Revision 2

Supplementary Material

Reexamination of the structure of opal-A: A combined study of synchrotron X-ray diffraction and pair distribution function analysis

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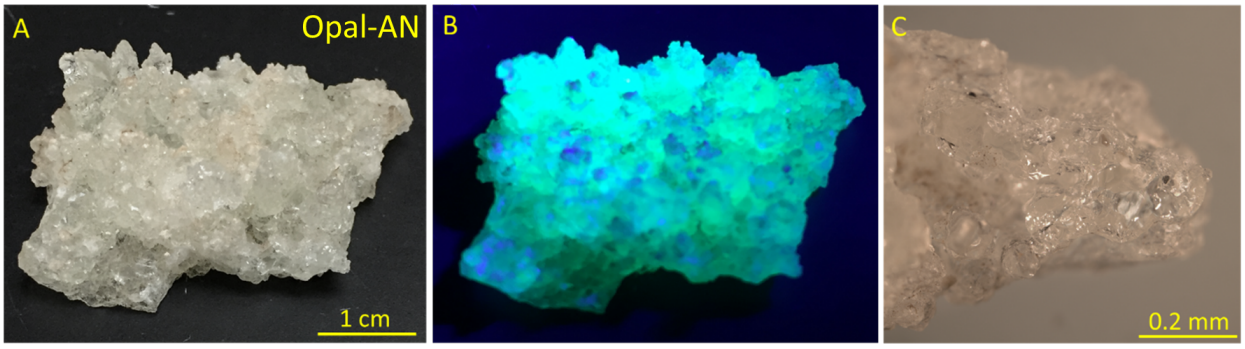

Figure S1. (A) Opal-AN (hyalite) from Chalice mine, North Carolina, (B) its UV light image and (C) close-up image of opal-AN showing globular and botryoidal shapes.

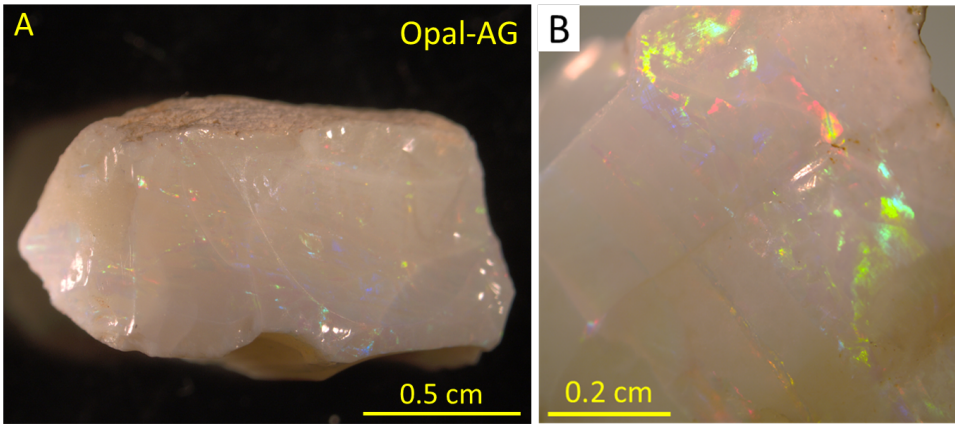

Figure S2. (A) Opal-AG (precious opal) from Spencer mine, Idaho and (B) close-up image of opal-AG displaying iridescent colors.

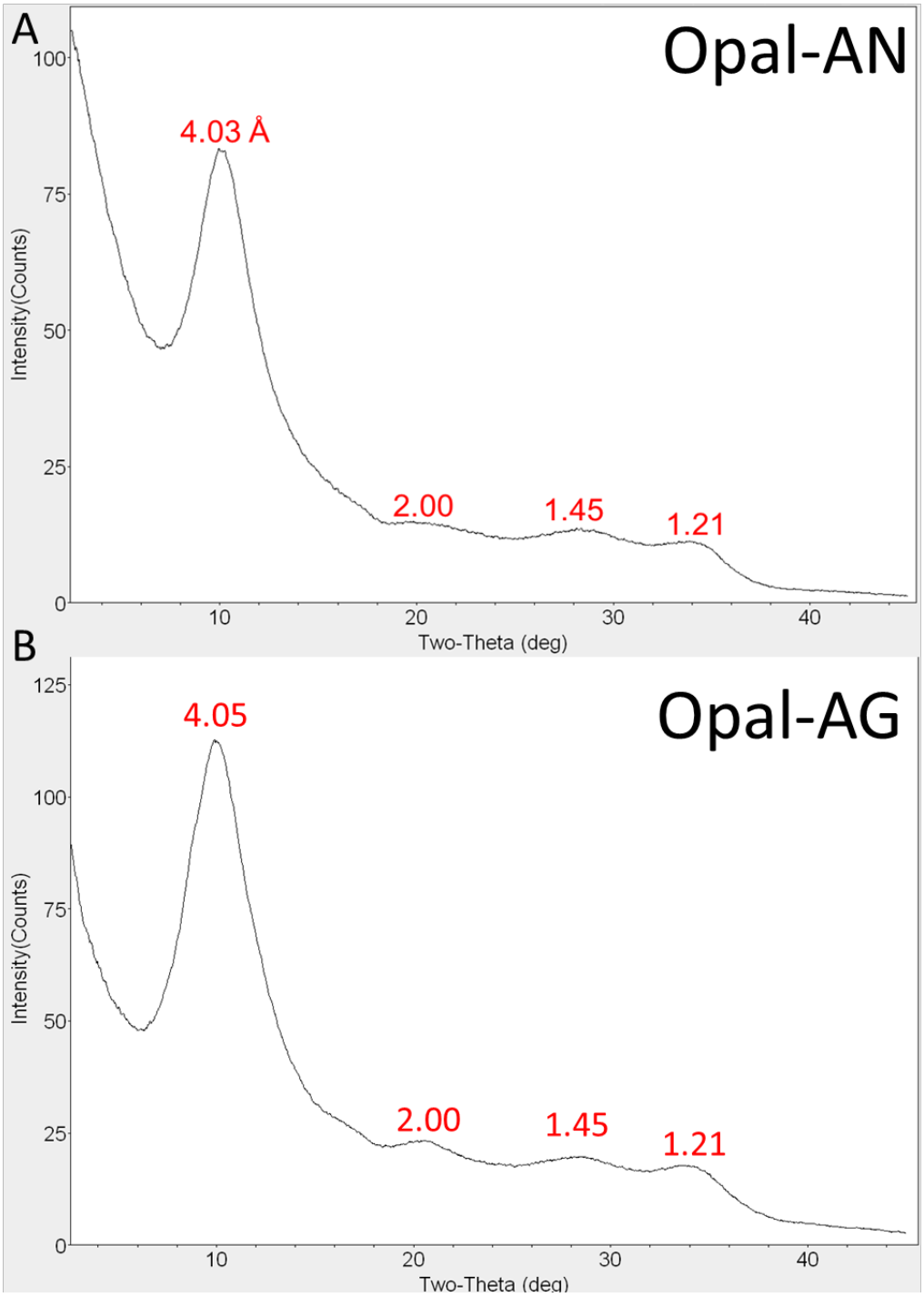

Figure S3. Laboratory XRD patterns (Mo-Kα radiation) of (A) opal-AN and (B) opal-AG.

