Supplementary Material (ESI) for Chemical Science

Reversible NO_x storage over Ru/Na-Y zeolite

*Sylvia Smeekens Steven Heylen, Kenneth Villani, Kristof Houthoofd, Eric Godard, Moniek Tromp, Jin Won Seo, Michaël DeMarco, Christine E. A. Kirschhock, Johan A. Martens**

Electronic Supporting Information

* johan.martens@biw.kuleuven.be

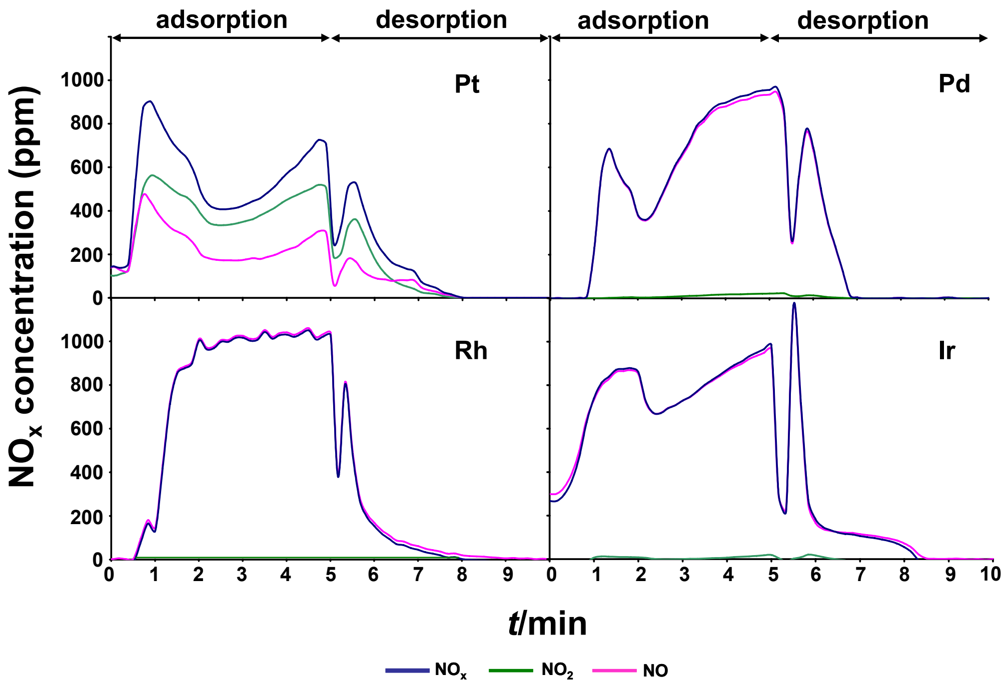

Fig. S1 Detailed NO_x adsorption-desorption patterns recorded at the outlet of a Pt(3%)/Na-Y, Pd(3%)/Na-Y, Rh(3%)/Na-Y and Ir(3%)/Na-Y adsorbent bed at 250 °C. All the catalysts were pretreated at 450 °C for 1 h under a flow of 5% O_2, 3% H_2O and balance N_2. Shown are typical reproducible cycles after some time of operation. Gas composition during lean phase was 1000 ppm NO, 5% O_2, 3% H_2O and balance N_2. Regeneration of the bed during desorption phase was done with 1% H_2, 3% H_2O and balance N_2.

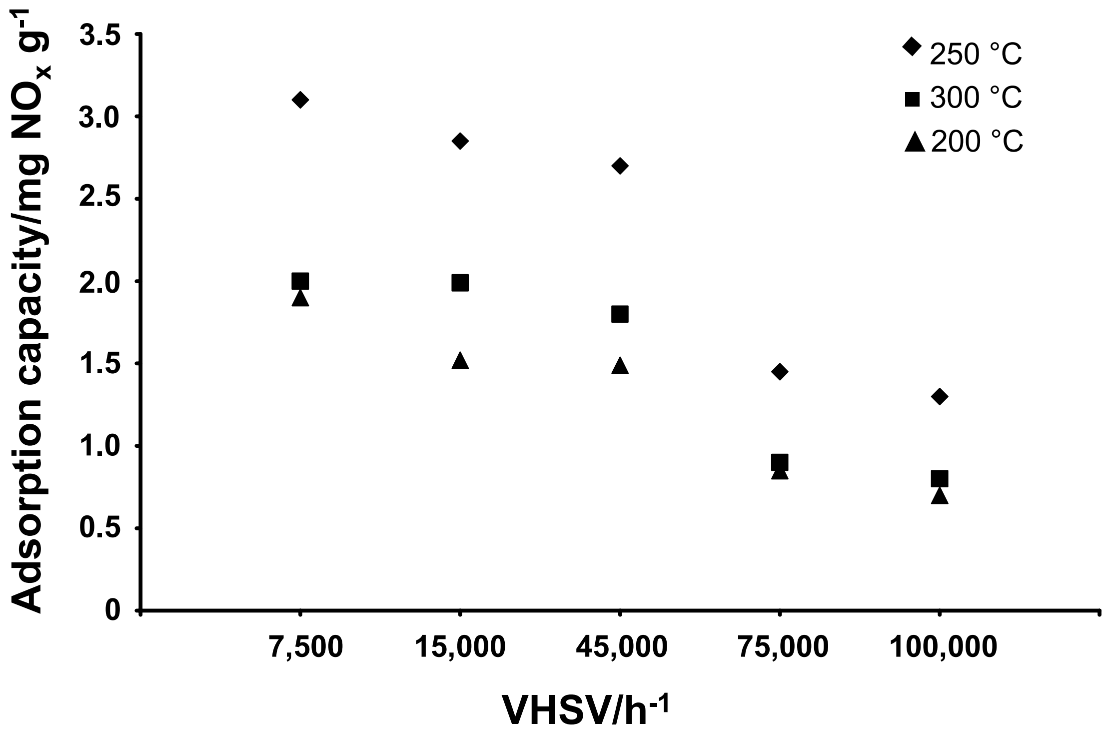

Fig. S2 NO_x adsorption capacity of a Ru(3%)/NaY zeolite at different volumetric space velocities and different reaction temperatures (♦ 250 °C, ■ 300 °C, ▲ 200 °C). The NO_x adsorption capacities were calculated based on an average of 10 cycles. The standard deviation of the NO_x adsorption capacities was less than ± 0.1 mg NO_x/g in all data points.

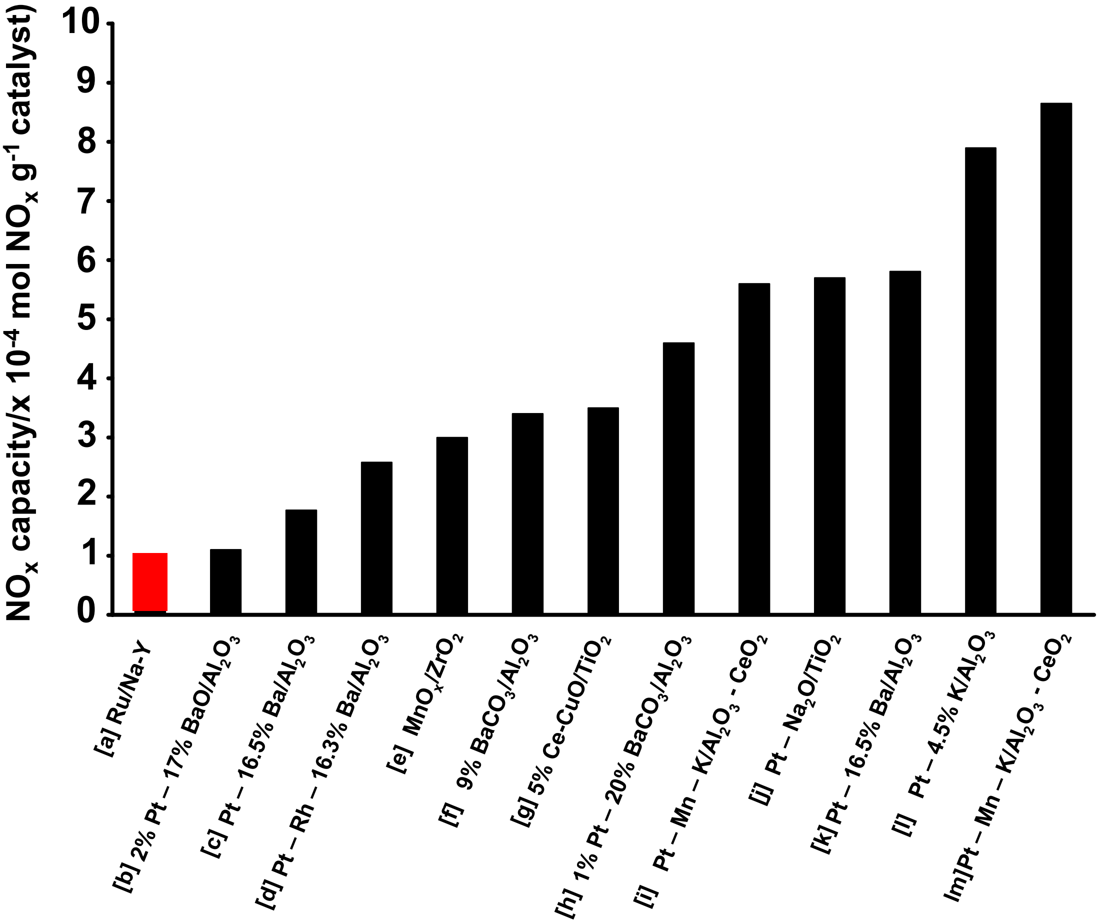

Fig. S3 Comparison of the NO_x adsorption capacity of the Ru/Na-Y zeolite with literature data on alternative formulations.[1,5,7] Feed gas comprised at least NO and O_2. The reaction temperatures were [a] 275 °C; [b][2] 300 °C; [c][3] 200 °C; [d][4] 300 °C; [e][5] 200 °C; [f][6] 400 °C; [g][7] 200 °C; [h][8] 350 °C; [i][9] 200 °C; [j][10] 300 °C; [k][3] 300 °C; [l][11] 250 °C; [m][9] 300 °C.

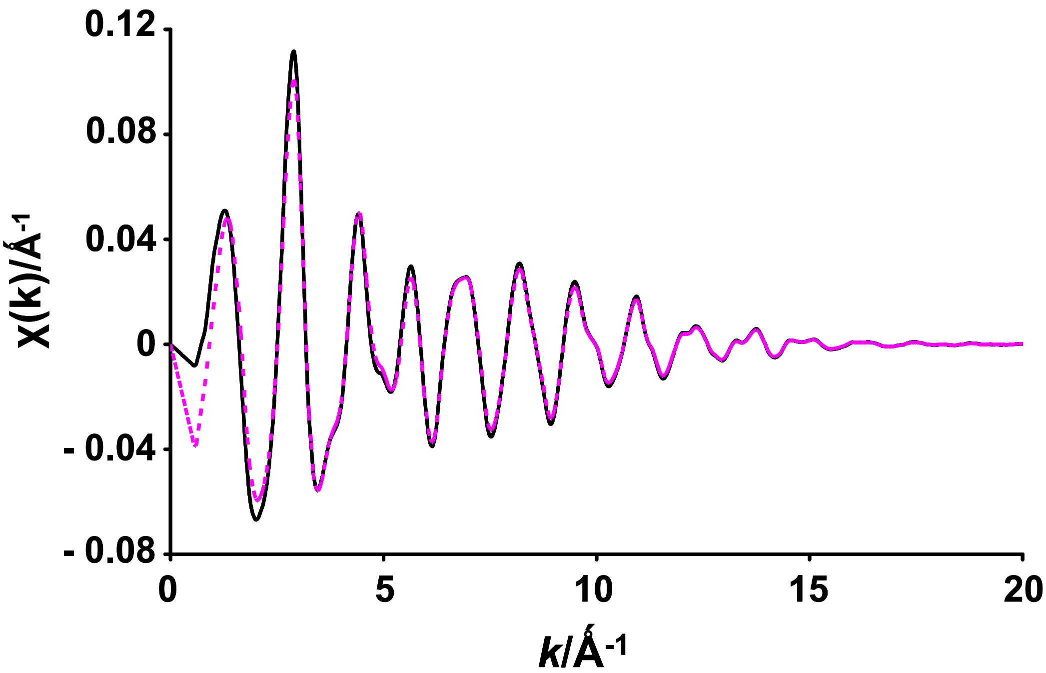

Fig. S4 Experimentally χ(k) EXAFS function of the Ru(3%)/Na-Y sample after NO_x saturation (—) and after regeneration (– – –) at the Ru K-edge.

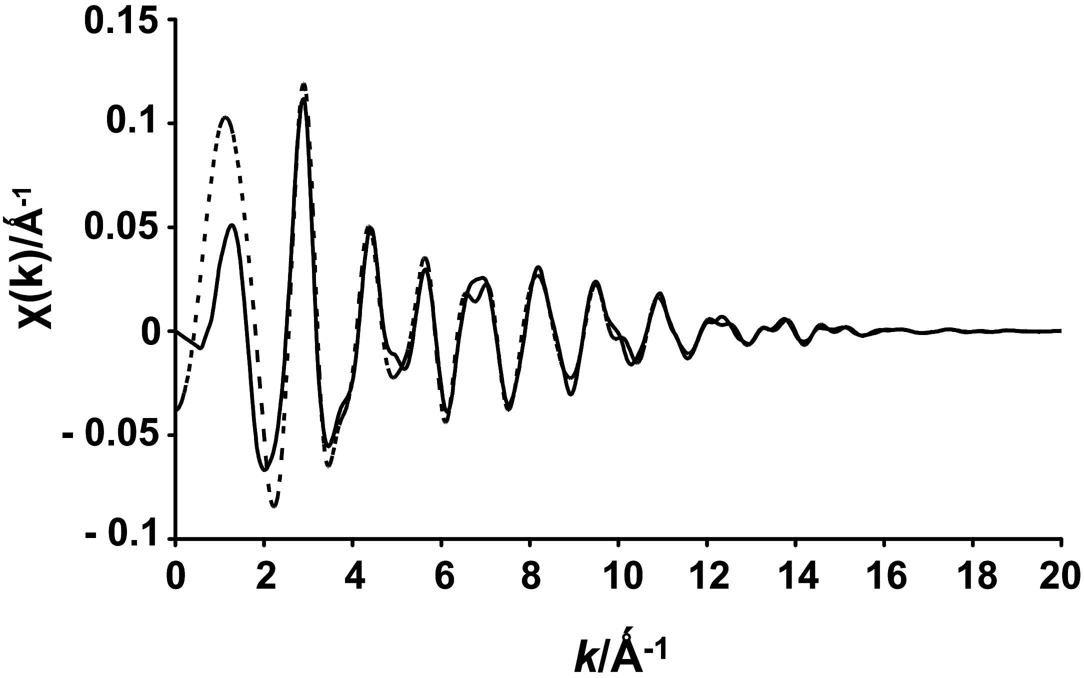

Fig. S5 Experimentally (—) and calculated (– – –) χ(k) EXAFS function of the NO_x saturated Ru(3%)/Na-Y sample at the Ru K-edge.

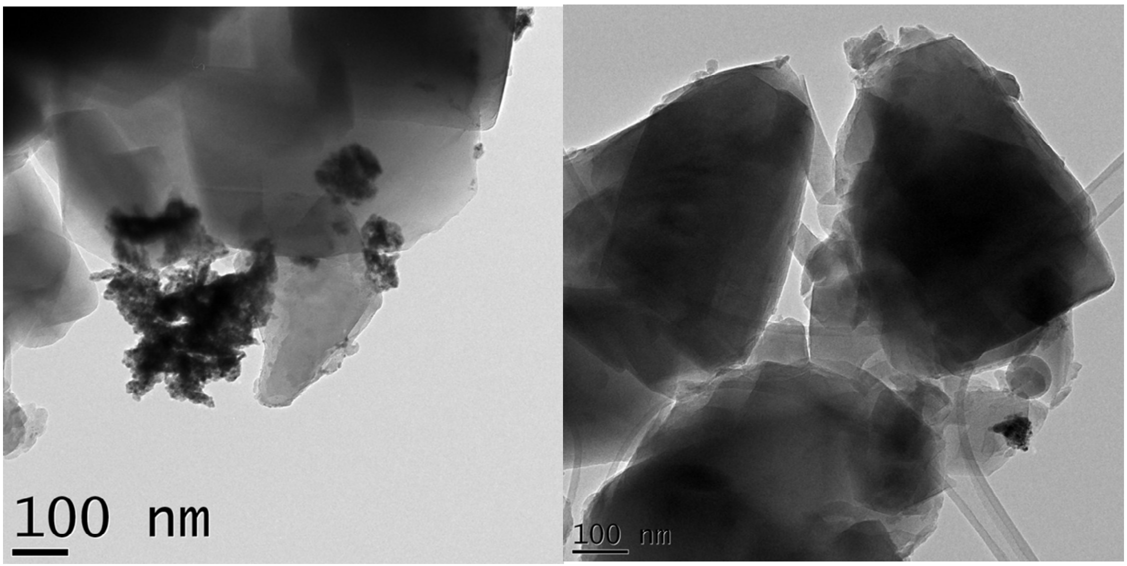

Fig S6 TEM images of NO_x saturated Ru(1%)/Na-Y zeolite.

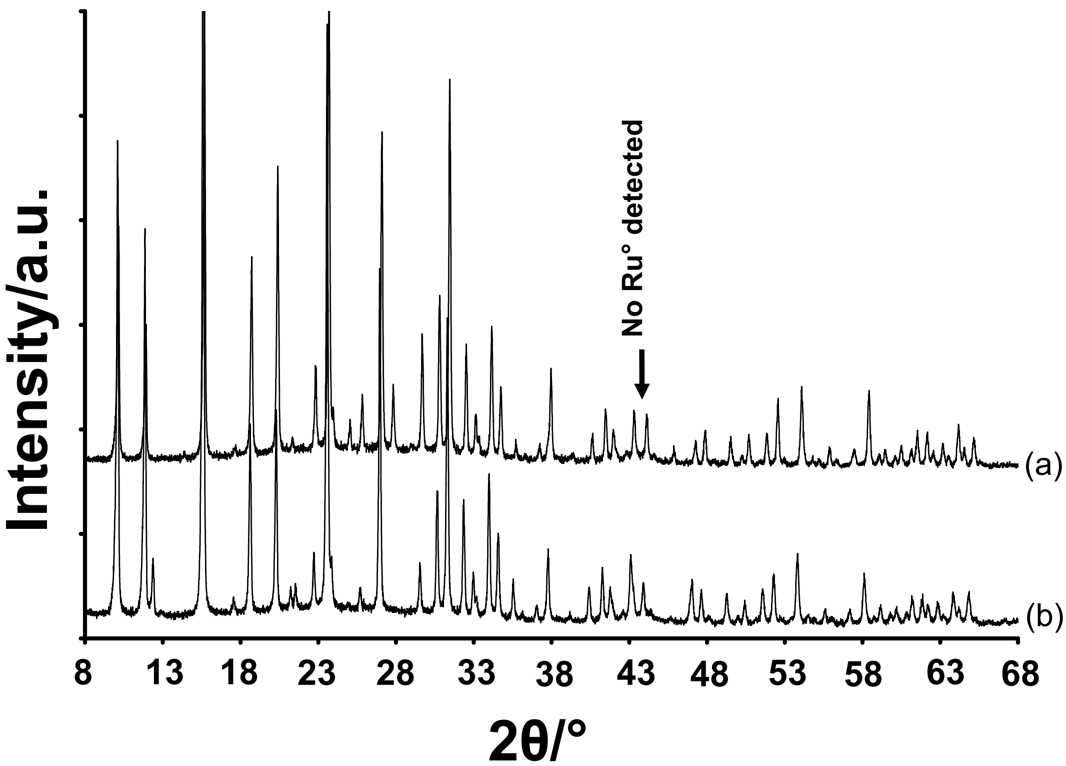

Fig S7 XRD pattern of Ru(1%)/Na-Y after (a) NO_x saturation and after (b) NO_x release.

Strategy of Rietveld refinement

Refinement of the structures occurred as follows: At first the structure cycled in oxidising conditions only, after desorption of NOx was investigated. This pattern resembled the data obtained in absence of Ruthenium rather closely. The positions of the framework atoms were obtained from the IZA website. Right from the start sodium cations were included on typical positions SII and SI'and SII'. SI was not occupied, as it is known from literature this site is unfavourable for Na^+. Typical publications in literature are for example [12, 13, 14]. Initially, the framework positions were kept fixed, while background, profileshape, unit cell scaling and cation position and occupation were refined. In a second step the environment of the SII cation was inspected on observed and difference electron density Fourier maps. Electron density at a distance of around 2.3-2.4 Å, typical for Na^+-oxygen distances, was assigned to water. The obtained positions for water were found to be in accordance with literature on the water surrounding Na^+ on SII and SII* positions in Faujasite[15,16,17,18] . After inclusion of these positions and refinement, not all sodium ions and water molecules in the structure were accounted for. Further typical sites like SIII, and SV were inspected for residual electron density. SV sodium ions were assumed to be coordinated with water and at first included as rigid bodies describing an octahedron of oxygen molecules centred by a sodium ion. Orientation and occupation of this rigid body was refined while the SIII position initially was kept fixed and at later stages left free to refinement. The obtained result closely resembled structures observed previously in samples without Ruthenium, with water molecules pointing towards the sodium ions on SIII [17,18]. The orientation of the SV-rigid body was then inspected for symmetry and replaced by water and sodium atoms on the respective positions. Initially occupation numbers of water molecules around SV and the corresponding Na^+ were constrained but later left to refinement. Refinement of this model resulted in a reasonable agreement between chemical composition and occupation factors. Also the octahedral environment of the sodium ions on SV far removed from the zeolite framwork was essentially retained.At this point the Fourier maps were inspected for possible positions of the Ruthenium ions. Electron density on SI finally was assigned to this species and refinement of the occupation number resulted in good agreement with the actual content of this cation in the material. As final step in all structure refinements the framework atoms were left to refine. Bond angles and distances refined to typical values for faujasite frameworks even though the temperature factors were treated as isotropic.

This structure then served as starting parameters for refinement of the sample cycled in absence of hydrogen after NOx adsorption. Already the comparison of the very similar diffraction patterns indicated the structure could be described very well with this set of parameters. An attempt was made to identify a possible adsorption site for the N_2O_3 molecule. A probable location in the vicinity of the position found in the system without Ruthenium and with similar characteristics was determined and N_2O_3 was inserted as rigid body. Refinement of position and orientation of the molecule led to a slight improvement of the goodness of fit and a physically sensible position. While the very low occupation factors of the adsorbed species does not allow final proof of this adsorption site we are nontheless confident the obtained position is close to the real situation as it also corroborates the observed reversible replacement of 2-3 water molecules by the NOx.

In a next step the samples cycled in presence of hydrogen were tackled. Already the comparison of the diffraction patterns revealed that a different decoration of the cavities in these samples was about to be encountered. Especially noteworthy was the very strong change of diffraction patterns between adsorption and desorption which – according to NMR – was directly related to a drastic change of sodium positions. Attempts to directly refine the structures with the above obtained models failed. Therefore, the same strategy as explained for samples obtained in absence of hydrogen was applied. The sample without NOx showed a similar distribution of cations compared to samples without hydrogen, except that the electron density previously assigned to SIII cations now was displaced significantly towards the framework, so that no significant interaction with water molecules around SV could be assumed. No electron density which could account for Ruthenium was found in this sample on position SI. This was in accordance with the reducing conditions used to prepare this sample, as a reduced Ru species is too large to be accomodated on this site. Furthermore, no indication for occupation of SII' by sodium was observed on Fourier maps and occupation number of any sodium inserted on this site immediately refined either to zero or caused the atom to shift either on SII or SI', or, most noteworthy, into the center of the sodalite cage. Occupation of this site by sodium is highly unlikely as sodium strongly prefers interaction with 6-rings of the framework. Accordingly, refinement of this electron density with Ruthenium was attempted and resulted in occupation factors in agreement with the chemical composition.
The sample after adsorption of NOx cycled under alternating reducing and oxidising conditions was analysed next. Biggest surprise in this sample were the very low occupation of SII by sodium and the very high occupation of SV and SIII. The latter also was found considerably shifted into the cavity which also explained the comparatively low intensity of the first reflection in the powder pattern. As before, the refinement successively introduced cations and water molecules, discarding intermediate solutions which were unstable or resulted in gross deviations of known chemical composition. Finally, possible positions for Ruthenium and the guest molecule were sought. The electron density in the center of the sodalite cage assigned in the desorbed sample to Ru was not observed. Instead, similar as for the samples cycled entirely under oxidising conditions, Ru was assigned to electron density on position SI. In correspondence to the positions assumed for N_2O_3 in previous studies the region in vicinity to SII, SIII, and SV cations was studied and the molecule was inserted on a likely site. As before the refinement remained stable and while the low occupation does not allow a final conclusion if this site is correct, the authors are confident the molecule is likely to adsorb on a site not far from the proposed structure.

