Electronic Supplementary Information (ESI) for

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On the Structure of Superbasic $(MgO)_n$ sites solvated in a Faujasite Zeolite

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Contents

S1. Experimental Section.

ATR-FTIR spectroscopy. Infrared spectra in Attenuated Total Reflection (ATR-IR) were collected on loose powder on a Bruker Alpha spectrophotometer (2 cm^{-1} resolution, average on 256 scans), equipped with an internal reflection element in diamond and placed in the glove box. The spectrum intensity was corrected for the effective thickness value for the different incident wavelengths.

S2. MgOHY synthesis: FTIR spectra at intermediate temperatures.

The ATR-IR spectrum of the HY zeolite impregnated with $Mg(NO_3)_2 \cdot 6\ H_2O$ after activation at 80°C in vacuum is reported in Figure S1 (dark blue line). It is evident from the comparison with the HY spectrum (black line in Figure S1) the presence of additional bands at about 1350 cm^{-1} associated with nitrate group (see Figure S2 for the spectrum of the pure salt). The comparison of these bands with the ones present in the bulk $Mg(NO_3)_2 \cdot 6\ H_2O$ activated at the same temperature (blue line in Figure S2) suggests a different environments around the NO_3^{2-} groups in the two cases. The thermal decomposition of $Mg(NO_3)_2 \cdot 6\ H_2O$ after the impregnation of HY was followed by IR spectroscopy (see Figure S1). The comparison with the spectra recorded for the pure $Mg(NO_3)_2 \cdot 6\ H_2O$ after a treatment at the same temperatures (Figure S2), evidences that the nitrate encapsulated in the HY zeolite is significantly less stable. In fact, the bands corresponding to the nitrate start to decrease in intensity already at 200°C, whereas for the bulk compound no decomposition is observed for $T < 400$°C.

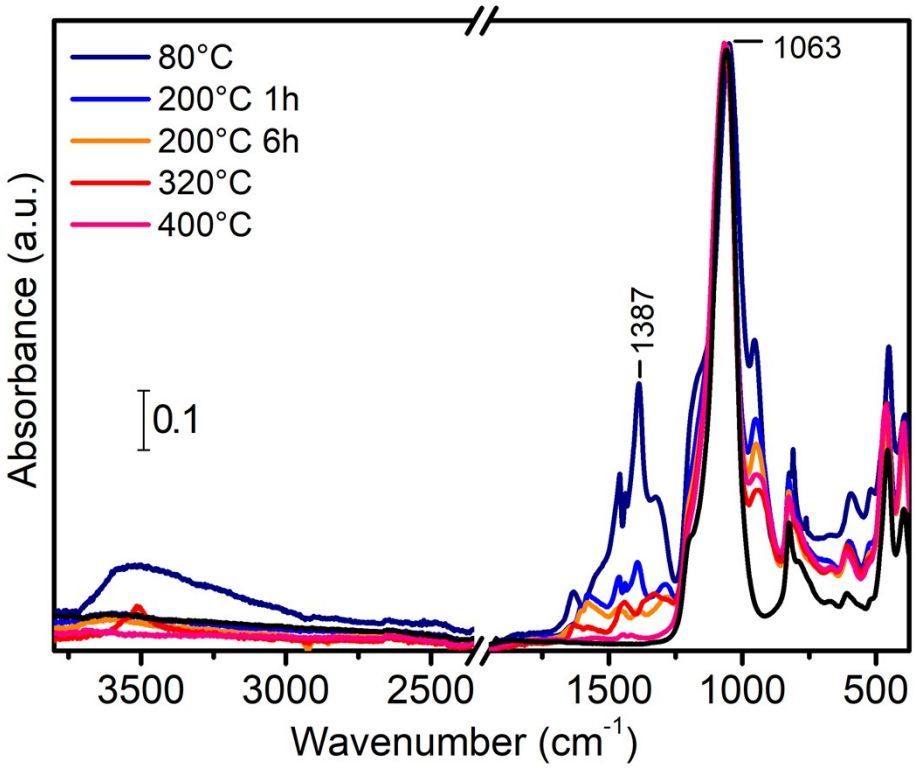

Figure S1. ATR-FTIR spectra of HY impregnated with $Mg(NO_3)_2 \cdot 6\ H_2O$ after activation in vacuum at increasing temperatures from 80°c to 400°C. At 200°C, the spectra obtained after 1 h (light blue line) and 6 h (orange line) are also reported. All the spectra have been recorded in a glove box and normalized at the intensity of the zeolite band at 1063 cm^{-1}. Spectrum of pristine HY activated at 400°C in vacuum is also reported (black curve).

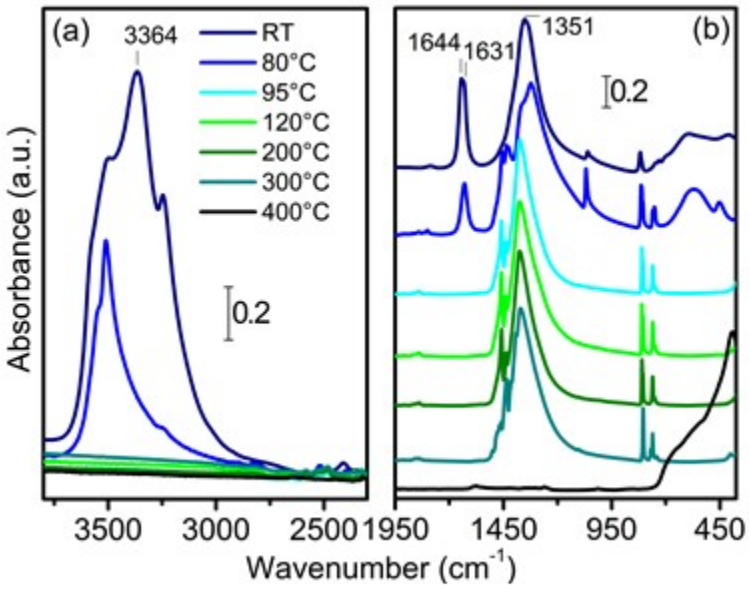

Figure S2. ATR-FTIR spectra of $Mg(NO_3)_2 \cdot 6\ H_2O$ after activation in vacuum at increasing temperatures from 25°C to 400°C recorded in a glove box. The spectra in the RT-300°C range have been normalized at the intensity of the band at 1351 cm^{-1}, whereas the spectrum recorded after the 400°C treatment has been normalized with respect to the intensity at 400 cm^{-1}.

S3. MgOHY synthesis: SEM images

Low resolution SEM images of the samples show that no appreciable change in gross sample morphology or particle aggregation is observed upon MgO addition (b and c). Under identical synthesis conditions, MgO adopts a disordered but recognizably different morphology (a)

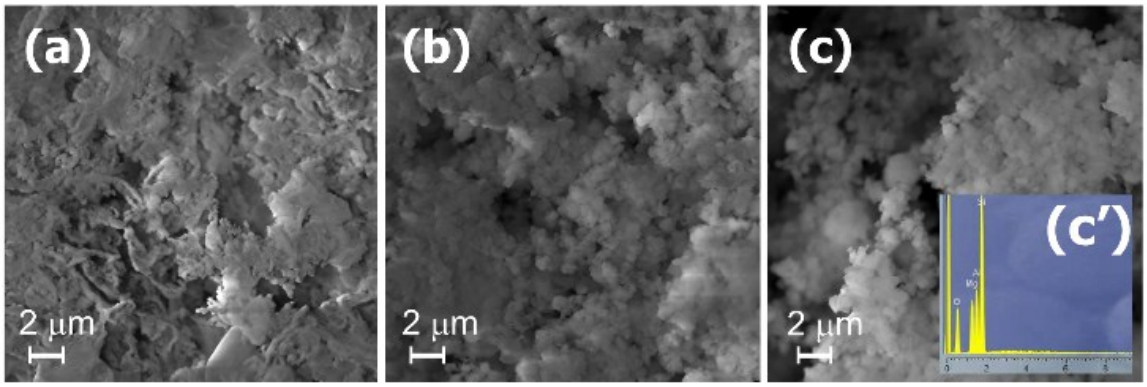

Figure S3. SEM images (secondary electrons signal) obtained for (a) MgO, (b) HY and (c) MgO/HY. In (c') one exemplicative EDS spectrum obtained for MgO/HY sample is reported.

S4. Additional XRPD data.

The patters recorded for the reference materials (MgO, $Mg(OH)_2$ and $Mg(NO_3)_2 \cdot 6\ H_2O$ are reported in Figure S4. Besides the MgO samples (synthetized as reported in the Experimental Section of the main text), the two other samples were used as received from Sigma-Aldrich.

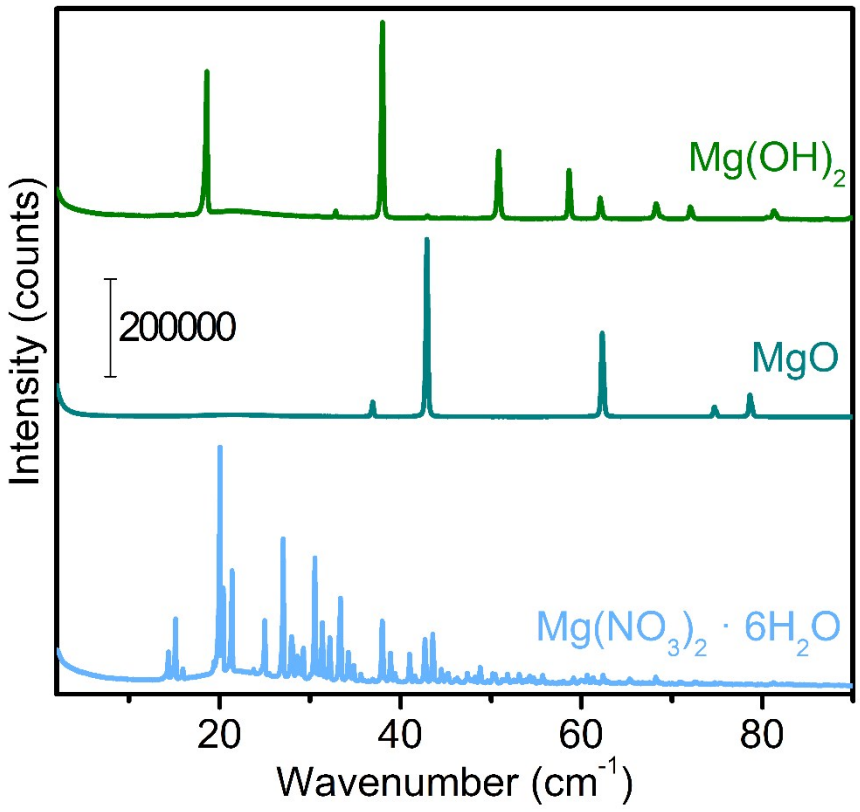

Figure S4. XRPD pattern of $Mg(NO_3)_2 \cdot 6\ H_2O$, $Mg(OH)_2$ and MgO recorded in air.

In Figure S5 it is reported a comparison between the pattern recorded for HY zeolite before (grey curve) and after the synthetic procedure to insert the MgO functionalities (blue curve). The two patterns are almost indistinguishable. It is evident from the comparison with the curves reported in Figure S4 that in the blue pattern are absent clear peaks associated to $Mg(OH)_2$ or MgO, suggesting a subnanometric dimensions of these species in the zeolite channels.

