Combined PDF and Rietveld studies of ADORable zeolites and the disordered intermediate IPC-1P

Supplementary Information

Synthesis

Ge- B-UTL - was produced according to the method given by Roth et al.[1] A molar composition of the reaction mixture was as follows: 0.692 - 0.764 SiO_2: 0.036 -0.108 H_3BO_3: 0.4 GeO_2: 0.6 - 0.7 ROH/Br: 30 H_2O.[1] Where ROH is the structural directing agent (SDA), (6R,10S)-6,10-dimethyl-5-azoniaspiro[4,5] decane hydroxide. Typically, the SDAOH/Br was dissolved in water and germanium dioxide and/or boric acid was added and left to stir for some hours. Adding in Silica (Aerosil) forms a fluid gel, which was given adequate stirring time before being charged into a Teflon-lined autoclave and heated between 2 - 23 days at 175 °C. Solid products were obtained by filtration, washed with distilled water and dried overnight.

Calcination - The solid zeolitic product was calcined in order to remove the structural directing agent in a stream of air at 550 °C for 6 hours with a ramp rate of 1 °C/min.

IPC-1P - was made by refluxing calcined Ge-B-UTL in HCl (0.1M, solid to liquid 1:200 w/w) at 95 °C overnight, this process is referred to as hydrolysis. The product was collected by filtration, washed with distilled water until the filtrate reached neutral pH, then dried overnight.

IPC-2 – IPC-1P, HNO_3 (1M, 1:20 w/w ratio solid IPC-1P to liquid) and $Si(CH_3)_2(OCH2CH2)_2$ (1:5 w/w ratio of IPC-1P to $Si(CH_3)_2(OCH2CH2)_2$) were charged inside an autoclave and heated to 170 °C overnight. The product was obtained by filtration, washed with distilled water and calcined as above.

IPC-4 - IPC-1P was heated at 70 °C with octylamine (1:66 w/w solid IPC-1P to octylamine) for several hours before being stirred at room temperature overnight. This organised the layers. The solid was collected by centrifugation, dried at 90 °C and calcined as above.

Synchrotron PXRD

IPC-2 Synchrotron Collection

Synchrotron data was collected at beamline I11, Diamond Light Source (UK). The powdered samples were placed in 0.5 mm borosilicate glass capillary tubes. The sample was cooled to 150 K using an Oxford Cryostream Plus. Data was collected in Debye-Scherrer geometry using the MAC detector system with monochromatic synchrotron radiation wavelength of 0.825698 Å, data was collected between 0 – 40 °2θ.

IPC-4 Synchrotron Collection

Synchrotron data for IPC-4 was collected at the Swiss Light Source (SLS) on the Material Science beamline. The powdered sample was placed inside a rotating 0.3 mm- borosilicate capillary. Data was

collected in Debye-Scherrer geometry using the MYTHEN II detector with Si 111 monochromator system with monochromatic radiation of 0.7086 Å, data was collected between 4 - 50 °2θ using 4 detector positions collecting for 10 s per pattern and a nominal step size of 0.004 °2θ.

Total Scattering Experiments

Total scattering data sets were collected using beamline I15 at Diamond Light Source, UK, which uses a Perkin-Elmer area detector and was set up an X-ray wavelength of 0.173 Å and sample to detector distance of 204 mm calibrated using a CeO_2 standard. This allows the collection of data to a high momentum range of Q ~22 $Å^{-1}$. Ground samples were packed into 1 mm external diameter Kapton capillaries. The program FIT2D was used to integrate the data followed by the use of PDFgetx2 to apply standard corrections and produce the total scattering data, G(*r*).

PDF refinement

PDFgui refinements were performed using C 2/m symmetry constraints applied to atomic positions, occupancies and ADP values. The latter were refined isotropically by element type to reduce over-parameterisation. s_{ratio} cutoff by r_{cut} was used to model the correlated motion of the framework, which defines the low-*r* to high-*r* PDF peak ratio, allowing low-*r* peaks to be sharpened. An r_{cut} value of 3.38 Å was used (The upper limit of Si-O-Si distance), a conservative estimate of correlated motion considering zeolites framework rigidity.
All structures used for both Rietveld and PDF analyses were refined in C 2/m to allow direct comparison of the final structures. All initial model refinements, excluding IPC-1P, use the idealised structure obtained from the IZA structure commission. The initial IPC-1P model was calculated using Density Function Theory using details given below.

Computational Details

The IPC-1P structure has been modelled theoretically using periodic models at the density functional theory (DFT) level. There are several possible structures of the interacting IPC-1P layers due to the high concentration and low symmetry of surface silanol groups as has been shown by Grajciar et al.[2] These structures differ in the inter-layer lateral shifts and/or orientation of interlayer hydrogen bond networks. Only the most stable inter-layer arrangement of IPC-1P layers has been considered herein. This energetically the most stable structure determined by Grajciar et al. has been re-optimized using an infinite (periodic) stack of interacting layers. The unit cell (UC) contains just one layer of IPC-1P with the $Si_{30}O_{64}H_8$ composition. The geometry of the system has been fully optimized, including lattice parameters; the final structural parameters are: *a*=14.47081, *b*=14.16853, *c*=12.54491, α=89.98132, β=117.03476, γ=119.50552. All calculations have been performed at the DFT level using the PBE functional[3] and projector augmented wave approximation[4] using VASP 5.3.3 program suite.[5-8] The energy cut-off has been set to 800 eV. Brillouin-zone sampling has been restricted to the Γ-point.

Full structural comparison tables

Full comparison tables:

Table 1: % Differences for the OKO structure calculated by different sources.

