Supporting Information of

Tunable Selectivity of Phenol Hydrogenation to Cyclohexane or Cyclohexanol by Solvent-Driven effect over Bifunctional Pd/NaY Catalyst

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1. Experimental Section

1.1 Chemical Materials

NaY zeolite (Si/Al=3.83) was purchased from Nankai Zeolite Factory. $Pd(OAc)_2$ (Pd content: 46.0%~48.0%), SiO_2 with purity of 99.99%, acetone (99.9%), were bought from Sinopharm Chemical Reagent Co., Ltd). phenol (>99%) was purchased from Sigma–Aldrich. N,N-dimethylformamide (99.5%), methanol (99.5%), ethanol (99.5%), and n-butanol (99%), n-octane (99%) were bought from Aladdin Chemical Reagent Co., Ltd). All the chemical reagents were of analytical grade and used directly without further purification.

1.2 Catalyst Preparation

Preparation of Pd/NaY catalyst: Firstly, 42.0 mg $Pd(OAc)_2$ was ultrasonically dissolved in 20 mL acetone, and then 1.0 g NaY zeolite was added and left stirring for overnight at room temperature. The suspension was evaporated under vacuum at 60 °C to remove the solvent and followed by calcination at 450 °C in air atmosphere for 2 h. Finally, the sample was reduced at 400 °C in H_2 atmosphere for 2 h, which was denoted as Pd/NaY.

Preparation of Pd/SiO_2 catalyst: The preparation procedure of Pd/SiO_2 catalyst was nearly identical to that of Pd/NaY catalyst except replacing NaY zeolite with SiO_2.

1.3 Catalyst Characterization

Inductively coupled plasma (ICP) spectroscopy was performed on an Ultima 2 plasma emission spectrometer from Jobin Yvon.

The Brunauer–Emmett–Teller (BET) surface areas were calculated from the N_2 adsorption-desorption isotherms that were acquired on an ASAP 2020 instrument (Micromeritics) at 77 K. Prior to measurement, the samples were subject to evacuation at 200°C overnight.

Powder X-ray diffraction (PXRD) were collected on a Rigaku MiniFlex II diffractometer operated at 40 kV with a Cu K_α X-ray source (λ=1.5406 Å). The silicon wafer was used and the test of 2θ was in the range of 5~85° with a ramp rate of 0.5°·min^{-1}. The diffraction data were analyzed by comparison with reference

patterns in the database (PDF2-2004).

X-ray photoelectron spectroscopy (XPS) were measured on an ESCALAB 250 Xi spectrometer equipped with an Al anode (K_α=1486.6 eV). All samples were pressed into a wafer for analysis.

Transmission electron microscopy (TEM) and high-resolution TEM (HRTEM) analysis were performed on a Tecnai G^2 F20 field-emission transmission electron microscope operating at an acceleration voltage of 200 kV. The samples were prepared by dropping an ethanol dispersion of samples onto carbon-coated copper grids with a pipettor, and the solvent was allowed to evaporate at room temperature.

NH_3 temperature programmed desorption (NH_3-TPD) was carried out using an Altamira AMI-300 instrument equipped with a thermal conductivity detector. 100 mg sample was treated in a flow of He at 600 °C for 1.0 h to remove the adsorbed impurities. After cooling to 30 °C in a flow of He, the sample was exposed to 10% NH_3/He mixture for 2.0 h (30 mL·min^{-1}), followed by purging with He for 30 min, and then heated to 800 °C by ramping at 10 °C·min^{-1} under a flow of He.

Extended X-ray absorption fine structure (EXAFS) and X-ray absorption near-edge structure (XANES) spectroscopy of the Pd K edge were measured at the BL14W1 beamline, Shanghai Synchrotron Radiation Facility (SSRF), with electron beam energy of 3.5 GeV under ‘‘top-up’’ mode (current: 220 mA). The samples were measured at room temperature using a fixed-exit monochromator equipped with two flat Si (311) crystals. Data on the catalysts and reference samples (Pd foil and PdO powder) were collected in the fluorescence mode (32-element HPGe detector) or the transmission mode (Oxford ion chamber). The Fourier-transformed curves were fitted in real space with Dk=2~13 $Å^{-1}$ and DR=1.1~3.3 $Å^{-1}$ for Pd (k^2 weighted).

1.4 Catalyst Evaluation

Catalytic performance of the prepared catalysts was evaluated in a 100 mL autoclave. Typically, 0.1 g of catalyst, 1.0 g of phenol and 70 mL of solvent were mixed

in the reactor under mechanical stirring at 600 rpm. After purged three times with 0.2 MPa of N_2, the autoclave was heated to the desired temperature, and then pressurized with 5.0 MPa of H_2 as the initial point. After reaction, the autoclave was quenched with tap water to room temperature. The products were analyzed by a gas chromatograph (GC, Agilent 6890) equipped with a flame ionization detector and an HP-INNOWAX capillary column (Hewlett–Packard Company, 30 m × 0.32 mm × 0.50 μm). The conversion of phenol and the selectivity to product were defined as follows:

$$\text{Conversion of phenol}\ (\%) = \frac{(\text{moles of phenol})_{\text{in}} - (\text{moles of phenol})_{\text{out}}}{(\text{moles of phenol})_{\text{in}}} \times 100\%$$

$$\text{Selectivity to product } i\ (\%) = \frac{moles\ of\ product\ i}{\sum moles\ of\ product} \times 100\%$$

2. Computational Methods and Models

The zeolites model was built by cutting out a portion of the NaY catalyst lattice near $Na_{(SII)}$ site. As shown in Figure S1, the considered cluster model is composed by 120 atoms (36T model) for description of the six member rings (6-MR) which is the so-called sodalite cage of Y zeolites. The silicon atoms located at the cluster edge were terminated by H atoms oriented in the direction of the next tetrahedral atom, in which the Si-H bond length was fixed to 1.47 Å. During optimization sequences all atoms were allowed to relax except for the Si and H terminations that were kept frozen (represented as stick model). Two silicon atoms of 6-MR were replaced by aluminum atoms to study the influence of the aluminum content, and meanwhile two oxygen atoms were protonated (Bronsted acid sites) to maintain the electric neutrality.

All geometry optimizations were performed with the density functional theory at the level of dispersion corrected PBE-D3(BJ)[1-3] using 6-31G(d) all-electron basis set.[4] The solvation effects were considered using the SMD model.[5] Analytical frequencies were calculated to confirm the correctness of the structure of either a local minimum or a transition state (TS). A step size of 0.1 $amu^{1/2}$ bohr was used in the IRC (intrinsic reaction coordinate) procedure[6] to check the connectivity between a transition state and the reactant as well as the product.

The optimized structures were then adopted to calculate the free energies at the level of M062X functional[7] with 6-311+G(2d,p) basis set[8]. The free energy at M062X/6-311+G(2d,p) level in solution phase was calculated according to Eq. (1):[9-10]

$$G_{\text{soln}}^{\text{M062X/6-311+G(2d,p)}} = E_{\text{gas}}^{\text{M062X/6-311+G(2d,p)}} + \Delta G_{\text{thermo(soln)}}^{\text{PBE-D3/6-31G(d)}} + \Delta G_{\text{solv}} + RT\ln\left(\frac{RT}{P}\right) \qquad (1)$$

The first term in the right-hand side is the electronic energy computed at M062X/6-311+G(2d,p) level in gas phase. The second term is the thermal correction to the free energy of the solute in the solution phase at PBE-D3/6-31G(d) level. The third term is the solvation free energy. The last term denotes the free energy correction from the gas-phase standard state (1 atm) to the solution phase standard state of 1 M. It should be noted that the solvation free energy ΔG_{solv} was obtained by using SMD model[5] at the level of B3LYP[11-12]/6-31G(d) to make it consistent with the specific methods used in the development of such solvation model.[9-10] All calculations were carried out using the Gaussian 09 program.[13]