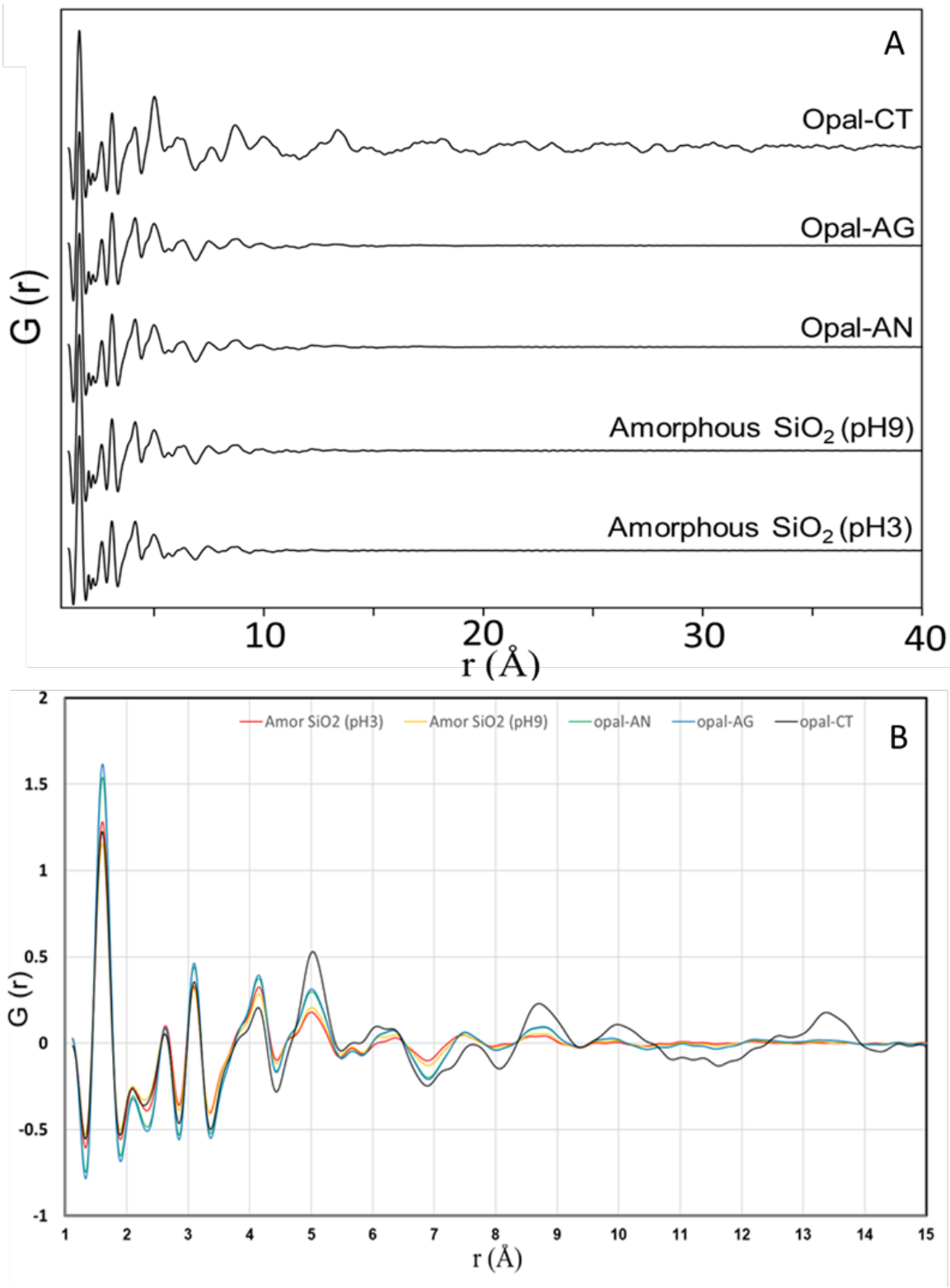

Figure S4. (A) PDF patterns of amorphous silica gels (pH 3 and pH 9), opal-AN, opal-AG, and opal-CT from 1 to 40 Å range. (B) The overlapped PDF patterns of samples from 1 to 15 Å range, indicating that the cluster size of opal-A is bigger than silica gels based on the dumping function.