% Differences	PDF Refinement from Rietveld refinement	PDF Refinement from IZA OKO	Rietveld Refinement from IZA OKO
Si-O Bonds / %	3.31	3.28	1.36
Si-O-Si Angles / %	5.30	4.59	3.06
O-Si-O Angles / %	4.49	4.33	2.44

Table 2: % Differences for the PCR structure calculated by different sources.

% Differences	PDF Refinement from Rietveld Refinement	PDF Refinement from IZA PCR	Rietveld Refinement from IZA PCR
Si-O Bonds / %	4.44	4.32	0.89
Si-O-Si Angles / %	6.82	5.61	2.19
O-Si-O Angles / %	6.33	6.17	0.63

Crystallographic Table for IPC-1P PDF refinement

Unit Cell: P1 a = 25.031 Å, b = 14.0983 Å, c = 12.244 Å, β = 119.076 °

Site Label	Atom Type Symbol	Frac x	Frac y	Frac z	Uiso	Occupancy
Si1	Si	0.768304	0	0.846536	0.01921	1
Si2	Si	0.231696	0	0.153464	0.01921	1
Si3	Si	0.268304	0.5	0.846536	0.01921	1
Si4	Si	0.731696	0.5	0.153464	0.01921	1
Si5	Si	0.774775	0	0.486865	0.01921	1
Si6	Si	0.225225	0	0.513135	0.01921	1
Si7	Si	0.274775	0.5	0.486865	0.01921	1
Si8	Si	0.725225	0.5	0.513135	0.01921	1
Si9	Si	0.778226	0	0.236117	0.01921	1
Si10	Si	0.221774	0	0.763883	0.01921	1
Si11	Si	0.278226	0.5	0.236117	0.01921	1
Si12	Si	0.721774	0.5	0.763883	0.01921	1
Si13	Si	0.815716	0.200977	0.595942	0.01921	1
Si14	Si	0.184284	0.200977	0.404058	0.01921	1
Si15	Si	0.184284	0.799023	0.404058	0.01921	1
Si16	Si	0.815716	0.799023	0.595942	0.01921	1
Si17	Si	0.315716	0.700977	0.595942	0.01921	1

Si18	Si	0.684284	0.700977	0.404058	0.01921	1
Si19	Si	0.684284	0.299023	0.404058	0.01921	1
Si20	Si	0.315716	0.299023	0.595942	0.01921	1
Si21	Si	0.810595	0.20419	0.842851	0.01921	1
Si22	Si	0.189405	0.20419	0.157149	0.01921	1
Si23	Si	0.189405	0.79581	0.157149	0.01921	1
Si24	Si	0.810595	0.79581	0.842851	0.01921	1
Si25	Si	0.310595	0.70419	0.842851	0.01921	1
Si26	Si	0.689405	0.70419	0.157149	0.01921	1
Si27	Si	0.689405	0.29581	0.157149	0.01921	1
Si28	Si	0.310595	0.29581	0.842851	0.01921	1
Si29	Si	0.67757	0	0.962667	0.01921	1
Si30	Si	0.32243	0	0.037333	0.01921	1
Si31	Si	0.17757	0.5	0.962667	0.01921	1
Si32	Si	0.82243	0.5	0.037333	0.01921	1
Si33	Si	0.677345	0.291923	0.757954	0.01921	1
Si34	Si	0.322655	0.291923	0.242046	0.01921	1
Si35	Si	0.322655	0.708077	0.242046	0.01921	1
Si36	Si	0.677345	0.708077	0.757954	0.01921	1
Si37	Si	0.177345	0.791923	0.757954	0.01921	1
Si38	Si	0.822655	0.791923	0.242046	0.01921	1
Si39	Si	0.822655	0.208077	0.242046	0.01921	1
Si40	Si	0.177345	0.208077	0.757954	0.01921	1
Si41	Si	0.670589	0	0.560148	0.01921	1
Si42	Si	0.329411	0	0.439852	0.01921	1
Si43	Si	0.170589	0.5	0.560148	0.01921	1
Si44	Si	0.829411	0.5	0.439852	0.01921	1
Si45	Si	0.615584	0.201502	0.905912	0.01921	1
Si46	Si	0.384416	0.201502	0.094088	0.01921	1
Si47	Si	0.384416	0.798498	0.094088	0.01921	1
Si48	Si	0.615584	0.798498	0.905912	0.01921	1
Si49	Si	0.115584	0.701502	0.905912	0.01921	1
Si50	Si	0.884416	0.701502	0.094088	0.01921	1
Si51	Si	0.884416	0.298498	0.094088	0.01921	1
Si52	Si	0.115584	0.298498	0.905912	0.01921	1
Si53	Si	0.6038	0.199742	0.498434	0.01921	1
Si54	Si	0.3962	0.199742	0.501566	0.01921	1
Si55	Si	0.3962	0.800258	0.501566	0.01921	1
Si56	Si	0.6038	0.800258	0.498434	0.01921	1
Si57	Si	0.1038	0.699742	0.498434	0.01921	1
Si58	Si	0.8962	0.699742	0.501566	0.01921	1
Si59	Si	0.8962	0.300258	0.501566	0.01921	1
Si60	Si	0.1038	0.300258	0.498434	0.01921	1
O1	O	0.75	0.25	0.5	0.025935	1
O2	O	0.25	0.25	0.5	0.025935	1
O3	O	0.25	0.75	0.5	0.025935	1

