.690475
O	14.673522	9.114738	9.882543
O	17.268373	13.499084	10.044611
O	16.182981	13.083593	7.708073
O	13.956334	12.765805	6.189370
O	11.840409	13.345861	7.709947
O	12.181986	13.362377	10.548748
O	14.674523	13.013946	9.866884
O	16.440264	11.042552	9.454555
O	12.017405	10.873809	9.206032
O	18.931002	7.462324	12.047511
O	18.354767	9.952883	12.550042
O	18.096884	12.612583	12.466666
O	14.103095	7.226720	11.711061
O	13.847014	9.774986	12.371647
O	13.924700	12.436079	12.383022
O	9.856030	9.369842	9.617693
O	9.688445	12.677256	9.533916
O	12.844514	18.737297	3.681931
O	13.678229	18.655512	1.167265
O	15.982361	19.065233	13.298821
O	18.111700	18.392248	1.341780
O	17.927898	18.899473	3.948521
O	15.441767	18.822065	3.107666
O	12.588633	3.156777	3.176857
O	13.773133	2.991019	0.866014
O	16.175373	2.820086	12.961971
O	18.187384	3.409097	1.181853
O	17.950924	3.131705	3.839449

O	15.274384	3.314377	3.014521
O	13.936313	1.008083	2.664288
O	18.186983	0.992960	2.185578
O	11.419747	17.336407	5.363371
O	11.598543	0.079596	5.767003
O	12.432461	2.664277	5.832847
O	16.258863	17.087471	4.933242
O	16.093884	19.574646	5.688980
O	15.771529	2.329974	5.680682
O	0.175993	19.229996	2.843888
O	0.233657	2.648358	2.758236
O	17.256561	1.080317	10.373967
O	16.336349	1.064795	7.925279
O	13.947725	0.670397	6.782639
O	11.689043	1.401487	8.023108
O	12.092486	1.157724	10.627173
O	14.611655	1.080317	9.946781
O	17.516647	16.654070	9.787122
O	16.259266	17.011854	7.557782
O	13.879651	17.154530	6.282248
O	11.845615	16.431202	7.860773
O	12.344764	16.509205	10.456674
O	14.862931	16.488510	9.768520
O	15.948924	18.819080	9.537261
O	11.762123	18.825052	9.120247
O	18.687334	2.480211	12.120984
O	18.364779	19.816021	12.545359
O	17.681229	17.237907	12.382889
O	13.773334	2.889733	11.697813
O	13.837605	0.337089	12.445120
O	14.101694	17.576588	12.137444
O	9.761725	0.732880	9.700534
O	9.982368	16.910767	9.780029
O	7.254170	9.617187	9.464859
O	5.508852	8.624824	12.071868
O	3.757929	9.044494	0.585908
O	1.901890	8.614676	12.021146
O	2.185201	9.120707	9.429528
O	4.838717	8.878337	9.713650
O	7.179088	13.253132	10.120091
O	6.251469	13.109063	12.524347
O	3.860041	12.778542	0.249058
O	1.754528	13.526942	12.122589
O	2.157370	13.096328	9.456696

O	4.590044	13.101900	10.379052
O	5.922107	10.954598	11.122076
O	1.751324	11.106030	11.205318
O	8.520362	7.619725	8.117326
O	8.667124	10.191273	7.360249
O	7.763330	12.688199	7.599135
O	3.499845	7.220153	8.185177
O	3.751922	9.787721	7.444427
O	4.171183	12.430905	7.774988
O	19.866629	9.365067	10.454533
O	19.795750	12.772173	10.456941
O	2.903390	11.115582	2.841345
O	3.843623	11.350788	5.348650
O	6.081282	10.853512	6.774609
O	8.093493	11.527889	5.185779
O	7.925308	10.857094	2.597239
O	5.426563	10.604376	3.351103
O	3.072776	6.555328	3.014119
O	3.673836	6.715515	5.596503
O	5.912096	7.285820	7.024202
O	8.176784	6.470160	5.435104
O	8.002393	7.047629	2.765597
O	5.518663	7.135185	3.694110
O	3.518867	8.927289	4.178708
O	8.344569	8.971265	4.515424
O	1.402941	12.504134	1.175161
O	1.338270	9.869705	0.922892
O	1.825606	7.207816	0.760824
O	6.095497	12.672678	1.770169
O	6.096298	10.286987	0.748645
O	5.931918	7.698525	1.168871
O	10.238449	10.692927	3.757277
O	10.308526	7.212193	4.008208
O	8.593242	14.916091	8.617313
O	3.832611	14.910917	8.531395
O	5.343872	14.942557	0.834296
O	2.409848	14.922460	0.917003
O	1.257782	4.942514	1.928892
O	6.254272	5.219906	1.842705
O	4.595049	4.996440	7.364933
O	7.586135	4.973556	7.767092
O	11.672225	4.985495	4.770905
O	16.507738	5.055739	5.101868
O	14.774834	5.047978	12.807531

O	17.845608	4.946692	12.468139
O	18.770624	15.008424	11.543508
O	14.013198	14.935593	11.710794
O	15.347864	14.994891	6.109340
O	12.427855	14.931613	5.694868
O	9.679035	1.071760	12.626995
O	9.933715	8.034619	14.467291
O	10.507345	3.407505	11.969890
O	11.598744	5.882741	13.292263
Al	4.539588	18.881565	7.017376
Al	6.357585	3.559135	2.463275
Al	17.860023	6.464787	13.278880
Al	11.338658	12.449014	9.078091
Al	16.171370	3.480335	4.477551
Al	7.520263	6.624576	7.028752
H	10.247660	5.845331	9.391654
H	19.873035	7.197468	11.994246
H	11.608755	14.075558	10.898714
H	18.607244	3.594157	4.398591
H	2.977071	17.124880	7.066090
H	7.926710	3.170906	12.429328
H	8.797667	1.150560	13.036514
H	9.510650	0.672387	11.749337
H	9.202311	7.659921	15.031919
H	9.671827	8.955744	14.285282
H	10.956238	3.385616	11.104545
H	10.252464	2.438025	12.224167
H	11.532671	4.919033	13.426764
H	12.162964	6.275548	13.994068
Pt	7.073972	5.066087	-3.530837
Pt	9.757320	6.838490	-0.817835
Pt	9.128630	6.627362	-3.247519
Pt	6.407240	5.497298	-1.134477
Pt	7.545691	7.769365	-1.341110
Pt	8.652307	4.467126	-1.435728

312

#### Pt6H2@H-MFI-4W\_FS

Si	8.461698	1.080118	8.740572
Si	6.057456	0.643534	10.791783
Si	5.601955	1.251050	0.287868
Si	2.462906	1.276919	0.158187
Si	1.408948	0.541651	10.818952
Si	3.659421	1.339004	9.044901
Si	8.589638	16.468613	9.040886

Si	6.119724	17.317900	10.890684
Si	5.427563	16.518160	0.466665
Si	2.378213	16.476173	0.432405
Si	1.364099	17.360683	11.014477
Si	3.577731	16.384836	9.141526
Si	1.539692	18.839378	2.049607
Si	3.932521	19.369289	4.068298
Si	7.743909	18.544674	6.927309
Si	8.638291	19.376055	4.143109
Si	6.407640	18.771124	2.215690
Si	1.634396	3.399943	2.314456
Si	3.916103	2.683579	4.342516
Si	4.522769	3.393177	7.249839
Si	7.576725	3.431782	7.178240
Si	8.633687	2.611545	4.339839
Si	11.589734	10.937685	4.626369
Si	14.143741	10.515627	2.713805
Si	14.435061	11.074590	13.117348
Si	17.644987	11.256865	13.237528
Si	18.720770	10.536122	2.679009
Si	16.457483	11.344221	4.519707
Si	11.731091	6.574232	4.470056
Si	14.177177	7.354073	2.566458
Si	14.854722	6.651440	13.038255
Si	18.907175	7.394468	2.709388
Si	16.488916	6.522295	4.458413
Si	18.558191	8.960320	11.303415
Si	16.179577	9.432723	9.370375
Si	15.619362	8.922314	6.429060
Si	12.452082	8.653279	6.613210
Si	11.479213	9.376011	9.393394
Si	13.719675	8.695067	11.154463
Si	18.479704	13.463265	11.131444
Si	16.147743	12.630891	9.249795
Si	15.452378	13.410334	6.287601
Si	12.418645	13.377501	6.227511
Si	13.789952	13.435009	11.142552
Si	11.535274	18.796795	4.642161
Si	13.952930	19.298250	2.649031
Si	14.390011	18.859278	13.100485
Si	17.530260	18.617504	13.227490
Si	18.613852	19.345211	2.559633
Si	16.397017	18.626060	4.414516
Si	11.720677	3.379447	4.530815

Si	13.941518	2.624280	2.453104
Si	14.658505	3.448895	12.962106
Si	17.702650	3.444318	12.991280
Si	18.686333	2.512647	2.404925
Si	18.518747	1.041713	11.383714
Si	16.058846	0.540457	9.430465
Si	15.532065	0.985995	6.489149
Si	12.432860	1.215033	6.574399
Si	11.346467	0.502052	9.330895
Si	13.610954	1.349351	11.190330
Si	18.434055	16.545422	11.117928
Si	16.158154	17.263577	9.149155
Si	15.417541	16.587408	6.229787
Si	12.390413	16.443140	6.309415
Si	11.485821	17.209253	9.246047
Si	13.856826	16.430206	11.032946
Si	8.565011	9.164683	8.633909
Si	6.088690	9.402476	10.614459
Si	5.346074	8.922513	0.309549
Si	2.220840	8.691286	0.237950
Si	1.447591	9.572613	10.775055
Si	3.601157	8.753769	8.697880
Si	8.342967	13.348647	8.979725
Si	6.016211	12.567413	11.004439
Si	5.379110	13.370337	0.483662
Si	2.361395	13.436004	0.256820
Si	1.365300	12.644820	10.811591
Si	3.715482	13.344866	9.030849
Si	1.515265	11.102845	2.000357
Si	3.914101	10.488365	3.953472
Si	4.476519	11.112597	6.847814
Si	7.644199	11.317159	6.744497
Si	8.643897	10.501299	4.036982
Si	6.380411	11.112796	2.136596
Si	1.648411	6.494039	2.238441
Si	3.961153	7.344721	4.134544
Si	4.470111	6.571247	7.024469
Si	8.695955	7.387305	4.248433
Si	6.412646	6.706361	2.386992
O	7.171479	1.077929	9.706155
O	6.419253	1.319503	12.226576
O	4.023821	0.914757	0.002141
O	1.831012	1.502972	12.056746
O	2.110919	0.997537	9.441974

O	4.581834	1.156530	10.382933
O	7.415548	16.748789	10.121296
O	6.160569	16.737646	12.402161
O	3.892677	17.093639	0.411661
O	1.752125	16.495077	12.315706
O	2.097304	16.582434	9.766378
O	4.751421	16.833160	10.125578
O	6.091093	18.920168	10.882654
O	1.841023	18.899473	11.198627
O	8.601050	2.570553	8.117326
O	8.424056	19.910938	7.527938
O	8.506146	17.320290	7.679968
O	3.753124	2.904458	8.604734
O	4.165977	0.407333	7.861175
O	3.588343	17.408838	7.778869
O	19.841202	0.664229	10.530949
O	19.793949	17.332626	10.714163
O	2.758631	18.816893	3.087592
O	3.755927	18.666256	5.502554
O	6.179590	18.476818	7.202062
O	8.102303	18.411350	5.346642
O	7.918900	18.982054	2.747798
O	5.392725	18.984243	3.451476
O	2.590647	3.326317	3.600830
O	3.679443	2.910229	5.948074
O	6.067267	2.814316	7.272322
O	8.093092	3.414867	5.661277
O	7.999189	3.221648	3.007829
O	5.274996	3.328904	3.834631
O	3.834613	1.079521	4.092923
O	8.337961	1.008282	4.591708
O	1.415756	17.332626	1.421007
O	1.675040	0.013730	0.832824
O	2.251474	2.654726	1.004929
O	6.257676	17.242285	1.654139
O	6.178789	19.803684	0.997435
O	5.845022	2.583288	1.097005
O	10.200607	19.073193	3.770259
O	10.263677	2.736511	4.339170
O	12.834101	10.705662	3.616890
O	13.841208	11.113392	1.235920
O	16.051237	11.032006	13.057259
O	18.105894	11.362727	1.401735
O	17.949722	11.017479	4.014365

O	15.425149	11.344022	3.262240
O	12.765626	6.960472	3.263445
O	13.932308	6.965446	0.995428
O	16.330744	7.279850	13.215714
O	18.675520	6.478319	1.410702
O	18.021801	6.898187	3.996699
O	15.447573	6.547567	3.173243
O	14.522157	8.940820	2.678875
O	18.523352	8.955346	2.351661
O	11.531870	12.459759	5.193809
O	11.672424	9.868711	5.855330
O	12.266078	7.227118	5.858944
O	16.431654	12.851371	5.116455
O	16.093884	10.284599	5.688712
O	15.940715	7.626889	5.528116
O	0.246871	10.946241	3.003814
O	0.493943	7.288009	3.095354
O	17.269375	8.708001	10.372495
O	16.423044	8.868387	7.865457
O	14.026212	9.040115	6.695916
O	11.843614	8.450509	8.099392
O	12.167569	8.643131	10.690475
O	14.673522	9.114738	9.882543
O	17.268373	13.499084	10.044611
O	16.182981	13.083593	7.708073
O	13.956334	12.765805	6.189370
O	11.840409	13.345861	7.709947
O	12.181986	13.362377	10.548748
O	14.674523	13.013946	9.866884
O	16.440264	11.042552	9.454555
O	12.017405	10.873809	9.206032
O	18.931002	7.462324	12.047511
O	18.354767	9.952883	12.550042
O	18.096884	12.612583	12.466666
O	14.103095	7.226720	11.711061
O	13.847014	9.774986	12.371647
O	13.924700	12.436079	12.383022
O	9.856030	9.369842	9.617693
O	9.688445	12.677256	9.533916
O	12.844514	18.737297	3.681931
O	13.678229	18.655512	1.167265
O	15.982361	19.065233	13.298821
O	18.111700	18.392248	1.341780
O	17.927898	18.899473	3.948521

O	15.441767	18.822065	3.107666
O	12.588633	3.156777	3.176857
O	13.773133	2.991019	0.866014
O	16.175373	2.820086	12.961971
O	18.187384	3.409097	1.181853
O	17.950924	3.131705	3.839449
O	15.274384	3.314377	3.014521
O	13.936313	1.008083	2.664288
O	18.186983	0.992960	2.185578
O	11.419747	17.336407	5.363371
O	11.598543	0.079596	5.767003
O	12.432461	2.664277	5.832847
O	16.258863	17.087471	4.933242
O	16.093884	19.574646	5.688980
O	15.771529	2.329974	5.680682
O	0.175993	19.229996	2.843888
O	0.233657	2.648358	2.758236
O	17.256561	1.080317	10.373967
O	16.336349	1.064795	7.925279
O	13.947725	0.670397	6.782639
O	11.689043	1.401487	8.023108
O	12.092486	1.157724	10.627173
O	14.611655	1.080317	9.946781
O	17.516647	16.654070	9.787122
O	16.259266	17.011854	7.557782
O	13.879651	17.154530	6.282248
O	11.845615	16.431202	7.860773
O	12.344764	16.509205	10.456674
O	14.862931	16.488510	9.768520
O	15.948924	18.819080	9.537261
O	11.762123	18.825052	9.120247
O	18.687334	2.480211	12.120984
O	18.364779	19.816021	12.545359
O	17.681229	17.237907	12.382889
O	13.773334	2.889733	11.697813
O	13.837605	0.337089	12.445120
O	14.101694	17.576588	12.137444
O	9.761725	0.732880	9.700534
O	9.982368	16.910767	9.780029
O	7.254170	9.617187	9.464859
O	5.508852	8.624824	12.071868
O	3.757929	9.044494	0.585908
O	1.901890	8.614676	12.021146
O	2.185201	9.120707	9.429528

O	4.838717	8.878337	9.713650
O	7.179088	13.253132	10.120091
O	6.251469	13.109063	12.524347
O	3.860041	12.778542	0.249058
O	1.754528	13.526942	12.122589
O	2.157370	13.096328	9.456696
O	4.590044	13.101900	10.379052
O	5.922107	10.954598	11.122076
O	1.751324	11.106030	11.205318
O	8.520362	7.619725	8.117326
O	8.667124	10.191273	7.360249
O	7.763330	12.688199	7.599135
O	3.499845	7.220153	8.185177
O	3.751922	9.787721	7.444427
O	4.171183	12.430905	7.774988
O	19.866629	9.365067	10.454533
O	19.795750	12.772173	10.456941
O	2.903390	11.115582	2.841345
O	3.843623	11.350788	5.348650
O	6.081282	10.853512	6.774609
O	8.093493	11.527889	5.185779
O	7.925308	10.857094	2.597239
O	5.426563	10.604376	3.351103
O	3.072776	6.555328	3.014119
O	3.673836	6.715515	5.596503
O	5.912096	7.285820	7.024202
O	8.176784	6.470160	5.435104
O	8.002393	7.047629	2.765597
O	5.518663	7.135185	3.694110
O	3.518867	8.927289	4.178708
O	8.344569	8.971265	4.515424
O	1.402941	12.504134	1.175161
O	1.338270	9.869705	0.922892
O	1.825606	7.207816	0.760824
O	6.095497	12.672678	1.770169
O	6.096298	10.286987	0.748645
O	5.931918	7.698525	1.168871
O	10.238449	10.692927	3.757277
O	10.308526	7.212193	4.008208
O	8.593242	14.916091	8.617313
O	3.832611	14.910917	8.531395
O	5.343872	14.942557	0.834296
O	2.409848	14.922460	0.917003
O	1.257782	4.942514	1.928892

O	6.254272	5.219906	1.842705
O	4.595049	4.996440	7.364933
O	7.586135	4.973556	7.767092
O	11.672225	4.985495	4.770905
O	16.507738	5.055739	5.101868
O	14.774834	5.047978	12.807531
O	17.845608	4.946692	12.468139
O	18.770624	15.008424	11.543508
O	14.013198	14.935593	11.710794
O	15.347864	14.994891	6.109340
O	12.427855	14.931613	5.694868
O	9.679035	1.071760	12.626995
O	9.933715	8.034619	14.467291
O	10.507345	3.407505	11.969890
O	11.598744	5.882741	13.292263
Al	4.539588	18.881565	7.017376
Al	6.357585	3.559135	2.463275
Al	17.860023	6.464787	13.278880
Al	11.338658	12.449014	9.078091
Al	16.171370	3.480335	4.477551
Al	7.520263	6.624576	7.028752
H	10.247660	5.845331	9.391654
H	19.873035	7.197468	11.994246
H	11.608755	14.075558	10.898714
H	18.607244	3.594157	4.398591
H	2.977071	17.124880	7.066090
H	7.926710	3.170906	12.429328
H	8.797667	1.150560	13.036514
H	9.510650	0.672387	11.749337
H	9.202311	7.659921	15.031919
H	10.349171	8.580449	13.054850
H	10.956238	3.385616	11.104545
H	10.252464	2.438025	12.224167
H	11.532671	4.919033	13.426764
H	12.162964	6.275548	13.994068
Pt	7.073972	5.066087	-3.530837
Pt	9.757320	6.838490	-0.817835
Pt	9.128630	6.627362	-3.247519
Pt	6.407240	5.497298	-1.134477
Pt	7.545691	7.769365	-1.341110
Pt	8.652307	4.467126	-1.435728

318

### Pt6H2@H-MFI-6W\_IS

Si	8.440474	1.077133	8.753419
----	----------	----------	----------

Si	6.063462	0.629604	10.825241
Si	5.597350	1.174837	0.374189
Si	2.439280	1.277715	0.180135
Si	1.423764	0.540258	10.818015
Si	3.682246	1.328258	9.036871
Si	8.607457	16.467417	9.052796
Si	6.159768	17.302179	10.913837
Si	5.423159	16.495476	0.470948
Si	2.384420	16.470999	0.444717
Si	1.397936	17.352724	11.020098
Si	3.628387	16.372700	9.143266
Si	1.538691	18.834204	2.052551
Si	3.939328	19.367300	4.061740
Si	7.696857	18.516218	6.929049
Si	8.633687	19.369289	4.145117
Si	6.415449	18.705656	2.213013
Si	1.650213	3.407107	2.336940
Si	3.947337	2.676018	4.373431
Si	4.538386	3.398749	7.260411
Si	7.598549	3.434767	7.200589
Si	8.641695	2.595824	4.360984
Si	11.602549	10.931714	4.619946
Si	14.160559	10.499508	2.713805
Si	14.442869	11.078769	13.124040
Si	17.652596	11.257263	13.238732
Si	18.727577	10.534730	2.678607
Si	16.463289	11.345216	4.517030
Si	11.758921	6.560502	4.465640
Si	14.259268	7.333975	2.564852
Si	14.871340	6.652236	13.031429
Si	18.917185	7.394269	2.701225
Si	16.543777	6.525877	4.456004
Si	18.565199	8.961117	11.302345
Si	16.184584	9.432126	9.371312
Si	15.633577	8.919926	6.423037
Si	12.469501	8.656463	6.600228
Si	11.489425	9.353127	9.386167
Si	13.723879	8.707802	11.165972
Si	18.486313	13.462668	11.131980
Si	16.151346	12.631288	9.254077
Si	15.476805	13.416305	6.290144
Si	12.450279	13.374317	6.232998
Si	13.789752	13.433218	11.142954
Si	11.534274	18.793013	4.641224

Si	13.954132	19.298647	2.649031
Si	14.398420	18.857487	13.100619
Si	17.538269	18.614918	13.225883
Si	18.616455	19.346006	2.558696
Si	16.400219	18.623873	4.412107
Si	11.722281	3.382631	4.540183
Si	13.940317	2.626867	2.456985
Si	14.662511	3.445114	12.966253
Si	17.707256	3.434368	12.996231
Si	18.695541	2.513443	2.408940
Si	18.530359	1.039325	11.383312
Si	16.078667	0.544835	9.424577
Si	15.551287	0.987786	6.482859
Si	12.459691	1.204288	6.564362
Si	11.370293	0.459070	9.320457
Si	13.624570	1.340596	11.177616
Si	18.456079	16.549999	11.114582
Si	16.162359	17.265766	9.155712
Si	15.422946	16.589598	6.233534
Si	12.396821	16.439360	6.307140
Si	11.507243	17.201094	9.242969
Si	13.861231	16.426825	11.036024
Si	8.550395	9.128865	8.654118
Si	6.108111	9.372429	10.633597
Si	5.315240	8.900226	0.379140
Si	2.241863	8.698648	0.263645
Si	1.462207	9.567638	10.784557
Si	3.611969	8.752774	8.708051
Si	8.337961	13.344270	8.981332
Si	6.010404	12.557065	10.996276
Si	5.388120	13.329942	0.493297
Si	2.364398	13.430830	0.258024
Si	1.372108	12.643029	10.812393
Si	3.721689	13.344668	9.034595
Si	1.521271	11.100657	2.001562
Si	3.907093	10.481799	3.969666
Si	4.476919	11.107821	6.853836
Si	7.651608	11.286513	6.757479
Si	8.649103	10.494931	4.044209
Si	6.369598	11.110408	2.188790
Si	1.676242	6.506575	2.240582
Si	3.990985	7.340741	4.146455
Si	4.471714	6.575624	7.030224
Si	8.703564	7.366411	4.233177

Si	6.402235	6.657410	2.422457
O	7.256373	1.160908	9.864610
O	6.350177	1.323681	12.281981
O	4.007603	0.913364	0.154975
O	1.842424	1.499390	12.062232
O	2.144556	0.992562	9.449335
O	4.586640	1.087679	10.379990
O	7.491231	16.751177	10.195571
O	6.171782	16.749386	12.431736
O	3.897683	17.092247	0.417148
O	1.751925	16.495874	12.334041
O	2.162576	16.586016	9.786721
O	4.830908	16.758739	10.121161
O	6.096498	18.910618	10.879041
O	1.846829	18.899473	11.200367
O	8.666522	2.561797	8.118530
O	8.179788	19.971035	7.524190
O	8.512353	17.332428	7.693084
O	3.762134	2.897892	8.611292
O	4.177190	0.393602	7.851405
O	3.587942	17.405855	7.784624
O	19.852814	0.664627	10.531217
O	19.829788	17.323671	10.711084
O	2.760633	18.817490	3.086387
O	3.757729	18.666855	5.493721
O	6.144151	18.316832	7.198180
O	8.099499	18.409958	5.354271
O	7.916899	18.976881	2.746861
O	5.401936	18.986034	3.438762
O	2.654316	3.330098	3.589187
O	3.680444	2.906448	5.970023
O	6.083284	2.811530	7.279148
O	8.098498	3.405913	5.674392
O	8.011202	3.152997	3.011175
O	5.334261	3.313979	3.927777
O	3.837817	1.078128	4.093057
O	8.340965	0.996940	4.599604
O	1.415756	17.330637	1.424085
O	1.665029	0.003980	0.833761
O	2.178193	2.654726	0.999442
O	6.262481	17.167664	1.679834
O	6.172983	19.655039	0.922089
O	5.923108	2.493743	1.178507
O	10.199006	19.071798	3.772266

O	10.269484	2.736113	4.343319
O	12.843111	10.692131	3.608325
O	13.845013	11.109015	1.240604
O	16.057243	11.032404	13.057259
O	18.106094	11.362528	1.404011
O	17.953527	11.015489	4.013829
O	15.427551	11.348399	3.263311
O	12.847116	6.881074	3.268932
O	14.014799	6.968431	1.002654
O	16.345961	7.285820	13.132069
O	18.607645	6.476328	1.419535
O	18.085670	6.892218	4.020923
O	15.584324	6.555328	3.105258
O	14.588029	8.931467	2.687173
O	18.523754	8.954351	2.351527
O	11.594940	12.449412	5.187786
O	11.673827	9.866123	5.860683
O	12.272084	7.229904	5.855999
O	16.439463	12.852565	5.113511
O	16.096085	10.285993	5.687508
O	15.944921	7.621914	5.519551
O	0.249274	10.947236	3.005019
O	0.500150	7.284029	3.086521
O	17.271778	8.708200	10.372896
O	16.424246	8.867193	7.865725
O	14.039025	9.040912	6.693374
O	11.921098	8.386036	8.113578
O	12.176579	8.630992	10.690876
O	14.674323	9.112150	9.884282
O	17.270376	13.499084	10.047421
O	16.189789	13.084986	7.713426
O	13.990373	12.766005	6.193653
O	11.845416	13.342877	7.706868
O	12.183187	13.358397	10.546607
O	14.674925	13.013549	9.867019
O	16.439463	11.041756	9.454688
O	12.012599	10.860277	9.200412
O	18.937609	7.460732	12.046307
O	18.355167	9.952683	12.549373
O	18.097485	12.613976	12.466666
O	14.099893	7.220949	11.701962
O	13.849216	9.778567	12.376197
O	13.925100	12.434885	12.384093
O	9.876852	9.293032	9.608058

O	9.690448	12.677652	9.533246
O	12.844112	18.738092	3.681797
O	13.679231	18.657104	1.165927
O	15.990170	19.065233	13.298688
O	18.112701	18.391850	1.342449
O	17.928900	18.899672	3.946781
O	15.441767	18.822065	3.107533
O	12.587030	3.161155	3.182344
O	13.771932	2.989427	0.866951
O	16.174973	2.817698	12.962641
O	18.188585	3.406510	1.185466
O	17.952925	3.132500	3.840252
O	15.273982	3.315173	3.014922
O	13.934912	1.009476	2.664689
O	18.189186	0.994552	2.186782
O	11.421949	17.335014	5.364308
O	11.600346	0.079397	5.769545
O	12.433461	2.661093	5.842483
O	16.260466	17.087471	4.933643
O	16.097689	19.572258	5.686705
O	15.773932	2.333755	5.677069
O	0.176194	19.229399	2.846029
O	0.240464	2.655124	2.768408
O	17.268373	1.078924	10.374101
O	16.347763	1.065194	7.918855
O	13.970951	0.668208	6.780765
O	11.756317	1.401487	8.038365
O	12.098894	1.091858	10.636943
O	14.664913	1.154540	9.951599
O	17.523054	16.658846	9.789665
O	16.259865	17.014242	7.564474
O	13.884856	17.155127	6.282248
O	11.848418	16.425232	7.856089
O	12.350571	16.504431	10.460153
O	14.866535	16.489305	9.770928
O	15.944319	18.824852	9.537930
O	11.843012	18.807938	9.113020
O	18.689735	2.476430	12.121117
O	18.368584	19.815622	12.544957
O	17.686832	17.238304	12.378071
O	13.765124	2.885355	11.702229
O	13.843410	0.335696	12.440703
O	14.102896	17.576786	12.138381
O	9.764929	0.592393	9.616756

O	10.005795	16.913952	9.777486
O	7.255972	9.623554	9.448800
O	5.259579	8.705613	12.131021
O	3.738708	9.047081	0.753597
O	1.914904	8.621043	12.041354
O	2.188004	9.119115	9.433543
O	4.846125	8.875551	9.711241
O	7.179288	13.258904	10.122232
O	6.256875	13.027875	12.541209
O	3.858239	12.770183	0.251868
O	1.754728	13.527539	12.124330
O	2.160574	13.096128	9.457097
O	4.598853	13.171148	10.391231
O	5.913497	10.957185	11.044723
O	1.751925	11.106230	11.206791
O	8.510350	7.551671	8.193875
O	8.664320	10.123815	7.350345
O	7.772541	12.674270	7.598198
O	3.498644	7.220551	8.185846
O	3.750521	9.785134	7.446435
O	4.172785	12.429911	7.779136
O	19.875439	9.363276	10.458280
O	19.800556	12.773169	10.456941
O	2.908195	11.114587	2.845761
O	3.838217	11.352380	5.356947
O	6.081882	10.852318	6.774742
O	8.097297	11.520725	5.194077
O	7.929713	10.857491	2.606741
O	5.438776	10.607361	3.422836
O	3.092398	6.560302	3.021346
O	3.673036	6.713724	5.602124
O	5.915699	7.285223	7.023934
O	8.185193	6.472349	5.441795
O	8.007999	6.976390	2.765463
O	5.570921	7.127822	3.768251
O	3.523872	8.916344	4.179779
O	8.350575	8.957535	4.506056
O	1.402541	12.503935	1.177303
O	1.331663	9.873287	0.923427
O	1.822402	7.207816	0.759218
O	6.085287	12.678051	1.826378
O	6.088890	10.267883	0.820913
O	5.853832	7.638629	1.237928
O	10.246258	10.693922	3.762229

O	10.337558	7.209408	3.999644
O	8.592641	14.917485	8.617313
O	3.832211	14.904749	8.519083
O	5.340668	14.917882	0.762028
O	2.411450	14.918678	0.920081
O	1.321652	4.948483	1.932505
O	6.181392	5.153443	1.919256
O	4.596050	4.996838	7.365602
O	7.588538	4.965994	7.780341
O	11.674227	4.982112	4.840230
O	16.511742	5.059122	5.102001
O	14.769028	5.045590	12.798698
O	17.845407	4.929778	12.465730
O	18.771626	15.009617	11.543105
O	14.014398	14.933404	11.711999
O	15.350867	14.998274	6.110009
O	12.431659	14.928628	5.694601
O	8.925407	2.326790	12.375260
O	11.192498	4.217394	9.280575
O	9.753517	8.527517	14.303617
O	11.096792	4.224359	11.791628
O	13.269179	5.732305	9.032321
O	11.514451	6.451852	13.371223
Al	4.537586	18.854700	7.012826
Al	6.374003	3.515556	2.536480
Al	17.862427	6.459614	13.256397
Al	11.336656	12.443243	9.073406
Al	16.176775	3.486305	4.474740
Al	7.514256	6.603284	7.039860
H	12.050641	4.708103	9.062031
H	19.895260	7.245226	12.051392
H	11.598945	14.056653	10.908618
H	18.606844	3.601520	4.397253
H	2.951643	17.110950	7.099547
H	6.427463	6.337434	12.109875
H	7.985775	2.010595	12.454220
H	9.254970	1.868317	11.575225
H	9.888865	5.739071	9.454555
H	11.130429	3.428200	8.710326
H	9.125627	8.111231	14.946268
H	9.325847	9.371633	14.059243
H	11.202109	4.144962	10.744408
H	11.372896	3.362334	12.157653
H	12.873144	6.578609	8.740170

H	13.617162	5.914182	9.926706
H	11.683837	5.555204	13.006938
H	11.745106	6.452251	14.317534
Pt	7.060157	4.783521	-3.443312
Pt	9.502040	7.038873	-0.742890
Pt	8.863739	6.619203	-3.176188
Pt	6.465504	4.732380	-0.989271
Pt	7.244560	7.882591	-1.304039
Pt	8.955039	4.532197	-1.384739

318

Pt6H2@H-MFI-6W\_FS

Si	8.440474	1.077133	8.753419
Si	6.063462	0.629604	10.825241
Si	5.597350	1.174837	0.374189
Si	2.439280	1.277715	0.180135
Si	1.423764	0.540258	10.818015
Si	3.682246	1.328258	9.036871
Si	8.607457	16.467417	9.052796
Si	6.159768	17.302179	10.913837
Si	5.423159	16.495476	0.470948
Si	2.384420	16.470999	0.444717
Si	1.397936	17.352724	11.020098
Si	3.628387	16.372700	9.143266
Si	1.538691	18.834204	2.052551
Si	3.939328	19.367300	4.061740
Si	7.696857	18.516218	6.929049
Si	8.633687	19.369289	4.145117
Si	6.415449	18.705656	2.213013
Si	1.650213	3.407107	2.336940
Si	3.947337	2.676018	4.373431
Si	4.538386	3.398749	7.260411
Si	7.598549	3.434767	7.200589
Si	8.641695	2.595824	4.360984
Si	11.602549	10.931714	4.619946
Si	14.160559	10.499508	2.713805
Si	14.442869	11.078769	13.124040
Si	17.652596	11.257263	13.238732
Si	18.727577	10.534730	2.678607
Si	16.463289	11.345216	4.517030
Si	11.758921	6.560502	4.465640
Si	14.259268	7.333975	2.564852
Si	14.871340	6.652236	13.031429
Si	18.917185	7.394269	2.701225
Si	16.543777	6.525877	4.456004

Si	18.565199	8.961117	11.302345
Si	16.184584	9.432126	9.371312
Si	15.633577	8.919926	6.423037
Si	12.469501	8.656463	6.600228
Si	11.489425	9.353127	9.386167
Si	13.723879	8.707802	11.165972
Si	18.486313	13.462668	11.131980
Si	16.151346	12.631288	9.254077
Si	15.476805	13.416305	6.290144
Si	12.450279	13.374317	6.232998
Si	13.789752	13.433218	11.142954
Si	11.534274	18.793013	4.641224
Si	13.954132	19.298647	2.649031
Si	14.398420	18.857487	13.100619
Si	17.538269	18.614918	13.225883
Si	18.616455	19.346006	2.558696
Si	16.400219	18.623873	4.412107
Si	11.722281	3.382631	4.540183
Si	13.940317	2.626867	2.456985
Si	14.662511	3.445114	12.966253
Si	17.707256	3.434368	12.996231
Si	18.695541	2.513443	2.408940
Si	18.530359	1.039325	11.383312
Si	16.078667	0.544835	9.424577
Si	15.551287	0.987786	6.482859
Si	12.459691	1.204288	6.564362
Si	11.370293	0.459070	9.320457
Si	13.624570	1.340596	11.177616
Si	18.456079	16.549999	11.114582
Si	16.162359	17.265766	9.155712
Si	15.422946	16.589598	6.233534
Si	12.396821	16.439360	6.307140
Si	11.507243	17.201094	9.242969
Si	13.861231	16.426825	11.036024
Si	8.550395	9.128865	8.654118
Si	6.108111	9.372429	10.633597
Si	5.315240	8.900226	0.379140
Si	2.241863	8.698648	0.263645
Si	1.462207	9.567638	10.784557
Si	3.611969	8.752774	8.708051
Si	8.337961	13.344270	8.981332
Si	6.010404	12.557065	10.996276
Si	5.388120	13.329942	0.493297
Si	2.364398	13.430830	0.258024