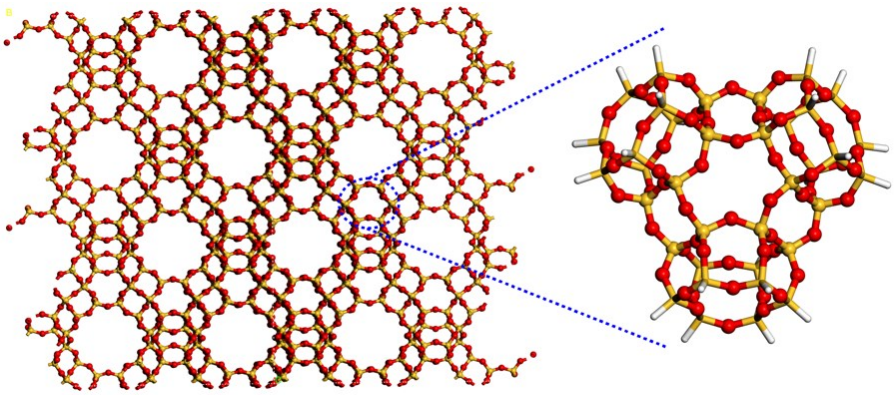

Figure S1. Selected cluster model composed by 120 atoms (36T) for description of the sodalite cage of Y zeolites.

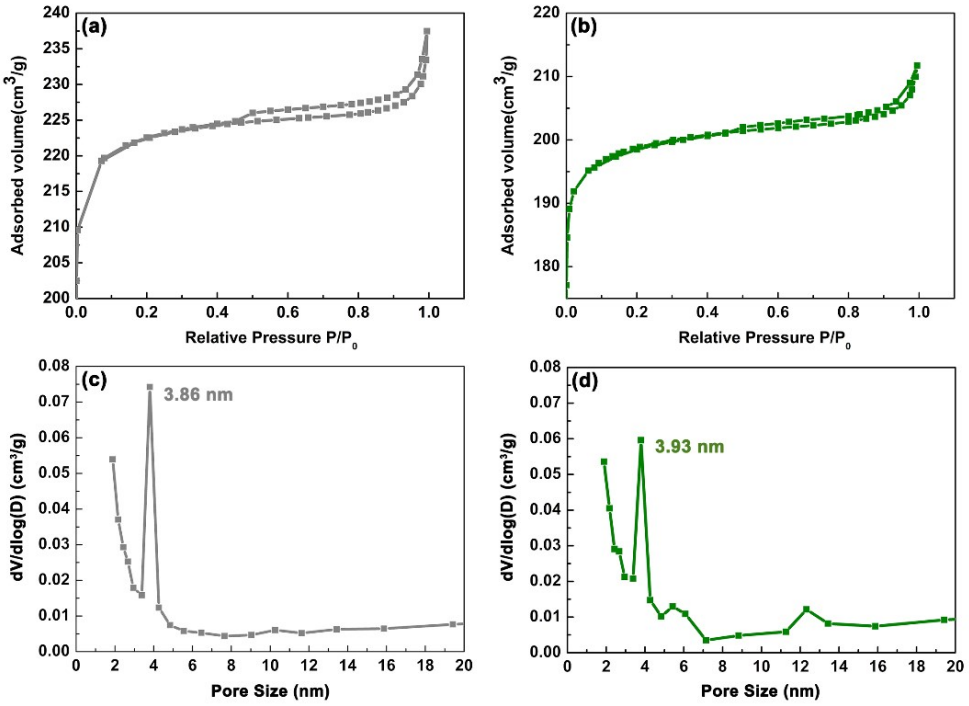

Figure S2. N_2 adsorption-desorption measurements at 77 K for (a) Pd/NaY catalyst and (b) NaY zeolite; pore size distribution of (c) Pd/NaY catalyst and (d) NaY zeolite.

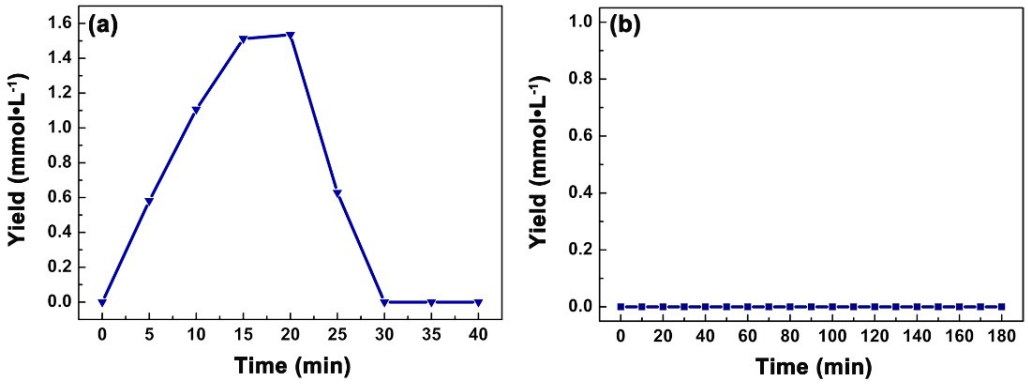

Figure S3. The variation tendency of benzene yield over Pd/NaY catalyst in (a) n-octane and (b) EtOH as a function of time. Reaction condition: 0.1 g catalyst, 1.0 g phenol, 70 mL solvent, 5.0 MPa H_2, 235 °C.

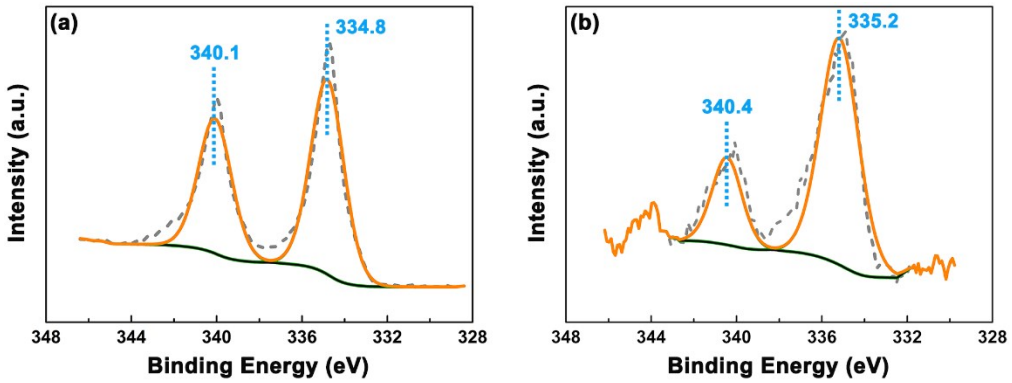

Figure S4. Pd 3d XPS of spent Pd/NaY catalyst in the solvent of (a) n-octane and (b) EtOH.

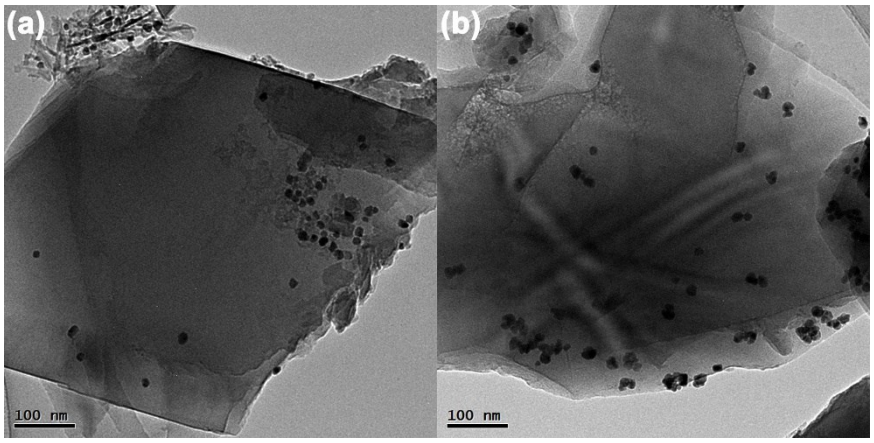

Figure S5. TEM image of spent Pd/NaY catalyst in the solvent of (a) n-octane and (b) EtOH.