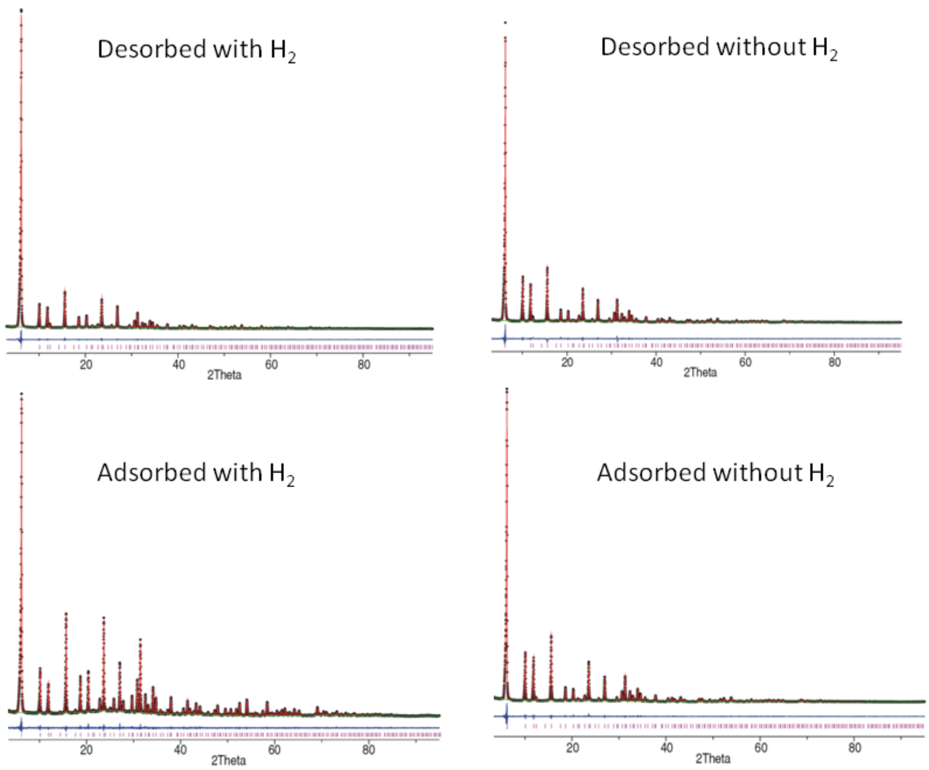

Fig. S8 Refined XRD patterns of the Ru(1%)/Na-Y zeolite.

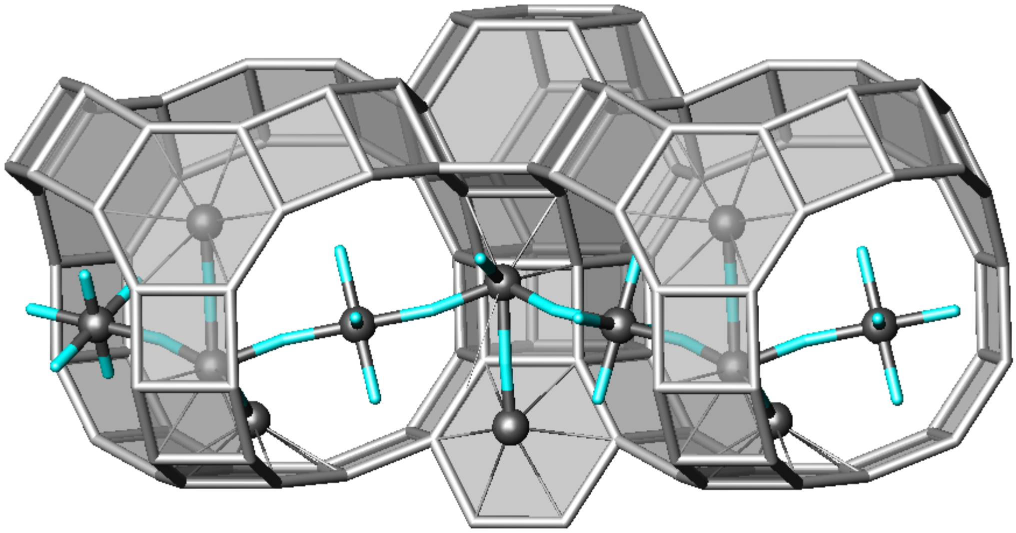

Fig. S9 Representation of the sodium cation distribution in a Ru(1%)/Na-Y zeolite during NO_x adsorption-desorption cycles without using a reducing agent during regeneration. A close contact between the frame and Na^+ cations on position SIII is observed.

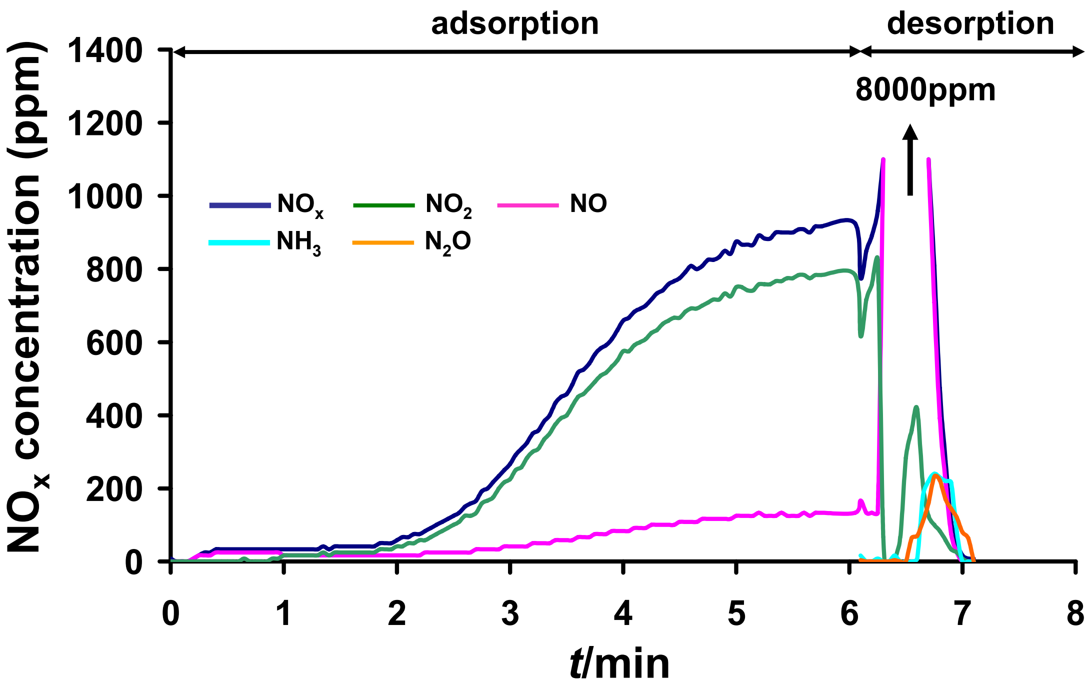

Fig. S10 A detailed NO_x adsorption-desorption pattern recorded at the outlet of a Ru(3%)/Na-Y adsorbent bed at 250 °C. The catalyst was pretreated at 450 °C for 1 h under a flow of 5% O_2, 3% H_2O and balance N_2 before adsorption-desorption cycles started. Gas composition during lean phase was 50 ppm SO_2, 1000 ppm NO, 5% O_2, 3% H_2O and balance N_2. Regeneration of the bed during rich phase was done with 1% H_2, 3% H_2O and balance N_2. When SO_x was absent in the lean phase, but present in the rich phase (50 ppm SO_2), a very similar NO_x adsorption-desorption pattern was obtained.

Rietveld refinements of Ru(3%)/Na-Y samples after Ru ion-exchange and after pretreatment

We performed Rietveld refinement in combination with analysis of difference electron density charts of the corresponding powder X-ray patterns on more samples: freshly Ru ion-exchanged sample and pretreated sample (Fig. S11). In the freshly Ru ion-exchanged sample electron density was found on SV in an octahedral environment with bond lengths typically found between Ru^{+3} and NH_3 (Fig. S12). Other electron density assigned to Na^+ was found at position SII' in the sodalite cage and SII* and SIII, linked by water molecules in the supercages. To become an active NO_x adsorbent, the Ru ion first need to migrate into the small cage system of the zeolite. After a pretreatment at 450 °C, electron density was found in the hexagonal prism at cation position SI (Fig. S13). The sodalite cages were crowded, occupied by cations on position SI'. Other electron density was found at position SII, in the 6-ring of the sodalite cage and interacting with one water molecule, resulting in tetrahedral environment. This indicates that after a pretreatment the NH_3 ligands have disappeared, resulting in a redistribution of the cations in the zeolite. Ru is already found in the hexagonal prism at position SI. However, because the large number of Na^+ cations in the sodalite cage, some cycles are necessary to push these cations into the supercage creating the NO_x adsorption site.

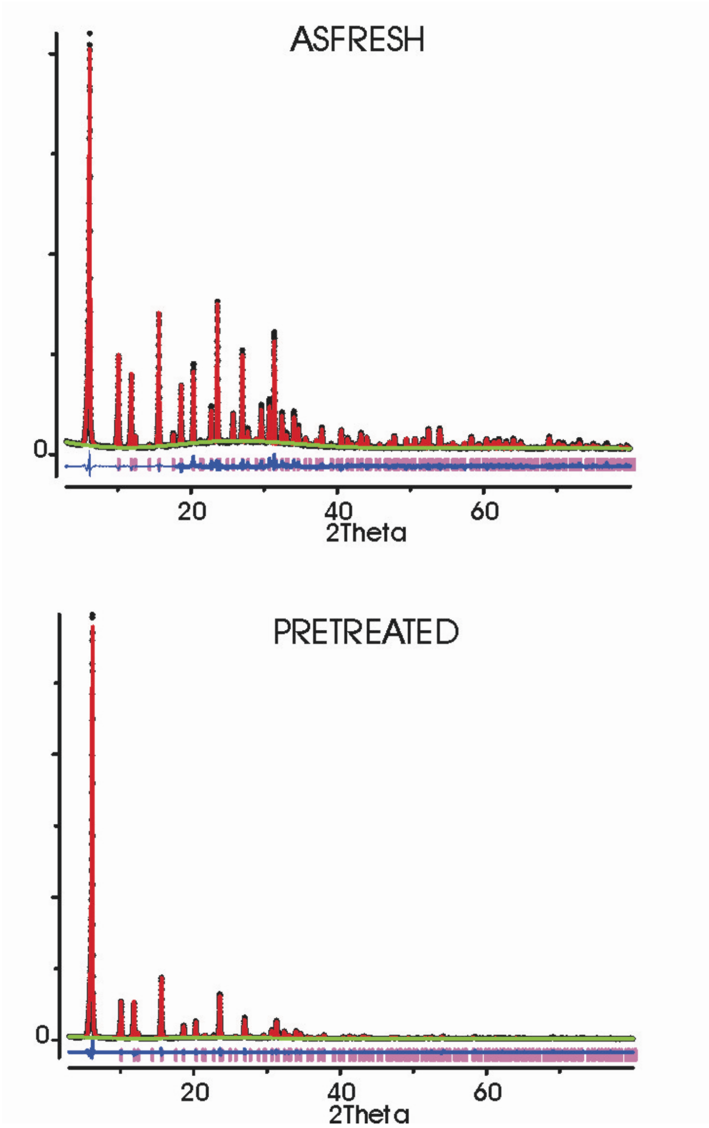

Fig. S11 Refined XRD patterns of the Ru(3%)/Na-Y zeolite after Ru ion-exchange and after pretreatment at 450°C.

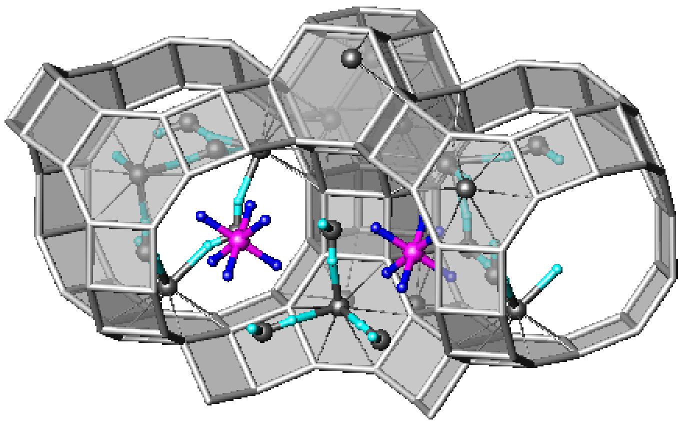

Fig. S12 Representation of the cation distribution in a Ru(3%)/Na-Y zeolite after fresh Ru ion-exchange. Ru^{+3} cations (purple spheres) are found on position SV in an octahedral environment. Na^{+} cations are represented as the grey spheres and found at position SII' in the sodalite cages and SII* and SIII in the supercages.

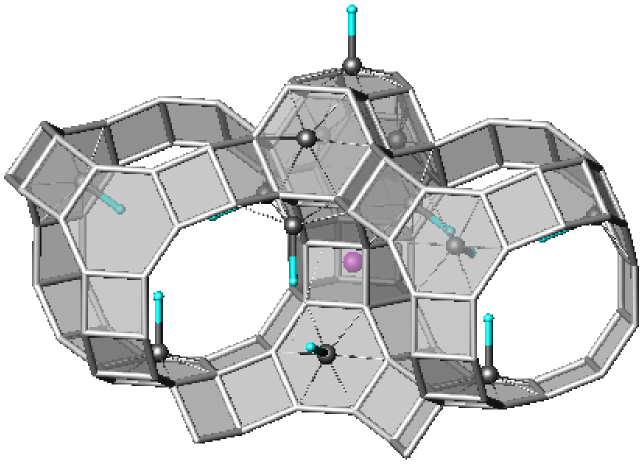

Fig. S13 Representation of the cation distribution in a Ru(3%)/Na-Y zeolite after pretreatment at 450 °C. Ru^{+3} cations (purple spheres) are found in the hexagonal prism at cation position SI. Na^{+} cations are found at position SI' and at position SII in the 6-ring of the sodalite cage interacting with a water molecule, resulting in tetrahedral environment.

Table S1 EXAFS fitting parameters at the Ru K-edge for the Ru(3%)/Na-Y sample.

Abs-Sca[1]	CN	R/Å	$\Delta\ \sigma^2$/Å^2
Ru-Ru	6	2.70 ± 0.01	0.005 ± 0.001
Ru-Ru	6	3.78 ± 0.01	0.005 ± 0.001
Ru-Ru	2	4.28 ± 0.01	0.005 ± 0.001
Ru-Ru	12	4.65 ± 0.01	0.005 ± 0.001
Ru-Ru	6	4.68 ± 0.01	0.005 ± 0.001
Ru-Ru	12	5.06 ± 0.01	0.005 ± 0.001
Ru-Ru-Ru	24	4.00 ± 0.01	0.005 ± 0.001
Ru-Ru-Ru	24	5.00 ± 0.01	0.005 ± 0.001
Ru-Ru-Ru	24	5.04 ± 0.01	0.005 ± 0.001
Ru-Ru-Ru	12	5.06 ± 0.01	0.005 ± 0.001

[1]Abbreviations: Abs-Sca: Absorber – Scatterer, CN: coordination number,

R: interatomic distance, $\Delta\sigma^2$: Debye-Waller factor

Fit: R-space, 2.5 Å^{-1} < k < 19.2 Å^{-1} and 1.39 Å < R < 5.83 Å

S_0^2: 0.82 ± 0.05

ΔE_0: -7.0 ± 0.5 eV

R-factor: 0.05

Table S2 Rietveld parameters for the refined Ru(1%)/Na-Y structures.

Rietveld parameters	Ru(1%)/Na-Y			
	With H_2 during cycling		No H_2 during cycling	
	NO_x saturated	regenerated	NO_x saturated	
R_p	0.0342	0.0318	0.0407	0.0444
R_{wp}	0.0486	0.0431	0.0550	0.0606
R_e	0.0442	0.043	0.0599	0.0598
R_F	0.0982	0.105	0.12834	0.11349
χ^2	0.93	1.01	0.92	1.02

Table S3 CIF files for Ru(1%)/Na-Y zeolite after (a) NO_x saturation and after (b) NO_x regeneration. H_2 was used during regeneration.

(a)

```
data_ADSHREV2_publ

_pd_block_id
  2010-08-06T09:28|ADSHREV2|ceak|stadip

_audit_creation_method  "from EXP file using GSAS2CIF"
_audit_creation_date                 2010-08-06T09:28
_audit_author_name                    ceak
_audit_update_record
; 2010-08-06T09:28  Initial CIF as created by GSAS2CIF
;
_refine_ls_shift/su_max              0.92
_refine_ls_shift/su_mean             0.07
_computing_structure_refinement       GSAS
_refine_ls_number_parameters          57
_refine_ls_goodness_of_fit_all        0.93
_refine_ls_number_restraints          0
_refine_ls_matrix_type               full

_pd_phase_name
   "Ru1% NaY adsorbed NOx with H2"
_cell_length_a                       24.60508(8)
_cell_length_b                       24.60508
_cell_length_c                       24.60508
_cell_angle_alpha                      90.0
_cell_angle_beta                       90.0
_cell_angle_gamma                      90.0
_cell_volume                         14896.16(14)
_symmetry_cell_setting                cubic
_symmetry_space_group_name_H-M        "F d -3 m"

loop_
     _atom_site_type_symbol
     _atom_site_label
     _atom_site_fract_x
     _atom_site_fract_y
     _atom_site_fract_z
     _atom_site_occupancy
     _atom_site_thermal_displace_type
     _atom_site_U_iso_or_equiv
     _atom_site_symmetry_multiplicity
O
O1     0.89306(10)  0.10694(10)  0.0         1.0       Uiso   0.0017(5)    96
O
O2     0.96580(18)  0.07523(12)  0.07523(12)  1.0       Uiso   0.0017(5)    96
O
O3     0.99602(13)  0.14239(14)  0.99602(13)  1.0       Uiso   0.0017(5)    96
O
O4     0.92629(16)  0.17841(12)  0.07159(12)  1.0       Uiso   0.0017(5)    96
Si
```

T1 0.94578(6) 0.12757(6) 0.03571(6) 1.0 Uiso 0.00133(26) 192
O
ow1 0.3087(8) 0.3087(8) 0.5405(17) 0.1773(21) Uiso 0.096(8) 96
Na
Sii' 0.17289(26) 0.17289(26) 0.17289(26) 0.507(10) Uiso 0.101(7) 32
Na
SI' 0.07344(29) 0.07344(29) 0.07344(29) 0.469(10) Uiso 0.055(6) 32
Na
siii 0.375 0.375 0.5098(12) 0.1773(21) Uiso 0.101(14) 48
Na
sV 0.5 0.5 0.5 0.532(6) Uiso 0.056(6) 16
Ru
ru 0.0 0.0 0.0 0.0639(27) Uiso 0.071(28) 16
O
ow2 0.3171(12) 0.3171(12) 0.2274(21) 0.185(11) Uiso 0.089(18) 96
N
n1 0.247(7) 0.398(11) 0.454(10) 0.0212(21) Uiso 0.025 192
N
n2 0.299(9) 0.346(5) 0.437(10) 0.0219(12) Uiso 0.025 192
N
on1 0.270(5) 0.438(6) 0.456(8) 0.0219(12) Uiso 0.025 192
N
on2 0.345(10) 0.363(6) 0.432(7) 0.0219(12) Uiso 0.025 192
N
on3 0.282(6) 0.300(9) 0.432(5) 0.0219(12) Uiso 0.025 192
O
ow3 0.375 0.375 0.4221(18) 0.1780(12) Uiso 0.09(4) 48
O
ow4 0.375 0.375 0.6000(15) 0.170(9) Uiso 0.085(25) 48
O
ow5 0.2457(11) 0.2457(11) 0.5903(15) 0.1774(21) Uiso 0.090(8) 96
O
ow6 0.4405(9) 0.5595(9) 0.5 0.1774(21) Uiso 0.090(8) 96
Na
SII 0.251(4) 0.251(4) 0.251(4) 0.0353(21) Uiso 0.090(8) 32

_chemical_formula_sum "N0.11 Na0.26 O2.45 Ru0.01 Si"
_chemical_formula_weight 74.94
_cell_formula_units_Z 192

loop_ _atom_type_symbol
_atom_type_number_in_cell
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_Cromer_Mann_a1
_atom_type_scat_Cromer_Mann_a2
_atom_type_scat_Cromer_Mann_a3
_atom_type_scat_Cromer_Mann_a4
_atom_type_scat_Cromer_Mann_b1
_atom_type_scat_Cromer_Mann_b2
_atom_type_scat_Cromer_Mann_b3
_atom_type_scat_Cromer_Mann_b4
_atom_type_scat_Cromer_Mann_c
_atom_type_scat_source

```
 O       469.58    0.000    0.000
3.04850 13.2771 2.28680 5.70110 1.54630 0.32390 0.86700 32.9089 0.25080
 International_Tables_Vol_C
 Si      192.0    0.000    0.000
6.29150 2.43860 3.03530 32.3337 1.98910 0.67850 1.54100 81.6937 1.14070
 International_Tables_Vol_C
 Na       49.389    0.000    0.000
4.76260 3.28500 3.17360 8.84220 1.26740 0.31360 1.11280 129.424 0.67600
 International_Tables_Vol_C
 Ru        1.022    0.000    0.000
19.2674 0.80852 12.9182 8.43467 4.86337 24.7997 1.56756 94.2928 5.37874
 International_Tables_Vol_C
 N        20.869    0.000    0.000
12.2126 0.00570 3.13220 9.89330 2.01250 28.9975 1.16630 0.58260 -11.529
 International_Tables_Vol_C
_diffrn_radiation_probe              x-ray
_diffrn_radiation_polarisn_ratio      0.0
_diffrn_radiation_wavelength          1.5405
_diffrn_radiation_type               Cu_K\a~1~
_pd_proc_ls_prof_R_factor             0.0342
_pd_proc_ls_prof_wR_factor            0.0486
_pd_proc_ls_prof_wR_expected          0.0442
_refine_ls_R_Fsqd_factor             0.09816

_pd_proc_ls_background_function
;   GSAS Background function number 1 with 20 terms.
 Shifted Chebyshev function of 1st kind
      1:    263.659     2:   -132.615     3:    22.6845     4:    24.5332
      5:   -17.5921     6:   -31.2151     7:    43.6860     8:   -14.6541
      9:   -1.82601    10:    10.9365    11:   -12.5844    12:   -1.62933
     13:    9.25131    14:   -15.1842    15:   0.557432    16:    7.62129
     17:   -2.06372    18:    1.86382    19:    7.24730    20:    1.59525
;

_pd_spec_mounting
;sealed glass capillary 1mm outer diameter packing density 50%
;
_pd_spec_mount_mode              'transmission'
_pd_spec_shape                  'cylinder'
_exptl_absorpt_process_details
;   GSAS Absorption/surface roughness correction: function number 0
 Debye-Scherrer absorption correction
Term (= MU.r/wave) =      3.0000
Correction is not refined.
;
_exptl_absorpt_correction_T_min       0.00381
_exptl_absorpt_correction_T_max       0.03700

_pd_proc_ls_profile_function
;
 CW Profile function number 3 with  19 terms
 Pseudovoigt profile coefficients as parameterized in
 P. Thompson, D.E. Cox & J.B. Hastings (1987). J. Appl. Cryst.,20,79-83.
 Asymmetry correction of L.W. Finger, D.E. Cox & A. P. Jephcoat (1994).
 J. Appl. Cryst.,27,892-900.
 #1(GU)   =    9.816 #2(GV)   =   32.491 #3(GW)   =    1.438
```

```
 #4(GP)   =    3.633 #5(LX)   =    2.885 #6(LY)   =    1.756
 #7(S/L)  =   0.0266 #8(H/L)  =   0.0274
 #9(trns) =     0.00 #10(shft)=   0.0000
 #11(stec)=     0.00 #12(ptec)=     0.00 #13(sfec)=     0.00
 #14(L11) =    0.054 #15(L22) =    0.138 #16(L33) =   -0.161
 #17(L12) =   -0.082 #18(L13) =    0.008 #19(L23) =    0.081
 Peak tails are ignored  where the intensity is below 0.0010 times the peak
   Aniso. broadening axis   0.0   0.0   1.0
;
_pd_proc_ls_peak_cutoff 0.00100
_pd_proc_info_datetime              2010-08-06T09:28:53
_pd_calc_method                     "Rietveld Refinement"

_pd_meas_2theta_range_min            3.41
_pd_meas_2theta_range_max            95.0
_pd_meas_2theta_range_inc            0.01
_pd_proc_2theta_range_min            3.39792
_pd_proc_2theta_range_max            94.98792
_pd_proc_2theta_range_inc            0.01


loop_
      _refln_index_h
      _refln_index_k
      _refln_index_l
      _refln_observed_status
      _refln_F_squared_meas
      _refln_F_squared_calc
      _refln_phase_calc
      _refln_d_spacing
      _gsas_i100_meas
   1   1   1 o  1382589.4  1373154.3  180.00  14.20575  100.00
   2   2   0 o  264332.00  260189.44   0.00    8.69921  11.68
   3   1   1 o  118604.48  119938.63   0.00    7.41871   7.99
   2   2   2 o  11187.445  10754.289   0.00    7.10287   0.23
   4   0   0 o  40595.34   34839.734  180.00   6.15127   0.50
   3   3   1 o  621576.6   630092.8   180.00   5.64479  26.88
   4   2   2 o  17030.764  16207.318   0.00    5.02249   0.61
   5   1   1 o  255227.61  252875.28   0.00    4.73525   8.48
   3   3   3 o  64255.17   63677.49    0.00    4.73525   0.72
   4   4   0 o  627228.4   597319.8   180.00   4.34960   9.17
   4   4   2 o  10676.085  10470.126  180.00   4.10085   0.28
   5   3   1 o  4101.588   3591.914    0.00    4.15902   0.23
   6   2   0 o  109159.76  105059.59   0.00    3.89040   2.73
   5   3   3 o  877998.6   872803.1   180.00   3.75224  20.73
   6   2   2 o  16585.871  15232.650   0.00    3.70936   0.38
   4   4   4 o  77614.30   71672.70   180.00   3.55144   0.57
   7   1   1 o  7961.906   8227.182   180.00   3.44540   0.17
   5   5   1 o  144841.67  149594.80   0.00    3.44540   3.04
   6   4   2 o  299289.44  294806.78  180.00   3.28799  11.67
   5   5   3 o  10968.317  10682.683  180.00   3.20331   0.20
   7   3   1 o  56833.21   55232.16    0.00    3.20331   2.14
   8   0   0 o  20650.693  12569.461  180.00   3.07564   0.09
   7   3   3 o  222379.66  208791.58  180.00   3.00599   3.82
   6   4   4 o  2626.077   2491.409   180.00   2.98380   0.04
   8   2   2 o  198269.22  199133.20   0.00    2.89974   3.25
```