Si	1.372108	12.643029	10.812393
Si	3.721689	13.344668	9.034595
Si	1.521271	11.100657	2.001562
Si	3.907093	10.481799	3.969666
Si	4.476919	11.107821	6.853836
Si	7.651608	11.286513	6.757479
Si	8.649103	10.494931	4.044209
Si	6.369598	11.110408	2.188790
Si	1.676242	6.506575	2.240582
Si	3.990985	7.340741	4.146455
Si	4.471714	6.575624	7.030224
Si	8.703564	7.366411	4.233177
Si	6.402235	6.657410	2.422457
O	7.256373	1.160908	9.864610
O	6.350177	1.323681	12.281981
O	4.007603	0.913364	0.154975
O	1.842424	1.499390	12.062232
O	2.144556	0.992562	9.449335
O	4.586640	1.087679	10.379990
O	7.491231	16.751177	10.195571
O	6.171782	16.749386	12.431736
O	3.897683	17.092247	0.417148
O	1.751925	16.495874	12.334041
O	2.162576	16.586016	9.786721
O	4.830908	16.758739	10.121161
O	6.096498	18.910618	10.879041
O	1.846829	18.899473	11.200367
O	8.666522	2.561797	8.118530
O	8.179788	19.971035	7.524190
O	8.512353	17.332428	7.693084
O	3.762134	2.897892	8.611292
O	4.177190	0.393602	7.851405
O	3.587942	17.405855	7.784624
O	19.852814	0.664627	10.531217
O	19.829788	17.323671	10.711084
O	2.760633	18.817490	3.086387
O	3.757729	18.666855	5.493721
O	6.144151	18.316832	7.198180
O	8.099499	18.409958	5.354271
O	7.916899	18.976881	2.746861
O	5.401936	18.986034	3.438762
O	2.654316	3.330098	3.589187
O	3.680444	2.906448	5.970023
O	6.083284	2.811530	7.279148

O	8.098498	3.405913	5.674392
O	8.011202	3.152997	3.011175
O	5.334261	3.313979	3.927777
O	3.837817	1.078128	4.093057
O	8.340965	0.996940	4.599604
O	1.415756	17.330637	1.424085
O	1.665029	0.003980	0.833761
O	2.178193	2.654726	0.999442
O	6.262481	17.167664	1.679834
O	6.172983	19.655039	0.922089
O	5.923108	2.493743	1.178507
O	10.199006	19.071798	3.772266
O	10.269484	2.736113	4.343319
O	12.843111	10.692131	3.608325
O	13.845013	11.109015	1.240604
O	16.057243	11.032404	13.057259
O	18.106094	11.362528	1.404011
O	17.953527	11.015489	4.013829
O	15.427551	11.348399	3.263311
O	12.847116	6.881074	3.268932
O	14.014799	6.968431	1.002654
O	16.345961	7.285820	13.132069
O	18.607645	6.476328	1.419535
O	18.085670	6.892218	4.020923
O	15.584324	6.555328	3.105258
O	14.588029	8.931467	2.687173
O	18.523754	8.954351	2.351527
O	11.594940	12.449412	5.187786
O	11.673827	9.866123	5.860683
O	12.272084	7.229904	5.855999
O	16.439463	12.852565	5.113511
O	16.096085	10.285993	5.687508
O	15.944921	7.621914	5.519551
O	0.249274	10.947236	3.005019
O	0.500150	7.284029	3.086521
O	17.271778	8.708200	10.372896
O	16.424246	8.867193	7.865725
O	14.039025	9.040912	6.693374
O	11.921098	8.386036	8.113578
O	12.176579	8.630992	10.690876
O	14.674323	9.112150	9.884282
O	17.270376	13.499084	10.047421
O	16.189789	13.084986	7.713426
O	13.990373	12.766005	6.193653

O	11.845416	13.342877	7.706868
O	12.183187	13.358397	10.546607
O	14.674925	13.013549	9.867019
O	16.439463	11.041756	9.454688
O	12.012599	10.860277	9.200412
O	18.937609	7.460732	12.046307
O	18.355167	9.952683	12.549373
O	18.097485	12.613976	12.466666
O	14.099893	7.220949	11.701962
O	13.849216	9.778567	12.376197
O	13.925100	12.434885	12.384093
O	9.876852	9.293032	9.608058
O	9.690448	12.677652	9.533246
O	12.844112	18.738092	3.681797
O	13.679231	18.657104	1.165927
O	15.990170	19.065233	13.298688
O	18.112701	18.391850	1.342449
O	17.928900	18.899672	3.946781
O	15.441767	18.822065	3.107533
O	12.587030	3.161155	3.182344
O	13.771932	2.989427	0.866951
O	16.174973	2.817698	12.962641
O	18.188585	3.406510	1.185466
O	17.952925	3.132500	3.840252
O	15.273982	3.315173	3.014922
O	13.934912	1.009476	2.664689
O	18.189186	0.994552	2.186782
O	11.421949	17.335014	5.364308
O	11.600346	0.079397	5.769545
O	12.433461	2.661093	5.842483
O	16.260466	17.087471	4.933643
O	16.097689	19.572258	5.686705
O	15.773932	2.333755	5.677069
O	0.176194	19.229399	2.846029
O	0.240464	2.655124	2.768408
O	17.268373	1.078924	10.374101
O	16.347763	1.065194	7.918855
O	13.970951	0.668208	6.780765
O	11.756317	1.401487	8.038365
O	12.098894	1.091858	10.636943
O	14.664913	1.154540	9.951599
O	17.523054	16.658846	9.789665
O	16.259865	17.014242	7.564474
O	13.884856	17.155127	6.282248

O	11.848418	16.425232	7.856089
O	12.350571	16.504431	10.460153
O	14.866535	16.489305	9.770928
O	15.944319	18.824852	9.537930
O	11.843012	18.807938	9.113020
O	18.689735	2.476430	12.121117
O	18.368584	19.815622	12.544957
O	17.686832	17.238304	12.378071
O	13.765124	2.885355	11.702229
O	13.843410	0.335696	12.440703
O	14.102896	17.576786	12.138381
O	9.764929	0.592393	9.616756
O	10.005795	16.913952	9.777486
O	7.255972	9.623554	9.448800
O	5.259579	8.705613	12.131021
O	3.738708	9.047081	0.753597
O	1.914904	8.621043	12.041354
O	2.188004	9.119115	9.433543
O	4.846125	8.875551	9.711241
O	7.179288	13.258904	10.122232
O	6.256875	13.027875	12.541209
O	3.858239	12.770183	0.251868
O	1.754728	13.527539	12.124330
O	2.160574	13.096128	9.457097
O	4.598853	13.171148	10.391231
O	5.913497	10.957185	11.044723
O	1.751925	11.106230	11.206791
O	8.510350	7.551671	8.193875
O	8.664320	10.123815	7.350345
O	7.772541	12.674270	7.598198
O	3.498644	7.220551	8.185846
O	3.750521	9.785134	7.446435
O	4.172785	12.429911	7.779136
O	19.875439	9.363276	10.458280
O	19.800556	12.773169	10.456941
O	2.908195	11.114587	2.845761
O	3.838217	11.352380	5.356947
O	6.081882	10.852318	6.774742
O	8.097297	11.520725	5.194077
O	7.929713	10.857491	2.606741
O	5.438776	10.607361	3.422836
O	3.092398	6.560302	3.021346
O	3.673036	6.713724	5.602124
O	5.915699	7.285223	7.023934

O	8.185193	6.472349	5.441795
O	8.007999	6.976390	2.765463
O	5.570921	7.127822	3.768251
O	3.523872	8.916344	4.179779
O	8.350575	8.957535	4.506056
O	1.402541	12.503935	1.177303
O	1.331663	9.873287	0.923427
O	1.822402	7.207816	0.759218
O	6.085287	12.678051	1.826378
O	6.088890	10.267883	0.820913
O	5.853832	7.638629	1.237928
O	10.246258	10.693922	3.762229
O	10.337558	7.209408	3.999644
O	8.592641	14.917485	8.617313
O	3.832211	14.904749	8.519083
O	5.340668	14.917882	0.762028
O	2.411450	14.918678	0.920081
O	1.321652	4.948483	1.932505
O	6.181392	5.153443	1.919256
O	4.596050	4.996838	7.365602
O	7.588538	4.965994	7.780341
O	11.674227	4.982112	4.840230
O	16.511742	5.059122	5.102001
O	14.769028	5.045590	12.798698
O	17.845407	4.929778	12.465730
O	18.771626	15.009617	11.543105
O	14.014398	14.933404	11.711999
O	15.350867	14.998274	6.110009
O	12.431659	14.928628	5.694601
O	8.925407	2.326790	12.375260
O	11.192498	4.217394	9.280575
O	9.753517	8.527517	14.303617
O	11.096792	4.224359	11.791628
O	13.269179	5.732305	9.032321
O	11.514451	6.451852	13.371223
Al	4.537586	18.854700	7.012826
Al	6.374003	3.515556	2.536480
Al	17.862427	6.459614	13.256397
Al	11.336656	12.443243	9.073406
Al	16.176775	3.486305	4.474740
Al	7.514256	6.603284	7.039860
H	12.050641	4.708103	9.062031
H	19.895260	7.245226	12.051392
H	11.598945	14.056653	10.908618

H	18.606844	3.601520	4.397253
H	2.951643	17.110950	7.099547
H	6.427463	6.337434	12.109875
H	7.985775	2.010595	12.454220
H	9.254970	1.868317	11.575225
H	9.888865	5.739071	9.454555
H	11.130429	3.428200	8.710326
H	9.125627	8.111231	14.946268
H	10.021811	8.345043	12.588987
H	11.202109	4.144962	10.744408
H	11.372896	3.362334	12.157653
H	12.873144	6.578609	8.740170
H	13.617162	5.914182	9.926706
H	11.683837	5.555204	13.006938
H	11.745106	6.452251	14.317534
Pt	7.060157	4.783521	-3.443312
Pt	9.502040	7.038873	-0.742890
Pt	8.863739	6.619203	-3.176188
Pt	6.465504	4.732380	-0.989271
Pt	7.244560	7.882591	-1.304039
Pt	8.955039	4.532197	-1.384739

324

#### Pt6H2@H-MFI-8W\_IS

Si	8.399429	1.004502	8.764393
Si	6.028624	0.633186	10.861376
Si	5.609964	1.185383	0.384360
Si	2.448290	1.277317	0.180804
Si	1.414354	0.539462	10.825643
Si	3.658620	1.318906	9.069927
Si	8.600850	16.451696	9.056410
Si	6.156965	17.305166	10.924811
Si	5.422358	16.494480	0.484465
Si	2.383819	16.472391	0.445922
Si	1.398937	17.353123	11.020901
Si	3.629988	16.369713	9.146746
Si	1.539492	18.836592	2.050945
Si	3.934723	19.369886	4.064551
Si	7.669227	18.477018	6.925837
Si	8.630683	19.359539	4.151674
Si	6.404837	18.710234	2.212745
Si	1.630592	3.407704	2.326635
Si	3.882266	2.676415	4.406353
Si	4.491936	3.379049	7.271653
Si	7.537482	3.368702	7.200991

Si	8.646100	2.592840	4.396717
Si	11.598744	10.931517	4.623291
Si	14.152550	10.504881	2.715545
Si	14.448475	11.082151	13.123505
Si	17.656200	11.259650	13.241141
Si	18.726175	10.533535	2.680213
Si	16.461687	11.343425	4.517967
Si	11.738898	6.559109	4.474606
Si	14.219825	7.329996	2.580242
Si	14.912186	6.665170	13.070507
Si	18.918186	7.396259	2.710994
Si	16.515547	6.524683	4.469655
Si	18.562395	8.986190	11.292174
Si	16.182581	9.484659	9.355922
Si	15.618561	8.924502	6.427320
Si	12.450279	8.652483	6.612407
Si	11.481014	9.369643	9.395535
Si	13.749508	8.733274	11.147236
Si	18.485710	13.466648	11.132381
Si	16.147743	12.665913	9.248322
Si	15.474803	13.420283	6.282784
Si	12.451080	13.374914	6.228448
Si	13.791754	13.438990	11.146701
Si	11.535274	18.789829	4.637343
Si	13.953932	19.300636	2.646756
Si	14.395417	18.858879	13.100753
Si	17.535868	18.615116	13.226686
Si	18.617056	19.345610	2.557893
Si	16.400822	18.623672	4.410100
Si	11.721279	3.384422	4.526131
Si	13.939517	2.627862	2.455781
Si	14.660508	3.449890	12.972142
Si	17.706856	3.445711	12.992752
Si	18.685331	2.513244	2.406397
Si	18.526556	1.041116	11.386524
Si	16.077065	0.544238	9.426718
Si	15.561499	0.988383	6.481655
Si	12.468499	1.191751	6.557269
Si	11.360883	0.444544	9.329557
Si	13.620366	1.339402	11.178018
Si	18.456478	16.551989	11.114716
Si	16.162359	17.265965	9.155444
Si	15.420544	16.592781	6.232731
Si	12.394818	16.438963	6.307542

Si	11.502838	17.194925	9.244174
Si	13.860430	16.429609	11.035622
Si	8.536779	9.134238	8.649700
Si	6.095898	9.356510	10.646846
Si	5.311036	8.900624	0.368568
Si	2.236858	8.694470	0.264850
Si	1.468413	9.567439	10.788839
Si	3.609366	8.751580	8.704705
Si	8.370398	13.313625	8.985748
Si	6.013808	12.532391	10.996142
Si	5.381913	13.354617	0.470145
Si	2.361795	13.432621	0.256954
Si	1.369104	12.643427	10.812126
Si	3.717685	13.334917	9.031786
Si	1.516466	11.102448	1.999153
Si	3.912699	10.498513	3.952803
Si	4.471714	11.108617	6.847948
Si	7.647402	11.259451	6.734861
Si	8.646300	10.494534	4.032967
Si	6.375004	11.107622	2.133518
Si	1.671837	6.508963	2.251154
Si	3.959551	7.371584	4.165727
Si	4.465306	6.553537	7.033570
Si	8.741405	7.388897	4.234783
Si	6.407640	6.709146	2.471037
O	7.161469	1.083899	9.789799
O	6.336762	1.323681	12.295364
O	4.011608	0.915951	0.161131
O	1.840622	1.498992	12.065177
O	2.099307	0.995547	9.440637
O	4.519766	1.080317	10.446235
O	7.484624	16.748194	10.195972
O	6.171381	16.743814	12.444450
O	3.897683	17.091251	0.417550
O	1.751725	16.495674	12.335380
O	2.162576	16.585020	9.787256
O	4.831709	16.755554	10.123035
O	6.089891	18.906637	10.885599
O	1.846028	18.899275	11.201169
O	8.589638	2.490957	8.115049
O	8.185794	19.905964	7.524592
O	8.507548	17.315313	7.693084
O	3.753725	2.890330	8.636184
O	4.170783	0.403751	7.867197

O	3.584739	17.401875	7.786230
O	19.845806	0.664030	10.534161
O	19.830589	17.323473	10.710816
O	2.760433	18.817291	3.086521
O	3.753725	18.669441	5.496666
O	6.112115	18.306683	7.193496
O	8.093893	18.403391	5.352932
O	7.917699	18.984243	2.742980
O	5.399533	18.986830	3.443847
O	2.595452	3.322536	3.605246
O	3.593148	2.900080	6.007093
O	6.024419	2.747654	7.270851
O	8.094093	3.402331	5.692192
O	7.985975	3.231399	3.084246
O	5.273995	3.330297	3.997101
O	3.834814	1.080715	4.096537
O	8.339764	0.996542	4.596927
O	1.415355	17.331034	1.424754
O	1.665029	0.004975	0.833226
O	2.176391	2.655323	0.999844
O	6.265484	17.170448	1.687329
O	6.176386	19.648472	0.920081
O	5.920506	2.408774	1.333884
O	10.194401	19.071600	3.771597
O	10.266080	2.734322	4.278143
O	12.836905	10.698498	3.607388
O	13.842811	11.111204	1.238463
O	16.062248	11.032404	13.057526
O	18.106094	11.363523	1.406152
O	17.952124	11.015489	4.014499
O	15.426750	11.343425	3.262508
O	12.852722	6.880875	3.325542
O	14.006189	6.962660	1.009614
O	16.369987	7.284427	13.289587
O	18.685129	6.473543	1.417260
O	18.040821	6.901371	4.005131
O	15.517651	6.550751	3.164143
O	14.522157	8.930472	2.682622
O	18.523352	8.954152	2.351527
O	11.593739	12.451202	5.186716
O	11.672626	9.868312	5.856267
O	12.262273	7.228710	5.862825
O	16.439062	12.852365	5.110700
O	16.093884	10.285993	5.688177

O	15.942718	7.626292	5.531595
O	0.247872	10.947037	3.005153
O	0.498948	7.289402	3.097362
O	17.265171	8.783618	10.368880
O	16.420042	8.873362	7.867599
O	14.025611	9.039718	6.696184
O	11.845416	8.447325	8.101533
O	12.186391	8.636365	10.696898
O	14.671521	9.193537	9.875584
O	17.271976	13.512218	10.047555
O	16.188988	13.094537	7.705128
O	13.990973	12.766005	6.191779
O	11.848820	13.346260	7.702184
O	12.188191	13.363173	10.550622
O	14.670719	13.018523	9.867019
O	16.445068	11.088519	9.449470
O	12.022010	10.866049	9.207772
O	18.875740	7.452374	11.982470
O	18.358971	9.952883	12.554860
O	18.097685	12.614772	12.465997
O	14.258266	7.295172	11.705040
O	13.845013	9.785931	12.379810
O	13.926302	12.436676	12.384360
O	9.855629	9.370240	9.611403
O	9.738300	12.683025	9.540071
O	12.844514	18.737495	3.680325
O	13.679030	18.656307	1.166061
O	15.987767	19.064835	13.298821
O	18.112501	18.391253	1.342315
O	17.929300	18.899672	3.946112
O	15.441167	18.821867	3.107265
O	12.595840	3.158170	3.186358
O	13.776537	2.989029	0.867352
O	16.175573	2.823469	12.960767
O	18.186583	3.409495	1.182254
O	17.948921	3.133297	3.839583
O	15.275584	3.314576	3.013450
O	13.935913	1.009476	2.664288
O	18.186983	0.993358	2.185444
O	11.420548	17.334219	5.362836
O	11.601147	0.075815	5.762452
O	12.423651	2.656715	5.841948
O	16.259865	17.087870	4.933375
O	16.099890	19.571264	5.686169

O	15.775934	2.335944	5.677738
O	0.176394	19.229597	2.846029
O	0.227650	2.654925	2.765999
O	17.266771	1.079720	10.374769
O	16.349564	1.067382	7.922067
O	13.983564	0.668805	6.778490
O	11.758719	1.339601	8.027793
O	12.097692	1.088674	10.636139
O	14.663111	1.155535	9.951599
O	17.522854	16.659046	9.789665
O	16.258863	17.014641	7.563938
O	13.881652	17.156321	6.281847
O	11.847818	16.423441	7.855687
O	12.349770	16.502041	10.460554
O	14.866535	16.488909	9.770661
O	15.944118	18.824852	9.537930
O	11.841210	18.796993	9.116901
O	18.687733	2.481206	12.121385
O	18.365980	19.816420	12.546429
O	17.686434	17.238903	12.378205
O	13.769129	2.887743	11.700757
O	13.844412	0.337288	12.440436
O	14.102695	17.577583	12.138247
O	9.755319	0.587617	9.615552
O	10.000588	16.909575	9.775345
O	7.246562	9.625545	9.460443
O	5.257977	8.628007	12.127274
O	3.740109	9.044095	0.752660
O	1.918708	8.621441	12.042024
O	2.188605	9.118518	9.433678
O	4.843522	8.877143	9.710437
O	7.196307	13.179705	10.108983
O	6.248065	13.113441	12.502398
O	3.857639	12.773765	0.247318
O	1.753927	13.528534	12.122724
O	2.157170	13.096128	9.456829
O	4.593447	13.099710	10.378116
O	5.918704	10.932312	11.125957
O	1.752325	11.107423	11.206924
O	8.510151	7.550278	8.199898
O	8.597446	10.037852	7.284903
O	7.847222	12.609797	7.605291
O	3.501447	7.217766	8.187318
O	3.750120	9.784537	7.445231

O	4.170983	12.428319	7.773650
O	19.883646	9.362281	10.457075
O	19.797152	12.772372	10.456941
O	2.900587	11.122148	2.842148
O	3.842222	11.354967	5.349720
O	6.074275	10.854307	6.773003
O	8.095695	11.522716	5.182968
O	7.926909	10.857491	2.592689
O	5.426563	10.606565	3.352843
O	3.069373	6.559109	3.068722
O	3.669432	6.715117	5.610689
O	5.926712	7.214581	7.023800
O	8.339563	6.539011	5.521424
O	7.989178	6.962660	2.839471
O	5.525471	7.207617	3.768653
O	3.507054	8.945396	4.185400
O	8.351776	8.968878	4.504986
O	1.399938	12.505328	1.175027
O	1.331863	9.873486	0.923159
O	1.826207	7.207020	0.767783
O	6.096699	12.669495	1.765218
O	6.093295	10.280023	0.750652
O	5.930917	7.699918	1.249972
O	10.245057	10.696906	3.757143
O	10.352574	7.211795	3.932060
O	8.588237	14.896988	8.623470
O	3.834213	14.897387	8.525105
O	5.338866	14.924250	0.834162
O	2.410849	14.918878	0.919814
O	1.321852	4.953458	1.929962
O	6.171782	5.202793	1.988179
O	4.591044	4.976342	7.365067
O	7.591742	4.906497	7.777665
O	11.668621	4.976939	4.846252
O	16.511543	5.055739	5.107221
O	14.767226	5.057729	12.794951
O	17.845808	4.948881	12.467603
O	18.772627	15.011408	11.544176
O	14.015800	14.937184	11.714006
O	15.349866	15.001260	6.108135
O	12.431859	14.929423	5.692995
O	10.095893	3.569880	14.888321
O	8.923605	2.488967	11.792832
O	10.854326	3.814837	9.280308

O	9.679035	1.163296	13.807376
O	9.844216	8.703226	14.216227
O	11.182487	4.149339	12.292018
O	12.431059	5.547244	10.533626
O	11.681636	6.876697	13.050165
Al	4.513359	18.864849	7.023533
Al	6.306730	3.551971	2.594696
Al	17.889856	6.466379	13.283431
Al	11.372295	12.448814	9.074076
Al	16.175173	3.486902	4.472331
Al	7.538083	6.571247	7.047622
H	10.176382	6.202120	9.486138
H	19.775127	7.107923	11.805279
H	11.600947	14.066205	10.898046
H	9.288406	3.611470	2.081458
H	18.607044	3.595948	4.396583
H	2.952644	17.100006	7.100217
H	9.875852	4.181576	14.150783
H	9.881658	1.982338	14.362636
H	6.396828	3.654849	12.465060
H	9.508648	2.168991	11.080723
H	9.922703	4.112328	9.261036
H	10.979665	3.284728	8.472109
H	9.122423	1.893390	12.620571
H	9.073369	0.601746	14.323423
H	9.103602	9.330045	14.333461
H	10.651302	9.236121	14.096046
H	11.768129	4.604032	11.591686
H	11.346868	3.191800	12.207438
H	11.972755	5.022110	9.816966
H	13.387109	5.389843	10.449580
H	12.043033	6.584380	12.182813
H	11.955336	6.209284	13.707807
Pt	7.186096	4.941916	-3.476100
Pt	9.536879	7.101954	-0.757344
Pt	8.942025	6.804861	-3.180738
Pt	6.641297	5.179511	-1.057257
Pt	7.242558	7.821103	-1.293735
Pt	9.103803	4.613782	-1.361051

324

#### Pt6H2@H-MFI-8W\_FS

Si	8.399429	1.004502	8.764393
Si	6.028624	0.633186	10.861376
Si	5.609964	1.185383	0.384360

Si	2.448290	1.277317	0.180804
Si	1.414354	0.539462	10.825643
Si	3.658620	1.318906	9.069927
Si	8.600850	16.451696	9.056410
Si	6.156965	17.305166	10.924811
Si	5.422358	16.494480	0.484465
Si	2.383819	16.472391	0.445922
Si	1.398937	17.353123	11.020901
Si	3.629988	16.369713	9.146746
Si	1.539492	18.836592	2.050945
Si	3.934723	19.369886	4.064551
Si	7.669227	18.477018	6.925837
Si	8.630683	19.359539	4.151674
Si	6.404837	18.710234	2.212745
Si	1.630592	3.407704	2.326635
Si	3.882266	2.676415	4.406353
Si	4.491936	3.379049	7.271653
Si	7.537482	3.368702	7.200991
Si	8.646100	2.592840	4.396717
Si	11.598744	10.931517	4.623291
Si	14.152550	10.504881	2.715545
Si	14.448475	11.082151	13.123505
Si	17.656200	11.259650	13.241141
Si	18.726175	10.533535	2.680213
Si	16.461687	11.343425	4.517967
Si	11.738898	6.559109	4.474606
Si	14.219825	7.329996	2.580242
Si	14.912186	6.665170	13.070507
Si	18.918186	7.396259	2.710994
Si	16.515547	6.524683	4.469655
Si	18.562395	8.986190	11.292174
Si	16.182581	9.484659	9.355922
Si	15.618561	8.924502	6.427320
Si	12.450279	8.652483	6.612407
Si	11.481014	9.369643	9.395535
Si	13.749508	8.733274	11.147236
Si	18.485710	13.466648	11.132381
Si	16.147743	12.665913	9.248322
Si	15.474803	13.420283	6.282784
Si	12.451080	13.374914	6.228448
Si	13.791754	13.438990	11.146701
Si	11.535274	18.789829	4.637343
Si	13.953932	19.300636	2.646756
Si	14.395417	18.858879	13.100753

Si	17.535868	18.615116	13.226686
Si	18.617056	19.345610	2.557893
Si	16.400822	18.623672	4.410100
Si	11.721279	3.384422	4.526131
Si	13.939517	2.627862	2.455781
Si	14.660508	3.449890	12.972142
Si	17.706856	3.445711	12.992752
Si	18.685331	2.513244	2.406397
Si	18.526556	1.041116	11.386524
Si	16.077065	0.544238	9.426718
Si	15.561499	0.988383	6.481655
Si	12.468499	1.191751	6.557269
Si	11.360883	0.444544	9.329557
Si	13.620366	1.339402	11.178018
Si	18.456478	16.551989	11.114716
Si	16.162359	17.265965	9.155444
Si	15.420544	16.592781	6.232731
Si	12.394818	16.438963	6.307542
Si	11.502838	17.194925	9.244174
Si	13.860430	16.429609	11.035622
Si	8.536779	9.134238	8.649700
Si	6.095898	9.356510	10.646846
Si	5.311036	8.900624	0.368568
Si	2.236858	8.694470	0.264850
Si	1.468413	9.567439	10.788839
Si	3.609366	8.751580	8.704705
Si	8.370398	13.313625	8.985748
Si	6.013808	12.532391	10.996142
Si	5.381913	13.354617	0.470145
Si	2.361795	13.432621	0.256954
Si	1.369104	12.643427	10.812126
Si	3.717685	13.334917	9.031786
Si	1.516466	11.102448	1.999153
Si	3.912699	10.498513	3.952803
Si	4.471714	11.108617	6.847948
Si	7.647402	11.259451	6.734861
Si	8.646300	10.494534	4.032967
Si	6.375004	11.107622	2.133518
Si	1.671837	6.508963	2.251154
Si	3.959551	7.371584	4.165727
Si	4.465306	6.553537	7.033570
Si	8.741405	7.388897	4.234783
Si	6.407640	6.709146	2.471037
O	7.161469	1.083899	9.789799

O	6.336762	1.323681	12.295364
O	4.011608	0.915951	0.161131
O	1.840622	1.498992	12.065177
O	2.099307	0.995547	9.440637
O	4.519766	1.080317	10.446235
O	7.484624	16.748194	10.195972
O	6.171381	16.743814	12.444450
O	3.897683	17.091251	0.417550
O	1.751725	16.495674	12.335380
O	2.162576	16.585020	9.787256
O	4.831709	16.755554	10.123035
O	6.089891	18.906637	10.885599
O	1.846028	18.899275	11.201169
O	8.589638	2.490957	8.115049
O	8.185794	19.905964	7.524592
O	8.507548	17.315313	7.693084
O	3.753725	2.890330	8.636184
O	4.170783	0.403751	7.867197
O	3.584739	17.401875	7.786230
O	19.845806	0.664030	10.534161
O	19.830589	17.323473	10.710816
O	2.760433	18.817291	3.086521
O	3.753725	18.669441	5.496666
O	6.112115	18.306683	7.193496
O	8.093893	18.403391	5.352932
O	7.917699	18.984243	2.742980
O	5.399533	18.986830	3.443847
O	2.595452	3.322536	3.605246
O	3.593148	2.900080	6.007093
O	6.024419	2.747654	7.270851
O	8.094093	3.402331	5.692192
O	7.985975	3.231399	3.084246
O	5.273995	3.330297	3.997101
O	3.834814	1.080715	4.096537
O	8.339764	0.996542	4.596927
O	1.415355	17.331034	1.424754
O	1.665029	0.004975	0.833226
O	2.176391	2.655323	0.999844
O	6.265484	17.170448	1.687329
O	6.176386	19.648472	0.920081
O	5.920506	2.408774	1.333884
O	10.194401	19.071600	3.771597
O	10.266080	2.734322	4.278143
O	12.836905	10.698498	3.607388

O	13.842811	11.111204	1.238463
O	16.062248	11.032404	13.057526
O	18.106094	11.363523	1.406152
O	17.952124	11.015489	4.014499
O	15.426750	11.343425	3.262508
O	12.852722	6.880875	3.325542
O	14.006189	6.962660	1.009614
O	16.369987	7.284427	13.289587
O	18.685129	6.473543	1.417260
O	18.040821	6.901371	4.005131
O	15.517651	6.550751	3.164143
O	14.522157	8.930472	2.682622
O	18.523352	8.954152	2.351527
O	11.593739	12.451202	5.186716
O	11.672626	9.868312	5.856267
O	12.262273	7.228710	5.862825
O	16.439062	12.852365	5.110700
O	16.093884	10.285993	5.688177
O	15.942718	7.626292	5.531595
O	0.247872	10.947037	3.005153
O	0.498948	7.289402	3.097362
O	17.265171	8.783618	10.368880
O	16.420042	8.873362	7.867599
O	14.025611	9.039718	6.696184
O	11.845416	8.447325	8.101533
O	12.186391	8.636365	10.696898
O	14.671521	9.193537	9.875584
O	17.271976	13.512218	10.047555
O	16.188988	13.094537	7.705128
O	13.990973	12.766005	6.191779
O	11.848820	13.346260	7.702184
O	12.188191	13.363173	10.550622
O	14.670719	13.018523	9.867019
O	16.445068	11.088519	9.449470
O	12.022010	10.866049	9.207772
O	18.875740	7.452374	11.982470
O	18.358971	9.952883	12.554860
O	18.097685	12.614772	12.465997
O	14.258266	7.295172	11.705040
O	13.845013	9.785931	12.379810
O	13.926302	12.436676	12.384360
O	9.855629	9.370240	9.611403
O	9.738300	12.683025	9.540071
O	12.844514	18.737495	3.680325

O	13.679030	18.656307	1.166061
O	15.987767	19.064835	13.298821
O	18.112501	18.391253	1.342315
O	17.929300	18.899672	3.946112
O	15.441167	18.821867	3.107265
O	12.595840	3.158170	3.186358
O	13.776537	2.989029	0.867352
O	16.175573	2.823469	12.960767
O	18.186583	3.409495	1.182254
O	17.948921	3.133297	3.839583
O	15.275584	3.314576	3.013450
O	13.935913	1.009476	2.664288
O	18.186983	0.993358	2.185444
O	11.420548	17.334219	5.362836
O	11.601147	0.075815	5.762452
O	12.423651	2.656715	5.841948
O	16.259865	17.087870	4.933375
O	16.099890	19.571264	5.686169
O	15.775934	2.335944	5.677738
O	0.176394	19.229597	2.846029
O	0.227650	2.654925	2.765999
O	17.266771	1.079720	10.374769
O	16.349564	1.067382	7.922067
O	13.983564	0.668805	6.778490
O	11.758719	1.339601	8.027793
O	12.097692	1.088674	10.636139
O	14.663111	1.155535	9.951599
O	17.522854	16.659046	9.789665
O	16.258863	17.014641	7.563938
O	13.881652	17.156321	6.281847
O	11.847818	16.423441	7.855687
O	12.349770	16.502041	10.460554
O	14.866535	16.488909	9.770661
O	15.944118	18.824852	9.537930
O	11.841210	18.796993	9.116901
O	18.687733	2.481206	12.121385
O	18.365980	19.816420	12.546429
O	17.686434	17.238903	12.378205
O	13.769129	2.887743	11.700757
O	13.844412	0.337288	12.440436
O	14.102695	17.577583	12.138247
O	9.755319	0.587617	9.615552
O	10.000588	16.909575	9.775345
O	7.246562	9.625545	9.460443

O	5.257977	8.628007	12.127274
O	3.740109	9.044095	0.752660
O	1.918708	8.621441	12.042024
O	2.188605	9.118518	9.433678
O	4.843522	8.877143	9.710437
O	7.196307	13.179705	10.108983
O	6.248065	13.113441	12.502398
O	3.857639	12.773765	0.247318
O	1.753927	13.528534	12.122724
O	2.157170	13.096128	9.456829
O	4.593447	13.099710	10.378116
O	5.918704	10.932312	11.125957
O	1.752325	11.107423	11.206924
O	8.510151	7.550278	8.199898
O	8.597446	10.037852	7.284903
O	7.847222	12.609797	7.605291
O	3.501447	7.217766	8.187318
O	3.750120	9.784537	7.445231
O	4.170983	12.428319	7.773650
O	19.883646	9.362281	10.457075
O	19.797152	12.772372	10.456941
O	2.900587	11.122148	2.842148
O	3.842222	11.354967	5.349720
O	6.074275	10.854307	6.773003
O	8.095695	11.522716	5.182968
O	7.926909	10.857491	2.592689
O	5.426563	10.606565	3.352843
O	3.069373	6.559109	3.068722
O	3.669432	6.715117	5.610689
O	5.926712	7.214581	7.023800
O	8.339563	6.539011	5.521424
O	7.989178	6.962660	2.839471
O	5.525471	7.207617	3.768653
O	3.507054	8.945396	4.185400
O	8.351776	8.968878	4.504986
O	1.399938	12.505328	1.175027
O	1.331863	9.873486	0.923159
O	1.826207	7.207020	0.767783
O	6.096699	12.669495	1.765218
O	6.093295	10.280023	0.750652
O	5.930917	7.699918	1.249972
O	10.245057	10.696906	3.757143
O	10.352574	7.211795	3.932060
O	8.588237	14.896988	8.623470

O	3.834213	14.897387	8.525105
O	5.338866	14.924250	0.834162
O	2.410849	14.918878	0.919814
O	1.321852	4.953458	1.929962
O	6.171782	5.202793	1.988179
O	4.591044	4.976342	7.365067
O	7.591742	4.906497	7.777665
O	11.668621	4.976939	4.846252
O	16.511543	5.055739	5.107221
O	14.767226	5.057729	12.794951
O	17.845808	4.948881	12.467603
O	18.772627	15.011408	11.544176
O	14.015800	14.937184	11.714006
O	15.349866	15.001260	6.108135
O	12.431859	14.929423	5.692995
O	10.095893	3.569880	14.888321
O	8.923605	2.488967	11.792832
O	10.854326	3.814837	9.280308
O	9.679035	1.163296	13.807376
O	9.844216	8.703226	14.216227
O	11.182487	4.149339	12.292018
O	12.431059	5.547244	10.533626
O	11.681636	6.876697	13.050165
Al	4.513359	18.864849	7.023533
Al	6.306730	3.551971	2.594696
Al	17.889856	6.466379	13.283431
Al	11.372295	12.448814	9.074076
Al	16.175173	3.486902	4.472331
Al	7.538083	6.571247	7.047622
H	10.176382	6.202120	9.486138
H	19.775127	7.107923	11.805279
H	11.600947	14.066205	10.898046
H	9.288406	3.611470	2.081458
H	18.607044	3.595948	4.396583
H	2.952644	17.100006	7.100217
H	9.875852	4.181576	14.150783
H	9.881658	1.982338	14.362636
H	6.396828	3.654849	12.465060
H	9.508648	2.168991	11.080723
H	9.922703	4.112328	9.261036
H	10.979665	3.284728	8.472109
H	9.122423	1.893390	12.620571
H	9.073369	0.601746	14.323423
H	9.674230	8.981812	12.404703