O4	O	0.75	0.75	0.5	0.025935	1
O5	O	0.746579	0.245846	0.807907	0.025935	1
O6	O	0.253421	0.245846	0.192093	0.025935	1
O7	O	0.253421	0.754154	0.192093	0.025935	1
O8	O	0.746579	0.754154	0.807907	0.025935	1
O9	O	0.246579	0.745846	0.807907	0.025935	1
O10	O	0.753421	0.745846	0.192093	0.025935	1
O11	O	0.753421	0.254154	0.192093	0.025935	1
O12	O	0.246579	0.254154	0.807907	0.025935	1
O13	O	0.762644	0	0.348176	0.025935	1
O14	O	0.237356	0	0.651824	0.025935	1
O15	O	0.262644	0.5	0.348176	0.025935	1
O16	O	0.737356	0.5	0.651824	0.025935	1
O17	O	0.730909	0	0.921739	0.025935	1
O18	O	0.269091	0	0.078261	0.025935	1
O19	O	0.230909	0.5	0.921739	0.025935	1
O20	O	0.769091	0.5	0.078261	0.025935	1
O21	O	0.721911	0	0.703194	0.025935	1
O22	O	0.278089	0	0.296806	0.025935	1
O23	O	0.221911	0.5	0.703194	0.025935	1
O24	O	0.778089	0.5	0.296806	0.025935	1
O25	O	0.71149	0	0.110803	0.025935	1
O26	O	0.28851	0	0.889197	0.025935	1
O27	O	0.21149	0.5	0.110803	0.025935	1
O28	O	0.78851	0.5	0.889197	0.025935	1
O29	O	0.706996	0	0.47962	0.025935	1
O30	O	0.293004	0	0.52038	0.025935	1
O31	O	0.206996	0.5	0.47962	0.025935	1
O32	O	0.793004	0.5	0.52038	0.025935	1
O33	O	0.815663	0.090162	0.562021	0.025935	1
O34	O	0.184337	0.090162	0.437979	0.025935	1
O35	O	0.184337	0.909838	0.437979	0.025935	1
O36	O	0.815663	0.909838	0.562021	0.025935	1
O37	O	0.315663	0.590162	0.562021	0.025935	1
O38	O	0.684337	0.590162	0.437979	0.025935	1
O39	O	0.684337	0.409838	0.437979	0.025935	1
O40	O	0.315663	0.409838	0.562021	0.025935	1
O41	O	0.811667	0.093359	0.875307	0.025935	1
O42	O	0.188333	0.093359	0.124693	0.025935	1
O43	O	0.188333	0.906641	0.124693	0.025935	1
O44	O	0.811667	0.906641	0.875307	0.025935	1
O45	O	0.311667	0.593359	0.875307	0.025935	1
O46	O	0.688333	0.593359	0.124693	0.025935	1
O47	O	0.688333	0.406641	0.124693	0.025935	1
O48	O	0.311667	0.406641	0.875307	0.025935	1
O49	O	0.818711	0.910014	0.242588	0.025935	1

O50	O	0.181289	0.910014	0.757412	0.025935	1
O51	O	0.181289	0.089986	0.757412	0.025935	1
O52	O	0.818711	0.089986	0.242588	0.025935	1
O53	O	0.318711	0.410014	0.242588	0.025935	1
O54	O	0.681289	0.410014	0.757412	0.025935	1
O55	O	0.681289	0.589986	0.757412	0.025935	1
O56	O	0.318711	0.589986	0.242588	0.025935	1
O57	O	0.822656	0.217613	0.727889	0.025935	1
O58	O	0.177344	0.217613	0.272111	0.025935	1
O59	O	0.177344	0.782387	0.272111	0.025935	1
O60	O	0.822656	0.782387	0.727889	0.025935	1
O61	O	0.322656	0.717613	0.727889	0.025935	1
O62	O	0.677344	0.717613	0.272111	0.025935	1
O63	O	0.677344	0.282387	0.272111	0.025935	1
O64	O	0.322656	0.282387	0.727889	0.025935	1
O65	O	0.652148	0.266261	0.851377	0.025935	1
O66	O	0.347852	0.266261	0.148623	0.025935	1
O67	O	0.347852	0.733739	0.148623	0.025935	1
O68	O	0.652148	0.733739	0.851377	0.025935	1
O69	O	0.152148	0.766261	0.851377	0.025935	1
O70	O	0.847852	0.766261	0.148623	0.025935	1
O71	O	0.847852	0.233739	0.148623	0.025935	1
O72	O	0.152148	0.233739	0.851377	0.025935	1
O73	O	0.633143	0.090629	0.910458	0.025935	1
O74	O	0.366857	0.090629	0.089542	0.025935	1
O75	O	0.366857	0.909371	0.089542	0.025935	1
O76	O	0.633143	0.909371	0.910458	0.025935	1
O77	O	0.133143	0.590629	0.910458	0.025935	1
O78	O	0.866857	0.590629	0.089542	0.025935	1
O79	O	0.866857	0.409371	0.089542	0.025935	1
O80	O	0.133143	0.409371	0.910458	0.025935	1
O81	O	0.629524	0.253764	0.622969	0.025935	1
O82	O	0.370476	0.253764	0.377031	0.025935	1
O83	O	0.370476	0.746236	0.377031	0.025935	1
O84	O	0.629524	0.746236	0.622969	0.025935	1
O85	O	0.129524	0.753764	0.622969	0.025935	1
O86	O	0.870476	0.753764	0.377031	0.025935	1
O87	O	0.870476	0.246236	0.377031	0.025935	1
O88	O	0.129524	0.246236	0.622969	0.025935	1
O89	O	0.866075	0.258688	0.959043	0.025935	1
O90	O	0.133925	0.258688	0.040957	0.025935	1
O91	O	0.133925	0.741312	0.040957	0.025935	1
O92	O	0.866075	0.741312	0.959043	0.025935	1
O93	O	0.366075	0.758688	0.959043	0.025935	1
O94	O	0.633925	0.758688	0.040957	0.025935	1
O95	O	0.633925	0.241312	0.040957	0.025935	1