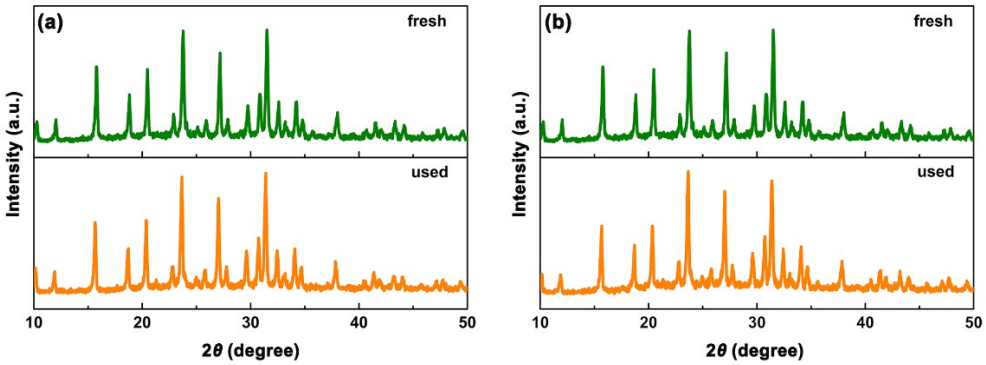

Figure S6. PXRD patterns of fresh and spent Pd/NaY catalyst in the solvent of (a) n-octane and (b) EtOH.

Optimized Cartesian coordinates (Unit in Å)

In the solvent of n-octane:

Cyclohexanol

C	-5.18471800	1.29417300	0.00675300
C	-3.64872000	1.27642000	-0.04216900

C	-3.07835400	2.69436900	-0.09521100
C	-3.58397500	3.53130600	1.08865900
C	-5.12032100	3.56150500	1.14179700
C	-5.69937000	2.13867800	1.18322800
H	-3.24711600	0.78056600	0.86295300
H	-3.28434900	0.70218700	-0.91261000
H	-5.57660500	1.71447400	-0.94081300
H	-5.57158800	0.26144400	0.07446800
H	-3.18032900	3.08509500	2.01832400
H	-3.17863300	4.56026800	1.02110800
H	-5.45952900	4.14510300	2.01661100
H	-5.50699100	4.08554200	0.24508300
H	-5.40323400	1.65423200	2.13475400
H	-6.80406900	2.17416400	1.17601100
H	-3.42712300	3.17617400	-1.03868800
O	-1.64917600	2.57665100	-0.10060100
H	-1.29898700	3.49158000	-0.08549200

Cyclohexene

C	-5.17204400	1.30157800	-0.02583200
C	-3.70270700	1.52770800	-0.28471500
C	-2.99754500	2.53033600	0.27294100
C	-3.60663000	3.56738800	1.18436400
C	-5.14319400	3.55177100	1.12910000
C	-5.67605800	2.11283300	1.17916600
H	-3.19935000	0.82377100	-0.96050700
H	-5.75265800	1.56865700	-0.93377300
H	-5.36125000	0.22241600	0.13303200
H	-3.26173400	3.39289200	2.22522900
H	-3.22402700	4.57098000	0.91594400
H	-5.56158100	4.15390200	1.95533500
H	-5.47653000	4.02667500	0.18619800
H	-5.32534100	1.63110300	2.11223900
H	-6.78024700	2.10441900	1.21074700
H	-1.92387700	2.61896500	0.06084200

TS1

C	-5.21134300	1.31201200	-0.05841100
C	-3.80783200	1.62355900	-0.56289400
C	-3.11730900	2.80603100	-0.13453500
C	-3.68055500	3.72425500	0.93286700
C	-5.18311700	3.50168700	1.17937900
C	-5.50688900	2.00567200	1.27942100
H	-2.79910900	1.14456000	0.23681100

H	-3.57261800	1.28188200	-1.58130100
H	-5.96728900	1.64390000	-0.80151400
H	-5.34670500	0.21875800	0.04047300
H	-3.12110100	3.55778500	1.86806700
H	-3.48114200	4.77124500	0.63843200
H	-5.48532900	4.03758100	2.09668000
H	-5.76763900	3.94054800	0.34752500
H	-4.89488800	1.55018200	2.08206700
H	-6.56570100	1.85612500	1.55726200
H	-2.35031000	3.23682900	-0.78909400
O	-1.79901700	1.72382100	0.90145200
H	-1.01007300	1.62585900	0.31988300

Zeolites model

Si	22.94994200	15.16833300	12.99890000
Si	21.21791400	13.43710000	11.25789200
Si	23.38654300	9.08916500	13.43650900
Si	23.38678800	13.43652000	9.08918500
Si	21.21802400	11.25789400	13.43703300
Si	22.94985400	12.99894700	15.16846000
O	21.63152900	14.78415400	12.09944600
O	21.65284200	12.06847100	14.79930100
O	24.16123500	15.77061200	12.06304600
O	24.23886700	12.10716300	15.68917300
O	20.70649600	12.24257300	12.24585400
O	23.46243000	13.86541500	13.86438300
O	22.46793900	12.87537900	10.34414700
O	22.47811700	10.34487800	12.86117300
Si	31.60348000	15.15333600	12.99603400
Si	31.51860400	15.09708800	17.30661700
Si	25.10474100	10.83119700	15.16195100
Si	29.45118500	19.50101300	15.16816500
Si	29.34835500	10.71959700	15.17135600
Al	27.24423500	12.87790000	11.08683600
Si	27.28255800	12.99897100	19.50110600
Si	27.26607100	17.31969300	10.85135700
Si	33.36048700	16.88523900	11.25653200
Si	33.36075800	13.43649700	19.06433500
Si	29.01424500	19.06445800	9.08919200
Si	25.56563700	11.25726500	9.08927400
Si	29.01397900	11.25788500	21.23296600
Si	31.19314700	21.23297300	13.43719200
Si	31.19388300	9.08915100	16.88528300
Si	25.56570400	9.08913100	11.25706000

Si	29.01381400	21.23297400	11.25786400
Si	29.01450100	9.08923500	19.06442300
Si	31.19467500	16.88524500	9.08967100
Si	31.19308600	13.43708300	21.23305500
Si	33.36084400	11.25710500	16.88535800
Si	33.36078700	19.06440400	13.43651800
Si	27.28241500	19.50121600	12.99889900
Si	27.30385600	10.76238200	13.06292600
Si	27.27348200	10.84752100	17.35342000
Si	31.58382200	17.29730300	15.12595500
Al	31.53145300	12.99245500	15.16215400
Si	29.51210400	15.20047200	10.90306700
Si	29.45110600	15.16834200	19.50104100
Si	25.14589400	15.13580200	10.91901000
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O	32.84812200	14.75899600	18.22434600
O	24.14797300	9.54621500	14.83164400
O	30.38635300	20.79847100	14.80185600
O	30.52208800	9.65625600	15.47670300
O	26.90883600	12.01650600	9.62164500
O	27.63824400	12.03423600	20.77628300
O	27.66140400	18.25489300	9.56980300
O	26.96699500	9.61049100	11.95991500
O	27.64132500	20.78545000	12.04424800
O	27.61559900	9.57985500	18.32486900
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O	30.37229700	14.79377900	20.80681000
O	32.77245100	11.85795100	15.50542900
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O	30.35119700	15.75573800	18.25643000
O	30.06469500	12.06528900	14.38054100
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O	26.74910800	12.13843300	18.19265700
O	33.88113200	12.26878300	18.05549300
O	24.35519100	12.22807700	8.56368600
O	30.18193300	12.26379900	21.74694600
O	30.07864800	8.57538100	17.94972100
O	24.45181400	8.57454500	12.32244700
O	30.18716700	21.74284100	12.26147600
O	30.14691500	18.01273100	8.57082800
O	33.87270100	18.03526900	12.28045700
O	26.76143100	18.20316000	12.12019600
O	30.33636100	18.20474900	15.66824000