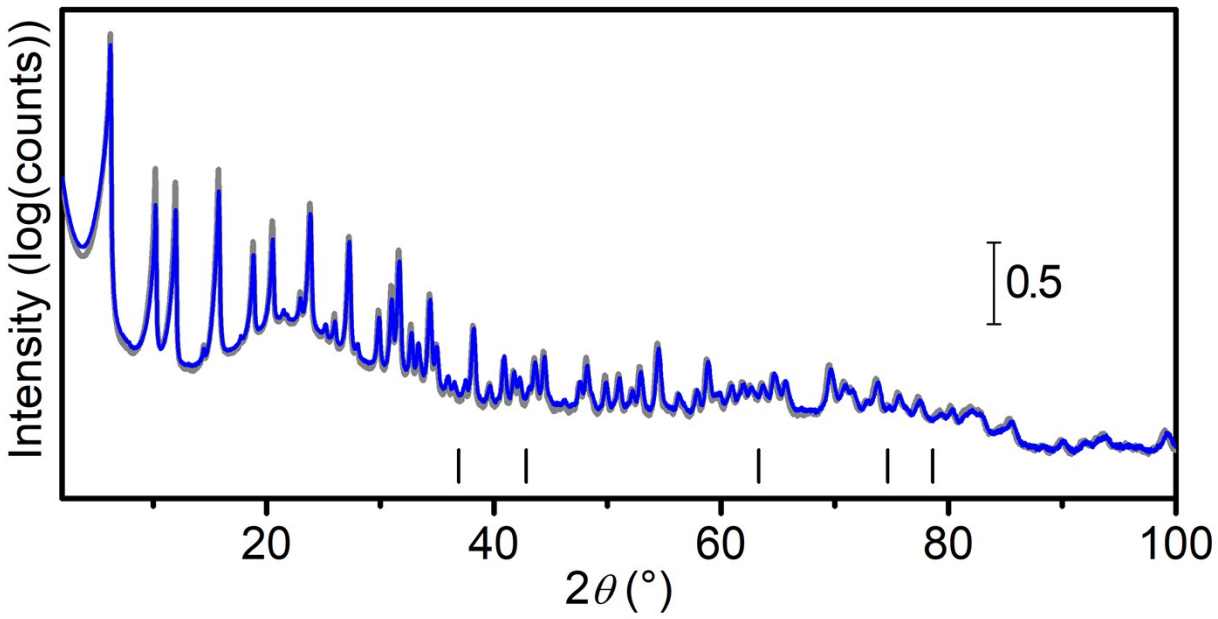

Figure S5. XRPD patterns of the HY (grey curve) and MgOHY (blue curve) samples in inert atmosphere after activation at 400°C overnight.

CIF file as obtained by Rietveld refinement of the MgOHY pattern.

The refined structures of the Y zeolite without and with MgO were deposited within the COD database (http://www.crystallography.net/cod/) with entry numbers 3000174 and 3000175.

S5. Modeling Results

The coordinates of the optimized structures displayed in Figs. 6, 7 and 8 are listed below (in CIF Format). Cut and paste to an ASCII text file with .cif extension for visualization with any molecular graphics program.

CIF file relative to the structure reported in Fig. 6a.

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CIF file relative to the structure reported in Fig. 6b.

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Si9	Si	-0.398659391338	-0.202705768734	-0.045917090829
Si10	Si	-0.747499890948	0.153575663786	-0.405841806607
Si11	Si	-0.570297897361	-0.379199447404	0.122009242584
Si12	Si	-0.910603894412	-0.031509869118	-0.221055038321
Si13	Si	-0.748393079520	-0.020982909728	0.120091752824
Si14	Si	-0.574886746240	0.153911973669	-0.225510270256
Si15	Si	-0.563562197340	-0.216693102494	-0.415477139665
Si16	Si	-0.923494235976	-0.200705973852	0.121776970499
Si17	Si	-0.390860034248	-0.383913525898	-0.230077823027
Si18	Si	-0.406595752244	-0.024380243921	-0.400347080328

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Si19   Si     -0.931962771618   0.160864236997   -0.043586099464
Si20   Si     -0.923361837224   -0.023378643591   0.118738470198
Si21   Si     -0.567728069618   -0.384105263384   -0.233612245748
Si22   Si     -0.741425462412   -0.374312820905   0.112654649728
Si23   Si     -0.925595040975   -0.206252786631   -0.047726631087
Si24   Si     -0.668068418408   0.224337859556   0.021783978993
Si25   Si     -0.324772397311   -0.127298385814   0.370191092104
Si26   Si     -0.493323973544   0.396689212173   -0.156973757899
Si27   Si     -0.139591083902   0.046607280063   0.199983796320
Si28   Si     -0.313748148637   0.049945248144   -0.163065431606
Si29   Si     -0.492547802038   -0.127175316155   0.194215891434
Si30   Si     -0.149153867398   0.219489219957   -0.143366310481
Si31   Si     -0.677165559955   0.407665037749   0.189819275260
Si32   Si     -0.675018214893   0.043870778868   0.368614027681
Si33   Si     -0.143029614870   -0.142049185563   0.022789073240
Si34   Si     -0.329018018928   0.397006596064   0.024941587889
Si35   Si     -0.504495268836   0.234038676772   0.375429787318
Si36   Si     0.678327481826   -0.132599414439   0.018253684487
Si37   Si     0.501344891868   0.403676972454   0.193859796487
Si38   Si     0.503653568761   0.222225915338   -0.152113480169
Si39   Si     0.320787044932   0.048127043316   0.194710222285
Si40   Si     0.678874332480   0.397844615437   -0.149846089811
Si41   Si     0.498692450337   -0.135836782251   0.375410420440
Si42   Si     0.336702341079   0.398400114156   0.016854503914
Si43   Si     0.852239756006   0.226406624403   0.022412101270
Si44   Si     0.601340608662   -0.202705768734   -0.045917090829
Si45   Si     0.252500109052   0.153575663786   -0.405841806607
Si46   Si     0.429702102639   -0.379199447404   0.122009242584
Si47   Si     0.089396105588   -0.031509869118   -0.221055038321
Si48   Si     0.251606920480   -0.020982909728   0.120091752824
Si49   Si     0.425113253760   0.153911973669   -0.225510270256
Si50   Si     0.436437802660   -0.216693102494   -0.415477139665
Si51   Si     0.076505764024   -0.200705973852   0.121776970499
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Si57   Si     0.258574537588   -0.374312820905   0.112654649728
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Si61   Si     0.506676026456   0.396689212173   -0.156973757899
Si62   Si     0.860408916098   0.046607280063   0.199983796320
Si63   Si     0.686251851363   0.049945248144   -0.163065431606
Si64   Si     0.507452197962   -0.127175316155   0.194215891434
Si65   Si     0.850846132602   0.219489219957   -0.143366310481
Si66   Si     0.322834440045   0.407665037749   0.189819275260
Si67   Si     0.324981785107   0.043870778868   0.368614027681
Si68   Si     0.856970385130   -0.142049185563   0.022789073240
Si69   Si     0.670981981073   0.397006596064   0.024941587889
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CIF file relative to the structure reported in Fig.7a