6	6	0	o	619646.9	623163.6	0.00	2.89974	5.06
6	6	2	o	2006.788	1974.021	0.00	2.82240	0.03
7	5	1	o	54328.63	54188.55	0.00	2.84115	1.71
5	5	5	o	2991939.3	2984181.5	180.00	2.84115	15.67
9	1	1	o	56418.07	55738.55	0.00	2.70076	0.82
8	4	0	o	271118.53	262712.13	0.00	2.75093	4.10
7	5	3	o	47261.43	46857.71	0.00	2.70076	1.39
8	4	2	o	23827.662	23270.939	0.00	2.68463	0.67
6	6	4	o	552509.2	556719.9	180.00	2.62291	7.79
9	3	1	o	156342.75	158206.42	0.00	2.57931	4.28
7	7	1	o	3792.458	3596.323	0.00	2.47290	0.04
8	4	4	o	69320.98	69289.43	0.00	2.51125	0.94
9	3	3	o	950.759	904.032	180.00	2.47290	0.01
7	5	5	o	23968.391	22995.740	180.00	2.47290	0.34
8	6	2	o	26929.551	27120.621	0.00	2.41273	0.71
10	2	0	o	37068.16	37158.87	0.00	2.41273	0.43
7	7	3	o	16647.758	16019.349	0.00	2.37866	0.21
10	2	2	o	17045.570	16752.359	180.00	2.36762	0.20
9	5	1	o	21158.240	20504.016	0.00	2.37866	0.51
6	6	6	o	1057343.3	1043566.8	0.00	2.36762	4.04
8	6	4	o	18464.668	18554.021	180.00	2.28452	0.39
9	5	3	o	15148.684	15040.277	180.00	2.29444	0.30
11	1	1	o	79574.24	80255.80	180.00	2.21857	0.89
10	4	2	o	467.135	464.639	0.00	2.24613	0.01
7	7	5	o	85383.19	86262.98	0.00	2.21857	0.89
8	8	0	o	763459.1	779626.9	0.00	2.17480	3.68
8	8	2	o	3162.710	2927.732	180.00	2.14160	0.03
11	3	1	o	49810.27	48265.34	180.00	2.14976	0.99
9	7	1	o	16218.581	15782.628	0.00	2.14976	0.30
9	5	5	o	7883.169	7674.750	180.00	2.14976	0.08
10	4	4	o	14699.570	13602.644	0.00	2.14160	0.14
12	0	0	o	187698.53	175610.56	180.00	2.05042	0.46
8	6	6	o	2957.958	2995.686	0.00	2.10987	0.03
9	7	3	o	51328.37	50171.12	180.00	2.08698	0.96
11	3	3	o	253735.70	251862.00	0.00	2.08698	2.23
10	6	0	o	72296.48	73882.20	0.00	2.10987	0.71
8	8	4	o	262347.94	248715.73	180.00	2.05042	2.36
10	6	2	o	11189.457	11340.618	180.00	2.07951	0.20
7	7	7	o	50190.54	46569.44	0.00	2.02939	0.14
12	2	2	o	1910.988	1813.560	180.00	1.99574	0.02
11	5	1	o	12066.240	11162.248	0.00	2.02939	0.22
10	6	4	o	8371.099	8161.130	0.00	1.99574	0.14
9	7	5	o	45297.14	44761.68	180.00	1.97633	0.76
11	5	3	o	278.942	276.234	180.00	1.97633	0.00
12	4	0	o	6290.609	5795.040	180.00	1.94520	0.05
9	9	1	o	30657.766	30931.377	180.00	1.92722	0.22
8	8	6	o	137125.33	137501.25	0.00	1.92133	1.04
12	4	2	o	25322.066	25429.941	0.00	1.92133	0.38
13	1	1	o	3313.388	3124.144	180.00	1.88160	0.02
9	9	3	o	18204.217	17184.619	0.00	1.88160	0.14
10	8	2	o	193387.92	198565.19	0.00	1.89832	2.92
11	5	5	o	247.653	219.879	0.00	1.88160	0.00
11	7	1	o	2160.061	2064.480	0.00	1.88160	0.03
10	6	6	o	1628.776	1366.812	180.00	1.87612	0.01
12	4	4	o	28084.170	27477.434	0.00	1.85468	0.21
13	3	1	o	53188.32	53659.70	180.00	1.83907	0.75

10	8	4	o	36877.28	37224.39	180.00	1.83395	0.50
11	7	3	o	17036.920	17244.787	0.00	1.83907	0.24
9	7	7	o	118642.31	120581.61	0.00	1.83907	0.82
9	9	5	o	322328.66	321842.16	0.00	1.79930	2.09
12	6	2	o	30568.521	29467.717	180.00	1.81391	0.42
13	3	3	o	14776.219	14772.984	0.00	1.79930	0.10
8	8	8	o	209413.56	208340.17	0.00	1.77572	0.44
14	2	0	o	136121.75	135421.59	180.00	1.73984	0.83
11	7	5	o	118857.17	117955.80	180.00	1.76201	1.48
13	5	1	o	31113.861	30894.359	180.00	1.76201	0.39
12	6	4	o	11485.400	11270.489	180.00	1.75751	0.14
14	2	2	o	17749.762	17040.813	0.00	1.72270	0.10
10	8	6	o	11856.271	11846.711	0.00	1.73984	0.14
10	10	2	o	8525.201	8192.695	0.00	1.72270	0.05
10	10	0	o	997148.6	998792.4	180.00	1.73984	2.98
13	5	3	o	1006.898	961.412	180.00	1.72694	0.02
11	9	1	o	21259.563	20526.049	180.00	1.72694	0.25
11	9	3	o	474630.1	477624.7	180.00	1.69388	5.17
9	9	7	o	2049.595	2061.256	0.00	1.69388	0.01
10	10	4	o	654.353	621.600	180.00	1.67416	0.00
12	8	0	o	11096.272	10567.970	0.00	1.70606	0.06
12	8	2	o	59049.46	59601.84	180.00	1.68988	0.63
14	4	2	o	13975.672	13344.466	180.00	1.67416	0.15
12	6	6	o	43096.34	41298.38	180.00	1.67416	0.24
15	1	1	o	782.882	761.439	180.00	1.63310	0.00
13	7	1	o	2592.607	2582.942	180.00	1.66266	0.03
13	5	5	o	1618.579	1604.635	0.00	1.66266	0.01
11	7	7	o	110878.66	110592.97	180.00	1.66266	0.58
12	8	4	o	98976.08	95547.64	180.00	1.64400	0.99
11	9	5	o	10468.164	10268.700	0.00	1.63310	0.10
13	7	3	o	13562.112	13358.782	0.00	1.63310	0.13
14	4	4	o	89050.21	89245.09	0.00	1.62951	0.43
15	3	1	o	45019.31	43572.25	0.00	1.60506	0.42
10	8	8	o	26850.969	27183.619	0.00	1.62951	0.13
10	10	6	o	8034.338	7942.859	180.00	1.60165	0.04
14	6	2	o	151912.02	152295.94	0.00	1.60165	1.34
14	6	0	o	416.397	322.311	180.00	1.61540	0.00
15	3	3	o	45718.61	45402.02	180.00	1.57842	0.20
11	11	1	o	910337.8	905932.8	0.00	1.57842	3.95
16	0	0	o	942220.9	935349.6	0.00	1.53782	0.90
9	9	9	o	293009.53	292147.44	0.00	1.57842	0.42
13	7	5	o	25561.748	25486.494	0.00	1.57842	0.22
12	8	6	o	0.012	0.001	0.00	1.57518	0.00
11	11	3	o	9004.659	8752.307	0.00	1.55306	0.04
12	10	2	o	131.299	129.552	0.00	1.56242	0.00
14	6	4	o	70955.45	70143.86	0.00	1.56242	0.60
11	9	7	o	83095.61	80769.11	0.00	1.55306	0.66
15	5	1	o	14280.349	13884.371	0.00	1.55306	0.11
13	9	1	o	8654.576	8401.486	180.00	1.55306	0.07
16	2	2	o	350.275	351.780	180.00	1.51434	0.00
15	5	3	o	157815.36	160247.22	0.00	1.52889	1.19
12	10	4	o	4447.500	4471.191	180.00	1.52594	0.03
11	11	5	o	619318.6	620334.7	180.00	1.50581	2.17
10	10	8	o	256746.02	257567.66	0.00	1.51434	0.93
13	9	3	o	47729.34	48498.52	180.00	1.52889	0.37
14	8	2	o	7780.187	7814.076	180.00	1.51434	0.06

16	4	0	o	52559.63	52725.23	0.00	1.49190	0.18
13	7	7	o	39740.13	39752.23	180.00	1.50581	0.14
16	4	2	o	30085.428	30024.584	180.00	1.48105	0.19
14	6	6	o	996.989	1008.485	0.00	1.50299	0.00
13	9	5	o	28325.277	28369.521	180.00	1.48374	0.19
12	10	6	o	218771.52	215843.19	180.00	1.47043	1.38
12	8	8	o	538533.0	541966.4	0.00	1.49190	1.82
15	5	5	o	133278.39	133589.58	180.00	1.48374	0.44
17	1	1	o	80506.39	76334.28	180.00	1.44238	0.23
14	8	4	o	2943.160	2940.289	0.00	1.48105	0.02
15	7	1	o	23811.344	23903.305	180.00	1.48374	0.16
11	11	7	o	3916.990	3700.720	180.00	1.44238	0.01
15	7	3	o	46360.00	44932.20	0.00	1.46262	0.29
16	4	4	o	11639.464	11397.981	180.00	1.44987	0.03
11	9	9	o	57377.07	55630.11	0.00	1.46262	0.18
12	12	2	o	2775.327	2644.463	0.00	1.43990	0.01
12	12	0	o	1381437.3	1355706.9	0.00	1.44987	2.04
17	3	1	o	25371.662	24667.090	180.00	1.42295	0.13
13	11	1	o	58348.07	54904.75	0.00	1.44238	0.34
13	11	3	o	10070.784	9802.386	0.00	1.42295	0.06
16	6	2	o	12249.090	12030.151	0.00	1.43014	0.07
12	12	4	o	631.926	516.460	0.00	1.41120	0.00
14	8	6	o	284188.03	279245.75	180.00	1.43014	1.56
13	9	7	o	939.011	918.558	180.00	1.42295	0.00
17	3	3	o	30625.424	27345.822	180.00	1.40429	0.07
15	7	5	o	4248.880	4154.523	0.00	1.42295	0.02
14	10	2	o	16383.570	15677.204	180.00	1.42057	0.08
10	10	10	o	6573.692	6275.688	180.00	1.42057	0.01
14	10	0	o	14378.768	14173.026	180.00	1.43014	0.04
12	10	8	o	368.657	323.867	180.00	1.40200	0.00
16	6	4	o	424.115	372.123	180.00	1.40200	0.00
13	11	5	o	8878.890	8803.234	180.00	1.38634	0.04
14	10	4	o	26497.479	25667.041	0.00	1.39299	0.12
15	9	1	o	13830.822	12393.058	180.00	1.40429	0.07
12	12	6	o	14023.628	13700.698	0.00	1.36695	0.03
15	9	3	o	8517.784	8490.918	180.00	1.38634	0.04
17	5	1	o	8763.521	8717.235	180.00	1.38634	0.04
18	2	0	o	716.131	700.984	180.00	1.35859	0.00
11	11	9	o	9480.165	9267.192	0.00	1.36906	0.02
17	5	3	o	2672.975	2617.138	180.00	1.36906	0.01
18	2	2	o	39689.71	38388.45	180.00	1.35038	0.07
16	8	0	o	5200.873	4541.380	180.00	1.37547	0.01
15	7	7	o	24019.379	23606.262	180.00	1.36906	0.05
16	8	2	o	70303.16	68902.61	0.00	1.36695	0.28
14	10	6	o	935.251	905.972	0.00	1.35038	0.00
14	8	8	o	0.110	0.099	0.00	1.36695	0.00
16	6	6	o	1439649.0	1413547.4	0.00	1.35859	2.86
15	9	5	o	62172.37	60075.70	180.00	1.35242	0.24
13	9	9	o	110143.26	106428.59	180.00	1.35242	0.21
13	13	1	o	95029.33	94084.16	0.00	1.33636	0.17
13	11	7	o	1747.267	1731.158	0.00	1.33636	0.01
17	5	5	o	718054.4	710891.4	0.00	1.33636	1.26
16	8	4	o	109815.41	105717.32	180.00	1.34232	0.40
18	4	2	o	30184.459	29777.080	0.00	1.32662	0.10
13	13	3	o	111324.21	108327.73	0.00	1.32087	0.18
14	12	2	o	208093.55	205122.30	0.00	1.32662	0.69

12	12	8	o	49298.20	51003.37	180.00	1.31146	0.07
17	7	1	o	1.686	1.466	180.00	1.33636	0.00
19	1	1	o	2058.335	2002.486	0.00	1.29143	0.00
12	10	10	o	145052.39	142771.67	0.00	1.32662	0.24
17	7	3	o	286.584	273.391	180.00	1.32087	0.00
14	12	4	o	3585.828	3617.998	0.00	1.30407	0.01
18	4	4	o	3922.595	3958.332	180.00	1.30407	0.01
15	11	1	o	2592.746	2478.697	0.00	1.32087	0.01
13	13	5	o	15500.298	15036.750	180.00	1.29143	0.02
15	11	3	o	211980.22	207610.33	0.00	1.30590	0.61
15	9	7	o	24518.449	23964.377	0.00	1.30590	0.07
16	8	6	o	34.643	34.968	180.00	1.30407	0.00
14	10	8	o	90952.17	87917.23	180.00	1.29680	0.25
18	6	0	o	100482.70	96997.16	180.00	1.29680	0.14
19	3	1	o	61900.33	64070.24	180.00	1.27743	0.15
18	6	2	o	1656.668	1655.497	180.00	1.28966	0.00
16	10	2	o	53561.90	51714.07	180.00	1.29680	0.14
11	11	11	o	1688750.0	1612611.6	0.00	1.29143	0.73
17	7	5	o	206030.22	196833.25	0.00	1.29143	0.54
15	11	5	o	6970.864	7186.145	180.00	1.27743	0.02
13	11	9	o	123587.78	127095.41	180.00	1.27743	0.29
19	3	3	o	48848.09	47530.59	0.00	1.26388	0.05
14	12	6	o	4628.953	4494.249	0.00	1.26891	0.01
16	10	4	o	6562.528	6978.902	0.00	1.27571	0.01
18	6	4	o	50572.52	48875.36	0.00	1.26891	0.11
20	0	0	o	46021.52	47387.86	180.00	1.23025	0.01
13	13	7	o	41908.46	43736.60	0.00	1.25075	0.04
17	9	1	o	26918.820	27506.887	180.00	1.27743	0.06
17	9	3	o	359693.1	347892.59	180.00	1.26388	0.73
19	5	1	o	14.802	15.683	180.00	1.25075	0.00
12	12	10	o	795.980	846.747	0.00	1.24913	0.00
17	7	7	o	14406.760	15181.440	180.00	1.25075	0.01
16	8	8	o	367561.6	355645.7	0.00	1.25562	0.35
19	5	3	o	373649.3	347047.41	180.00	1.23802	0.59
16	10	6	o	84554.37	81653.81	180.00	1.24274	0.14
14	14	2	o	422.586	414.567	180.00	1.23645	0.00
20	2	2	o	99230.95	90264.30	180.00	1.21813	0.06
15	9	9	o	12903.682	13609.981	0.00	1.25075	0.01
15	11	7	o	78413.91	72515.04	180.00	1.23802	0.12
17	9	5	o	896.689	822.056	0.00	1.23802	0.00
14	14	0	o	166839.80	160728.22	0.00	1.24274	0.07
18	8	2	o	59364.23	57194.95	180.00	1.24274	0.10
18	6	6	o	1955.482	1918.595	0.00	1.23645	0.00
15	13	1	o	155.503	140.874	0.00	1.23802	0.00
15	13	3	o	11467.690	11631.074	0.00	1.22567	0.02
14	12	8	o	20433.002	20869.826	180.00	1.22415	0.03
14	14	4	o	85667.96	77112.34	0.00	1.21813	0.05
14	10	10	o	19108.957	18750.479	180.00	1.23645	0.01
18	8	4	o	37322.05	38146.46	180.00	1.22415	0.05
16	12	2	o	254.585	260.741	180.00	1.22415	0.00
19	5	5	o	4388.782	4151.122	0.00	1.21368	0.00
20	4	0	o	14900.120	14794.469	180.00	1.20636	0.01
16	12	0	o	43109.25	44377.25	180.00	1.23025	0.03
13	13	9	o	21370.395	20440.678	0.00	1.20204	0.01
15	13	5	o	137584.89	131015.41	0.00	1.20204	0.14
16	12	4	o	35005.281	34589.785	180.00	1.20636	0.04

20	4	2	o	7276.947	7751.815	180.00	1.20061	0.01
19	7	1	o	84325.25	79253.44	0.00	1.21368	0.10
13	11	11	o	126941.79	118805.48	180.00	1.21368	0.08
14	14	6	o	782334.7	789188.6	0.00	1.18933	0.31
17	11	1	o	59474.24	55443.50	180.00	1.21368	0.07
21	1	1	o	63171.39	74866.02	0.00	1.16902	0.02
19	7	3	o	120994.18	112831.45	180.00	1.20204	0.12
17	11	3	o	1619.663	1499.889	180.00	1.20204	0.00
16	10	8	o	22083.920	23429.754	0.00	1.20061	0.02
17	9	7	o	55683.30	51520.11	0.00	1.20204	0.06
18	8	6	o	1767.201	2964.486	0.00	1.19493	0.00
20	4	4	o	139421.97	124103.91	180.00	1.18381	0.05
15	11	9	o	11291.755	11339.039	0.00	1.19072	0.01
18	10	2	o	1364.882	1334.822	0.00	1.18933	0.00
12	12	12	o	599684.4	522860.5	180.00	1.18381	0.07
16	12	6	o	35417.16	34727.598	180.00	1.17837	0.02
18	10	0	o	3781.583	6242.375	0.00	1.19493	0.00
19	7	5	o	608.710	521.090	0.00	1.17972	0.00
17	11	5	o	436307.2	378504.9	180.00	1.17972	0.30
21	3	1	o	1860.427	23047.855	180.00	1.15861	0.00
15	13	7	o	1123.906	1207.500	0.00	1.16902	0.00
20	6	2	o	230544.48	207437.55	180.00	1.17300	0.14
14	12	10	o	54952.24	49263.57	0.00	1.17300	0.03
18	10	4	o	4287.638	3795.650	180.00	1.17300	0.00
21	3	3	o	64824.33	54525.20	0.00	1.14847	0.01
14	14	8	o	12669.525	13597.711	180.00	1.15224	0.00
19	9	1	o	346057.38	339613.56	0.00	1.16902	0.19
15	15	1	o	1558.905	11032.013	180.00	1.15861	0.00
15	15	3	o	22761.734	18660.736	0.00	1.14847	0.00
20	6	4	o	296.608	3632.676	0.00	1.15733	0.00
19	9	3	o	-0.896	0.880	0.00	1.15861	0.00
13	13	11	o	1555.791	1269.763	180.00	1.14847	0.00
16	14	2	o	117352.93	115077.06	0.00	1.15224	0.04
17	9	9	o	2282.937	12034.660	180.00	1.15861	0.00
18	8	8	o	383.847	2931.899	0.00	1.15733	0.00
17	11	7	o	23668.818	18513.270	0.00	1.14847	0.01
19	7	7	o	3936.891	3025.729	0.00	1.14847	0.00
16	10	10	o	6967.676	6306.784	180.00	1.15224	0.00
15	15	5	o	82.558	12714.532	0.00	1.12896	0.00
21	5	1	o	50418.59	44463.59	180.00	1.13859	0.01
18	10	6	o	23854.025	21393.313	180.00	1.14722	0.01
16	12	8	o	1620.064	1014.693	0.00	1.14226	0.00
16	14	4	o	13211.588	20768.498	180.00	1.13737	0.00
17	13	1	o	23515.664	17713.188	0.00	1.14847	0.01
17	13	3	o	42861.59	36016.57	0.00	1.13859	0.01
19	9	5	o	5099.930	4133.288	0.00	1.13859	0.00
20	8	0	o	1859593.4	1129215.8	0.00	1.14226	0.24
21	5	3	o	17.950	360.477	0.00	1.12896	0.00
15	13	9	o	-948.817	16056.077	0.00	1.12896	0.00
20	8	2	o	2883.435	4309.497	0.00	1.13737	0.00
22	2	0	o	434523.2	141421.67	0.00	1.11382	0.01
20	6	6	o	-536.965	6217.801	0.00	1.13254	0.00
15	11	11	o	2011.163	1585.428	180.00	1.13859	0.00
18	12	2	o	8.468	296.419	0.00	1.13254	0.00
22	2	2	o	34644.832	24866.334	0.00	1.10928	0.00
17	13	5	o	1557.649	2632.559	180.00	1.11957	0.00