H	10.651302	9.236121	14.096046
H	11.768129	4.604032	11.591686
H	11.346868	3.191800	12.207438
H	11.972755	5.022110	9.816966
H	13.387109	5.389843	10.449580
H	12.043033	6.584380	12.182813
H	11.955336	6.209284	13.707807
Pt	7.186096	4.941916	-3.476100
Pt	9.536879	7.101954	-0.757344
Pt	8.942025	6.804861	-3.180738
Pt	6.641297	5.179511	-1.057257
Pt	7.242558	7.821103	-1.293735
Pt	9.103803	4.613782	-1.361051

330

#### Pt6H2@H-MFI-10W\_IS

Si	8.431664	1.061214	8.759843
Si	6.042439	0.616471	10.834208
Si	5.599152	1.196925	0.378471
Si	2.440281	1.279307	0.180001
Si	1.413954	0.538865	10.820825
Si	3.661423	1.329253	9.039949
Si	8.610661	16.459856	9.055340
Si	6.159167	17.295017	10.915577
Si	5.418353	16.493286	0.471483
Si	2.381617	16.469805	0.442843
Si	1.396134	17.352526	11.017823
Si	3.628387	16.368519	9.143801
Si	1.533685	18.834602	2.050543
Si	3.912699	19.380831	4.073652
Si	7.695255	18.513830	6.936944
Si	8.626078	19.371876	4.155020
Si	6.386217	18.706255	2.221578
Si	1.627789	3.410092	2.327705
Si	3.904089	2.697906	4.385342
Si	4.538386	3.406510	7.272992
Si	7.573321	3.471978	7.219594
Si	8.644898	2.615922	4.382264
Si	11.593739	10.936491	4.620080
Si	14.166766	10.500902	2.723441
Si	14.473102	11.089712	13.121095
Si	17.679426	11.237363	13.244084
Si	18.727777	10.532540	2.684897
Si	16.461687	11.345613	4.517967
Si	11.768531	6.581396	4.497759

Si	14.255864	7.363426	2.577164
Si	14.880350	6.665170	13.092857
Si	18.927797	7.398846	2.709924
Si	16.535168	6.529857	4.447171
Si	18.562395	8.960320	11.311713
Si	16.188988	9.486252	9.351907
Si	15.619362	8.920523	6.420628
Si	12.450480	8.657061	6.623381
Si	11.483417	9.403471	9.399149
Si	13.756716	8.743222	11.146566
Si	18.492517	13.460878	11.129169
Si	16.147743	12.667106	9.245378
Si	15.452378	13.412921	6.281044
Si	12.419847	13.374317	6.221221
Si	13.790954	13.439983	11.144827
Si	11.536877	18.794008	4.644838
Si	13.957736	19.298647	2.650369
Si	14.398821	18.857088	13.102359
Si	17.537870	18.613724	13.226018
Si	18.613653	19.346006	2.558696
Si	16.401020	18.623075	4.415319
Si	11.729688	3.392978	4.556109
Si	13.939716	2.626668	2.471706
Si	14.653300	3.455262	12.982180
Si	17.702650	3.444119	12.992484
Si	18.683329	2.514438	2.407468
Si	18.520950	1.040519	11.383714
Si	16.054640	0.550406	9.433142
Si	15.558695	0.989776	6.486205
Si	12.465697	1.195333	6.574265
Si	11.376101	0.475586	9.350167
Si	13.608552	1.341193	11.195817
Si	18.454077	16.548407	11.113645
Si	16.160757	17.268551	9.154240
Si	15.417140	16.589001	6.233132
Si	12.391816	16.438963	6.310486
Si	11.507243	17.212437	9.245512
Si	13.859828	16.430206	11.034685
Si	8.586034	9.170653	8.636184
Si	6.119925	9.340392	10.570027
Si	5.335863	8.918931	0.374456
Si	2.241262	8.693873	0.250664
Si	1.465410	9.557092	10.770505
Si	3.592347	8.754765	8.696407

Si	8.375603	13.325167	8.992171
Si	6.047245	12.523635	11.002700
Si	5.386118	13.329345	0.489952
Si	2.362195	13.429238	0.259229
Si	1.380717	12.637856	10.812261
Si	3.741311	13.340091	9.041689
Si	1.519269	11.098269	1.999286
Si	3.911698	10.489161	3.958156
Si	4.481724	11.109612	6.849554
Si	7.650806	11.309795	6.748779
Si	8.647302	10.489559	4.038321
Si	6.379810	11.115382	2.156670
Si	1.667632	6.510157	2.232954
Si	3.964556	7.349298	4.138157
Si	4.481524	6.581196	7.025808
Si	8.718780	7.368998	4.251244
Si	6.438074	6.716709	2.399304
O	7.246762	1.086286	9.864877
O	6.348776	1.324080	12.283319
O	4.011007	0.916150	0.157250
O	1.842424	1.498594	12.061696
O	2.111921	0.996940	9.441707
O	4.574026	1.087679	10.381461
O	7.491031	16.750181	10.195839
O	6.173783	16.749586	12.438026
O	3.895280	17.093241	0.417683
O	1.752325	16.495476	12.331097
O	2.162376	16.586016	9.786185
O	4.830107	16.756948	10.121563
O	6.090492	18.901663	10.886401
O	1.845828	18.899872	11.200233
O	8.590439	2.574533	8.182901
O	8.182190	19.971235	7.516830
O	8.511352	17.329842	7.694556
O	3.756928	2.898289	8.616778
O	4.172184	0.397184	7.856491
O	3.587942	17.404461	7.785694
O	19.845205	0.665224	10.533224
O	19.827986	17.323671	10.711084
O	2.753025	18.819281	3.088261
O	3.753324	18.671829	5.502019
O	6.140747	18.317429	7.197378
O	8.097697	18.410954	5.356278
O	7.902283	18.977278	2.751143

O	5.359488	18.984045	3.429929
O	2.593850	3.322735	3.605916
O	3.672035	2.904259	5.990365
O	6.074275	2.811728	7.277676
O	8.094093	3.401734	5.687775
O	8.011803	3.227618	3.021212
O	5.263584	3.397356	3.920550
O	3.839819	1.093251	4.093592
O	8.337562	1.008879	4.585953
O	1.415355	17.330637	1.423550
O	1.665830	0.004577	0.833092
O	2.177593	2.654925	1.000647
O	6.261680	17.170250	1.680102
O	6.181592	19.662203	0.922223
O	5.921306	2.474441	1.252381
O	10.192199	19.071798	3.766378
O	10.268884	2.741087	4.343319
O	12.850720	10.768146	3.606183
O	13.847615	11.108617	1.233645
O	16.082672	11.029419	13.052441
O	18.108696	11.364319	1.410702
O	17.953327	11.016484	4.016774
O	15.431755	11.356160	3.262106
O	12.926804	7.032704	3.432070
O	13.937914	6.970222	1.013628
O	16.347963	7.281044	13.299356
O	18.684330	6.474139	1.419803
O	18.083469	6.891621	4.018513
O	15.584723	6.556124	3.093347
O	14.660308	8.952361	2.678741
O	18.523754	8.953953	2.353267
O	11.530670	12.458764	5.193943
O	11.677431	9.868711	5.852654
O	12.254866	7.212790	5.928401
O	16.434258	12.852764	5.115920
O	16.094284	10.285793	5.687508
O	15.944719	7.622312	5.520220
O	0.249674	10.946241	3.005286
O	0.506156	7.289203	3.094551
O	17.267374	8.786801	10.370621
O	16.421242	8.871770	7.864788
O	14.028614	9.040315	6.696854
O	11.845416	8.457672	8.114782
O	12.193798	8.636365	10.693018

O	14.676326	9.194134	9.874781
O	17.274179	13.510824	10.047823
O	16.183582	13.094537	7.701783
O	13.959538	12.766005	6.187764
O	11.846016	13.348051	7.704192
O	12.188592	13.364964	10.551693
O	14.672722	13.018921	9.867955
O	16.445671	11.089911	9.449335
O	12.097492	10.875002	9.211519
O	18.856920	7.403025	11.968952
O	18.359173	9.874481	12.623650
O	18.103092	12.600047	12.462518
O	14.255664	7.299948	11.707582
O	13.847415	9.791303	12.383558
O	13.928905	12.435680	12.384093
O	9.870445	9.458194	9.615150
O	9.747710	12.683025	9.528028
O	12.841310	18.737495	3.678719
O	13.678430	18.656109	1.168336
O	15.990970	19.064238	13.299891
O	18.113302	18.391054	1.342315
O	17.929100	18.899473	3.947316
O	15.442968	18.821470	3.109272
O	12.587430	3.159563	3.193050
O	13.775937	2.992810	0.887025
O	16.170568	2.824862	12.961971
O	18.186382	3.409097	1.181050
O	17.948921	3.135088	3.840118
O	15.276786	3.314377	3.018000
O	13.934310	1.007884	2.666697
O	18.186583	0.993955	2.185578
O	11.418746	17.335611	5.362167
O	11.600947	0.079198	5.762720
O	12.433062	2.654328	5.847702
O	16.258863	17.087072	4.934446
O	16.100090	19.572855	5.687508
O	15.777135	2.335347	5.678541
O	0.173991	19.230394	2.845627
O	0.226849	2.654129	2.765463
O	17.258963	1.080118	10.375037
O	16.345760	1.069173	7.929160
O	13.983765	0.667014	6.777285
O	11.762324	1.332039	8.032878
O	12.086081	1.073551	10.695560

O	14.624069	1.148371	9.946648
O	17.521852	16.659641	9.788996
O	16.257263	17.015238	7.562734
O	13.878449	17.156122	6.280776
O	11.847017	16.427422	7.858364
O	12.349969	16.502838	10.459885
O	14.867135	16.489107	9.771062
O	15.942718	18.826843	9.538867
O	11.841411	18.811918	9.121050
O	18.686533	2.481007	12.120448
O	18.367182	19.816420	12.545627
O	17.687035	17.237707	12.378071
O	13.764924	2.892121	11.709188
O	13.848817	0.337885	12.453953
O	14.103095	17.577583	12.139452
O	9.759323	0.586424	9.619165
O	10.005593	16.913355	9.777888
O	7.239555	9.634499	9.375194
O	5.434371	8.693475	12.153772
O	3.754325	9.037529	0.742623
O	1.926517	8.625818	12.030515
O	2.153566	9.124089	9.384695
O	4.755024	8.887093	9.780699
O	7.271790	13.184680	10.185400
O	6.256875	13.023498	12.543753
O	3.856037	12.770382	0.252002
O	1.755529	13.526147	12.124463
O	2.173989	13.095929	9.461782
O	4.663925	13.176322	10.372227
O	5.922708	10.926540	11.041912
O	1.751925	11.099861	11.203043
O	8.591440	7.613756	8.120270
O	8.678535	10.186696	7.346598
O	7.767735	12.686408	7.608369
O	3.499645	7.220353	8.180894
O	3.754325	9.786726	7.442554
O	4.172585	12.428518	7.777531
O	19.868031	9.362679	10.461759
O	19.810368	12.774960	10.456139
O	2.903390	11.118169	2.843754
O	3.842622	11.352380	5.351193
O	6.083885	10.856098	6.772601
O	8.094294	11.524704	5.184440
O	7.927310	10.859680	2.600049

O	5.425361	10.598606	3.360739
O	3.080985	6.556720	3.018402
O	3.677040	6.715913	5.597841
O	5.922708	7.288606	7.027146
O	8.191801	6.474737	5.455179
O	8.006197	6.880676	2.840274
O	5.516861	7.130409	3.690496
O	3.516864	8.928881	4.181385
O	8.346371	8.957734	4.505387
O	1.398737	12.503338	1.176767
O	1.336468	9.870899	0.921687
O	1.827608	7.209806	0.758816
O	6.085887	12.684420	1.823166
O	6.102505	10.299126	0.762697
O	6.017011	7.711260	1.181987
O	10.243256	10.692927	3.757277
O	10.345367	7.213984	4.013829
O	8.591240	14.909923	8.623604
O	3.833012	14.901765	8.520823
O	5.339867	14.917882	0.762296
O	2.410849	14.918480	0.919814
O	1.316647	4.950871	1.927821
O	6.179590	5.203987	1.834542
O	4.593647	5.003404	7.367342
O	7.588138	4.980521	7.780609
O	11.678832	4.988082	4.845181
O	16.511141	5.062902	5.101466
O	14.767426	5.059918	12.798565
O	17.846409	4.949479	12.467336
O	18.772026	15.008621	11.544310
O	14.015800	14.937782	11.714140
O	15.347463	14.998274	6.108403
O	12.428455	14.931414	5.692325
O	11.002089	5.395614	15.225573
O	10.177382	2.731337	14.638193
O	9.007697	2.238837	11.967748
O	10.767230	3.485310	9.703612
O	5.050750	-16.570494	13.290390
O	9.251164	8.536671	14.135794
O	11.090185	4.055217	12.626059
O	12.416842	5.549234	10.615797
O	11.340861	6.796901	13.045347
O	11.754716	9.038524	14.633106
Al	4.533381	18.857288	7.022194

Al	6.334560	3.563314	2.552807
Al	17.868834	6.462797	13.300294
Al	11.383508	12.436875	9.071801
Al	16.175173	3.490683	4.478354
Al	7.535079	6.609453	7.055250
H	10.439671	7.067926	9.917473
H	19.414131	6.812223	11.424800
H	11.615562	14.097447	10.861376
H	9.325646	2.975697	1.690005
H	18.603239	3.617638	4.384806
H	2.950842	17.110353	7.101154
H	10.058251	5.600772	15.375194
H	11.050542	4.418573	15.164947
H	8.256672	4.742728	13.043875
H	10.055048	1.776782	14.369729
H	8.051046	2.010794	12.040819
H	9.381108	1.703553	11.235163
H	10.247259	3.619230	8.891532
H	11.450981	4.190531	9.737204
H	4.077880	-16.590792	13.248100
H	5.299823	-16.133512	12.454488
H	8.664520	9.298205	13.983362
H	10.181187	8.880326	14.358754
H	11.690044	3.540828	12.051793
H	10.763627	3.447900	13.381930
H	12.044434	6.304600	10.119020
H	13.373895	5.722156	10.667857
H	11.716073	6.282512	12.283854
H	11.318837	6.148194	13.833606
H	12.083676	9.867914	14.245803
H	12.017605	8.335293	13.997012
Pt	6.974463	4.821130	-2.989628
Pt	9.251765	7.052803	-0.834430
Pt	9.011301	6.453246	-3.362479
Pt	6.627482	5.020518	-0.419691
Pt	6.917601	7.310097	-1.892490
Pt	9.182489	4.395888	-1.773381

330

#### Pt6H2@H-MFI-10W\_FS

Si	8.431664	1.061214	8.759843
Si	6.042439	0.616471	10.834208
Si	5.599152	1.196925	0.378471
Si	2.440281	1.279307	0.180001
Si	1.413954	0.538865	10.820825

Si	3.661423	1.329253	9.039949
Si	8.610661	16.459856	9.055340
Si	6.159167	17.295017	10.915577
Si	5.418353	16.493286	0.471483
Si	2.381617	16.469805	0.442843
Si	1.396134	17.352526	11.017823
Si	3.628387	16.368519	9.143801
Si	1.533685	18.834602	2.050543
Si	3.912699	19.380831	4.073652
Si	7.695255	18.513830	6.936944
Si	8.626078	19.371876	4.155020
Si	6.386217	18.706255	2.221578
Si	1.627789	3.410092	2.327705
Si	3.904089	2.697906	4.385342
Si	4.538386	3.406510	7.272992
Si	7.573321	3.471978	7.219594
Si	8.644898	2.615922	4.382264
Si	11.593739	10.936491	4.620080
Si	14.166766	10.500902	2.723441
Si	14.473102	11.089712	13.121095
Si	17.679426	11.237363	13.244084
Si	18.727777	10.532540	2.684897
Si	16.461687	11.345613	4.517967
Si	11.768531	6.581396	4.497759
Si	14.255864	7.363426	2.577164
Si	14.880350	6.665170	13.092857
Si	18.927797	7.398846	2.709924
Si	16.535168	6.529857	4.447171
Si	18.562395	8.960320	11.311713
Si	16.188988	9.486252	9.351907
Si	15.619362	8.920523	6.420628
Si	12.450480	8.657061	6.623381
Si	11.483417	9.403471	9.399149
Si	13.756716	8.743222	11.146566
Si	18.492517	13.460878	11.129169
Si	16.147743	12.667106	9.245378
Si	15.452378	13.412921	6.281044
Si	12.419847	13.374317	6.221221
Si	13.790954	13.439983	11.144827
Si	11.536877	18.794008	4.644838
Si	13.957736	19.298647	2.650369
Si	14.398821	18.857088	13.102359
Si	17.537870	18.613724	13.226018
Si	18.613653	19.346006	2.558696

Si	16.401020	18.623075	4.415319
Si	11.729688	3.392978	4.556109
Si	13.939716	2.626668	2.471706
Si	14.653300	3.455262	12.982180
Si	17.702650	3.444119	12.992484
Si	18.683329	2.514438	2.407468
Si	18.520950	1.040519	11.383714
Si	16.054640	0.550406	9.433142
Si	15.558695	0.989776	6.486205
Si	12.465697	1.195333	6.574265
Si	11.376101	0.475586	9.350167
Si	13.608552	1.341193	11.195817
Si	18.454077	16.548407	11.113645
Si	16.160757	17.268551	9.154240
Si	15.417140	16.589001	6.233132
Si	12.391816	16.438963	6.310486
Si	11.507243	17.212437	9.245512
Si	13.859828	16.430206	11.034685
Si	8.586034	9.170653	8.636184
Si	6.119925	9.340392	10.570027
Si	5.335863	8.918931	0.374456
Si	2.241262	8.693873	0.250664
Si	1.465410	9.557092	10.770505
Si	3.592347	8.754765	8.696407
Si	8.375603	13.325167	8.992171
Si	6.047245	12.523635	11.002700
Si	5.386118	13.329345	0.489952
Si	2.362195	13.429238	0.259229
Si	1.380717	12.637856	10.812261
Si	3.741311	13.340091	9.041689
Si	1.519269	11.098269	1.999286
Si	3.911698	10.489161	3.958156
Si	4.481724	11.109612	6.849554
Si	7.650806	11.309795	6.748779
Si	8.647302	10.489559	4.038321
Si	6.379810	11.115382	2.156670
Si	1.667632	6.510157	2.232954
Si	3.964556	7.349298	4.138157
Si	4.481524	6.581196	7.025808
Si	8.718780	7.368998	4.251244
Si	6.438074	6.716709	2.399304
O	7.246762	1.086286	9.864877
O	6.348776	1.324080	12.283319
O	4.011007	0.916150	0.157250

O	1.842424	1.498594	12.061696
O	2.111921	0.996940	9.441707
O	4.574026	1.087679	10.381461
O	7.491031	16.750181	10.195839
O	6.173783	16.749586	12.438026
O	3.895280	17.093241	0.417683
O	1.752325	16.495476	12.331097
O	2.162376	16.586016	9.786185
O	4.830107	16.756948	10.121563
O	6.090492	18.901663	10.886401
O	1.845828	18.899872	11.200233
O	8.590439	2.574533	8.182901
O	8.182190	19.971235	7.516830
O	8.511352	17.329842	7.694556
O	3.756928	2.898289	8.616778
O	4.172184	0.397184	7.856491
O	3.587942	17.404461	7.785694
O	19.845205	0.665224	10.533224
O	19.827986	17.323671	10.711084
O	2.753025	18.819281	3.088261
O	3.753324	18.671829	5.502019
O	6.140747	18.317429	7.197378
O	8.097697	18.410954	5.356278
O	7.902283	18.977278	2.751143
O	5.359488	18.984045	3.429929
O	2.593850	3.322735	3.605916
O	3.672035	2.904259	5.990365
O	6.074275	2.811728	7.277676
O	8.094093	3.401734	5.687775
O	8.011803	3.227618	3.021212
O	5.263584	3.397356	3.920550
O	3.839819	1.093251	4.093592
O	8.337562	1.008879	4.585953
O	1.415355	17.330637	1.423550
O	1.665830	0.004577	0.833092
O	2.177593	2.654925	1.000647
O	6.261680	17.170250	1.680102
O	6.181592	19.662203	0.922223
O	5.921306	2.474441	1.252381
O	10.192199	19.071798	3.766378
O	10.268884	2.741087	4.343319
O	12.850720	10.768146	3.606183
O	13.847615	11.108617	1.233645
O	16.082672	11.029419	13.052441

O	18.108696	11.364319	1.410702
O	17.953327	11.016484	4.016774
O	15.431755	11.356160	3.262106
O	12.926804	7.032704	3.432070
O	13.937914	6.970222	1.013628
O	16.347963	7.281044	13.299356
O	18.684330	6.474139	1.419803
O	18.083469	6.891621	4.018513
O	15.584723	6.556124	3.093347
O	14.660308	8.952361	2.678741
O	18.523754	8.953953	2.353267
O	11.530670	12.458764	5.193943
O	11.677431	9.868711	5.852654
O	12.254866	7.212790	5.928401
O	16.434258	12.852764	5.115920
O	16.094284	10.285793	5.687508
O	15.944719	7.622312	5.520220
O	0.249674	10.946241	3.005286
O	0.506156	7.289203	3.094551
O	17.267374	8.786801	10.370621
O	16.421242	8.871770	7.864788
O	14.028614	9.040315	6.696854
O	11.845416	8.457672	8.114782
O	12.193798	8.636365	10.693018
O	14.676326	9.194134	9.874781
O	17.274179	13.510824	10.047823
O	16.183582	13.094537	7.701783
O	13.959538	12.766005	6.187764
O	11.846016	13.348051	7.704192
O	12.188592	13.364964	10.551693
O	14.672722	13.018921	9.867955
O	16.445671	11.089911	9.449335
O	12.097492	10.875002	9.211519
O	18.856920	7.403025	11.968952
O	18.359173	9.874481	12.623650
O	18.103092	12.600047	12.462518
O	14.255664	7.299948	11.707582
O	13.847415	9.791303	12.383558
O	13.928905	12.435680	12.384093
O	9.870445	9.458194	9.615150
O	9.747710	12.683025	9.528028
O	12.841310	18.737495	3.678719
O	13.678430	18.656109	1.168336
O	15.990970	19.064238	13.299891

O	18.113302	18.391054	1.342315
O	17.929100	18.899473	3.947316
O	15.442968	18.821470	3.109272
O	12.587430	3.159563	3.193050
O	13.775937	2.992810	0.887025
O	16.170568	2.824862	12.961971
O	18.186382	3.409097	1.181050
O	17.948921	3.135088	3.840118
O	15.276786	3.314377	3.018000
O	13.934310	1.007884	2.666697
O	18.186583	0.993955	2.185578
O	11.418746	17.335611	5.362167
O	11.600947	0.079198	5.762720
O	12.433062	2.654328	5.847702
O	16.258863	17.087072	4.934446
O	16.100090	19.572855	5.687508
O	15.777135	2.335347	5.678541
O	0.173991	19.230394	2.845627
O	0.226849	2.654129	2.765463
O	17.258963	1.080118	10.375037
O	16.345760	1.069173	7.929160
O	13.983765	0.667014	6.777285
O	11.762324	1.332039	8.032878
O	12.086081	1.073551	10.695560
O	14.624069	1.148371	9.946648
O	17.521852	16.659641	9.788996
O	16.257263	17.015238	7.562734
O	13.878449	17.156122	6.280776
O	11.847017	16.427422	7.858364
O	12.349969	16.502838	10.459885
O	14.867135	16.489107	9.771062
O	15.942718	18.826843	9.538867
O	11.841411	18.811918	9.121050
O	18.686533	2.481007	12.120448
O	18.367182	19.816420	12.545627
O	17.687035	17.237707	12.378071
O	13.764924	2.892121	11.709188
O	13.848817	0.337885	12.453953
O	14.103095	17.577583	12.139452
O	9.759323	0.586424	9.619165
O	10.005593	16.913355	9.777888
O	7.239555	9.634499	9.375194
O	5.434371	8.693475	12.153772
O	3.754325	9.037529	0.742623

O	1.926517	8.625818	12.030515
O	2.153566	9.124089	9.384695
O	4.755024	8.887093	9.780699
O	7.271790	13.184680	10.185400
O	6.256875	13.023498	12.543753
O	3.856037	12.770382	0.252002
O	1.755529	13.526147	12.124463
O	2.173989	13.095929	9.461782
O	4.663925	13.176322	10.372227
O	5.922708	10.926540	11.041912
O	1.751925	11.099861	11.203043
O	8.591440	7.613756	8.120270
O	8.678535	10.186696	7.346598
O	7.767735	12.686408	7.608369
O	3.499645	7.220353	8.180894
O	3.754325	9.786726	7.442554
O	4.172585	12.428518	7.777531
O	19.868031	9.362679	10.461759
O	19.810368	12.774960	10.456139
O	2.903390	11.118169	2.843754
O	3.842622	11.352380	5.351193
O	6.083885	10.856098	6.772601
O	8.094294	11.524704	5.184440
O	7.927310	10.859680	2.600049
O	5.425361	10.598606	3.360739
O	3.080985	6.556720	3.018402
O	3.677040	6.715913	5.597841
O	5.922708	7.288606	7.027146
O	8.191801	6.474737	5.455179
O	8.006197	6.880676	2.840274
O	5.516861	7.130409	3.690496
O	3.516864	8.928881	4.181385
O	8.346371	8.957734	4.505387
O	1.398737	12.503338	1.176767
O	1.336468	9.870899	0.921687
O	1.827608	7.209806	0.758816
O	6.085887	12.684420	1.823166
O	6.102505	10.299126	0.762697
O	6.017011	7.711260	1.181987
O	10.243256	10.692927	3.757277
O	10.345367	7.213984	4.013829
O	8.591240	14.909923	8.623604
O	3.833012	14.901765	8.520823
O	5.339867	14.917882	0.762296

O	2.410849	14.918480	0.919814
O	1.316647	4.950871	1.927821
O	6.179590	5.203987	1.834542
O	4.593647	5.003404	7.367342
O	7.588138	4.980521	7.780609
O	11.678832	4.988082	4.845181
O	16.511141	5.062902	5.101466
O	14.767426	5.059918	12.798565
O	17.846409	4.949479	12.467336
O	18.772026	15.008621	11.544310
O	14.015800	14.937782	11.714140
O	15.347463	14.998274	6.108403
O	12.428455	14.931414	5.692325
O	11.002089	5.395614	15.225573
O	10.177382	2.731337	14.638193
O	9.007697	2.238837	11.967748
O	10.767230	3.485310	9.703612
O	5.910094	-16.843708	12.095422
O	9.251164	8.536671	14.135794
O	11.090185	4.055217	12.626059
O	12.416842	5.549234	10.615797
O	11.340861	6.796901	13.045347
O	11.754716	9.038524	14.633106
Al	4.533381	18.857288	7.022194
Al	6.334560	3.563314	2.552807
Al	17.868834	6.462797	13.300294
Al	11.383508	12.436875	9.071801
Al	16.175173	3.490683	4.478354
Al	7.535079	6.609453	7.055250
H	10.439671	7.067926	9.917473
H	19.414131	6.812223	11.424800
H	11.615562	14.097447	10.861376
H	9.325646	2.975697	1.690005
H	18.603239	3.617638	4.384806
H	2.950842	17.110353	7.101154
H	10.058251	5.600772	15.375194
H	11.050542	4.418573	15.164947
H	8.256672	4.742728	13.043875
H	10.055048	1.776782	14.369729
H	8.051046	2.010794	12.040819
H	9.381108	1.703553	11.235163
H	10.247259	3.619230	8.891532
H	11.450981	4.190531	9.737204
H	4.943832	-16.935640	12.016194

H	6.132538	-17.455603	12.821851
H	9.475411	7.981290	12.139987
H	10.181187	8.880326	14.358754
H	11.690044	3.540828	12.051793
H	10.763627	3.447900	13.381930
H	12.044434	6.304600	10.119020
H	13.373895	5.722156	10.667857
H	11.716073	6.282512	12.283854
H	11.318837	6.148194	13.833606
H	12.083676	9.867914	14.245803
H	12.017605	8.335293	13.997012
Pt	6.974463	4.821130	-2.989628
Pt	9.251765	7.052803	-0.834430
Pt	9.011301	6.453246	-3.362479
Pt	6.627482	5.020518	-0.419691
Pt	6.917601	7.310097	-1.892490
Pt	9.182489	4.395888	-1.773381

303

#### Pt6@H-MFI-1W

Si	8.454890	1.043106	8.771486
Si	6.072672	0.542646	10.824438
Si	5.590943	1.209660	0.383021
Si	2.370204	1.372633	0.225771
Si	1.406145	0.529114	10.841434
Si	3.619777	1.182797	9.001808
Si	8.503343	16.636162	9.047310
Si	6.137343	17.204676	10.972186
Si	5.491434	16.459061	0.585774
Si	1.447390	17.336208	10.879710
Si	3.742312	16.384836	9.048648
Si	1.510860	18.834801	2.073161
Si	3.942732	19.277754	4.064685
Si	4.391625	18.713020	6.982179
Si	7.553500	18.567558	6.862803
Si	8.626078	19.365509	4.187274
Si	6.415449	18.698891	2.311378
Si	1.449593	3.500035	2.316731
Si	4.521968	3.479539	7.358911
Si	7.592542	3.471978	7.216783
Si	8.605455	2.564583	4.421342
Si	6.530375	3.502821	2.400375
Si	11.558099	10.939277	4.642697
Si	14.036223	10.648354	2.660273
Si	14.446474	11.158961	13.101289

Si	17.674019	11.333874	13.230032
Si	18.739590	10.504682	2.639529
Si	11.685840	6.591544	4.456138
Si	14.070460	7.438445	2.506234
Si	14.768228	6.726260	12.996901
Si	17.756710	6.583982	13.194568
Si	18.769224	7.405413	2.592689
Si	16.419641	6.498815	4.397654
Si	18.518747	8.884108	11.413290
Si	16.216618	9.502568	9.394331
Si	15.653600	8.750983	6.503469
Si	12.471904	8.612088	6.627262
Si	11.438168	9.447051	9.330359
Si	13.737694	8.866596	11.141080
Si	18.550383	13.512417	11.200099
Si	16.215015	12.671086	9.316308
Si	15.462990	13.450530	6.406710
Si	12.439668	13.344866	6.279036
Si	11.443173	12.481848	9.139920
Si	13.676628	13.394017	11.005778
Si	11.523862	18.829031	4.719515
Si	13.987968	19.414660	2.811902
Si	17.642586	18.644766	13.277275
Si	18.722971	19.386202	2.578101
Si	16.456682	18.674019	4.441952
Si	11.663416	3.412877	4.489729
Si	13.864033	2.696115	2.482279
Si	17.766321	3.526501	13.066224
Si	18.568401	2.542296	2.531394
Si	16.238441	3.455461	4.374501
Si	18.509939	1.114145	11.370867
Si	16.082672	0.621446	9.349632
Si	15.598539	1.118722	6.431602
Si	12.505341	1.276919	6.561819
Si	11.423553	0.560555	9.286865
Si	13.635782	1.430937	11.061451
Si	18.520149	16.592781	11.086076
Si	16.121714	17.286263	9.191980
Si	15.405127	16.570694	6.250530
Si	12.384007	16.451101	6.330561
Si	11.473207	17.370434	9.207103
Si	13.703056	16.434982	11.041912
Si	8.493933	9.088669	8.619590
Si	5.985978	9.723448	10.463901

Si	5.666626	8.625620	0.223630
Si	2.461304	8.569902	0.083644
Si	1.413954	9.411829	10.748289
Si	3.563516	9.026385	8.678742
Si	6.153762	12.774960	10.930431
Si	5.407341	13.333723	0.491290
Si	2.396833	13.327354	0.309281
Si	1.393331	12.526023	10.875294
Si	3.687451	13.279201	9.017867
Si	1.598757	10.924153	1.895434
Si	4.015011	10.445981	3.901145
Si	4.372604	11.101652	6.771665
Si	7.541687	11.356559	6.739813
Si	8.584232	10.473242	4.065622
Si	6.462701	11.016087	2.052551
Si	1.595153	6.546174	2.278590
Si	3.938928	7.242042	4.316419
Si	4.548398	6.618805	7.251712
Si	7.637992	6.620198	7.056053
Si	8.664120	7.405413	4.280017
Si	6.341768	6.593136	2.585730
Al	2.161175	16.352201	0.415542
Al	3.763135	2.648955	4.333817
Al	16.457281	11.108218	4.441684
Al	14.474103	18.877186	12.959161
Al	14.449476	3.551176	12.872305
Al	8.414246	13.299298	8.926729
O	7.256773	1.083501	9.858052
O	6.262281	1.239111	12.287869
O	3.986380	1.167673	0.333237
O	1.917907	1.491430	12.051124
O	2.083089	0.989179	9.447061
O	4.591445	0.908389	10.285104
O	7.498639	16.583031	10.291928
O	6.164173	16.814058	12.546429
O	3.921709	17.161892	0.670756
O	1.839221	16.419661	12.120850
O	2.253876	16.831171	9.535655
O	4.819896	16.582434	10.281892
O	6.179790	18.818684	10.871144
O	1.834015	18.902657	11.205720
O	8.603854	2.493544	8.024982
O	8.265882	19.815424	7.610912
O	7.828001	17.180996	7.687597

O	3.764937	2.741286	8.590949
O	3.919907	0.158794	7.772043
O	4.167379	17.328646	7.787033
O	19.842203	0.748998	10.537239
O	19.862425	17.328646	10.539247
O	2.920409	18.660686	2.926862
O	3.664626	18.584473	5.524235
O	5.993586	18.905443	6.766044
O	8.178987	18.337923	5.372070
O	7.934118	18.997375	2.770816
O	5.427563	18.750629	3.593336
O	2.594851	3.474763	3.422836
O	3.846627	3.162349	5.955569
O	6.084285	2.908239	7.360785
O	7.923306	3.475957	5.598511
O	7.990380	3.081758	2.993108
O	5.505449	3.235975	3.763835
O	3.909896	0.965301	4.087436
O	8.256872	0.989975	4.677626
O	1.248171	17.409039	1.416457
O	1.672037	0.082979	0.917940
O	1.914303	2.750838	0.930119
O	6.345172	17.170052	1.755314
O	6.082683	19.731848	1.100083
O	6.082083	2.552843	1.184396
O	10.201009	19.158159	3.846542
O	10.193600	2.736709	4.351884
O	12.691144	10.930720	3.513573
O	13.766326	11.265820	1.177303
O	16.071459	11.110806	13.055786
O	18.110699	11.376457	1.402806
O	18.103891	11.019669	4.011822
O	15.277787	11.440929	3.261169
O	12.696350	6.961466	3.250998
O	13.852221	7.056186	0.933464
O	16.286295	7.292188	13.297215
O	18.439661	6.474538	1.280218
O	17.924894	6.811428	3.855509
O	15.343859	6.640893	3.168827
O	14.345762	9.032753	2.674726
O	18.353567	8.945396	2.264404
O	11.520259	12.451999	5.287623
O	11.768531	9.867517	5.854126
O	12.179783	7.213388	5.859746