O	30.27107900	14.54590400	12.17758800
O	30.88328000	13.80184300	16.55708800
O	25.93325200	11.29004200	13.80728800
O	28.63399800	11.31183900	16.51389500
O	25.99405200	13.94189800	11.61603700
O	28.59247900	13.85464900	19.00749300
O	32.11932800	12.85498600	19.99854400
O	24.94424700	10.29955800	10.31491300
O	29.60713700	10.32925100	19.98591300
O	32.16024700	10.25936500	17.54703400
O	29.59669200	19.97982500	10.33705200
O	32.12946300	17.49981000	10.30551400
O	32.11194100	19.98437500	12.85554300
O	28.59397900	19.01486000	13.85217900
O	31.08400100	16.52846500	13.74488800
O	28.58824900	16.44896900	11.36474200
O	32.17126300	14.00112500	13.92925700
O	32.06464100	16.25093700	16.26891100
O	26.12284700	10.32327100	16.32933800
O	28.31222800	10.02791900	14.13359400
O	28.56172100	13.92709300	10.28183300
O	26.11004700	16.32301800	10.31317500
H	28.63327800	22.42721600	10.49001600
H	28.63304800	19.83176300	7.89471700
H	31.95983300	16.50394100	7.89415100
H	34.55572800	16.50425500	10.49082500
H	34.55555400	19.83138500	13.81787100
H	31.96028900	22.42760600	13.81789900
H	28.68415800	19.88176000	16.36293600
H	26.08849900	19.88158800	13.76660700
H	28.63320300	10.49002700	22.42720000
H	28.63301400	7.89472200	19.83175500
H	31.96011200	7.89433100	16.50394300
H	34.55561100	10.49065100	16.50423900
H	34.55557100	13.81780400	19.83139000
H	31.96031700	13.81790600	22.42758600
H	28.68410100	16.36289700	19.88176900
H	26.08847700	13.76655000	19.88163200
H	20.02379400	13.81778300	10.49003000
H	22.61918300	13.81796600	7.89475500
H	25.94697900	10.49021000	7.89474100
H	25.94694100	7.89471400	10.49023500
H	22.61923200	7.89472900	13.81797900
H	20.02380300	10.49002300	13.81779500

H	22.56937900	16.36252400	13.76655600
H	22.56938300	13.76656500	16.36252000
H	29.57039600	12.37128600	13.56128900
H	28.66362000	13.72963700	9.32323900

LM1

Si	22.95008800	15.16818500	12.99875000
Si	21.21787400	13.43715300	11.25792000
Si	23.38655300	9.08917300	13.43646900
Si	23.38690800	13.43676500	9.08913100
Si	21.21800900	11.25786300	13.43703200
Si	22.94975600	12.99900700	15.16845500
O	21.64329700	14.79020700	12.07966400
O	21.65909800	12.05565700	14.80412900
O	24.18694400	15.75597500	12.08778000
O	24.23858000	12.11027100	15.69704900
O	20.70535200	12.25238100	12.25553500
O	23.44930100	13.85952000	13.86160900
O	22.45763800	12.84886200	10.32865900
O	22.47052000	10.33626400	12.85195100
Si	31.59235100	15.15085500	12.97180200
Si	31.51975200	15.09811400	17.29945800
Si	25.09319300	10.82747300	15.16733400
Si	29.45116400	19.50102900	15.16812100
Si	29.34445400	10.72768000	15.15242800
Al	27.29843600	12.96181500	11.04437100
Si	27.28252800	12.99899200	19.50114700
Si	27.29483600	17.30591300	10.85837200
Si	33.36047200	16.88520300	11.25647700
Si	33.36078700	13.43649000	19.06432700
Si	29.01437800	19.06424700	9.08942900
Si	25.56588200	11.25728400	9.08898100
Si	29.01398700	11.25786500	21.23297600
Si	31.19319000	21.23301500	13.43715800
Si	31.19382200	9.08924100	16.88535000
Si	25.56574400	9.08948800	11.25715800
Si	29.01377600	21.23304800	11.25790300
Si	29.01451500	9.08923400	19.06440500
Si	31.19427600	16.88532700	9.08973400
Si	31.19308600	13.43707200	21.23307000
Si	33.36093100	11.25705900	16.88536300
Si	33.36076800	19.06436200	13.43641900
Si	27.28252400	19.50095500	12.99885500
Si	27.28579700	10.80064200	13.04581100

Si	27.27366100	10.85096200	17.34340700
Si	31.58697100	17.29848400	15.12030300
Al	31.54085800	13.00098900	15.14574700
Si	29.45582100	15.16266500	10.88110400
Si	29.45111300	15.16837100	19.50101000
Si	25.11370300	15.11598800	10.89278700
O	32.79822900	15.49612800	11.91290500
O	32.84736700	14.75494200	18.22093100
O	24.12769100	9.54616800	14.84202000
O	30.38511500	20.79987400	14.80153700
O	30.50679000	9.65411500	15.47925200
O	26.99310200	11.88406400	9.64392300
O	27.63782800	12.03392200	20.77694500
O	27.65947100	18.24676500	9.56293200
O	26.96751700	9.64263300	11.93385600
O	27.64674200	20.79689600	12.05959700
O	27.62584500	9.58127100	18.30983100
O	24.17848100	14.79796400	9.57009000
O	30.46066300	15.51330800	9.62788500
O	30.37055600	14.79296400	20.80851700
O	32.77132100	11.85528500	15.50395300
O	32.88296900	18.25850000	14.79628400
O	30.35209900	15.74937700	18.25553000
O	30.07949600	12.06199200	14.35866500
O	28.03881200	12.11188200	12.42541600
O	26.75139700	12.13605700	18.19293000
O	33.88178000	12.26507700	18.05824400
O	24.43762400	12.30104200	8.56869400
O	30.18315600	12.26221200	21.74718700
O	30.08837900	8.57120700	17.95889400
O	24.46257600	8.57590800	12.33047300
O	30.19244900	21.74528000	12.25756200
O	30.16111300	18.02924400	8.56620800
O	33.87696300	18.02626100	12.29162100
O	26.76057000	18.21462900	12.10560600
O	30.33733200	18.20391000	15.66589000
O	30.27082600	14.54431200	12.16768000
O	30.88840800	13.80399200	16.54400700
O	25.90488700	11.27335600	13.80291700
O	28.62163100	11.32414300	16.48980500
O	25.83915300	13.78745300	11.47446600
O	28.59263200	13.85368000	19.00924600
O	32.12059300	12.85417800	20.00010700
O	24.93003000	10.28976100	10.29460800