20	8	4	o	14250.973	33379.434	0.00	1.12306	0.00
16	14	6	o	35450.93	10634.270	180.00	1.11382	0.00
18	12	4	o	555.960	2020.203	0.00	1.11841	0.00
14	14	10	o	19912.291	14865.208	0.00	1.10928	0.00
15	15	7	o	730592.7	67270.84	180.00	1.10147	0.01
21	5	5	o	114274.41	43960.29	180.00	1.11041	0.00
14	12	12	o	4009.179	16451.443	180.00	1.11841	0.00
19	11	1	o	6444.791	9349.010	180.00	1.11957	0.00
21	7	1	o	2906.118	1038.661	0.00	1.11041	0.00
18	10	8	o	5943.831	1670.468	180.00	1.11382	0.00
22	4	2	o	3206216.3	101458.89	0.00	1.09600	0.01
19	11	3	o	4801.356	1432.664	180.00	1.11041	0.00
19	9	7	o	117051.32	41302.91	180.00	1.11041	0.01
17	11	9	o	39430.66	13971.546	180.00	1.11041	0.00
21	7	3	o	73143.36	6798.811	0.00	1.10147	0.00
20	8	6	o	213965.78	16943.299	180.00	1.10037	0.00
16	12	10	o	71367.54	5842.029	180.00	1.10037	0.00
17	13	7	o	278.888	8.049	180.00	1.09275	0.00
22	4	4	o	-1582.033	21905.373	0.00	1.08318	0.00
18	12	6	o	2401410.3	66901.76	0.00	1.09600	0.01
23	1	1	o	219562.56	212229.44	0.00	1.06777	0.01
13	13	13	o	1220744.5	134442.63	180.00	1.09275	0.00
19	11	5	o	71320.48	7750.123	0.00	1.09275	0.00
20	10	2	o	3386263.5	85981.78	180.00	1.09600	0.02
16	16	2	o	-123.950	1452.357	180.00	1.08318	0.00
16	14	8	o	-434.086	16895.537	0.00	1.08318	0.00
15	13	11	o	-1441.774	20239.908	180.00	1.08423	0.00
21	7	5	o	-154.170	3135.082	0.00	1.08423	0.00
15	15	9	o	35851.96	27066.129	0.00	1.06777	0.00
17	15	1	o	-51.123	458.746	180.00	1.08423	0.00
16	16	0	o	-6637.277	73635.21	180.00	1.08740	0.00
16	16	4	o	-8402.842	97267.59	0.00	1.07080	0.00
20	10	4	o	-112.444	1723.068	0.00	1.08318	0.00
22	6	0	o	1842750.3	290951.59	180.00	1.07900	0.01
17	15	3	o	297728.34	91277.89	180.00	1.07591	0.01
22	6	2	o	-22.760	549.880	0.00	1.07488	0.00
23	3	1	o	49902.48	42709.21	0.00	1.05982	0.01
18	14	2	o	-21.619	9.823	0.00	1.07488	0.00
21	9	1	o	64773.91	16110.661	180.00	1.07591	0.00
19	9	9	o	8129.820	2013.940	180.00	1.07591	0.00
18	14	0	o	318770.63	40900.08	180.00	1.07900	0.00
17	15	5	o	130678.01	106618.99	0.00	1.05982	0.01
18	12	8	o	7435.911	9180.756	0.00	1.06677	0.00
14	14	12	o	247970.80	121117.32	180.00	1.06278	0.01
22	6	4	o	135969.59	66556.41	180.00	1.06278	0.01
23	3	3	o	396675.5	257159.20	0.00	1.05204	0.03
18	10	10	o	-191.058	1834.407	180.00	1.07488	0.00
19	11	7	o	18426.975	10069.465	0.00	1.06777	0.00
21	9	3	o	93892.71	50914.70	180.00	1.06777	0.01
20	8	8	o	-437.426	5005.379	180.00	1.07080	0.00
16	16	6	o	47435.23	35051.488	0.00	1.05108	0.00
18	14	4	o	197642.88	94795.55	180.00	1.06278	0.02
17	13	9	o	181810.80	148009.22	0.00	1.05982	0.02
20	10	6	o	46930.58	21729.619	180.00	1.06278	0.00
17	11	11	o	1789.041	997.297	180.00	1.06777	0.00
19	13	1	o	130510.66	64075.57	180.00	1.06777	0.01

```
  19  13   3 o  6795.745   5321.949    0.00    1.05982   0.00
  21   7   7 o  7514.474   5993.589   180.00   1.05982   0.00
  16  14  10 o  4549.924   4585.568    0.00    1.04726   0.00
  21   9   5 o  13732.551  7640.153   180.00   1.05204   0.00
  16  12  12 o  17867.943  40250.26    0.00    1.05493   0.00
  20  12   2 o  2916.319   2001.818    0.00    1.05108   0.00
  22   8   2 o  13660.693  13884.042  180.00   1.04726   0.00
  20  12   0 o  490.310    1155.964   180.00   1.05493   0.00
_reflns_number_total                369
_reflns_limit_h_min                 1
_reflns_limit_h_max                 23
_reflns_limit_k_min                 0
_reflns_limit_k_max                 16
_reflns_limit_l_min                 0
_reflns_limit_l_max                 13
_reflns_d_resolution_high           1.047
_reflns_d_resolution_low            14.206
#--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--#
```

(b)

```
data_DESHREV2_publ

_pd_block_id
  2010-08-06T11:07|DESHREV2|ceak|stadip

_audit_creation_method  "from EXP file using GSAS2CIF"
_audit_creation_date                2010-08-06T11:07
_audit_author_name                  ceak
_audit_update_record
; 2010-08-06T11:07  Initial CIF as created by GSAS2CIF
;

_refine_ls_shift/su_max             0.59
_refine_ls_shift/su_mean            0.02
_computing_structure_refinement     GSAS
_refine_ls_number_parameters        41
_refine_ls_goodness_of_fit_all      1.01
_refine_ls_number_restraints        0
_refine_ls_matrix_type              full

_pd_phase_name
   "Ru1% NaY desobed NOx with H2"
_cell_length_a                      24.73623(9)
_cell_length_b                      24.73623
_cell_length_c                      24.73623
_cell_angle_alpha                   90.0
_cell_angle_beta                    90.0
_cell_angle_gamma                   90.0
_cell_volume                        15135.63(17)
_symmetry_cell_setting              cubic
_symmetry_space_group_name_H-M      "F d -3 m"

loop_
      _atom_site_type_symbol
      _atom_site_label
      _atom_site_fract_x
```

```
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_occupancy
    _atom_site_thermal_displace_type
    _atom_site_U_iso_or_equiv
    _atom_site_symmetry_multiplicity
O
O1     0.8963(4)   0.1037(4)   0.0        1.0       Uiso   0.029(7)    96
O
O2     0.9667(6)   0.07587(35)  0.07587(35)  1.0       Uiso   0.023(5)    96
O
O3     0.9962(5)   0.1396(7)   0.9962(5)   1.0       Uiso   0.081(7)    96
O
O4     0.9318(5)   0.1784(4)   0.0716(4)   1.0       Uiso   0.013(6)    96
Si
T1     0.94820(22)  0.12442(24)  0.03579(22)  1.0       Uiso   0.0278(14)  192
O
ow1    0.4483(10)   0.4483(10)   0.5434(15)   0.127(7)   Uiso   0.077(28)   96
Na
SII    0.23290(15)  0.23290(15)  0.23290(15)  0.861(14)  Uiso   0.082(6)    32
Na
SI'    0.06752(24)  0.06752(24)  0.06752(24)  0.483(13)  Uiso   0.055(7)    32
Na
siii   0.375       0.375       0.6210(27)   0.115(13)  Uiso   0.072(7)    48
Na
sV     0.5         0.5         0.5          0.159(10)  Uiso   0.019(4)    16
Ru
ru     0.125       0.125       0.125        0.142(8)   Uiso   0.0834(3)   8
O
ow2    0.3133(5)   0.3133(5)   0.2068(7)    0.638(13)  Uiso   0.117(12)   96
O
ow3    0.2801(11)   0.2801(11)   0.2801(11)   0.219(24)  Uiso   0.11(4)     32

_chemical_formula_sum                "Na0.27 O2.37 Ru0.01 Si"
_chemical_formula_weight              72.84
_cell_formula_units_Z               192


loop_ _atom_type_symbol
    _atom_type_number_in_cell
    _atom_type_scat_dispersion_real
    _atom_type_scat_dispersion_imag
    _atom_type_scat_Cromer_Mann_a1
    _atom_type_scat_Cromer_Mann_a2
    _atom_type_scat_Cromer_Mann_a3
    _atom_type_scat_Cromer_Mann_a4
    _atom_type_scat_Cromer_Mann_b1
    _atom_type_scat_Cromer_Mann_b2
    _atom_type_scat_Cromer_Mann_b3
    _atom_type_scat_Cromer_Mann_b4
    _atom_type_scat_Cromer_Mann_c
    _atom_type_scat_source
 O      454.203   0.000   0.000
 3.04850 13.2771 2.28680 5.70110 1.54630 0.32390 0.86700 32.9089 0.25080
 International_Tables_Vol_C
 Si     192.0   0.000   0.000
```

```
 6.29150 2.43860 3.03530 32.3337 1.98910 0.67850 1.54100 81.6937 1.14070
  International_Tables_Vol_C
  Na       52.657    0.000    0.000
 4.76260 3.28500 3.17360 8.84220 1.26740 0.31360 1.11280 129.424 0.67600
  International_Tables_Vol_C
  Ru        1.137    0.000    0.000
 19.2674 0.80852 12.9182 8.43467 4.86337 24.7997 1.56756 94.2928 5.37874
  International_Tables_Vol_C
_diffrn_radiation_probe              x-ray
_diffrn_radiation_polarisn_ratio      0.0
_diffrn_radiation_wavelength          1.540562
_diffrn_radiation_type               Cu_K\a~1~
_pd_proc_ls_prof_R_factor            0.0318
_pd_proc_ls_prof_wR_factor           0.0431
_pd_proc_ls_prof_wR_expected         0.0430
_refine_ls_R_Fsqd_factor             0.10536

_pd_proc_ls_background_function
;   GSAS Background function number 1 with 18 terms.
 Shifted Chebyshev function of 1st kind
      1:    294.374     2:   -201.102     3:    60.4383     4:   -11.2548
      5:   -12.1908     6:   -15.5667     7:    38.3328     8:   -23.6268
      9:    1.30625    10:    5.76620    11:   -15.6537    12:    2.51078
     13:    2.17043    14:   -13.5866    15:    4.08970    16:    3.01348
     17:   -1.50847    18:   -1.53944
;

_pd_spec_mounting
;sealed glass capillary .7mm outer diameter packing density 40%
;
_pd_spec_mount_mode              'transmission'
_pd_spec_shape                 'cylinder'
_exptl_absorpt_process_details
;   GSAS Absorption/surface roughness correction: function number 0
 Debye-Scherrer absorption correction
Term (= MU.r/wave) =       1.7234
Correction is not refined.
;
_exptl_absorpt_correction_T_min        0.02124
_exptl_absorpt_correction_T_max        0.07490

_pd_proc_ls_profile_function
;
 CW Profile function number 3 with  19 terms
 Pseudovoigt profile coefficients as parameterized in
 P. Thompson, D.E. Cox & J.B. Hastings (1987). J. Appl. Cryst.,20,79-83.
 Asymmetry correction of L.W. Finger, D.E. Cox & A. P. Jephcoat (1994).
 J. Appl. Cryst.,27,892-900.
 #1(GU)   =    0.000 #2(GV)   =    6.338 #3(GW)   =    4.936
 #4(GP)   =    3.355 #5(LX)   =    2.602 #6(LY)   =    3.376
 #7(S/L)  =   0.0249 #8(H/L)  =   0.0269
 #9(trns) =     0.00 #10(shft)=   0.0000
 #11(stec)=     0.00 #12(ptec)=     0.00 #13(sfec)=     0.00
 #14(L11) =    0.036 #15(L22) =    0.032 #16(L33) =   -0.045
 #17(L12) =   -0.017 #18(L13) =    0.010 #19(L23) =    0.015
 Peak tails are ignored  where the intensity is below 0.0005 times the peak
```

```
  Aniso. broadening axis   0.0   0.0   1.0
;
_pd_proc_ls_peak_cutoff 0.00050
_pd_proc_info_datetime              2010-08-06T11:07:20
_pd_calc_method                    "Rietveld Refinement"

_pd_meas_2theta_range_min            3.01
_pd_meas_2theta_range_max             95.0
_pd_meas_2theta_range_inc            0.01
_pd_proc_2theta_range_min            2.99985
_pd_proc_2theta_range_max            94.98985
_pd_proc_2theta_range_inc            0.01


loop_
     _refln_index_h
     _refln_index_k
     _refln_index_l
     _refln_observed_status
     _refln_F_squared_meas
     _refln_F_squared_calc
     _refln_phase_calc
     _refln_d_spacing
     _gsas_i100_meas
   1   1   1 o  2497974.3  2496519.5  180.00  14.28147 100.00
   2   2   0 o  274097.47  271738.34   0.00    8.74558   6.24
   3   1   1 o  166889.67  166418.28   0.00    7.45825   5.57
   2   2   2 o  92352.23   89812.51   180.00  7.14074   0.93
   4   0   0 o  5592.597   3753.370    0.00   6.18406   0.03
   3   3   1 o  458189.0   455704.6   180.00  5.67488   8.97
   4   2   2 o  7222.535   4206.879   180.00  5.04926   0.11
   5   1   1 o  186469.08  186936.39   0.00   4.76049   2.60
   3   3   3 o  1386.526   1388.429    0.00   4.76049   0.01
   4   4   0 o  464355.5   459447.8   180.00  4.37279   2.73
   5   3   1 o  760.004    257.172    180.00  4.18119   0.02
   4   4   2 o  36147.39   34495.734  180.00  4.12271   0.37
   6   2   0 o  68739.50   66586.31    0.00   3.91114   0.66
   5   3   3 o  783752.0   778260.4   180.00  3.77224   6.92
   6   2   2 o  38632.80   38220.75   180.00  3.72913   0.33
   4   4   4 o  28745.502  27856.016  180.00   3.57037   0.08
   7   1   1 o  12029.757  11685.793  180.00   3.46377   0.09
   5   5   1 o  60031.78   58440.78    0.00   3.46377   0.45
   6   4   2 o  396942.2   394657.3   180.00  3.30552   5.40
   5   5   3 o  18664.697  15971.466  180.00   3.22038   0.12
   7   3   1 o  577.487    487.131     0.00   3.22038   0.01
   8   0   0 o  28537.539  28586.979  180.00   3.09203   0.04
   7   3   3 o  102016.17  98872.61   180.00   3.02201   0.59
   6   4   4 o  16855.811  18067.436   0.00    2.99971   0.09
   8   2   2 o  60495.51   58791.73    0.00    2.91519   0.33
   6   6   0 o  543139.7   531366.3    0.00    2.91519   1.45
   7   5   1 o  14976.570  14735.022   0.00    2.85629   0.16
   6   6   2 o  49600.14   48216.73   180.00   2.83744   0.24
   5   5   5 o  1929517.9  1904171.6  180.00   2.85629   3.28
   9   1   1 o  21009.258  21107.697  180.00   2.71515   0.09
   8   4   0 o  271707.94  270213.66   0.00    2.76559   1.31
   7   5   3 o  102363.07  103397.44   0.00    2.71515   0.94
```

8	4	2	o	46575.39	45829.46	0.00	2.69894	0.41
6	6	4	o	422732.8	422591.9	180.00	2.63689	1.85
9	3	1	o	190077.64	190803.69	0.00	2.59306	1.59
8	4	4	o	210213.06	208566.02	0.00	2.52463	0.84
9	3	3	o	4584.304	4359.965	0.00	2.48608	0.02
7	7	1	o	21703.912	20702.326	180.00	2.48608	0.08
7	5	5	o	31468.625	29962.592	180.00	2.48608	0.13
10	2	0	o	1249.337	1159.148	0.00	2.42559	0.00
8	6	2	o	14457.450	13193.655	0.00	2.42559	0.11
10	2	2	o	1025.360	993.475	0.00	2.38024	0.00
9	5	1	o	1136.676	1101.876	0.00	2.39134	0.01
7	7	3	o	30416.080	29498.355	0.00	2.39134	0.11
6	6	6	o	877145.1	853233.8	0.00	2.38024	0.98
9	5	3	o	46.975	36.001	180.00	2.30667	0.00
8	6	4	o	13137.244	11972.955	180.00	2.29670	0.08
10	4	2	o	590.917	740.996	180.00	2.25810	0.00
11	1	1	o	51536.42	53226.30	180.00	2.23039	0.16
7	7	5	o	158354.94	162491.31	0.00	2.23039	0.47
8	8	0	o	444941.0	437435.6	0.00	2.18639	0.60
11	3	1	o	46623.26	45968.13	180.00	2.16121	0.26
10	4	4	o	28310.174	26962.561	0.00	2.15301	0.08
9	7	1	o	15322.054	15126.481	0.00	2.16121	0.08
9	5	5	o	27602.797	27239.025	180.00	2.16121	0.08
8	8	2	o	455.749	432.513	0.00	2.15301	0.00
10	6	0	o	28734.609	29168.361	0.00	2.12111	0.08
8	6	6	o	31777.275	32130.650	0.00	2.12111	0.08
11	3	3	o	187250.22	186379.23	0.00	2.09810	0.45
9	7	3	o	72784.91	72475.01	180.00	2.09810	0.37
12	0	0	o	298018.16	284942.69	180.00	2.06135	0.19
10	6	2	o	56717.58	56105.46	180.00	2.09059	0.28
8	8	4	o	126940.80	122430.97	180.00	2.06135	0.31
11	5	1	o	10992.308	10748.995	0.00	2.04021	0.06
12	2	2	o	6109.491	5347.641	180.00	2.00637	0.02
7	7	7	o	65725.20	64949.36	0.00	2.04021	0.05
10	6	4	o	382.020	342.315	180.00	2.00637	0.00
11	5	3	o	4885.815	5890.600	0.00	1.98686	0.02
9	7	5	o	3240.629	3940.842	180.00	1.98686	0.02
12	4	0	o	9062.313	10439.397	180.00	1.95557	0.02
12	4	2	o	139177.47	139608.73	0.00	1.93157	0.56
9	9	1	o	59676.39	58782.96	180.00	1.93749	0.12
13	1	1	o	7.085	8.174	180.00	1.89163	0.00
8	8	6	o	67357.27	67366.44	0.00	1.93157	0.13
10	8	2	o	73219.58	76334.28	0.00	1.90844	0.29
11	5	5	o	2590.930	2733.239	180.00	1.89163	0.00
11	7	1	o	8043.176	8589.621	180.00	1.89163	0.03
9	9	3	o	51163.47	54587.44	0.00	1.89163	0.10
10	6	6	o	5315.026	5044.011	180.00	1.88612	0.01
12	4	4	o	1137.648	1741.977	0.00	1.86456	0.00
13	3	1	o	18001.412	18340.420	180.00	1.84887	0.07
11	7	3	o	41885.69	42475.87	0.00	1.84887	0.15
10	8	4	o	101.885	102.559	180.00	1.84373	0.00
9	7	7	o	69242.84	69900.23	0.00	1.84887	0.12
12	6	2	o	46627.81	50483.76	180.00	1.82358	0.16
13	3	3	o	87162.23	89240.79	0.00	1.80889	0.15
9	9	5	o	161140.89	164524.81	0.00	1.80889	0.27
13	5	1	o	39520.43	40838.82	180.00	1.77140	0.13

12	6	4	o	8079.923	8494.992	180.00	1.76687	0.02
14	2	0	o	77951.76	79136.86	180.00	1.74912	0.12
8	8	8	o	199385.17	194779.16	0.00	1.78518	0.11
11	7	5	o	95472.45	98617.01	180.00	1.77140	0.30
14	2	2	o	2417.637	2275.566	180.00	1.73188	0.00
10	8	6	o	9293.488	9432.561	0.00	1.74912	0.03
13	5	3	o	38944.14	38205.43	180.00	1.73614	0.11
10	10	0	o	767969.7	779610.8	180.00	1.74912	0.57
11	9	1	o	14339.095	14095.006	180.00	1.73614	0.04
10	10	2	o	1146.771	1073.345	0.00	1.73188	0.00
12	8	0	o	5733.256	5437.688	0.00	1.71515	0.01
12	8	2	o	19070.744	19093.926	180.00	1.69889	0.05
14	4	2	o	19461.422	19206.045	180.00	1.68309	0.05
11	9	3	o	327846.22	329206.38	180.00	1.70291	0.89
9	9	7	o	37079.91	37243.19	0.00	1.70291	0.05
12	6	6	o	38543.97	38087.66	180.00	1.68309	0.05
10	10	4	o	43077.77	42600.01	180.00	1.68309	0.06
13	5	5	o	170.771	145.503	180.00	1.67152	0.00
13	7	1	o	2191.285	1867.343	180.00	1.67152	0.01
15	1	1	o	2255.957	1865.749	180.00	1.64180	0.00
11	7	7	o	28060.639	23580.611	180.00	1.67152	0.04
12	8	4	o	113403.23	120729.89	180.00	1.65276	0.28
14	4	4	o	16513.971	13741.272	180.00	1.63820	0.02
13	7	3	o	5330.226	4334.867	0.00	1.64180	0.01
11	9	5	o	6.913	5.720	0.00	1.64180	0.00
10	8	8	o	3986.096	3257.941	0.00	1.63820	0.00
15	3	1	o	2693.746	2783.866	0.00	1.61361	0.01
14	6	0	o	6162.771	6563.440	180.00	1.62401	0.01
10	10	6	o	11100.396	11792.243	180.00	1.61019	0.01
14	6	2	o	50230.89	53410.14	0.00	1.61019	0.11
15	3	3	o	57164.05	56660.62	180.00	1.58683	0.06
13	7	5	o	4616.004	4556.317	0.00	1.58683	0.01
12	8	6	o	13260.555	13379.494	0.00	1.58357	0.03
14	6	4	o	49064.09	53908.86	0.00	1.57075	0.10
16	0	0	o	446089.8	484450.0	0.00	1.54601	0.10
11	11	1	o	597503.6	588512.8	0.00	1.58683	0.62
15	5	1	o	101.817	103.911	0.00	1.56134	0.00
12	10	2	o	318.746	348.886	0.00	1.57075	0.00
9	9	9	o	12759.521	12546.324	180.00	1.58683	0.00
13	9	1	o	47467.36	48123.98	180.00	1.56134	0.09
11	11	3	o	1109.167	1124.881	0.00	1.56134	0.00
11	9	7	o	46200.81	46759.52	0.00	1.56134	0.09
15	5	3	o	73200.65	84082.66	0.00	1.53703	0.13
16	2	2	o	637.450	694.903	180.00	1.52241	0.00
13	9	3	o	17391.340	20007.049	180.00	1.53703	0.03
12	10	4	o	1586.358	1942.627	0.00	1.53408	0.00
14	8	2	o	55089.42	58348.42	180.00	1.52241	0.09
14	6	6	o	7322.623	8545.669	180.00	1.51101	0.01
13	7	7	o	11754.853	12128.087	180.00	1.51383	0.01
11	11	5	o	267109.22	275671.97	180.00	1.51383	0.22
10	10	8	o	33879.129	35743.13	0.00	1.52241	0.03
16	4	0	o	19688.123	20705.162	0.00	1.49985	0.02
16	4	2	o	10398.124	10611.491	180.00	1.48895	0.02
13	9	5	o	2011.140	1787.482	180.00	1.49165	0.00
15	5	5	o	27367.867	24928.424	180.00	1.49165	0.02
15	7	1	o	66142.64	59831.37	180.00	1.49165	0.10

12	8	8	o	244944.81	255673.48	0.00	1.49985	0.20
14	8	4	o	399.295	406.441	0.00	1.48895	0.00
15	7	3	o	2357.570	2654.433	0.00	1.47042	0.00
12	10	6	o	100810.94	100037.52	180.00	1.47827	0.15
17	1	1	o	129267.29	133420.25	180.00	1.45006	0.09
16	4	4	o	10509.092	10809.168	0.00	1.45760	0.01
11	9	9	o	72115.75	78516.10	0.00	1.47042	0.05
12	12	0	o	1212793.3	1231148.1	0.00	1.45760	0.42
16	6	2	o	3609.920	3754.522	0.00	1.43776	0.00
13	11	1	o	71873.05	72330.07	0.00	1.45006	0.10
11	11	7	o	803.021	808.733	0.00	1.45006	0.00
17	3	1	o	72.723	95.605	0.00	1.43053	0.00
12	12	2	o	761.750	843.568	0.00	1.44758	0.00
14	8	6	o	177853.05	182813.81	180.00	1.43776	0.23
13	9	7	o	13756.104	18474.963	180.00	1.43053	0.02
15	7	5	o	4864.334	6617.506	180.00	1.43053	0.01
13	11	3	o	5370.638	7380.779	0.00	1.43053	0.01
17	3	3	o	3906.896	8736.073	180.00	1.41177	0.00
14	10	0	o	44490.50	45066.05	180.00	1.43776	0.03
14	10	2	o	74.388	137.811	0.00	1.42815	0.00
12	12	4	o	-136.356	4425.332	180.00	1.41872	0.00
16	6	4	o	2287.953	8921.359	180.00	1.40948	0.00
10	10	10	o	26039.877	45407.86	0.00	1.42815	0.01
15	9	1	o	19202.990	45140.50	180.00	1.41177	0.02
17	5	1	o	4736.669	14501.015	180.00	1.39373	0.01
12	10	8	o	975.761	3444.238	180.00	1.40948	0.00
14	10	4	o	-249.416	4421.743	0.00	1.40041	0.00
13	11	5	o	2147.586	6002.125	180.00	1.39373	0.00
15	9	3	o	1517.313	3790.261	0.00	1.39373	0.00
17	5	3	o	348.706	414.877	0.00	1.37636	0.00
16	8	0	o	40637.37	81867.02	180.00	1.38280	0.02
18	2	2	o	0.730	1.114	0.00	1.35758	0.00
16	8	2	o	34359.293	35757.50	0.00	1.37424	0.03
18	2	0	o	4224.046	3846.409	180.00	1.36583	0.00
15	7	7	o	4890.965	5717.678	180.00	1.37636	0.00
14	8	8	o	4180.478	4300.302	180.00	1.37424	0.00
12	12	6	o	91414.20	94254.36	0.00	1.37424	0.04
16	6	6	o	766020.6	688246.1	0.00	1.36583	0.35
11	11	9	o	453.423	527.404	0.00	1.37636	0.00
15	9	5	o	70502.02	68966.97	180.00	1.35963	0.06
17	5	5	o	296574.59	293419.66	0.00	1.34349	0.12
14	10	6	o	8244.829	8654.954	180.00	1.35758	0.01
16	8	4	o	19132.484	16386.277	180.00	1.34947	0.02
13	9	9	o	150037.25	145890.97	180.00	1.35963	0.07
17	7	1	o	2.244	2.062	0.00	1.34349	0.00
18	4	2	o	337.403	323.855	0.00	1.33369	0.00
13	11	7	o	6987.583	6791.881	0.00	1.34349	0.01
13	13	1	o	17962.160	17362.734	0.00	1.34349	0.01
17	7	3	o	3683.446	4165.302	180.00	1.32791	0.00
14	12	2	o	145038.72	136249.89	0.00	1.33369	0.11
13	13	3	o	135570.45	150237.97	0.00	1.32791	0.05
15	11	1	o	2656.939	2932.744	0.00	1.32791	0.00
12	10	10	o	12158.741	11164.903	0.00	1.33369	0.00
18	4	4	o	437.286	449.222	0.00	1.31102	0.00
19	1	1	o	88.279	84.130	180.00	1.29832	0.00
15	11	3	o	130752.88	121028.93	0.00	1.31286	0.08