O96	O	0.366075	0.241312	0.959043	0.025935	1
O97	O	0.87246	0.254332	0.590625	0.025935	1
O98	O	0.12754	0.254332	0.409375	0.025935	1
O99	O	0.12754	0.745668	0.409375	0.025935	1
O100	O	0.87246	0.745668	0.590625	0.025935	1
O101	O	0.37246	0.754332	0.590625	0.025935	1
O102	O	0.62754	0.754332	0.409375	0.025935	1
O103	O	0.62754	0.245668	0.409375	0.025935	1
O104	O	0.37246	0.245668	0.590625	0.025935	1
O105	O	0.631219	0.09414	0.536834	0.025935	1
O106	O	0.368781	0.09414	0.463166	0.025935	1
O107	O	0.368781	0.90586	0.463166	0.025935	1
O108	O	0.631219	0.90586	0.536834	0.025935	1
O109	O	0.131219	0.59414	0.536834	0.025935	1
O110	O	0.868781	0.59414	0.463166	0.025935	1
O111	O	0.868781	0.40586	0.463166	0.025935	1
O112	O	0.131219	0.40586	0.536834	0.025935	1
O113	O	0.540621	0.214642	0.817466	0.025935	1
O114	O	0.459379	0.214642	0.182534	0.025935	1
O115	O	0.459379	0.785358	0.182534	0.025935	1
O116	O	0.540621	0.785358	0.817466	0.025935	1
O117	O	0.040621	0.714642	0.817466	0.025935	1
O118	O	0.959379	0.714642	0.182534	0.025935	1
O119	O	0.959379	0.285358	0.182534	0.025935	1
O120	O	0.040621	0.285358	0.817466	0.025935	1
O121	O	0.528697	0.19966	0.425517	0.025935	1
O122	O	0.471303	0.19966	0.574483	0.025935	1
O123	O	0.471303	0.80034	0.574483	0.025935	1
O124	O	0.528697	0.80034	0.425517	0.025935	1
O125	O	0.028697	0.69966	0.425517	0.025935	1
O126	O	0.971303	0.69966	0.574483	0.025935	1
O127	O	0.971303	0.30034	0.574483	0.025935	1
O128	O	0.028697	0.30034	0.425517	0.025935	1

Crystallographic table for IPC-4 PDF refinement

Unit Cell: P1 a = 20.0659 Å, b = 14.0200 Å, c = 12.4396 Å, β = 115.651 °

Site Label	Atom Type Symbol	Frac x	Frac y	Frac z	Uiso	Occupancy
O1	O	0.81836	0.898898	0.732124	0.018438	1
O2	O	0.31836	0.398898	0.732124	0.018438	1
O3	O	0.18164	0.898898	0.267876	0.018438	1
O4	O	0.68164	0.398898	0.267876	0.018438	1
O5	O	0.18164	0.101102	0.267876	0.018438	1

O6	O	0.68164	0.601102	0.267876	0.018438	1
O7	O	0.81836	0.101102	0.732124	0.018438	1
O8	O	0.31836	0.601102	0.732124	0.018438	1
O9	O	0.868889	0.725379	0.723178	0.018438	1
O10	O	0.368889	0.225379	0.723178	0.018438	1
O11	O	0.131111	0.725379	0.276822	0.018438	1
O12	O	0.631111	0.225379	0.276822	0.018438	1
O13	O	0.131111	0.274621	0.276822	0.018438	1
O14	O	0.631111	0.774621	0.276822	0.018438	1
O15	O	0.868889	0.274621	0.723178	0.018438	1
O16	O	0.368889	0.774621	0.723178	0.018438	1
O17	O	0.850075	0.771214	0.91926	0.018438	1
O18	O	0.350075	0.271214	0.91926	0.018438	1
O19	O	0.149925	0.771214	0.08074	0.018438	1
O20	O	0.649925	0.271214	0.08074	0.018438	1
O21	O	0.149925	0.228786	0.08074	0.018438	1
O22	O	0.649925	0.728786	0.08074	0.018438	1
O23	O	0.850075	0.228786	0.91926	0.018438	1
O24	O	0.350075	0.728786	0.91926	0.018438	1
O25	O	0.740783	0.780528	0.703319	0.018438	1
O26	O	0.240783	0.280528	0.703319	0.018438	1
O27	O	0.259217	0.780528	0.296681	0.018438	1
O28	O	0.759217	0.280528	0.296681	0.018438	1
O29	O	0.259217	0.219472	0.296681	0.018438	1
O30	O	0.759217	0.719472	0.296681	0.018438	1
O31	O	0.740783	0.219472	0.703319	0.018438	1
O32	O	0.240783	0.719472	0.703319	0.018438	1
O33	O	0.401613	0.256557	0.122989	0.018438	1
O34	O	0.901613	0.756557	0.122989	0.018438	1
O35	O	0.598387	0.256557	0.877011	0.018438	1
O36	O	0.098387	0.756557	0.877011	0.018438	1
O37	O	0.598387	0.743443	0.877011	0.018438	1
O38	O	0.098387	0.243443	0.877011	0.018438	1
O39	O	0.401613	0.743443	0.122989	0.018438	1
O40	O	0.901613	0.243443	0.122989	0.018438	1
O41	O	0.39952	0.089081	0.266713	0.018438	1
O42	O	0.89952	0.589081	0.266713	0.018438	1
O43	O	0.60048	0.089081	0.733287	0.018438	1
O44	O	0.10048	0.589081	0.733287	0.018438	1
O45	O	0.60048	0.910919	0.733287	0.018438	1
O46	O	0.10048	0.410919	0.733287	0.018438	1
O47	O	0.39952	0.910919	0.266713	0.018438	1
O48	O	0.89952	0.410919	0.266713	0.018438	1
O49	O	0.400343	0.25442	0.363689	0.018438	1
O50	O	0.900343	0.75442	0.363689	0.018438	1
O51	O	0.599657	0.25442	0.636311	0.018438	1