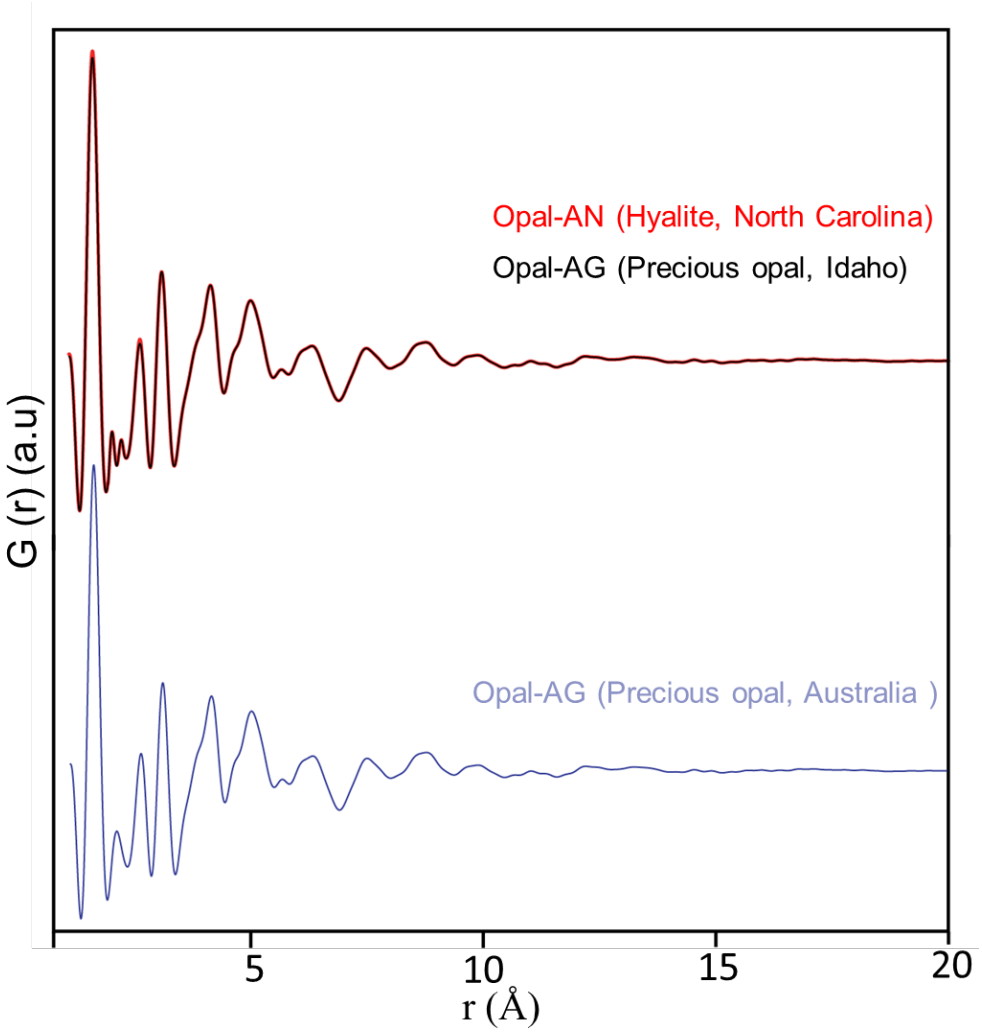

Figure S5. PDF patterns of opal-AN and opal-AG, Idaho (upper, overlapped) and Australian opal-AG (below). The three opals show nearly identical PDF patterns.

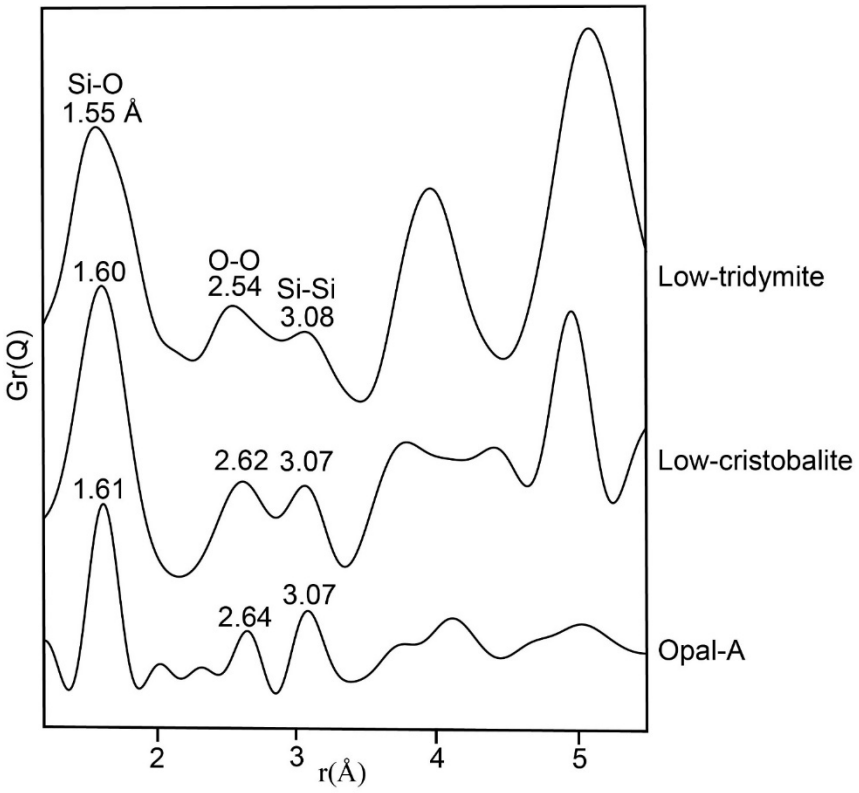

Figure S6. The experimental PDF patterns of low-tridymite (Lee and Xu 2019), low-cristobalite (Lee and Xu 2019) and opal-A (This study) from 1 to 5.5 Å range.