O	29.60600000	10.32852700	19.98655300
O	32.16128900	10.25776900	17.54478700
O	29.59242700	19.98289600	10.33730500
O	32.15801600	17.51655100	10.28552900
O	32.11499300	19.98716900	12.85458200
O	28.58971600	19.01288000	13.85779900
O	31.10038700	16.52863300	13.74055000
O	28.64107200	16.49727600	11.37796100
O	32.17929500	14.00314300	13.91038400
O	32.06752200	16.25738800	16.27173600
O	26.11598700	10.31858000	16.33055200
O	28.31017500	10.05202600	14.10090500
O	28.51487500	13.98537200	10.26381900
O	26.14710500	16.27250500	10.35395700
H	28.63330100	22.42722100	10.49001400
H	28.63301300	19.83173500	7.89471100
H	31.95979700	16.50393600	7.89413000
H	34.55579300	16.50432100	10.49089300
H	34.55554500	19.83138000	13.81791100
H	31.96026700	22.42761800	13.81790400
H	28.68418300	19.88176400	16.36295200
H	26.08849100	19.88164700	13.76656700
H	28.63320300	10.49003400	22.42720400
H	28.63302200	7.89471100	19.83174300
H	31.96009100	7.89432000	16.50393500
H	34.55561100	10.49064200	16.50425900
H	34.55557400	13.81779900	19.83138800
H	31.96031200	13.81790000	22.42759100
H	28.68408900	16.36289400	19.88175900
H	26.08846300	13.76653300	19.88161900
H	20.02376000	13.81775000	10.49006600
H	22.61910200	13.81789200	7.89478400
H	25.94684600	10.49007700	7.89478500
H	25.94692500	7.89467500	10.49028800
H	22.61925500	7.89472000	13.81799800
H	20.02380700	10.49002500	13.81781100
H	22.56938500	16.36252500	13.76655900
H	22.56939600	13.76652200	16.36255100
H	29.55270800	12.41002100	13.57560300
H	29.12313300	13.17788300	9.03871000
C	32.88872400	11.61636400	8.94375200
C	31.60848400	12.36905500	8.53282000
C	30.38423600	11.51485800	8.83060100
C	30.30456900	11.07487400	10.28837800

C	31.58984900	10.32536000	10.68844100
C	32.83497600	11.18055800	10.41546500
H	31.53958400	13.30931200	9.11163300
H	31.62843000	12.63942700	7.46312400
H	33.01468600	10.72542700	8.29826600
H	33.76096200	12.26657200	8.75922400
H	30.20543100	11.96946800	10.92820000
H	29.41470200	10.44292200	10.45508400
H	31.52668300	10.05204500	11.75656800
H	31.65660000	9.37627800	10.12213800
H	32.81746400	12.07676100	11.06628400
H	33.74706100	10.61757100	10.67912300
H	30.32724200	10.65105400	8.14793500
O	29.16857700	12.33135300	8.43697600
H	28.27099400	11.89896900	8.77805800

TS2

Si	22.94997900	15.16823400	12.99893200
Si	21.21790900	13.43711500	11.25786700
Si	23.38653600	9.08915400	13.43651800
Si	23.38688600	13.43665200	9.08925400
Si	21.21805500	11.25791200	13.43701300
Si	22.94979400	12.99895200	15.16845000
O	21.63006000	14.78548600	12.09867400
O	21.65481000	12.06334600	14.80163300
O	24.16869600	15.75191500	12.06405800
O	24.24316800	12.11128400	15.68547400
O	20.70567700	12.24383100	12.24723900
O	23.45534800	13.86276100	13.86279800
O	22.46577300	12.87399000	10.34190200
O	22.47240000	10.33928000	12.85748500
Si	31.60066700	15.16387500	12.98969600
Si	31.52078100	15.10174200	17.30296300
Si	25.11141100	10.83913000	15.15005400
Si	29.45116300	19.50102200	15.16815800
Si	29.34965200	10.72794900	15.15913800
Al	27.34142500	12.93578800	11.03574500
Si	27.28252000	12.99898100	19.50113300
Si	27.27204600	17.31765300	10.84278600
Si	33.36045900	16.88526200	11.25651700
Si	33.36078100	13.43650000	19.06433200
Si	29.01429800	19.06429500	9.08928500
Si	25.56560800	11.25723700	9.08915900
Si	29.01398000	11.25788600	21.23297300

Si	31.19318100	21.23297800	13.43716900
Si	31.19385900	9.08917900	16.88535000
Si	25.56572800	9.08914300	11.25710700
Si	29.01379400	21.23298300	11.25793800
Si	29.01449100	9.08922900	19.06443200
Si	31.19469500	16.88546800	9.08964600
Si	31.19309100	13.43707800	21.23307900
Si	33.36087300	11.25709300	16.88534300
Si	33.36075900	19.06436300	13.43645100
Si	27.28247300	19.50114700	12.99882100
Si	27.30742000	10.78498200	13.04090900
Si	27.27969800	10.85271000	17.34316500
Si	31.59159100	17.30973800	15.13007500
Al	31.53717000	13.00509400	15.15206800
Si	29.48344500	15.13949900	10.88954400
Si	29.45110000	15.16838600	19.50102700
Si	25.15830800	15.13869800	10.90957300
O	32.78864200	15.49705700	11.90738200
O	32.84934600	14.75672700	18.22190000
O	24.14964400	9.55424400	14.82745900
O	30.39090800	20.79666500	14.80392100
O	30.51452800	9.65529700	15.47868600
O	26.90220700	11.97985700	9.64783800
O	27.63856000	12.03575700	20.77810700
O	27.64805400	18.28023700	9.57238700
O	26.96793400	9.61989600	11.94796200
O	27.64109500	20.78842900	12.04672900
O	27.62432800	9.58113700	18.31086800
O	24.27720700	14.72663000	9.57796800
O	30.50585000	15.50545000	9.65984900
O	30.36955800	14.79248900	20.80920100
O	32.76915800	11.85980200	15.50691600
O	32.88360200	18.27528500	14.80746900
O	30.35449900	15.75454600	18.25939400
O	30.07718800	12.06646400	14.36461600
O	28.10023700	12.06005200	12.39273100
O	26.75244400	12.13586200	18.19335300
O	33.88220700	12.26533300	18.05849600
O	24.35562900	12.22780700	8.55957700
O	30.18411200	12.26140000	21.74737500
O	30.08757400	8.57171300	17.95833900
O	24.45587100	8.57229900	12.32661900
O	30.18488700	21.74567800	12.26454400
O	30.14493100	18.01168600	8.57308000

O	33.87588700	18.01745900	12.30058600
O	26.77364800	18.19788400	12.12202100
O	30.33340700	18.20427800	15.67283300
O	30.26644500	14.55681600	12.20435500
O	30.88503700	13.80883100	16.54993500
O	25.93417600	11.29854500	13.79364500
O	28.63673800	11.32382900	16.50258900
O	26.04029500	13.95673400	11.57128000
O	28.59237200	13.85458500	19.00826900
O	32.12004200	12.85499000	19.99948400
O	24.92895700	10.26972800	10.28830800
O	29.60576300	10.32854700	19.98681700
O	32.16306800	10.25668500	17.54615400
O	29.60019100	19.98587300	10.33379900
O	32.16771000	17.52593400	10.27591700
O	32.11575100	19.98795700	12.85058400
O	28.59447500	19.01939300	13.85345900
O	31.11286300	16.55147700	13.74041300
O	28.58002300	16.42972400	11.32401100
O	32.18947100	14.02403600	13.93463300
O	32.06956000	16.26211700	16.27542100
O	26.12896800	10.32991000	16.31866800
O	28.31188800	10.04254200	14.11864600
O	28.62895100	13.89315900	10.24052500
O	26.07679500	16.36188100	10.29208900
H	28.63327400	22.42721500	10.49001800
H	28.63299100	19.83172700	7.89471300
H	31.95973300	16.50386600	7.89411200
H	34.55575300	16.50427800	10.49085200
H	34.55556200	19.83137000	13.81787800
H	31.96026200	22.42762400	13.81789700
H	28.68418800	19.88175700	16.36295700
H	26.08849100	19.88158100	13.76660000
H	28.63320400	10.49003500	22.42720500
H	28.63301100	7.89471600	19.83174500
H	31.96009900	7.89432700	16.50393000
H	34.55561400	10.49064800	16.50425600
H	34.55557500	13.81779900	19.83138600
H	31.96031200	13.81789600	22.42759200
H	28.68410200	16.36289800	19.88177100
H	26.08847700	13.76654700	19.88163600
H	20.02378000	13.81777300	10.49004700
H	22.61920200	13.81795700	7.89474100
H	25.94695000	10.49022400	7.89472400