O52	O	0.099657	0.75442	0.636311	0.018438	1
O53	O	0.599657	0.74558	0.636311	0.018438	1
O54	O	0.099657	0.24558	0.636311	0.018438	1
O55	O	0.400343	0.74558	0.363689	0.018438	1
O56	O	0.900343	0.24558	0.363689	0.018438	1
O57	O	0.51474	0.197607	0.283292	0.018438	1
O58	O	0.01474	0.697607	0.283292	0.018438	1
O59	O	0.48526	0.197607	0.716708	0.018438	1
O60	O	0.98526	0.697607	0.716708	0.018438	1
O61	O	0.48526	0.802393	0.716708	0.018438	1
O62	O	0.98526	0.302393	0.716708	0.018438	1
O63	O	0.51474	0.802393	0.283292	0.018438	1
O64	O	0.01474	0.302393	0.283292	0.018438	1
O65	O	0.167553	0.907479	0.946904	0.018438	1
O66	O	0.667553	0.407479	0.946904	0.018438	1
O67	O	0.832447	0.907479	0.053096	0.018438	1
O68	O	0.332447	0.407479	0.053096	0.018438	1
O69	O	0.832447	0.092521	0.053096	0.018438	1
O70	O	0.332447	0.592521	0.053096	0.018438	1
O71	O	0.167553	0.092521	0.946904	0.018438	1
O72	O	0.667553	0.592521	0.946904	0.018438	1
O73	O	0.25	0.75	0	0.018438	1
O74	O	0.75	0.25	0	0.018438	1
O75	O	0.75	0.75	0	0.018438	1
O76	O	0.25	0.25	0	0.018438	1
O77	O	0.160576	0.903497	0.649578	0.018438	1
O78	O	0.660576	0.403497	0.649578	0.018438	1
O79	O	0.839424	0.903497	0.350422	0.018438	1
O80	O	0.339424	0.403497	0.350422	0.018438	1
O81	O	0.839424	0.096503	0.350422	0.018438	1
O82	O	0.339424	0.596503	0.350422	0.018438	1
O83	O	0.160576	0.096503	0.649578	0.018438	1
O84	O	0.660576	0.596503	0.649578	0.018438	1
O85	O	0.129323	0.768041	0.495292	0.018438	1
O86	O	0.629323	0.268041	0.495292	0.018438	1
O87	O	0.870677	0.768041	0.504708	0.018438	1
O88	O	0.370677	0.268041	0.504708	0.018438	1
O89	O	0.870677	0.231959	0.504708	0.018438	1
O90	O	0.370677	0.731959	0.504708	0.018438	1
O91	O	0.129323	0.231959	0.495292	0.018438	1
O92	O	0.629323	0.731959	0.495292	0.018438	1
O93	O	0.129945	0.592691	0.413617	0.018438	1
O94	O	0.629945	0.092691	0.413617	0.018438	1
O95	O	0.870055	0.592691	0.586383	0.018438	1
O96	O	0.370055	0.092691	0.586383	0.018438	1
O97	O	0.870055	0.407309	0.586383	0.018438	1

O98	O	0.370055	0.907309	0.586383	0.018438	1
O99	O	0.129945	0.407309	0.413617	0.018438	1
O100	O	0.629945	0.907309	0.413617	0.018438	1
O101	O	0.700926	0	0.312969	0.018438	1
O102	O	0.200926	0.5	0.312969	0.018438	1
O103	O	0.299074	0	0.687031	0.018438	1
O104	O	0.799074	0.5	0.687031	0.018438	1
O105	O	0.7567	0	0.1543	0.018438	1
O106	O	0.2567	0.5	0.1543	0.018438	1
O107	O	0.2433	0	0.8457	0.018438	1
O108	O	0.7433	0.5	0.8457	0.018438	1
O109	O	0.792114	0.5	0.287389	0.018438	1
O110	O	0.292114	0	0.287389	0.018438	1
O111	O	0.207886	0.5	0.712611	0.018438	1
O112	O	0.707886	0	0.712611	0.018438	1
O113	O	0.751763	0.5	0.457845	0.018438	1
O114	O	0.251763	0	0.457845	0.018438	1
O115	O	0.248237	0.5	0.542155	0.018438	1
O116	O	0.748237	0	0.542155	0.018438	1
O117	O	0.801303	0.5	0.088469	0.018438	1
O118	O	0.301303	0	0.088469	0.018438	1
O119	O	0.198697	0.5	0.911531	0.018438	1
O120	O	0.698697	0	0.911531	0.018438	1
Si1	Si	0.82761	0.797346	0.772772	0.014997	1
Si2	Si	0.32761	0.297346	0.772772	0.014997	1
Si3	Si	0.17239	0.797346	0.227228	0.014997	1
Si4	Si	0.67239	0.297346	0.227228	0.014997	1
Si5	Si	0.17239	0.202654	0.227228	0.014997	1
Si6	Si	0.67239	0.702654	0.227228	0.014997	1
Si7	Si	0.82761	0.202654	0.772772	0.014997	1
Si8	Si	0.32761	0.702654	0.772772	0.014997	1
Si9	Si	0.425536	0.205559	0.259837	0.014997	1
Si10	Si	0.925536	0.705559	0.259837	0.014997	1
Si11	Si	0.574464	0.205559	0.740163	0.014997	1
Si12	Si	0.074464	0.705559	0.740163	0.014997	1
Si13	Si	0.574464	0.794441	0.740163	0.014997	1
Si14	Si	0.074464	0.294441	0.740163	0.014997	1
Si15	Si	0.425536	0.794441	0.259837	0.014997	1
Si16	Si	0.925536	0.294441	0.259837	0.014997	1
Si17	Si	0.175053	0.801106	0.978953	0.014997	1
Si18	Si	0.675053	0.301106	0.978953	0.014997	1
Si19	Si	0.824947	0.801106	0.021047	0.014997	1
Si20	Si	0.324947	0.301106	0.021047	0.014997	1
Si21	Si	0.824947	0.198894	0.021047	0.014997	1
Si22	Si	0.324947	0.698894	0.021047	0.014997	1
Si23	Si	0.175053	0.198894	0.978953	0.014997	1