15	9	7	o	38187.24	35352.90	0.00	1.31286	0.03
12	12	8	o	31990.455	47651.41	180.00	1.31845	0.01
14	12	4	o	38188.40	39015.99	0.00	1.31102	0.02
16	8	6	o	3924.260	4017.922	0.00	1.31102	0.00
17	7	5	o	249283.63	227310.94	0.00	1.29832	0.15
18	6	2	o	24.802	27.185	180.00	1.29653	0.00
16	10	2	o	23732.211	20186.268	180.00	1.30371	0.01
18	6	0	o	79778.81	68259.33	180.00	1.30371	0.02
19	3	1	o	32225.713	43510.92	180.00	1.28424	0.02
13	13	5	o	26397.607	23675.111	0.00	1.29832	0.01
14	10	8	o	30103.369	25359.760	180.00	1.30371	0.02
11	11	11	o	626556.0	545283.2	0.00	1.29832	0.06
19	3	3	o	22136.928	23043.689	0.00	1.27061	0.01
17	9	1	o	19398.268	24736.307	180.00	1.28424	0.01
15	11	5	o	441.811	584.134	180.00	1.28424	0.00
18	6	4	o	37517.64	56773.49	0.00	1.27567	0.02
16	10	4	o	0.871	1.844	180.00	1.28251	0.00
13	11	9	o	35826.49	44534.77	180.00	1.28424	0.02
14	12	6	o	13756.503	20598.154	0.00	1.27567	0.01
17	9	3	o	205629.84	205598.42	180.00	1.27061	0.10
17	7	7	o	3936.256	13554.758	180.00	1.25741	0.00
19	5	1	o	1643.289	5258.175	180.00	1.25741	0.00
16	8	8	o	210021.94	230236.52	0.00	1.26232	0.05
19	5	3	o	129942.38	105004.80	180.00	1.24461	0.05
20	0	0	o	-1390.947	43186.55	180.00	1.23681	0.00
13	13	7	o	87.874	280.189	180.00	1.25741	0.00
15	9	9	o	1255.137	3670.417	0.00	1.25741	0.00
18	8	2	o	99115.20	124365.27	180.00	1.24937	0.04
17	9	5	o	948.105	738.343	180.00	1.24461	0.00
18	6	6	o	3560.587	4272.795	0.00	1.24304	0.00
12	12	10	o	3032.806	21371.691	0.00	1.25579	0.00
16	10	6	o	6747.894	8429.432	180.00	1.24937	0.00
20	2	2	o	-2187.037	25578.018	180.00	1.22463	0.00
15	11	7	o	11703.477	8642.239	180.00	1.24461	0.00
14	14	0	o	92016.80	112283.89	0.00	1.24937	0.01
14	14	2	o	364.775	408.797	0.00	1.24304	0.00
15	13	1	o	15108.701	10828.710	0.00	1.24461	0.01
18	8	4	o	-59.380	3819.141	180.00	1.23067	0.00
14	10	10	o	3069.736	3320.509	180.00	1.24304	0.00
19	5	5	o	3823.041	17549.412	0.00	1.22015	0.00
15	13	3	o	-3.889	0.774	0.00	1.23220	0.00
16	12	0	o	-1787.825	18331.102	180.00	1.23681	0.00
16	12	2	o	-549.494	11420.653	0.00	1.23067	0.00
14	12	8	o	-915.377	26052.135	180.00	1.23067	0.00
20	4	2	o	352.586	1128.007	0.00	1.20700	0.00
19	7	1	o	3021.027	11676.045	0.00	1.22015	0.00
20	4	0	o	15260.179	52836.45	180.00	1.21279	0.00
14	14	4	o	-118.635	907.997	0.00	1.22463	0.00
19	7	3	o	48112.12	49758.31	180.00	1.20844	0.01
17	11	1	o	11009.990	36142.34	180.00	1.22015	0.00
16	12	4	o	4024.432	12653.277	180.00	1.21279	0.00
17	9	7	o	37595.47	36300.41	0.00	1.20844	0.01
17	11	3	o	2664.210	2527.752	0.00	1.20844	0.00
13	11	11	o	6903.303	19989.246	180.00	1.22015	0.00
20	4	4	o	120349.77	92309.20	180.00	1.19012	0.01
15	13	5	o	34240.766	32196.037	0.00	1.20844	0.01

13	13	9	o	16991.742	15071.945	0.00	1.20844	0.00
18	8	6	o	-1.644	87.272	180.00	1.20130	0.00
16	10	8	o	642.083	1553.956	0.00	1.20700	0.00
18	10	2	o	142.020	117.988	180.00	1.19567	0.00
14	14	6	o	220800.53	180563.77	0.00	1.19567	0.02
18	10	0	o	-831.857	16294.994	180.00	1.20130	0.00
21	1	1	o	19074.604	39843.75	0.00	1.17525	0.00
19	7	5	o	2147.510	1481.227	180.00	1.18601	0.00
15	11	9	o	46.196	71.722	0.00	1.19707	0.00
17	11	5	o	220313.52	145227.81	180.00	1.18601	0.03
20	6	2	o	152444.50	89723.34	180.00	1.17925	0.02
16	12	6	o	11375.646	10706.395	180.00	1.18465	0.00
18	10	4	o	1052.141	583.106	180.00	1.17925	0.00
12	12	12	o	528343.1	361538.1	180.00	1.19012	0.02
21	3	1	o	-633.597	5712.232	180.00	1.16478	0.00
20	6	4	o	-386.695	7822.500	0.00	1.16349	0.00
19	9	1	o	26148.148	32800.539	0.00	1.17525	0.00
15	13	7	o	2879.440	3393.149	180.00	1.17525	0.00
14	12	10	o	14054.198	7204.763	0.00	1.17925	0.00
21	3	3	o	24773.867	12581.939	0.00	1.15459	0.00
19	9	3	o	-504.852	6848.065	0.00	1.16478	0.00
17	9	9	o	-1980.243	20999.467	180.00	1.16478	0.00
18	8	8	o	-967.185	22200.213	0.00	1.16349	0.00
19	7	7	o	112244.90	55026.14	0.00	1.15459	0.00
15	15	1	o	-506.731	6942.636	180.00	1.16478	0.00
18	10	6	o	20.071	9.748	0.00	1.15333	0.00
14	14	8	o	4230.742	1780.311	180.00	1.15838	0.00
16	14	2	o	73297.41	29780.602	0.00	1.15838	0.01
21	5	1	o	3008.472	990.315	180.00	1.14466	0.00
15	15	3	o	23829.441	11184.695	0.00	1.15459	0.00
17	11	7	o	52231.68	24916.412	0.00	1.15459	0.00
20	8	0	o	1611188.5	411955.5	0.00	1.14835	0.05
16	10	10	o	7026.784	2745.721	180.00	1.15838	0.00
19	9	5	o	5267.865	1568.518	0.00	1.14466	0.00
20	6	6	o	-3.747	234.853	0.00	1.13858	0.00
17	13	1	o	58794.08	26828.730	0.00	1.15459	0.00
13	13	11	o	35807.05	16394.678	180.00	1.15459	0.00
20	8	2	o	1380.524	1601.004	180.00	1.14343	0.00
16	12	8	o	8355.021	1953.843	0.00	1.14835	0.00
21	5	3	o	-721.075	9390.445	180.00	1.13498	0.00
17	13	3	o	15737.676	4391.105	0.00	1.14466	0.00
16	14	4	o	428.348	437.039	0.00	1.14343	0.00
20	8	4	o	-2646.759	28561.264	0.00	1.12905	0.00
15	11	11	o	8453.088	2243.156	180.00	1.14466	0.00
18	12	2	o	-62.314	1051.699	0.00	1.13858	0.00
22	2	2	o	-128.915	4241.732	0.00	1.11520	0.00
22	2	0	o	-3907.114	56216.17	0.00	1.11976	0.00
15	15	5	o	-638.031	29143.365	0.00	1.13498	0.00
15	13	9	o	-225.956	2915.499	0.00	1.13498	0.00
21	5	5	o	-50.672	517.839	180.00	1.11633	0.00
17	13	5	o	-177.225	3435.452	180.00	1.12554	0.00
18	12	4	o	-97.421	1811.623	180.00	1.12437	0.00
21	7	1	o	-2.592	17.392	0.00	1.11633	0.00
19	11	1	o	-905.552	11887.913	180.00	1.12554	0.00
18	10	8	o	308.280	300.753	180.00	1.11976	0.00
16	14	6	o	13493.415	11416.340	180.00	1.11976	0.00

19	11	3	o	-279.568	1101.583	180.00	1.11633	0.00
19	9	7	o	-1230.318	13829.672	180.00	1.11633	0.00
14	12	12	o	-26.864	957.111	180.00	1.12437	0.00
21	7	3	o	-915.922	14828.898	0.00	1.10735	0.00
22	4	2	o	639324.3	24144.439	0.00	1.10184	0.00
20	8	6	o	-26.783	352.466	0.00	1.10624	0.00
17	11	9	o	-6.618	1.118	180.00	1.11633	0.00
14	14	10	o	3.000	30.111	0.00	1.11520	0.00
15	15	7	o	-1611.260	29605.473	180.00	1.10735	0.00
22	4	4	o	-420.172	12725.728	0.00	1.08895	0.00
18	12	6	o	1962159.9	62077.74	0.00	1.10184	0.01
20	10	2	o	1513957.9	48208.75	180.00	1.10184	0.00
16	12	10	o	-74.519	1735.601	180.00	1.10624	0.00
21	7	5	o	-43.931	622.363	180.00	1.09001	0.00
17	13	7	o	-4.476	0.008	0.00	1.09857	0.00
19	11	5	o	-1254.817	17169.373	0.00	1.09857	0.00
23	1	1	o	848564.8	55487.71	0.00	1.07346	0.00
20	10	4	o	-79.848	2076.732	0.00	1.08895	0.00
22	6	2	o	3208.280	118.913	0.00	1.08061	0.00
22	6	0	o	11696103.	75534.98	180.00	1.08476	0.00
16	14	8	o	-252.581	5260.558	0.00	1.08895	0.00
16	16	0	o	-279.953	1160.140	180.00	1.09320	0.00
21	9	1	o	3915722.	73211.30	180.00	1.08164	0.01
15	13	11	o	-386.415	4415.642	180.00	1.09001	0.00
17	15	1	o	-88.934	2255.903	0.00	1.09001	0.00
13	13	13	o	-141.408	472.166	180.00	1.09857	0.00
16	16	2	o	-58.902	851.202	0.00	1.08895	0.00
17	15	3	o	1694578.6	30825.813	180.00	1.08164	0.00
19	9	9	o	269776.81	4943.006	180.00	1.08164	0.00
20	8	8	o	22856.309	60635.60	180.00	1.07651	0.00
18	14	2	o	110300.22	4775.297	180.00	1.08061	0.00
18	10	10	o	336052.22	14416.889	0.00	1.08061	0.00
23	3	1	o	30809.498	7753.623	0.00	1.06546	0.00
18	14	0	o	155905.86	829.349	180.00	1.08476	0.00
21	9	3	o	152274.20	8870.828	180.00	1.07346	0.00
19	11	7	o	231427.11	12996.703	0.00	1.07346	0.00
22	6	4	o	268630.84	15897.639	180.00	1.06844	0.00
16	16	4	o	-2654.105	39138.70	0.00	1.07651	0.00
21	7	7	o	3080.408	697.093	180.00	1.06546	0.00
19	13	1	o	782990.6	42364.52	180.00	1.07346	0.00
15	15	9	o	48937.18	2617.770	0.00	1.07346	0.00
20	10	6	o	45992.20	2519.854	180.00	1.06844	0.00
18	12	8	o	1534.691	156.204	180.00	1.07245	0.00
23	3	3	o	-8396.249	138615.69	0.00	1.05764	0.00
17	11	11	o	6206.060	195.022	0.00	1.07346	0.00
18	14	4	o	1269347.0	69496.41	180.00	1.06844	0.01
21	9	5	o	-655.285	7729.662	180.00	1.05764	0.00
17	13	9	o	124100.01	23451.785	0.00	1.06546	0.00
17	15	5	o	13528.660	2521.516	0.00	1.06546	0.00
19	13	3	o	1343.300	271.765	180.00	1.06546	0.00
23	5	1	o	128099.50	25294.229	180.00	1.04999	0.00
14	14	12	o	799500.4	40160.75	180.00	1.06844	0.00
22	6	6	o	168381.48	36100.55	0.00	1.04905	0.00
22	8	2	o	-981.384	8077.358	180.00	1.05284	0.00
20	12	2	o	-184.861	3564.161	0.00	1.05668	0.00
20	12	0	o	-2088.219	42237.53	180.00	1.06056	0.00

```
  16  16   6 o -70.928     2754.914   180.00   1.05668   0.00
  16  12  12 o -2981.276   38478.96    0.00    1.06056   0.00
  19  13   5 o  109192.79  18928.904  180.00   1.04999   0.00
  18  14   6 o  5741.820   1166.955   180.00   1.04905   0.00
  16  14  10 o -158.963    1537.741    0.00    1.05284   0.00
  20  12   4 o  34756.754  6370.162    0.00    1.04530   0.00
_reflns_number_total                 374
_reflns_limit_h_min                  1
_reflns_limit_h_max                  24
_reflns_limit_k_min                  0
_reflns_limit_k_max                  17
_reflns_limit_l_min                  0
_reflns_limit_l_max                  13
_reflns_d_resolution_high            1.045
_reflns_d_resolution_low             14.281
#--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--#
```

Table S4 CIF files for Ru(1%)/Na-Y zeolite after (a) NO_x saturation and after (b) NO_x regeneration. No H_2 was used during regeneration.

(a)

```
data_ADSREV_publ

_pd_block_id
  2010-07-27T10:33|ADSHRGB|CEAK|stadip

_audit_creation_method  "from EXP file using GSAS2CIF"
_audit_creation_date                 2010-07-27T10:33
_audit_author_name                   CEAK
_audit_update_record
; 2010-07-27T10:33  Initial CIF as created by GSAS2CIF
;

_refine_ls_shift/su_max              3.57
_refine_ls_shift/su_mean             0.85
_computing_structure_refinement      GSAS
_refine_ls_number_parameters         49
_refine_ls_goodness_of_fit_all       0.92
_refine_ls_number_restraints         0
_refine_ls_matrix_type               full

_pd_phase_name
   "Ru1% NaY adsorbed NOx no H2"
_cell_length_a                       24.70180(18)
_cell_length_b                       24.7018
_cell_length_c                       24.7018
_cell_angle_alpha                    90.0
_cell_angle_beta                     90.0
_cell_angle_gamma                    90.0
_cell_volume                         15072.52(32)
_symmetry_cell_setting               cubic
_symmetry_space_group_name_H-M       "F d -3 m"

loop_
```

```
    _atom_site_type_symbol
    _atom_site_label
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_occupancy
    _atom_site_thermal_displace_type
    _atom_site_U_iso_or_equiv
    _atom_site_symmetry_multiplicity
O
O1    0.89305(15)  0.10694(15)  0.0        1.0       Uiso   0.0008(24)   96
O
O2    0.96627(25)  0.07873(15)  0.07873(15)  1.0       Uiso   0.0098(25)   96
O
O3    1.00023(15)  0.14204(21)  1.00023(15)  1.0       Uiso   0.0043(23)   96
O
O4    0.92696(18)  0.17756(15)  0.07244(15)  1.0       Uiso   0.0145(26)   96
Si
T1    0.94646(9)   0.12572(9)   0.03614(8)   1.0       Uiso   0.0040(4)   192
Na
sii   0.23499(13)  0.23499(13)  0.23499(13)  0.915(11)  Uiso   0.0102(34)   32
Na
SI'   0.0675(6)    0.0675(6)    0.0675(6)    0.257(10)  Uiso   0.088(16)    32
Na
siii  0.375        0.375        0.2101(17)   0.186(16)  Uiso   0.037(23)    48
Na
sV    0.5          0.5          0.5          0.243(14)  Uiso   0.002(19)    16
Ru
ru    0.0          0.0          0.0          0.0970(33) Uiso   0.002(11)    16
O
ow1   0.3196(7)    0.3196(7)    0.5207(9)    0.245(10)  Uiso   0.016(14)    96
O
ow2   0.3090(10)   0.3090(10)   0.2163(12)   0.180(9)   Uiso   0.036(19)    96
O
O14   0.375        0.375        0.6016(22)   0.188(19)  Uiso   0.045(31)    48
O
O15   0.375        0.375        0.4644(19)   0.188(13)  Uiso   0.040(25)    48
N
N16   0.248(7)     0.398(6)     0.459(10)    0.01       Uiso   0.025       192
N
N17   0.300(7)     0.347(6)     0.440(6)     0.01       Uiso   0.025       192
N
on1   0.271(7)     0.438(6)     0.462(11)    0.01       Uiso   0.025       192
N
on2   0.345(7)     0.364(6)     0.435(7)     0.01       Uiso   0.025       192
N
on3   0.282(7)     0.301(6)     0.435(7)     0.01       Uiso   0.025       192

_chemical_formula_sum              "N0.05 Na0.26 O2.31 Ru0.01 Si"
_chemical_formula_weight            72.54
_cell_formula_units_Z              192

loop_ _atom_type_symbol
    _atom_type_number_in_cell
    _atom_type_scat_dispersion_real
    _atom_type_scat_dispersion_imag
```

```
    _atom_type_scat_Cromer_Mann_a1
    _atom_type_scat_Cromer_Mann_a2
    _atom_type_scat_Cromer_Mann_a3
    _atom_type_scat_Cromer_Mann_a4
    _atom_type_scat_Cromer_Mann_b1
    _atom_type_scat_Cromer_Mann_b2
    _atom_type_scat_Cromer_Mann_b3
    _atom_type_scat_Cromer_Mann_b4
    _atom_type_scat_Cromer_Mann_c
    _atom_type_scat_source
  O       442.937    0.000    0.000
 3.04850 13.2771 2.28680 5.70110 1.54630 0.32390 0.86700 32.9089 0.25080
  International_Tables_Vol_C
  Si       192.0    0.000    0.000
 6.29150 2.43860 3.03530 32.3337 1.98910 0.67850 1.54100 81.6937 1.14070
  International_Tables_Vol_C
  Na       50.322    0.000    0.000
 4.76260 3.28500 3.17360 8.84220 1.26740 0.31360 1.11280 129.424 0.67600
  International_Tables_Vol_C
  Ru        1.552    0.000    0.000
 19.2674 0.80852 12.9182 8.43467 4.86337 24.7997 1.56756 94.2928 5.37874
  International_Tables_Vol_C
  N         9.6    0.000    0.000
 12.2126 0.00570 3.13220 9.89330 2.01250 28.9975 1.16630 0.58260 -11.529
  International_Tables_Vol_C
_diffrn_radiation_probe              x-ray
_diffrn_radiation_polarisn_ratio      0.0
_diffrn_radiation_wavelength          1.540562
_diffrn_radiation_type               Cu_K\a~1~
_pd_proc_ls_prof_R_factor            0.0407
_pd_proc_ls_prof_wR_factor            0.0550
_pd_proc_ls_prof_wR_expected          0.0599
_refine_ls_R_Fsqd_factor             0.12834

_pd_proc_ls_background_function
;   GSAS Background function number 1 with 10 terms.
 Shifted Chebyshev function of 1st kind
     1:    153.372     2:   -117.997     3:    70.3842     4:   -38.2430
     5:    24.3030     6:   -29.1598     7:    36.6038     8:   -20.2819
     9:    9.56488    10:   0.510292
;

_pd_spec_mounting
;sealed glass capillary .7mm outer diameter packing density 40%
;
_pd_spec_mount_mode              'transmission'
_pd_spec_shape                  'cylinder'
_exptl_absorpt_process_details
;   GSAS Absorption/surface roughness correction: function number 0
 Debye-Scherrer absorption correction
Term (= MU.r/wave) =       1.7234
Correction is not refined.
;
_exptl_absorpt_correction_T_min       0.02124
_exptl_absorpt_correction_T_max        0.07327
```

```
_pd_proc_ls_profile_function
;
 CW Profile function number 3 with  19 terms
 Pseudovoigt profile coefficients as parameterized in
 P. Thompson, D.E. Cox & J.B. Hastings (1987). J. Appl. Cryst.,20,79-83.
 Asymmetry correction of L.W. Finger, D.E. Cox & A. P. Jephcoat (1994).
 J. Appl. Cryst.,27,892-900.
 #1(GU)   =    0.000 #2(GV)   =   -1.425 #3(GW)   =    3.831
 #4(GP)   =    0.000 #5(LX)   =    1.489 #6(LY)   =    0.130
 #7(S/L)  =   0.0329 #8(H/L)  =   0.0181
 #9(trns) =     0.00 #10(shft)=   0.0000
 #11(stec)=     0.00 #12(ptec)=     0.00 #13(sfec)=     0.00
 #14(L11) =    0.066 #15(L22) =    0.066 #16(L33) =    0.016
 #17(L12) =    0.000 #18(L13) =   -0.003 #19(L23) =    0.003
 Peak tails are ignored  where the intensity is below 0.0010 times the peak
   Aniso. broadening axis   0.0   0.0   1.0
;
_pd_proc_ls_peak_cutoff 0.00100
_pd_proc_info_datetime              2010-07-27T10:33:47
_pd_calc_method                     "Rietveld Refinement"

_pd_meas_2theta_range_min           3.0
_pd_meas_2theta_range_max           94.99
_pd_meas_2theta_range_inc           0.01
_pd_proc_2theta_range_min           2.99081
_pd_proc_2theta_range_max           94.9808
_pd_proc_2theta_range_inc           0.01

loop_
      _refln_index_h
      _refln_index_k
      _refln_index_l
      _refln_observed_status
      _refln_F_squared_meas
      _refln_F_squared_calc
      _refln_phase_calc
      _refln_d_spacing
      _gsas_i100_meas
   1   1   1 o  1659701.5  1659874.6  180.00  14.26159 100.00
   2   2   0 o  439506.7   437285.9    0.00    8.73341  15.02
   3   1   1 o  252171.97  253988.53   0.00    7.44787  12.59
   2   2   2 o  60336.45   62568.59   180.00   7.13080   0.93
   4   0   0 o  1095.797   842.791     0.00    6.17545   0.01
   3   3   1 o  665876.9   666811.1   180.00   5.66698  19.54
   4   2   2 o  7652.867   6505.881   180.00   5.04223   0.18
   5   1   1 o  134157.78  130738.27   0.00    4.75386   2.82
   3   3   3 o  119036.22  116049.80   0.00    4.75386   0.83
   4   4   0 o  360415.8   350634.84  180.00   4.36670   3.20
   5   3   1 o  17516.734  16833.367   0.00    4.17537   0.57
   4   4   2 o  17360.129  17613.088  180.00   4.11697   0.27
   6   2   0 o  104739.51  104983.48   0.00    3.90570   1.50
   5   3   3 o  833736.6   807448.3   180.00   3.76699  11.08
   6   2   2 o  19020.016  18692.617  180.00   3.72394   0.25
   4   4   4 o  2086.574   1655.291    0.00    3.56540   0.01
   5   5   1 o  62501.12   65090.15    0.00    3.45894   0.71
   7   1   1 o  2593.827   2702.169   180.00   3.45894   0.03
```