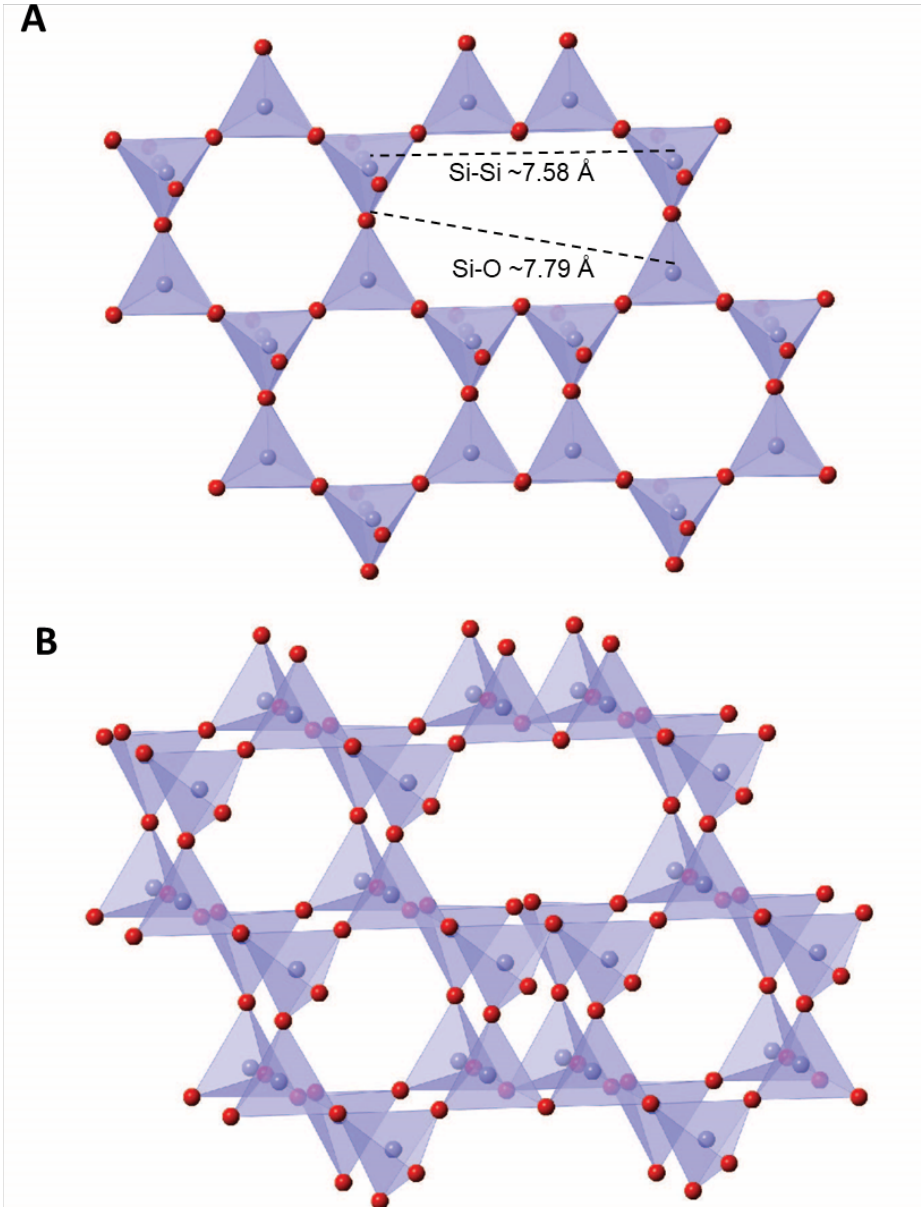

Figure S7. The opal-twinning/stacking faults model showing mixture of four-, six- and eight-membered ring. The eight-members rings can provide additional Si-Si and Si-O correlations around ~7 to ~8 Å.

Table S1. Major element compositions of opal-AN and opal-AG obtained via EPMA.

	Opal-AN						Opal-AG					
	1	2	3	4	5	Average	1	2	3	4	5	Average
Elemental composition (wt. %)												
Si	40.75	40.64	40.87	40.98	41.05	40.86	41.72	41.42	41.29	41.80	42.42	41.73
Al	0.02	0.00	0.02	0.02	0.01	0.01	0.92	0.93	0.93	0.95	0.92	0.93
Fe	0.00	0.01	0.00	0.02	0.03	0.01	0.09	0.05	0.04	0.06	0.08	0.06
Mg	0.26	0.31	0.13	0.28	0.28	0.25	0.03	0.04	0.03	0.02	0.02	0.03
Ca	0.18	0.19	0.17	0.21	0.18	0.19	0.26	0.27	0.28	0.27	0.26	0.27
Na	0.02	0.02	0.02	0.01	0.00	0.01	0.04	0.14	0.12	0.10	0.13	0.11
K	0.00	0.00	0.00	0.02	0.00	0.00	0.07	0.11	0.10	0.09	0.09	0.09
O	53.44	53.87	52.52	55.52	55.84	54.24	54.96	54.16	54.19	54.51	54.80	54.52
Total	94.67	95.05	93.73	97.05	97.39	95.58	98.08	97.12	96.97	97.80	98.72	97.74
Oxide composition (wt. %)												
SiO_2	87.19	86.95	87.43	87.66	87.83	87.41	89.24	88.61	88.32	89.42	90.75	89.27
Al_2O_3	0.03	0.01	0.03	0.03	0.02	0.02	1.73	1.77	1.75	1.79	1.73	1.75
Fe_2O_3	0.00	0.02	0.00	0.02	0.03	0.01	0.12	0.07	0.05	0.08	0.10	0.08
MgO	0.44	0.52	0.21	0.46	0.46	0.42	0.06	0.06	0.05	0.04	0.04	0.05
CaO	0.25	0.26	0.24	0.29	0.26	0.26	0.36	0.37	0.39	0.38	0.36	0.37
Na_2O	0.03	0.03	0.03	0.02	0.00	0.02	0.05	0.18	0.17	0.13	0.18	0.14
K_2O	0.00	0.00	0.00	0.02	0.00	0.00	0.08	0.13	0.12	0.11	0.11	0.11
*H_2O	7.61	8.18	6.52	9.62	9.92	8.37	7.25	6.66	6.89	6.59	6.14	6.71
Total	95.54	95.97	94.46	98.13	98.51	96.52	98.90	97.86	97.74	98.53	99.41	98.49

*Note: H_2O is calculated by analysing the O by EPMA and assigning the excessive O to H_2O.

Table S2. The mass fractions of each phases of opal-A based on scale factors from PDF refinement (Fig. 5)

Phases	Fig. 5A	Fig. 5B	Fig. 5C	Fig. 5D
Cristobalite	47.3%	44.3%	46.9%	46.1%
Tridymite	35.1%	32.9%	31.3%	32.6%
Coesite	17.6%	15.7%	14.3%	14.9%
Twinning/Stacking model		7.1%	7.5%	6.4%
	100.0%	100.0%	100.0%	100.0%

Supplementary Data. Crystal structure data of cristobalite, tridymite, mixed layers, and twinning supercell for opal-A refinement.

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_cell_length_b                         7.424(5)
_cell_length_c                         7.424(5)
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_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           409.179486
_space_group_name_H-M_alt              'F d -3 m'
_space_group_IT_number                 227

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  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
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  O1          1.0     0.000000     0.000000     0.000000    Biso  1.000000 O


#=============================================================================
# CRYSTAL DATA
#-----------------------------------------------------------------------
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_cell_length_c                         8.5819(8)
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   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
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   _atom_site_type_symbol
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   O1         1.0     0.500000     0.500000     0.000000     Biso  1.000000 O
   O2         1.0     0.000000     0.500000     0.000000     Biso  1.000000 O
   O3         1.0     0.000000     0.500000     0.500000     Biso  1.000000 O
   O4         1.0     0.333333     0.666667     0.250000     Biso  1.000000 O
   O5         1.0     0.666667     0.333333     0.750000     Biso  1.000000 O
   O6         1.0     0.500000     0.000000     0.000000     Biso  1.000000 O
   O7         1.0     0.500000     0.500000     0.500000     Biso  1.000000 O
   Si8        1.0     0.333333     0.666667     0.437576     Biso  1.000000 Si
   Si9        1.0     0.666667     0.333333     0.937576     Biso  1.000000 Si
   Si10       1.0     0.666667     0.333333     0.562424     Biso  1.000000 Si
   Si11       1.0     0.333333     0.666667     0.062424     Biso  1.000000 Si
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   O4         1.0     0.613200     0.270700     0.318500    Uiso  0.012700 O
   O5         1.0     0.616500     0.274900     0.684800    Uiso  0.012700 O
   O6         1.0     0.724400     0.465700     0.315300    Uiso  0.012700 O
   O7         1.0     0.727800     0.469800     0.681700    Uiso  0.012700 O
   O8         1.0     0.835800     0.660700     0.312100    Uiso  0.012700 O
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O14	1.0	0.502500	0.469200	0.683700	Uiso	0.012700 O
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O80	1.0	0.212800	0.487200	0.586100	Uiso	0.012700	O
O81	1.0	0.324100	0.682100	0.582900	Uiso	0.012700	O
O82	1.0	0.283800	0.218300	0.422100	Uiso	0.012700	O