Si24	Si	0.675053	0.698894	0.978953	0.014997	1
Si25	Si	0.16511	0.794549	0.625155	0.014997	1
Si26	Si	0.66511	0.294549	0.625155	0.014997	1
Si27	Si	0.83489	0.794549	0.374845	0.014997	1
Si28	Si	0.33489	0.294549	0.374845	0.014997	1
Si29	Si	0.83489	0.205451	0.374845	0.014997	1
Si30	Si	0.33489	0.705451	0.374845	0.014997	1
Si31	Si	0.16511	0.205451	0.625155	0.014997	1
Si32	Si	0.66511	0.705451	0.625155	0.014997	1
Si33	Si	0.101328	0.697639	0.377556	0.014997	1
Si34	Si	0.601328	0.197639	0.377556	0.014997	1
Si35	Si	0.898672	0.697639	0.622444	0.014997	1
Si36	Si	0.398672	0.197639	0.622444	0.014997	1
Si37	Si	0.898672	0.302361	0.622444	0.014997	1
Si38	Si	0.398672	0.802361	0.622444	0.014997	1
Si39	Si	0.101328	0.302361	0.377556	0.014997	1
Si40	Si	0.601328	0.802361	0.377556	0.014997	1
Si41	Si	0.781229	0	0.306132	0.014997	1
Si42	Si	0.281229	0.5	0.306132	0.014997	1
Si43	Si	0.218771	0	0.693868	0.014997	1
Si44	Si	0.718771	0.5	0.693868	0.014997	1
Si45	Si	0.218428	0	0.307631	0.014997	1
Si46	Si	0.718428	0.5	0.307631	0.014997	1
Si47	Si	0.781572	0	0.692369	0.014997	1
Si48	Si	0.281572	0.5	0.692369	0.014997	1
Si49	Si	0.352803	0	0.225362	0.014997	1
Si50	Si	0.852803	0.5	0.225362	0.014997	1
Si51	Si	0.647197	0	0.774638	0.014997	1
Si52	Si	0.147197	0.5	0.774638	0.014997	1
Si53	Si	0.223658	0	0.954956	0.014997	1
Si54	Si	0.723658	0.5	0.954956	0.014997	1
Si55	Si	0.776342	0	0.045044	0.014997	1
Si56	Si	0.276342	0.5	0.045044	0.014997	1
Si57	Si	0.330019	0	0.583366	0.014997	1
Si58	Si	0.830019	0.5	0.583366	0.014997	1
Si59	Si	0.669981	0	0.416634	0.014997	1
Si60	Si	0.169981	0.5	0.416634	0.014997	1

Crystallographic table for IPC-2

Unit Cell: P1 a = 23.7842 Å, b = 14.0815 Å, c = 12.3963 Å, β = 109.13 °

Site Label	Atom Type Symbol	Frac x	Frac y	Frac z	Uiso	Occupancy
Si1	Si	0.307302	0.794321	0.251705	0.015764	1
Si2	Si	0.692698	0.794321	0.748295	0.015764	1
Si3	Si	0.692698	0.205679	0.748295	0.015764	1
Si4	Si	0.307302	0.205679	0.251705	0.015764	1
Si5	Si	0.807302	0.294321	0.251705	0.015764	1
Si6	Si	0.192698	0.294321	0.748295	0.015764	1
Si7	Si	0.192698	0.705679	0.748295	0.015764	1
Si8	Si	0.807302	0.705679	0.251705	0.015764	1
Si9	Si	0.316153	0.788051	0.51389	0.015764	1
Si10	Si	0.683847	0.788051	0.48611	0.015764	1
Si11	Si	0.683847	0.211949	0.48611	0.015764	1
Si12	Si	0.316153	0.211949	0.51389	0.015764	1
Si13	Si	0.816153	0.288051	0.51389	0.015764	1
Si14	Si	0.183847	0.288051	0.48611	0.015764	1
Si15	Si	0.183847	0.711949	0.48611	0.015764	1
Si16	Si	0.816153	0.711949	0.51389	0.015764	1
Si17	Si	0.320016	0.794835	0.862459	0.015764	1
Si18	Si	0.679984	0.794835	0.137541	0.015764	1
Si19	Si	0.679984	0.205165	0.137541	0.015764	1
Si20	Si	0.320016	0.205165	0.862459	0.015764	1
Si21	Si	0.820016	0.294835	0.862459	0.015764	1
Si22	Si	0.179984	0.294835	0.137541	0.015764	1
Si23	Si	0.179984	0.705165	0.137541	0.015764	1
Si24	Si	0.820016	0.705165	0.862459	0.015764	1
Si25	Si	0.36289	0.691533	0.093711	0.015764	1
Si26	Si	0.63711	0.691533	0.906289	0.015764	1
Si27	Si	0.63711	0.308467	0.906289	0.015764	1
Si28	Si	0.36289	0.308467	0.093711	0.015764	1
Si29	Si	0.86289	0.191533	0.093711	0.015764	1
Si30	Si	0.13711	0.191533	0.906289	0.015764	1
Si31	Si	0.13711	0.808467	0.906289	0.015764	1
Si32	Si	0.86289	0.808467	0.093711	0.015764	1
Si33	Si	0.389572	0.691409	0.730857	0.015764	1
Si34	Si	0.610428	0.691409	0.269143	0.015764	1
Si35	Si	0.610428	0.308591	0.269143	0.015764	1
Si36	Si	0.389572	0.308591	0.730857	0.015764	1
Si37	Si	0.889572	0.191409	0.730857	0.015764	1
Si38	Si	0.110428	0.191409	0.269143	0.015764	1
Si39	Si	0.110428	0.808591	0.269143	0.015764	1
Si40	Si	0.889572	0.808591	0.730857	0.015764	1
Si41	Si	0.990261	0.889129	0.122973	0.015764	1
Si42	Si	0.009739	0.889129	0.877027	0.015764	1
Si43	Si	0.009739	0.110871	0.877027	0.015764	1