6	4	2	o	362334.0	368144.4	180.00	3.30092	7.43
7	3	1	o	8986.820	9393.815	0.00	3.21590	0.18
5	5	3	o	1204.662	1261.039	180.00	3.21590	0.01
8	0	0	o	67224.92	65891.47	0.00	3.08773	0.15
7	3	3	o	121954.70	124253.71	180.00	3.01781	1.06
6	4	4	o	2353.725	2259.445	180.00	2.99553	0.02
6	6	0	o	531278.6	531554.8	0.00	2.91114	2.13
8	2	2	o	136558.16	136427.91	0.00	2.91114	1.10
7	5	1	o	52544.52	52751.55	0.00	2.85232	0.80
6	6	2	o	1039.128	1033.973	180.00	2.83349	0.01
5	5	5	o	2667860.8	2683572.8	180.00	2.85232	6.81
8	4	0	o	462007.8	463532.4	0.00	2.76175	3.32
9	1	1	o	8704.093	8520.556	180.00	2.71138	0.06
7	5	3	o	104103.21	101794.16	0.00	2.71138	1.43
8	4	2	o	49745.85	50645.00	0.00	2.69519	0.67
6	6	4	o	614533.2	609207.3	180.00	2.63322	4.03
9	3	1	o	201840.34	196578.69	0.00	2.58945	2.54
8	4	4	o	202289.97	196892.02	0.00	2.52112	1.21
7	7	1	o	2084.855	1986.674	180.00	2.48263	0.01
9	3	3	o	87.359	84.083	0.00	2.48262	0.00
7	5	5	o	52418.31	50218.91	180.00	2.48263	0.32
8	6	2	o	5489.810	4920.390	0.00	2.42221	0.07
10	2	0	o	1878.635	1737.079	0.00	2.42221	0.01
9	5	1	o	3678.798	3660.051	180.00	2.38801	0.03
7	7	3	o	69326.80	68979.33	0.00	2.38801	0.37
10	2	2	o	21713.326	21532.553	180.00	2.37693	0.11
6	6	6	o	1034780.6	1028456.7	0.00	2.37693	1.74
9	5	3	o	898.140	876.776	0.00	2.30346	0.01
8	6	4	o	10151.340	9789.740	180.00	2.29351	0.09
10	4	2	o	54.716	51.542	0.00	2.25496	0.00
11	1	1	o	167422.11	163917.91	180.00	2.22729	0.77
7	7	5	o	101665.87	99736.77	0.00	2.22729	0.45
8	8	0	o	754891.1	744740.1	0.00	2.18335	1.53
9	7	1	o	23399.248	23102.742	0.00	2.15821	0.19
11	3	1	o	49205.42	48550.23	180.00	2.15821	0.41
8	8	2	o	3786.622	3747.255	180.00	2.15002	0.01
9	5	5	o	26304.680	25947.857	180.00	2.15821	0.11
10	4	4	o	38317.62	37920.69	0.00	2.15002	0.15
10	6	0	o	33795.059	33079.121	0.00	2.11816	0.14
8	6	6	o	7898.516	7728.902	0.00	2.11816	0.03
11	3	3	o	337010.06	336166.81	0.00	2.09518	1.23
9	7	3	o	61883.96	61717.29	180.00	2.09518	0.48
10	6	2	o	45439.39	45138.92	180.00	2.08768	0.34
12	0	0	o	293862.84	288888.88	180.00	2.05848	0.29
8	8	4	o	99275.19	97636.36	180.00	2.05848	0.37
11	5	1	o	1069.671	1042.332	0.00	2.03737	0.01
7	7	7	o	131132.45	128962.74	0.00	2.03737	0.15
10	6	4	o	397.385	373.734	0.00	2.00358	0.00
12	2	2	o	4501.238	4278.404	0.00	2.00358	0.01
9	7	5	o	26680.506	25427.840	180.00	1.98410	0.18
11	5	3	o	2.547	1.686	0.00	1.98410	0.00
12	4	0	o	10213.274	9732.139	0.00	1.95285	0.03
9	9	1	o	64116.25	63814.76	180.00	1.93479	0.19
12	4	2	o	91413.31	91438.74	0.00	1.92889	0.55
8	8	6	o	176396.89	176592.47	0.00	1.92889	0.53
10	8	2	o	200877.88	200155.13	0.00	1.90579	1.20

9	9	3	o	50053.78	49776.76	0.00	1.88899	0.14
13	1	1	o	32495.561	32319.861	180.00	1.88899	0.09
11	7	1	o	170.317	169.627	0.00	1.88899	0.00
11	5	5	o	243.493	242.268	180.00	1.88899	0.00
10	6	6	o	10469.378	10325.482	180.00	1.88349	0.03
12	4	4	o	34348.238	34266.395	0.00	1.86197	0.10
11	7	3	o	66398.41	66179.90	0.00	1.84630	0.36
13	3	1	o	17833.176	17771.516	180.00	1.84630	0.10
10	8	4	o	5787.169	5780.381	180.00	1.84116	0.03
9	7	7	o	133589.05	133190.67	0.00	1.84630	0.36
12	6	2	o	45833.75	45040.05	180.00	1.82104	0.24
9	9	5	o	176051.22	172164.55	0.00	1.80638	0.44
13	3	3	o	13575.191	13266.121	0.00	1.80637	0.04
13	5	1	o	95548.59	95072.88	180.00	1.76893	0.45
11	7	5	o	134148.53	133514.95	180.00	1.76893	0.64
12	6	4	o	453.332	450.802	180.00	1.76441	0.00
14	2	0	o	154833.14	152948.66	180.00	1.74668	0.35
10	10	0	o	1177342.3	1163275.5	180.00	1.74668	1.32
8	8	8	o	402319.0	399189.3	0.00	1.78270	0.32
11	9	1	o	267.282	259.502	180.00	1.73373	0.00
10	8	6	o	8432.680	8330.354	0.00	1.74668	0.04
14	2	2	o	2377.648	2319.620	0.00	1.72947	0.01
10	10	2	o	8789.574	8576.805	180.00	1.72947	0.02
13	5	3	o	691.918	678.629	0.00	1.73373	0.00
12	8	0	o	42309.98	41501.84	0.00	1.71276	0.09
11	9	3	o	488954.0	485788.8	180.00	1.70054	1.99
12	8	2	o	14460.031	14405.974	180.00	1.69653	0.06
9	9	7	o	22959.188	22811.596	0.00	1.70054	0.05
10	10	4	o	46456.78	45619.82	180.00	1.68074	0.09
14	4	2	o	32977.105	32379.859	180.00	1.68075	0.13
13	7	1	o	10571.652	10340.885	0.00	1.66919	0.04
12	6	6	o	40188.62	39443.34	180.00	1.68074	0.08
11	7	7	o	45443.04	44461.38	180.00	1.66919	0.09
13	5	5	o	20902.715	20460.365	180.00	1.66919	0.04
12	8	4	o	73282.38	70515.55	180.00	1.65046	0.27
13	7	3	o	50945.95	49290.12	0.00	1.63952	0.18
11	9	5	o	4049.220	3917.313	0.00	1.63952	0.01
15	1	1	o	34966.781	33813.219	180.00	1.63952	0.06
14	4	4	o	29577.520	28339.377	0.00	1.63592	0.05
14	6	0	o	1486.177	1386.672	180.00	1.62175	0.00
10	8	8	o	19365.266	18553.652	0.00	1.63592	0.03
15	3	1	o	4375.027	4240.417	0.00	1.61137	0.02
14	6	2	o	150402.66	147092.13	0.00	1.60795	0.48
10	10	6	o	13390.821	13100.627	180.00	1.60795	0.02
11	11	1	o	523772.6	516387.8	0.00	1.58462	0.83
13	7	5	o	27793.631	27395.211	0.00	1.58462	0.09
15	3	3	o	71047.69	70046.18	180.00	1.58462	0.11
12	8	6	o	13270.509	13188.052	0.00	1.58137	0.04
12	10	2	o	2358.637	2314.568	180.00	1.56857	0.01
15	5	1	o	3415.644	3395.632	0.00	1.55916	0.01
13	9	1	o	62628.63	62249.86	180.00	1.55916	0.18
11	11	3	o	17398.514	17298.057	0.00	1.55916	0.02
14	6	4	o	39213.56	38427.79	0.00	1.56857	0.12
9	9	9	o	3324.078	3264.669	0.00	1.58462	0.00
11	9	7	o	66571.56	66219.26	0.00	1.55916	0.19
16	0	0	o	774209.4	761914.7	0.00	1.54386	0.27

15	5	3	o	119658.63	117510.89	0.00	1.53490	0.32
13	9	3	o	41033.78	40285.70	180.00	1.53490	0.11
12	10	4	o	3023.461	2973.249	0.00	1.53194	0.01
16	2	2	o	134.604	131.668	0.00	1.52029	0.00
14	8	2	o	46699.05	45520.54	180.00	1.52029	0.12
11	11	5	o	485979.3	475899.5	180.00	1.51173	0.60
13	7	7	o	5009.804	4899.337	180.00	1.51173	0.01
10	10	8	o	117414.77	114368.62	0.00	1.52029	0.15
14	6	6	o	2425.378	2390.225	0.00	1.50890	0.00
16	4	0	o	87117.26	85613.77	0.00	1.49777	0.11
13	9	5	o	77710.91	75949.02	180.00	1.48957	0.18
15	7	1	o	42105.25	41177.13	180.00	1.48957	0.10
15	5	5	o	78184.14	76393.48	180.00	1.48957	0.09
12	8	8	o	519778.0	510903.1	0.00	1.49777	0.62
16	4	2	o	8809.799	8668.583	180.00	1.48687	0.02
14	8	4	o	12.731	12.475	0.00	1.48687	0.00
12	10	6	o	291108.09	287819.88	180.00	1.47622	0.65
15	7	3	o	46277.48	45409.68	0.00	1.46837	0.10
12	12	0	o	1626263.3	1597509.3	0.00	1.45557	0.84
13	11	1	o	70531.15	69368.00	0.00	1.44805	0.14
17	1	1	o	190679.56	187553.81	180.00	1.44805	0.19
16	4	4	o	3602.969	3538.694	180.00	1.45557	0.00
12	12	2	o	31504.430	31048.553	0.00	1.44556	0.03
11	9	9	o	52252.84	51258.55	0.00	1.46837	0.06
11	11	7	o	33.497	32.669	180.00	1.44805	0.00
16	6	2	o	1844.883	1809.967	0.00	1.43576	0.00
14	10	0	o	65251.41	64076.97	180.00	1.43576	0.06
17	3	1	o	1530.467	1479.207	180.00	1.42854	0.00
13	11	3	o	59630.96	57686.93	0.00	1.42854	0.11
14	8	6	o	309988.41	304493.88	180.00	1.43576	0.59
14	10	2	o	7822.325	7480.926	180.00	1.42616	0.01
13	9	7	o	26.698	26.128	0.00	1.42854	0.00
15	7	5	o	353.587	341.867	0.00	1.42854	0.00
12	12	4	o	2954.044	2694.320	0.00	1.41675	0.00
17	3	3	o	2208.924	2061.394	180.00	1.40981	0.00
15	9	1	o	12718.249	11633.651	180.00	1.40981	0.02
16	6	4	o	1144.660	1049.674	180.00	1.40752	0.00
10	10	10	o	33.578	30.996	180.00	1.42616	0.00
12	10	8	o	349.730	322.080	180.00	1.40752	0.00
14	10	4	o	703.837	617.777	0.00	1.39846	0.00
13	11	5	o	4424.837	4097.711	180.00	1.39179	0.01
17	5	1	o	47492.81	44111.92	180.00	1.39179	0.07
15	9	3	o	16116.273	14963.827	180.00	1.39179	0.03
16	8	0	o	32.337	31.863	0.00	1.38087	0.00
17	5	3	o	108.626	103.997	0.00	1.37445	0.00
16	8	2	o	119722.91	115780.57	0.00	1.37232	0.17
12	12	6	o	99439.68	96184.50	0.00	1.37232	0.07
11	11	9	o	7816.751	7487.292	0.00	1.37445	0.01
15	7	7	o	16496.150	15831.494	180.00	1.37445	0.01
14	8	8	o	232.668	225.374	180.00	1.37232	0.00
18	2	0	o	8002.108	7871.741	180.00	1.36393	0.01
15	9	5	o	104123.88	102472.98	180.00	1.35773	0.14
16	6	6	o	1406431.9	1382897.9	0.00	1.36393	0.96
18	2	2	o	14653.742	14433.203	180.00	1.35569	0.01
14	10	6	o	3428.109	3378.732	0.00	1.35569	0.00
13	13	1	o	45672.16	45047.40	0.00	1.34162	0.03

17	7	1	o	5110.455	5045.901	0.00	1.34162	0.01
13	9	9	o	254872.94	250855.72	180.00	1.35773	0.17
16	8	4	o	63596.01	62234.00	180.00	1.34759	0.08
17	5	5	o	673825.4	664480.7	0.00	1.34162	0.41
13	11	7	o	13644.638	13464.316	0.00	1.34162	0.02
14	12	2	o	198547.83	194211.91	0.00	1.33183	0.22
18	4	2	o	8381.719	8188.179	0.00	1.33183	0.01
13	13	3	o	181198.41	175446.53	0.00	1.32606	0.10
17	7	3	o	2251.344	2187.067	0.00	1.32606	0.00
15	11	1	o	68.742	66.271	0.00	1.32606	0.00
12	10	10	o	115365.00	112711.52	0.00	1.33183	0.07
15	11	3	o	196021.38	191219.75	0.00	1.31104	0.19
14	12	4	o	21132.031	20766.105	0.00	1.30919	0.02
18	4	4	o	2092.370	2055.968	180.00	1.30919	0.00
12	12	8	o	13218.251	12707.861	180.00	1.31661	0.01
15	9	7	o	48509.70	47298.02	0.00	1.31104	0.05
16	10	2	o	41530.52	40659.36	180.00	1.30190	0.04
18	6	0	o	102209.50	100028.08	180.00	1.30190	0.05
16	8	6	o	1138.374	1118.472	0.00	1.30919	0.00
19	1	1	o	7771.260	7596.541	0.00	1.29651	0.00
17	7	5	o	243462.56	237987.63	0.00	1.29651	0.22
13	13	5	o	21315.232	20873.654	180.00	1.29651	0.01
18	6	2	o	792.850	777.188	0.00	1.29473	0.00
14	10	8	o	134661.16	131769.44	180.00	1.30190	0.12
19	3	1	o	81168.46	77983.27	180.00	1.28245	0.06
15	11	5	o	1285.270	1226.822	180.00	1.28245	0.00
17	9	1	o	77018.84	74025.95	180.00	1.28245	0.06
11	11	11	o	1859946.0	1816713.8	0.00	1.29651	0.27
16	10	4	o	3502.288	3370.545	0.00	1.28073	0.00
13	11	9	o	89571.74	86085.47	180.00	1.28245	0.07
14	12	6	o	14734.795	14063.822	0.00	1.27390	0.01
18	6	4	o	39761.20	37910.55	0.00	1.27390	0.03
17	9	3	o	287717.09	277411.81	180.00	1.26885	0.20
19	3	3	o	96826.83	93331.13	0.00	1.26885	0.03
19	5	1	o	3228.863	3056.238	180.00	1.25566	0.00
13	13	7	o	33914.441	32162.188	0.00	1.25566	0.01
18	8	2	o	112842.77	107642.01	180.00	1.24763	0.06
14	14	0	o	69308.05	66018.04	0.00	1.24763	0.01
16	8	8	o	344807.41	329374.56	0.00	1.26056	0.11
19	5	3	o	347815.81	329892.00	180.00	1.24288	0.19
15	13	1	o	4366.667	4134.965	0.00	1.24288	0.00
17	7	7	o	4569.578	4306.491	180.00	1.25566	0.00
15	9	9	o	225.985	213.503	180.00	1.25566	0.00
14	14	2	o	10074.568	9570.426	0.00	1.24131	0.00
16	10	6	o	52954.55	50513.14	180.00	1.24763	0.03
12	12	10	o	23786.592	22479.438	0.00	1.25404	0.01
17	9	5	o	2.096	1.791	0.00	1.24288	0.00
15	11	7	o	43433.16	41179.80	180.00	1.24288	0.02
16	12	0	o	52750.00	47240.41	180.00	1.23509	0.01
20	0	0	o	26426.689	23696.205	180.00	1.23509	0.00
18	6	6	o	7352.269	6989.270	0.00	1.24131	0.00
15	13	3	o	8955.322	7965.602	0.00	1.23048	0.00
18	8	4	o	29402.936	25943.848	180.00	1.22896	0.01
16	12	2	o	17258.455	15224.454	0.00	1.22896	0.01
14	10	10	o	20215.455	19259.469	180.00	1.24131	0.01
14	14	4	o	8779.578	7684.938	0.00	1.22292	0.00

20	2	2	o	119245.14	104968.56	180.00	1.22292	0.03
14	12	8	o	16028.252	14136.175	180.00	1.22896	0.01
19	7	1	o	52080.10	47060.29	0.00	1.21845	0.02
17	11	1	o	55189.00	49713.34	180.00	1.21845	0.02
19	5	5	o	11337.997	10236.681	0.00	1.21845	0.00
16	12	4	o	32710.182	29631.859	180.00	1.21111	0.01
20	4	0	o	32695.209	29566.838	180.00	1.21111	0.01
17	11	3	o	1334.984	1214.666	180.00	1.20676	0.00
15	13	5	o	107595.09	98068.08	0.00	1.20676	0.04
19	7	3	o	66652.27	60597.65	180.00	1.20676	0.02
20	4	2	o	1677.318	1531.588	0.00	1.20532	0.00
13	11	11	o	107863.86	97124.88	180.00	1.21845	0.02
13	13	9	o	18921.047	17160.771	0.00	1.20676	0.00
17	9	7	o	109247.60	99514.72	0.00	1.20676	0.04
18	8	6	o	203.429	177.121	0.00	1.19963	0.00
18	10	0	o	22519.010	20050.809	180.00	1.19963	0.00
16	10	8	o	16340.896	14927.419	0.00	1.20532	0.01
14	14	6	o	763805.8	699718.2	0.00	1.19401	0.10
18	10	2	o	401.092	364.186	0.00	1.19401	0.00
15	11	9	o	19934.748	18042.381	0.00	1.19540	0.01
20	4	4	o	141784.25	128982.67	180.00	1.18847	0.02
19	7	5	o	4136.714	3730.584	0.00	1.18436	0.00
17	11	5	o	379984.9	342620.88	180.00	1.18436	0.09
20	6	2	o	230059.70	198832.73	180.00	1.17761	0.05
16	12	6	o	3691.471	3329.428	180.00	1.18300	0.00
21	1	1	o	13205.937	10776.478	0.00	1.17362	0.00
19	9	1	o	166379.88	136893.42	0.00	1.17362	0.03
18	10	4	o	24961.506	21524.994	180.00	1.17761	0.01
12	12	12	o	815748.9	738182.1	180.00	1.18847	0.03
15	13	7	o	2158.888	1808.450	0.00	1.17362	0.00
14	12	10	o	17882.086	15447.253	0.00	1.17761	0.00
15	15	1	o	6785.820	4835.597	180.00	1.16316	0.00
19	9	3	o	2003.785	1460.250	180.00	1.16316	0.00
21	3	1	o	9269.698	6601.179	180.00	1.16316	0.00
20	6	4	o	35077.64	24998.242	0.00	1.16188	0.00
16	14	2	o	117036.91	79854.31	0.00	1.15677	0.01
18	8	8	o	29290.309	20932.111	0.00	1.16188	0.00
17	13	1	o	10113.345	6967.917	0.00	1.15298	0.00
21	3	3	o	135929.83	95506.31	0.00	1.15298	0.01
15	15	3	o	52127.22	36287.79	0.00	1.15298	0.00
17	9	9	o	74821.15	53647.55	180.00	1.16316	0.01
14	14	8	o	34371.719	23473.340	180.00	1.15677	0.00
17	11	7	o	76710.35	53802.46	0.00	1.15298	0.01
19	7	7	o	49555.78	34798.223	0.00	1.15298	0.00
20	8	0	o	1438982.1	982777.9	0.00	1.14675	0.07
18	10	6	o	9851.891	7046.129	180.00	1.15173	0.00
16	10	10	o	7813.422	5190.095	180.00	1.15677	0.00
19	9	5	o	59.261	1.789	180.00	1.14306	0.00
17	13	3	o	37123.91	21830.783	0.00	1.14306	0.00
21	5	1	o	89532.08	53097.01	180.00	1.14306	0.01
16	14	4	o	75.813	44.951	0.00	1.14184	0.00
20	8	2	o	3101.644	1690.918	0.00	1.14184	0.00
13	13	11	o	246.489	172.007	180.00	1.15298	0.00
16	12	8	o	17795.117	12302.395	0.00	1.14675	0.00
18	12	2	o	252.655	94.738	0.00	1.13699	0.00
20	6	6	o	27710.938	10214.401	0.00	1.13699	0.00

15	15	5	o	61618.97	20523.854	0.00	1.13340	0.00
21	5	3	o	3.883	0.442	0.00	1.13340	0.00
15	11	11	o	10411.838	6397.077	0.00	1.14306	0.00
19	11	1	o	53353.75	12950.229	180.00	1.12397	0.00
15	13	9	o	2693.337	862.697	0.00	1.13340	0.00
20	8	4	o	141703.72	40671.61	0.00	1.12748	0.01
22	2	0	o	390608.1	81474.29	0.00	1.11820	0.00
17	13	5	o	15753.599	3911.227	180.00	1.12397	0.00
18	12	4	o	33.861	6.360	0.00	1.12281	0.00
19	11	3	o	8111.278	1216.725	180.00	1.11478	0.00
21	7	1	o	20847.299	3940.600	0.00	1.11478	0.00
22	2	2	o	160456.50	27602.895	0.00	1.11364	0.00
16	14	6	o	45685.02	9532.403	180.00	1.11820	0.00
19	9	7	o	99049.63	18266.660	180.00	1.11478	0.00
21	5	5	o	89851.26	17069.445	180.00	1.11478	0.00
18	10	8	o	35660.62	7647.455	180.00	1.11820	0.00
14	12	12	o	2.839	0.073	180.00	1.12281	0.00
21	7	3	o	336968.47	43933.86	0.00	1.10580	0.00
17	11	9	o	36784.71	6858.638	180.00	1.11478	0.00
14	14	10	o	28155.859	4889.941	0.00	1.11364	0.00
22	4	2	o	608543.8	71471.26	0.00	1.10031	0.00
20	10	2	o	772305.0	88951.52	180.00	1.10031	0.00
15	15	7	o	385263.2	49583.52	180.00	1.10580	0.00
20	8	6	o	4452.505	597.198	180.00	1.10470	0.00
19	11	5	o	94904.16	8232.167	0.00	1.09705	0.00
18	12	6	o	517149.3	60495.57	0.00	1.10031	0.00
16	12	10	o	1356.660	196.170	180.00	1.10470	0.00
16	16	0	o	679746.8	39541.77	180.00	1.09168	0.00
17	13	7	o	13527.054	1097.488	180.00	1.09705	0.00
17	15	1	o	2536.340	220.046	0.00	1.08849	0.00
21	7	5	o	46994.36	3659.026	0.00	1.08849	0.00
16	16	2	o	45042.07	4559.482	0.00	1.08744	0.00
20	10	4	o	3817.642	382.754	0.00	1.08744	0.00
22	4	4	o	86710.88	8940.392	0.00	1.08744	0.00
22	6	0	o	2476951.5	311029.25	180.00	1.08325	0.00
18	14	0	o	463509.9	57996.11	180.00	1.08325	0.00
16	14	8	o	129089.60	13644.249	0.00	1.08744	0.00
13	13	13	o	899420.3	76945.64	180.00	1.09705	0.00
21	9	1	o	491328.7	68825.25	180.00	1.08013	0.00
17	15	3	o	634999.9	87674.11	180.00	1.08013	0.00
18	14	2	o	295.524	21.289	180.00	1.07910	0.00
22	6	2	o	102472.58	15790.104	0.00	1.07910	0.00
15	13	11	o	51693.88	3709.805	180.00	1.08849	0.00
23	1	1	o	604394.3	150979.03	0.00	1.07197	0.00
19	13	1	o	278994.09	70176.56	180.00	1.07197	0.00
16	16	4	o	433802.5	96529.32	0.00	1.07501	0.00
19	9	9	o	5692.887	770.931	180.00	1.08013	0.00
18	10	10	o	10822.252	1698.307	0.00	1.07910	0.00
19	11	7	o	109915.34	27024.715	0.00	1.07197	0.00
21	9	3	o	63445.20	15523.093	180.00	1.07197	0.00
18	12	8	o	2521.101	724.116	0.00	1.07096	0.00
20	8	8	o	697.765	112.150	180.00	1.07501	0.00
19	13	3	o	9969.833	3974.233	0.00	1.06398	0.00
23	3	1	o	80754.13	32302.893	0.00	1.06398	0.00
18	14	4	o	413376.8	157275.86	180.00	1.06696	0.01
20	10	6	o	34530.883	13046.674	180.00	1.06696	0.00

```
  22   6   4 o  200697.73  76457.73   180.00   1.06696   0.00
  15  15   9 o  115734.99  28817.621   0.00    1.07197   0.00
  20  12   0 o  373.194    135.110     0.00    1.05908   0.00
  21   7   7 o  10526.186  4293.823    0.00    1.06398   0.00
  17  15   5 o  147136.36  58442.23    0.00    1.06398   0.00
  17  11  11 o  12462.910  2616.516    0.00    1.07197   0.00
  23   3   3 o  476209.0   208287.22   0.00    1.05617   0.01
  20  12   2 o  54944.97   24981.332   0.00    1.05521   0.00
  17  13   9 o  131793.69  52807.77    0.00    1.06398   0.00
  14  14  12 o  335865.38  131749.86  180.00   1.06696   0.00
  22   8   2 o  64753.43   30826.156  180.00   1.05138   0.00
  21   9   5 o  49017.35   21356.266  180.00   1.05617   0.00
  16  16   6 o  84821.97   38884.14    0.00    1.05521   0.00
  19  13   5 o  127512.11  68512.45   180.00   1.04853   0.01
  23   5   1 o  157846.56  84313.51   180.00   1.04853   0.01
  18  14   6 o  5318.913   2927.855   180.00   1.04759   0.00
  16  12  12 o  155081.45  61167.04    0.00    1.05908   0.00
  22   6   6 o  349014.72  195080.47   0.00    1.04759   0.01
  16  14  10 o  73.110     24.411      0.00    1.05138   0.00
_reflns_number_total                  373
_reflns_limit_h_min                   1
_reflns_limit_h_max                   23
_reflns_limit_k_min                   0
_reflns_limit_k_max                   16
_reflns_limit_l_min                   0
_reflns_limit_l_max                   13
_reflns_d_resolution_high             1.048
_reflns_d_resolution_low              14.262
#--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--#
```