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H2   H     0.696089939633   0.280791839763   0.479296698308
H3   H     0.365130235099   0.823805071950   0.518676043430
H4   H     0.380031885795   0.992456424976   0.099927488789
H5   H     0.793981032289   0.820211861238   0.696660911172
H6   H     0.982049188189   0.724663950787   0.267338156747
H7   H     0.158519238117   0.187835345103   0.281896852454
H8   H     0.949623097515   0.015304379323   0.611635513099
H9   H     0.696272331351   0.286050644692   0.002873916821
H10  H     0.277966759121   0.655417534365   0.833819263747
H11  H     0.244029643505   0.996729568295   0.734119205216
H12  H     0.928092887599   0.566369975635   0.977403386545
H13  H     0.289007179214   0.018505184867   0.000392415547
O1   O     0.363470425480   0.761030433080   0.555113580467
O2   O     0.368094788595   0.576665423921   0.639797868894
O3   O     0.183014230110   0.692111330436   0.671376786284
O4   O     0.282424142291   0.665372042468   0.772749853676
O5   O     0.189712153498   0.809627560204   0.967678113956
O6   O     0.746221680223   0.220300192419   0.485484452185
O7   O     0.475573757212   0.999537886030   0.777448850802
O8   O     0.758107003099   0.005206945856   0.206465679189
O9   O     0.166469776103   0.997628907382   0.497531647828
O10  O     0.157279682336   0.507925411686   0.819305280801
O11  O     0.487975695210   0.784771031110   0.205154899462
O12  O     0.955148578657   0.800462300077   0.485631175648
O13  O     0.764437749958   0.505561160389   0.985097042577
O14  O     0.464952681498   0.221182335081   0.997795758430
O15  O     0.201053367107   0.784302902356   0.494989539421
O16  O     0.479395863837   0.997104225972   0.198769550588
O17  O     0.973515320222   0.507429685503   0.786369142752
O18  O     0.983206448449   0.780579701183   0.211630763629
O19  O     0.785966949276   0.999674947686   0.480516097616
O20  O     0.764440148878   0.513017445557   0.193353996248
O21  O     0.460344762707   0.243679577589   0.774704696469
O22  O     0.191808151804   0.495545841648   0.973305894703
O23  O     0.470871407264   0.813170304034   0.970387951422
O24  O     0.150665810358   0.979994258046   0.957091936416
O25  O     0.941250711285   0.180067600731   0.391793695665
O26  O     0.342168231110   0.981229835264   0.963341968636
O27  O     0.940837237069   0.393814367456   0.169063604869
O28  O     0.932567327445   0.197768015647   0.955394278348
O29  O     0.940535025363   0.961090732333   0.172754154486
O30  O     0.154657292401   0.957268640268   0.370825284468
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O35	O	0.356805192286	0.193998303861	0.956276724055
O36	O	0.019529170748	0.809802309943	0.024972822783
O37	O	0.804277885311	0.049614550153	0.600629035482
O38	O	0.566610032472	0.050897199676	0.813383498769
O39	O	0.791786037117	0.044476657702	0.030285376110
O40	O	0.009790021031	0.812471240126	0.594391155256
O41	O	0.569107088981	0.840213005605	0.023891787895
O42	O	0.996015208286	0.534506658645	0.948659536661
O43	O	0.584392458685	0.047155012064	0.023491687507
O44	O	0.812145943670	0.618236776885	0.014597087409
O45	O	0.117981617954	0.852135891856	0.123470280300
O46	O	0.838905828729	0.142953652279	0.337393912171
O47	O	0.334773310902	0.161755191380	0.839723128399
O48	O	0.110687453485	0.380916193242	0.137249090701
O49	O	0.103432532725	0.153721476083	0.841259110944
O50	O	0.832803476151	0.138313070506	0.131783804138
O51	O	0.122681122627	0.149752116592	0.337411310618
O52	O	0.109670669962	0.367787459768	0.852329334270
O53	O	0.341343202325	0.849332711731	0.127703467712
O54	O	0.118822915579	0.824904172853	0.378647701761
O55	O	0.825643725565	0.375217914359	0.131673183442
O56	O	0.338352155892	0.137514603229	0.132315874886
O57	O	0.118069231100	0.851348493320	0.840550682776
O58	O	0.823290735447	0.190834762612	0.601123295054
O59	O	0.831713851419	0.644028947823	0.140651104585
O60	O	0.615746502715	0.870535524809	0.845128964812
O61	O	0.829079445882	0.867506847973	0.144023537999
O62	O	0.822912932261	0.175629139381	0.841719901568
O63	O	0.830223371491	0.853907904385	0.636023013405
O64	O	0.616357682405	0.867052919829	0.126795834658
O65	O	0.091404272399	0.657577949897	0.859985952480
O66	O	0.100242979039	0.864998187049	0.650855973263
O67	O	0.598870112799	0.170639074739	0.853364397014
O68	O	0.828512306622	0.655272687446	0.832347979836
O69	O	0.292881089063	0.836482690167	0.014355776360
O70	O	0.800921527388	0.335249807146	0.306300433809
O71	O	0.283044488501	0.050634390022	0.810900063946
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O73	O	0.303039501204	0.021425481654	0.309179062049
O74	O	0.284194486956	0.341295671193	0.822755560390
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O76	O	0.022552216327	0.823501139665	0.305196479041
O77	O	0.794509159723	0.323901164618	0.038307576246
O78	O	0.286750437069	0.317754335467	0.040414803199
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O80	O	0.651431561335	0.188508937720	0.662727191386
O81	O	0.932077021290	0.673218877175	0.191533612073
O82	O	0.652990025825	0.985147676851	0.671836093477
O83	O	0.652815160583	0.975924282259	0.161289676026
O84	O	0.946521662312	0.184278319825	0.672085094544
O85	O	0.937892393229	0.677509790802	0.657130180302
O86	O	0.664575017955	0.692615506802	0.139101988516
O87	O	0.004314373773	0.648158392990	0.774531717365
O88	O	0.131549831071	0.986797077999	0.666245007379
O89	O	0.636401269167	0.192639757266	0.968611174508
O90	O	0.645210894035	0.696038470989	0.965351103647
O91	O	0.183970251728	0.004138356764	0.783028322312
O92	O	0.752791750627	0.231603066895	0.997865237361
O93	O	0.958191117543	0.499657010047	0.222126776441
O94	O	0.961694296866	0.234952405983	0.778316690927
O95	O	0.003727211930	0.211253330081	0.480499991852
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O98  O     0.987592220432   0.039321940834   0.614154821479
O99  O     0.010372773452   0.321144352343   0.306939974414
O100 O     0.003669103108   0.332632940806   0.816812070885
Mg1  Mg    0.303895829989   0.691613006403   0.552737091745
Mg2  Mg    0.392562846141   0.656202467402   0.660862856669
Mg3  Mg    0.151339745233   0.761285009544   0.761162846423
Mg4  Mg    0.255710395476   0.572302061253   0.742632814513
Al1  Al    0.839052052173   0.218011582098   0.370566868864
Al2  Al    0.365500218108   0.053983305149   0.834216055702
Al3  Al    0.190244305451   0.024192999063   0.381965624059
Al4  Al    0.373437660252   0.839260147781   0.211340882495
Al5  Al    0.759139353140   0.620186846733   0.949415717453
Al6  Al    0.752731811044   0.153280835804   0.953738989402
Al7  Al    0.112918846183   0.786617823288   0.605174738475
Al8  Al    0.936339654609   0.785007712131   0.132387633758
Al9  Al    0.096547257079   0.974183031017   0.780343098763
Al10 Al    0.761113160824   0.983824693921   0.592895753330
Al11 Al    0.583573521304   0.152846211039   0.776910569990
Al12 Al    0.933336294463   0.170410721494   0.592391015564
Al13 Al    0.114771860754   0.608404508037   0.969787931438
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Si2  Si    0.003110722963   0.400988370838   0.206974403479
Si3  Si    0.998473222125   0.230883130965   0.847096559356
Si4  Si    0.832927029652   0.032829323416   0.206578645829
Si5  Si    0.173094626465   0.392548143967   0.871477540772
Si6  Si    0.013546617468   0.856776019806   0.381619158509
Si7  Si    0.827823198338   0.401655915604   0.029109031820
Si8  Si    0.363092139030   0.218368615368   0.030937167253
Si9  Si    0.120510155707   0.786928745838   0.949769472552
Si10 Si    0.756967433072   0.157697557378   0.596397125213
Si11 Si    0.932380625446   0.609233794724   0.151817819189
Si12 Si    0.578507160069   0.978519173133   0.774401559388
Si13 Si    0.758967824126   0.972703167226   0.133045430268
Si14 Si    0.930055529802   0.160555349249   0.778183471155
Si15 Si    0.939668382231   0.783187402824   0.590461690200
Si16 Si    0.585016811685   0.795209570748   0.124520051544
Si17 Si    0.054912951244   0.593613485634   0.852068446318
Si18 Si    0.103061657223   0.972070881203   0.603308426648
Si19 Si    0.574879598520   0.157971890599   0.958047925108
Si20 Si    0.586924597483   0.970556852236   0.126362510329
Si21 Si    0.931731709236   0.619951562446   0.766816286770
Si22 Si    0.769434213152   0.617719770957   0.120084638596
Si23 Si    0.578911200125   0.802534707639   0.950748904970
Si24 Si    0.832917939590   0.221813712449   0.033449306663
Si25 Si    0.193024224786   0.847007134757   0.388282178670
Si26 Si    0.002944262793   0.398889368923   0.855438761373
Si27 Si    0.372403938454   0.033230756900   0.206279705906
Si28 Si    0.179539861118   0.050935203857   0.851161868154
Si29 Si    0.017157296118   0.859980961330   0.203386077646
Si30 Si    0.354687155565   0.232129932828   0.852017700724
Si31 Si    0.830851677277   0.404697105917   0.201545304942
Si32 Si    0.845337926934   0.036707817035   0.372892261446
Si33 Si    0.364728129286   0.860334349317   0.024600226459
Si34 Si    0.183748446034   0.392215036963   0.033483598104
Si35 Si    0.009677853347   0.219371012709   0.384439341251
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CIF file relative to the structure reported in Fig.7b