O	16.521954	12.779934	5.268486
O	16.021204	10.051581	5.686036
O	16.020203	7.382529	5.692995
O	0.318150	10.687554	2.846698
O	0.329162	7.304923	2.994179
O	17.197096	8.783419	10.466978
O	16.428852	8.785010	7.952045
O	14.055243	8.791577	6.784110
O	11.836805	8.452896	8.109563
O	12.170973	8.943008	10.694891
O	14.663712	9.367852	9.884015
O	17.332644	13.515600	10.117146
O	16.268675	13.196420	7.768297
O	14.001985	12.767199	6.273416
O	11.844814	13.350039	7.785962
O	12.181584	13.258904	10.381193
O	14.698550	13.009768	9.788193
O	16.597637	11.099861	9.365558
O	11.997983	10.949823	8.957510
O	18.690536	7.467100	12.207170
O	18.435057	10.117249	12.467603
O	18.096483	12.764612	12.564764
O	14.173573	7.380141	11.623537
O	13.862031	9.792895	12.461715
O	13.924700	12.451004	12.284389
O	9.819590	9.361684	9.543015
O	9.869043	12.517665	9.371982
O	12.775638	18.816296	3.679656
O	13.591133	18.821270	1.256931
O	16.096687	18.990412	13.471997
O	18.358772	18.402197	1.339504
O	17.954529	18.903254	3.925636
O	15.429152	18.814106	3.174716
O	12.429256	3.148818	3.093614
O	13.764324	2.899881	0.918074
O	16.192392	2.809938	12.961838
O	18.112101	3.476554	1.261749
O	17.676823	2.901075	3.840519
O	15.110003	3.480335	3.182745
O	14.093886	1.100216	2.841211
O	18.269875	0.991567	2.100194
O	11.419547	17.334219	5.355475
O	11.666618	0.072830	5.852520
O	12.438267	2.654726	5.707047

O	16.267075	17.169653	5.017421
O	16.180979	19.742794	5.614169
O	15.762519	2.492947	5.601856
O	0.267494	19.318546	3.012246
O	0.103314	2.746858	2.909330
O	17.206707	1.172250	10.390428
O	16.363579	1.236524	7.863316
O	14.029015	0.754769	6.689760
O	11.844214	1.498793	8.023644
O	12.082677	1.149366	10.630117
O	14.594236	1.084893	9.780029
O	17.438160	16.654070	9.871167
O	16.189789	16.850872	7.625634
O	13.866635	17.152939	6.282382
O	11.759321	16.492491	7.847791
O	12.173575	16.595964	10.443156
O	14.741397	16.675562	9.792341
O	16.107698	18.897285	9.366494
O	11.935715	18.916388	9.027102
O	18.682728	2.574533	12.125132
O	18.357571	19.915714	12.548704
O	17.855019	17.318697	12.378606
O	13.682034	2.982860	11.451699
O	14.021006	0.492500	12.304999
O	13.859628	17.424360	12.289074
O	9.827799	0.662836	9.542213
O	9.854228	17.414211	9.454688
O	7.108611	9.116329	9.453484
O	5.675836	8.714170	11.712802
O	4.019416	8.866596	0.247050
O	2.076682	8.448319	11.880491
O	2.073278	9.122697	9.291148
O	4.590844	9.867914	9.626659
O	7.252169	13.605543	10.125846
O	6.175585	13.343872	12.453953
O	3.920308	12.687404	0.332300
O	1.845428	13.426453	12.147348
O	2.165980	13.016932	9.530704
O	4.662123	12.942907	10.279080
O	6.505949	11.179656	10.958000
O	1.669835	10.956389	11.207594
O	8.599449	7.589678	7.933844
O	8.499139	10.203213	7.434926
O	7.753119	12.775356	7.440145

O	3.929117	7.447201	8.510920
O	3.599154	9.719269	7.204738
O	3.933121	12.362453	7.698303
O	19.852013	9.118319	10.527603
O	19.835196	12.768990	10.540451
O	2.921010	10.944450	2.828899
O	3.847627	11.356160	5.250552
O	5.986778	10.855502	6.853033
O	8.006998	11.510975	5.177481
O	7.991180	10.778094	2.586399
O	5.515059	10.686957	3.338791
O	2.834314	6.549557	3.342003
O	3.680244	6.799488	5.874468
O	6.097300	7.128021	7.024068
O	8.182791	6.466578	5.530391
O	7.916698	6.880477	2.929806
O	5.426162	6.627163	3.947985
O	3.838017	8.855055	4.188478
O	8.259275	8.948780	4.596927
O	1.415555	12.355886	1.164455
O	1.589747	9.778170	0.747173
O	2.005404	7.198264	0.843530
O	6.258076	12.597260	1.663239
O	6.182794	10.119637	0.739545
O	5.666225	7.630869	1.594986
O	10.184391	10.618903	3.858720
O	10.252464	7.213786	4.012224
O	9.018909	15.077273	8.614102
O	3.835614	14.844057	8.537551
O	5.334261	14.916091	0.924364
O	2.412451	14.768440	0.998238
O	1.089998	5.036835	1.924476
O	6.337764	5.044596	1.995272
O	4.587641	5.060913	7.698839
O	7.759926	5.058127	7.691210
O	11.584929	4.992460	4.766490
O	16.423044	4.958035	4.937123
O	14.852320	5.168168	12.736735
O	17.688835	5.051162	12.555128
O	18.857719	15.074089	11.541901
O	13.925701	14.910321	11.544176
O	15.351668	14.985340	5.948744
O	12.424252	14.918678	5.780519
O	10.928808	3.721312	12.470547

Pt	7.251768	5.081409	-3.523075
Pt	9.440773	6.631143	-0.011108
Pt	9.271988	6.348378	-2.570205
Pt	6.439275	5.091756	-1.178909
Pt	7.331455	7.552466	-0.990743
Pt	8.788055	4.282265	-0.982848
H	11.341261	3.671764	11.584593
H	11.124423	2.862073	12.886625
H	16.182781	1.853791	13.186538
H	5.957946	3.566896	17.955437
H	3.804780	17.706131	14.877748
H	9.870646	15.094386	8.122411
H	17.449373	13.073644	18.754669
H	12.842911	18.192461	14.659872

306

Pt6@H-MFI-2W

Si	8.430863	1.037136	8.744587
Si	6.055254	0.526130	10.812126
Si	5.575726	1.187174	0.391720
Si	2.359993	1.373230	0.216002
Si	1.382519	0.535880	10.835680
Si	3.610768	1.190955	8.997659
Si	8.491330	16.602930	9.062031
Si	6.090692	17.193333	10.971384
Si	5.488431	16.454285	0.586711
Si	1.415155	17.334816	10.881316
Si	3.686450	16.384836	9.060559
Si	1.508458	18.837191	2.075302
Si	3.942131	19.267406	4.065086
Si	4.381214	18.722174	6.988336
Si	7.548894	18.546267	6.860929
Si	8.626879	19.364513	4.187541
Si	6.417050	18.689341	2.314322
Si	1.449392	3.498443	2.318069
Si	4.517163	3.472774	7.345795
Si	7.575724	3.473171	7.218523
Si	8.611061	2.561996	4.431914
Si	6.535581	3.469988	2.424063
Si	11.552894	10.938878	4.643633
Si	14.032018	10.647757	2.661076
Si	14.450277	11.158165	13.102225
Si	17.678625	11.332282	13.235119
Si	18.748199	10.506076	2.649968
Si	11.659210	6.604478	4.465238

Si	14.060248	7.438644	2.514934
Si	14.766425	6.725464	13.008410
Si	17.758112	6.587564	13.198048
Si	18.766819	7.408597	2.596837
Si	16.416637	6.499810	4.398056
Si	18.523352	8.885501	11.414093
Si	16.218620	9.500977	9.396740
Si	15.686436	8.765510	6.490756
Si	12.489122	8.623431	6.620838
Si	11.451982	9.455606	9.325007
Si	13.739496	8.863612	11.142552
Si	18.549181	13.510626	11.204247
Si	16.219421	12.669295	9.315237
Si	15.462990	13.451325	6.406443
Si	12.438267	13.343872	6.279170
Si	11.468201	12.479857	9.147816
Si	13.686638	13.397002	11.009257
Si	11.524262	18.827639	4.719381
Si	13.987369	19.413664	2.811635
Si	17.637779	18.645761	13.277007
Si	18.720369	19.386003	2.578369
Si	16.455681	18.673620	4.443156
Si	11.664617	3.419643	4.491870
Si	13.864433	2.694524	2.483885
Si	17.771126	3.530282	13.067429
Si	18.567602	2.542097	2.532465
Si	16.238243	3.456257	4.375037
Si	18.496122	1.116533	11.370732
Si	16.065853	0.625227	9.352710
Si	15.597538	1.119120	6.432137
Si	12.503939	1.277118	6.560748
Si	11.397723	0.556575	9.280040
Si	13.590533	1.428549	11.059979
Si	18.503931	16.587807	11.086209
Si	16.104294	17.291834	9.194790
Si	15.403325	16.571091	6.252002
Si	12.382205	16.449509	6.332033
Si	11.462996	17.366455	9.207371
Si	13.687639	16.442545	11.046597
Si	8.501141	9.094440	8.633508
Si	6.051850	9.518886	10.656214
Si	5.534481	8.697057	0.289207
Si	2.400638	8.632982	0.177860
Si	1.418158	9.447846	10.804230

Si	3.589544	8.963305	8.784735
Si	6.117522	12.615370	10.997480
Si	5.404538	13.325366	0.508554
Si	2.398035	13.357801	0.370308
Si	1.392530	12.559254	10.923875
Si	3.688453	13.291536	9.056276
Si	1.579736	10.968130	1.944818
Si	4.017014	10.472844	3.938483
Si	4.385018	11.091105	6.835233
Si	7.556503	11.333277	6.745166
Si	8.577024	10.473839	4.077532
Si	6.460899	11.045537	2.111034
Si	1.582539	6.546174	2.286084
Si	3.940730	7.257762	4.308925
Si	4.521368	6.628755	7.255861
Si	7.597348	6.616020	7.068499
Si	8.600250	7.418347	4.292597
Si	6.318142	6.559307	2.554146
Al	2.160374	16.381454	0.403765
Al	3.758330	2.635623	4.330471
Al	16.465092	11.118566	4.433253
Al	14.462690	18.884350	12.958090
Al	14.467296	3.535654	12.874179
Al	8.416247	13.205773	8.970224
O	7.253370	1.083899	9.863940
O	6.266085	1.241698	12.284524
O	3.982376	1.166081	0.258961
O	1.910900	1.491629	12.044299
O	2.079084	0.987985	9.447729
O	4.585238	0.909981	10.283765
O	7.438974	16.572285	10.275869
O	6.157766	16.815649	12.546027
O	3.923711	17.167067	0.671157
O	1.838019	16.423639	12.114024
O	2.189806	16.823212	9.529366
O	4.755625	16.589397	10.299022
O	6.176187	18.813311	10.871680
O	1.764339	18.904846	11.208129
O	8.598448	2.493345	8.024179
O	8.261477	19.805275	7.602882
O	7.835609	17.166668	7.692014
O	3.763735	2.747256	8.590548
O	3.920308	0.171529	7.770706
O	4.095700	17.395109	7.853011

O	19.821178	0.755565	10.529209
O	19.840799	17.326458	10.538444
O	2.919608	18.658895	2.926327
O	3.665027	18.581289	5.526778
O	5.988580	18.897484	6.770192
O	8.177185	18.333546	5.370197
O	7.933116	18.997576	2.770816
O	5.428164	18.747446	3.594005
O	2.596052	3.471779	3.421632
O	3.840019	3.151604	5.947004
O	6.076076	2.896299	7.358242
O	7.924507	3.474763	5.602392
O	8.000992	3.073997	3.001673
O	5.502245	3.232792	3.773605
O	3.908094	0.952565	4.082886
O	8.257273	0.987388	4.679901
O	1.243967	17.415009	1.416724
O	1.674240	0.084372	0.918341
O	1.916506	2.748450	0.929985
O	6.345572	17.166071	1.754913
O	6.076076	19.716526	1.097005
O	6.082884	2.481206	1.245556
O	10.200607	19.157364	3.847211
O	10.197804	2.736113	4.354025
O	12.688142	10.931714	3.513841
O	13.766726	11.265223	1.177436
O	16.074863	11.110607	13.057392
O	18.118708	11.374069	1.406687
O	18.105293	11.026633	4.010617
O	15.273982	11.439736	3.264248
O	12.680332	6.964252	3.257556
O	13.848617	7.061956	0.940557
O	16.285694	7.292585	13.297215
O	18.438459	6.474936	1.284768
O	17.921091	6.811826	3.856312
O	15.339054	6.641092	3.169764
O	14.344562	9.032753	2.676466
O	18.355768	8.948381	2.264939
O	11.519657	12.452795	5.286553
O	11.765527	9.869308	5.853456
O	12.184788	7.218163	5.863092
O	16.522154	12.783715	5.268486
O	16.172169	10.038648	5.693664
O	16.018200	7.380340	5.694199

O	0.320752	10.692529	2.919234
O	0.322955	7.303132	3.006357
O	17.199898	8.783220	10.468451
O	16.424646	8.780235	7.957264
O	14.076467	8.869979	6.704081
O	11.848418	8.455085	8.105146
O	12.173777	8.944004	10.694757
O	14.664713	9.366261	9.885487
O	17.334646	13.515003	10.117548
O	16.269075	13.196818	7.767895
O	14.002185	12.767199	6.273282
O	11.844614	13.350239	7.787167
O	12.194199	13.262286	10.387618
O	14.704356	13.009967	9.789531
O	16.597837	11.098667	9.365424
O	12.015202	10.952011	8.952559
O	18.690336	7.466702	12.207839
O	18.434654	10.117448	12.468540
O	18.095284	12.765208	12.570117
O	14.174574	7.375166	11.628221
O	13.862832	9.792498	12.462251
O	13.927503	12.451401	12.286665
O	9.836207	9.445260	9.529633
O	9.911691	12.517665	9.439432
O	12.775638	18.816296	3.680191
O	13.590733	18.820673	1.258404
O	16.090479	18.994989	13.468652
O	18.357170	18.402994	1.338701
O	17.953728	18.903454	3.925903
O	15.429152	18.814306	3.174983
O	12.429256	3.149813	3.094016
O	13.760519	2.899881	0.918074
O	16.197798	2.802376	12.961168
O	18.112301	3.476753	1.262552
O	17.676422	2.901075	3.840787
O	15.109802	3.479738	3.182477
O	14.094087	1.099420	2.841345
O	18.269674	0.991567	2.099927
O	11.418746	17.334219	5.356010
O	11.665618	0.072631	5.852520
O	12.438666	2.656516	5.708385
O	16.266672	17.169853	5.018625
O	16.180578	19.743389	5.614972
O	15.762319	2.492748	5.601856

O	0.265692	19.319939	3.012915
O	0.103113	2.745067	2.909464
O	17.193090	1.174240	10.393105
O	16.358574	1.237917	7.866126
O	14.027213	0.755167	6.690162
O	11.839609	1.496405	8.024580
O	12.026215	1.157923	10.631857
O	14.573813	1.085889	9.786185
O	17.420942	16.650091	9.872238
O	16.185984	16.850075	7.629783
O	13.864635	17.153734	6.282114
O	11.759321	16.493685	7.849532
O	12.160361	16.596165	10.446368
O	14.689140	16.746799	9.784445
O	16.108900	18.902857	9.366226
O	11.927106	18.916985	9.028708
O	18.682127	2.574931	12.125534
O	18.355768	19.916910	12.549239
O	17.851816	17.319294	12.380881
O	13.677629	2.983656	11.453573
O	13.952531	0.485735	12.307676
O	13.856826	17.424559	12.295096
O	9.790958	0.666815	9.546362
O	9.841213	17.407047	9.453885
O	7.100202	9.354520	9.374524
O	5.268589	8.694470	11.954098
O	3.914501	8.954550	0.587514
O	2.085291	8.518961	11.963466
O	2.085091	9.124686	9.365825
O	4.657517	9.625345	9.780699
O	7.266984	13.366158	10.195304
O	6.165774	13.283179	12.477908
O	3.909095	12.691185	0.410457
O	1.837419	13.432025	12.214932
O	2.167582	13.096527	9.601634
O	4.670331	12.933952	10.292598
O	6.343370	11.027629	11.212010
O	1.667232	10.996784	11.267683
O	8.599850	7.558038	7.951510
O	8.508949	10.128193	7.357438
O	7.765933	12.760831	7.447773
O	3.839419	7.370988	8.522696
O	3.669231	9.713696	7.341914
O	3.932921	12.353896	7.760133

O	19.860622	9.122697	10.537106
O	19.836996	12.772969	10.547009
O	2.925615	10.943455	2.844423
O	3.834613	11.340838	5.312783
O	5.996589	10.860277	6.854639
O	8.008599	11.519730	5.179489
O	7.997187	10.781477	2.593492
O	5.522067	10.768542	3.413067
O	2.833513	6.554731	3.340129
O	3.679843	6.868936	5.872862
O	6.075876	7.145930	7.099280
O	8.099899	6.468568	5.529187
O	7.853429	6.950522	2.923516
O	5.420155	6.628158	3.927376
O	3.913700	8.867193	4.181786
O	8.187797	8.958331	4.597730
O	1.409749	12.426925	1.257868
O	1.498847	9.860353	0.756943
O	1.923313	7.213786	0.843129
O	6.263883	12.605419	1.675552
O	6.173182	10.111676	0.831218
O	5.671632	7.463120	1.419803
O	10.179986	10.612535	3.861531
O	10.196203	7.210801	4.085428
O	9.006495	15.019567	8.698548
O	3.834213	14.852414	8.539960
O	5.335463	14.914699	0.923026
O	2.418858	14.821174	1.006803
O	1.090398	5.033054	1.926215
O	6.342569	4.996440	1.996878
O	4.585438	5.055739	7.620147
O	7.688047	5.053550	7.682377
O	11.581726	4.998629	4.765687
O	16.422443	4.957836	4.936989
O	14.851918	5.158617	12.798698
O	17.688635	5.052754	12.555797
O	18.855318	15.073891	11.542972
O	13.930105	14.917684	11.541366
O	15.351067	14.986534	5.949011
O	12.424452	14.918281	5.780921
O	8.769035	2.567568	12.221356
O	11.187693	4.307735	12.556065
Pt	7.119823	5.088572	-3.558540
Pt	9.564309	7.204433	-0.555528

Pt	9.032525	6.698004	-3.021346
Pt	6.556804	5.287961	-1.165258
Pt	7.234149	7.864682	-1.225214
Pt	9.009500	4.765413	-0.971204
H	7.816588	2.335944	12.155244
H	9.157863	2.299329	11.368055
H	11.637788	3.989352	11.746126
H	11.374298	3.639925	13.242345
H	16.200602	1.841254	13.162181
H	5.928113	3.604107	17.961594
H	3.805982	17.697176	14.886982
H	9.861435	15.017776	8.212880
H	17.454779	13.051953	18.781702
H	12.853924	18.178732	14.662416

312

Pt6@H-MFI-4W

Si	8.444077	1.039922	8.753285
Si	6.058457	0.529711	10.816543
Si	5.578129	1.195532	0.398010
Si	2.361795	1.377807	0.224834
Si	1.392730	0.534288	10.839160
Si	3.613370	1.188766	8.998863
Si	8.488527	16.602531	9.063102
Si	6.089291	17.194527	10.971919
Si	5.488831	16.456076	0.587246
Si	1.419159	17.331234	10.886804
Si	3.687051	16.386030	9.059756
Si	1.510259	18.837587	2.074499
Si	3.942532	19.278152	4.064952
Si	4.381614	18.723167	6.987131
Si	7.550096	18.550644	6.865345
Si	8.623675	19.369289	4.187541
Si	6.415649	18.692524	2.313251
Si	1.453597	3.513169	2.307765
Si	4.519166	3.479340	7.358376
Si	7.577326	3.477151	7.223341
Si	8.603453	2.576722	4.421877
Si	6.530976	3.513964	2.405460
Si	11.553694	10.943057	4.645106
Si	14.036022	10.650145	2.665492
Si	14.464293	11.161348	13.110924
Si	17.703651	11.339446	13.253453
Si	18.761414	10.516025	2.661745
Si	11.673225	6.595325	4.455469

Si	14.086878	7.440037	2.542235
Si	14.818282	6.756506	13.021793
Si	17.821983	6.589355	13.192962
Si	18.779835	7.424118	2.597641
Si	16.432255	6.491253	4.416256
Si	18.577011	8.888884	11.417573
Si	16.251257	9.496599	9.403297
Si	15.689439	8.767500	6.494235
Si	12.492326	8.621441	6.607857
Si	11.449982	9.452622	9.300382
Si	13.762922	8.868188	11.130775
Si	18.555788	13.511620	11.201437
Si	16.225227	12.670092	9.314836
Si	15.463591	13.452918	6.406978
Si	12.439868	13.346260	6.281178
Si	11.463595	12.482643	9.149690
Si	13.691043	13.396803	11.008990
Si	11.522059	18.828634	4.718444
Si	13.988170	19.415056	2.813107
Si	17.642185	18.644567	13.278078
Si	18.722771	19.385607	2.578369
Si	16.456882	18.673023	4.441818
Si	11.663416	3.414469	4.485714
Si	13.884056	2.700891	2.498740
Si	17.778734	3.531276	13.056456
Si	18.560595	2.541699	2.522562
Si	16.254259	3.463620	4.407290
Si	18.507135	1.113747	11.370732
Si	16.082069	0.622242	9.351372
Si	15.598739	1.113946	6.435216
Si	12.504740	1.276919	6.558339
Si	11.421148	0.557570	9.282850
Si	13.629776	1.427554	11.062522
Si	18.507135	16.588800	11.086477
Si	16.106297	17.290440	9.195459
Si	15.404125	16.571886	6.251869
Si	12.382404	16.451498	6.331899
Si	11.460393	17.364464	9.207236
Si	13.687240	16.442942	11.045794
Si	8.477315	9.093843	8.656124
Si	6.025220	9.516697	10.688869
Si	5.436373	8.731682	0.249727
Si	2.369403	8.665815	0.234203
Si	1.463608	9.455606	10.820825

Si	3.603559	8.986787	8.757835
Si	6.120925	12.645217	10.996678
Si	5.405540	13.333723	0.503602
Si	2.395632	13.357203	0.421431
Si	1.403342	12.573780	10.948097
Si	3.688052	13.298304	9.055741
Si	1.562517	10.968528	1.998751
Si	4.021619	10.462098	3.937412
Si	4.382215	11.095284	6.822386
Si	7.556303	11.325118	6.754534
Si	8.581228	10.477818	4.082886
Si	6.443480	11.041159	2.099257
Si	1.579135	6.564481	2.294114
Si	3.943133	7.245823	4.315616
Si	4.525573	6.616418	7.267237
Si	7.607358	6.601096	7.048291
Si	8.641094	7.409791	4.267838
Si	6.306129	6.597911	2.531796
Al	2.162776	16.367523	0.416880
Al	3.760732	2.649552	4.333416
Al	16.463490	11.120755	4.436732
Al	14.473303	18.877186	12.962641
Al	14.493324	3.560329	12.868959
Al	8.407238	13.210947	8.977049
O	7.258776	1.082506	9.865680
O	6.264483	1.239907	12.289742
O	3.980373	1.167076	0.328820
O	1.916506	1.491231	12.048849
O	2.080686	0.987388	9.448532
O	4.587240	0.909782	10.284836
O	7.439174	16.574076	10.277207
O	6.158166	16.816446	12.546429
O	3.922910	17.166470	0.670756
O	1.838220	16.420057	12.122456
O	2.189806	16.823212	9.531641
O	4.755225	16.590195	10.298755
O	6.176786	18.814505	10.871680
O	1.767142	18.902458	11.209869
O	8.600049	2.493345	8.025249
O	8.264080	19.808460	7.608235
O	7.836210	17.167465	7.691611
O	3.762935	2.744669	8.595767
O	3.920908	0.171927	7.770304
O	4.095099	17.397696	7.853144

O	19.831991	0.754371	10.531351
O	19.843603	17.326458	10.539515
O	2.920209	18.661680	2.927397
O	3.665427	18.584473	5.525306
O	5.989781	18.898279	6.770728
O	8.178386	18.339516	5.373542
O	7.933317	18.997375	2.771352
O	5.427363	18.750629	3.593871
O	2.591447	3.474167	3.421632
O	3.844224	3.159762	5.954498
O	6.077077	2.897892	7.359312
O	7.923506	3.476156	5.604935
O	8.001792	3.150609	3.006089
O	5.506450	3.241945	3.765843
O	3.910296	0.965698	4.087035
O	8.256071	0.996343	4.672541
O	1.244367	17.415407	1.416457
O	1.671837	0.085765	0.918341
O	1.919509	2.761185	0.923962
O	6.345973	17.167862	1.755314
O	6.081282	19.719709	1.096202
O	6.087889	2.486778	1.253318
O	10.198606	19.158159	3.847345
O	10.195202	2.736113	4.350947
O	12.686740	10.931714	3.511833
O	13.761121	11.260247	1.179042
O	16.088276	11.109612	13.134077
O	18.195793	11.431180	1.412174
O	18.099287	11.028225	4.013696
O	15.275384	11.442720	3.264649
O	12.694148	6.963854	3.252738
O	13.936713	7.065936	0.976959
O	16.350565	7.297163	13.293335
O	18.510738	6.477721	1.277541
O	17.928299	6.807249	3.850423
O	15.354470	6.634327	3.186626
O	14.346163	9.037728	2.681686
O	18.352766	8.959923	2.263065
O	11.520458	12.454983	5.287623
O	11.765727	9.870700	5.850780
O	12.183387	7.215577	5.857471
O	16.521553	12.785506	5.268352
O	16.170368	10.040239	5.695270
O	16.020002	7.383524	5.697946

O	0.322955	10.694519	2.999130
O	0.336169	7.369595	3.007695
O	17.261166	8.785807	10.457477
O	16.428051	8.779040	7.959138
O	14.078069	8.869581	6.702742
O	11.846817	8.452498	8.087214
O	12.193798	8.868587	10.641091
O	14.685135	9.367653	9.881472
O	17.338451	13.515600	10.116879
O	16.269075	13.196420	7.767895
O	14.002787	12.767398	6.273416
O	11.844814	13.349046	7.788103
O	12.196802	13.259300	10.390562
O	14.709763	13.008772	9.791405
O	16.600639	11.099066	9.366761
O	12.016803	10.951415	8.956707
O	18.764818	7.466503	12.208107
O	18.434654	10.117448	12.472154
O	18.092880	12.765607	12.563158
O	14.187789	7.381136	11.634645
O	13.862832	9.800058	12.453685
O	13.932509	12.447422	12.287869
O	9.842215	9.445458	9.531641
O	9.907887	12.517068	9.440234
O	12.775037	18.816692	3.679656
O	13.591133	18.822065	1.257734
O	16.096085	18.991207	13.471597
O	18.358772	18.402197	1.339638
O	17.954329	18.903254	3.925903
O	15.429152	18.813908	3.174849
O	12.432461	3.149017	3.086789
O	13.840406	2.901871	0.927710
O	16.208410	2.809341	12.885421
O	18.102291	3.477947	1.255459
O	17.679226	2.904657	3.840386
O	15.100992	3.483519	3.247787
O	14.094486	1.100415	2.843085
O	18.266670	0.989975	2.100328
O	11.419147	17.334417	5.355475
O	11.666018	0.072233	5.852520
O	12.438467	2.654726	5.703567
O	16.266672	17.169455	5.018358
O	16.180979	19.741598	5.614570
O	15.765122	2.487972	5.610823

O	0.266293	19.320337	3.013183
O	0.100711	2.742679	2.849375
O	17.201099	1.174638	10.395112
O	16.363180	1.236325	7.865859
O	14.027813	0.754371	6.690563
O	11.842812	1.497798	8.023108
O	12.075869	1.149963	10.629448
O	14.591433	1.088276	9.782036
O	17.422342	16.649693	9.872640
O	16.186184	16.849480	7.630184
O	13.865234	17.153536	6.282114
O	11.759321	16.493286	7.848728
O	12.160562	16.595369	10.446771
O	14.689741	16.746599	9.784579
O	16.110102	18.901264	9.366226
O	11.929908	18.913601	9.028975
O	18.688934	2.573140	12.123794
O	18.356770	19.916512	12.549106
O	17.852215	17.318895	12.380346
O	13.678430	2.988034	11.459729
O	14.021406	0.493893	12.304732
O	13.855624	17.425356	12.294829
O	9.816786	0.672387	9.549975
O	9.840612	17.407446	9.454153
O	7.086787	9.375813	9.371848
O	4.995689	8.799338	11.954900
O	3.849630	9.029768	0.738340
O	2.082488	8.537666	12.016730
O	2.100107	9.127472	9.368770
O	4.673935	9.702752	9.705486
O	7.263181	13.430631	10.199318
O	6.166375	13.346856	12.471351
O	3.910296	12.692975	0.413936
O	1.830011	13.429636	12.263914
O	2.169384	13.099511	9.613544
O	4.675737	13.005986	10.298352
O	6.339566	11.057278	11.209601
O	1.674240	11.010514	11.282538
O	8.598047	7.547890	7.952446
O	8.511553	10.120432	7.360383
O	7.768335	12.757648	7.450182
O	3.842622	7.381932	8.518280
O	3.662624	9.703151	7.283965
O	3.930719	12.351110	7.763478

O	19.908674	9.126876	10.540585
O	19.845606	12.775356	10.550890
O	2.932622	10.941863	2.849375
O	3.840019	11.351981	5.294315
O	5.994987	10.861670	6.851293
O	8.007999	11.517740	5.181095
O	7.996587	10.775308	2.587469
O	5.529075	10.759191	3.411862
O	2.832712	6.554133	3.342271
O	3.686050	6.797299	5.869115
O	6.084285	7.134985	7.092321
O	8.176384	6.469165	5.529588
O	7.849024	6.950323	2.925122
O	5.423359	6.624974	3.921888
O	3.913500	8.858040	4.189682
O	8.259475	8.953157	4.597997
O	1.412552	12.435084	1.329200
O	1.415756	9.852194	0.826534
O	1.921712	7.212990	0.845940
O	6.264483	12.605419	1.672340
O	6.177788	10.108294	0.819307
O	5.672032	7.539930	1.433185
O	10.184190	10.618505	3.853635
O	10.236648	7.210004	4.012625
O	9.006896	15.021158	8.696675
O	3.830609	14.857390	8.534340
O	5.333260	14.918678	0.928379
O	2.417056	14.820178	1.072380
O	1.087195	5.049371	1.931167
O	6.336963	5.038029	1.926483
O	4.587040	5.054346	7.695359
O	7.686045	5.054346	7.689336
O	11.585529	4.993455	4.765151
O	16.429052	4.959826	4.999086
O	14.851519	5.191649	12.794817
O	17.695444	5.056734	12.554860
O	18.855516	15.074886	11.543240
O	13.930306	14.917286	11.541767
O	15.350667	14.987131	5.949145
O	12.424651	14.918878	5.780921
O	8.920602	2.478420	12.296836
O	9.590939	8.547019	14.385522
O	11.273787	4.152325	12.544154
O	11.590335	6.958879	12.881004

Pt	7.119622	5.002608	-3.445454
Pt	9.239152	7.182544	-0.716258
Pt	8.885763	6.836501	-3.168961
Pt	6.501744	5.019722	-1.061272
Pt	6.884965	7.754640	-1.346731
Pt	8.985873	4.685020	-1.173421
H	7.961948	2.256348	12.265387
H	9.289807	2.120437	11.466020
H	8.932415	9.268158	14.469566
H	10.469104	8.968480	14.346845
H	11.849420	3.736833	11.858141
H	11.271785	3.530680	13.295074
H	11.711468	7.179360	11.936699
H	11.679833	5.981441	12.914595
H	16.192791	1.850209	13.098745
H	5.940928	3.599132	17.956240
H	3.805582	17.698967	14.885108
H	9.829400	15.024940	8.158678
H	17.454378	13.055734	18.774342
H	12.838506	18.198233	14.659471

318

#### Pt6@H-MFI-6W

Si	8.427259	1.044101	8.742579
Si	6.053652	0.525931	10.814402
Si	5.567918	1.186378	0.392791
Si	2.353586	1.375021	0.223362
Si	1.383320	0.534686	10.837152
Si	3.610167	1.188965	8.998863
Si	8.490529	16.599945	9.061897
Si	6.089691	17.191940	10.971116
Si	5.488230	16.455080	0.586309
Si	1.416556	17.331432	10.886804
Si	3.685249	16.384439	9.060157
Si	1.508458	18.835796	2.075034
Si	3.944134	19.274967	4.064819
Si	4.381014	18.722570	6.988737
Si	7.548494	18.547262	6.863605
Si	8.624677	19.366701	4.190485
Si	6.416650	18.689739	2.313118
Si	1.446990	3.499438	2.322084
Si	4.528376	3.473967	7.358376
Si	7.583933	3.481529	7.204203
Si	8.599648	2.570951	4.420807
Si	6.484925	3.492673	2.417505

Si	11.555097	10.928132	4.643499
Si	14.061049	10.661088	2.673254
Si	14.452279	11.165329	13.110254
Si	17.678024	11.325715	13.246493
Si	18.709358	10.497320	2.670578
Si	11.668221	6.617014	4.501506
Si	14.102495	7.468891	2.588005
Si	14.815278	6.740985	13.063013
Si	17.815174	6.588957	13.215178
Si	18.750002	7.406408	2.650102
Si	16.426849	6.501601	4.483573
Si	18.568401	8.882317	11.426406
Si	16.223024	9.501971	9.448265
Si	15.664412	8.792374	6.524882
Si	12.478511	8.630594	6.633552
Si	11.455788	9.458989	9.331966
Si	13.729685	8.854259	11.185913
Si	18.542974	13.508835	11.241587
Si	16.226629	12.667504	9.326747
Si	15.459586	13.461275	6.427855
Si	12.438666	13.341882	6.277430
Si	11.467800	12.480453	9.147549
Si	13.688239	13.397400	11.008990
Si	11.524062	18.826843	4.720586
Si	13.990772	19.413862	2.813776
Si	17.638580	18.644369	13.279015
Si	18.721371	19.385805	2.578770
Si	16.457483	18.672823	4.445164
Si	11.653805	3.431185	4.479424
Si	13.896469	2.704672	2.502086
Si	17.777533	3.532670	13.069839
Si	18.566801	2.542495	2.535945
Si	16.255661	3.466207	4.416256
Si	18.502932	1.116334	11.384919
Si	16.070658	0.631793	9.370509
Si	15.599740	1.113747	6.443245
Si	12.502738	1.280899	6.556332
Si	11.396722	0.556774	9.277364
Si	13.591934	1.426559	11.062790
Si	18.504131	16.588404	11.086612
Si	16.105698	17.303772	9.202151
Si	15.402123	16.593975	6.264047
Si	12.381003	16.448912	6.332033
Si	11.461394	17.366056	9.207103

Si	13.688440	16.442942	11.045927
Si	8.477514	9.096828	8.658533
Si	6.048646	9.476302	10.720719
Si	5.449588	8.714170	0.262976
Si	2.376011	8.664621	0.237281
Si	1.448391	9.454413	10.830327
Si	3.594149	8.962509	8.806014
Si	6.113917	12.616563	11.004172
Si	5.407141	13.332927	0.502799
Si	2.399436	13.357602	0.431334
Si	1.406946	12.573780	10.964425
Si	3.684649	13.297507	9.063235
Si	1.558512	10.964946	2.006915
Si	4.020818	10.432847	3.963376
Si	4.389022	11.075982	6.864409
Si	7.559706	11.324919	6.754266
Si	8.573020	10.476624	4.072045
Si	6.433469	11.041756	2.102469
Si	1.573729	6.546373	2.287021
Si	3.945535	7.213388	4.312003
Si	4.485729	6.609851	7.281690
Si	7.555902	6.605871	7.078537
Si	8.595445	7.391683	4.302501
Si	6.334360	6.558114	2.534071
Al	2.161375	16.366331	0.416211
Al	3.748719	2.638607	4.352285
Al	16.451477	11.156573	4.455469
Al	14.464693	18.884350	12.957823
Al	14.478909	3.550579	12.869494
Al	8.411843	13.199205	8.973168
O	7.253170	1.083501	9.866349
O	6.260679	1.238514	12.288137
O	3.971564	1.165285	0.327750
O	1.914303	1.490833	12.047109
O	2.078083	0.987189	9.448666
O	4.584638	0.908787	10.284836
O	7.439374	16.572683	10.276271
O	6.158767	16.817043	12.546429
O	3.923111	17.166470	0.670622
O	1.838420	16.420456	12.122188
O	2.189005	16.823809	9.531908
O	4.754825	16.590195	10.298487
O	6.176786	18.812914	10.871680
O	1.764138	18.903652	11.209333