(b)

```
data_DESREV_publ

_pd_block_id
  2010-07-26T11:56|DESHR|CEAK|stadip

_audit_creation_method  "from EXP file using GSAS2CIF"
_audit_creation_date                  2010-07-26T11:56
_audit_author_name                    CEAK
_audit_update_record
; 2010-07-26T11:56  Initial CIF as created by GSAS2CIF
;

_refine_ls_shift/su_max               1.03
_refine_ls_shift/su_mean              0.32
_computing_structure_refinement       GSAS
_refine_ls_number_parameters          45
_refine_ls_goodness_of_fit_all        1.02
_refine_ls_number_restraints          0
_refine_ls_matrix_type                full

_pd_phase_name
   "Ru1% NaY desorbed NOx no H2"
_cell_length_a                        24.72590(21)
```

```
_cell_length_b                    24.7259
_cell_length_c                    24.7259
_cell_angle_alpha                 90.0
_cell_angle_beta                  90.0
_cell_angle_gamma                 90.0
_cell_volume                      15116.7(4)
_symmetry_cell_setting            cubic
_symmetry_space_group_name_H-M    "F d -3 m"

loop_
    _atom_site_type_symbol
    _atom_site_label
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_occupancy
    _atom_site_thermal_displace_type
    _atom_site_U_iso_or_equiv
    _atom_site_symmetry_multiplicity
O
O1    0.89300(16)  0.10700(16)  0.0         1.0       Uiso   0.0059(27)   96
O
O2    0.96719(28)  0.07828(16)  0.07828(16)  1.0      Uiso   0.0111(27)   96
O
O3    0.99997(16)  0.14416(23)  0.99997(16)  1.0      Uiso   0.0012(29)   96
O
O4    0.92931(20)  0.17802(17)  0.07198(17)  1.0      Uiso   0.0029(32)   96
Si
T1    0.94682(10)  0.12453(10)  0.03568(9)   1.0      Uiso   0.0024(5)   192
Na
sii   0.23504(16)  0.23504(16)  0.23504(16)  0.916(12)  Uiso   0.017(4)    32
Na
SI'   0.0679(6)    0.0679(6)    0.0679(6)    0.262(9)   Uiso   0.010(12)   32
Na
siii  0.375        0.375        0.2105(17)   0.191(18)  Uiso   0.021(23)   48
Na
sV    0.5          0.5          0.5          0.237(30)  Uiso   0.042(8)    16
Ru
ru    0.0          0.0          0.0          0.0967(34) Uiso   0.026(13)   16
O
ow1   0.3196(8)    0.3196(8)    0.5200(9)    0.244(12)  Uiso   0.017(16)   96
O
ow2   0.3086(6)    0.3086(6)    0.2181(8)    0.194(7)   Uiso   0.077(10)   96
O
O14   0.375        0.375        0.6030(29)   0.181(21)  Uiso   0.08(4)     48
O
O15   0.375        0.375        0.4628(30)   0.174(14)  Uiso   0.10(5)     48

_chemical_formula_sum             "Na0.26 O2.31 Ru0.01 Si"
_chemical_formula_weight          71.89
_cell_formula_units_Z             192


loop_ _atom_type_symbol
    _atom_type_number_in_cell
    _atom_type_scat_dispersion_real
```

```
    _atom_type_scat_dispersion_imag
    _atom_type_scat_Cromer_Mann_a1
    _atom_type_scat_Cromer_Mann_a2
    _atom_type_scat_Cromer_Mann_a3
    _atom_type_scat_Cromer_Mann_a4
    _atom_type_scat_Cromer_Mann_b1
    _atom_type_scat_Cromer_Mann_b2
    _atom_type_scat_Cromer_Mann_b3
    _atom_type_scat_Cromer_Mann_b4
    _atom_type_scat_Cromer_Mann_c
    _atom_type_scat_source
 O        443.167    0.000    0.000
 3.04850 13.2771 2.28680 5.70110 1.54630 0.32390 0.86700 32.9089 0.25080
 International_Tables_Vol_C
 Si       192.0    0.000    0.000
 6.29150 2.43860 3.03530 32.3337 1.98910 0.67850 1.54100 81.6937 1.14070
 International_Tables_Vol_C
 Na       50.631    0.000    0.000
 4.76260 3.28500 3.17360 8.84220 1.26740 0.31360 1.11280 129.424 0.67600
 International_Tables_Vol_C
 Ru        1.547    0.000    0.000
 19.2674 0.80852 12.9182 8.43467 4.86337 24.7997 1.56756 94.2928 5.37874
 International_Tables_Vol_C
_diffrn_radiation_probe              x-ray
_diffrn_radiation_polarisn_ratio       0.0
_diffrn_radiation_wavelength          1.540562
_diffrn_radiation_type               Cu_K\a~1~
_pd_proc_ls_prof_R_factor            0.0444
_pd_proc_ls_prof_wR_factor           0.0606
_pd_proc_ls_prof_wR_expected         0.0598
_refine_ls_R_Fsqd_factor             0.11349

_pd_proc_ls_background_function
;   GSAS Background function number 1 with 10 terms.
 Shifted Chebyshev function of 1st kind
     1:    148.093    2:   -103.222    3:    49.0362    4:   -16.3916
     5:    4.92265    6:   -16.1140    7:    26.6737    8:   -14.4236
     9:    6.88823   10:    1.34373
;

_pd_spec_mounting
;sealed glass capillary .7mm outer diameter packing density 40%
;
_pd_spec_mount_mode              'transmission'
_pd_spec_shape                   'cylinder'
_exptl_absorpt_process_details
;   GSAS Absorption/surface roughness correction: function number 0
 Debye-Scherrer absorption correction
Term (= MU.r/wave) =      1.7234
Correction is not refined.
;
_exptl_absorpt_correction_T_min       0.02124
_exptl_absorpt_correction_T_max       0.07318

_pd_proc_ls_profile_function
;
```

```
 CW Profile function number 3 with  19 terms
 Pseudovoigt profile coefficients as parameterized in
 P. Thompson, D.E. Cox & J.B. Hastings (1987). J. Appl. Cryst.,20,79-83.
 Asymmetry correction of L.W. Finger, D.E. Cox & A. P. Jephcoat (1994).
 J. Appl. Cryst.,27,892-900.
 #1(GU)   =    0.000 #2(GV)   =   -1.448 #3(GW)   =    3.938
 #4(GP)   =    0.002 #5(LX)   =    1.436 #6(LY)   =    0.195
 #7(S/L)  =   0.0325 #8(H/L)  =   0.0180
 #9(trns) =     0.00 #10(shft)=   0.0000
 #11(stec)=     0.00 #12(ptec)=     0.00 #13(sfec)=     0.00
 #14(L11) =    0.063 #15(L22) =    0.064 #16(L33) =    0.019
 #17(L12) =    0.007 #18(L13) =    0.000 #19(L23) =    0.003
 Peak tails are ignored  where the intensity is below 0.0010 times the peak
   Aniso. broadening axis   0.0   0.0   1.0
;
_pd_proc_ls_peak_cutoff 0.00100
_pd_proc_info_datetime              2010-07-26T11:56:11
_pd_calc_method                    "Rietveld Refinement"

_pd_meas_2theta_range_min            3.0
_pd_meas_2theta_range_max            94.99
_pd_meas_2theta_range_inc            0.01
_pd_proc_2theta_range_min            2.99179
_pd_proc_2theta_range_max            94.9818
_pd_proc_2theta_range_inc            0.01

loop_
      _refln_index_h
      _refln_index_k
      _refln_index_l
      _refln_observed_status
      _refln_F_squared_meas
      _refln_F_squared_calc
      _refln_phase_calc
      _refln_d_spacing
      _gsas_i100_meas
   1   1   1 o  1794474.6  1781148.6  180.00  14.27553  100.00
   2   2   0 o  457061.5   454049.3    0.00    8.74194  14.45
   3   1   1 o  254877.70  251366.73   0.00    7.45515  11.78
   2   2   2 o  86607.31   65151.80   180.00   7.13777   1.22
   4   0   0 o  6486.916   5957.100    0.00    6.18149   0.05
   3   3   1 o  609491.4   638402.6   180.00   5.67252  16.57
   4   2   2 o  10695.398  6001.079   180.00   5.04716   0.23
   5   1   1 o  132770.45  120558.19   0.00    4.75851   2.58
   3   3   3 o  152188.48  138599.97   0.00    4.75851   0.98
   4   4   0 o  380291.1   374563.7   180.00   4.37097   3.12
   5   3   1 o  11651.406  13778.230   0.00    4.17945   0.35
   4   4   2 o  19336.451  15354.152  180.00   4.12099   0.28
   6   2   0 o  127398.81  119188.40   0.00    3.90952   1.69
   5   3   3 o  808412.9   807097.4   180.00   3.77067   9.95
   6   2   2 o  24433.246  24196.420  180.00   3.72758   0.30
   4   4   4 o  564.164    378.070     0.00    3.56888   0.00
   5   5   1 o  62249.29   57746.86    0.00    3.46233   0.65
   7   1   1 o  3234.019   3010.740   180.00   3.46233   0.03
   6   4   2 o  386291.9   373666.7   180.00   3.30414   7.32
   5   5   3 o  307.299    227.236    180.00   3.21904   0.00
```

7	3	1	o	10998.896	8215.928	0.00	3.21904	0.20
8	0	0	o	41782.89	36753.22	0.00	3.09074	0.08
7	3	3	o	118821.44	118208.51	180.00	3.02076	0.95
6	4	4	o	1205.160	1127.315	180.00	2.99846	0.01
6	6	0	o	561565.7	556853.2	0.00	2.91398	2.08
8	2	2	o	138612.33	138104.13	0.00	2.91398	1.04
7	5	1	o	60962.93	59458.11	0.00	2.85511	0.86
5	5	5	o	2724553.8	2752775.3	180.00	2.85511	6.44
6	6	2	o	878.839	946.972	180.00	2.83626	0.01
8	4	0	o	408479.2	396755.1	0.00	2.76445	2.72
9	1	1	o	7092.707	6876.389	180.00	2.71403	0.04
7	5	3	o	111742.07	108192.84	0.00	2.71403	1.42
8	4	2	o	41495.60	42263.93	0.00	2.69782	0.51
6	6	4	o	631800.7	610932.2	180.00	2.63579	3.83
9	3	1	o	203393.19	201408.83	0.00	2.59198	2.37
8	4	4	o	194596.13	182522.64	0.00	2.52358	1.08
9	3	3	o	3.244	3.493	180.00	2.48505	0.00
7	7	1	o	959.373	990.941	180.00	2.48505	0.01
7	5	5	o	56168.47	58508.15	180.00	2.48505	0.32
8	6	2	o	4321.663	3616.721	0.00	2.42458	0.05
10	2	0	o	10773.963	9419.001	0.00	2.42458	0.05
9	5	1	o	3288.089	2957.728	180.00	2.39035	0.03
7	7	3	o	61740.97	54767.75	0.00	2.39035	0.31
10	2	2	o	19494.648	18412.025	180.00	2.37926	0.09
6	6	6	o	1106368.6	1052873.9	0.00	2.37926	1.72
9	5	3	o	632.480	684.372	0.00	2.30571	0.01
8	6	4	o	9720.134	11087.825	180.00	2.29575	0.08
10	4	2	o	57.070	51.145	0.00	2.25716	0.00
11	1	1	o	169162.31	162764.03	180.00	2.22946	0.72
7	7	5	o	141453.13	136473.22	0.00	2.22946	0.58
8	8	0	o	758913.8	751917.1	0.00	2.18549	1.43
11	3	1	o	43904.59	44986.38	180.00	2.16032	0.34
9	7	1	o	32829.555	33541.445	0.00	2.16032	0.24
8	8	2	o	1223.750	1152.545	180.00	2.15212	0.00
10	4	4	o	52341.29	49098.91	0.00	2.15212	0.19
9	5	5	o	48606.88	49946.82	180.00	2.16032	0.19
10	6	0	o	51947.61	46831.14	0.00	2.12023	0.20
8	6	6	o	454.619	404.585	0.00	2.12023	0.00
11	3	3	o	376379.0	362175.4	0.00	2.09723	1.28
9	7	3	o	72010.23	69104.04	180.00	2.09723	0.51
10	6	2	o	64396.45	61245.00	180.00	2.08972	0.44
12	0	0	o	336194.31	312159.34	180.00	2.06050	0.30
8	8	4	o	121725.68	113259.90	180.00	2.06050	0.42
11	5	1	o	4477.294	3664.092	0.00	2.03936	0.03
7	7	7	o	136527.89	115840.77	0.00	2.03936	0.15
12	2	2	o	5638.066	3534.009	0.00	2.00554	0.02
10	6	4	o	173.785	101.732	0.00	2.00554	0.00
11	5	3	o	2943.781	2339.571	0.00	1.98604	0.02
9	7	5	o	25069.404	19978.078	180.00	1.98604	0.16
12	4	0	o	8757.883	6835.030	0.00	1.95476	0.03
9	9	1	o	48279.93	45296.62	180.00	1.93669	0.13
12	4	2	o	97919.20	91637.00	0.00	1.93077	0.54
8	8	6	o	154213.39	144477.41	0.00	1.93077	0.43
10	8	2	o	200429.92	197482.97	0.00	1.90765	1.11
11	7	1	o	1237.303	1152.245	0.00	1.89084	0.01
13	1	1	o	42422.84	39246.10	180.00	1.89084	0.11

9	9	3	o	38344.04	35315.48	0.00	1.89084	0.10
11	5	5	o	122.273	92.197	0.00	1.89084	0.00
10	6	6	o	9607.492	8439.593	180.00	1.88534	0.03
12	4	4	o	34470.133	35323.72	0.00	1.86379	0.09
11	7	3	o	74051.99	68405.13	0.00	1.84810	0.37
13	3	1	o	14981.793	13784.277	180.00	1.84810	0.08
10	8	4	o	219.442	199.625	180.00	1.84296	0.00
9	7	7	o	102800.97	94954.18	0.00	1.84810	0.26
12	6	2	o	42732.95	43601.49	180.00	1.82282	0.21
9	9	5	o	203756.55	199889.98	0.00	1.80814	0.47
13	3	3	o	21774.100	21354.010	0.00	1.80814	0.05
13	5	1	o	112962.34	111098.02	180.00	1.77066	0.49
8	8	8	o	252939.66	231705.06	0.00	1.78444	0.19
11	7	5	o	117095.90	115163.31	180.00	1.77066	0.51
12	6	4	o	3840.611	3748.686	180.00	1.76614	0.02
10	10	0	o	1186337.9	1219962.6	180.00	1.74839	1.24
14	2	0	o	156259.84	160750.86	180.00	1.74839	0.33
11	9	1	o	2024.102	2230.506	180.00	1.73542	0.01
13	5	3	o	231.609	245.195	0.00	1.73542	0.00
10	8	6	o	9888.354	10168.797	0.00	1.74839	0.04
10	10	2	o	45676.39	53367.41	180.00	1.73116	0.09
14	2	2	o	973.882	1155.427	180.00	1.73116	0.00
12	8	0	o	36852.38	36692.40	0.00	1.71444	0.07
11	9	3	o	501166.7	494675.6	180.00	1.70220	1.89
12	8	2	o	13088.890	12779.273	180.00	1.69819	0.05
9	9	7	o	16810.318	16560.912	0.00	1.70220	0.03
10	10	4	o	57274.99	58236.26	180.00	1.68239	0.10
14	4	2	o	28788.221	29267.375	180.00	1.68239	0.11
13	7	1	o	9532.213	10620.989	0.00	1.67082	0.03
13	5	5	o	41837.66	46765.98	180.00	1.67082	0.07
12	6	6	o	38010.90	38646.25	180.00	1.68239	0.07
11	7	7	o	38274.44	43045.75	180.00	1.67082	0.07
12	8	4	o	77096.27	81139.45	180.00	1.65207	0.27
15	1	1	o	36810.55	40857.92	180.00	1.64112	0.06
11	9	5	o	7407.931	8208.342	0.00	1.64112	0.02
13	7	3	o	49370.54	54636.99	0.00	1.64112	0.16
14	4	4	o	598.600	631.971	0.00	1.63752	0.00
14	6	0	o	592.159	589.202	180.00	1.62334	0.00
10	8	8	o	18774.477	19901.682	0.00	1.63752	0.03
15	3	1	o	248.229	241.980	0.00	1.61294	0.00
14	6	2	o	144409.70	140435.14	0.00	1.60952	0.43
10	10	6	o	26167.838	25420.885	180.00	1.60952	0.04
11	11	1	o	588554.0	593161.5	0.00	1.58617	0.86
15	3	3	o	81880.30	82450.77	180.00	1.58617	0.12
13	7	5	o	28842.135	29044.510	0.00	1.58617	0.08
12	8	6	o	16587.229	16718.281	0.00	1.58292	0.05
14	6	4	o	48350.49	48531.30	0.00	1.57010	0.14
12	10	2	o	3586.154	3596.512	180.00	1.57010	0.01
9	9	9	o	3505.911	3527.594	0.00	1.58617	0.00
13	9	1	o	45686.09	43072.26	180.00	1.56069	0.13
15	5	1	o	7999.591	7550.922	0.00	1.56069	0.02
11	11	3	o	3165.579	2990.471	0.00	1.56069	0.00
11	9	7	o	65596.88	61795.19	0.00	1.56069	0.17
16	0	0	o	828674.4	814427.1	0.00	1.54537	0.26
15	5	3	o	123319.96	108394.67	0.00	1.53640	0.31
13	9	3	o	26594.984	23345.039	180.00	1.53640	0.07

12	10	4	o	4309.573	3831.480	0.00	1.53344	0.01
16	2	2	o	374.609	381.058	0.00	1.52178	0.00
14	8	2	o	38776.82	39598.82	180.00	1.52178	0.09
11	11	5	o	521878.9	505446.1	180.00	1.51320	0.60
10	10	8	o	169704.39	174175.30	0.00	1.52178	0.20
14	6	6	o	2920.200	2822.915	0.00	1.51038	0.00
13	7	7	o	11.518	10.844	180.00	1.51320	0.00
15	7	1	o	50945.56	46716.03	180.00	1.49103	0.11
16	4	0	o	77333.20	73096.81	0.00	1.49923	0.09
15	5	5	o	81614.59	74580.16	180.00	1.49103	0.09
13	9	5	o	57388.65	52492.48	180.00	1.49103	0.13
12	8	8	o	494254.4	467618.4	0.00	1.49923	0.55
16	4	2	o	14206.404	13359.854	180.00	1.48833	0.03
14	8	4	o	860.164	808.885	180.00	1.48833	0.00
15	7	3	o	23461.477	22698.574	0.00	1.46981	0.05
12	10	6	o	317551.19	311734.72	180.00	1.47766	0.65
12	12	0	o	1702925.6	1711386.8	0.00	1.45699	0.82
11	9	9	o	68896.24	66573.21	0.00	1.46981	0.07
17	1	1	o	221510.78	233166.20	180.00	1.44946	0.21
13	11	1	o	67641.84	71096.18	0.00	1.44946	0.13
16	4	4	o	9799.470	9833.723	180.00	1.45699	0.01
12	12	2	o	18944.119	19983.646	0.00	1.44698	0.02
11	11	7	o	56.778	60.883	180.00	1.44946	0.00
16	6	2	o	11132.253	10918.330	0.00	1.43717	0.02
14	10	0	o	112276.38	110230.02	180.00	1.43717	0.10
13	11	3	o	41338.06	39674.39	0.00	1.42994	0.07
17	3	1	o	1671.741	1600.563	180.00	1.42994	0.00
15	7	5	o	659.896	632.941	180.00	1.42994	0.00
14	8	6	o	293877.91	287957.34	180.00	1.43717	0.52
14	10	2	o	7932.486	7758.830	180.00	1.42755	0.01
13	9	7	o	226.950	218.773	0.00	1.42994	0.00
12	12	4	o	3511.321	3898.905	0.00	1.41813	0.00
17	3	3	o	5496.913	5595.740	180.00	1.41118	0.00
15	9	1	o	8014.131	8246.719	180.00	1.41118	0.01
10	10	10	o	520.717	504.211	0.00	1.42755	0.00
16	6	4	o	1769.401	1887.700	180.00	1.40889	0.00
12	10	8	o	2027.416	2160.596	180.00	1.40889	0.00
14	10	4	o	566.210	669.058	0.00	1.39983	0.00
15	9	3	o	6578.887	7159.144	180.00	1.39315	0.01
17	5	1	o	46011.93	49945.43	180.00	1.39315	0.07
13	11	5	o	518.987	572.082	180.00	1.39315	0.00
16	8	0	o	12251.143	14311.442	180.00	1.38222	0.01
16	8	2	o	108279.13	117963.30	0.00	1.37366	0.14
15	7	7	o	24805.799	27626.908	180.00	1.37579	0.02
17	5	3	o	3035.906	3380.308	0.00	1.37579	0.00
12	12	6	o	103352.05	112593.96	0.00	1.37366	0.07
11	11	9	o	9937.942	11127.765	0.00	1.37579	0.01
18	2	2	o	17789.557	18650.688	180.00	1.35701	0.01
14	8	8	o	845.819	919.935	180.00	1.37366	0.00
18	2	0	o	12364.775	12651.846	180.00	1.36526	0.01
16	6	6	o	1486288.9	1520859.3	0.00	1.36526	0.94
15	9	5	o	118226.71	122162.86	180.00	1.35906	0.14
16	8	4	o	104162.00	117671.38	180.00	1.34891	0.12
14	10	6	o	944.741	989.827	0.00	1.35701	0.00
17	7	1	o	348.555	364.948	0.00	1.34293	0.00
13	13	1	o	19576.393	20738.852	0.00	1.34293	0.01