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H2   H     0.681866981614   0.273466557192   0.487545160549
H3   H     0.236284729071   0.719131318424   0.488240519943
H4   H     0.362235660946   0.002511535833   0.090624562246
H5   H     0.789132022499   0.816009398688   0.698826680371
H6   H     0.990176912800   0.722187138730   0.254358873097
H7   H     0.146872922171   0.193035229539   0.273526700815
H8   H     0.961737944113   0.004355473378   0.607145057282
H9   H     0.489412898917   0.463486169897   0.918208275993
H10  H     0.289213524409   0.555415697191   0.782236686627
H11  H     0.225451713224   0.025819893141   0.717028554893
H12  H     0.864231331957   0.632904921135   0.978166295706
H13  H     0.277106585994   0.017057863353   0.000798666530
O1   O     0.533223913791   0.394670218467   0.734826525119
O2   O     0.467877138066   0.450786867081   0.886653283170
O3   O     0.407903276425   0.323332699504   0.905281227488
O4   O     0.348330983897   0.507616439247   0.790511070911
O5   O     0.181919630002   0.784867772603   0.999402242289
O6   O     0.740183636894   0.221409442088   0.489928795752
O7   O     0.468977901219   0.990950303018   0.784064147546
O8   O     0.746748097162   0.009451381797   0.205033631865
O9   O     0.172448389199   0.013936269922   0.490256082500
O10  O     0.168943256161   0.499569246922   0.792567863365
O11  O     0.476676331932   0.783060171027   0.209848221352
O12  O     0.953724470014   0.797652225227   0.490399579889
O13  O     0.756464100233   0.504055533082   0.992752477757
O14  O     0.471190597784   0.181064901436   0.023512786491
O15  O     0.189563915429   0.780323852052   0.489061994179
O16  O     0.471451547104   0.003152214819   0.183189219009
O17  O     0.972381031512   0.503266354536   0.784370484788
O18  O     0.976508462800   0.784292555132   0.207277010846
O19  O     0.770932922593   0.998208433661   0.483886856694
O20  O     0.757480740237   0.510751548508   0.188115262299
O21  O     0.451397565268   0.244436763792   0.773422874079
O22  O     0.194680419780   0.490109506742   0.987954804163
O23  O     0.463862184676   0.812381725654   0.972727132292
O24  O     0.142703190420   0.968913615139   0.953100346900
O25  O     0.933653569949   0.181496515856   0.389607419629
O26  O     0.335332039316   0.979977642877   0.966898525877
O27  O     0.931623734963   0.395037485402   0.169125023013
O28  O     0.924455239650   0.195465942519   0.961429427023
O29  O     0.927132146223   0.964351455989   0.175688344216
O30  O     0.141805806074   0.961216146422   0.385534033439
O31  O     0.146562043399   0.379252514862   0.970369790488
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O32	O	0.354116096956	0.973780861541	0.156738891067
O33	O	0.940359506822	0.970731784715	0.360824987661
O34	O	0.931077759942	0.387711610100	0.961002881895
O35	O	0.352879705865	0.184660942118	0.955696441528
O36	O	0.008642758679	0.824149800731	0.018621915598
O37	O	0.788195704946	0.047989035750	0.605892119500
O38	O	0.561787421838	0.050420241572	0.809767270548
O39	O	0.762962208536	0.046647682509	0.032329442090
O40	O	0.999950733078	0.828214614815	0.592477118588
O41	O	0.562566260834	0.836275307938	0.028937026226
O42	O	0.995732944226	0.623485239646	0.812214873940
O43	O	0.610559750362	0.021504467382	0.019899364857
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O45	O	0.108112421757	0.861663860884	0.129644899508
O46	O	0.821972722565	0.144475388638	0.344922252813
O47	O	0.326945671232	0.157293008691	0.836763671534
O48	O	0.101319248589	0.372763992517	0.141197665831
O49	O	0.097247606584	0.149951499681	0.853378807557
O50	O	0.819905407244	0.143522022625	0.133867415644
O51	O	0.114374625223	0.155792025836	0.333701338801
O52	O	0.106036371023	0.360212489936	0.856289854758
O53	O	0.334259632974	0.845673730452	0.130148571295
O54	O	0.106973815293	0.840508730319	0.367517963689
O55	O	0.821349033795	0.368203094204	0.133067552769
O56	O	0.324765628191	0.148112750167	0.121482869297
O57	O	0.130890110450	0.856693144878	0.850254328341
O58	O	0.822483048364	0.179154675089	0.606658735224
O59	O	0.826098074775	0.643608882638	0.137037187002
O60	O	0.610893997658	0.868514689245	0.849892782613
O61	O	0.819212582225	0.869147258056	0.145754252372
O62	O	0.814737900176	0.174712491857	0.841690774645
O63	O	0.823905955442	0.850875996014	0.638045315358
O64	O	0.609973004372	0.854530953584	0.139617109598
O65	O	0.123367338171	0.635365875098	0.844893603012
O66	O	0.121888569755	0.864304253176	0.622991605236
O67	O	0.581666843793	0.170581368906	0.858830822201
O68	O	0.825653427903	0.650143122829	0.833083697751
O69	O	0.284665226937	0.836870460314	0.017034064753
O70	O	0.791601363869	0.335858004841	0.307800374103
O71	O	0.276294954410	0.041916626125	0.816308449671
O72	O	0.794933792834	0.030324688278	0.310727241370
O73	O	0.296071513994	0.027931250135	0.296985689727
O74	O	0.283747152035	0.333767674536	0.825656247155
O75	O	0.283254387118	0.826513039893	0.315466551491
O76	O	0.005940471534	0.825319041154	0.310146090831
O77	O	0.788645782595	0.325719098380	0.033348885373
O78	O	0.279026568053	0.319067795257	0.044433269722
O79	O	0.150119733521	0.678484047813	0.963878008753
O80	O	0.645081539073	0.194492033554	0.665596705691
O81	O	0.939009634353	0.677173523075	0.165728292662
O82	O	0.643557226926	0.977103289179	0.674565321970
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O84	O	0.939889717998	0.183854065933	0.673025923704
O85	O	0.947363438676	0.677976355586	0.664366620103
O86	O	0.653756280377	0.686338414617	0.143954713406
O87	O	0.142610688727	0.671394024603	0.672673846945
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O89	O	0.628052343479	0.200697948850	0.949323955001
O90	O	0.637719250874	0.694549353947	0.967261931818
O91	O	0.170732298648	0.022937289367	0.772044252382
O92	O	0.744007523132	0.230332621013	0.997045331069
O93	O	0.956710371654	0.503633444866	0.212416573035
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O95  O     0.995525761145   0.210648120471   0.481108449262
O96  O     0.001914859094   0.604275167726   0.033040976302
O97  O     0.986769621137   0.046755191688   0.822573293850
O98  O     0.994973129977   0.032696950822   0.610356271404
O99  O     0.994309803126   0.326469553016   0.311270713017
O100 O     0.995969385272   0.328607636060   0.820986784793
Mg1  Mg     0.541546959814   0.304865622018   0.870947022721
Mg2  Mg     0.468427679632   0.511550282489   0.758949701045
Mg3  Mg     0.400654347692   0.372983346778   0.781263935142
Mg4  Mg     0.334114400289   0.435443296798   0.939610708789
Al1  Al     0.828878054704   0.218359082265   0.374012253347
Al2  Al     0.358102176907   0.047383977172   0.836820610379
Al3  Al     0.187500496555   0.031810455325   0.380288496950
Al4  Al     0.364448710994   0.846365599363   0.208179618834
Al5  Al     0.749775557823   0.618641740863   0.944938718513
Al6  Al     0.744120571286   0.160726529892   0.954870372679
Al7  Al     0.107711858551   0.787750863999   0.604433678898
Al8  Al     0.929563562496   0.792745004082   0.124725281145
Al9  Al     0.093440875352   0.971451266086   0.781567295170
Al10 Al     0.750291479488   0.980449784962   0.595451769078
Al11 Al     0.567268927525   0.157889863450   0.774540860517
Al12 Al     0.933452214867   0.161077071619   0.595161379935
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Si1  Si     0.178189561071   0.862219341224   0.024458793822
Si2  Si     0.993064371467   0.401059933175   0.208760839707
Si3  Si     0.991369461972   0.224639602549   0.854887273304
Si4  Si     0.819657210565   0.038936394884   0.206296244211
Si5  Si     0.171183660939   0.394184508132   0.862870592880
Si6  Si     0.999879463656   0.860571428400   0.383210152548
Si7  Si     0.822433636240   0.397636917335   0.029499040829
Si8  Si     0.366703574093   0.225265331469   0.013406032856
Si9  Si     0.115324541621   0.786088523625   0.956272617510
Si10 Si     0.750321413798   0.154358447321   0.601447156078
Si11 Si     0.933745651345   0.609943908635   0.134968273500
Si12 Si     0.571676253814   0.974368424463   0.776830136281
Si13 Si     0.745256374039   0.973421678233   0.136407303837
Si14 Si     0.923565055114   0.155477011876   0.780847590136
Si15 Si     0.937386701209   0.785661468856   0.594163817137
Si16 Si     0.574669688324   0.790618403249   0.131116892326
Si17 Si     0.105774436337   0.611288771076   0.780681214161
Si18 Si     0.114196550850   0.969397624221   0.596139671611
Si19 Si     0.578718690081   0.132669899171   0.965595557175
Si20 Si     0.583481633640   0.960021947151   0.132333577367
Si21 Si     0.933764901805   0.612771488097   0.774814057764
Si22 Si     0.759049028635   0.616154157324   0.126226217778
Si23 Si     0.571053972401   0.801420231947   0.954187465492
Si24 Si     0.816844729840   0.223263986695   0.031289951067
Si25 Si     0.179358511932   0.860284421556   0.380606282444
Si26 Si     0.999343207969   0.394742253222   0.856064081340
Si27 Si     0.362380862651   0.044749326862   0.192184551617
Si28 Si     0.171258373140   0.047776800584   0.852551006635
Si29 Si     0.005258768369   0.864755794873   0.205113026560
Si30 Si     0.355016885127   0.220632164858   0.849756841929
Si31 Si     0.823889215248   0.400295902831   0.201627109634
Si32 Si     0.828664403476   0.038906479080   0.376311006501
Si33 Si     0.356919468161   0.859277556309   0.026732943183
Si34 Si     0.174048613645   0.390306158008   0.038616016813
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CIF file relative to the structure reported in Fig.7c

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loop_
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_atom_site_type_symbol
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_atom_site_fract_z
H1   H     0.247609499553   0.500765131268   0.155906774984
H2   H     0.683700211592   0.271945807653   0.479070254897
H3   H     0.244585642018   0.719275064851   0.477192276610
H4   H     0.366900022124   0.009400518101   0.082653002274
H5   H     0.792032137059   0.808903167677   0.683479812776
H6   H     0.952928807164   0.737495213134   0.265090552973
H7   H     0.144751754720   0.190772799024   0.268078458967
H8   H     0.960090068158   0.999229386399   0.597681289776
H9   H     0.613978850873   0.335894046888   0.007113524159
H10  H     0.478481202210   0.623910142868   0.971268285940
H11  H     0.213742130153   0.025295020484   0.709531553024
H12  H     0.867393451895   0.633829896783   0.967986145092
H13  H     0.296306413352   0.009971581929   0.985621356987
O1   O     0.553077910291   0.378222553586   0.996821879382
O2   O     0.297384388913   0.487893049377   0.101915871982
O3   O     0.419551018473   0.467083617279   0.934893211725
O4   O     0.476699220310   0.570864918959   0.970149402185
O5   O     0.200781874356   0.771105532950   0.981156965010
O6   O     0.739983824103   0.216989133428   0.477804510993
O7   O     0.470269072615   0.991831274609   0.765419809569
O8   O     0.759507171053   0.999469026999   0.187686641268
O9   O     0.169236376630   0.012429582467   0.486038909798
O10  O     0.177063660425   0.494119900616   0.775525311534
O11  O     0.482487172159   0.791908842157   0.191092187334
O12  O     0.960219046415   0.792194339373   0.475796129340
O13  O     0.764914279005   0.499935739171   0.979912555694
O14  O     0.458962129159   0.231881290639   0.970993285171
O15  O     0.192008110886   0.777502618118   0.477422398750
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O18  O     0.964617022830   0.786010192395   0.204333826550
O19  O     0.771771928296   0.990930503260   0.468627661802
O20  O     0.750831477305   0.509475232101   0.172684150520
O21  O     0.456742497273   0.220361068832   0.778328932223
O22  O     0.183464251350   0.491761276223   0.989655501450
O23  O     0.466595826858   0.794089312648   0.970258131235
O24  O     0.152408599753   0.954774365816   0.945295706467
O25  O     0.932976912272   0.181725817471   0.374524334799
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O27  O     0.927970446433   0.402683224057   0.158756597247
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O29	O	0.937662892985	0.965223432316	0.157682166629
O30	O	0.142194641859	0.958769649062	0.377444134241
O31	O	0.136084432804	0.392351017932	0.954909544196
O32	O	0.354384838959	0.978737035144	0.149658950417
O33	O	0.943372595415	0.967803523262	0.349030437788
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O35	O	0.354002186980	0.169687807037	0.959074551667
O36	O	0.027663517434	0.792782874905	0.021443106484
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O43	O	0.570056466158	0.055589554631	0.025563648403
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O46	O	0.821926994064	0.140766238122	0.333228741241
O47	O	0.324537667747	0.145261238534	0.842392986318
O48	O	0.107623160407	0.358010043180	0.128170802100
O49	O	0.093252428742	0.136588260144	0.857232799505
O50	O	0.819553742711	0.141576410074	0.119046589930
O51	O	0.112263734004	0.153393329818	0.327943554392
O52	O	0.107266550631	0.360825508487	0.840305234558
O53	O	0.338055027335	0.849209983106	0.118096023146
O54	O	0.111907145448	0.839847525500	0.352668251639
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O62	O	0.814586773262	0.181701480843	0.832785355941
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O67	O	0.603005650762	0.148026340324	0.843421612847
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O71	O	0.276104441319	0.040432488952	0.803134582764
O72	O	0.801333327196	0.025859996940	0.294236375545
O73	O	0.293121035893	0.027262284503	0.295457807263
O74	O	0.279655200284	0.317987600397	0.832347323392
O75	O	0.287457544511	0.828578732314	0.303702810397
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O77	O	0.785619072671	0.325084248728	0.025508802383
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O79	O	0.170907354202	0.659797440047	0.949188022393
O80	O	0.644905569319	0.175876519688	0.653427610158
O81	O	0.926582201746	0.673477045606	0.170672649333
O82	O	0.647769573423	0.965683065777	0.660846588425
O83	O	0.647573893828	0.961987899201	0.161292734020
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O87	O	0.144852270523	0.667532504681	0.660296082868
O88	O	0.126300117374	0.977137412615	0.664315319379
O89	O	0.617378997113	0.215012230577	0.940871301754
O90	O	0.642295210042	0.684808955263	0.958388709429