O	8.596645	2.496727	8.027258
O	8.261878	19.806469	7.604221
O	7.835810	17.166668	7.692014
O	3.765938	2.743276	8.596571
O	3.920107	0.171529	7.770572
O	4.094899	17.396502	7.853278
O	19.819977	0.755764	10.531083
O	19.841801	17.325861	10.539648
O	2.920209	18.662676	2.927933
O	3.665027	18.585667	5.525306
O	5.988580	18.897285	6.769924
O	8.177586	18.334740	5.371669
O	7.934318	18.998770	2.770950
O	5.428565	18.749834	3.593737
O	2.591247	3.471978	3.427654
O	3.833612	3.161951	5.964402
O	6.084886	2.898488	7.358643
O	8.005997	3.482922	5.617782
O	7.931515	3.069222	3.008097
O	5.415751	3.412877	3.759820
O	3.921309	0.965897	4.083421
O	8.259074	0.990771	4.677493
O	1.244367	17.414610	1.416724
O	1.670235	0.083178	0.918743
O	1.912902	2.753226	0.931858
O	6.346173	17.166866	1.755181
O	6.080481	19.717123	1.095666
O	6.079880	2.474441	1.251846
O	10.200607	19.159155	3.846140
O	10.193801	2.737108	4.267838
O	12.687740	10.856297	3.511699
O	13.766927	11.266615	1.186938
O	16.074261	11.109810	13.056723
O	18.108297	11.362727	1.416858
O	18.087275	11.038373	4.026543
O	15.268977	11.512169	3.273214
O	12.686339	7.120459	3.335311
O	13.942921	7.054991	1.026476
O	16.346762	7.297163	13.296011
O	18.436058	6.470757	1.333348
O	17.930099	6.806453	3.930989
O	15.343258	6.638307	3.261169
O	14.432858	9.057627	2.679812
O	18.281687	8.936840	2.342694

O	11.524862	12.447422	5.278389
O	11.757118	9.868312	5.855196
O	12.182985	7.203438	5.926528
O	16.522154	12.847590	5.265809
O	16.171768	10.042429	5.697812
O	16.016598	7.382131	5.775568
O	0.270097	10.692529	2.936899
O	0.318350	7.307510	3.011844
O	17.261166	8.782225	10.463231
O	16.353769	8.778245	8.010127
O	14.051640	8.943208	6.701672
O	11.846617	8.456876	8.115585
O	12.175978	8.940820	10.700377
O	14.678728	9.368250	9.959361
O	17.344257	13.512018	10.127853
O	16.272680	13.189257	7.777263
O	14.004388	12.768194	6.272880
O	11.844814	13.349443	7.785025
O	12.195801	13.262485	10.387484
O	14.708961	13.010762	9.792608
O	16.598639	11.097474	9.371179
O	12.016803	10.953603	8.953897
O	18.762415	7.461528	12.221490
O	18.435656	10.118443	12.471619
O	18.095682	12.775954	12.623114
O	14.172572	7.380539	11.701427
O	13.854623	9.802446	12.483931
O	13.926903	12.453391	12.288672
O	9.840212	9.445458	9.532845
O	9.912891	12.517665	9.440101
O	12.774837	18.817091	3.679388
O	13.590533	18.821270	1.259207
O	16.091080	18.994789	13.469053
O	18.356970	18.402197	1.340307
O	17.953926	18.903454	3.926572
O	15.430756	18.813709	3.176054
O	12.438066	3.143644	3.087993
O	13.840007	2.899085	0.934401
O	16.206005	2.808943	12.956885
O	18.112701	3.475957	1.265764
O	17.676222	2.904657	3.844535
O	15.104596	3.485708	3.253274
O	14.093485	1.099420	2.842549
O	18.269073	0.991965	2.101532

O	11.417544	17.333422	5.355475
O	11.665217	0.072432	5.852386
O	12.428857	2.655920	5.695939
O	16.264872	17.167664	5.017822
O	16.180578	19.742395	5.616845
O	15.764321	2.485385	5.614035
O	0.265892	19.319939	3.013584
O	0.101311	2.743873	2.912810
O	17.176073	1.170459	10.444629
O	16.361979	1.235728	7.876966
O	14.025810	0.756162	6.690697
O	11.839408	1.497201	8.022975
O	12.025414	1.159714	10.631054
O	14.569808	1.086684	9.786052
O	17.419741	16.649494	9.872104
O	16.188187	16.922508	7.624965
O	13.858827	17.158907	6.280107
O	11.759121	16.493286	7.849398
O	12.160961	16.596762	10.446235
O	14.690742	16.747198	9.783776
O	16.110300	18.910618	9.373989
O	11.926504	18.917183	9.028975
O	18.686731	2.577318	12.128076
O	18.359972	19.913527	12.555530
O	17.850815	17.320089	12.380747
O	13.682634	2.983059	11.453975
O	13.948727	0.484143	12.309550
O	13.856826	17.424759	12.295364
O	9.788956	0.668009	9.548771
O	9.840612	17.406849	9.454020
O	7.084584	9.374618	9.372918
O	5.006501	8.716757	11.972432
O	3.857839	9.023997	0.742221
O	2.080086	8.537666	12.022217
O	2.086493	9.128667	9.379610
O	4.670732	9.624748	9.776149
O	7.267986	13.362776	10.197177
O	6.165774	13.344070	12.469075
O	3.912299	12.691781	0.416077
O	1.834616	13.431029	12.277699
O	2.164578	13.098915	9.619567
O	4.675137	13.002007	10.302769
O	6.333158	11.032006	11.216962
O	1.675241	11.008524	11.285082

O	8.590839	7.547492	7.944952
O	8.512153	10.119239	7.359178
O	7.768936	12.758642	7.446033
O	3.768140	7.360839	8.517076
O	3.668431	9.702752	7.355163
O	3.930919	12.353101	7.769902
O	19.893457	9.126677	10.542994
O	19.843002	12.771776	10.620080
O	2.904191	10.938083	2.913881
O	3.835214	11.279350	5.342360
O	6.000193	10.859879	6.856111
O	8.008399	11.512567	5.179489
O	7.989579	10.781477	2.580912
O	5.515260	10.764564	3.417081
O	2.829909	6.546771	3.337051
O	3.678442	6.789340	5.865367
O	6.032028	7.143741	7.108916
O	8.024217	6.474936	5.528651
O	7.910292	6.802274	2.929806
O	5.422158	6.531250	3.922691
O	3.924913	8.817247	4.183526
O	8.176985	8.944999	4.518235
O	1.416957	12.432896	1.334687
O	1.423764	9.851597	0.828542
O	1.920911	7.211398	0.848750
O	6.263282	12.605818	1.672875
O	6.175185	10.106106	0.822653
O	5.675836	7.551273	1.502911
O	10.177983	10.613928	3.854706
O	10.193399	7.217964	4.174158
O	9.005896	15.018173	8.698548
O	3.830008	14.855797	8.535945
O	5.333861	14.918480	0.927843
O	2.418658	14.822765	1.077198
O	1.087595	5.032059	1.927420
O	6.340767	5.010966	1.908416
O	4.585438	5.049571	7.696965
O	7.678637	5.055341	7.694958
O	11.595941	5.005593	4.771709
O	16.428452	4.955050	5.016082
O	14.852520	5.178317	12.803650
O	17.699648	5.057331	12.564095
O	18.853716	15.077074	11.546987
O	13.930105	14.918281	11.541499

O	15.346863	15.003846	6.024358
O	12.424252	14.917485	5.780118
O	10.511549	5.385864	15.307074
O	9.732894	3.627986	12.794282
O	8.466903	4.025568	13.635001
O	10.157360	7.809761	13.666319
O	11.264378	4.313108	12.126336
O	10.605253	6.657410	10.239869
Pt	7.118221	5.035243	-3.420963
Pt	9.314434	7.218163	-0.733656
Pt	8.915195	6.857395	-3.194388
Pt	6.563211	5.031263	-1.011755
Pt	6.953440	7.757824	-1.315147
Pt	9.036129	4.728998	-1.290389
H	9.624375	5.790808	15.250463
H	10.394621	4.488617	14.922179
H	9.280797	2.767951	12.689627
H	10.394020	3.578238	13.503715
H	7.929913	4.848989	13.711152
H	8.101101	3.405515	14.297327
H	9.694252	8.314996	14.368122
H	11.089785	8.095311	13.704459
H	11.738098	3.918511	11.365914
H	11.314832	3.642910	12.859859
H	11.343063	7.289800	10.352420
H	11.035926	5.780262	10.440747
H	16.199600	1.856179	13.194434
H	5.395329	4.318282	17.544043
H	3.805181	17.696180	14.886178
H	9.856630	15.015586	8.205385
H	17.457983	13.085383	18.812885
H	12.878551	18.151867	14.669776

324

#### Pt6@H-MFI-8W

Si	8.427259	1.037534	8.739768
Si	6.051649	0.523941	10.814802
Si	5.555705	1.189562	0.386635
Si	2.342974	1.376215	0.222693
Si	1.364299	0.534885	10.839695
Si	3.594149	1.182996	9.004350
Si	8.491330	16.601139	9.062031
Si	6.090092	17.191143	10.970982
Si	5.486228	16.453487	0.587112
Si	1.414554	17.333025	10.887071

Si	3.683848	16.384239	9.061361
Si	1.509258	18.835199	2.074231
Si	3.919106	19.292080	4.069770
Si	4.363394	18.725754	6.991413
Si	7.535880	18.546663	6.864810
Si	8.626078	19.368095	4.199184
Si	6.399031	18.697697	2.316865
Si	1.441384	3.501030	2.320880
Si	4.523370	3.473967	7.384204
Si	7.578126	3.484514	7.218657
Si	8.601050	2.572145	4.426427
Si	6.477117	3.474763	2.425535
Si	11.553094	10.933704	4.643901
Si	14.054644	10.686957	2.680749
Si	14.475506	11.157966	13.100886
Si	17.688835	11.318353	13.249437
Si	18.738789	10.504484	2.674592
Si	11.673426	6.618607	4.494279
Si	14.112507	7.509883	2.583321
Si	14.803866	6.773421	13.042805
Si	17.821783	6.589355	13.215847
Si	18.762014	7.401831	2.653180
Si	16.418840	6.500606	4.457476
Si	18.567802	8.881123	11.422525
Si	16.246050	9.492221	9.409588
Si	15.689039	8.791180	6.501729
Si	12.507342	8.629201	6.619366
Si	11.465598	9.449040	9.319520
Si	13.751910	8.867193	11.136262
Si	18.546577	13.510028	11.243862
Si	16.253458	12.662728	9.315372
Si	15.458586	13.461474	6.424242
Si	12.437466	13.343673	6.277430
Si	11.478012	12.484035	9.150760
Si	13.724480	13.398195	11.006447
Si	11.524862	18.828634	4.719649
Si	13.987770	19.417444	2.813241
Si	17.650793	18.643970	13.287178
Si	18.733183	19.387993	2.582116
Si	16.455881	18.673620	4.441149
Si	11.663014	3.428001	4.488257
Si	13.879250	2.702483	2.501818
Si	17.783339	3.531476	13.070107
Si	18.563396	2.541898	2.538621

Si	16.247652	3.467003	4.409832
Si	18.479906	1.117329	11.374346
Si	16.045630	0.633186	9.360472
Si	15.596336	1.114543	6.437357
Si	12.502337	1.279705	6.558741
Si	11.396923	0.557968	9.281244
Si	13.584927	1.414023	11.075905
Si	18.501728	16.589996	11.086879
Si	16.103695	17.305563	9.201348
Si	15.402324	16.595566	6.262977
Si	12.380404	16.450502	6.331096
Si	11.462996	17.366455	9.207638
Si	13.688440	16.442545	11.045124
Si	8.474711	9.078321	8.645017
Si	6.041638	9.466352	10.714028
Si	5.436974	8.711782	0.274619
Si	2.369403	8.663427	0.237281
Si	1.447390	9.454214	10.829123
Si	3.591947	8.960122	8.801999
Si	6.114518	12.602833	10.997079
Si	5.406741	13.320988	0.508955
Si	2.398636	13.359194	0.431736
Si	1.408347	12.573382	10.964692
Si	3.684849	13.297308	9.062433
Si	1.574730	10.965741	2.007316
Si	4.017414	10.405983	3.976892
Si	4.388422	11.076181	6.862401
Si	7.554901	11.343425	6.757746
Si	8.572820	10.469262	4.082618
Si	6.431667	11.029221	2.111570
Si	1.578534	6.543587	2.287556
Si	3.946336	7.189310	4.325252
Si	4.479522	6.599105	7.280754
Si	7.546291	6.608657	7.057793
Si	8.586034	7.402428	4.303839
Si	6.309333	6.548562	2.545447
Al	2.157971	16.366331	0.414873
Al	3.712479	2.650945	4.373698
Al	16.458084	11.163139	4.443290
Al	14.472902	18.860670	12.972544
Al	14.460489	3.568488	12.872038
Al	8.417249	13.200002	8.975041
O	7.251368	1.084098	9.863807
O	6.252470	1.231350	12.287333

O	3.959551	1.164291	0.329088
O	1.910299	1.490236	12.045504
O	2.064068	0.987189	9.453216
O	4.583236	0.905604	10.280151
O	7.439374	16.572086	10.276404
O	6.159167	16.817640	12.548303
O	3.922910	17.165674	0.670890
O	1.838420	16.420656	12.121117
O	2.188204	16.823809	9.532443
O	4.754825	16.589796	10.299155
O	6.177588	18.811520	10.871144
O	1.761335	18.905045	11.209200
O	8.596445	2.496529	8.025652
O	8.258875	19.804281	7.600741
O	7.833807	17.167465	7.691880
O	3.760332	2.738898	8.610757
O	3.853634	0.166157	7.762007
O	4.094699	17.395506	7.854349
O	19.800957	0.751983	10.529209
O	19.840799	17.325462	10.539515
O	2.921610	18.657700	2.924989
O	3.664426	18.581089	5.522763
O	5.973763	18.900866	6.773806
O	8.171779	18.334343	5.373007
O	7.930914	18.998173	2.768809
O	5.426963	18.824654	3.596012
O	2.586842	3.479539	3.424576
O	3.835814	3.154389	5.992372
O	6.080281	2.897494	7.362792
O	7.923906	3.477549	5.605202
O	7.930914	3.073003	3.016394
O	5.435572	3.245328	3.770527
O	3.831810	0.974454	4.093592
O	8.256872	0.990373	4.677894
O	1.245168	17.414013	1.416858
O	1.668633	0.081984	0.918609
O	1.911100	2.755215	0.931858
O	6.341368	17.171843	1.759865
O	6.085086	19.721104	1.090982
O	6.076677	2.473247	1.244351
O	10.195202	19.155972	3.847345
O	10.189596	2.740689	4.352018
O	12.690143	10.935894	3.512502
O	13.768728	11.272585	1.173689

O	16.088678	11.041756	13.057927
O	18.113703	11.361932	1.420070
O	18.095083	11.037777	4.023064
O	15.272982	11.524903	3.268396
O	12.768830	7.132796	3.415609
O	13.937514	7.135383	1.005732
O	16.346560	7.292785	13.291461
O	18.435856	6.472150	1.334820
O	17.931902	6.808641	3.928848
O	15.365283	6.648256	3.202820
O	14.441868	9.099813	2.687440
O	18.349962	8.941815	2.339215
O	11.519857	12.450605	5.284947
O	11.762924	9.867317	5.852921
O	12.178382	7.204234	5.930543
O	16.524357	12.848586	5.264605
O	16.176575	10.053771	5.688177
O	16.017599	7.376360	5.761783
O	0.300330	10.696906	2.952692
O	0.326559	7.302137	3.014253
O	17.257563	8.781827	10.460554
O	16.428452	8.783816	7.964758
O	14.083074	8.945596	6.696988
O	11.920298	8.458269	8.120938
O	12.180984	8.945993	10.700244
O	14.681732	9.366459	9.889368
O	17.353268	13.513013	10.127050
O	16.276884	13.189854	7.771776
O	14.003986	12.768392	6.273282
O	11.845015	13.350239	7.785962
O	12.243453	13.255322	10.375840
O	14.753611	13.013746	9.801709
O	16.605246	11.091702	9.367699
O	12.012400	10.951216	8.954030
O	18.763016	7.464115	12.220017
O	18.440462	10.116055	12.468807
O	18.090878	12.772969	12.623381
O	14.184785	7.385116	11.641871
O	13.858827	9.798467	12.462651
O	13.935311	12.446426	12.290145
O	9.848021	9.367057	9.532176
O	9.920900	12.519654	9.446123
O	12.772834	18.818483	3.679121
O	13.591535	18.822065	1.261348

O	16.099890	18.990610	13.477485
O	18.421440	18.403391	1.328664
O	17.954529	18.902458	3.922423
O	15.428753	18.813709	3.173110
O	12.436064	3.149614	3.097362
O	13.840007	2.898488	0.933063
O	16.200800	2.824663	12.956885
O	18.112301	3.474565	1.266701
O	17.674221	2.905254	3.845203
O	15.101193	3.483917	3.247385
O	14.095287	1.102007	2.847100
O	18.269674	0.990572	2.102469
O	11.416545	17.334616	5.355341
O	11.663014	0.072432	5.852787
O	12.434663	2.655720	5.704237
O	16.265472	17.168459	5.017019
O	16.180779	19.741997	5.614436
O	15.764121	2.486778	5.612028
O	0.276504	19.322725	3.020275
O	0.099309	2.743475	2.913613
O	17.178074	1.181802	10.399261
O	16.355772	1.236524	7.871613
O	14.024809	0.753575	6.690162
O	11.838408	1.496206	8.024580
O	12.019607	1.160311	10.635470
O	14.539375	1.081113	9.778557
O	17.418139	16.649891	9.872372
O	16.188187	16.922707	7.624563
O	13.858827	17.159107	6.280107
O	11.758719	16.493484	7.848996
O	12.160961	16.594770	10.445833
O	14.690341	16.746004	9.782973
O	16.107899	18.911612	9.374123
O	11.925903	18.917582	9.029243
O	18.684130	2.573339	12.125668
O	18.354767	19.916512	12.550979
O	17.851414	17.320290	12.382219
O	13.680832	2.974701	11.458391
O	13.943721	0.437977	12.296836
O	13.856424	17.417793	12.294829
O	9.785752	0.667412	9.545559
O	9.840412	17.407248	9.453752
O	7.080179	9.294624	9.378539
O	5.001696	8.717155	11.974172

O	3.850231	9.028176	0.744630
O	2.079685	8.537666	12.021012
O	2.086292	9.128468	9.379208
O	4.668329	9.624948	9.773204
O	7.268186	13.359592	10.198783
O	6.167576	13.278603	12.480452
O	3.909296	12.691582	0.417550
O	1.834616	13.431228	12.277966
O	2.165179	13.098915	9.619835
O	4.675938	13.000016	10.302903
O	6.337563	11.018873	11.207995
O	1.675641	11.007928	11.284814
O	8.593843	7.565600	7.873888
O	8.517960	10.189880	7.431313
O	7.765532	12.773565	7.447372
O	3.766739	7.359248	8.514399
O	3.668030	9.703350	7.354361
O	3.931119	12.352702	7.769768
O	19.892857	9.126677	10.540585
O	19.844404	12.771178	10.621284
O	2.916204	10.933704	2.917360
O	3.837016	11.281141	5.340754
O	6.000793	10.860476	6.857048
O	8.008199	11.515352	5.184307
O	7.986175	10.778294	2.591484
O	5.516261	10.692728	3.414672
O	2.830310	6.547766	3.334910
O	3.672635	6.716311	5.864431
O	6.022217	7.140358	7.107711
O	8.019611	6.464588	5.517677
O	7.862839	6.868737	2.936096
O	5.418554	6.546174	3.927509
O	3.917104	8.802522	4.261950
O	8.182190	8.952361	4.592510
O	1.418559	12.432696	1.335088
O	1.422964	9.854184	0.828542
O	1.920510	7.210801	0.847545
O	6.260879	12.597858	1.682779
O	6.177588	10.102324	0.819173
O	5.671431	7.546298	1.497825
O	10.177182	10.613331	3.857382
O	10.188595	7.217367	4.173757
O	9.006096	15.018970	8.698816
O	3.830209	14.855599	8.536481

O	5.337064	14.913903	0.923695
O	2.418658	14.823959	1.077332
O	1.086193	5.032457	1.924743
O	6.334560	4.992460	1.922200
O	4.587841	5.044993	7.709277
O	7.679638	5.059719	7.695760
O	11.591937	5.006588	4.770772
O	16.424246	4.958433	5.008187
O	14.777236	5.210752	12.802713
O	17.760115	5.057529	12.560615
O	18.853916	15.077870	11.548058
O	13.933910	14.918081	11.542436
O	15.346662	15.004244	6.024625
O	12.424051	14.918281	5.780252
O	10.998085	5.709620	15.299713
O	10.268482	3.164538	14.627218
O	8.682340	2.553440	12.119645
O	9.434366	0.659652	14.136865
O	9.346469	8.457473	14.463677
O	11.189495	4.227742	12.375929
O	11.592938	6.965247	12.977495
O	11.751913	9.281491	14.473045
Pt	7.148054	5.059320	-3.424309
Pt	9.274190	7.252389	-0.736868
Pt	8.979867	6.834710	-3.184485
Pt	6.526971	5.004599	-1.037852
Pt	6.912996	7.740512	-1.311802
Pt	9.016507	4.746707	-1.151072
H	10.087083	6.060240	15.241632
H	10.883759	4.733176	15.214464
H	9.476612	3.581024	14.191602
H	10.050844	2.195059	14.663620
H	7.706868	2.679002	11.978990
H	9.037930	2.268088	11.254835
H	8.940223	1.015247	13.372026
H	8.829501	0.078203	14.631500
H	8.625678	9.117324	14.442666
H	10.243455	8.950172	14.519083
H	11.620769	3.713551	11.662348
H	11.134634	3.633757	13.184130
H	11.819986	6.358526	12.251334
H	11.576719	6.395738	13.800683
H	11.997182	10.176747	14.181966
H	12.048038	8.674173	13.759866

H	16.181379	1.885032	13.241274
H	5.861440	3.639328	17.947807
H	3.799575	17.692001	14.888721
H	9.846820	15.018770	8.188925
H	17.459183	13.082199	18.823860
H	12.700554	18.420902	14.613032
		330	

Pt6@H-MFI-10W

Si	8.465502	1.032161	8.760512
Si	6.057255	0.520160	10.796869
Si	5.555904	1.184190	0.369237
Si	2.343175	1.375419	0.214797
Si	1.362497	0.534089	10.836617
Si	3.594349	1.184786	9.002075
Si	8.491130	16.604919	9.060559
Si	6.090893	17.189951	10.969377
Si	5.485627	16.456871	0.586443
Si	1.413353	17.333820	10.886804
Si	3.683447	16.387026	9.060826
Si	1.510660	18.835995	2.074097
Si	3.918305	19.293673	4.070841
Si	4.367198	18.727348	6.990745
Si	7.541687	18.554623	6.869628
Si	8.625278	19.369488	4.199719
Si	6.399031	18.698692	2.318069
Si	1.440383	3.500234	2.320211
Si	4.523370	3.476753	7.384338
Si	7.576525	3.473370	7.221869
Si	8.598248	2.574135	4.421609
Si	6.461299	3.471779	2.404256
Si	11.557499	10.932510	4.642161
Si	14.058647	10.675416	2.678072
Si	14.474904	11.223433	13.102760
Si	17.692240	11.327904	13.249973
Si	18.741392	10.501299	2.673254
Si	11.671624	6.609453	4.488524
Si	14.107500	7.492172	2.575291
Si	14.829894	6.758297	13.049362
Si	17.826788	6.583783	13.215847
Si	18.764017	7.399244	2.650771
Si	16.418039	6.508565	4.442353
Si	18.557791	8.880326	11.424800
Si	16.245451	9.497395	9.403832
Si	15.680029	8.843314	6.495306

Si	12.498733	8.625818	6.616957
Si	11.463395	9.452423	9.325676
Si	13.764524	8.912364	11.154731
Si	18.542173	13.510028	11.240784
Si	16.228031	12.668699	9.322464
Si	15.458385	13.463663	6.426383
Si	12.438666	13.342877	6.275155
Si	11.466599	12.483041	9.144872
Si	13.689240	13.428640	10.997748
Si	11.528467	18.839178	4.704392
Si	13.993776	19.424807	2.806148
Si	17.650394	18.641582	13.299089
Si	18.737589	19.389387	2.584124
Si	16.457684	18.671829	4.437134
Si	11.663014	3.421434	4.484242
Si	13.882653	2.709249	2.494859
Si	17.772327	3.528690	13.072381
Si	18.559793	2.543291	2.537952
Si	16.247051	3.470386	4.417193
Si	18.492319	1.126084	11.392948
Si	16.110300	0.629405	9.380815
Si	15.617961	1.106981	6.448866
Si	12.512348	1.277118	6.560347
Si	11.429358	0.529910	9.278435
Si	13.643991	1.423574	11.066403
Si	18.505333	16.581837	11.091028
Si	16.157953	17.316507	9.207638
Si	15.401723	16.606512	6.267928
Si	12.368190	16.453487	6.290278
Si	11.452584	17.364265	9.152233
Si	13.700053	16.469009	11.005778
Si	8.482320	9.085087	8.659738
Si	5.992985	9.496599	10.685122
Si	5.453992	8.718946	0.288136
Si	2.361795	8.652881	0.190306
Si	1.433775	9.460780	10.803828
Si	3.571524	8.970072	8.734147
Si	6.112316	12.613379	10.994938
Si	5.403937	13.327157	0.507082
Si	2.397234	13.362975	0.426784
Si	1.404343	12.574575	10.961481
Si	3.682446	13.298900	9.056946
Si	1.565520	10.956788	1.959673
Si	4.013210	10.460506	3.932862

Si	4.379012	11.100259	6.816497
Si	7.549095	11.337256	6.757612
Si	8.582230	10.444387	4.066291
Si	6.443680	11.048720	2.109964
Si	1.580737	6.545776	2.285147
Si	3.941331	7.243833	4.306784
Si	4.492736	6.603881	7.250910
Si	7.561508	6.624576	7.066358
Si	8.587436	7.369197	4.282426
Si	6.300323	6.539209	2.545447
Al	2.156970	16.368320	0.414070
Al	3.712679	2.654526	4.375304
Al	16.458282	11.184233	4.448777
Al	14.500532	18.884947	12.973347
Al	14.445872	3.582417	12.853703
Al	8.415246	13.207166	8.966611
O	7.261579	1.083103	9.862201
O	6.258877	1.232942	12.271542
O	3.964556	1.162699	0.259363
O	1.903491	1.491032	12.041890
O	2.064468	0.987189	9.452011
O	4.584237	0.905206	10.277876
O	7.439374	16.570892	10.276136
O	6.159167	16.817640	12.547500
O	3.922710	17.166470	0.671291
O	1.838620	16.420656	12.120582
O	2.187604	16.823610	9.532443
O	4.754624	16.589001	10.299022
O	6.177187	18.809729	10.870744
O	1.761536	18.905045	11.208665
O	8.597647	2.486380	8.018693
O	8.259475	19.809256	7.605559
O	7.832806	17.168459	7.691076
O	3.759931	2.740888	8.610757
O	3.853834	0.166356	7.761337
O	4.094899	17.396502	7.854082
O	19.798754	0.750391	10.530012
O	19.839798	17.325064	10.540585
O	2.922812	18.657700	2.924721
O	3.664827	18.581089	5.523031
O	5.976767	18.900866	6.773806
O	8.172179	18.336729	5.374613
O	7.929913	18.997974	2.768408
O	5.426362	18.825249	3.595878

O	2.586442	3.479539	3.423639
O	3.833812	3.153594	5.994781
O	6.076477	2.896101	7.359981
O	7.921905	3.475758	5.603998
O	7.917299	3.074595	3.012379
O	5.433170	3.236175	3.765173
O	3.831410	0.976046	4.093458
O	8.255672	0.991965	4.676154
O	1.245569	17.414412	1.417260
O	1.671637	0.083178	0.918074
O	1.914504	2.751634	0.932260
O	6.341368	17.173037	1.759463
O	6.083684	19.724485	1.090581
O	6.084085	2.489962	1.185199
O	10.193000	19.161741	3.843999
O	10.187194	2.739694	4.353088
O	12.695149	10.930919	3.512502
O	13.768128	11.276166	1.176901
O	16.086676	11.114388	13.056188
O	18.115305	11.361533	1.421542
O	18.095083	11.031209	4.024536
O	15.274183	11.520327	3.265854
O	12.769230	7.132000	3.418955
O	13.940317	7.057578	1.011621
O	16.359575	7.295769	13.300294
O	18.438860	6.470956	1.335490
O	17.935907	6.807050	3.926439
O	15.365082	6.637908	3.191310
O	14.443670	9.082898	2.681953
O	18.350563	8.940422	2.339348
O	11.519857	12.448417	5.284010
O	11.761724	9.867317	5.853590
O	12.175578	7.199458	5.929606
O	16.527359	12.860922	5.262865
O	16.099689	10.191073	5.772757
O	16.019402	7.464712	5.688177
O	0.310942	10.690340	2.933554
O	0.328961	7.303331	3.013049
O	17.252155	8.782622	10.458548
O	16.427851	8.784613	7.957398
O	14.071861	8.936840	6.703277
O	11.919697	8.455682	8.125890
O	12.190194	8.947983	10.702251
O	14.680931	9.369046	9.881472

O	17.344257	13.510227	10.128790
O	16.273081	13.190649	7.775925
O	14.004388	12.769786	6.273148
O	11.845615	13.349842	7.785025
O	12.195801	13.262286	10.387349
O	14.710163	13.010563	9.793144
O	16.601242	11.098468	9.369305
O	12.012198	10.952807	8.954565
O	18.764618	7.464911	12.219349
O	18.435856	10.117646	12.470547
O	18.098085	12.776950	12.623783
O	14.254663	7.467896	11.693798
O	13.853222	9.877466	12.451009
O	13.934310	12.518063	12.302189
O	9.850224	9.373822	9.534986
O	9.910890	12.516670	9.440502
O	12.780043	18.824057	3.673366
O	13.593335	18.823658	1.255192
O	16.106697	18.982054	13.552161
O	18.431652	18.401798	1.332813
O	17.958132	18.901264	3.922557
O	15.429152	18.813908	3.172039
O	12.437466	3.149017	3.095756
O	13.841809	2.908239	0.927977
O	16.196796	2.828842	12.956618
O	18.111700	3.476156	1.268307
O	17.672218	2.907045	3.847345
O	15.101994	3.485310	3.252872
O	14.095888	1.109568	2.845627
O	18.270876	0.990373	2.104343
O	11.421350	17.326059	5.286686
O	11.668820	0.070840	5.852386
O	12.434062	2.654726	5.706645
O	16.264671	17.167465	5.015146
O	16.181580	19.739212	5.608682
O	15.767325	2.486579	5.622734
O	0.282510	19.324715	3.022551
O	0.098108	2.744470	2.912676
O	17.178474	1.248861	10.448109
O	16.428852	1.162898	7.864788
O	14.038626	0.759346	6.696318
O	11.841011	1.501380	8.026990
O	12.098093	1.072158	10.631857
O	14.601644	1.078526	9.767316

O	17.431353	16.576862	9.867955
O	16.188387	16.999716	7.614927
O	13.851419	17.158112	6.280776
O	11.678832	16.495674	7.778066
O	12.180984	16.588404	10.369148
O	14.752210	16.747595	9.781501
O	16.267075	18.910618	9.458838
O	11.932711	18.902657	8.946402
O	18.690336	2.579309	12.134902
O	18.352964	19.910938	12.552586
O	17.848812	17.322678	12.379677
O	13.683234	2.976691	11.447283
O	14.100693	0.501654	12.300316
O	13.852020	17.495399	12.215869
O	9.822993	0.592592	9.536592
O	9.840212	17.406849	9.455090
O	7.102804	9.280893	9.448934
O	5.085788	8.718150	11.951286
O	3.851632	9.025988	0.667009
O	2.085692	8.527915	11.969355
O	2.086092	9.134039	9.361676
O	4.666928	9.626340	9.702541
O	7.269187	13.359393	10.196508
O	6.167176	13.279201	12.479113
O	3.908494	12.692975	0.416211
O	1.835817	13.431626	12.272211
O	2.165179	13.098318	9.618228
O	4.674136	12.997828	10.299155
O	6.331758	11.021857	11.207326
O	1.674640	11.006733	11.279460
O	8.589437	7.612960	7.862915
O	8.509350	10.193661	7.444561
O	7.762529	12.771378	7.441751
O	3.755727	7.375166	8.457119
O	3.661423	9.709319	7.280219
O	3.929317	12.351310	7.765218
O	19.878441	9.129462	10.535500
O	19.842001	12.770581	10.619143
O	2.923212	10.936888	2.841880
O	3.837617	11.354171	5.288962
O	5.990783	10.862068	6.854372
O	8.005796	11.452671	5.186582
O	7.993182	10.783070	2.583187
O	5.520466	10.765558	3.413200

O	2.832512	6.553537	3.334642
O	3.672435	6.794116	5.853724
O	6.032628	7.146129	7.104098
O	8.022815	6.464588	5.521157
O	7.866643	6.791927	2.930476
O	5.421557	6.622387	3.928848
O	3.912699	8.857841	4.187942
O	8.178185	8.924105	4.516629
O	1.413153	12.437075	1.325720
O	1.421362	9.862144	0.758281
O	1.921111	7.215377	0.841925
O	6.264483	12.608006	1.676087
O	6.173584	10.112672	0.826802
O	5.668428	7.547890	1.495417
O	10.181787	10.612535	3.854973
O	10.191399	7.215377	4.174292
O	9.005695	15.020760	8.697344
O	3.830409	14.856395	8.536079
O	5.336463	14.916689	0.922758
O	2.418858	14.825152	1.076395
O	1.088396	5.034646	1.923940
O	6.255874	4.989475	1.927955
O	4.584237	5.052754	7.697367
O	7.687046	5.057928	7.682645
O	11.592737	4.998828	4.773047
O	16.422846	4.969576	5.012335
O	14.849917	5.210354	12.726431
O	17.764118	5.056535	12.561284
O	18.858120	15.072298	11.554213
O	13.927503	14.945144	11.532935
O	15.348865	15.011010	6.032655
O	12.425653	14.913505	5.773561
O	11.007093	5.712008	15.299713
O	10.185591	3.149216	14.719829
O	8.601251	2.643980	12.202084
O	10.188395	3.478544	10.117281
O	9.434366	0.658259	14.135526
O	9.426558	8.546223	14.559098
O	10.933613	4.309328	12.545894
O	12.084078	5.805334	10.375037
O	11.671425	6.967237	12.886625
O	11.843614	9.201497	14.472777
Pt	7.064762	5.109068	-3.556131
Pt	9.393321	7.318654	-0.646667

Pt	9.017308	6.727852	-3.090536
Pt	6.355583	5.300895	-1.171146
Pt	7.065763	7.835430	-1.204470
Pt	8.814285	4.852769	-0.937747
H	10.105503	6.065813	15.164010
H	10.890766	4.737753	15.232398
H	9.358283	3.571671	14.378428
H	9.983569	2.175757	14.725717
H	7.659215	2.510060	11.962396
H	9.106806	2.599605	11.349052
H	9.646599	4.313108	10.021324
H	10.817486	3.474763	9.374390
H	8.971257	1.030768	13.358643
H	8.811281	0.069845	14.597641
H	8.742206	9.242290	14.545447
H	10.348169	8.989772	14.620393
H	11.088984	3.898015	11.656192
H	10.926005	3.609480	13.261884
H	11.145647	6.093074	10.149400
H	12.650300	6.325295	9.781367
H	11.902478	6.496426	12.034395
H	11.685240	6.302212	13.620950
H	12.119316	10.059741	14.107690
H	12.056248	8.531099	13.779940
H	16.162958	1.867123	13.150002
H	5.911896	3.544410	17.951555
H	3.797973	17.690609	14.890595
H	9.846219	15.026731	8.185310
H	17.457380	13.120804	18.806997
H	12.689543	18.453537	14.600718