Si44	Si	0.990261	0.110871	0.122973	0.015764	1
Si45	Si	0.490261	0.389129	0.122973	0.015764	1
Si46	Si	0.509739	0.389129	0.877027	0.015764	1
Si47	Si	0.509739	0.610871	0.877027	0.015764	1
Si48	Si	0.490261	0.610871	0.122973	0.015764	1
Si49	Si	0.270846	0	0.779684	0.015764	1
Si50	Si	0.729154	0	0.220316	0.015764	1
Si51	Si	0.770846	0.5	0.779684	0.015764	1
Si52	Si	0.229154	0.5	0.220316	0.015764	1
Si53	Si	0.209435	0.5	0.827023	0.015764	1
Si54	Si	0.790565	0.5	0.172977	0.015764	1
Si55	Si	0.709435	0	0.827023	0.015764	1
Si56	Si	0.290565	0	0.172977	0.015764	1
Si57	Si	0.311493	0.5	0.711845	0.015764	1
Si58	Si	0.688507	0.5	0.288155	0.015764	1
Si59	Si	0.811493	0	0.711845	0.015764	1
Si60	Si	0.188507	0	0.288155	0.015764	1
Si61	Si	0.216985	0.5	0.45902	0.015764	1
Si62	Si	0.783015	0.5	0.54098	0.015764	1
Si63	Si	0.716985	0	0.45902	0.015764	1
Si64	Si	0.283015	0	0.54098	0.015764	1
Si65	Si	0.299111	0.5	0.063681	0.015764	1
Si66	Si	0.700889	0.5	0.936319	0.015764	1
Si67	Si	0.799111	0	0.063681	0.015764	1
Si68	Si	0.200889	0	0.936319	0.015764	1
O1	O	0.323894	0.902966	0.226131	0.010802	1
O2	O	0.676106	0.902966	0.773869	0.010802	1
O3	O	0.676106	0.097034	0.773869	0.010802	1
O4	O	0.323894	0.097034	0.226131	0.010802	1
O5	O	0.823894	0.402966	0.226131	0.010802	1
O6	O	0.176106	0.402966	0.773869	0.010802	1
O7	O	0.176106	0.597034	0.773869	0.010802	1
O8	O	0.823894	0.597034	0.226131	0.010802	1
O9	O	0.348466	0.723594	0.20332	0.010802	1
O10	O	0.651534	0.723594	0.79668	0.010802	1
O11	O	0.651534	0.276406	0.79668	0.010802	1
O12	O	0.348466	0.276406	0.20332	0.010802	1
O13	O	0.848466	0.223594	0.20332	0.010802	1
O14	O	0.151534	0.223594	0.79668	0.010802	1
O15	O	0.151534	0.776406	0.79668	0.010802	1
O16	O	0.848466	0.776406	0.20332	0.010802	1
O17	O	0.327606	0.773651	0.396527	0.010802	1
O18	O	0.672394	0.773651	0.603473	0.010802	1
O19	O	0.672394	0.226349	0.603473	0.010802	1
O20	O	0.327606	0.226349	0.396527	0.010802	1
O21	O	0.827606	0.273651	0.396527	0.010802	1

O22	O	0.172394	0.273651	0.603473	0.010802	1
O23	O	0.172394	0.726349	0.603473	0.010802	1
O24	O	0.827606	0.726349	0.396527	0.010802	1
O25	O	0.237703	0.760223	0.202792	0.010802	1
O26	O	0.762297	0.760223	0.797208	0.010802	1
O27	O	0.762297	0.239778	0.797208	0.010802	1
O28	O	0.237703	0.239778	0.202792	0.010802	1
O29	O	0.737703	0.260223	0.202792	0.010802	1
O30	O	0.262297	0.260223	0.797208	0.010802	1
O31	O	0.262297	0.739777	0.797208	0.010802	1
O32	O	0.737703	0.739777	0.202792	0.010802	1
O33	O	0.322108	0.90299	0.545336	0.010802	1
O34	O	0.677892	0.90299	0.454664	0.010802	1
O35	O	0.677892	0.09701	0.454664	0.010802	1
O36	O	0.322108	0.09701	0.545336	0.010802	1
O37	O	0.822108	0.40299	0.545336	0.010802	1
O38	O	0.177892	0.40299	0.454664	0.010802	1
O39	O	0.177892	0.59701	0.454664	0.010802	1
O40	O	0.822108	0.59701	0.545336	0.010802	1
O41	O	0.25	0.75	0.5	0.010802	1
O42	O	0.75	0.75	0.5	0.010802	1
O43	O	0.75	0.25	0.5	0.010802	1
O44	O	0.25	0.25	0.5	0.010802	1
O45	O	0.374525	0.75084	0.604944	0.010802	1
O46	O	0.625475	0.75084	0.395056	0.010802	1
O47	O	0.625475	0.24916	0.395056	0.010802	1
O48	O	0.374525	0.24916	0.604944	0.010802	1
O49	O	0.874525	0.25084	0.604944	0.010802	1
O50	O	0.125475	0.25084	0.395056	0.010802	1
O51	O	0.125475	0.74916	0.395056	0.010802	1
O52	O	0.874525	0.74916	0.604944	0.010802	1
O53	O	0.351835	0.769779	0.000351	0.010802	1
O54	O	0.648165	0.769779	0.999649	0.010802	1
O55	O	0.648165	0.230221	0.999649	0.010802	1
O56	O	0.351835	0.230221	0.000351	0.010802	1
O57	O	0.851835	0.269779	0.000351	0.010802	1
O58	O	0.148165	0.269779	0.999649	0.010802	1
O59	O	0.148165	0.730221	0.999649	0.010802	1
O60	O	0.851835	0.730221	0.000351	0.010802	1
O61	O	0.308094	0.907879	0.86389	0.010802	1
O62	O	0.691906	0.907879	0.13611	0.010802	1
O63	O	0.691906	0.092121	0.13611	0.010802	1
O64	O	0.308094	0.092121	0.86389	0.010802	1
O65	O	0.808094	0.407879	0.86389	0.010802	1
O66	O	0.191906	0.407879	0.13611	0.010802	1
O67	O	0.191906	0.592121	0.13611	0.010802	1