O91	O	0.165992185011	0.013932893527	0.769847199147
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O93	O	0.979237549692	0.498529934904	0.190867214837
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O96	O	0.993208943729	0.624941458505	0.020512176873
O97	O	0.979709993995	0.038384827471	0.818852513102
O98	O	0.992626665226	0.028204773138	0.601076195482
O99	O	0.996570786187	0.324504583391	0.298999470611
O100	O	0.002585543249	0.319662809088	0.807430495819
Mg1	Mg	0.498661908920	0.328837319857	0.960282279078
Mg2	Mg	0.426995382374	0.467684635285	0.057605417001
Mg3	Mg	0.525767307499	0.505416796865	0.890046433113
Mg4	Mg	0.279166189523	0.529983456358	0.981806531792
Al1	Al	0.826928025441	0.216283365779	0.362250799701
Al2	Al	0.359957275811	0.044763185430	0.823121540152
Al3	Al	0.183486071082	0.029909681124	0.376834854766
Al4	Al	0.368211656128	0.849219939691	0.196225297729
Al5	Al	0.756822061729	0.614896845841	0.932442838162
Al6	Al	0.736933578968	0.169732646471	0.942159407171
Al7	Al	0.109182132618	0.783139440806	0.593747199378
Al8	Al	0.932096174667	0.784749120806	0.117241187411
Al9	Al	0.087815050523	0.962832462032	0.779358601642
Al10	Al	0.752823959257	0.972672096492	0.580208808828
Al11	Al	0.571712313729	0.142616392623	0.766681374412
Al12	Al	0.928388556661	0.156109176044	0.586942142746
Al13	Al	0.105460066364	0.610209564943	0.945203791194
Si1	Si	0.187168294608	0.847825051592	0.015103308296
Si2	Si	0.000418665139	0.396521685510	0.194430414952
Si3	Si	0.993606563907	0.217663773645	0.843340589665
Si4	Si	0.827315133250	0.034798206906	0.189785362544
Si5	Si	0.174641858805	0.390747174094	0.849630561103
Si6	Si	0.004615604829	0.858123882943	0.370096676839
Si7	Si	0.828113136280	0.392704849095	0.017854798181
Si8	Si	0.358059475121	0.214449651117	0.016023777803
Si9	Si	0.129036176082	0.769765296036	0.947021640851
Si10	Si	0.750356437658	0.144062010945	0.589439057132
Si11	Si	0.933375415854	0.607659680928	0.129257253188
Si12	Si	0.574825549616	0.965088106918	0.762618668635
Si13	Si	0.751651472841	0.973022710743	0.115609266805
Si14	Si	0.923444265392	0.149599920438	0.772259774895
Si15	Si	0.941339796943	0.778907125324	0.580996444350
Si16	Si	0.579785819498	0.797105667361	0.109323124943
Si17	Si	0.110951878103	0.603404157853	0.766846584309
Si18	Si	0.110604181233	0.965008849066	0.590768872943
Si19	Si	0.571581810565	0.153848514910	0.940154697325
Si20	Si	0.580142845893	0.966543099803	0.121596054043
Si21	Si	0.936648178878	0.606035218163	0.760915255498
Si22	Si	0.759120906992	0.612933908740	0.116120555082
Si23	Si	0.573808935136	0.791681753407	0.941449281607
Si24	Si	0.811962847317	0.225313872566	0.019766586328
Si25	Si	0.182590774605	0.858450410685	0.369754875248
Si26	Si	0.002732509840	0.388690363563	0.842031196388
Si27	Si	0.367810062144	0.035338835008	0.196144938237
Si28	Si	0.172822868175	0.039241386183	0.846500365398
Si29	Si	0.007593021928	0.860646905661	0.193138279932
Si30	Si	0.356966906077	0.212574075030	0.846827458745
Si31	Si	0.823701982505	0.399924500851	0.189816855494
Si32	Si	0.831217374406	0.034602136899	0.363054647985
Si33	Si	0.361264807669	0.850993211163	0.018860833169
Si34	Si	0.175010775776	0.390347000893	0.021792349318
Si35	Si	0.997298059981	0.220280252446	0.374983441780

CIF file relative to the structure reported in Fig. 8a

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H2   H     0.691753200821   0.855933987379   0.894910994822
H3   H     0.990510501263   0.506481885947   0.945684627251
H4   H     0.268988889956   0.773186661565   0.372516532146
H5   H     0.524769893979   0.583113262592   0.149875317707
H6   H     0.782273331333   0.770673885105   0.445344183719
H7   H     0.776922833936   0.765571716897   0.889185904487
H8   H     0.695109751805   0.030428550867   0.084289079262
H9   H     0.208666238592   0.060259203067   0.438040244789
H10  H     0.780984241886   0.218699060466   0.433261050252
H11  H     0.691621774444   0.855943494732   0.444529528818
H12  H     0.690622546622   0.231517742566   0.513155747302
H13  H     0.252994587993   0.790377672655   0.457079556474
C1   C     0.618377694459   0.625834589882   0.284051838527
O1   O     0.910350454873   0.570836323412   0.453827312657
O2   O     0.480356633936   0.980451143600   0.949761282435
O3   O     0.211414862173   0.786000167010   0.238218416139
O4   O     0.496556037396   0.795081850263   0.642457512575
O5   O     0.913242515746   0.779219904307   0.952716944098
O6   O     0.916722212116   0.275600013452   0.245396482774
O7   O     0.221762299613   0.577990655961   0.651018412699
O8   O     0.698856718230   0.572043816923   0.944396225320
O9   O     0.520296336206   0.272793467786   0.439467746762
O10  O     0.204818081442   0.008894442001   0.434295121648
O11  O     0.932045341523   0.559302178036   0.946934894573
O12  O     0.214241011519   0.757246764534   0.659593823472
O13  O     0.705010343907   0.275059062638   0.245663496981
O14  O     0.720949725310   0.551667248635   0.670017217504
O15  O     0.516465456223   0.772608985724   0.935499565906
O16  O     0.488269248930   0.284487044411   0.635716080631
O17  O     0.201746747463   0.983950571454   0.247015673315
O18  O     0.911458947468   0.273412418913   0.455775336496
O19  O     0.206944488204   0.564988215882   0.446334912011
O20  O     0.897154105941   0.743366625151   0.413454387754
O21  O     0.665352187975   0.964544837069   0.849568025417
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O23	O	0.664571822615	0.179276715015	0.625847549410
O24	O	0.662917798998	0.976393790085	0.405861334550
O25	O	0.671405965640	0.730149275771	0.646109115349
O26	O	0.887181165330	0.739695645502	0.835643203135
O27	O	0.898340060969	0.151906728133	0.417071825180
O28	O	0.086356826896	0.761199702557	0.611893073246
O29	O	0.682996812083	0.742496686411	0.809048773420
O30	O	0.683958982740	0.137334327974	0.417090375909
O31	O	0.085401547502	0.964941249336	0.425621155059
O32	O	0.729810984763	0.598123866121	0.490103291225
O33	O	0.537580485500	0.804705457425	0.069998375801
O34	O	0.342090830296	0.792641517846	0.266481415868
O35	O	0.536992858556	0.803022016130	0.470885770459
O36	O	0.732683255751	0.596208636005	0.061014142941
O37	O	0.323893926423	0.599263044276	0.472281819321
O38	O	0.738405975538	0.397054884640	0.260739442150
O39	O	0.304757444708	0.825589881575	0.485876913158
O40	O	0.544024107071	0.406882016486	0.467445382410
O41	O	0.849653970660	0.635785623397	0.587707682255
O42	O	0.570986391295	0.918156126462	0.796588557775
O43	O	0.063563790926	0.909419535086	0.339252935463
O44	O	0.844640345987	0.131231461519	0.588913128770
O45	O	0.841026731662	0.920754230955	0.316471562450
O46	O	0.583593665405	0.912033015062	0.584012469156
O47	O	0.844977361914	0.929204455697	0.806114418833
O48	O	0.850544212069	0.142630413873	0.302378050448
O49	O	0.074113175155	0.622803525217	0.589421277825
O50	O	0.849743247176	0.617244417281	0.828574349589
O51	O	0.573618640034	0.134429174533	0.586866175335
O52	O	0.094314582775	0.917493464606	0.588386472379
O53	O	0.819106856389	0.655977485316	0.329764210499
O54	O	0.553761003434	0.941158294572	0.077834452140
O55	O	0.564868785121	0.395034174168	0.612111595068
O56	O	0.343527236591	0.628093625067	0.302934631568
O57	O	0.557103055184	0.638599312190	0.609477118770
O58	O	0.555608604958	0.957003072104	0.300047884017
O59	O	0.563379538767	0.618359681031	0.093403840524
O60	O	0.361695460505	0.644174818332	0.568887677311
O61	O	0.826746085690	0.412982670098	0.319169034037
O62	O	0.822247937930	0.657426945660	0.081445724880
O63	O	0.348106991247	0.926248117250	0.307749370959
O64	O	0.568573165903	0.430717336161	0.288784784430
O65	O	0.029994183481	0.593928119419	0.483230592150
O66	O	0.526020444881	0.112815870311	0.763772567573
O67	O	0.021619923852	0.823022676455	0.266878200578
O68	O	0.530460988929	0.812474862035	0.764082517209
O69	O	0.036096259955	0.803416219419	0.761106575557
O70	O	0.029158878331	0.097994899104	0.276275031505
O71	O	0.031611401567	0.601284450894	0.772558514870
O72	O	0.760904501090	0.589005220756	0.768112758579
O73	O	0.529202270233	0.098858236022	0.490689220732
O74	O	0.025586835603	0.100194996743	0.490563514728
O75	O	0.878461257780	0.466824440494	0.415476627750
O76	O	0.381647343728	0.951611202141	0.118479843717
O77	O	0.667566807229	0.445746861026	0.638017399398
O78	O	0.386763397439	0.742559265114	0.127493575002
O79	O	0.386639759638	0.758859658413	0.609199957697
O80	O	0.669820830266	0.979034876328	0.122489100115
O81	O	0.688444546119	0.445616586226	0.117437465831
O82	O	0.395523773278	0.464897978627	0.605800134557
O83	O	0.887093224091	0.450716936666	0.133197858010
O84	O	0.874921307508	0.742953252895	0.129736461664

O85	O	0.374024338674	0.960489061818	0.424750442922
O86	O	0.383330238544	0.454690512679	0.422834047477
O87	O	0.902538015482	0.797121061600	0.239177934328
O88	O	0.487180707555	0.988077823083	0.469812711927
O89	O	0.725618739211	0.274192822824	0.647731061883
O90	O	0.715181566651	0.993703733845	0.231354748927
O91	O	0.714722287704	0.006751699057	0.938795930839
O92	O	0.722336301779	0.407175814449	0.485208083890
O93	O	0.715232262859	0.824109360469	0.266818414095
O94	O	0.730700141822	0.820271716892	0.067896667107
O95	O	0.731416899364	0.105364150330	0.764810283454
O96	O	0.747441238817	0.102800883122	0.264769521416
O97	O	0.711212380618	0.785726156653	0.928401279476
O98	O	0.717194983041	0.790347169874	0.449506752002
O99	O	0.219585096974	0.788255150879	0.428198369973
O100	O	0.717470311083	0.262979508084	0.445856958980
O101	O	0.619973587801	0.560966503626	0.351408132308
O102	O	0.615932330515	0.691863992536	0.217706078419
Mg1	Mg	0.682358839405	0.739282011758	0.062889746470
Mg2	Mg	0.678437013383	0.733630974524	0.408847914664
Mg3	Mg	0.083965994080	0.814325353369	0.477962989313
Mg4	Mg	0.679807020295	0.402955831281	0.401374022132
Al1	Al	0.558885503117	0.996819604792	0.835232277308
Al2	Al	0.097557801112	0.813277197541	0.306374747551
Al3	Al	0.922975447277	0.817456668026	0.837810004954
Al4	Al	0.105830072313	0.632907695441	0.660113192359
Al5	Al	0.498766327587	0.389844057141	0.405353883604
Al6	Al	0.488087408172	0.930271372790	0.416370650941
Al7	Al	0.847699412270	0.561775087139	0.060419724723
Al8	Al	0.666464590544	0.554439837574	0.610341993253
Al9	Al	0.839733629432	0.753403005941	0.232836592277
Al10	Al	0.492165246536	0.748282440302	0.048312055079
Al11	Al	0.315290063410	0.910120309496	0.241412584849
Al12	Al	0.664899354180	0.939326150594	0.046160558568
Al13	Al	0.843565406074	0.390090252201	0.420382816639
Si1	Si	0.922890007769	0.633885019172	0.485937176362
Si2	Si	0.741486186232	0.170861097172	0.659526672361
Si3	Si	0.742305017455	0.998874664271	0.304611452183
Si4	Si	0.569699469687	0.811479834797	0.660336890241
Si5	Si	0.923740357128	0.166805451513	0.309045570166
Si6	Si	0.746607104213	0.633458674123	0.835522696958
Si7	Si	0.573905580849	0.164303316369	0.483814090263
Si8	Si	0.094664872233	0.997282282584	0.490006871123
Si9	Si	0.839143696821	0.567450452142	0.422714698204
Si10	Si	0.496958490675	0.919817823620	0.047378327128
Si11	Si	0.668734182415	0.383191974210	0.598273286346
Si12	Si	0.319273377411	0.737462970788	0.231650859652
Si13	Si	0.495183732543	0.746461201365	0.585977087026
Si14	Si	0.661657473777	0.936666398607	0.237572018907
Si15	Si	0.676807993392	0.553947447045	0.049862729235
Si16	Si	0.323250099632	0.571043912465	0.575970139207
Si17	Si	0.849139355959	0.383758632757	0.236258393857
Si18	Si	0.843293380111	0.751589550469	0.055154688907
Si19	Si	0.321417696587	0.923312014200	0.408006252922
Si20	Si	0.319424244146	0.741678158350	0.586539623478
Si21	Si	0.671922907000	0.384757430212	0.228845659360
Si22	Si	0.497098775719	0.388475839395	0.580590501377
Si23	Si	0.314358211928	0.560078417712	0.411750194733
Si24	Si	0.561360625131	0.995847542616	0.490015632514
Si25	Si	0.926855353724	0.636741600105	0.833977394492
Si26	Si	0.745200793933	0.165232591102	0.308963371665
Si27	Si	0.105590268103	0.806972673680	0.660360213490
Si28	Si	0.919597361721	0.819829746776	0.304542920001