H	25.94694600	7.89472300	10.49022400
H	22.61924300	7.89471700	13.81796600
H	20.02379500	10.49003700	13.81779700
H	22.56939600	16.36254400	13.76653400
H	22.56938800	13.76655500	16.36252700
H	29.56230800	12.38774500	13.56033100
H	27.73800800	14.66075600	8.69294000
C	30.70365200	11.11614900	9.40486600
C	30.55272100	12.49686700	8.80218900
C	29.78399700	12.72825700	7.66815300
C	28.91858100	11.69296200	7.05834500
C	29.29274000	10.25893800	7.46817300
C	29.58717900	10.15247600	8.97283900
H	29.49611200	13.09107200	9.29851400
H	31.28066500	13.26837400	9.09123900
H	31.69656200	10.73783900	9.09333600
H	30.74712000	11.20312500	10.50541900
H	27.87781000	11.94660800	7.34786000
H	28.94025800	11.84381800	5.96190900
H	28.47336600	9.57575600	7.18903600
H	30.18222200	9.94392300	6.89151700
H	28.66959900	10.38663500	9.53795000
H	29.87219300	9.11972300	9.23446900
H	29.72358800	13.75122600	7.27202600
O	27.56958200	15.07423500	7.81974500
H	26.80068800	15.65335400	7.99890600

In the solvent of EtOH:

Cyclohexanol

C	-5.18494800	1.29393100	0.00703000
C	-3.64876500	1.27619600	-0.04008400
C	-3.08031000	2.69499100	-0.09050300
C	-3.58446200	3.53096100	1.09292000
C	-5.12091400	3.56080500	1.14227300
C	-5.70083400	2.13851100	1.18257800
H	-3.25101400	0.77754500	0.86612800
H	-3.28714000	0.70155600	-0.91258000
H	-5.57403300	1.71465100	-0.94146900
H	-5.57067100	0.26042600	0.07470600
H	-3.18543300	3.08322600	2.02454700
H	-3.17575500	4.55753100	1.02331100
H	-5.46078000	4.14396200	2.01751000

H	-5.50500300	4.08539500	0.24473400
H	-5.40728000	1.65341100	2.13485400
H	-6.80583400	2.17454500	1.17147600
H	-3.42067700	3.17862500	-1.03382500
O	-1.64456500	2.58079500	-0.09450800
H	-1.29477000	3.49687000	-0.11493300

Cyclohexene

C	-5.17230800	1.30116900	-0.02554600
C	-3.70286400	1.52731100	-0.28528000
C	-2.99690400	2.53060400	0.27324700
C	-3.60671100	3.56789000	1.18433500
C	-5.14324300	3.55180900	1.12961300
C	-5.67654400	2.11297800	1.17894400
H	-3.19986800	0.82279400	-0.96168000
H	-5.75295300	1.56698200	-0.93399800
H	-5.36001700	0.22147600	0.13274100
H	-3.26081400	3.39424200	2.22514700
H	-3.22289800	4.57097500	0.91498400
H	-5.56043500	4.15317900	1.95725300
H	-5.47812500	4.02783600	0.18734700
H	-5.32749100	1.63141300	2.11320500
H	-6.78098100	2.10503200	1.20853100
H	-1.92261800	2.61970500	0.06146800

TS1

C	-5.20808400	1.33388600	-0.08453600
C	-3.80410500	1.64579900	-0.58736800
C	-3.11763500	2.81794000	-0.13526400
C	-3.70243700	3.76817400	0.88143600
C	-5.17976200	3.48567900	1.21314900
C	-5.46647000	1.98042900	1.28407100
H	-2.87538800	1.14801800	0.20861800
H	-3.54672000	1.30090200	-1.59940900
H	-5.96687400	1.70585900	-0.80432000
H	-5.35338500	0.23884000	-0.02813300
H	-3.08822200	3.74272200	1.79667300
H	-3.58430300	4.79199500	0.47661400
H	-5.44310200	3.98656300	2.16137300
H	-5.82375800	3.93003300	0.43005100
H	-4.81429400	1.51273100	2.04782100
H	-6.51069000	1.80205800	1.59779900
H	-2.27615700	3.19393100	-0.72681200
O	-1.84239500	1.63451900	1.00795600

H	-1.06418700	1.54221300	0.41284900

Zeolites model

Si	22.94993700	15.16834500	12.99889300
Si	21.21790600	13.43709500	11.25789300
Si	23.38654500	9.08916300	13.43651400
Si	23.38679300	13.43651400	9.08917500
Si	21.21802000	11.25789600	13.43703400
Si	22.94986800	12.99895400	15.16848900
O	21.63893900	14.79129000	12.08566000
O	21.66160700	12.05512100	14.80443000
O	24.17409000	15.76770800	12.07155700
O	24.24955300	12.11667400	15.69036500
O	20.70721400	12.24948400	12.25240300
O	23.46092400	13.85386100	13.85231800
O	22.47285600	12.86571900	10.34928400
O	22.48302300	10.34960700	12.85213600
Si	31.60133300	15.15836300	12.99597100
Si	31.51293100	15.08979100	17.30233400
Si	25.11051700	10.83980700	15.15445000
Si	29.45116100	19.50101300	15.16820900
Si	29.35058500	10.71854900	15.16671700
Al	27.26546400	12.88688400	11.07526200
Si	27.28253900	12.99896600	19.50111000
Si	27.28537000	17.30992200	10.86573100
Si	33.36053200	16.88525600	11.25649300
Si	33.36077000	13.43648800	19.06434000
Si	29.01424800	19.06447700	9.08918200
Si	25.56562000	11.25721000	9.08918300
Si	29.01397700	11.25788900	21.23297900
Si	31.19315500	21.23298700	13.43718800
Si	31.19390100	9.08912200	16.88532700
Si	25.56569500	9.08909400	11.25706400
Si	29.01381100	21.23298300	11.25786400
Si	29.01450400	9.08922000	19.06443900
Si	31.19470900	16.88528500	9.08965600
Si	31.19309100	13.43707800	21.23307500
Si	33.36088900	11.25706200	16.88536900
Si	33.36079300	19.06440900	13.43651800
Si	27.28239500	19.50123100	12.99890300
Si	27.30594700	10.77141800	13.05539400
Si	27.28092900	10.85111400	17.34867600
Si	31.57490000	17.29660100	15.11886400
Al	31.51695100	12.99086400	15.15982900

Si	29.51381800	15.19924100	10.90726700
Si	29.45109300	15.16838000	19.50104100
Si	25.15610300	15.11851300	10.92864200
O	32.80855000	15.50170200	11.94262300
O	32.84742900	14.76010600	18.21969200
O	24.14959000	9.55492300	14.83141300
O	30.40545000	20.78608600	14.81021100
O	30.53096300	9.65892400	15.47351800
O	26.90736500	11.99630100	9.63358300
O	27.63515800	12.02378900	20.76868200
O	27.66618800	18.24574200	9.57935500
O	26.96621900	9.60746700	11.96351500
O	27.63757200	20.77957300	12.03587100
O	27.61367600	9.58432700	18.32640000
O	24.28115900	14.72235400	9.59094100
O	30.44486200	15.50870900	9.61314200
O	30.39269300	14.80276200	20.79486700
O	32.78204500	11.87034700	15.50278500
O	32.87745300	18.24583600	14.79302200
O	30.34587400	15.75902300	18.24663700
O	30.07249200	12.05767900	14.38550800
O	28.08223900	12.05223100	12.40043100
O	26.75420600	12.14608800	18.18214700
O	33.88383300	12.26861700	18.05474200
O	24.35239500	12.22602700	8.56262400
O	30.17659500	12.27091700	21.74429400
O	30.07974500	8.57995400	17.94939900
O	24.45360400	8.57424300	12.32516300
O	30.18024800	21.74138400	12.26991500
O	30.15459700	18.02160900	8.57386100
O	33.87416000	18.03070600	12.28714500
O	26.75802100	18.19534300	12.12740300
O	30.32791100	18.19452300	15.67886900
O	30.28568300	14.54352200	12.17519600
O	30.87698900	13.77944100	16.57749000
O	25.93142800	11.30166900	13.79828900
O	28.65004800	11.30789500	16.52127000
O	25.97537400	13.90557800	11.62767400
O	28.60663300	13.84338900	19.00896500
O	32.11281500	12.84639400	19.98929400
O	24.92927600	10.29645100	10.31452400
O	29.61631500	10.33586800	19.97936200
O	32.15454100	10.27008500	17.55180900
O	29.60261500	19.97605800	10.34289500