300

### Pt<sub>6</sub>@H-MFI

Si	8.419651	1.020620	8.757032
Si	6.040437	0.631793	10.841301
Si	5.621577	1.171056	0.347958
Si	2.435276	1.284281	0.172908
Si	1.375511	0.536875	10.821494
Si	3.656818	1.255229	9.079027
Si	8.615267	16.459259	9.062968
Si	6.162371	17.304569	10.917718
Si	5.418954	16.476969	0.467067
Si	2.378814	16.469208	0.436554
Si	1.370906	17.354116	11.014343
Si	3.624182	16.307629	9.184217

Si	1.535888	18.834204	2.050008
Si	3.935724	19.355558	4.068566
Si	7.670028	18.460501	6.936275
Si	8.641094	19.257854	4.147392
Si	6.401834	18.689341	2.205117
Si	1.611771	3.410092	2.322218
Si	3.853634	2.660894	4.412241
Si	4.498943	3.361538	7.265631
Si	7.534278	3.349002	7.140500
Si	8.713975	2.472252	4.446100
Si	11.616963	11.014296	4.625432
Si	14.181783	10.510851	2.749671
Si	14.473102	11.068421	13.126449
Si	17.669214	11.228209	13.242613
Si	18.730980	10.530949	2.682756
Si	16.503132	11.351385	4.555841
Si	11.768531	6.569257	4.511811
Si	14.246654	7.334374	2.573952
Si	14.794655	6.655221	13.054582
Si	18.924795	7.396458	2.706846
Si	16.535368	6.530056	4.448242
Si	18.550783	8.950769	11.318807
Si	16.176575	9.482271	9.359670
Si	15.618561	8.917737	6.426651
Si	12.444273	8.675367	6.589656
Si	11.478211	9.473914	9.304263
Si	13.710065	8.749591	11.136663
Si	18.473497	13.465056	11.159950
Si	16.105896	12.662728	9.301586
Si	15.504235	13.417100	6.322130
Si	12.503539	13.441774	6.264047
Si	13.777739	13.427845	11.193274
Si	11.552694	18.795601	4.646042
Si	13.956135	19.313971	2.640198
Si	14.383404	18.871813	13.084425
Si	17.522453	18.619495	13.223207
Si	18.612452	19.344416	2.556287
Si	16.397617	18.623474	4.409698
Si	11.746507	3.404520	4.484777
Si	13.946123	2.645771	2.417371
Si	14.655903	3.452079	12.925971
Si	17.699047	3.450089	12.989675
Si	18.671915	2.515831	2.405728
Si	18.480705	1.055244	11.381037

Si	16.083872	0.528716	9.405037
Si	15.542477	0.987985	6.472554
Si	12.452482	1.215630	6.566905
Si	11.358280	0.502848	9.326345
Si	13.617962	1.344376	11.127698
Si	18.441862	16.517962	11.131310
Si	16.211412	17.232534	9.164411
Si	15.441566	16.585220	6.236210
Si	12.415442	16.478760	6.320256
Si	11.503839	17.246464	9.251801
Si	13.861430	16.439360	11.030670
Si	8.615066	9.143989	8.522830
Si	6.186598	9.307757	10.494413
Si	5.335663	8.829783	0.333638
Si	2.250273	8.692879	0.253742
Si	1.438781	9.554704	10.787768
Si	3.569722	8.906395	8.727591
Si	8.376804	13.327952	8.922581
Si	6.137944	12.440854	10.951844
Si	5.370701	13.309247	0.454621
Si	2.338770	13.427447	0.259630
Si	1.354889	12.625119	10.814802
Si	3.738107	13.232836	9.031919
Si	1.507056	11.112398	1.985636
Si	3.911698	10.499707	3.899271
Si	4.481324	11.121751	6.771397
Si	7.655411	11.312383	6.669150
Si	8.678135	10.566567	3.998439
Si	6.383414	11.047527	2.108090
Si	1.681648	6.517719	2.254233
Si	4.013410	7.394468	4.144180
Si	4.487531	6.564481	7.118418
Si	8.751016	7.454762	4.176032
Si	6.453891	6.712331	2.421921
O	7.169077	1.091858	9.778958
O	6.347975	1.325075	12.277164
O	4.014411	0.989179	0.161934
O	1.834416	1.495609	12.056210
O	2.087894	0.994751	9.445990
O	4.522970	1.080516	10.454265
O	7.489429	16.748194	10.195437
O	6.172182	16.746403	12.436287
O	3.896081	17.086079	0.416880
O	1.750523	16.495874	12.322665

O	2.153366	16.584623	9.789129
O	4.830708	16.755356	10.124105
O	6.089891	18.906836	10.882521
O	1.834816	18.899872	11.197958
O	8.588838	2.485783	8.033146
O	8.175983	19.900990	7.519908
O	8.515356	17.312527	7.697500
O	3.768741	2.824265	8.610889
O	4.167179	0.254906	7.948298
O	3.591346	17.255816	7.767493
O	19.803360	0.664030	10.527738
O	19.795950	17.322477	10.711084
O	2.760033	18.817888	3.086387
O	3.753124	18.662676	5.501484
O	6.115520	18.235443	7.190017
O	8.094494	18.329964	5.356412
O	7.917299	18.906239	2.748467
O	5.402135	18.988422	3.441037
O	2.592649	3.322735	3.600295
O	3.582336	2.907244	6.006960
O	6.015209	2.739296	7.114938
O	8.091290	3.395167	5.596503
O	7.937321	2.998183	3.009971
O	5.260380	3.319352	4.004729
O	3.835814	1.074944	4.097072
O	8.342767	0.915553	4.600272
O	1.416156	17.330637	1.422345
O	1.669835	0.005970	0.832556
O	2.172787	2.658307	1.002253
O	6.256074	17.157116	1.677158
O	6.172582	19.649267	0.924230
O	5.998391	2.419719	1.259073
O	10.210819	19.067820	3.770393
O	10.273889	2.734521	4.178976
O	12.847116	10.781079	3.600696
O	13.929505	11.104439	1.256931
O	16.086075	11.026832	12.978030
O	18.102489	11.360340	1.412040
O	17.991369	11.016484	4.031897
O	15.434559	11.356758	3.336783
O	12.931007	6.879482	3.419356
O	13.918492	6.974998	1.018982
O	16.280289	7.225725	13.288248
O	18.678524	6.478517	1.414717

O	18.086273	6.891024	4.019718
O	15.591331	6.556124	3.092811
O	14.582422	8.934452	2.758236
O	18.523954	8.953157	2.353133
O	11.595741	12.510303	5.271965
O	11.676630	9.863537	5.779315
O	12.258269	7.211398	5.922112
O	16.518751	12.847192	5.190061
O	16.098690	10.280221	5.695939
O	15.944519	7.622113	5.521157
O	0.252878	10.944450	3.003948
O	0.506156	7.289800	3.097763
O	17.265770	8.785010	10.369148
O	16.418039	8.871770	7.869204
O	14.023008	9.040514	6.696050
O	11.763926	8.471801	8.045324
O	12.169170	8.786801	10.625031
O	14.671120	9.187568	9.880134
O	17.204905	13.512018	10.137088
O	16.184183	13.104685	7.766557
O	14.016001	12.770183	6.188701
O	12.010197	13.509829	7.781010
O	12.165566	13.284970	10.631188
O	14.603045	13.011758	9.872773
O	16.440264	11.088320	9.454420
O	12.094689	10.932909	9.039815
O	18.849112	7.396259	11.974305
O	18.362377	9.869108	12.627530
O	18.108898	12.592087	12.479648
O	14.096889	7.289402	11.711999
O	13.846614	9.790308	12.379542
O	13.929706	12.452596	12.454086
O	9.842614	9.537192	9.529499
O	9.743106	12.614175	9.376130
O	12.849117	18.742073	3.677381
O	13.677028	18.666655	1.160975
O	15.976154	19.067421	13.300829
O	18.111101	18.393839	1.337765
O	17.928699	18.899672	3.945576
O	15.439565	18.825052	3.105124
O	12.587030	3.237169	3.112217
O	13.776537	2.983258	0.833359
O	16.178577	2.824066	12.963711
O	18.187183	3.412678	1.180648

O	17.944317	3.135287	3.840386
O	15.272581	3.316367	3.011844
O	13.928704	1.029375	2.665760
O	18.186382	0.993557	2.185444
O	11.424552	17.343571	5.362836
O	11.597342	0.083576	5.766066
O	12.427254	2.647363	5.767404
O	16.265272	17.086874	4.931100
O	16.096487	19.571661	5.683493
O	15.772330	2.336939	5.673991
O	0.175393	19.230194	2.844691
O	0.217839	2.657114	2.768006
O	17.201500	1.165285	10.389625
O	16.349564	1.060020	7.898781
O	13.962541	0.672387	6.772333
O	11.756518	1.408451	8.025517
O	12.086279	1.158918	10.623827
O	14.597439	0.993159	9.872238
O	17.521051	16.502241	9.792476
O	16.270277	17.007477	7.568756
O	13.914889	17.165674	6.281579
O	11.849821	16.499653	7.853546
O	12.357778	16.574474	10.465239
O	14.881951	16.505623	9.773337
O	16.186184	18.807541	9.541678
O	11.838408	18.840773	9.117303
O	18.688334	2.484788	12.124195
O	18.358171	19.819204	12.540809
O	17.681427	17.241091	12.376733
O	13.854223	2.879584	11.619389
O	13.845013	0.329328	12.383692
O	14.108102	17.573603	12.145876
O	9.751114	0.587418	9.602436
O	10.007195	16.914747	9.780564
O	7.087388	9.371633	9.031651
O	5.333060	8.549008	12.123526
O	3.757929	9.034544	0.746905
O	1.925716	8.622834	12.032254
O	2.090096	9.120707	9.367833
O	4.674136	9.364668	9.788728
O	7.261979	13.258306	10.115674
O	6.182393	13.024492	12.467871
O	3.832811	12.766999	0.251868
O	1.752325	13.525549	12.114426

O	2.169984	13.016732	9.454956
O	4.672935	12.842417	10.296746
O	6.421455	10.854706	11.042849
O	1.746319	11.092300	11.208262
O	8.762428	7.538935	8.116790
O	8.670927	10.120035	7.195905
O	7.765332	12.681234	7.538242
O	3.672435	7.316663	8.292776
O	3.749920	9.780955	7.359713
O	4.165377	12.430309	7.692014
O	19.855017	9.362082	10.464302
O	19.782936	12.776950	10.456272
O	2.896382	11.184432	2.830505
O	3.843223	11.362130	5.283608
O	6.083084	10.849531	6.690430
O	8.089289	11.603306	5.121273
O	7.925909	10.860277	2.583187
O	5.434772	10.530749	3.337051
O	3.082587	6.553736	3.099369
O	3.838217	6.804065	5.665158
O	6.074074	7.288407	7.195103
O	8.180989	6.546174	5.372338
O	8.020613	7.044644	2.765463
O	5.581533	7.206224	3.749917
O	3.505251	8.945596	4.179244
O	8.432064	9.033548	4.505922
O	1.339071	12.515476	1.165793
O	1.339272	9.871695	0.921420
O	1.835217	7.210004	0.777017
O	6.083885	12.610593	1.748355
O	6.098701	10.206396	0.746504
O	5.996989	7.619925	1.164856
O	10.257471	10.855502	3.755002
O	10.364187	7.216771	4.000179
O	8.598648	14.913107	8.614102
O	3.841221	14.820377	8.616913
O	5.343671	14.897187	0.760690
O	2.406644	14.917684	0.917672
O	1.328059	4.960025	1.934245
O	6.260679	5.166576	2.014543
O	4.599453	4.988281	7.368412
O	7.513455	4.904507	7.617872
O	11.592338	4.977138	4.843040
O	16.511543	5.062107	5.100931

O	14.764823	5.052555	12.797226
O	17.850815	4.954453	12.465596
O	18.775431	14.998672	11.619925
O	14.010594	14.942557	11.710661
O	15.354872	14.995090	6.110277
O	12.443272	14.979967	5.691389
Al	4.501946	18.753216	7.042403
Al	6.163172	3.539037	2.554413
Al	17.822783	6.461802	13.309260
Al	11.422951	12.511894	9.033525
Al	16.167564	3.492076	4.473268
Al	7.797568	6.532245	7.032499
H	6.147154	8.057702	7.825843
H	19.253155	6.748547	11.363104
H	11.496832	13.756178	11.166776
H	18.594431	3.626394	4.381594
H	2.967661	16.920916	7.091250
H	8.438472	2.788646	15.579552
Pt	7.038333	4.848193	-3.603641
Pt	9.374901	8.178290	-1.194433
Pt	8.983271	6.486279	-3.176455
Pt	6.711174	4.715068	-1.130997
Pt	6.934219	7.374968	-1.978811
Pt	8.989677	5.706237	-0.796556

300

#### Pt6H1@H-MFI

Si	8.419651	1.020620	8.757032
Si	6.040437	0.631793	10.841301
Si	5.621577	1.171056	0.347958
Si	2.435276	1.284281	0.172908
Si	1.375511	0.536875	10.821494
Si	3.656818	1.255229	9.079027
Si	8.615267	16.459259	9.062968
Si	6.162371	17.304569	10.917718
Si	5.418954	16.476969	0.467067
Si	2.378814	16.469208	0.436554
Si	1.370906	17.354116	11.014343
Si	3.624182	16.307629	9.184217
Si	1.535888	18.834204	2.050008
Si	3.935724	19.355558	4.068566
Si	7.670028	18.460501	6.936275
Si	8.641094	19.257854	4.147392
Si	6.401834	18.689341	2.205117
Si	1.611771	3.410092	2.322218

Si	3.853634	2.660894	4.412241
Si	4.498943	3.361538	7.265631
Si	7.534278	3.349002	7.140500
Si	8.713975	2.472252	4.446100
Si	11.616963	11.014296	4.625432
Si	14.181783	10.510851	2.749671
Si	14.473102	11.068421	13.126449
Si	17.669214	11.228209	13.242613
Si	18.730980	10.530949	2.682756
Si	16.503132	11.351385	4.555841
Si	11.768531	6.569257	4.511811
Si	14.246654	7.334374	2.573952
Si	14.794655	6.655221	13.054582
Si	18.924795	7.396458	2.706846
Si	16.535368	6.530056	4.448242
Si	18.550783	8.950769	11.318807
Si	16.176575	9.482271	9.359670
Si	15.618561	8.917737	6.426651
Si	12.444273	8.675367	6.589656
Si	11.478211	9.473914	9.304263
Si	13.710065	8.749591	11.136663
Si	18.473497	13.465056	11.159950
Si	16.105896	12.662728	9.301586
Si	15.504235	13.417100	6.322130
Si	12.503539	13.441774	6.264047
Si	13.777739	13.427845	11.193274
Si	11.552694	18.795601	4.646042
Si	13.956135	19.313971	2.640198
Si	14.383404	18.871813	13.084425
Si	17.522453	18.619495	13.223207
Si	18.612452	19.344416	2.556287
Si	16.397617	18.623474	4.409698
Si	11.746507	3.404520	4.484777
Si	13.946123	2.645771	2.417371
Si	14.655903	3.452079	12.925971
Si	17.699047	3.450089	12.989675
Si	18.671915	2.515831	2.405728
Si	18.480705	1.055244	11.381037
Si	16.083872	0.528716	9.405037
Si	15.542477	0.987985	6.472554
Si	12.452482	1.215630	6.566905
Si	11.358280	0.502848	9.326345
Si	13.617962	1.344376	11.127698
Si	18.441862	16.517962	11.131310

Si	16.211412	17.232534	9.164411
Si	15.441566	16.585220	6.236210
Si	12.415442	16.478760	6.320256
Si	11.503839	17.246464	9.251801
Si	13.861430	16.439360	11.030670
Si	8.615066	9.143989	8.522830
Si	6.186598	9.307757	10.494413
Si	5.335663	8.829783	0.333638
Si	2.250273	8.692879	0.253742
Si	1.438781	9.554704	10.787768
Si	3.569722	8.906395	8.727591
Si	8.376804	13.327952	8.922581
Si	6.137944	12.440854	10.951844
Si	5.370701	13.309247	0.454621
Si	2.338770	13.427447	0.259630
Si	1.354889	12.625119	10.814802
Si	3.738107	13.232836	9.031919
Si	1.507056	11.112398	1.985636
Si	3.9111698	10.499707	3.899271
Si	4.481324	11.121751	6.771397
Si	7.655411	11.312383	6.669150
Si	8.678135	10.566567	3.998439
Si	6.383414	11.047527	2.108090
Si	1.681648	6.517719	2.254233
Si	4.013410	7.394468	4.144180
Si	4.487531	6.564481	7.118418
Si	8.751016	7.454762	4.176032
Si	6.453891	6.712331	2.421921
O	7.169077	1.091858	9.778958
O	6.347975	1.325075	12.277164
O	4.014411	0.989179	0.161934
O	1.834416	1.495609	12.056210
O	2.087894	0.994751	9.445990
O	4.522970	1.080516	10.454265
O	7.489429	16.748194	10.195437
O	6.172182	16.746403	12.436287
O	3.896081	17.086079	0.416880
O	1.750523	16.495874	12.322665
O	2.153366	16.584623	9.789129
O	4.830708	16.755356	10.124105
O	6.089891	18.906836	10.882521
O	1.834816	18.899872	11.197958
O	8.588838	2.485783	8.033146
O	8.175983	19.900990	7.519908

O	8.515356	17.312527	7.697500
O	3.768741	2.824265	8.610889
O	4.167179	0.254906	7.948298
O	3.591346	17.255816	7.767493
O	19.803360	0.664030	10.527738
O	19.795950	17.322477	10.711084
O	2.760033	18.817888	3.086387
O	3.753124	18.662676	5.501484
O	6.115520	18.235443	7.190017
O	8.094494	18.329964	5.356412
O	7.917299	18.906239	2.748467
O	5.402135	18.988422	3.441037
O	2.592649	3.322735	3.600295
O	3.582336	2.907244	6.006960
O	6.015209	2.739296	7.114938
O	8.091290	3.395167	5.596503
O	7.937321	2.998183	3.009971
O	5.260380	3.319352	4.004729
O	3.835814	1.074944	4.097072
O	8.342767	0.915553	4.600272
O	1.416156	17.330637	1.422345
O	1.669835	0.005970	0.832556
O	2.172787	2.658307	1.002253
O	6.256074	17.157116	1.677158
O	6.172582	19.649267	0.924230
O	5.998391	2.419719	1.259073
O	10.210819	19.067820	3.770393
O	10.273889	2.734521	4.178976
O	12.847116	10.781079	3.600696
O	13.929505	11.104439	1.256931
O	16.086075	11.026832	12.978030
O	18.102489	11.360340	1.412040
O	17.991369	11.016484	4.031897
O	15.434559	11.356758	3.336783
O	12.931007	6.879482	3.419356
O	13.918492	6.974998	1.018982
O	16.280289	7.225725	13.288248
O	18.678524	6.478517	1.414717
O	18.086273	6.891024	4.019718
O	15.591331	6.556124	3.092811
O	14.582422	8.934452	2.758236
O	18.523954	8.953157	2.353133
O	11.595741	12.510303	5.271965
O	11.676630	9.863537	5.779315

O	12.258269	7.211398	5.922112
O	16.518751	12.847192	5.190061
O	16.098690	10.280221	5.695939
O	15.944519	7.622113	5.521157
O	0.252878	10.944450	3.003948
O	0.506156	7.289800	3.097763
O	17.265770	8.785010	10.369148
O	16.418039	8.871770	7.869204
O	14.023008	9.040514	6.696050
O	11.763926	8.471801	8.045324
O	12.169170	8.786801	10.625031
O	14.671120	9.187568	9.880134
O	17.204905	13.512018	10.137088
O	16.184183	13.104685	7.766557
O	14.016001	12.770183	6.188701
O	12.010197	13.509829	7.781010
O	12.165566	13.284970	10.631188
O	14.603045	13.011758	9.872773
O	16.440264	11.088320	9.454420
O	12.094689	10.932909	9.039815
O	18.849112	7.396259	11.974305
O	18.362377	9.869108	12.627530
O	18.108898	12.592087	12.479648
O	14.096889	7.289402	11.711999
O	13.846614	9.790308	12.379542
O	13.929706	12.452596	12.454086
O	9.842614	9.537192	9.529499
O	9.743106	12.614175	9.376130
O	12.849117	18.742073	3.677381
O	13.677028	18.666655	1.160975
O	15.976154	19.067421	13.300829
O	18.111101	18.393839	1.337765
O	17.928699	18.899672	3.945576
O	15.439565	18.825052	3.105124
O	12.587030	3.237169	3.112217
O	13.776537	2.983258	0.833359
O	16.178577	2.824066	12.963711
O	18.187183	3.412678	1.180648
O	17.944317	3.135287	3.840386
O	15.272581	3.316367	3.011844
O	13.928704	1.029375	2.665760
O	18.186382	0.993557	2.185444
O	11.424552	17.343571	5.362836
O	11.597342	0.083576	5.766066

O	12.427254	2.647363	5.767404
O	16.265272	17.086874	4.931100
O	16.096487	19.571661	5.683493
O	15.772330	2.336939	5.673991
O	0.175393	19.230194	2.844691
O	0.217839	2.657114	2.768006
O	17.201500	1.165285	10.389625
O	16.349564	1.060020	7.898781
O	13.962541	0.672387	6.772333
O	11.756518	1.408451	8.025517
O	12.086279	1.158918	10.623827
O	14.597439	0.993159	9.872238
O	17.521051	16.502241	9.792476
O	16.270277	17.007477	7.568756
O	13.914889	17.165674	6.281579
O	11.849821	16.499653	7.853546
O	12.357778	16.574474	10.465239
O	14.881951	16.505623	9.773337
O	16.186184	18.807541	9.541678
O	11.838408	18.840773	9.117303
O	18.688334	2.484788	12.124195
O	18.358171	19.819204	12.540809
O	17.681427	17.241091	12.376733
O	13.854223	2.879584	11.619389
O	13.845013	0.329328	12.383692
O	14.108102	17.573603	12.145876
O	9.751114	0.587418	9.602436
O	10.007195	16.914747	9.780564
O	7.087388	9.371633	9.031651
O	5.333060	8.549008	12.123526
O	3.757929	9.034544	0.746905
O	1.925716	8.622834	12.032254
O	2.090096	9.120707	9.367833
O	4.674136	9.364668	9.788728
O	7.261979	13.258306	10.115674
O	6.182393	13.024492	12.467871
O	3.832811	12.766999	0.251868
O	1.752325	13.525549	12.114426
O	2.169984	13.016732	9.454956
O	4.672935	12.842417	10.296746
O	6.421455	10.854706	11.042849
O	1.746319	11.092300	11.208262
O	8.762428	7.538935	8.116790
O	8.670927	10.120035	7.195905

O	7.765332	12.681234	7.538242
O	3.672435	7.316663	8.292776
O	3.749920	9.780955	7.359713
O	4.165377	12.430309	7.692014
O	19.855017	9.362082	10.464302
O	19.782936	12.776950	10.456272
O	2.896382	11.184432	2.830505
O	3.843223	11.362130	5.283608
O	6.083084	10.849531	6.690430
O	8.089289	11.603306	5.121273
O	7.925909	10.860277	2.583187
O	5.434772	10.530749	3.337051
O	3.082587	6.553736	3.099369
O	3.838217	6.804065	5.665158
O	6.074074	7.288407	7.195103
O	8.180989	6.546174	5.372338
O	8.020613	7.044644	2.765463
O	5.581533	7.206224	3.749917
O	3.505251	8.945596	4.179244
O	8.432064	9.033548	4.505922
O	1.339071	12.515476	1.165793
O	1.339272	9.871695	0.921420
O	1.835217	7.210004	0.777017
O	6.083885	12.610593	1.748355
O	6.098701	10.206396	0.746504
O	5.996989	7.619925	1.164856
O	10.257471	10.855502	3.755002
O	10.364187	7.216771	4.000179
O	8.598648	14.913107	8.614102
O	3.841221	14.820377	8.616913
O	5.343671	14.897187	0.760690
O	2.406644	14.917684	0.917672
O	1.328059	4.960025	1.934245
O	6.260679	5.166576	2.014543
O	4.599453	4.988281	7.368412
O	7.513455	4.904507	7.617872
O	11.592338	4.977138	4.843040
O	16.511543	5.062107	5.100931
O	14.764823	5.052555	12.797226
O	17.850815	4.954453	12.465596
O	18.775431	14.998672	11.619925
O	14.010594	14.942557	11.710661
O	15.354872	14.995090	6.110277
O	12.443272	14.979967	5.691389

Al	4.501946	18.753216	7.042403
Al	6.163172	3.539037	2.554413
Al	17.822783	6.461802	13.309260
Al	11.422951	12.511894	9.033525
Al	16.167564	3.492076	4.473268
Al	7.797568	6.532245	7.032499
H	6.147154	8.057702	7.825843
H	19.253155	6.748547	11.363104
H	11.496832	13.756178	11.166776
H	18.594431	3.626394	4.381594
H	2.967661	16.920916	7.091250
H	8.438472	5.431432	13.199118
Pt	7.038333	4.848193	-3.603641
Pt	9.374901	8.178290	-1.194433
Pt	8.983271	6.486279	-3.176455
Pt	6.711174	4.715068	-1.130997
Pt	6.934219	7.374968	-1.978811
Pt	8.989677	5.706237	-0.796556

300

#### Pt6H2@H-MFI

Si	8.419651	1.020620	8.757032
Si	6.040437	0.631793	10.841301
Si	5.621577	1.171056	0.347958
Si	2.435276	1.284281	0.172908
Si	1.375511	0.536875	10.821494
Si	3.656818	1.255229	9.079027
Si	8.615267	16.459259	9.062968
Si	6.162371	17.304569	10.917718
Si	5.418954	16.476969	0.467067
Si	2.378814	16.469208	0.436554
Si	1.370906	17.354116	11.014343
Si	3.624182	16.307629	9.184217
Si	1.535888	18.834204	2.050008
Si	3.935724	19.355558	4.068566
Si	7.670028	18.460501	6.936275
Si	8.641094	19.257854	4.147392
Si	6.401834	18.689341	2.205117
Si	1.611771	3.410092	2.322218
Si	3.853634	2.660894	4.412241
Si	4.498943	3.361538	7.265631
Si	7.534278	3.349002	7.140500
Si	8.713975	2.472252	4.446100
Si	11.616963	11.014296	4.625432
Si	14.181783	10.510851	2.749671

Si	14.473102	11.068421	13.126449
Si	17.669214	11.228209	13.242613
Si	18.730980	10.530949	2.682756
Si	16.503132	11.351385	4.555841
Si	11.768531	6.569257	4.511811
Si	14.246654	7.334374	2.573952
Si	14.794655	6.655221	13.054582
Si	18.924795	7.396458	2.706846
Si	16.535368	6.530056	4.448242
Si	18.550783	8.950769	11.318807
Si	16.176575	9.482271	9.359670
Si	15.618561	8.917737	6.426651
Si	12.444273	8.675367	6.589656
Si	11.478211	9.473914	9.304263
Si	13.710065	8.749591	11.136663
Si	18.473497	13.465056	11.159950
Si	16.105896	12.662728	9.301586
Si	15.504235	13.417100	6.322130
Si	12.503539	13.441774	6.264047
Si	13.777739	13.427845	11.193274
Si	11.552694	18.795601	4.646042
Si	13.956135	19.313971	2.640198
Si	14.383404	18.871813	13.084425
Si	17.522453	18.619495	13.223207
Si	18.612452	19.344416	2.556287
Si	16.397617	18.623474	4.409698
Si	11.746507	3.404520	4.484777
Si	13.946123	2.645771	2.417371
Si	14.655903	3.452079	12.925971
Si	17.699047	3.450089	12.989675
Si	18.671915	2.515831	2.405728
Si	18.480705	1.055244	11.381037
Si	16.083872	0.528716	9.405037
Si	15.542477	0.987985	6.472554
Si	12.452482	1.215630	6.566905
Si	11.358280	0.502848	9.326345
Si	13.617962	1.344376	11.127698
Si	18.441862	16.517962	11.131310
Si	16.211412	17.232534	9.164411
Si	15.441566	16.585220	6.236210
Si	12.415442	16.478760	6.320256
Si	11.503839	17.246464	9.251801
Si	13.861430	16.439360	11.030670
Si	8.615066	9.143989	8.522830

Si	6.186598	9.307757	10.494413
Si	5.335663	8.829783	0.333638
Si	2.250273	8.692879	0.253742
Si	1.438781	9.554704	10.787768
Si	3.569722	8.906395	8.727591
Si	8.376804	13.327952	8.922581
Si	6.137944	12.440854	10.951844
Si	5.370701	13.309247	0.454621
Si	2.338770	13.427447	0.259630
Si	1.354889	12.625119	10.814802
Si	3.738107	13.232836	9.031919
Si	1.507056	11.112398	1.985636
Si	3.911698	10.499707	3.899271
Si	4.481324	11.121751	6.771397
Si	7.655411	11.312383	6.669150
Si	8.678135	10.566567	3.998439
Si	6.383414	11.047527	2.108090
Si	1.681648	6.517719	2.254233
Si	4.013410	7.394468	4.144180
Si	4.487531	6.564481	7.118418
Si	8.751016	7.454762	4.176032
Si	6.453891	6.712331	2.421921
O	7.169077	1.091858	9.778958
O	6.347975	1.325075	12.277164
O	4.014411	0.989179	0.161934
O	1.834416	1.495609	12.056210
O	2.087894	0.994751	9.445990
O	4.522970	1.080516	10.454265
O	7.489429	16.748194	10.195437
O	6.172182	16.746403	12.436287
O	3.896081	17.086079	0.416880
O	1.750523	16.495874	12.322665
O	2.153366	16.584623	9.789129
O	4.830708	16.755356	10.124105
O	6.089891	18.906836	10.882521
O	1.834816	18.899872	11.197958
O	8.588838	2.485783	8.033146
O	8.175983	19.900990	7.519908
O	8.515356	17.312527	7.697500
O	3.768741	2.824265	8.610889
O	4.167179	0.254906	7.948298
O	3.591346	17.255816	7.767493
O	19.803360	0.664030	10.527738
O	19.795950	17.322477	10.711084

O	2.760033	18.817888	3.086387
O	3.753124	18.662676	5.501484
O	6.115520	18.235443	7.190017
O	8.094494	18.329964	5.356412
O	7.917299	18.906239	2.748467
O	5.402135	18.988422	3.441037
O	2.592649	3.322735	3.600295
O	3.582336	2.907244	6.006960
O	6.015209	2.739296	7.114938
O	8.091290	3.395167	5.596503
O	7.937321	2.998183	3.009971
O	5.260380	3.319352	4.004729
O	3.835814	1.074944	4.097072
O	8.342767	0.915553	4.600272
O	1.416156	17.330637	1.422345
O	1.669835	0.005970	0.832556
O	2.172787	2.658307	1.002253
O	6.256074	17.157116	1.677158
O	6.172582	19.649267	0.924230
O	5.998391	2.419719	1.259073
O	10.210819	19.067820	3.770393
O	10.273889	2.734521	4.178976
O	12.847116	10.781079	3.600696
O	13.929505	11.104439	1.256931
O	16.086075	11.026832	12.978030
O	18.102489	11.360340	1.412040
O	17.991369	11.016484	4.031897
O	15.434559	11.356758	3.336783
O	12.931007	6.879482	3.419356
O	13.918492	6.974998	1.018982
O	16.280289	7.225725	13.288248
O	18.678524	6.478517	1.414717
O	18.086273	6.891024	4.019718
O	15.591331	6.556124	3.092811
O	14.582422	8.934452	2.758236
O	18.523954	8.953157	2.353133
O	11.595741	12.510303	5.271965
O	11.676630	9.863537	5.779315
O	12.258269	7.211398	5.922112
O	16.518751	12.847192	5.190061
O	16.098690	10.280221	5.695939
O	15.944519	7.622113	5.521157
O	0.252878	10.944450	3.003948
O	0.506156	7.289800	3.097763

O	17.265770	8.785010	10.369148
O	16.418039	8.871770	7.869204
O	14.023008	9.040514	6.696050
O	11.763926	8.471801	8.045324
O	12.169170	8.786801	10.625031
O	14.671120	9.187568	9.880134
O	17.204905	13.512018	10.137088
O	16.184183	13.104685	7.766557
O	14.016001	12.770183	6.188701
O	12.010197	13.509829	7.781010
O	12.165566	13.284970	10.631188
O	14.603045	13.011758	9.872773
O	16.440264	11.088320	9.454420
O	12.094689	10.932909	9.039815
O	18.849112	7.396259	11.974305
O	18.362377	9.869108	12.627530
O	18.108898	12.592087	12.479648
O	14.096889	7.289402	11.711999
O	13.846614	9.790308	12.379542
O	13.929706	12.452596	12.454086
O	9.842614	9.537192	9.529499
O	9.743106	12.614175	9.376130
O	12.849117	18.742073	3.677381
O	13.677028	18.666655	1.160975
O	15.976154	19.067421	13.300829
O	18.111101	18.393839	1.337765
O	17.928699	18.899672	3.945576
O	15.439565	18.825052	3.105124
O	12.587030	3.237169	3.112217
O	13.776537	2.983258	0.833359
O	16.178577	2.824066	12.963711
O	18.187183	3.412678	1.180648
O	17.944317	3.135287	3.840386
O	15.272581	3.316367	3.011844
O	13.928704	1.029375	2.665760
O	18.186382	0.993557	2.185444
O	11.424552	17.343571	5.362836
O	11.597342	0.083576	5.766066
O	12.427254	2.647363	5.767404
O	16.265272	17.086874	4.931100
O	16.096487	19.571661	5.683493
O	15.772330	2.336939	5.673991
O	0.175393	19.230194	2.844691
O	0.217839	2.657114	2.768006

O	17.201500	1.165285	10.389625
O	16.349564	1.060020	7.898781
O	13.962541	0.672387	6.772333
O	11.756518	1.408451	8.025517
O	12.086279	1.158918	10.623827
O	14.597439	0.993159	9.872238
O	17.521051	16.502241	9.792476
O	16.270277	17.007477	7.568756
O	13.914889	17.165674	6.281579
O	11.849821	16.499653	7.853546
O	12.357778	16.574474	10.465239
O	14.881951	16.505623	9.773337
O	16.186184	18.807541	9.541678
O	11.838408	18.840773	9.117303
O	18.688334	2.484788	12.124195
O	18.358171	19.819204	12.540809
O	17.681427	17.241091	12.376733
O	13.854223	2.879584	11.619389
O	13.845013	0.329328	12.383692
O	14.108102	17.573603	12.145876
O	9.751114	0.587418	9.602436
O	10.007195	16.914747	9.780564
O	7.087388	9.371633	9.031651
O	5.333060	8.549008	12.123526
O	3.757929	9.034544	0.746905
O	1.925716	8.622834	12.032254
O	2.090096	9.120707	9.367833
O	4.674136	9.364668	9.788728
O	7.261979	13.258306	10.115674
O	6.182393	13.024492	12.467871
O	3.832811	12.766999	0.251868
O	1.752325	13.525549	12.114426
O	2.169984	13.016732	9.454956
O	4.672935	12.842417	10.296746
O	6.421455	10.854706	11.042849
O	1.746319	11.092300	11.208262
O	8.762428	7.538935	8.116790
O	8.670927	10.120035	7.195905
O	7.765332	12.681234	7.538242
O	3.672435	7.316663	8.292776
O	3.749920	9.780955	7.359713
O	4.165377	12.430309	7.692014
O	19.855017	9.362082	10.464302
O	19.782936	12.776950	10.456272