O83	1.0	0.395200	0.413300	0.418800	Uiso	0.012700 O
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O85	1.0	0.267200	0.585700	0.601300	Uiso	0.012700 O
O86	1.0	0.378400	0.780700	0.598100	Uiso	0.012700 O
O87	1.0	0.112500	0.315800	0.405700	Uiso	0.012700 O
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O89	1.0	0.335200	0.705800	0.399300	Uiso	0.012700 O
O90	1.0	0.326700	0.292800	0.587200	Uiso	0.012700 O
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O92	1.0	0.550100	0.680900	0.582400	Uiso	0.012700 O
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O94	1.0	0.101400	0.292100	0.589300	Uiso	0.012700 O
O95	1.0	0.392500	0.802700	0.414400	Uiso	0.012700 O
O96	1.0	0.269700	0.196300	0.605600	Uiso	0.012700 O
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Si3	1.0	0.392800	0.345600	0.434100	Uiso	0.012700 Si
Si4	1.0	0.158400	0.458700	0.618100	Uiso	0.012700 Si
Si5	1.0	0.269700	0.653700	0.614900	Uiso	0.012700 Si
Si6	1.0	0.280500	0.279700	0.390100	Uiso	0.012700 Si
Si7	1.0	0.391800	0.474700	0.386900	Uiso	0.012700 Si
Si8	1.0	0.158400	0.328600	0.573900	Uiso	0.012700 Si
Si9	1.0	0.166600	0.474000	0.389000	Uiso	0.012700 Si
Si10	1.0	0.383700	0.459400	0.616100	Uiso	0.012700 Si
Si11	1.0	0.381100	0.718700	0.567500	Uiso	0.012700 Si
Si12	1.0	0.167400	0.344900	0.436100	Uiso	0.012700 Si
Si13	1.0	0.278800	0.540000	0.432900	Uiso	0.012700 Si
Si14	1.0	0.272300	0.264400	0.619300	Uiso	0.012700 Si
Si15	1.0	0.269800	0.523600	0.570700	Uiso	0.012700 Si
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Si19	1.0	0.493800	0.719000	0.566500	Uiso	0.012700 Si
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Si21	1.0	0.833000	0.525300	0.565700	Uiso	0.012700 Si
Si22	1.0	0.502800	0.735400	0.428700	Uiso	0.012700 Si
Si23	1.0	0.730700	0.346700	0.431000	Uiso	0.012700 Si

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  Si24      1.0   0.842000   0.541600   0.427800   Uiso  0.012700 Si
  Si25      1.0   0.496300   0.459700   0.615100   Uiso  0.012700 Si
  Si26      1.0   0.607700   0.654700   0.611900   Uiso  0.012700 Si
  Si27      1.0   0.618500   0.280700   0.387100   Uiso  0.012700 Si
  Si28      1.0   0.729700   0.475700   0.383900   Uiso  0.012700 Si
  Si29      1.0   0.841100   0.670800   0.380700   Uiso  0.012700 Si
  Si30      1.0   0.496500   0.329600   0.570900   Uiso  0.012700 Si
  Si31      1.0   0.607800   0.524600   0.567700   Uiso  0.012700 Si
  Si32      1.0   0.719000   0.719700   0.564500   Uiso  0.012700 Si
  Si33      1.0   0.505500   0.345900   0.433100   Uiso  0.012700 Si
  Si34      1.0   0.616700   0.541000   0.429800   Uiso  0.012700 Si
  Si35      1.0   0.728000   0.736000   0.426600   Uiso  0.012700 Si
  Si36      1.0   0.610300   0.265400   0.616200   Uiso  0.012700 Si
  Si37      1.0   0.721600   0.460400   0.613000   Uiso  0.012700 Si
  Si38      1.0   0.832900   0.655400   0.609900   Uiso  0.012700 Si


#=============================================================================
# CRYSTAL DATA
#-----------------------------------------------------------------------
data_Opal_mixed_layers

_chemical_name_common                  'Opal_mixed layers'
_cell_length_a                         30.120001
_cell_length_b                         30.014999
_cell_length_c                         20.010000
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           18090.076861
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'
```