O	32.12659200	17.50591400	10.31557000
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O	28.60535300	19.01511200	13.84303000
O	31.07153200	16.53820300	13.73593600
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O	32.05907600	16.23772000	16.25688800
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H	31.95982900	16.50395600	7.89414400
H	34.55573300	16.50427400	10.49082300
H	34.55555400	19.83138500	13.81787100
H	31.96028900	22.42760800	13.81789100
H	28.68415800	19.88175600	16.36293800
H	26.08849800	19.88159500	13.76660200
H	28.63320500	10.49003400	22.42720500
H	28.63301600	7.89472000	19.83175400
H	31.96011000	7.89432400	16.50396000
H	34.55561600	10.49065000	16.50425800
H	34.55557700	13.81780100	19.83138200
H	31.96031400	13.81789700	22.42759100
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H	26.08847600	13.76654800	19.88163300
H	20.02379000	13.81777700	10.49003300
H	22.61918500	13.81796000	7.89475200
H	25.94691900	10.49022100	7.89471500
H	25.94691900	7.89470700	10.49023500
H	22.61922900	7.89473000	13.81797800
H	20.02380000	10.49002600	13.81779100
H	22.56937400	16.36252800	13.76654700
H	22.56938500	13.76656500	16.36252000
H	29.57313800	12.38761700	13.57627800
H	28.62373600	13.81472300	9.29906600

LM1

Si	22.95008800	15.16818500	12.99875000
Si	21.21787400	13.43715300	11.25792000
Si	23.38655300	9.08917300	13.43646900
Si	23.38690800	13.43676500	9.08913100
Si	21.21800900	11.25786300	13.43703200

Si	22.94975600	12.99900700	15.16845500
O	21.63372500	14.78909700	12.09209400
O	21.66055900	12.05538700	14.80430600
O	24.17276700	15.75731900	12.06894100
O	24.24567200	12.11460400	15.69566500
O	20.70567600	12.24727500	12.25078600
O	23.46067100	13.85376400	13.85395100
O	22.47099800	12.86471700	10.34884200
O	22.48194800	10.34840800	12.85096200
Si	31.59294900	15.18402100	12.99001900
Si	31.51549500	15.09491200	17.29690400
Si	25.10690700	10.84102900	15.14947800
Si	29.45116400	19.50102900	15.16812100
Si	29.34599400	10.73218900	15.15884400
Al	27.34583300	12.95272300	11.02382100
Si	27.28252800	12.99899200	19.50114700
Si	27.27693900	17.31159900	10.84512300
Si	33.36047200	16.88520300	11.25647700
Si	33.36078700	13.43649000	19.06432700
Si	29.01437800	19.06424700	9.08942900
Si	25.56588200	11.25728400	9.08898100
Si	29.01398700	11.25786500	21.23297600
Si	31.19319000	21.23301500	13.43715800
Si	31.19382200	9.08924100	16.88535000
Si	25.56574400	9.08948800	11.25715800
Si	29.01377600	21.23304800	11.25790300
Si	29.01451500	9.08923400	19.06440500
Si	31.19427600	16.88532700	9.08973400
Si	31.19308600	13.43707200	21.23307000
Si	33.36093100	11.25705900	16.88536300
Si	33.36076800	19.06436200	13.43641900
Si	27.28252400	19.50095500	12.99885500
Si	27.29373000	10.79695800	13.04019300
Si	27.28514300	10.85755500	17.33979100
Si	31.59430200	17.32035700	15.13224400
Al	31.52110200	13.00350300	15.14225800
Si	29.47376800	15.13229500	10.87923100
Si	29.45111300	15.16837100	19.50101000
Si	25.16242100	15.13298800	10.91365400
O	32.80088100	15.49566400	11.92113700
O	32.84836200	14.75622800	18.21518100
O	24.14309700	9.55440600	14.83614500
O	30.40406700	20.78793800	14.80924700
O	30.51689400	9.66211000	15.47900300

O	26.89919800	11.97170700	9.65432900
O	27.63609000	12.02664900	20.77109500
O	27.64795400	18.27598300	9.57188100
O	26.96544200	9.61345700	11.96096100
O	27.64038400	20.78648400	12.04437000
O	27.62343900	9.58513400	18.31009800
O	24.27124800	14.72769000	9.58597000
O	30.50308700	15.51379600	9.66169400
O	30.38938600	14.80148700	20.79738100
O	32.78006800	11.87752200	15.50481000
O	32.88931100	18.28771500	14.82458400
O	30.34919400	15.75698000	18.24870600
O	30.07927600	12.06131100	14.36641600
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O	26.75246100	12.14249600	18.18567400
O	33.88494300	12.26416400	18.05905200
O	24.34923400	12.22431300	8.55973900
O	30.17913100	12.26830800	21.74459200
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O	26.77013000	18.19743400	12.12207700
O	30.33268100	18.20235500	15.68996200
O	30.25405400	14.60502000	12.22329600
O	30.87751300	13.79207900	16.56133600
O	25.90900800	11.30388400	13.78487900
O	28.65024800	11.32959300	16.51448100
O	26.01949000	13.94055200	11.59048100
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O	32.11276700	12.84722600	19.98953400
O	24.91410300	10.27536400	10.29795200
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O	32.15648300	10.26870400	17.54982000
O	29.60596400	19.97822800	10.34247900
O	32.16026500	17.53599100	10.28910300
O	32.10610300	19.97611700	12.84560900
O	28.60447900	19.01421800	13.84620900
O	31.12081600	16.58575800	13.73327000
O	28.58260100	16.43527100	11.33374300
O	32.18811600	14.06137100	13.96233500
O	32.06986500	16.25508000	16.26932400
O	26.13516300	10.33339200	16.31281600

O	28.28502200	10.05545900	14.13760400
O	28.64079100	13.88388400	10.25215600
O	26.07356200	16.36138900	10.30474700
H	28.63330100	22.42722100	10.49001400
H	28.63301300	19.83173500	7.89471100
H	31.95979700	16.50393600	7.89413000
H	34.55579300	16.50432100	10.49089300
H	34.55554500	19.83138000	13.81791100
H	31.96026700	22.42761800	13.81790400
H	28.68418300	19.88176400	16.36295200
H	26.08849100	19.88164700	13.76656700
H	28.63320300	10.49003400	22.42720400
H	28.63302200	7.89471100	19.83174300
H	31.96009100	7.89432000	16.50393500
H	34.55561100	10.49064200	16.50425900
H	34.55557400	13.81779900	19.83138800
H	31.96031200	13.81790000	22.42759100
H	28.68408900	16.36289400	19.88175900
H	26.08846300	13.76653300	19.88161900
H	20.02376000	13.81775000	10.49006600
H	22.61910200	13.81789200	7.89478400
H	25.94684600	10.49007700	7.89478500
H	25.94692500	7.89467500	10.49028800
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H	20.02380700	10.49002500	13.81781100
H	22.56938500	16.36252500	13.76655900
H	22.56939600	13.76652200	16.36255100
H	29.56303100	12.40266600	13.56898300
H	29.50915800	12.97683200	9.37325800
C	32.21591400	10.72738100	11.49832500
C	31.47668900	11.85260900	10.74829700
C	30.87005000	11.29133100	9.47363600
C	29.90438000	10.14752100	9.72726600
C	30.64050800	9.01959100	10.47748800
C	31.28127800	9.54092100	11.77169000
H	30.66546400	12.23013600	11.39451700
H	32.15493600	12.69217900	10.51739200
H	33.08145800	10.38913100	10.89742700
H	32.62005100	11.13267000	12.44318200
H	29.06683100	10.51130500	10.34598700
H	29.48587300	9.77777500	8.77387300
H	29.92300200	8.20937000	10.69585500
H	31.42257400	8.59111600	9.82186200
H	30.47880500	9.86338100	12.46078300