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Si30 Si    0.097410785641   0.991308762799   0.313823427952
Si31 Si    0.558998216742   0.175388465761   0.658393777244
Si32 Si    0.573061291834   0.814926121904   0.826956976628
Si33 Si    0.099360637775   0.625825611070   0.488195511586
Si34 Si    0.917885082394   0.168680274650   0.489183278990
Si35 Si    0.741740260521   0.998833813731   0.840281953164
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CIF file relative to the structure reported in Fig. 8b

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H2   H     0.698748546698   0.284134640560   0.470094530767
H3   H     0.280635984780   0.889642477850   0.514383384070
H4   H     0.384096436377   0.997787504788   0.088389588362
H5   H     0.796457705692   0.822722220870   0.686339011271
H6   H     0.983609195364   0.728242361920   0.258439799667
H7   H     0.156556100536   0.195653927832   0.273275336792
H8   H     0.946787933790   0.024135826153   0.594017072371
H9   H     0.705957327256   0.290832049738   0.987276067164
H10  H     0.269844862299   0.648563403821   0.836709051937
H11  H     0.251842121260   0.991225009288   0.720502906737
H12  H     0.934534043861   0.568305494659   0.967525265672
H13  H     0.292274917806   0.018409215083   0.990840870384
C1   C     0.368711842081   0.838378284736   0.581307064748
O1   O     0.323470077376   0.826675465622   0.539123927437
O2   O     0.374901190278   0.599523581768   0.622437328329
O3   O     0.186991386037   0.699406228349   0.659841762242
O4   O     0.281885541558   0.656539493107   0.773627636578
O5   O     0.194313641889   0.807797186069   0.958684627913
O6   O     0.747294298805   0.222583459121   0.477327260562
O7   O     0.481041298124   0.003816267488   0.769009129539
O8   O     0.761406355842   0.006134783266   0.199333866440
O9   O     0.169193830557   0.994648509072   0.489579514766
O10  O     0.165965458569   0.510547269857   0.807568743913
O11  O     0.488985686492   0.789867825915   0.196047443743
O12  O     0.957883089722   0.800961469049   0.475387534249
O13  O     0.773314109321   0.506089523501   0.977098007992
O14  O     0.467642100575   0.227021390842   0.988655276344
O15  O     0.203097819379   0.796461222243   0.484943207959
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O16	O	0.479259342632	0.001888011870	0.190771454634
O17	O	0.972945088138	0.508083893477	0.776400992734
O18	O	0.986138189678	0.783465782368	0.202129821489
O19	O	0.789529421062	0.002561924287	0.471857147572
O20	O	0.756290122176	0.513599477875	0.184286183616
O21	O	0.465875843892	0.241236796151	0.765532571052
O22	O	0.175950785922	0.498448192264	0.979966508883
O23	O	0.475050723132	0.812205250725	0.963855575090
O24	O	0.157650181721	0.979201382499	0.943139827368
O25	O	0.942105558564	0.182958150682	0.386178802563
O26	O	0.345656583959	0.981379014167	0.953655613370
O27	O	0.936154500278	0.406892248307	0.160761213920
O28	O	0.940743857811	0.196086585610	0.947246663586
O29	O	0.944117556639	0.963420271188	0.164084374270
O30	O	0.152429439875	0.966332728153	0.358451857302
O31	O	0.159834103477	0.362045028736	0.967117107814
O32	O	0.363444293829	0.973993341345	0.155983626604
O33	O	0.960444525752	0.969366105242	0.348022826290
O34	O	0.945625194312	0.380588400880	0.951731689207
O35	O	0.363705070596	0.196422043054	0.944986840068
O36	O	0.021535434010	0.815649206889	0.015572378921
O37	O	0.809364056328	0.052683459912	0.590707808642
O38	O	0.576155419539	0.047097897257	0.808972912085
O39	O	0.792857120192	0.046649050690	0.023830721281
O40	O	0.013125990123	0.811417392466	0.583949828682
O41	O	0.572872867219	0.841926996736	0.015205837832
O42	O	0.000916003886	0.535707579531	0.935903616100
O43	O	0.585487383838	0.052214162883	0.016481536018
O44	O	0.816048840153	0.621049265564	0.009486300917
O45	O	0.121385726908	0.855077275315	0.111814115747
O46	O	0.843588827423	0.144519071098	0.328404419318
O47	O	0.335970174308	0.162853537633	0.832605422530
O48	O	0.114387459983	0.361691432256	0.133480929284
O49	O	0.109564963148	0.152440694339	0.827546118825
O50	O	0.836107966392	0.140057867277	0.122657636089
O51	O	0.121737585181	0.157959707453	0.330865741352
O52	O	0.115288011688	0.374973964480	0.835398471172
O53	O	0.343191960947	0.852238629018	0.118761793304
O54	O	0.121256441461	0.827159918867	0.372506048874
O55	O	0.834284463349	0.371541000568	0.122808368754
O56	O	0.340191805885	0.143998317608	0.121637440836
O57	O	0.121516897135	0.852254490466	0.830691017091
O58	O	0.822225046812	0.196692400538	0.593230413686
O59	O	0.829603074466	0.630287785082	0.151495888552
O60	O	0.619673078470	0.869208977581	0.837064864878
O61	O	0.830202575419	0.869453382479	0.136019950771
O62	O	0.826281217376	0.173132252548	0.834323796541
O63	O	0.833664671432	0.855816150910	0.626098398086
O64	O	0.617024880704	0.871945369569	0.118330796347
O65	O	0.091498460329	0.661171472178	0.849301940418
O66	O	0.095649257742	0.869167648354	0.644082632197
O67	O	0.601583083494	0.173944790523	0.845815529590
O68	O	0.834988333552	0.657070344723	0.825871326209
O69	O	0.297194133277	0.835891546621	0.005525528240
O70	O	0.803169657871	0.336741975981	0.298155506987
O71	O	0.289476940202	0.051015144586	0.798721932288
O72	O	0.813651177957	0.028745835148	0.300347508040
O73	O	0.301143670716	0.028570310129	0.298355473544
O74	O	0.290260555496	0.342461207013	0.810482854947
O75	O	0.297689880976	0.820650490467	0.310913836827
O76	O	0.029090239339	0.825610622731	0.294033507743
O77	O	0.802096345133	0.325167461524	0.026288759025
O78	O	0.289912846916	0.324600634772	0.024950047382

O79	O	0.164203008480	0.682020140362	0.943462771164
O80	O	0.652962560082	0.188556548439	0.655272440418
O81	O	0.934388977621	0.676498592781	0.181865181246
O82	O	0.658654625603	0.986542512550	0.664828907267
O83	O	0.653554973098	0.978859134813	0.155035683016
O84	O	0.949442988110	0.182384600611	0.665941951605
O85	O	0.937399310652	0.678859087182	0.648368344895
O86	O	0.666430238558	0.696517149422	0.132825775749
O87	O	0.013654163574	0.644856362759	0.759681449819
O88	O	0.124184727321	0.993207485147	0.657579347502
O89	O	0.639242526563	0.197072318542	0.960254815117
O90	O	0.650619218924	0.695798189670	0.958977403778
O91	O	0.191541641241	0.003008746101	0.768904095223
O92	O	0.760052878746	0.233737089324	0.985992921697
O93	O	0.984437373245	0.503075358817	0.196921829047
O94	O	0.962255391959	0.236249159569	0.771767889082
O95	O	0.002263144071	0.218879026489	0.473404328037
O96	O	0.993397207526	0.639121360583	0.033018953303
O97	O	0.001959978129	0.054183685536	0.815691895627
O98	O	0.986324111343	0.045677123508	0.597645788427
O99	O	0.002574313772	0.329655566113	0.301833049596
O100	O	0.010863354945	0.330896293136	0.807287381052
O101	O	0.427498845232	0.761003694293	0.613500912322
O102	O	0.343551634303	0.915485529475	0.581389296384
Mg1	Mg	0.305431647269	0.712904852170	0.544434257079
Mg2	Mg	0.405374265133	0.645408316652	0.675172163405
Mg3	Mg	0.150799349760	0.763935037151	0.754910608803
Mg4	Mg	0.262439203504	0.579904279264	0.726148532775
Al1	Al	0.841364300680	0.219783484805	0.362823807088
Al2	Al	0.369289656217	0.055088586569	0.824894117167
Al3	Al	0.188461369999	0.031606776016	0.371561994403
Al4	Al	0.374727400650	0.845193902888	0.201205896866
Al5	Al	0.765414688626	0.621401470299	0.942916486853
Al6	Al	0.755785751957	0.154883768600	0.945992092675
Al7	Al	0.113189661952	0.790825430895	0.595902741541
Al8	Al	0.938465111033	0.788528477049	0.122821798852
Al9	Al	0.100155527257	0.975758128022	0.770428464506
Al10	Al	0.765648053000	0.986049651564	0.584124152390
Al11	Al	0.588640902859	0.151710759091	0.771149626323
Al12	Al	0.932771244067	0.174810596455	0.584717402009
Al13	Al	0.105390716149	0.614786150856	0.963303592462
Si1	Si	0.192110862480	0.867599039736	0.005518396116
Si2	Si	0.006834204884	0.402567627837	0.197032648646
Si3	Si	0.004412256001	0.229623873941	0.837727242606
Si4	Si	0.836311300345	0.034677968232	0.198043411434
Si5	Si	0.179472171632	0.395326655707	0.857947174216
Si6	Si	0.017214952289	0.858152237964	0.372402249066
Si7	Si	0.836139196754	0.401151699931	0.019378099964
Si8	Si	0.366499385420	0.223718081856	0.019749032111
Si9	Si	0.122138980751	0.788826927186	0.941087845015
Si10	Si	0.758573887067	0.160674991888	0.588002076526
Si11	Si	0.933761726157	0.613695420676	0.141415677743
Si12	Si	0.584423956806	0.978550978718	0.767733603334
Si13	Si	0.760292101713	0.974596230102	0.126383436993
Si14	Si	0.933393313427	0.159747312541	0.771636929122
Si15	Si	0.941643641851	0.783511229660	0.580556776873
Si16	Si	0.586885680434	0.799011943158	0.116339876844
Si17	Si	0.060502629365	0.594509112717	0.839468167490
Si18	Si	0.098916294020	0.976100909217	0.594556997944
Si19	Si	0.577335428731	0.162498989064	0.950196720317
Si20	Si	0.587403172579	0.974889102723	0.119277322994
Si21	Si	0.935127566572	0.620150017241	0.757076318814
Si22	Si	0.768702426250	0.616941310632	0.116731555603