```
loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  O1      1.0   0.311600   0.550100   0.759800   Biso  1.000000 O
  O2      1.0   0.311600   0.551200   0.499400   Biso  1.000000 O
  O3      1.0   0.311600   0.552400   0.238900   Biso  1.000000 O
  O4      1.0   0.613900   0.554400   0.759800   Biso  1.000000 O
  O5      1.0   0.613900   0.555600   0.499300   Biso  1.000000 O
  O6      1.0   0.613900   0.556700   0.238900   Biso  1.000000 O
  O7      1.0   0.415500   0.410000   0.758500   Biso  1.000000 O
  O8      1.0   0.411300   0.693000   0.761200   Biso  1.000000 O
  O9      1.0   0.415500   0.411100   0.497900   Biso  1.000000 O
  O10     1.0   0.411300   0.694100   0.500700   Biso  1.000000 O
  O11     1.0   0.415500   0.412200   0.237400   Biso  1.000000 O
  O12     1.0   0.411300   0.695300   0.240200   Biso  1.000000 O
  O13     1.0   0.717800   0.414400   0.758500   Biso  1.000000 O
  O14     1.0   0.713600   0.697400   0.761100   Biso  1.000000 O
  O15     1.0   0.717800   0.415600   0.497900   Biso  1.000000 O
  O16     1.0   0.713600   0.698600   0.500700   Biso  1.000000 O
  O17     1.0   0.717800   0.416700   0.237400   Biso  1.000000 O
  O18     1.0   0.713600   0.699700   0.240200   Biso  1.000000 O
  O19     1.0   0.462700   0.552800   0.629600   Biso  1.000000 O
  O20     1.0   0.462700   0.553900   0.369100   Biso  1.000000 O
  O21     1.0   0.264300   0.408400   0.628100   Biso  1.000000 O
  O22     1.0   0.260200   0.691400   0.630900   Biso  1.000000 O
  O23     1.0   0.264300   0.409600   0.367700   Biso  1.000000 O
  O24     1.0   0.260200   0.692600   0.370500   Biso  1.000000 O
  O25     1.0   0.566600   0.412800   0.628100   Biso  1.000000 O
  O26     1.0   0.562500   0.695800   0.630900   Biso  1.000000 O
  O27     1.0   0.566600   0.413900   0.367700   Biso  1.000000 O
  O28     1.0   0.562500   0.696900   0.370500   Biso  1.000000 O
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O29	1.0	0.212400	0.478400	0.613700	Biso	1.000000	O
O30	1.0	0.212300	0.479600	0.353100	Biso	1.000000	O
O31	1.0	0.514700	0.482900	0.613600	Biso	1.000000	O
O32	1.0	0.514600	0.484000	0.353100	Biso	1.000000	O
O33	1.0	0.210400	0.619900	0.645500	Biso	1.000000	O
O34	1.0	0.210200	0.621000	0.385100	Biso	1.000000	O
O35	1.0	0.512700	0.624200	0.645500	Biso	1.000000	O
O36	1.0	0.512600	0.625400	0.385100	Biso	1.000000	O
O37	1.0	0.363600	0.480100	0.743900	Biso	1.000000	O
O38	1.0	0.363500	0.481200	0.483300	Biso	1.000000	O
O39	1.0	0.363500	0.482400	0.222800	Biso	1.000000	O
O40	1.0	0.665900	0.484500	0.743900	Biso	1.000000	O
O41	1.0	0.665800	0.485700	0.483300	Biso	1.000000	O
O42	1.0	0.665800	0.486800	0.222800	Biso	1.000000	O
O43	1.0	0.361500	0.621400	0.775800	Biso	1.000000	O
O44	1.0	0.361400	0.622600	0.515300	Biso	1.000000	O
O45	1.0	0.361400	0.623700	0.254800	Biso	1.000000	O
O46	1.0	0.663800	0.625900	0.775800	Biso	1.000000	O
O47	1.0	0.663700	0.627000	0.515300	Biso	1.000000	O
O48	1.0	0.663700	0.628100	0.254800	Biso	1.000000	O
O49	1.0	0.288600	0.485800	0.677400	Biso	1.000000	O
O50	1.0	0.288500	0.486900	0.416900	Biso	1.000000	O
O51	1.0	0.590900	0.490200	0.677400	Biso	1.000000	O
O52	1.0	0.590800	0.491300	0.416900	Biso	1.000000	O
O53	1.0	0.436300	0.629900	0.581900	Biso	1.000000	O
O54	1.0	0.436200	0.631000	0.321400	Biso	1.000000	O
O55	1.0	0.738600	0.634200	0.581900	Biso	1.000000	O
O56	1.0	0.738500	0.635400	0.321400	Biso	1.000000	O
O57	1.0	0.438600	0.475000	0.677300	Biso	1.000000	O
O58	1.0	0.438500	0.476100	0.416800	Biso	1.000000	O
O59	1.0	0.740900	0.479400	0.677300	Biso	1.000000	O
O60	1.0	0.740800	0.480500	0.416800	Biso	1.000000	O
O61	1.0	0.286600	0.614700	0.581800	Biso	1.000000	O
O62	1.0	0.286600	0.615800	0.321300	Biso	1.000000	O
O63	1.0	0.588900	0.619200	0.581800	Biso	1.000000	O
O64	1.0	0.588900	0.620300	0.321300	Biso	1.000000	O
O65	1.0	0.439700	0.487400	0.807600	Biso	1.000000	O

O66	1.0	0.439600	0.488600	0.547200	Biso	1.000000	O
O67	1.0	0.439600	0.489700	0.286700	Biso	1.000000	O
O68	1.0	0.742000	0.491800	0.807600	Biso	1.000000	O
O69	1.0	0.741900	0.492900	0.547200	Biso	1.000000	O
O70	1.0	0.741900	0.494000	0.286700	Biso	1.000000	O
O71	1.0	0.285200	0.627100	0.712100	Biso	1.000000	O
O72	1.0	0.285200	0.628200	0.451700	Biso	1.000000	O
O73	1.0	0.285000	0.629400	0.191200	Biso	1.000000	O
O74	1.0	0.587500	0.631500	0.712100	Biso	1.000000	O
O75	1.0	0.587500	0.632600	0.451600	Biso	1.000000	O
O76	1.0	0.587400	0.633700	0.191200	Biso	1.000000	O
O77	1.0	0.287400	0.472200	0.807500	Biso	1.000000	O
O78	1.0	0.287300	0.473400	0.547100	Biso	1.000000	O
O79	1.0	0.287300	0.474500	0.286600	Biso	1.000000	O
O80	1.0	0.589700	0.476600	0.807500	Biso	1.000000	O
O81	1.0	0.589600	0.477800	0.547000	Biso	1.000000	O
O82	1.0	0.589600	0.478900	0.286600	Biso	1.000000	O
O83	1.0	0.437900	0.616400	0.712000	Biso	1.000000	O
O84	1.0	0.437800	0.617500	0.451500	Biso	1.000000	O
O85	1.0	0.437800	0.618600	0.191100	Biso	1.000000	O
O86	1.0	0.740200	0.620700	0.712000	Biso	1.000000	O
O87	1.0	0.740100	0.621900	0.451500	Biso	1.000000	O
O88	1.0	0.740100	0.623100	0.191000	Biso	1.000000	O
O89	1.0	0.438500	0.477300	0.156300	Biso	1.000000	O
O90	1.0	0.740800	0.481600	0.156300	Biso	1.000000	O
O91	1.0	0.286700	0.613600	0.842200	Biso	1.000000	O
O92	1.0	0.589000	0.618000	0.842200	Biso	1.000000	O
O93	1.0	0.288500	0.488000	0.156500	Biso	1.000000	O
O94	1.0	0.590800	0.492500	0.156500	Biso	1.000000	O
O95	1.0	0.436300	0.628800	0.842400	Biso	1.000000	O
O96	1.0	0.738600	0.633100	0.842300	Biso	1.000000	O
O97	1.0	0.517300	0.272200	0.236100	Biso	1.000000	O
O98	1.0	0.517300	0.271100	0.496500	Biso	1.000000	O
O99	1.0	0.517300	0.270000	0.757000	Biso	1.000000	O
O100	1.0	0.668500	0.273900	0.366300	Biso	1.000000	O
O101	1.0	0.668500	0.272800	0.626800	Biso	1.000000	O
O102	1.0	0.366200	0.269500	0.366300	Biso	1.000000	O