H	31.83113100	8.72995700	12.28149300
H	31.64952700	11.01100000	8.74794400
O	30.17437000	12.44477500	8.75475800
H	29.63412400	12.09575500	8.00129900

TS2

Si	22.94997900	15.16823400	12.99893200
Si	21.21790900	13.43711500	11.25786700
Si	23.38653600	9.08915400	13.43651800
Si	23.38688600	13.43665200	9.08925400
Si	21.21805500	11.25791200	13.43701300
Si	22.94979400	12.99895200	15.16845000
O	21.63437300	14.78982500	12.09160200
O	21.66013900	12.05640300	14.80393000
O	24.17622200	15.75003600	12.07092300
O	24.24580400	12.11446100	15.69491600
O	20.70655500	12.24697400	12.25015200
O	23.46113200	13.85364300	13.85359100
O	22.47319700	12.86887200	10.35088500
O	22.48281800	10.34945800	12.85225500
Si	31.60094300	15.17729600	12.99248800
Si	31.51302200	15.09361900	17.29703500
Si	25.10984700	10.84247200	15.15050200
Si	29.45116300	19.50102200	15.16815800
Si	29.35092600	10.72693100	15.15630800
Al	27.36371900	12.94316100	11.03370900
Si	27.28252000	12.99898100	19.50113300
Si	27.26017000	17.31163700	10.84498300
Si	33.36045900	16.88526200	11.25651700
Si	33.36078100	13.43650000	19.06433200
Si	29.01429800	19.06429500	9.08928500
Si	25.56560800	11.25723700	9.08915900
Si	29.01398000	11.25788600	21.23297300
Si	31.19318100	21.23297800	13.43716900
Si	31.19385900	9.08917900	16.88535000
Si	25.56572800	9.08914300	11.25710700
Si	29.01379400	21.23298300	11.25793800
Si	29.01449100	9.08922900	19.06443200
Si	31.19469500	16.88546800	9.08964600
Si	31.19309100	13.43707800	21.23307900
Si	33.36087300	11.25709300	16.88534300
Si	33.36075900	19.06436300	13.43645100
Si	27.28247300	19.50114700	12.99882100
Si	27.29849400	10.79115300	13.04602300

Si	27.28757900	10.85790300	17.33919900
Si	31.58705900	17.31505400	15.12741200
Al	31.52054000	13.00262800	15.14711600
Si	29.48422000	15.12408300	10.88804200
Si	29.45110000	15.16838600	19.50102700
Si	25.17222300	15.15209500	10.91239000
O	32.80128900	15.49306200	11.91848000
O	32.84675600	14.75546000	18.21391300
O	24.14943300	9.55507900	14.83202900
O	30.41304000	20.78237200	14.81329000
O	30.52309000	9.65956100	15.47601000
O	26.87638300	12.00102100	9.66156500
O	27.63529600	12.02471300	20.76967300
O	27.65541900	18.28002500	9.58814100
O	26.96055100	9.61418400	11.96584300
O	27.63520100	20.77819500	12.03217300
O	27.62313300	9.58725500	18.31234700
O	24.29633600	14.70737500	9.59047100
O	30.49930300	15.52168000	9.67241300
O	30.39134200	14.80232900	20.79614900
O	32.77985100	11.87679600	15.50523600
O	32.88094000	18.28307000	14.81883400
O	30.34779500	15.75806500	18.24784600
O	30.08475200	12.05600800	14.36400100
O	28.08327600	12.06515600	12.40532900
O	26.75634400	12.14532900	18.18207900
O	33.88487700	12.26471800	18.05847000
O	24.33910500	12.21430300	8.55784600
O	30.17768400	12.26978500	21.74442900
O	30.08807700	8.57688900	17.95744900
O	24.45395100	8.57182600	12.32675500
O	30.17468200	21.74373200	12.27610200
O	30.14705600	18.01546800	8.57373700
O	33.87538200	18.00759700	12.31233600
O	26.77637900	18.18418900	12.13682600
O	30.32444200	18.19437600	15.68532200
O	30.27125400	14.57630200	12.21519600
O	30.87314500	13.78960200	16.56418900
O	25.91942000	11.31087700	13.79126400
O	28.65276900	11.32472500	16.51051600
O	26.10731900	14.01909000	11.58799700
O	28.60668800	13.84339900	19.00944700
O	32.11309400	12.84688400	19.98976800
O	24.91823200	10.27439100	10.29697900

O	29.61525200	10.33544800	19.98013900
O	32.15574300	10.26926900	17.55012800
O	29.61102500	19.98283600	10.33848800
O	32.15927600	17.53366100	10.29030800
O	32.10858900	19.97869800	12.84235000
O	28.60823200	19.02196700	13.84229000
O	31.11236400	16.57632800	13.72797600
O	28.52537300	16.37103600	11.33095100
O	32.19544800	14.06008800	13.96941500
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O	26.13589600	10.33289300	16.31448900
O	28.29287400	10.04523500	14.13529900
O	28.70492500	13.82789200	10.23536400
O	26.02734300	16.41166300	10.27785500
H	28.63327400	22.42721500	10.49001800
H	28.63299100	19.83172700	7.89471300
H	31.95973300	16.50386600	7.89411200
H	34.55575300	16.50427800	10.49085200
H	34.55556200	19.83137000	13.81787800
H	31.96026200	22.42762400	13.81789700
H	28.68418800	19.88175700	16.36295700
H	26.08849100	19.88158100	13.76660000
H	28.63320400	10.49003500	22.42720500
H	28.63301100	7.89471600	19.83174500
H	31.96009900	7.89432700	16.50393000
H	34.55561400	10.49064800	16.50425600
H	34.55557500	13.81779900	19.83138600
H	31.96031200	13.81789600	22.42759200
H	28.68410200	16.36289800	19.88177100
H	26.08847700	13.76654700	19.88163600
H	20.02378000	13.81777300	10.49004700
H	22.61920200	13.81795700	7.89474100
H	25.94695000	10.49022400	7.89472400
H	25.94694600	7.89472300	10.49022400
H	22.61924300	7.89471700	13.81796600
H	20.02379500	10.49003700	13.81779700
H	22.56939600	16.36254400	13.76653400
H	22.56938800	13.76655500	16.36252700
H	29.56494600	12.39487100	13.56799000
H	27.92763300	14.56995600	8.48426100
C	30.97453800	11.09701000	10.34260400
C	31.01238400	12.33182700	9.49327100
C	30.33267300	12.44598200	8.29909900
C	29.53700600	11.32211200	7.70375300

C	29.83599200	9.97033400	8.37319700
C	29.89208800	10.10148500	9.90185800
H	29.65313700	13.03234300	9.54458200
H	31.65264200	13.16318600	9.81779600
H	31.98524100	10.64603100	10.27304400
H	30.85394700	11.38807600	11.40274200
H	28.46235200	11.57570900	7.77144700
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H	30.07667400	9.12147100	10.37349500
H	30.42199900	13.38184700	7.73121700
O	27.66429700	15.23483100	7.81208900
H	26.83523800	15.60244000	8.18386700

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