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Si23 Si    0.583224081104   0.802177801134   0.943408587698
Si24 Si    0.839783950295   0.222309152870   0.023265389051
Si25 Si    0.193569677941   0.855092018999   0.378318533766
Si26 Si    0.008064848840   0.399863509407   0.844067110804
Si27 Si    0.372653168448   0.039434206196   0.196226594003
Si28 Si    0.186824711011   0.049967912066   0.836940646241
Si29 Si    0.021462465220   0.862345257994   0.192975237918
Si30 Si    0.359080319107   0.232739675036   0.842381730136
Si31 Si    0.830108994511   0.407227412944   0.193433167803
Si32 Si    0.849020415425   0.038587587877   0.364128935870
Si33 Si    0.368329970260   0.860590861999   0.016007091292
Si34 Si    0.182394496117   0.390693286021   0.027158629264
Si35 Si    0.007650059064   0.226258942022   0.377985606948
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CIF file relative to the structure reported in Fig. 8c

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_symmetry_cell_setting triclinic
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_symmetry_equiv_pos_as_xyz
1 x,y,z
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_cell_length_a  17.5704469
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_cell_angle_gamma  59.480639
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
H1   H     0.578109489262   0.388069177703   0.687345743715
H2   H     0.684058906527   0.272508172249   0.487617919411
H3   H     0.238479877275   0.717792766489   0.486713160862
H4   H     0.363829318491   0.001346328855   0.089502408086
H5   H     0.791357791354   0.813896751377   0.698599718627
H6   H     0.986998009700   0.722026946508   0.255984362978
H7   H     0.146116420303   0.191721512299   0.270765563733
H8   H     0.963607736381   0.001568705533   0.607015431765
H9   H     0.480355762335   0.461041282941   0.928748741509
H10  H     0.278329005299   0.549289011706   0.797248031765
H11  H     0.220678955469   0.032901148138   0.712944534015
H12  H     0.865709117250   0.630047618467   0.979840160277
H13  H     0.279812874961   0.015910665668   0.999773027559
C1   C     0.378310861806   0.742104486581   0.729534403479
O1   O     0.525599685744   0.404061115106   0.739092500880
O2   O     0.460578283208   0.448259725124   0.895771994053
O3   O     0.408470155871   0.318684117120   0.908068137025
O4   O     0.339255820336   0.503048174395   0.802134968650
O5   O     0.185782992558   0.782404028807   0.996340147103
O6   O     0.741377951838   0.218979135214   0.489746637613
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O7	O	0.470348329429	0.988894049249	0.782769948735
O8	O	0.749117283617	0.006416306961	0.204313825906
O9	O	0.173606333117	0.012850005173	0.489149527408
O10	O	0.168644994623	0.496541867151	0.789257128228
O11	O	0.477915484374	0.782385203430	0.209071124937
O12	O	0.955828100994	0.795327651408	0.489805780727
O13	O	0.757707277735	0.502488738194	0.992475098305
O14	O	0.472113975157	0.177305109180	0.024820166183
O15	O	0.191200598211	0.778672440566	0.487932824141
O16	O	0.472915370107	0.001322161862	0.182100971842
O17	O	0.974550960374	0.501307554621	0.784708917483
O18	O	0.976488601761	0.783119703426	0.206883103617
O19	O	0.771958320644	0.995296987231	0.483395328673
O20	O	0.753971317386	0.509044038795	0.188868610294
O21	O	0.452317464747	0.244859414911	0.772654927104
O22	O	0.191219089800	0.486406011505	0.995019712690
O23	O	0.465519428868	0.810666591257	0.971349103209
O24	O	0.144038303197	0.966475758913	0.951846421654
O25	O	0.934580231403	0.179233546735	0.388698882646
O26	O	0.337192654895	0.978546050587	0.965460528104
O27	O	0.928646921812	0.396954481690	0.170000449300
O28	O	0.925195887036	0.193613515194	0.961026728803
O29	O	0.929422185487	0.963134852489	0.174352648240
O30	O	0.143061467967	0.959776606327	0.384769989924
O31	O	0.144932718383	0.380220740156	0.969008113277
O32	O	0.355181232885	0.972350242102	0.155745093294
O33	O	0.941468293859	0.968554999895	0.360417367211
O34	O	0.932087299881	0.385593579377	0.960863943878
O35	O	0.355042993758	0.180903190673	0.955151183104
O36	O	0.011819481833	0.821198601750	0.018065002248
O37	O	0.790957904579	0.045323686043	0.604145490730
O38	O	0.560844766766	0.050292838687	0.809290631067
O39	O	0.763375810449	0.046844497616	0.031349450587
O40	O	0.001843547345	0.826170226316	0.591950350449
O41	O	0.563162114147	0.835169479864	0.028194082698
O42	O	0.997503652403	0.622988743935	0.811449657702
O43	O	0.612917914293	0.021279361769	0.018114631321
O44	O	0.803820518331	0.623803649827	0.012386239719
O45	O	0.109759967531	0.858285584414	0.128207808644
O46	O	0.822591927519	0.142064286200	0.344803352745
O47	O	0.329396886082	0.156341944196	0.834188964604
O48	O	0.100769679719	0.363894689695	0.143233262051
O49	O	0.098456165715	0.148244123210	0.853689126390
O50	O	0.820429669905	0.141871408168	0.133175443266
O51	O	0.115069868204	0.154984903946	0.332494860775
O52	O	0.107300436423	0.355755262724	0.856721437424
O53	O	0.335939359276	0.844057445647	0.128850731225
O54	O	0.108432888118	0.839061569191	0.366461277610
O55	O	0.822216292782	0.366065813065	0.132997597960
O56	O	0.325373723976	0.146150402390	0.121093007367
O57	O	0.132938984622	0.854003948456	0.848670304892
O58	O	0.824012970161	0.176024797164	0.606683605255
O59	O	0.826759300190	0.637388960862	0.140797852427
O60	O	0.612095689159	0.867802027732	0.849070490341
O61	O	0.821014141625	0.868525816002	0.142063019143
O62	O	0.815932901987	0.173229477260	0.841053403845
O63	O	0.825649789929	0.848627531309	0.637321837828
O64	O	0.611788834295	0.854037147796	0.137316130833
O65	O	0.130249201152	0.626939828716	0.844740508463
O66	O	0.125115414621	0.861953796244	0.621746046310
O67	O	0.582578249921	0.170448280913	0.857628035129
O68	O	0.827677887381	0.648299848520	0.833078775903
O69	O	0.286426127448	0.835417371940	0.015528742680

O70	O	0.791085480365	0.333600583870	0.308196483774
O71	O	0.277437819951	0.040463927513	0.815599680443
O72	O	0.796456172433	0.027908625453	0.309917300646
O73	O	0.297527956050	0.025974524368	0.296367022003
O74	O	0.284266476001	0.331532791308	0.826953969058
O75	O	0.284513962398	0.825269369167	0.314217950078
O76	O	0.007772023374	0.823450284166	0.309020008851
O77	O	0.789544059804	0.324133598848	0.033039881110
O78	O	0.277974902872	0.315943593760	0.044196151664
O79	O	0.152839276647	0.676053635834	0.961299118694
O80	O	0.646781122879	0.190817616418	0.665069906926
O81	O	0.939229469542	0.676061492978	0.164918371667
O82	O	0.644954475002	0.975972715833	0.673988722681
O83	O	0.641322723159	0.964922954585	0.175611580291
O84	O	0.941696765597	0.181299225175	0.672513991627
O85	O	0.949278056296	0.675891701930	0.664144504076
O86	O	0.654673645285	0.685664650976	0.143168586239
O87	O	0.144929409768	0.669764744364	0.672109079464
O88	O	0.134529888170	0.981268457686	0.665826500886
O89	O	0.627888582348	0.201562422004	0.948332551128
O90	O	0.639619549076	0.693493440769	0.966101568374
O91	O	0.171179306829	0.021501373796	0.771743184073
O92	O	0.744514251923	0.230141089458	0.995868203583
O93	O	0.963907703566	0.501358827718	0.208932766717
O94	O	0.962459070811	0.221072602178	0.783649859907
O95	O	0.996988473084	0.207223809184	0.480939228159
O96	O	0.000249459516	0.606962391968	0.030164277904
O97	O	0.987396385611	0.043545158560	0.821923211020
O98	O	0.996687985974	0.029675714958	0.610791129330
O99	O	0.991676422147	0.325649529631	0.312908145903
O100	O	0.995917612555	0.327152752439	0.820531220076
O101	O	0.419864268351	0.664281758428	0.730120580674
O102	O	0.340311617255	0.817692440555	0.727434629836
Mg1	Mg	0.539872592306	0.308368042404	0.872060210283
Mg2	Mg	0.453869075374	0.521798523879	0.768074894282
Mg3	Mg	0.399857984386	0.373455922252	0.783641995766
Mg4	Mg	0.331651741868	0.429947214632	0.945355107672
Al1	Al	0.829354099491	0.216021221084	0.373900667013
Al2	Al	0.359710878102	0.046290934064	0.835318910969
Al3	Al	0.188559916360	0.030891022601	0.379033322599
Al4	Al	0.365802807345	0.845148501150	0.206961044627
Al5	Al	0.751486609887	0.616939898406	0.944767880395
Al6	Al	0.744187517071	0.160804289595	0.953744048268
Al7	Al	0.109793579057	0.785790081830	0.603476115715
Al8	Al	0.930952561901	0.791257959726	0.123349300296
Al9	Al	0.094772351560	0.969314989717	0.780752117510
Al10	Al	0.751828703685	0.978242544403	0.594647175913
Al11	Al	0.567867722164	0.157384252507	0.773925974597
Al12	Al	0.934685624416	0.158405069766	0.595086844574
Al13	Al	0.112476416247	0.607554531659	0.958017088701
Si1	Si	0.180251181518	0.859833347026	0.022931916749
Si2	Si	0.993066226398	0.398672166045	0.209376685011
Si3	Si	0.992419886718	0.222601757877	0.854652784049
Si4	Si	0.821357510327	0.036935414098	0.205301335785
Si5	Si	0.171654028287	0.391706817175	0.862147312247
Si6	Si	0.001437856568	0.858556452817	0.382455786132
Si7	Si	0.823402063378	0.395904238702	0.029280610696
Si8	Si	0.368272413686	0.222621064415	0.012539978002
Si9	Si	0.117837318460	0.783349865202	0.954899007954
Si10	Si	0.751936326037	0.151417028699	0.601063115731
Si11	Si	0.934952876317	0.608245630623	0.134102596006
Si12	Si	0.572493595418	0.973607509319	0.776021198512
Si13	Si	0.746576637268	0.972365063626	0.134741613170