O68	O	0.808094	0.592121	0.86389	0.010802	1
O69	O	0.370202	0.771702	0.815912	0.010802	1
O70	O	0.629798	0.771702	0.184088	0.010802	1
O71	O	0.629798	0.228298	0.184088	0.010802	1
O72	O	0.370202	0.228298	0.815912	0.010802	1
O73	O	0.870202	0.271702	0.815912	0.010802	1
O74	O	0.129798	0.271702	0.184088	0.010802	1
O75	O	0.129798	0.728298	0.184088	0.010802	1
O76	O	0.870202	0.728298	0.815912	0.010802	1
O77	O	0.327954	0.595382	0.03547	0.010802	1
O78	O	0.672046	0.595382	0.96453	0.010802	1
O79	O	0.672046	0.404618	0.96453	0.010802	1
O80	O	0.327954	0.404618	0.03547	0.010802	1
O81	O	0.827954	0.095382	0.03547	0.010802	1
O82	O	0.172046	0.095382	0.96453	0.010802	1
O83	O	0.172046	0.904618	0.96453	0.010802	1
O84	O	0.827954	0.904618	0.03547	0.010802	1
O85	O	0.350868	0.588595	0.732602	0.010802	1
O86	O	0.649132	0.588595	0.267398	0.010802	1
O87	O	0.649132	0.411405	0.267398	0.010802	1
O88	O	0.350868	0.411405	0.732602	0.010802	1
O89	O	0.850868	0.088595	0.732602	0.010802	1
O90	O	0.149132	0.088595	0.267398	0.010802	1
O91	O	0.149132	0.911405	0.267398	0.010802	1
O92	O	0.850868	0.911405	0.732602	0.010802	1
O93	O	0.20897	0	0.815396	0.010802	1
O94	O	0.79103	0	0.184604	0.010802	1
O95	O	0.70897	0.5	0.815396	0.010802	1
O96	O	0.29103	0.5	0.184604	0.010802	1
O97	O	0.259988	0	0.64701	0.010802	1
O98	O	0.740012	0	0.35299	0.010802	1
O99	O	0.759988	0.5	0.64701	0.010802	1
O100	O	0.240012	0.5	0.35299	0.010802	1
O101	O	0.237865	0.5	0.957972	0.010802	1
O102	O	0.762135	0.5	0.042028	0.010802	1
O103	O	0.737865	0	0.957972	0.010802	1
O104	O	0.262135	0	0.042028	0.010802	1
O105	O	0.27509	0.5	0.797589	0.010802	1
O106	O	0.72491	0.5	0.202411	0.010802	1
O107	O	0.77509	0	0.797589	0.010802	1
O108	O	0.22491	0	0.202411	0.010802	1
O109	O	0.275875	0.5	0.585319	0.010802	1
O110	O	0.724125	0.5	0.414681	0.010802	1
O111	O	0.775875	0	0.585319	0.010802	1
O112	O	0.224125	0	0.414681	0.010802	1
O113	O	0.044076	0.835596	0.223492	0.010802	1

O114	O	0.955924	0.835596	0.776508	0.010802	1
O115	O	0.955924	0.164404	0.776508	0.010802	1
O116	O	0.044076	0.164404	0.223492	0.010802	1
O117	O	0.544076	0.335596	0.223492	0.010802	1
O118	O	0.455924	0.335596	0.776508	0.010802	1
O119	O	0.455924	0.664404	0.776508	0.010802	1
O120	O	0.544076	0.664404	0.223492	0.010802	1
O121	O	0.931721	0.814249	0.115597	0.010802	1
O122	O	0.068279	0.814249	0.884403	0.010802	1
O123	O	0.068279	0.185751	0.884403	0.010802	1
O124	O	0.931721	0.185751	0.115597	0.010802	1
O125	O	0.431721	0.314249	0.115597	0.010802	1
O126	O	0.568279	0.314249	0.884403	0.010802	1
O127	O	0.568279	0.685751	0.884403	0.010802	1
O128	O	0.431721	0.685751	0.115597	0.010802	1
O129	O	0	0.139491	0	0.010802	1
O130	O	0	0.860509	0	0.010802	1
O131	O	0.5	0.639491	0	0.010802	1
O132	O	0.5	0.360509	0	0.010802	1
O133	O	0.991444	0	0.16937	0.010802	1
O134	O	0.008556	0	0.83063	0.010802	1
O135	O	0.491444	0.5	0.16937	0.010802	1
O136	O	0.508556	0.5	0.83063	0.010802	1

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