13	9	9	o	286605.66	295429.28	180.00	1.35906	0.17
17	5	5	o	784554.1	832402.6	0.00	1.34293	0.44
13	11	7	o	18067.500	19119.020	0.00	1.34293	0.02
14	12	2	o	191727.59	174662.34	0.00	1.33313	0.20
18	4	2	o	7168.609	6463.324	0.00	1.33313	0.01
17	7	3	o	2293.484	2199.205	0.00	1.32736	0.00
13	13	3	o	223276.27	213201.53	0.00	1.32736	0.11
15	11	1	o	2463.248	2350.999	0.00	1.32736	0.00
12	10	10	o	131500.53	118121.41	0.00	1.33313	0.07
15	11	3	o	178333.75	166925.61	0.00	1.31232	0.16
16	8	6	o	1240.612	1179.504	0.00	1.31047	0.00
18	4	4	o	6116.802	5826.751	180.00	1.31047	0.00
14	12	4	o	46107.16	43929.48	0.00	1.31047	0.04
12	12	8	o	14982.764	15656.877	180.00	1.31790	0.01
15	9	7	o	66749.55	62189.97	0.00	1.31232	0.06
18	6	0	o	99471.66	93106.42	180.00	1.30317	0.04
16	10	2	o	30140.822	28266.037	180.00	1.30317	0.03
13	13	5	o	19683.123	19049.277	180.00	1.29778	0.01
17	7	5	o	264442.63	255109.38	0.00	1.29778	0.22
19	1	1	o	23332.027	22513.346	0.00	1.29778	0.01
18	6	2	o	59.935	58.835	0.00	1.29599	0.00
14	10	8	o	121891.67	113857.50	180.00	1.30317	0.10
17	9	1	o	54144.34	50686.28	180.00	1.28371	0.04
11	11	11	o	2163811.8	2084664.4	0.00	1.29778	0.29
15	11	5	o	8299.491	7735.267	180.00	1.28371	0.01
19	3	1	o	62091.47	57992.21	180.00	1.28371	0.05
16	10	4	o	719.605	674.904	0.00	1.28198	0.00
17	9	3	o	326337.69	263232.50	180.00	1.27009	0.21
13	11	9	o	86082.66	80309.21	180.00	1.28371	0.06
14	12	6	o	8439.897	7236.394	0.00	1.27514	0.01
18	6	4	o	39612.22	33808.477	0.00	1.27514	0.03
19	3	3	o	76668.57	61447.53	0.00	1.27009	0.02
19	5	1	o	369.765	344.176	180.00	1.25689	0.00
16	8	8	o	356204.5	300457.81	0.00	1.26179	0.11
15	9	9	o	2915.992	2738.802	180.00	1.25689	0.00
13	13	7	o	37929.34	35603.73	0.00	1.25689	0.01
17	7	7	o	2795.377	2596.885	180.00	1.25689	0.00
18	8	2	o	105413.38	92817.29	180.00	1.24885	0.06
16	10	6	o	49282.13	43362.96	180.00	1.24885	0.03
14	14	0	o	56654.85	49693.52	0.00	1.24885	0.01
12	12	10	o	11889.725	11589.223	0.00	1.25527	0.00
19	5	3	o	329660.38	285074.84	180.00	1.24410	0.16
17	9	5	o	3230.557	2788.012	0.00	1.24410	0.00
15	13	1	o	21562.121	18695.521	0.00	1.24410	0.01
14	14	2	o	16089.408	14578.457	0.00	1.24253	0.00
15	11	7	o	56463.73	48718.56	180.00	1.24410	0.03
16	12	0	o	48021.30	48337.83	180.00	1.23630	0.01
20	0	0	o	44953.63	45126.56	180.00	1.23630	0.00
14	10	10	o	26974.363	24356.494	180.00	1.24253	0.01
18	6	6	o	7325.387	6631.727	0.00	1.24253	0.00
15	13	3	o	9892.671	11042.923	0.00	1.23169	0.00
16	12	2	o	28239.414	31442.049	0.00	1.23016	0.01
18	8	4	o	26011.502	28977.229	180.00	1.23016	0.01
17	11	1	o	69744.89	62441.22	180.00	1.21964	0.03
14	14	4	o	9663.604	8972.976	0.00	1.22412	0.00
20	2	2	o	110663.41	102811.86	180.00	1.22412	0.02

14	12	8	o	11469.672	12803.827	180.00	1.23016	0.00
19	5	5	o	8412.190	7498.158	0.00	1.21964	0.00
19	7	1	o	50445.38	45183.18	0.00	1.21964	0.02
17	11	3	o	598.532	515.802	180.00	1.20794	0.00
13	11	11	o	61326.18	54117.60	180.00	1.21964	0.01
16	12	4	o	61296.66	58406.04	180.00	1.21229	0.02
20	4	0	o	26005.674	24757.482	180.00	1.21229	0.00
19	7	3	o	53266.30	45769.63	180.00	1.20794	0.02
15	13	5	o	131665.13	113750.61	0.00	1.20794	0.04
17	9	7	o	145044.69	124452.72	0.00	1.20794	0.05
13	13	9	o	3508.942	2935.886	0.00	1.20794	0.00
18	10	0	o	13716.390	14609.286	180.00	1.20080	0.00
20	4	2	o	4067.628	3687.606	0.00	1.20650	0.00
16	10	8	o	5609.600	5081.979	0.00	1.20650	0.00
14	14	6	o	717458.1	600475.3	0.00	1.19517	0.09
18	10	2	o	1692.234	1410.024	180.00	1.19517	0.00
18	8	6	o	316.377	342.785	0.00	1.20080	0.00
15	11	9	o	11982.727	10181.641	0.00	1.19657	0.00
17	11	5	o	481456.3	401733.6	180.00	1.18552	0.11
16	12	6	o	8304.665	7232.072	180.00	1.18416	0.00
20	4	4	o	170395.98	138994.92	180.00	1.18963	0.02
19	7	5	o	6910.327	5753.706	0.00	1.18552	0.00
20	6	2	o	231670.45	177855.14	180.00	1.17876	0.05
18	10	4	o	17542.842	13491.915	180.00	1.17876	0.00
12	12	12	o	935422.4	759426.0	180.00	1.18963	0.04
21	1	1	o	53561.55	45058.85	0.00	1.17477	0.00
15	13	7	o	922.944	799.577	0.00	1.17477	0.00
19	9	1	o	127686.20	108635.30	0.00	1.17477	0.02
14	12	10	o	44508.61	33706.738	0.00	1.17876	0.01
15	15	1	o	3108.938	3447.409	180.00	1.16430	0.00
16	14	2	o	93502.11	64313.80	0.00	1.15790	0.01
21	3	1	o	18419.744	20376.738	180.00	1.16430	0.00
19	9	3	o	36.502	40.519	180.00	1.16430	0.00
20	6	4	o	45466.36	45706.36	0.00	1.16301	0.01
17	13	1	o	8158.478	5374.149	0.00	1.15411	0.00
15	15	3	o	176652.67	118883.35	0.00	1.15411	0.01
17	9	9	o	49265.88	53744.16	180.00	1.16430	0.00
14	14	8	o	27850.945	18713.785	180.00	1.15790	0.00
18	8	8	o	29340.805	29082.957	0.00	1.16301	0.00
17	11	7	o	83024.19	55410.83	0.00	1.15411	0.01
19	7	7	o	31330.494	20718.205	0.00	1.15411	0.00
21	3	3	o	108062.04	72260.70	0.00	1.15411	0.01
18	10	6	o	5476.376	3904.839	180.00	1.15285	0.00
16	10	10	o	22189.854	14602.146	180.00	1.15790	0.00
17	13	3	o	9132.994	8235.295	0.00	1.14418	0.00
16	14	4	o	4438.928	4994.696	0.00	1.14296	0.00
13	13	11	o	717.233	478.039	180.00	1.15411	0.00
20	8	0	o	1679206.6	1085616.3	0.00	1.14787	0.07
16	12	8	o	6874.340	4363.304	0.00	1.14787	0.00
18	12	2	o	327.419	2714.001	0.00	1.13810	0.00
19	9	5	o	2748.420	2495.057	180.00	1.14418	0.00
21	5	1	o	76199.70	68238.70	180.00	1.14418	0.01
20	8	2	o	19.543	22.440	0.00	1.14296	0.00
15	15	5	o	-803.891	40038.31	0.00	1.13450	0.00
15	11	11	o	11700.014	10298.015	0.00	1.14418	0.00
20	6	6	o	3490.686	38361.32	0.00	1.13810	0.00

20	8	4	o	3498.571	27004.209	0.00	1.12858	0.00
15	13	9	o	-16.378	341.701	180.00	1.13450	0.00
21	5	3	o	-62.530	126.307	180.00	1.13450	0.00
19	11	1	o	-1258.680	16788.316	180.00	1.12507	0.00
17	13	5	o	-597.789	15054.224	180.00	1.12507	0.00
18	12	4	o	-0.080	0.162	0.00	1.12391	0.00
16	14	6	o	22197.105	26753.484	180.00	1.11929	0.00
22	2	0	o	50663.88	58115.84	0.00	1.11929	0.00
21	7	1	o	-368.948	8553.765	0.00	1.11587	0.00
21	5	5	o	-741.721	14937.479	180.00	1.11587	0.00
19	11	3	o	-63.792	58.150	0.00	1.11587	0.00
22	2	2	o	-287.174	9426.469	0.00	1.11473	0.00
18	10	8	o	12799.911	14425.771	180.00	1.11929	0.00
14	12	12	o	-14.056	844.357	180.00	1.12391	0.00
17	11	9	o	-1197.173	15363.178	180.00	1.11587	0.00
19	9	7	o	-607.341	4013.930	180.00	1.11587	0.00
14	14	10	o	-28.140	106.327	180.00	1.11473	0.00
15	15	7	o	40299.06	18202.596	180.00	1.10689	0.00
21	7	3	o	180554.30	82842.53	0.00	1.10689	0.00
20	8	6	o	425.791	118.075	0.00	1.10578	0.00
18	12	6	o	681185.0	63963.92	0.00	1.10138	0.00
20	10	2	o	1230333.8	116057.70	180.00	1.10138	0.01
22	4	2	o	688073.4	63884.79	0.00	1.10138	0.00
16	12	10	o	9815.265	3033.605	180.00	1.10578	0.00
16	16	0	o	82371.39	80040.11	180.00	1.09274	0.00
19	11	5	o	45258.73	11820.634	0.00	1.09812	0.00
17	13	7	o	265.571	51.817	180.00	1.09812	0.00
17	15	1	o	1709.729	321.645	0.00	1.08956	0.00
16	16	2	o	73093.09	8630.947	0.00	1.08850	0.00
22	6	0	o	8766049.	355220.4	180.00	1.08430	0.00
18	14	0	o	834721.6	34280.059	180.00	1.08430	0.00
21	7	5	o	5381.241	962.286	0.00	1.08956	0.00
16	14	8	o	173372.80	21407.588	0.00	1.08850	0.00
22	4	4	o	47698.55	5979.986	0.00	1.08850	0.00
20	10	4	o	227.413	29.743	180.00	1.08850	0.00
13	13	13	o	297302.22	81219.16	180.00	1.09812	0.00
21	9	1	o	1995581.5	149194.86	180.00	1.08119	0.00
17	15	3	o	1875438.3	139385.72	180.00	1.08119	0.00
22	6	2	o	42341.79	4235.038	0.00	1.08016	0.00
18	14	2	o	9776.321	940.382	180.00	1.08016	0.00
15	13	11	o	16395.539	2847.554	180.00	1.08956	0.00
16	16	4	o	433060.5	59735.41	0.00	1.07606	0.00
19	9	9	o	284.210	15.475	180.00	1.08119	0.00
23	1	1	o	1696311.8	195680.28	0.00	1.07301	0.01
19	13	1	o	561354.6	65903.45	180.00	1.07301	0.00
21	9	3	o	139849.14	15861.530	180.00	1.07301	0.00
20	8	8	o	39196.54	5444.754	180.00	1.07606	0.00
18	10	10	o	2646.611	261.264	0.00	1.08016	0.00
18	14	4	o	919977.4	139005.44	180.00	1.06800	0.01
20	10	6	o	154549.44	22925.746	180.00	1.06800	0.00
22	6	4	o	604165.7	90924.74	180.00	1.06800	0.01
15	15	9	o	256855.95	29540.145	0.00	1.07301	0.00
19	11	7	o	93140.04	10415.630	0.00	1.07301	0.00
18	12	8	o	21953.627	2912.239	0.00	1.07201	0.00
17	15	5	o	378714.1	86357.46	0.00	1.06502	0.01
23	3	1	o	160403.17	37078.34	0.00	1.06502	0.00

```
 19  13   3 o  19678.893  4532.001    0.00    1.06502   0.00
 17  11  11 o  44726.47   4405.381    0.00    1.07301   0.00
 20  12   0 o  24.446     0.671     180.00   1.06012   0.00
 21   7   7 o  60234.99   14003.844   0.00    1.06502   0.00
 17  13   9 o  246220.78  56211.24    0.00    1.06502   0.00
 14  14  12 o  675854.8   98658.60   180.00   1.06800   0.00
 23   3   3 o  581444.8   218985.36   0.00    1.05721   0.01
 21   9   5 o  116690.50  43935.98   180.00   1.05721   0.00
 16  16   6 o  80596.80   36324.39    0.00    1.05624   0.00
 20  12   2 o  6183.032   2744.461    0.00    1.05624   0.00
 22   8   2 o  59634.77   36488.45   180.00   1.05241   0.00
 16  12  12 o  131955.25  56027.30    0.00    1.06012   0.00
 23   5   1 o  126221.73  80398.55   180.00   1.04956   0.01
 19  13   5 o  64469.40   41115.32   180.00   1.04956   0.00
 22   6   6 o  213378.86  179758.97   0.00    1.04861   0.01
 18  14   6 o  10154.902  8459.910   180.00   1.04861   0.00
 16  14  10 o  774.459    510.503    180.00   1.05241   0.00
_reflns_number_total                373
_reflns_limit_h_min                 1
_reflns_limit_h_max                 23
_reflns_limit_k_min                 0
_reflns_limit_k_max                 16
_reflns_limit_l_min                 0
_reflns_limit_l_max                 13
_reflns_d_resolution_high           1.049
_reflns_d_resolution_low            14.276
#--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--#
```

Table S5 Representation of the occupation numbers received after Rietveld refinement of a Ru(1%)/Na-Y zeolite after adsorption-desorption cycles with and without H_2 during regeneration.

atom	site	no H_2	with H_2	
		ads/des*	des	ads
Ru	U	0.0	1.1	0.0
Ru	SI	1.6	0.0	1.3
Na	SII’	0.0	0.0	16.1
Na	SI’	16.1	15.3	15.2
Na	SIII	8.9	3.2	8.6
Na	SV	3.8	2.0	8.6
Na	SII	20.6	28.0	2.0
Na	sum	49.4	48.5	50.4
water		84.6	85.6	83.1

* patterns of ad- and desorbed samples refined with identical occupation numbers

Table S6 Average NO_x adsorption capacity of a Ru(3%)/Na-Y zeolite after 5 min. adsorption with and without SO_2 in lean or rich phases. The NO_x adsorption capacities were calculated over 10 stable and reversible NO_x cycles.

SO_2 in lean phase (ppm)	SO_2 in rich phase (ppm)	NO adsorption capacity (mg NO_x/g)
0	0	2.60 ± 0.03
0	50	2.70 ± 0.04
50	0	2.50 ± 0.04

Table S7 Rietveld parameters for the refined Ru(3%)/Na-Y structures after Ru ion exchange and after pretreatment.

Rietveld parameters	Ru(3%)/Na-Y Ion exchanged	Ru(3%)/Na-Y After pretreatment
R_p	0.0488	0.0472
R_{wp}	0.0645	0.0720
R_e	0.0559	0.0434
R_F	0.19703	0.18967
χ^2	1.15	1.67

Rietveld refinement was used to minimize $\sum w_i (I_{0,i} - I_{c,i})^2$ where $I_{0,i}$ and $I_{c,i}$ are the observed and calculated powder diffraction intensities for the i^{th} point respectively. Weights, w_i are $1/ I_{0,i}$. Weighted and unweighted profile R-factors are defined as $R_{wp} = \{[\sum w_i (I_{0,i} - I_{c,i})^2]/[\sum w_i (I_{0,i})^2]\}^{1/2}$ and $R_p = \sum| I_{0,i} - I_{c,i}|/\sum I_{0,i}$. The structure R-factor is defined as $R_F = \sum[(F_0-F_c)^2]/[\sum(F_0)^2]$. The expected R-factor (the statistically best possible value for R_{wp}) is defined as $R_e = [(N-P)/(\sum w_i I_{0,i}^2)]^{1/2}$ where N is the number of observed powder diffraction data points and P is the number of refined parameters. χ^2 was calculated from $(R_{wp}/R_e)^2$.

Table S8 Atomic coordinates, occupation parameters, isotropic type and displacements (Å^2) and symmetry multiplicity for Ru(3%)/Na-Y adsorbent after (a) Ru ion exchange and (b) after pretreatment at 450 °C for 1 h under a flow of 5% O_2, 3% H_2O and N_2.

(a)

Atom		x/a	y/b	z/c	Occupancy	thermal parameter type	u_{iso} or u_{equiv}	symmetry multiplicity
O	O1	0.89175(17)	0.10826(17)	0	1	Uiso	0.0045(24)	96
O	O2	0.96946(20)	0.07997(15)	0.07997(15)	1	Uiso	0.0426(17)	96
O	O3	1.00037(18)	0.14284(21)	1.00037(18)	1	Uiso	0.0102(27)	96
O	O4	0.93064(25)	0.17876(20)	0.07124(20)	1	Uiso	0.0372(32)	96
Si	T1	0.94664(9)	0.12646(9)	0.03651(9)	1	Uiso	0.01776	192
Na	SII'	-0.17581	-0.17581	-0.17581	0.2938(25)	Uiso	0.059(6)	32
Na	SII	0.26162	0.26162	0.26162	0.6083(33)	Uiso	0.295(14)	32
O	ow2	0.3379(5)	0.3379(5)	0.2393(5)	0.6083(33)	Uiso	0.251(13)	96
Na	SIII	0.375	0.375	0.5439(7)	0.6083(33)	Uiso	0.198(10)	48
Ru	Ru15	0.5	0.5	0.5	0.1480(18)	Uiso	0.02854	16
N	NH3	0.5	0.5	0.4086	0.1480(18)	Uiso	0.02792	96

(b)

Atom		x/a	y/b	z/c	Occupancy	thermal parameter type	u_{iso} or u_{equiv}	symmetry multiplicity
O	O1	0.89146(32)	0.10854(32)	0	1	Uiso	0.0702	96
O	O2	0.9670(4)	0.08008(31)	0.08008(31)	1	Uiso	0.01893	96
O	O3	0.99910(28)	0.1468(4)	0.99910(28)	1	Uiso	0.05696	96
O	O4	0.92874(32)	0.18016(25)	0.06984(25)	1	Uiso	0.00743	96
Si	T1	0.94445(21)	0.12702(18)	0.03481(17)	1	Uiso	0.03297	192
Na	SII	-0.2370(4)	-0.2370(4)	-0.2370(4)	0.61689	Uiso	0.025(8)	32
Na	SII*	-0.06774(27)	-0.06774(27)	-0.06774(27)	0.97804	Uiso	0.100(5)	32
O	ow	0.3046(11)	0.3046(11)	0.3046(11)	0.6169	Uiso	0.71(5)	32
Ru	Ru	0	0	0	0.09508	Uiso	0.272(33)	16

Table S9 Framework angles and bondlengths

NOx adsorbed on Ru1%NaY cycled with H2

Vector	Length /Å	Angle	Degrees /°	Angle	Degrees /°
T1_O1	1.6470(18)	T1_O1_T1	140.37(26)	O1_T1_O2	107.58(20)
T1_O2	1.6872(17)	T1_O2_T1	142.62(31)	O1_T1_O3	110.45(18)
T1_O3	1.6169(18)	T1_O3_T1	150.77(27)	O1_T1_O4	107.36(21)
T1_O4	1.6044(21)	T1_O4_T1	140.23(33)	O2_T1_O3	107.28(23)
Average:	1.639	Average:	143.5	O2_T1_O4	111.42(25)
				O3_T1_O4	112.66(23)
				Average:	109.5

Ru1%NaY cycled with H2

Vector	Length /Å	Angle	Degrees /°	Angle	Degrees /°
T1_O1	1.642(7)	T1_O1_T1	141.12(10)	O1_T1_O2	108.6(8)
T1_O2	1.623(6)	T1_O2_T1	145.52(11)	O1_T1_O3	109.1(7)
T1_O3	1.594(6)	T1_O3_T1	150.50(14)	O1_T1_O4	110.4(7)
T1_O4	1.654(7)	T1_O4_T1	143.64(10)	O2_T1_O3	110.0(9)
Average:	1.628	Average:	145.2	O2_T1_O4	109.9(8)
				O3_T1_O4	108.9(10)
				Average:	109.5

NOx adsorbed on Ru1%NaY cycled without H2

Vector	Length /Å	Angle	Degrees /°	Angle	Degrees /°
T1_O1	1.6592(28)	T1_O1_T1	137.2(4)	O1_T1_O2	112.60(31)
T1_O2	1.6412(23)	T1_O2_T1	144.9(5)	O1_T1_O3	114.83(22)
T1_O3	1.6472(28)	T1_O3_T1	143.9(4)	O1_T1_O4	106.23(27)
T1_O4	1.6360(25)	T1_O4_T1	140.5(4)	O2_T1_O3	106.13(33)
Average:	1.646	Average:	141.6	O2_T1_O4	106.86(30)
				O3_T1_O4	109.9(4)
				Average:	109.4

Ru1%NaY cycled without H2

Vector	Length /Å	Angle	Degrees /°	Angle	Degrees /°
T1_O1	1.6545(31)	T1_O1_T1	134.9(5)	O1_T1_O2	114.1(4)
T1_O2	1.6343(25)	T1_O2_T1	143.8(5)	O1_T1_O3	115.51(24)
T1_O3	1.6559(33)	T1_O3_T1	139.5(4)	O1_T1_O4	106.73(30)
T1_O4	1.6559(26)	T1_O4_T1	142.9(4)	O2_T1_O3	107.7(4)
Average:	1.650	Average:	140.3	O2_T1_O4	106.86(33)
				O3_T1_O4	105.2(4)
				Average:	109.4

References

1 R. Sounak and A. Baiker, *Chem. Rev.*, 2009, **109**, 4054-4091.

2 H. Mahzoul, J. F. Brilhac and P. Gilot, *Appl. Catal B*, 1999, **20**, 47-55.

3 L. Lietti, P. Forzatti, I. Nova and E. Tronconi, *J. Catal.*, 2001, **204**, 175-191.

4 T. Lesage, C. Verrier, P. Bazin, J. Saussey and M. Daturi, *Phys. Chem. Chem. Phys.*, 2003, **5**, 4435-4440.

5 K. Eguchi, M. Watabe, S. Ogata and H Arai, *J. Catal.*, 1996, **158**, 420-426.

6 F. Rodrigues, L. Juste, C. Potvin, J. F. Tempere, G. Blanchard and G. Djega-Mariadassou, **Catal. Lett.**, 2001, **72**, 59-64.

7 W. B. Li, R. T. Yang, K. Krist and J. R. Regalbuto, *Energy&Fuels*, 1997, **11**, 428-432.

8 I. Nova, L. Castoldi, L. Lietti, E. Tronconi, P. Forzatti, F. Prinetto and G. Ghiotti, *J. Catal.*, 2004, **222**, 377-388.

9 T. Lesage, J. Saussey, S. Malo, M. Hervieu, C. Hedouin, G. Blanchard and M. Daturi, *Appl. Catal. B*, 2007, **72**, 166-177.

10 K. Yamamoto, R. Kikuchi, T. Takeguchi and K. Eguchi, *J. Catal.*, 2006, **238**, 449-457.

11 T. J. Toops, D. B. Smith, W. S. Epling, J. E. Parks and W. P Patridge, *Appl. Catal. B*, 2005, **58**, 255-264.

12 W.J. Mortier, “Compilation of extra-framework sites in zeolites”, Butterworth, Guildford, 1982.

13 L. Zhou, K. Seff, *J. Phys. Chem. B*, 1999, **103**, 9512–9518.

14 W. T. Lim, S. M. Seo, G. H. K., H. S. Lee, K. Seff *J. Phys. Chem. C,* 2007, **111***,* 18294-18306.

15 D.H. Olson, *J. Phys. Chem.*, 1970, **74**, 2758-2764 (1970).

16 C. E. A. Kirschhock, B. Hunger, J. Martens, and P. A. Jacobs *J. Phys. Chem. B*, 2000, **104**, 439–448.

17 A. Sultana, R. Loenders, O. Monticelli, C. Kirschhock, P.A. Jacobs, J.A. Martens, *Angew. Chem. Int. Ed.* 2000, **39**, 2934-2937.

18 C.E.A. Kirschhock, A. Sultana, E. Godard, J.A. Martens, *Angew. Chem. Int. Ed.* 2004, **43**, 3722-3724.