O	2.896382	11.184432	2.830505
O	3.843223	11.362130	5.283608
O	6.083084	10.849531	6.690430
O	8.089289	11.603306	5.121273
O	7.925909	10.860277	2.583187
O	5.434772	10.530749	3.337051
O	3.082587	6.553736	3.099369
O	3.838217	6.804065	5.665158
O	6.074074	7.288407	7.195103
O	8.180989	6.546174	5.372338
O	8.020613	7.044644	2.765463
O	5.581533	7.206224	3.749917
O	3.505251	8.945596	4.179244
O	8.432064	9.033548	4.505922
O	1.339071	12.515476	1.165793
O	1.339272	9.871695	0.921420
O	1.835217	7.210004	0.777017
O	6.083885	12.610593	1.748355
O	6.098701	10.206396	0.746504
O	5.996989	7.619925	1.164856
O	10.257471	10.855502	3.755002
O	10.364187	7.216771	4.000179
O	8.598648	14.913107	8.614102
O	3.841221	14.820377	8.616913
O	5.343671	14.897187	0.760690
O	2.406644	14.917684	0.917672
O	1.328059	4.960025	1.934245
O	6.260679	5.166576	2.014543
O	4.599453	4.988281	7.368412
O	7.513455	4.904507	7.617872
O	11.592338	4.977138	4.843040
O	16.511543	5.062107	5.100931
O	14.764823	5.052555	12.797226
O	17.850815	4.954453	12.465596
O	18.775431	14.998672	11.619925
O	14.010594	14.942557	11.710661
O	15.354872	14.995090	6.110277
O	12.443272	14.979967	5.691389
Al	4.501946	18.753216	7.042403
Al	6.163172	3.539037	2.554413
Al	17.822783	6.461802	13.309260
Al	11.422951	12.511894	9.033525
Al	16.167564	3.492076	4.473268
Al	7.797568	6.532245	7.032499

H	9.008698	5.888910	9.361811
H	19.253155	6.748547	11.363104
H	11.496832	13.756178	11.166776
H	18.594431	3.626394	4.381594
H	2.967661	16.920916	7.091250
H	8.438472	5.431432	13.199118
Pt	7.038333	3.250303	-3.068990
Pt	9.374901	6.926643	-1.783954
Pt	8.983271	5.250351	-3.100172
Pt	6.711174	4.715068	-1.130997
Pt	6.934219	6.789539	-2.411483
Pt	8.989677	5.706237	-0.796556
	300		
	Pt6H3@H-MFI		
Si	8.419651	1.020620	8.757032
Si	6.040437	0.631793	10.841301
Si	5.621577	1.171056	0.347958
Si	2.435276	1.284281	0.172908
Si	1.375511	0.536875	10.821494
Si	3.656818	1.255229	9.079027
Si	8.615267	16.459259	9.062968
Si	6.162371	17.304569	10.917718
Si	5.418954	16.476969	0.467067
Si	2.378814	16.469208	0.436554
Si	1.370906	17.354116	11.014343
Si	3.624182	16.307629	9.184217
Si	1.535888	18.834204	2.050008
Si	3.935724	19.355558	4.068566
Si	7.670028	18.460501	6.936275
Si	8.641094	19.257854	4.147392
Si	6.401834	18.689341	2.205117
Si	1.611771	3.410092	2.322218
Si	3.853634	2.660894	4.412241
Si	4.498943	3.361538	7.265631
Si	7.534278	3.349002	7.140500
Si	8.713975	2.472252	4.446100
Si	11.616963	11.014296	4.625432
Si	14.181783	10.510851	2.749671
Si	14.473102	11.068421	13.126449
Si	17.669214	11.228209	13.242613
Si	18.730980	10.530949	2.682756
Si	16.503132	11.351385	4.555841
Si	11.768531	6.569257	4.511811
Si	14.246654	7.334374	2.573952

Si	14.794655	6.655221	13.054582
Si	18.924795	7.396458	2.706846
Si	16.535368	6.530056	4.448242
Si	18.550783	8.950769	11.318807
Si	16.176575	9.482271	9.359670
Si	15.618561	8.917737	6.426651
Si	12.444273	8.675367	6.589656
Si	11.478211	9.473914	9.304263
Si	13.710065	8.749591	11.136663
Si	18.473497	13.465056	11.159950
Si	16.105896	12.662728	9.301586
Si	15.504235	13.417100	6.322130
Si	12.503539	13.441774	6.264047
Si	13.777739	13.427845	11.193274
Si	11.552694	18.795601	4.646042
Si	13.956135	19.313971	2.640198
Si	14.383404	18.871813	13.084425
Si	17.522453	18.619495	13.223207
Si	18.612452	19.344416	2.556287
Si	16.397617	18.623474	4.409698
Si	11.746507	3.404520	4.484777
Si	13.946123	2.645771	2.417371
Si	14.655903	3.452079	12.925971
Si	17.699047	3.450089	12.989675
Si	18.671915	2.515831	2.405728
Si	18.480705	1.055244	11.381037
Si	16.083872	0.528716	9.405037
Si	15.542477	0.987985	6.472554
Si	12.452482	1.215630	6.566905
Si	11.358280	0.502848	9.326345
Si	13.617962	1.344376	11.127698
Si	18.441862	16.517962	11.131310
Si	16.211412	17.232534	9.164411
Si	15.441566	16.585220	6.236210
Si	12.415442	16.478760	6.320256
Si	11.503839	17.246464	9.251801
Si	13.861430	16.439360	11.030670
Si	8.615066	9.143989	8.522830
Si	6.186598	9.307757	10.494413
Si	5.335663	8.829783	0.333638
Si	2.250273	8.692879	0.253742
Si	1.438781	9.554704	10.787768
Si	3.569722	8.906395	8.727591
Si	8.376804	13.327952	8.922581

Si	6.137944	12.440854	10.951844
Si	5.370701	13.309247	0.454621
Si	2.338770	13.427447	0.259630
Si	1.354889	12.625119	10.814802
Si	3.738107	13.232836	9.031919
Si	1.507056	11.112398	1.985636
Si	3.911698	10.499707	3.899271
Si	4.481324	11.121751	6.771397
Si	7.655411	11.312383	6.669150
Si	8.678135	10.566567	3.998439
Si	6.383414	11.047527	2.108090
Si	1.681648	6.517719	2.254233
Si	4.013410	7.394468	4.144180
Si	4.487531	6.564481	7.118418
Si	8.751016	7.454762	4.176032
Si	6.453891	6.712331	2.421921
O	7.169077	1.091858	9.778958
O	6.347975	1.325075	12.277164
O	4.014411	0.989179	0.161934
O	1.834416	1.495609	12.056210
O	2.087894	0.994751	9.445990
O	4.522970	1.080516	10.454265
O	7.489429	16.748194	10.195437
O	6.172182	16.746403	12.436287
O	3.896081	17.086079	0.416880
O	1.750523	16.495874	12.322665
O	2.153366	16.584623	9.789129
O	4.830708	16.755356	10.124105
O	6.089891	18.906836	10.882521
O	1.834816	18.899872	11.197958
O	8.588838	2.485783	8.033146
O	8.175983	19.900990	7.519908
O	8.515356	17.312527	7.697500
O	3.768741	2.824265	8.610889
O	4.167179	0.254906	7.948298
O	3.591346	17.255816	7.767493
O	19.803360	0.664030	10.527738
O	19.795950	17.322477	10.711084
O	2.760033	18.817888	3.086387
O	3.753124	18.662676	5.501484
O	6.115520	18.235443	7.190017
O	8.094494	18.329964	5.356412
O	7.917299	18.906239	2.748467
O	5.402135	18.988422	3.441037

O	2.592649	3.322735	3.600295
O	3.582336	2.907244	6.006960
O	6.015209	2.739296	7.114938
O	8.091290	3.395167	5.596503
O	7.937321	2.998183	3.009971
O	5.260380	3.319352	4.004729
O	3.835814	1.074944	4.097072
O	8.342767	0.915553	4.600272
O	1.416156	17.330637	1.422345
O	1.669835	0.005970	0.832556
O	2.172787	2.658307	1.002253
O	6.256074	17.157116	1.677158
O	6.172582	19.649267	0.924230
O	5.998391	2.419719	1.259073
O	10.210819	19.067820	3.770393
O	10.273889	2.734521	4.178976
O	12.847116	10.781079	3.600696
O	13.929505	11.104439	1.256931
O	16.086075	11.026832	12.978030
O	18.102489	11.360340	1.412040
O	17.991369	11.016484	4.031897
O	15.434559	11.356758	3.336783
O	12.931007	6.879482	3.419356
O	13.918492	6.974998	1.018982
O	16.280289	7.225725	13.288248
O	18.678524	6.478517	1.414717
O	18.086273	6.891024	4.019718
O	15.591331	6.556124	3.092811
O	14.582422	8.934452	2.758236
O	18.523954	8.953157	2.353133
O	11.595741	12.510303	5.271965
O	11.676630	9.863537	5.779315
O	12.258269	7.211398	5.922112
O	16.518751	12.847192	5.190061
O	16.098690	10.280221	5.695939
O	15.944519	7.622113	5.521157
O	0.252878	10.944450	3.003948
O	0.506156	7.289800	3.097763
O	17.265770	8.785010	10.369148
O	16.418039	8.871770	7.869204
O	14.023008	9.040514	6.696050
O	11.763926	8.471801	8.045324
O	12.169170	8.786801	10.625031
O	14.671120	9.187568	9.880134

O	17.204905	13.512018	10.137088
O	16.184183	13.104685	7.766557
O	14.016001	12.770183	6.188701
O	12.010197	13.509829	7.781010
O	12.165566	13.284970	10.631188
O	14.603045	13.011758	9.872773
O	16.440264	11.088320	9.454420
O	12.094689	10.932909	9.039815
O	18.849112	7.396259	11.974305
O	18.362377	9.869108	12.627530
O	18.108898	12.592087	12.479648
O	14.096889	7.289402	11.711999
O	13.846614	9.790308	12.379542
O	13.929706	12.452596	12.454086
O	9.842614	9.537192	9.529499
O	9.743106	12.614175	9.376130
O	12.849117	18.742073	3.677381
O	13.677028	18.666655	1.160975
O	15.976154	19.067421	13.300829
O	18.111101	18.393839	1.337765
O	17.928699	18.899672	3.945576
O	15.439565	18.825052	3.105124
O	12.587030	3.237169	3.112217
O	13.776537	2.983258	0.833359
O	16.178577	2.824066	12.963711
O	18.187183	3.412678	1.180648
O	17.944317	3.135287	3.840386
O	15.272581	3.316367	3.011844
O	13.928704	1.029375	2.665760
O	18.186382	0.993557	2.185444
O	11.424552	17.343571	5.362836
O	11.597342	0.083576	5.766066
O	12.427254	2.647363	5.767404
O	16.265272	17.086874	4.931100
O	16.096487	19.571661	5.683493
O	15.772330	2.336939	5.673991
O	0.175393	19.230194	2.844691
O	0.217839	2.657114	2.768006
O	17.201500	1.165285	10.389625
O	16.349564	1.060020	7.898781
O	13.962541	0.672387	6.772333
O	11.756518	1.408451	8.025517
O	12.086279	1.158918	10.623827
O	14.597439	0.993159	9.872238

O	17.521051	16.502241	9.792476
O	16.270277	17.007477	7.568756
O	13.914889	17.165674	6.281579
O	11.849821	16.499653	7.853546
O	12.357778	16.574474	10.465239
O	14.881951	16.505623	9.773337
O	16.186184	18.807541	9.541678
O	11.838408	18.840773	9.117303
O	18.688334	2.484788	12.124195
O	18.358171	19.819204	12.540809
O	17.681427	17.241091	12.376733
O	13.854223	2.879584	11.619389
O	13.845013	0.329328	12.383692
O	14.108102	17.573603	12.145876
O	9.751114	0.587418	9.602436
O	10.007195	16.914747	9.780564
O	7.087388	9.371633	9.031651
O	5.333060	8.549008	12.123526
O	3.757929	9.034544	0.746905
O	1.925716	8.622834	12.032254
O	2.090096	9.120707	9.367833
O	4.674136	9.364668	9.788728
O	7.261979	13.258306	10.115674
O	6.182393	13.024492	12.467871
O	3.832811	12.766999	0.251868
O	1.752325	13.525549	12.114426
O	2.169984	13.016732	9.454956
O	4.672935	12.842417	10.296746
O	6.421455	10.854706	11.042849
O	1.746319	11.092300	11.208262
O	8.762428	7.538935	8.116790
O	8.670927	10.120035	7.195905
O	7.765332	12.681234	7.538242
O	3.672435	7.316663	8.292776
O	3.749920	9.780955	7.359713
O	4.165377	12.430309	7.692014
O	19.855017	9.362082	10.464302
O	19.782936	12.776950	10.456272
O	2.896382	11.184432	2.830505
O	3.843223	11.362130	5.283608
O	6.083084	10.849531	6.690430
O	8.089289	11.603306	5.121273
O	7.925909	10.860277	2.583187
O	5.434772	10.530749	3.337051

O	3.082587	6.553736	3.099369
O	3.838217	6.804065	5.665158
O	6.074074	7.288407	7.195103
O	8.180989	6.546174	5.372338
O	8.020613	7.044644	2.765463
O	5.581533	7.206224	3.749917
O	3.505251	8.945596	4.179244
O	8.432064	9.033548	4.505922
O	1.339071	12.515476	1.165793
O	1.339272	9.871695	0.921420
O	1.835217	7.210004	0.777017
O	6.083885	12.610593	1.748355
O	6.098701	10.206396	0.746504
O	5.996989	7.619925	1.164856
O	10.257471	10.855502	3.755002
O	10.364187	7.216771	4.000179
O	8.598648	14.913107	8.614102
O	3.841221	14.820377	8.616913
O	5.343671	14.897187	0.760690
O	2.406644	14.917684	0.917672
O	1.328059	4.960025	1.934245
O	6.260679	5.166576	2.014543
O	4.599453	4.988281	7.368412
O	7.513455	4.904507	7.617872
O	11.592338	4.977138	4.843040
O	16.511543	5.062107	5.100931
O	14.764823	5.052555	12.797226
O	17.850815	4.954453	12.465596
O	18.775431	14.998672	11.619925
O	14.010594	14.942557	11.710661
O	15.354872	14.995090	6.110277
O	12.443272	14.979967	5.691389
Al	4.501946	18.753216	7.042403
Al	6.163172	3.539037	2.554413
Al	17.822783	6.461802	13.309260
Al	11.422951	12.511894	9.033525
Al	16.167564	3.492076	4.473268
Al	7.797568	6.532245	7.032499
H	9.008698	5.888910	9.361811
H	19.253155	6.748547	11.363104
H	9.076373	7.648977	12.056344
H	18.594431	3.626394	4.381594
H	2.967661	16.920916	7.091250
H	8.438472	5.431432	13.199118

Pt	7.038333	3.250303	-3.068990
Pt	9.374901	6.926643	-1.783954
Pt	8.983271	5.250351	-3.100172
Pt	6.711174	4.159687	-2.241653
Pt	6.934219	4.938335	-1.532220
Pt	8.989677	5.706237	-0.796556
	330		
	Pt <sub>6</sub> H <sub>1</sub> @H-MFI	+ H <sub>B</sub>	+ (H <sub>2</sub> O) <sub>10</sub>
Si	8.403434	1.067382	8.745122
Si	6.047845	0.654876	10.850402
Si	5.587739	1.171852	0.354248
Si	2.461104	1.271546	0.153102
Si	1.388125	0.543442	10.815070
Si	3.674838	1.261597	9.075682
Si	8.610261	16.466024	9.056009
Si	6.161370	17.321283	10.908350
Si	5.420956	16.500051	0.459706
Si	2.377412	16.474979	0.436420
Si	1.375511	17.357899	11.013942
Si	3.624382	16.318573	9.178731
Si	1.542094	18.840773	2.048670
Si	3.941130	19.368095	4.064819
Si	7.674432	18.481594	6.930789
Si	8.621874	19.349192	4.134143
Si	6.405638	18.701878	2.203110
Si	1.690457	3.389596	2.320880
Si	3.927916	2.678405	4.386412
Si	4.527374	3.343828	7.224277
Si	7.561708	3.321143	6.999711
Si	8.716578	2.587666	4.189147
Si	11.634583	11.029021	4.623827
Si	14.194197	10.515228	2.747128
Si	14.475305	11.073992	13.132337
Si	17.671217	11.228011	13.252516
Si	18.730381	10.547464	2.714742
Si	16.506536	11.352777	4.545804
Si	11.744104	6.491452	4.453863
Si	14.257265	7.344124	2.575960
Si	14.803465	6.642485	13.047355
Si	18.920589	7.409989	2.725849
Si	16.535368	6.521499	4.448509
Si	18.556589	8.952958	11.320145
Si	16.204405	9.490828	9.345081
Si	15.615358	8.917737	6.415944

Si	12.438267	8.660841	6.537462
Si	11.495431	9.483267	9.247386
Si	13.781343	8.754963	11.125288
Si	18.475300	13.464459	11.164635
Si	16.108500	12.669495	9.299981
Si	15.501833	13.418096	6.319319
Si	12.502136	13.455107	6.259229
Si	13.779541	13.433019	11.191669
Si	11.540280	18.836592	4.636406
Si	13.987770	19.362921	2.659871
Si	14.391613	18.840174	13.102626
Si	17.529861	18.619097	13.223207
Si	18.616655	19.348793	2.555484
Si	16.404825	18.625067	4.417461
Si	11.765727	3.423424	4.469655
Si	14.144742	2.681788	2.478264
Si	14.742198	3.438547	12.967324
Si	17.802361	3.451481	13.052842
Si	18.767820	2.495136	2.435572
Si	18.509537	1.062607	11.397365
Si	16.129723	0.509812	9.425915
Si	15.546081	0.992761	6.485670
Si	12.453884	1.229559	6.556600
Si	11.349270	0.524538	9.320189
Si	13.659408	1.291246	11.129035
Si	18.448872	16.516966	11.133853
Si	16.237442	17.236912	9.166552
Si	15.441967	16.586214	6.237816
Si	12.409435	16.501842	6.312761
Si	11.502439	17.258402	9.251133
Si	13.859828	16.442743	11.039905
Si	8.584833	9.265372	8.566860
Si	6.208822	9.300992	10.563871
Si	5.468609	8.793368	0.351304
Si	2.312541	8.672183	0.253073
Si	1.444387	9.551122	10.792319
Si	3.595751	8.856050	8.774162
Si	8.369396	13.323972	8.924990
Si	6.106710	12.442248	10.982090
Si	5.348076	13.343473	0.446323
Si	2.332162	13.433019	0.257355
Si	1.354288	12.623727	10.813732
Si	3.734303	13.244576	9.033391
Si	1.523074	11.115183	1.987911

Si	3.906292	10.511646	3.924164
Si	4.482125	11.107622	6.811278
Si	7.640795	11.332878	6.667812
Si	8.689147	10.586864	3.998974
Si	6.357786	11.084937	2.126425
Si	1.656820	6.482895	2.268151
Si	3.930919	7.394468	4.170411
Si	4.426664	6.541797	7.080142
Si	8.785254	7.415362	4.258203
Si	6.384816	6.628954	2.513328
O	7.168476	1.160709	9.786854
O	6.352580	1.326666	12.291616
O	4.011407	0.900430	0.007093
O	1.823403	1.500186	12.052998
O	2.097505	1.000323	9.439298
O	4.526774	1.079123	10.454398
O	7.488628	16.748989	10.192091
O	6.168778	16.745605	12.419157
O	3.891476	17.090853	0.414070
O	1.749923	16.495275	12.321059
O	2.153366	16.584623	9.788193
O	4.830908	16.757147	10.121831
O	6.096298	18.920567	10.877568
O	1.835217	18.901861	11.196218
O	8.581228	2.513244	8.007986
O	8.178987	19.910145	7.535700
O	8.515156	17.317305	7.691076
O	3.840820	2.822673	8.604065
O	4.168180	0.251523	7.946960
O	3.593148	17.260193	7.763077
O	19.810167	0.661841	10.520243
O	19.798553	17.322081	10.711351
O	2.761434	18.818285	3.086923
O	3.754125	18.664267	5.495327
O	6.123728	18.235046	7.190686
O	8.095896	18.410954	5.354538
O	7.920503	18.903454	2.744318
O	5.403738	18.986631	3.440769
O	2.673137	3.396759	3.593603
O	3.586541	2.911025	5.976982
O	6.031827	2.723178	7.026610
O	8.184994	3.395366	5.513261
O	8.014606	3.145236	2.852587
O	5.339266	3.315372	4.014766

O	3.833612	1.082307	4.093860
O	8.349774	1.005297	4.506458
O	1.415155	17.332825	1.422747
O	1.670035	0.011939	0.832423
O	2.259483	2.650746	0.997837
O	6.257275	17.162092	1.675418
O	6.170780	19.651258	0.921152
O	5.758327	2.402804	1.328263
O	10.196604	19.074982	3.760890
O	10.350973	2.727556	4.097340
O	12.933611	10.863859	3.681797
O	13.927904	11.107622	1.255593
O	16.086676	11.026235	12.977630
O	18.104092	11.357553	1.422211
O	18.019600	11.024244	4.087971
O	15.508040	11.345216	3.264248
O	12.949227	6.881671	3.424576
O	13.930507	6.969227	1.013628
O	16.289497	7.222740	13.215445
O	18.674118	6.548562	1.401602
O	18.082668	6.886646	4.025205
O	15.593934	6.554532	3.090804
O	14.595838	8.939626	2.762787
O	18.519548	8.967882	2.426472
O	11.590735	12.519455	5.276381
O	11.673426	9.872491	5.774096
O	12.186790	7.221347	5.860549
O	16.514145	12.846596	5.187920
O	16.093483	10.283405	5.690853
O	15.943919	7.618929	5.520220
O	0.262689	10.945246	2.998060
O	0.498147	7.287611	3.097897
O	17.269375	8.786404	10.369148
O	16.421043	8.871969	7.860372
O	14.016601	9.033748	6.692839
O	11.769932	8.458667	8.017488
O	12.250660	8.786801	10.544065
O	14.695346	9.195128	9.865814
O	17.205305	13.512218	10.141370
O	16.183783	13.105680	7.764950
O	14.012997	12.773368	6.188701
O	12.011398	13.514207	7.778467
O	12.167369	13.345662	10.622355
O	14.602645	13.011559	9.871970

O	16.443266	11.094687	9.453484
O	12.099295	10.946441	9.035131
O	18.853115	7.398448	11.968283
O	18.361975	9.869705	12.629270
O	18.109497	12.590296	12.485002
O	14.093286	7.287412	11.710661
O	13.846414	9.789711	12.375929
O	13.926302	12.451401	12.449135
O	9.881057	9.546147	9.542615
O	9.742105	12.609200	9.374792
O	12.847116	18.825249	3.674972
O	13.671021	18.737696	1.174626
O	15.976754	19.070208	13.294806
O	18.108696	18.395233	1.339237
O	17.931301	18.901463	3.945175
O	15.447573	18.814106	3.111815
O	12.930608	3.318954	3.343743
O	13.855824	3.062257	0.905628
O	16.269276	2.831429	13.051638
O	18.343355	3.475559	1.239266
O	18.102291	3.064446	3.927777
O	15.587326	3.235577	2.926728
O	14.087479	1.067780	2.668972
O	18.193390	1.001716	2.183035
O	11.430960	17.391129	5.366449
O	11.595941	0.091137	5.774497
O	12.419446	2.650149	5.781857
O	16.267075	17.086674	4.933910
O	16.097887	19.574448	5.689515
O	15.780739	2.337934	5.675864
O	0.176394	19.228603	2.844022
O	0.325157	2.570951	2.767471
O	17.187885	1.177225	10.456539
O	16.348164	1.071959	7.927152
O	13.965944	0.675770	6.775546
O	11.761523	1.414222	8.026588
O	12.093287	1.241897	10.618742
O	14.593635	0.834365	9.880000
O	17.525658	16.485327	9.797561
O	16.268074	17.004492	7.574243
O	13.917292	17.168062	6.281445
O	11.850221	16.507215	7.853814
O	12.358779	16.582235	10.466443
O	14.868937	16.586613	9.780699

O	16.348164	18.805151	9.541142
O	11.831800	18.866440	9.133496
O	18.760612	2.486579	12.140388
O	18.361376	19.819405	12.544422
O	17.681229	17.241091	12.376465
O	14.011795	2.798197	11.635849
O	13.759118	0.251125	12.379275
O	14.107301	17.502764	12.227913
O	9.752916	0.666815	9.610332
O	10.007195	16.915941	9.778021
O	7.169477	9.703350	9.199474
O	5.669429	8.535676	12.148418
O	3.862244	8.954550	0.656168
O	1.928118	8.618456	12.039883
O	2.100908	9.117921	9.375729
O	4.695760	9.203884	9.876119
O	7.264782	13.176919	10.116343
O	6.183995	13.104884	12.466934
O	3.825804	12.768790	0.246916
O	1.750323	13.526544	12.111214
O	2.168583	13.016533	9.453752
O	4.666127	12.848387	10.295140
O	6.258276	10.856695	11.209601
O	1.746319	11.091305	11.209065
O	8.678135	7.706684	8.116656
O	8.679937	10.188487	7.202864
O	7.755521	12.693572	7.533425
O	3.668831	7.294178	8.291037
O	3.761733	9.783144	7.436130
O	4.171383	12.434089	7.696430
O	19.858820	9.362479	10.464704
O	19.781536	12.775356	10.456539
O	2.909797	11.193387	2.839070
O	3.843022	11.352977	5.327371
O	6.085086	10.777298	6.690162
O	8.082080	11.605892	5.119132
O	7.921905	10.945047	2.587469
O	5.430567	10.531547	3.345349
O	3.005302	6.540205	3.169095
O	3.674237	6.873313	5.693128
O	6.001595	7.281641	6.948989
O	8.429061	6.641092	5.597172
O	7.926109	6.798892	3.016127
O	5.491234	7.210801	3.774274

O	3.496642	8.962111	4.179244
O	8.425258	9.026982	4.359512
O	1.339071	12.514680	1.165793
O	1.426968	9.870103	0.923962
O	1.908897	7.210004	0.827739
O	6.010203	12.620344	1.752236
O	6.180791	10.209183	0.762296
O	6.158567	7.634848	1.240470
O	10.267682	10.861471	3.755404
O	10.384210	7.221546	3.914527
O	8.595845	14.909326	8.620793
O	3.840420	14.826347	8.615574
O	5.338666	14.919474	0.763500
O	2.404842	14.919474	0.917003
O	1.316847	4.926395	1.932104
O	6.095497	5.149065	2.006112
O	4.588642	4.983108	7.353423
O	7.419352	4.884807	7.444293
O	11.597743	4.964801	5.013138
O	16.514746	5.057132	5.102135
O	14.768228	5.041810	12.788795
O	17.924496	4.942514	12.479915
O	18.776831	14.996881	11.622869
O	14.017402	14.943751	11.707181
O	15.354671	14.996086	6.110678
O	12.437265	14.996483	5.690853
O	11.179084	4.975944	15.724490
O	9.260575	10.616117	12.214263
O	11.011498	0.920329	14.463276
O	9.175882	2.816106	13.215311
O	10.835305	8.543039	12.633820
O	9.105004	8.798940	14.640734
O	11.092989	3.975024	10.792586
O	11.094390	5.221498	8.209535
O	11.757718	8.959126	15.138181
O	9.432364	6.303804	14.308300
Al	4.511557	18.760977	7.031027
Al	6.302725	3.497448	2.562176
Al	17.836597	6.464588	13.294806
Al	11.426555	12.532391	9.036871
Al	16.301512	3.461630	4.484510
Al	7.758325	6.561894	7.161645
H	5.972963	8.230624	6.699263
H	19.292397	6.760685	11.371000

H	11.494229	13.761950	11.196218
H	8.337562	10.544878	-0.862267
H	18.799856	3.428797	4.506993
H	2.962054	16.936836	7.088038
H	11.758719	8.721533	14.182902
H	10.471706	5.450933	15.216471
H	9.944326	2.247791	13.465840
H	9.198507	10.621688	11.239445
H	10.533774	0.266249	15.005019
H	11.643994	0.398378	13.941206
H	8.749814	3.034598	14.069549
H	11.864636	4.750886	15.075280
H	10.112111	9.258806	12.607188
H	11.358880	8.693873	11.801665
H	8.444879	9.420187	14.990165
H	9.994382	9.127274	14.942121
H	11.162065	4.351314	9.875584
H	11.309827	3.020071	10.727813
H	11.469603	6.114366	8.091629
H	11.158661	4.807002	7.328531
H	6.324549	3.662411	12.309417
H	11.634784	8.110634	15.599627
H	8.616267	5.784241	14.182099
H	9.139041	7.240849	14.584660
Pt	6.842719	4.936743	-3.900877
Pt	9.961546	6.675717	-1.224009
Pt	8.999488	6.272563	-3.548369
Pt	6.642298	5.147274	-1.390895
Pt	7.522466	7.628282	-1.948966
Pt	9.050344	4.389520	-1.850066

330

Pt <sub>6</sub> H <sub>1</sub> @H-MFI + H <sup>+</sup> (H <sub>2</sub> O) <sub>10</sub>			
Si	8.413044	1.064198	8.727858
Si	6.098100	0.661841	10.858967
Si	5.603157	1.173444	0.345951
Si	2.468713	1.272342	0.149890
Si	1.407747	0.540457	10.811992
Si	3.716483	1.258811	9.082239
Si	8.568815	16.452892	9.002878
Si	6.102505	17.338993	10.868335
Si	5.425762	16.505424	0.438427
Si	2.375610	16.477566	0.421163
Si	1.357091	17.354713	10.990923
Si	3.566719	16.348223	9.138181

Si	1.548702	18.840572	2.035420
Si	3.955146	19.373865	4.030425
Si	7.668226	18.466074	6.916737
Si	8.627079	19.348196	4.127050
Si	6.414848	18.699289	2.194545
Si	1.687855	3.386611	2.318739
Si	3.926714	2.679600	4.379453
Si	4.521968	3.342634	7.219058
Si	7.557303	3.316964	6.978298
Si	8.720582	2.583686	4.181653
Si	11.642993	11.035986	4.626637
Si	14.200403	10.526969	2.740169
Si	14.456884	11.124735	13.113467
Si	17.654198	11.227812	13.259609
Si	18.724773	10.549058	2.716481
Si	16.506136	11.358350	4.550488
Si	11.758921	6.484686	4.460822
Si	14.265274	7.345915	2.577164
Si	14.800463	6.646664	13.042403
Si	18.918386	7.410786	2.725180
Si	16.536970	6.522494	4.452123
Si	18.550182	8.960320	11.318672
Si	16.193792	9.504559	9.350569
Si	15.619562	8.920324	6.420361
Si	12.442672	8.665418	6.538265
Si	11.519258	9.488441	9.247787
Si	13.762121	8.768892	11.136663
Si	18.470295	13.458689	11.188322
Si	16.086475	12.686807	9.326479
Si	15.498429	13.416701	6.336449
Si	12.484118	13.452123	6.283988
Si	13.624570	13.428244	11.165972
Si	11.544886	18.830822	4.638280
Si	13.989771	19.358543	2.656660
Si	14.384206	18.825647	13.094730
Si	17.522053	18.619694	13.221601
Si	18.621260	19.345409	2.555216
Si	16.405827	18.621683	4.418263
Si	11.770933	3.416260	4.472198
Si	14.146544	2.677809	2.476926
Si	14.741998	3.438547	12.965718
Si	17.803562	3.451481	13.049094
Si	18.765818	2.494340	2.434100
Si	18.518547	1.058428	11.393350

Si	16.131725	0.503047	9.427655
Si	15.550486	0.990970	6.487410
Si	12.456487	1.223788	6.559276
Si	11.345866	0.515782	9.319787
Si	13.661010	1.285077	11.130239
Si	18.435656	16.510599	11.134789
Si	16.221624	17.228355	9.175385
Si	15.442768	16.583229	6.243705
Si	12.411238	16.496868	6.315839
Si	11.476409	17.233530	9.254210
Si	13.841408	16.407721	11.047265
Si	8.587235	9.255025	8.553477
Si	6.247064	9.285869	10.576451
Si	5.472012	8.795956	0.351705
Si	2.311740	8.671388	0.259229
Si	1.441984	9.556097	10.812928
Si	3.629188	8.855851	8.789152
Si	8.309530	13.326758	8.909330
Si	6.077678	12.443840	10.989050
Si	5.342870	13.348051	0.453416
Si	2.327958	13.436004	0.257221
Si	1.344477	12.626513	10.817613
Si	3.720688	13.253927	9.027637
Si	1.517267	11.116577	1.989651
Si	3.902488	10.512045	3.922825
Si	4.476318	11.106427	6.812750
Si	7.637392	11.318353	6.652020
Si	8.695154	10.585273	3.989740
Si	6.354382	11.083345	2.127629
Si	1.652416	6.480507	2.268553
Si	3.928116	7.393275	4.167734
Si	4.423060	6.540403	7.079875
Si	8.792661	7.415761	4.258203
Si	6.384816	6.630745	2.512926
O	7.182892	1.173245	9.774007
O	6.418852	1.328059	12.301119
O	4.022820	0.903216	0.002141
O	1.829610	1.500186	12.052328
O	2.149762	0.995746	9.451879
O	4.585238	1.081909	10.452124
O	7.342668	16.732075	10.029087
O	6.161971	16.742422	12.378472
O	3.893878	17.090057	0.407914
O	1.754328	16.496071	12.300316

O	2.075881	16.586414	9.713917
O	4.684547	16.916140	10.129325
O	6.178389	18.935291	10.884662
O	1.836818	18.893902	11.189393
O	8.588838	2.492549	7.950037
O	8.178786	19.891239	7.535298
O	8.504344	17.246264	7.603819
O	3.846426	2.822673	8.603395
O	4.172585	0.247146	7.941071
O	3.586541	17.249449	7.693887
O	19.832392	0.666219	10.522117
O	19.781336	17.326059	10.712155
O	2.826906	18.818684	3.004885
O	3.754125	18.659889	5.449290
O	6.113317	18.236837	7.187072
O	8.094093	18.413540	5.344769
O	7.926909	18.904051	2.734816
O	5.421757	18.988024	3.435951
O	2.672136	3.397356	3.591863
O	3.585740	2.912219	5.969354
O	6.027823	2.724969	7.024737
O	8.183792	3.400341	5.498405
O	8.015007	3.145435	2.848572
O	5.340268	3.315770	4.013963
O	3.833212	1.084098	4.091719
O	8.349774	1.005098	4.503915
O	1.415555	17.330437	1.416858
O	1.669234	0.018108	0.826400
O	2.262085	2.649950	0.997034
O	6.257275	17.160101	1.665648
O	6.171381	19.651058	0.918341
O	5.759728	2.403998	1.325051
O	10.201209	19.075581	3.760623
O	10.352375	2.728153	4.096537
O	12.935412	10.862068	3.680861
O	13.925901	11.105234	1.253318
O	16.078066	11.022852	12.983518
O	18.103891	11.355364	1.426093
O	18.019400	11.024444	4.091049
O	15.512044	11.347206	3.265184
O	12.952831	6.881473	3.425245
O	13.927103	6.972809	1.015234
O	16.286695	7.221944	13.216516
O	18.674519	6.548562	1.400933

O	18.083870	6.886248	4.025741
O	15.596336	6.553736	3.091741
O	14.589831	8.942014	2.761448
O	18.520149	8.967683	2.427275
O	11.588734	12.520252	5.276248
O	11.672225	9.870700	5.772490
O	12.186991	7.222143	5.864029
O	16.508940	12.847988	5.193273
O	16.093483	10.282610	5.690318
O	15.943317	7.619725	5.521023
O	0.261087	10.944650	2.999933
O	0.497947	7.287213	3.098165
O	17.266972	8.787200	10.367007
O	16.416437	8.872766	7.865591
O	14.017402	9.033548	6.692437
O	11.771334	8.457075	8.020164
O	12.203609	8.798343	10.585686
O	14.682934	9.191945	9.869293
O	17.247150	13.503063	10.127585
O	16.184383	13.103691	7.774319
O	14.002185	12.777745	6.198872
O	11.919296	13.506645	7.779270
O	12.101097	13.271638	10.698103
O	14.601644	13.016932	9.889100
O	16.442066	11.100259	9.453885
O	12.088882	10.951614	9.029243
O	18.852915	7.404418	11.968417
O	18.361774	9.874282	12.629270
O	18.116106	12.604424	12.532376
O	14.089280	7.292785	11.709322
O	13.845013	9.802845	12.379410
O	13.939316	12.501945	12.463990
O	9.885262	9.533213	9.537529
O	9.682239	12.528809	9.452011
O	12.848317	18.825848	3.674704
O	13.669620	18.737892	1.173823
O	15.968946	19.070208	13.295609
O	18.109299	18.397024	1.338166
O	17.933506	18.901463	3.944505
O	15.449374	18.814306	3.112484
O	12.931007	3.319153	3.343341
O	13.855824	3.062854	0.905628
O	16.269476	2.833021	13.051370
O	18.343555	3.475161	1.237660