O103	1.0	0.366200	0.268300	0.626800	Biso	1.000000	O
O104	1.0	0.618500	0.202300	0.380900	Biso	1.000000	O
O105	1.0	0.618500	0.201200	0.641400	Biso	1.000000	O
O106	1.0	0.316200	0.197900	0.380900	Biso	1.000000	O
O107	1.0	0.316200	0.196800	0.641400	Biso	1.000000	O
O108	1.0	0.616500	0.343900	0.351700	Biso	1.000000	O
O109	1.0	0.616500	0.342800	0.612200	Biso	1.000000	O
O110	1.0	0.314200	0.339600	0.351700	Biso	1.000000	O
O111	1.0	0.314200	0.338400	0.612200	Biso	1.000000	O
O112	1.0	0.467400	0.200700	0.250700	Biso	1.000000	O
O113	1.0	0.467400	0.199600	0.511100	Biso	1.000000	O
O114	1.0	0.467400	0.198400	0.771600	Biso	1.000000	O
O115	1.0	0.767600	0.346700	0.221500	Biso	1.000000	O
O116	1.0	0.767600	0.345600	0.481900	Biso	1.000000	O
O117	1.0	0.767600	0.344400	0.742400	Biso	1.000000	O
O118	1.0	0.465300	0.342300	0.221500	Biso	1.000000	O
O119	1.0	0.465300	0.341200	0.482000	Biso	1.000000	O
O120	1.0	0.465400	0.340100	0.742400	Biso	1.000000	O
O121	1.0	0.542200	0.207900	0.317200	Biso	1.000000	O
O122	1.0	0.542200	0.206800	0.577600	Biso	1.000000	O
O123	1.0	0.692600	0.351200	0.415600	Biso	1.000000	O
O124	1.0	0.692600	0.350100	0.676000	Biso	1.000000	O
O125	1.0	0.390300	0.346900	0.415600	Biso	1.000000	O
O126	1.0	0.390300	0.345800	0.676100	Biso	1.000000	O
O127	1.0	0.694900	0.197200	0.317000	Biso	1.000000	O
O128	1.0	0.694900	0.196000	0.577500	Biso	1.000000	O
O129	1.0	0.392600	0.192800	0.317000	Biso	1.000000	O
O130	1.0	0.392600	0.191700	0.577500	Biso	1.000000	O
O131	1.0	0.540300	0.336000	0.415500	Biso	1.000000	O
O132	1.0	0.540300	0.334900	0.675900	Biso	1.000000	O
O133	1.0	0.238000	0.331700	0.415500	Biso	1.000000	O
O134	1.0	0.238000	0.330600	0.675900	Biso	1.000000	O
O135	1.0	0.693300	0.209600	0.447400	Biso	1.000000	O
O136	1.0	0.693400	0.208400	0.707900	Biso	1.000000	O
O137	1.0	0.391000	0.205200	0.447400	Biso	1.000000	O
O138	1.0	0.391100	0.204100	0.707900	Biso	1.000000	O
O139	1.0	0.541500	0.349600	0.285200	Biso	1.000000	O

O140	1.0	0.541500	0.348400	0.545800	Biso	1.000000	O
O141	1.0	0.541600	0.347300	0.806300	Biso	1.000000	O
O142	1.0	0.239200	0.345200	0.285400	Biso	1.000000	O
O143	1.0	0.239200	0.344100	0.545800	Biso	1.000000	O
O144	1.0	0.543700	0.195600	0.186800	Biso	1.000000	O
O145	1.0	0.543700	0.194500	0.447300	Biso	1.000000	O
O146	1.0	0.543700	0.193300	0.707700	Biso	1.000000	O
O147	1.0	0.691500	0.338800	0.285100	Biso	1.000000	O
O148	1.0	0.691500	0.337700	0.545700	Biso	1.000000	O
O149	1.0	0.691600	0.336600	0.806200	Biso	1.000000	O
O150	1.0	0.389200	0.334500	0.285100	Biso	1.000000	O
O151	1.0	0.389200	0.333400	0.545700	Biso	1.000000	O
O152	1.0	0.389300	0.332200	0.806200	Biso	1.000000	O
O153	1.0	0.540300	0.337200	0.154900	Biso	1.000000	O
O154	1.0	0.542300	0.205700	0.838100	Biso	1.000000	O
O155	1.0	0.692600	0.352400	0.155000	Biso	1.000000	O
O156	1.0	0.390300	0.348000	0.155000	Biso	1.000000	O
O157	1.0	0.610200	0.768400	0.386500	Biso	1.000000	O
O158	1.0	0.610400	0.767100	0.647000	Biso	1.000000	O
O159	1.0	0.307900	0.763900	0.386500	Biso	1.000000	O
O160	1.0	0.308000	0.762800	0.647000	Biso	1.000000	O
O161	1.0	0.761400	0.771000	0.256300	Biso	1.000000	O
O162	1.0	0.761400	0.769900	0.516700	Biso	1.000000	O
O163	1.0	0.761500	0.768800	0.777200	Biso	1.000000	O
O164	1.0	0.459100	0.766700	0.256300	Biso	1.000000	O
O165	1.0	0.459200	0.765600	0.516700	Biso	1.000000	O
O166	1.0	0.459200	0.764400	0.777200	Biso	1.000000	O
O167	1.0	0.533900	0.773900	0.322800	Biso	1.000000	O
O168	1.0	0.534000	0.772800	0.583200	Biso	1.000000	O
O169	1.0	0.231700	0.769600	0.322800	Biso	1.000000	O
O170	1.0	0.231700	0.768500	0.583200	Biso	1.000000	O
O171	1.0	0.686600	0.763200	0.322600	Biso	1.000000	O
O172	1.0	0.686600	0.762000	0.583100	Biso	1.000000	O
O173	1.0	0.384300	0.758800	0.322600	Biso	1.000000	O
O174	1.0	0.384300	0.757700	0.583100	Biso	1.000000	O
O175	1.0	0.685000	0.776700	0.192500	Biso	1.000000	O
O176	1.0	0.685200	0.775600	0.453000	Biso	1.000000	O