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Si14 Si    0.924804399632   0.152854642901   0.780520511519
Si15 Si    0.939301400550   0.783524437935   0.593621135242
Si16 Si    0.575780781104   0.789951114465   0.130053252192
Si17 Si    0.108484455784   0.607913708529   0.779419637554
Si18 Si    0.116077468381   0.967565473676   0.595094076102
Si19 Si    0.579471392985   0.132767029885   0.964138598698
Si20 Si    0.585026801412   0.959525473188   0.130373330867
Si21 Si    0.935757109111   0.611006039749   0.774741866064
Si22 Si    0.758924745329   0.613392078983   0.127285624403
Si23 Si    0.572506546749   0.800253808190   0.953130743095
Si24 Si    0.817501369262   0.221939459757   0.030662146804
Si25 Si    0.180752240358   0.858928861181   0.379553611479
Si26 Si    0.000422200461   0.392355706805   0.855982897605
Si27 Si    0.363736013193   0.042991089431   0.191410720568
Si28 Si    0.172433359401   0.046229916056   0.852045589421
Si29 Si    0.006765121996   0.862880737158   0.204066053369
Si30 Si    0.356893115493   0.219094522856   0.848813485587
Si31 Si    0.822254359022   0.399051494967   0.202341735069
Si32 Si    0.829683790313   0.036449843869   0.375914402933
Si33 Si    0.358647344659   0.857913938195   0.025342864127
Si34 Si    0.172538478772   0.386516482805   0.040285767265
Si35 Si    0.001076842322   0.218756497123   0.384641926827
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CIF file relative to the structure reported in Fig. 8d

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_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
H1   H     0.204488587083   0.480980244445   0.173693534150
H2   H     0.682417858709   0.277074358697   0.477354369917
H3   H     0.244205998151   0.724091199471   0.475253688542
H4   H     0.364562909907   0.014273188469   0.081480611525
H5   H     0.790827244729   0.813542654086   0.681400462988
H6   H     0.949993684109   0.743285641012   0.264416828233
H7   H     0.142602485970   0.194374664392   0.264994133817
H8   H     0.958558870211   0.003763128377   0.596072294656
H9   H     0.577253619096   0.308216691182   0.072346082108
H10  H     0.425724599962   0.592691802047   0.061473506730
H11  H     0.214185607260   0.025492105786   0.708907488107
H12  H     0.867146340199   0.636779365125   0.966882562613
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H13	H	0.292307008429	0.013674458690	0.984494437537
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O1	O	0.520788244689	0.350850080873	0.055476603198
O2	O	0.262253966175	0.475849289865	0.123448862941
O3	O	0.411791334391	0.463515113552	0.963041224253
O4	O	0.446447075534	0.533020101162	0.056556098670
O5	O	0.200609551634	0.774003082420	0.979772111829
O6	O	0.738761574121	0.222177406797	0.475881990411
O7	O	0.469939031812	0.996790133791	0.765087867662
O8	O	0.758639135609	0.004013869865	0.186089530483
O9	O	0.167543494116	0.017126333831	0.484913028706
O10	O	0.177967642262	0.498904586799	0.775391158047
O11	O	0.481794229769	0.796840076626	0.189089501958
O12	O	0.959216946359	0.796899527790	0.473642171657
O13	O	0.764649003393	0.504491462196	0.973858459531
O14	O	0.456326221483	0.236071787139	0.971351744573
O15	O	0.191012206141	0.781859171693	0.475602967554
O16	O	0.472421590668	0.991300641191	0.194050287887
O17	O	0.964980624259	0.501178100774	0.769623540572
O18	O	0.962106519999	0.791292449502	0.203372501001
O19	O	0.770820096272	0.995428691670	0.466763239635
O20	O	0.748160764923	0.514481815554	0.171046831859
O21	O	0.455509064480	0.223052308460	0.776716961873
O22	O	0.180006462635	0.496445762349	0.986182918242
O23	O	0.466054176732	0.799648842931	0.968320960394
O24	O	0.154242540194	0.957273812222	0.943731776076
O25	O	0.931519602504	0.187658205836	0.372060564322
O26	O	0.338667556128	0.971571485688	0.950041892733
O27	O	0.925510261096	0.408692017910	0.158032180480
O28	O	0.915044659122	0.203224683221	0.942607152723
O29	O	0.937091312340	0.970092057759	0.155384334519
O30	O	0.141223784120	0.963282466739	0.375799986175
O31	O	0.133903569812	0.394363330405	0.954018693050
O32	O	0.352966679627	0.983240371092	0.148359305445
O33	O	0.942552523235	0.972549145953	0.347207423768
O34	O	0.935996646947	0.379805255936	0.944827653492
O35	O	0.352683609431	0.173688690963	0.957644333290
O36	O	0.026601013824	0.797780904492	0.021193084994
O37	O	0.794419547683	0.044815021111	0.582724283741
O38	O	0.575937121550	0.033724719644	0.800318903181
O39	O	0.755085348406	0.061452418794	0.015252316744
O40	O	0.001115451214	0.826697024015	0.578789392100
O41	O	0.566546506760	0.838464617038	0.007496001484
O42	O	0.001745473701	0.613442759379	0.795549607396
O43	O	0.569562298979	0.061057552857	0.022819946108
O44	O	0.806096144846	0.628652544560	0.998598890028
O45	O	0.110254434305	0.846508077748	0.117162455807
O46	O	0.820930630991	0.145334549856	0.331515698684
O47	O	0.322008446576	0.149213240690	0.841913781719
O48	O	0.105672549331	0.361951914128	0.126678042658
O49	O	0.093179674070	0.138462468897	0.856017214022
O50	O	0.818303847471	0.146312584231	0.117043491256
O51	O	0.111075579308	0.158103883006	0.326506747193
O52	O	0.107152235471	0.367765471076	0.835194871535
O53	O	0.337089802756	0.853654576619	0.116620845882
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O55	O	0.829887396291	0.369454496600	0.115830143364
O56	O	0.343478694307	0.147935538199	0.122181401550
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O58	O	0.818764667830	0.173904081245	0.596929420091
O59	O	0.826458322677	0.628862959962	0.138927935438
O60	O	0.607428658260	0.858761697284	0.832102695229
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O62	O	0.813089155922	0.186653194803	0.831102873585
O63	O	0.826218241877	0.847859267567	0.620727498045
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O67	O	0.601001436882	0.155447715638	0.841260524395
O68	O	0.828551831267	0.652240255845	0.816803942177
O69	O	0.289418350566	0.821445110741	0.018653633843
O70	O	0.789333240797	0.338805881199	0.292366368990
O71	O	0.276412731271	0.044080542951	0.799857854014
O72	O	0.800740112037	0.030560475586	0.292170049720
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O78	O	0.278914664847	0.321024575520	0.015790247477
O79	O	0.168136986383	0.663117047469	0.950005481149
O80	O	0.643911204690	0.180441324485	0.651687025927
O81	O	0.924578133406	0.678670333818	0.168836552372
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O84	O	0.936026715553	0.179029492324	0.665002406685
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O86	O	0.657956989132	0.698021330054	0.126322704950
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O95	O	0.987093213915	0.214451215735	0.471337832692
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O97	O	0.978277793501	0.042482531438	0.817875247095
O98	O	0.991141236754	0.032466900746	0.599777249763
O99	O	0.995398156648	0.329742907916	0.297706890534
O100	O	0.006318562438	0.321715793099	0.803997398438
O101	O	0.645833780597	0.475461390475	0.865927759566
O102	O	0.807229331285	0.420079668501	0.812254830235
Mg1	Mg	0.491408757595	0.328317938490	0.973833834792
Mg2	Mg	0.389767720201	0.439213301012	0.106373860376
Mg3	Mg	0.514929726352	0.488572222406	0.955378159015
Mg4	Mg	0.271906422549	0.530718124860	0.990194316998
Al1	Al	0.825457029873	0.221269666093	0.360341202424
Al2	Al	0.358805489698	0.048802552589	0.821767834134
Al3	Al	0.182223926143	0.034412558039	0.375621786102
Al4	Al	0.367406277118	0.853626775944	0.194631806287
Al5	Al	0.756351310035	0.619628925149	0.929935980638
Al6	Al	0.734837981697	0.175795445542	0.940319601045
Al7	Al	0.108091931716	0.787380182543	0.591837717319
Al8	Al	0.930206864845	0.789859589033	0.115957221594
Al9	Al	0.086110422168	0.966165281481	0.778743837113
Al10	Al	0.751879700388	0.977450932606	0.578291288087
Al11	Al	0.571074351988	0.147245720712	0.765209157590
Al12	Al	0.927279697320	0.160438733926	0.585511343348
Al13	Al	0.103120907164	0.615459263467	0.942822611026
Si1	Si	0.187361007613	0.850279696220	0.014100876240
Si2	Si	0.999011607914	0.401522595078	0.193072426820
Si3	Si	0.994436925321	0.220825759333	0.841432242859
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Si5	Si	0.174248209052	0.395340696141	0.847483264523

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Si7	Si	0.828292745808	0.397706171959	0.014119212303
Si8	Si	0.355647035263	0.218858055982	0.014873863470
Si9	Si	0.127578426463	0.773274154010	0.946656547576
Si10	Si	0.749269189939	0.148910049348	0.587508897883
Si11	Si	0.932055545814	0.612527011479	0.127363597265
Si12	Si	0.574912823283	0.969611331667	0.761463661144
Si13	Si	0.750261105051	0.978417208248	0.113665383502
Si14	Si	0.922156252634	0.153725073432	0.771065022752
Si15	Si	0.940238582439	0.783520578322	0.578881213718
Si16	Si	0.578936540867	0.802509644072	0.107201615612
Si17	Si	0.109847333065	0.608054818271	0.764993770988
Si18	Si	0.109095245178	0.969134479584	0.589556642576
Si19	Si	0.569554748715	0.160402085959	0.938400110994
Si20	Si	0.578842607222	0.972409529141	0.119185933233
Si21	Si	0.935913156813	0.609812867326	0.758186821897
Si22	Si	0.757768220630	0.617405615283	0.114506295858
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Si25	Si	0.181735545070	0.862974412107	0.367993747458
Si26	Si	0.003078757129	0.393054736224	0.838083452639
Si27	Si	0.366049272545	0.040139283194	0.194735848520
Si28	Si	0.173439176173	0.041673481260	0.844579189433
Si29	Si	0.006592540364	0.865193620074	0.191209195875
Si30	Si	0.355557844165	0.216252625119	0.845451324899
Si31	Si	0.821906240256	0.405365936680	0.187662898920
Si32	Si	0.830379723746	0.039146611032	0.361298263592
Si33	Si	0.360426528309	0.854749591277	0.017628134495
Si34	Si	0.172477093621	0.394359528818	0.019956663219
Si35	Si	0.996115343965	0.225273237263	0.373332947165