O	18.102489	3.064446	3.927241
O	15.587127	3.235776	2.926996
O	14.086477	1.066188	2.669106
O	18.195793	1.000124	2.183972
O	11.431360	17.387150	5.366985
O	11.595941	0.090540	5.773962
O	12.419045	2.648159	5.785604
O	16.266872	17.086079	4.936052
O	16.099089	19.574646	5.688712
O	15.780939	2.337735	5.676667
O	0.187806	19.225618	2.843888
O	0.324757	2.570553	2.767471
O	17.192692	1.175235	10.455737
O	16.348965	1.072357	7.929427
O	13.969549	0.675770	6.775947
O	11.761724	1.411834	8.028194
O	12.092687	1.240106	10.616601
O	14.594836	0.834763	9.879465
O	17.521252	16.484531	9.796758
O	16.266474	17.004492	7.579997
O	13.916891	17.167664	6.280910
O	11.847818	16.504032	7.852475
O	12.344364	16.589397	10.462161
O	14.856524	16.587606	9.783240
O	16.348362	18.801968	9.541678
O	11.764326	18.848133	9.127340
O	18.762014	2.485783	12.138113
O	18.361574	19.819006	12.543218
O	17.679426	17.241688	12.378606
O	14.010594	2.795810	11.635983
O	13.758518	0.250329	12.380747
O	14.103296	17.499182	12.219349
O	9.749312	0.673581	9.608058
O	9.946328	16.919722	9.718200
O	7.181291	9.703151	9.198538
O	5.680041	8.537068	12.145876
O	3.866849	8.953555	0.654027
O	1.928519	8.617063	12.049251
O	2.166180	9.117722	9.439432
O	4.754624	9.203288	9.869025
O	7.253971	13.173934	10.123035
O	6.181392	13.103492	12.467603
O	3.825203	12.769587	0.246515
O	1.752926	13.529530	12.110544

O	2.165980	13.016932	9.454823
O	4.658719	12.845799	10.291795
O	6.335561	10.863461	11.212411
O	1.747921	11.097474	11.212411
O	8.678135	7.699719	8.112908
O	8.681338	10.188289	7.200456
O	7.756322	12.684420	7.525529
O	3.672836	7.295372	8.293713
O	3.762334	9.782547	7.442153
O	4.172184	12.436477	7.698035
O	19.863226	9.361684	10.464972
O	19.779932	12.774363	10.463633
O	2.908796	11.193784	2.838668
O	3.842822	11.352380	5.328843
O	6.083284	10.777896	6.690296
O	8.082480	11.604102	5.113377
O	7.920302	10.949823	2.585462
O	5.429365	10.531744	3.347222
O	3.004902	6.539011	3.168024
O	3.674638	6.874110	5.692727
O	6.001995	7.278855	6.948186
O	8.430062	6.641490	5.594897
O	7.931115	6.804264	3.012781
O	5.491834	7.211199	3.774943
O	3.497443	8.961913	4.179779
O	8.427259	9.025988	4.357371
O	1.339472	12.515277	1.166061
O	1.428770	9.870899	0.925836
O	1.910699	7.209010	0.830148
O	6.010004	12.620543	1.752504
O	6.179590	10.211370	0.762430
O	6.160569	7.633654	1.237660
O	10.270485	10.860277	3.755404
O	10.396824	7.223735	3.914260
O	8.610460	14.869528	8.618385
O	3.844424	14.839480	8.623604
O	5.340868	14.923654	0.758548
O	2.405443	14.922857	0.913925
O	1.317448	4.924206	1.931167
O	6.097300	5.150259	2.006246
O	4.588441	4.982710	7.354361
O	7.419152	4.880031	7.444026
O	11.597743	4.961020	5.013539
O	16.514545	5.056734	5.102269

O	14.766624	5.043601	12.789464
O	17.925896	4.944901	12.479113
O	18.779634	14.996881	11.626884
O	14.015600	14.931811	11.698883
O	15.354470	14.994692	6.110678
O	12.437065	14.990713	5.696742
O	11.180084	4.975347	15.724625
O	9.189898	11.188610	11.473782
O	11.010697	0.921523	14.462339
O	9.177283	2.816106	13.214375
O	10.917397	8.458467	12.717063
O	9.179286	9.033947	14.464213
O	11.094390	3.967860	10.791516
O	11.093389	5.221298	8.211140
O	11.613360	8.958331	15.236814
O	9.428159	6.315943	14.310709
Al	4.503949	18.769932	6.994759
Al	6.303526	3.495458	2.561506
Al	17.835798	6.468170	13.292933
Al	11.550892	12.605221	9.191980
Al	16.301311	3.460038	4.485312
Al	7.755722	6.555527	7.156158
H	5.976967	8.201373	6.615752
H	19.264769	6.761282	11.357617
H	9.722883	11.752748	11.534675
H	8.242456	11.145032	-1.651998
H	18.799255	3.432180	4.504852
H	2.976871	16.921314	7.001718
H	11.847217	8.575872	14.365045
H	10.480515	5.461679	15.225170
H	9.939121	2.237842	13.466511
H	9.355079	10.327184	11.014745
H	10.545787	0.256100	15.001674
H	11.664216	0.414894	13.950439
H	8.747011	3.033404	14.067006
H	11.871043	4.759841	15.077823
H	10.139542	8.971863	13.097006
H	11.279994	8.846498	11.877948
H	8.557403	9.744740	14.706713
H	10.048040	9.226569	14.941718
H	11.172676	4.344151	9.875049
H	11.324643	3.013703	10.732229
H	11.494029	6.100636	8.076373
H	11.148450	4.786306	7.339237

H	6.340767	3.655645	12.298308
H	11.503639	8.192617	15.830885
H	8.627079	5.779665	14.152389
H	9.096795	7.220750	14.565521
Pt	6.853530	4.931967	-3.901546
Pt	10.027819	6.639898	-1.259340
Pt	9.011301	6.258832	-3.562287
Pt	6.658316	5.141504	-1.391832
Pt	7.568516	7.625894	-1.937725
Pt	9.060555	4.371015	-1.861441

330



Si	8.423455	1.013058	8.755961
Si	6.040037	0.613287	10.843843
Si	5.602756	1.182001	0.384360
Si	2.440882	1.279108	0.180537
Si	1.414554	0.538069	10.822029
Si	3.660021	1.330447	9.042224
Si	8.606457	16.457867	9.057213
Si	6.156364	17.289644	10.923740
Si	5.419354	16.480949	0.485268
Si	2.383419	16.468214	0.445922
Si	1.397736	17.351332	11.020098
Si	3.628587	16.358770	9.146210
Si	1.536288	18.834404	2.050945
Si	3.930519	19.370880	4.065086
Si	7.667425	18.477814	6.930254
Si	8.633886	19.349588	4.157563
Si	6.398230	18.704464	2.213682
Si	1.626587	3.413275	2.326902
Si	3.872655	2.677609	4.417461
Si	4.490134	3.431583	7.274865
Si	7.537883	3.440338	7.226954
Si	8.662518	2.576921	4.457610
Si	11.591736	10.939277	4.624228
Si	14.158557	10.505677	2.726385
Si	14.467296	11.092300	13.122969
Si	17.668013	11.264029	13.253185
Si	18.731182	10.532740	2.685567
Si	16.463089	11.344420	4.518101
Si	11.764527	6.578609	4.504049
Si	14.244251	7.348701	2.576629
Si	14.867736	6.662981	13.086165
Si	18.930000	7.398448	2.710057

Si	16.535568	6.530653	4.446100
Si	18.557991	8.988976	11.321349
Si	16.190590	9.485058	9.353513
Si	15.619763	8.919726	6.421164
Si	12.451080	8.658453	6.623648
Si	11.463395	9.380787	9.395669
Si	13.742900	8.756157	11.142686
Si	18.487513	13.465653	11.129570
Si	16.146542	12.667106	9.244843
Si	15.449976	13.411528	6.280910
Si	12.415442	13.373522	6.227779
Si	13.785347	13.437795	11.140812
Si	11.541282	18.791222	4.643499
Si	13.956534	19.298647	2.646354
Si	14.395017	18.861267	13.097675
Si	17.535467	18.615316	13.225750
Si	18.614853	19.346006	2.558161
Si	16.400822	18.622679	4.412910
Si	11.740299	3.395167	4.554101
Si	13.943320	2.626469	2.462204
Si	14.651299	3.453272	12.969867
Si	17.701649	3.450089	12.990210
Si	18.683128	2.515234	2.405728
Si	18.524754	1.042708	11.386659
Si	16.074863	0.545631	9.427119
Si	15.561898	0.989577	6.483528
Si	12.469301	1.193343	6.572124
Si	11.366289	0.444544	9.334910
Si	13.619164	1.345968	11.175877
Si	18.455078	16.550795	11.114047
Si	16.161959	17.266361	9.153170
Si	15.417940	16.588005	6.232062
Si	12.393618	16.436773	6.308613
Si	11.506042	17.196119	9.244442
Si	13.861630	16.428616	11.035622
Si	8.562008	9.175827	8.595232
Si	6.174184	9.351336	10.595322
Si	5.323049	8.860626	0.350233
Si	2.244066	8.691684	0.262039
Si	1.461406	9.564056	10.794996
Si	3.609566	8.803914	8.714073
Si	8.331554	13.334917	8.959919
Si	6.033229	12.530400	10.992261
Si	5.386118	13.336906	0.472688

Si	2.361795	13.428244	0.256552
Si	1.371907	12.640442	10.811858
Si	3.723691	13.323575	9.037941
Si	1.527679	11.096678	2.002766
Si	3.938528	10.498513	3.962037
Si	4.479722	11.112597	6.846208
Si	7.645000	11.308403	6.726430
Si	8.650705	10.488365	4.037919
Si	6.383214	11.079963	2.167778
Si	1.683249	6.514733	2.253697
Si	4.024422	7.353477	4.141369
Si	4.486930	6.609055	7.048827
Si	8.709970	7.373773	4.226084
Si	6.455894	6.673130	2.367720
O	7.244960	1.088276	9.867821
O	6.344571	1.325472	12.288271
O	4.011407	0.917344	0.156849
O	1.842825	1.498594	12.062500
O	2.111120	0.996144	9.442242
O	4.575227	1.086286	10.380658
O	7.489429	16.751377	10.198649
O	6.171981	16.744411	12.448064
O	3.899284	17.089062	0.418353
O	1.752125	16.496868	12.335915
O	2.162977	16.585020	9.787256
O	4.830307	16.755554	10.122366
O	6.091293	18.898479	10.889480
O	1.846829	18.899275	11.200501
O	8.571618	2.500508	8.108358
O	8.179988	19.909348	7.526064
O	8.508348	17.321283	7.693619
O	3.750521	2.900677	8.625879
O	4.170582	0.400368	7.856624
O	3.583738	17.397896	7.786765
O	19.847008	0.665025	10.534161
O	19.829988	17.323671	10.711084
O	2.760834	18.817888	3.084514
O	3.752923	18.666855	5.493052
O	6.110114	18.308474	7.193496
O	8.092292	18.401003	5.354405
O	7.919502	18.984840	2.738296
O	5.399733	18.989218	3.443981
O	2.595852	3.321939	3.604578
O	3.595951	2.906647	6.014856

O	6.023619	2.817698	7.273527
O	8.087286	3.410689	5.701828
O	7.992982	3.157573	3.092410
O	5.270391	3.327312	4.002588
O	3.835614	1.082108	4.097206
O	8.340164	0.987587	4.600272
O	1.415956	17.330637	1.424353
O	1.666031	0.004577	0.833359
O	2.177793	2.655720	1.000915
O	6.265484	17.169256	1.684920
O	6.178389	19.649267	0.918743
O	5.924510	2.407580	1.328798
O	10.196002	19.071999	3.770928
O	10.271886	2.738699	4.341445
O	12.846715	10.773915	3.608860
O	13.845213	11.111601	1.235652
O	16.075863	11.032205	13.055652
O	18.106895	11.367502	1.416055
O	17.954529	11.015887	4.017309
O	15.431355	11.351981	3.261571
O	12.931409	6.962262	3.430732
O	13.934711	6.969028	1.011220
O	16.335348	7.282835	13.291461
O	18.682327	6.473145	1.421944
O	18.083870	6.892218	4.018781
O	15.585525	6.559905	3.091741
O	14.596438	8.946989	2.680213
O	18.524153	8.954351	2.352999
O	11.528266	12.461550	5.196352
O	11.677831	9.868910	5.852787
O	12.255466	7.213786	5.927063
O	16.432655	12.851969	5.115518
O	16.094284	10.285395	5.687641
O	15.944719	7.622511	5.519952
O	0.252678	10.946837	3.005554
O	0.506356	7.290397	3.096693
O	17.268974	8.787001	10.374234
O	16.421043	8.871969	7.865992
O	14.029214	9.040514	6.696452
O	11.848019	8.455682	8.111034
O	12.185188	8.641141	10.692883
O	14.675725	9.192940	9.876922
O	17.271778	13.511819	10.046752
O	16.183182	13.094337	7.701248

O	13.955533	12.766403	6.189370
O	11.842011	13.346459	7.711686
O	12.180383	13.363173	10.549150
O	14.670919	13.018125	9.867019
O	16.444870	11.089514	9.449602
O	12.018605	10.874406	9.211519
O	18.861925	7.462324	12.040150
O	18.365179	9.935769	12.607723
O	18.099686	12.612782	12.464659
O	14.185987	7.293381	11.712935
O	13.848016	9.792099	12.384495
O	13.926903	12.436875	12.383022
O	9.849622	9.372828	9.613277
O	9.684040	12.679047	9.529633
O	12.844112	18.737696	3.679522
O	13.679030	18.656904	1.165659
O	15.987967	19.064835	13.299223
O	18.112701	18.391850	1.341913
O	17.929300	18.899473	3.946647
O	15.442167	18.821867	3.108068
O	12.583226	3.156578	3.185288
O	13.776337	2.991815	0.879932
O	16.171968	2.826454	12.961971
O	18.186583	3.409694	1.180113
O	17.949121	3.134888	3.839851
O	15.275185	3.315173	3.018000
O	13.934111	1.008680	2.666964
O	18.187183	0.994154	2.185979
O	11.419347	17.335213	5.363237
O	11.601347	0.079397	5.763657
O	12.432660	2.654129	5.848104
O	16.259066	17.087072	4.933777
O	16.099890	19.571861	5.686303
O	15.776134	2.335944	5.677069
O	0.175793	19.229996	2.845895
O	0.227250	2.655124	2.764928
O	17.267374	1.079521	10.374368
O	16.350765	1.066984	7.922335
O	13.984966	0.667014	6.778624
O	11.756317	1.339402	8.033146
O	12.100096	1.082307	10.640823
O	14.663712	1.154739	9.951734
O	17.522654	16.659243	9.788996
O	16.258064	17.014044	7.561395

O	13.879049	17.155924	6.280910
O	11.847217	16.423243	7.856089
O	12.350370	16.501047	10.461357
O	14.867135	16.488710	9.770260
O	15.944719	18.824654	9.537663
O	11.843413	18.795004	9.116901
O	18.686731	2.483196	12.121653
O	18.367182	19.816618	12.546162
O	17.686832	17.238903	12.378071
O	13.769931	2.884758	11.705040
O	13.844011	0.337487	12.439499
O	14.102695	17.576986	12.138649
O	9.760725	0.577469	9.608994
O	10.003391	16.912758	9.777888
O	7.260578	9.707528	9.363684
O	5.342670	8.705215	12.130619
O	3.751922	9.033548	0.754132
O	1.921311	8.622834	12.043228
O	2.173789	9.120906	9.436086
O	4.823900	9.037728	9.707359
O	7.180289	13.257908	10.109385
O	6.249266	13.115829	12.504942
O	3.856637	12.772572	0.247853
O	1.753326	13.528733	12.123259
O	2.158572	13.096328	9.457499
O	4.597451	13.093144	10.383736
O	6.012806	10.936092	11.125154
O	1.749923	11.106627	11.208129
O	8.591640	7.628680	8.039035
O	8.684341	10.180726	7.292932
O	7.777346	12.700935	7.552027
O	3.507054	7.275472	8.184910
O	3.738708	9.799064	7.430644
O	4.172585	12.430110	7.772981
O	19.868631	9.361883	10.464837
O	19.798754	12.772770	10.456674
O	2.916204	11.113194	2.845761
O	3.840219	11.358150	5.351059
O	6.081683	10.855103	6.770996
O	8.093893	11.528485	5.170388
O	7.938723	10.856297	2.597373
O	5.479420	10.610744	3.428859
O	3.077181	6.555129	3.077421
O	3.745515	6.717106	5.596235

O	5.931918	7.293780	7.030358
O	8.185794	6.467175	5.428680
O	8.023816	6.953507	2.778445
O	5.575326	7.133593	3.681128
O	3.588343	8.931865	4.181385
O	8.347572	8.958729	4.506993
O	1.402941	12.501746	1.178373
O	1.336468	9.871894	0.923962
O	1.830011	7.206423	0.770861
O	6.088890	12.621737	1.757723
O	6.110314	10.203013	0.826400
O	6.009002	7.608582	1.103027
O	10.245858	10.692728	3.757411
O	10.344565	7.211995	4.012357
O	8.592641	14.914898	8.616645
O	3.834613	14.889228	8.526577
O	5.340868	14.914699	0.837241
O	2.410649	14.917286	0.919948
O	1.324856	4.956841	1.930899
O	6.255273	5.137325	1.915241
O	4.586039	5.025493	7.371758
O	7.586135	4.972561	7.782349
O	11.674027	4.983506	4.846654
O	16.510941	5.063500	5.100797
O	14.767026	5.059918	12.798297
O	17.847210	4.957239	12.468540
O	18.772226	15.011010	11.544176
O	14.014799	14.935194	11.712935
O	15.347263	14.997279	6.108135
O	12.428255	14.929623	5.692995
O	11.087783	5.548239	15.143267
O	9.683841	3.057083	14.717688
O	8.940623	2.489564	11.870052
O	10.431662	3.479539	9.863405
O	9.678034	0.582643	13.891554
O	9.179086	8.628406	14.132047
O	11.248158	4.141579	12.467336
O	12.353373	5.557591	10.705062
O	11.340060	6.970023	13.045882
O	11.672025	9.126876	14.638459
Al	4.508354	18.857088	7.021926
Al	6.292114	3.529884	2.611425
Al	17.858624	6.467573	13.307118
Al	11.328247	12.445034	9.073273

Al	16.176374	3.491678	4.477417
Al	7.533077	6.617214	7.024737
H	10.479515	6.353751	9.371579
H	19.546078	6.927439	11.590079
H	11.610357	14.086502	10.884127
H	8.920001	3.117178	2.087614
H	18.602039	3.622215	4.381862
H	2.953245	17.090057	7.101689
H	10.152756	5.772103	15.319788
H	11.093790	4.587715	14.960588
H	9.339061	3.698826	13.891286
H	9.697455	2.080042	14.385655
H	7.975964	2.335148	11.743984
H	9.371697	2.591447	10.963756
H	9.959543	4.348330	9.804118
H	10.542583	3.208515	8.934893
H	9.222333	0.629604	13.031027
H	9.167673	-0.038604	14.449091
H	8.483121	9.300593	14.238308
H	10.084480	8.999721	14.404258
H	11.744905	4.576571	11.696074
H	11.344465	3.188616	12.288003
H	11.716073	6.004523	10.091987
H	13.205710	6.032581	10.714698
H	11.741100	6.556323	12.242768
H	11.371294	6.296839	13.822364
H	12.016603	9.982533	14.331320
H	11.925103	8.471203	13.948566
Pt	7.048945	4.946892	-3.367430
Pt	9.223935	7.162247	-0.859055
Pt	9.065761	6.670145	-3.329289
Pt	6.573423	4.836253	-0.896126
Pt	6.879158	7.252589	-1.968773
Pt	9.058554	4.619752	-1.085361

330

		Pt <sub>6</sub> H <sub>2</sub> @H-MFI + (H <sub>2</sub> O) <sub>10</sub>	
Si	8.420452	1.015844	8.751813
Si	6.040437	0.610700	10.834743
Si	5.597550	1.193741	0.392925
Si	2.440481	1.279904	0.181072
Si	1.412552	0.538268	10.823368
Si	3.657018	1.327263	9.041956
Si	8.609860	16.464632	9.056276
Si	6.158166	17.292429	10.917450

Si	5.419354	16.492092	0.472955
Si	2.381617	16.470005	0.443513
Si	1.394732	17.352724	11.019028
Si	3.627386	16.370111	9.144605
Si	1.535487	18.835001	2.050677
Si	3.932121	19.371279	4.059465
Si	7.668226	18.479803	6.926238
Si	8.632285	19.364313	4.160641
Si	6.401834	18.706255	2.212477
Si	1.625586	3.414072	2.324493
Si	3.888673	2.680594	4.380122
Si	4.480924	3.406311	7.254255
Si	7.530875	3.410887	7.170611
Si	8.649504	2.594830	4.367542
Si	11.597342	10.937685	4.620481
Si	14.170370	10.499907	2.724377
Si	14.477707	11.090509	13.117749
Si	17.682230	11.236766	13.244487
Si	18.728979	10.530949	2.685031
Si	16.463089	11.345613	4.517833
Si	11.773136	6.580400	4.492539
Si	14.272682	7.364620	2.586666
Si	14.898570	6.659399	13.083756
Si	18.932001	7.397254	2.709388
Si	16.542776	6.527867	4.451454
Si	18.561594	8.957734	11.312783
Si	16.187185	9.485058	9.353378
Si	15.621164	8.919926	6.420628
Si	12.452282	8.656065	6.620303
Si	11.473005	9.383175	9.400487
Si	13.754113	8.736656	11.147638
Si	18.491318	13.461872	11.129972
Si	16.148142	12.666709	9.245111
Si	15.452178	13.413319	6.280910
Si	12.419446	13.375113	6.222827
Si	13.790552	13.439983	11.143489
Si	11.538278	18.792616	4.640555
Si	13.954733	19.300438	2.646221
Si	14.391613	18.862860	13.099012
Si	17.532665	18.615713	13.226553
Si	18.613852	19.346006	2.558428
Si	16.399418	18.623873	4.412241
Si	11.731091	3.393377	4.547811
Si	13.941118	2.628260	2.463944

Si	14.646493	3.453272	12.970135
Si	17.698246	3.442129	12.992484
Si	18.682327	2.515034	2.406665
Si	18.522551	1.041116	11.386391
Si	16.068655	0.547620	9.429528
Si	15.559496	0.989179	6.484331
Si	12.467098	1.194935	6.566102
Si	11.361282	0.450911	9.335847
Si	13.612157	1.350346	11.182433
Si	18.452675	16.549601	11.114849
Si	16.161358	17.267756	9.153705
Si	15.418741	16.589397	6.232062
Si	12.393417	16.439758	6.308211
Si	11.507645	17.201889	9.244174
Si	13.861430	16.431599	11.035890
Si	8.555600	9.158316	8.603395
Si	6.093495	9.360688	10.570964
Si	5.308833	8.903808	0.373252
Si	2.235656	8.692282	0.255348
Si	1.463208	9.555699	10.774787
Si	3.588343	8.754565	8.697612
Si	8.363189	13.345464	8.972365
Si	6.057856	12.556269	10.987041
Si	5.387920	13.326361	0.491290
Si	2.362996	13.429238	0.259095
Si	1.378314	12.637457	10.812796
Si	3.737106	13.342479	9.040751
Si	1.520070	11.097474	1.999286
Si	3.905892	10.495728	3.967792
Si	4.478721	11.111005	6.851427
Si	7.644800	11.315368	6.742222
Si	8.650505	10.490752	4.040596
Si	6.370400	11.111204	2.189459
Si	1.686253	6.514733	2.252091
Si	4.001196	7.372580	4.152477
Si	4.487330	6.580202	7.039458
Si	8.718579	7.378151	4.210292
Si	6.423458	6.704172	2.435171
O	7.247363	1.085689	9.870097
O	6.342569	1.322686	12.284925
O	4.010206	0.915155	0.156849
O	1.842825	1.498594	12.061964
O	2.108717	0.995945	9.442510
O	4.574226	1.087480	10.380390

O	7.490630	16.750381	10.196508
O	6.173783	16.748194	12.438829
O	3.896481	17.091848	0.417951
O	1.752526	16.495275	12.331899
O	2.161975	16.586016	9.786854
O	4.830107	16.756351	10.121696
O	6.089891	18.899076	10.886669
O	1.846429	18.899275	11.200233
O	8.519160	2.501901	8.108893
O	8.180388	19.908154	7.526064
O	8.507948	17.321880	7.692147
O	3.749520	2.897692	8.619590
O	4.170382	0.399771	7.855956
O	3.583537	17.403269	7.784624
O	19.845806	0.664826	10.533893
O	19.827385	17.323473	10.711219
O	2.760433	18.816692	3.082774
O	3.753524	18.666058	5.486897
O	6.110514	18.308474	7.193764
O	8.092692	18.402794	5.353066
O	7.918900	18.979864	2.743515
O	5.401135	18.987627	3.441572
O	2.591247	3.321740	3.601366
O	3.604360	2.909433	5.979926
O	6.015810	2.811928	7.267772
O	8.089488	3.402928	5.664890
O	8.010001	3.154986	3.007160
O	5.270191	3.321143	3.931123
O	3.835214	1.079521	4.094931
O	8.340164	0.996343	4.597462
O	1.415355	17.330437	1.423684
O	1.665630	0.004577	0.832824
O	2.176592	2.655522	0.999844
O	6.262881	17.168459	1.680637
O	6.176587	19.656830	0.920617
O	5.921506	2.474441	1.249169
O	10.193200	19.071201	3.771062
O	10.270885	2.739097	4.345192
O	12.852121	10.768542	3.605514
O	13.850018	11.109612	1.231771
O	16.085073	11.029419	13.051906
O	18.108898	11.364120	1.411371
O	17.954126	11.016286	4.016774
O	15.432557	11.357753	3.262374

O	12.932210	7.036685	3.430732
O	14.001384	6.971614	1.025539
O	16.359375	7.283233	13.293736
O	18.685129	6.473543	1.420606
O	18.088675	6.891024	4.019986
O	15.593934	6.553935	3.099637
O	14.670118	8.955346	2.682622
O	18.524353	8.953157	2.353802
O	11.530068	12.458764	5.195147
O	11.677431	9.868711	5.852921
O	12.254065	7.212193	5.926795
O	16.433857	12.852565	5.116321
O	16.094084	10.285993	5.687508
O	15.945920	7.622113	5.521157
O	0.250475	10.946837	3.005956
O	0.508759	7.290198	3.096291
O	17.266972	8.786801	10.370487
O	16.420643	8.871969	7.865591
O	14.029015	9.040315	6.697121
O	11.845816	8.453892	8.113043
O	12.188793	8.636962	10.694222
O	14.672922	9.194731	9.875049
O	17.273581	13.510824	10.047956
O	16.183382	13.094337	7.701649
O	13.957937	12.766204	6.188835
O	11.843813	13.347453	7.706601
O	12.184188	13.365561	10.551023
O	14.671921	13.018125	9.867152
O	16.444870	11.089314	9.449470
O	12.020207	10.874207	9.211386
O	18.858721	7.400637	11.967346
O	18.359774	9.874084	12.623381
O	18.103291	12.600047	12.462651
O	14.260869	7.300745	11.707716
O	13.847014	9.792099	12.382219
O	13.928704	12.435680	12.383156
O	9.847019	9.370639	9.616355
O	9.708868	12.676260	9.528428
O	12.843713	18.737495	3.679924
O	13.679030	18.656307	1.166462
O	15.985765	19.064436	13.298955
O	18.112501	18.391651	1.341780
O	17.928900	18.899275	3.946914
O	15.441367	18.821867	3.107934

O	12.592636	3.158369	3.193987
O	13.774936	2.992810	0.880735
O	16.169167	2.824862	12.962106
O	18.186382	3.409296	1.180648
O	17.948921	3.134490	3.840252
O	15.276986	3.314576	3.016796
O	13.934912	1.009078	2.666028
O	18.186983	0.993756	2.185712
O	11.419347	17.335611	5.362702
O	11.600947	0.077805	5.763657
O	12.431659	2.656715	5.848104
O	16.259266	17.087271	4.933777
O	16.099689	19.572060	5.686705
O	15.776334	2.335546	5.678139
O	0.175393	19.229797	2.845761
O	0.226249	2.655920	2.764259
O	17.266171	1.079322	10.373967
O	16.348965	1.067183	7.924075
O	13.982564	0.667412	6.778356
O	11.757919	1.341789	8.031673
O	12.098693	1.084296	10.637611
O	14.656505	1.154540	9.953339
O	17.522053	16.658846	9.788996
O	16.258265	17.013447	7.562332
O	13.879850	17.155724	6.281312
O	11.847217	16.424038	7.856624
O	12.350170	16.501047	10.460287
O	14.867135	16.488510	9.770527
O	15.944519	18.825249	9.537930
O	11.842011	18.800575	9.116232
O	18.686932	2.481405	12.121385
O	18.366581	19.815823	12.546295
O	17.686434	17.238504	12.378606
O	13.767727	2.889534	11.704237
O	13.843810	0.338681	12.441105
O	14.103095	17.577383	12.139050
O	9.754718	0.580056	9.611002
O	10.005193	16.913155	9.778155
O	7.166875	9.538386	9.300516
O	5.259179	8.708997	12.130754
O	3.737907	9.042902	0.756675
O	1.923714	8.624624	12.033726
O	2.152765	9.125085	9.387104
O	4.755225	8.878337	9.777754

O	7.243759	13.258704	10.143912
O	6.258276	13.021707	12.540005
O	3.857839	12.769985	0.251199
O	1.755729	13.525748	12.124330
O	2.171987	13.095929	9.461514
O	4.655916	13.175526	10.374234
O	5.995388	10.954001	10.974863
O	1.751925	11.099662	11.202910
O	8.593242	7.620521	8.034752
O	8.679737	10.199631	7.349810
O	7.764532	12.689394	7.599537
O	3.499445	7.219357	8.183972
O	3.754125	9.785931	7.443892
O	4.172785	12.429512	7.779136
O	19.867029	9.362679	10.461893
O	19.808165	12.774561	10.456139
O	2.906994	11.119164	2.843218
O	3.838017	11.357354	5.357750
O	6.082283	10.856098	6.772333
O	8.095494	11.526495	5.183236
O	7.929313	10.858287	2.602726
O	5.438175	10.609350	3.422167
O	3.081786	6.556920	3.078492
O	3.736105	6.714918	5.599581
O	5.925110	7.289999	7.030626
O	8.191801	6.471354	5.412621
O	8.014205	6.967237	2.771486
O	5.576927	7.217566	3.755404
O	3.510858	8.938631	4.184730
O	8.348974	8.961117	4.509134
O	1.400739	12.503338	1.177035
O	1.332664	9.872491	0.921955
O	1.830812	7.207417	0.768720
O	6.084686	12.678449	1.825441
O	6.089691	10.268282	0.819709
O	5.926712	7.633456	1.170076
O	10.245858	10.692728	3.756876
O	10.348169	7.213984	4.009815
O	8.596045	14.919275	8.615172
O	3.833012	14.903157	8.520555
O	5.341068	14.915694	0.762162
O	2.411450	14.918281	0.919814
O	1.324856	4.958831	1.929962
O	6.175585	5.196226	1.992461

O	4.592246	4.999027	7.369483
O	7.593743	4.967388	7.702051
O	11.678232	4.988679	4.843575
O	16.512545	5.061311	5.103206
O	14.768627	5.059122	12.797895
O	17.847410	4.946692	12.466666
O	18.772026	15.008821	11.544444
O	14.015199	14.936787	11.713470
O	15.347263	14.998075	6.108269
O	12.428455	14.930618	5.692460
O	11.087583	5.460485	15.147951
O	10.339962	2.898687	14.630028
O	8.738201	2.555429	12.052463
O	10.525765	3.476753	9.716326
O	9.766130	0.328930	14.052552
O	9.517457	8.550202	14.144360
O	10.925204	4.146952	12.299646
O	12.432660	5.556199	10.539782
O	11.604751	6.789340	13.029287
O	11.925503	9.036137	14.635650
Al	4.510756	18.859674	7.013896
Al	6.337563	3.552369	2.562979
Al	17.874239	6.458619	13.299891
Al	11.351273	12.451999	9.074076
Al	16.174572	3.490086	4.476346
Al	7.529673	6.630745	6.991413
H	10.106905	6.070787	9.358331
H	19.415133	6.810831	11.421721
H	11.620969	14.101625	10.870744
H	6.041438	3.823394	-1.047487
H	18.603642	3.614852	4.386011
H	2.948039	17.099012	7.102760
H	10.162166	5.745637	15.275759
H	11.043334	4.475086	15.058686
H	9.442175	3.080166	14.992440
H	10.339561	1.905130	14.561642
H	7.795766	2.239632	12.080031
H	9.098196	2.302911	11.176679
H	9.792760	4.082081	9.492294
H	10.991477	3.292886	8.881628
H	9.130032	0.574086	13.359847
H	9.266582	-0.233614	14.675665
H	8.831304	9.239702	14.174336
H	10.434464	8.918334	14.426206

H	11.186091	3.797724	11.405395
H	10.837908	3.436159	12.996499
H	12.044635	6.174660	9.896996
H	13.378901	5.778869	10.561462
H	11.925103	6.275349	12.237818
H	11.536076	6.141230	13.816476
H	12.252462	9.856174	14.225995
H	12.188392	8.312409	14.017220
Pt	7.079979	5.047183	-3.597350
Pt	9.512853	7.183340	-0.887694
Pt	8.947030	6.795110	-3.283653
Pt	6.413647	5.324973	-1.217987
Pt	7.218531	7.874233	-1.399594
Pt	8.886965	4.724022	-1.298954
		2	
		Pt <sub>2</sub>	
Pt	10.330750	7.494361	6.777151
Pt	11.810376	9.159709	7.548414
		3	
		Pt <sub>3</sub>	
Pt	9.404133	7.896321	8.073830
Pt	11.038128	9.679669	8.691723
Pt	10.861534	8.915151	6.321460
		4	
		Pt <sub>4</sub> _Upper	
Pt	9.181087	8.483541	7.577856
Pt	11.493428	9.616391	8.118262
Pt	10.978063	8.580050	5.923182
Pt	9.866841	10.207392	6.384226
		4	
		Pt <sub>4</sub> _Lower	
Pt	9.291208	7.118469	7.008275
Pt	11.493428	9.616391	8.118262
Pt	10.978063	8.580050	5.923182
Pt	9.806575	8.155208	9.203221
		5	
		Pt <sub>5</sub> _Upper	
Pt	8.674331	8.071433	6.812348
Pt	10.389615	8.935646	7.800416
Pt	10.414643	9.269949	6.034528
Pt	10.429259	7.501127	7.175295
Pt	8.466103	10.152471	6.982046
		5	
		Pt <sub>5</sub> _Lower	

Pt	8.296116	7.936120	6.693507
Pt	10.889565	10.875798	8.009057
Pt	10.414643	9.269949	6.034528
Pt	9.415345	8.906991	8.816854
Pt	8.419851	10.562190	7.080945
		6	
		$\text{Pt}_6\text{\_Upper}$	
Pt	10.319338	7.686984	6.360271
Pt	12.676929	10.359420	7.548414
Pt	12.124322	9.250846	5.198091
Pt	10.871945	8.795158	8.710593
Pt	10.176382	10.323999	6.651753
Pt	12.820286	7.723001	7.256932
		6	
		$\text{Pt}_6\text{\_Lower}$	
Pt	10.319338	7.686984	6.360271
Pt	12.676929	10.359420	7.548414
Pt	13.184286	8.920523	5.720563
Pt	10.945227	8.982807	5.043651
Pt	10.176382	10.323999	6.651753
Pt	12.820286	7.723001	7.256932