O177	1.0	0.685200	0.774500	0.713500	Biso	1.000000 O
O178	1.0	0.382700	0.772300	0.192500	Biso	1.000000 O
O179	1.0	0.382800	0.771100	0.453000	Biso	1.000000 O
O180	1.0	0.382800	0.770000	0.713500	Biso	1.000000 O
O181	1.0	0.535400	0.760400	0.452900	Biso	1.000000 O
O182	1.0	0.535600	0.759300	0.713300	Biso	1.000000 O
O183	1.0	0.233100	0.756100	0.452900	Biso	1.000000 O
O184	1.0	0.233200	0.754900	0.713400	Biso	1.000000 O
O185	1.0	0.686700	0.760900	0.843600	Biso	1.000000 O
O186	1.0	0.384400	0.756600	0.843600	Biso	1.000000 O
Si188	1.0	0.263200	0.462700	0.356200	Biso	1.000000 Si
Si189	1.0	0.565500	0.465900	0.616800	Biso	1.000000 Si
Si187	1.0	0.263200	0.461600	0.616800	Biso	1.000000 Si
Si190	1.0	0.565500	0.467000	0.356200	Biso	1.000000 Si
Si191	1.0	0.462300	0.605900	0.642000	Biso	1.000000 Si
Si192	1.0	0.462300	0.607100	0.381600	Biso	1.000000 Si
Si193	1.0	0.463900	0.499700	0.617100	Biso	1.000000 Si
Si194	1.0	0.463900	0.500900	0.356700	Biso	1.000000 Si
Si195	1.0	0.260600	0.638200	0.642400	Biso	1.000000 Si
Si196	1.0	0.365000	0.322600	0.354900	Biso	1.000000 Si
Si197	1.0	0.260600	0.639300	0.381900	Biso	1.000000 Si
Si198	1.0	0.667300	0.327000	0.354900	Biso	1.000000 Si
Si199	1.0	0.667300	0.325900	0.615300	Biso	1.000000 Si
Si200	1.0	0.565700	0.360900	0.355200	Biso	1.000000 Si
Si201	1.0	0.565700	0.359700	0.615700	Biso	1.000000 Si
Si202	1.0	0.263400	0.356400	0.355200	Biso	1.000000 Si
Si203	1.0	0.365000	0.321500	0.615300	Biso	1.000000 Si
Si204	1.0	0.668900	0.220600	0.377700	Biso	1.000000 Si
Si205	1.0	0.668900	0.219500	0.638200	Biso	1.000000 Si
Si206	1.0	0.366600	0.216300	0.377800	Biso	1.000000 Si
Si207	1.0	0.366600	0.215200	0.638200	Biso	1.000000 Si
Si208	1.0	0.562900	0.642600	0.642400	Biso	1.000000 Si
Si209	1.0	0.562900	0.643800	0.381900	Biso	1.000000 Si
Si210	1.0	0.263400	0.355300	0.615700	Biso	1.000000 Si
Si211	1.0	0.517600	0.219100	0.247500	Biso	1.000000 Si
Si212	1.0	0.716900	0.363500	0.225000	Biso	1.000000 Si
Si213	1.0	0.516200	0.324300	0.485100	Biso	1.000000 Si

Si214	1.0	0.516100	0.325400	0.224600	Biso	1.000000 Si
Si215	1.0	0.517700	0.218000	0.508000	Biso	1.000000 Si
Si216	1.0	0.516200	0.323100	0.745600	Biso	1.000000 Si
Si217	1.0	0.517700	0.216800	0.768500	Biso	1.000000 Si
Si218	1.0	0.716900	0.362400	0.485400	Biso	1.000000 Si
Si219	1.0	0.414500	0.358100	0.485400	Biso	1.000000 Si
Si220	1.0	0.414500	0.359200	0.225000	Biso	1.000000 Si
Si221	1.0	0.414500	0.356900	0.745900	Biso	1.000000 Si
Si222	1.0	0.716900	0.361300	0.745900	Biso	1.000000 Si
Si223	1.0	0.414300	0.463200	0.747000	Biso	1.000000 Si
Si224	1.0	0.414300	0.464400	0.486600	Biso	1.000000 Si
Si225	1.0	0.414300	0.465500	0.226000	Biso	1.000000 Si
Si226	1.0	0.716600	0.467600	0.747000	Biso	1.000000 Si
Si227	1.0	0.716600	0.468700	0.486500	Biso	1.000000 Si
Si228	1.0	0.716600	0.469800	0.226000	Biso	1.000000 Si
Si229	1.0	0.311200	0.603100	0.772300	Biso	1.000000 Si
Si230	1.0	0.311200	0.604300	0.511800	Biso	1.000000 Si
Si231	1.0	0.311200	0.605400	0.251300	Biso	1.000000 Si
Si232	1.0	0.613500	0.607500	0.772300	Biso	1.000000 Si
Si233	1.0	0.613500	0.608600	0.511800	Biso	1.000000 Si
Si234	1.0	0.257700	0.744500	0.643500	Biso	1.000000 Si
Si235	1.0	0.613500	0.609700	0.251300	Biso	1.000000 Si
Si236	1.0	0.560000	0.748800	0.643500	Biso	1.000000 Si
Si237	1.0	0.560000	0.750000	0.383000	Biso	1.000000 Si
Si238	1.0	0.257700	0.745600	0.383000	Biso	1.000000 Si
Si239	1.0	0.312700	0.496900	0.747400	Biso	1.000000 Si
Si240	1.0	0.711200	0.751600	0.513200	Biso	1.000000 Si
Si241	1.0	0.711200	0.750500	0.773700	Biso	1.000000 Si
Si242	1.0	0.711200	0.752700	0.252700	Biso	1.000000 Si
Si243	1.0	0.312700	0.498100	0.486900	Biso	1.000000 Si
Si244	1.0	0.408900	0.746000	0.773700	Biso	1.000000 Si
Si245	1.0	0.408900	0.747200	0.513300	Biso	1.000000 Si
Si246	1.0	0.408900	0.748300	0.252700	Biso	1.000000 Si
Si247	1.0	0.312700	0.499200	0.226400	Biso	1.000000 Si
Si248	1.0	0.615000	0.501400	0.747300	Biso	1.000000 Si
Si249	1.0	0.615000	0.502500	0.486900	Biso	1.000000 Si
Si251	1.0	0.411800	0.639800	0.772600	Biso	1.000000 Si

Si252	1.0	0.411800	0.641000	0.512100	Biso	1.000000 Si
Si253	1.0	0.411800	0.642100	0.251700	Biso	1.000000 Si
Si254	1.0	0.714100	0.644200	0.772600	Biso	1.000000 Si
Si255	1.0	0.714100	0.645400	0.512100	Biso	1.000000 Si
Si256	1.0	0.714100	0.646600	0.251700	Biso	1.000000 Si
Si250	1.0	0.615000	0.503700	0.226400	Biso	1.000000 Si

REFERENCES

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