

Electronic Supplementary Information

**DFT and SISSO studies on the CO₂ cycloaddition reaction to ethylene oxide catalyzed by
intraframework M(II)-BEA zeolites**

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Table S1. Optimized geometrical parameters and NBO charges of the species involved in the CO₂ cycloaddition to EO over Ni-DeAlBEA in the presence of TMAI.

Parameters	ISOLATED	ADS1	ADS2	TS1	INT1	CO ₂ -INT1	TS2	INT2	TS3	PROD
Distance (Å)										
Ni-Oa	1.83	1.89	1.90	1.91	1.93	1.94	1.95	1.95	1.93	1.91
Ni-Ob	1.81	1.88	1.89	1.88	1.92	1.91	1.94	1.92	1.89	1.85
Ni-Oc	1.96	1.99	1.99	2.03	2.06	2.04	2.01	2.00	1.99	2.01
C1-C2	1.46	1.45	1.44	1.45	1.52	1.52	1.51	1.52	1.50	1.53
C1-O1	1.42	1.45	1.47	1.42	1.38	1.38	1.39	1.42	1.43	1.46
C2-O1	1.42	1.45	1.47	1.82	2.30	2.31	-	-	-	-
C2-O2	-	-	-	-	-	-	-	3.44	2.00	1.47
C3-O1	-	-	-	-	-	2.63	1.83	1.54	1.38	1.33
C3-O2	1.17	-	-	-	-	1.17	1.19	1.21	1.26	1.31
C3-O3	1.17	-	-	-	-	1.17	1.21	1.25	1.25	1.23
I-C2	-	-	3.42	2.88	2.26	2.26	2.22	2.21	2.74	3.53
I-N	-	-	4.04	4.06	4.14	4.18	4.12	4.18	4.06	4.03
Ni-O1	-	2.02	1.97	1.96	1.89	1.91	2.00	2.20	2.26	2.54
Ni-O3	-	-	-	-	-	3.14	2.29	2.06	2.11	2.05
Angle (°)										
C2-O2-C3	59.1	60.0	60.7	78.9	104.9	-	-	-	-	-
C2-C1-O1	-	-	-	-	-	-	-	79.0	99.8	108.9
O1-C3-O2	-	-	-	-	-	93.6	109.8	118.3	115.4	114.2
O1-C3-O3	-	-	-	-	-	90.8	99.6	105.4	112.5	120.7
O2-C3-O3	180.0	-	-	-	-	175.5	150.6	136.2	132.1	125.2
I-C2-C1	-	-	79.2	108.8	113.5	113.6	111.9	109.9	94.9	72.7
NBO charge (e)										
Ni	+1.18	+1.15	+1.13	+1.10	+1.05	+1.06	+1.07	+1.06	+1.09	+1.10
C1	-0.15	-0.12	-0.12	-0.13	-0.10	-0.10	-0.10	-0.13	-0.16	-0.15
C2	-0.15	-0.12	-0.12	-0.25	-0.60	-0.59	-0.60	-0.63	-0.27	-0.15
C3	+1.03	-	-	-	-	+1.05	+1.03	+1.02	+1.05	+1.08
O1	-0.53	-0.60	-0.62	-0.66	-0.77	-0.80	-0.75	-0.66	-0.59	-0.54
O2	-0.51	-	-	-	-	-0.52	-0.58	-0.63	-0.59	-0.50
O3	-0.51	-	-	-	-	-0.53	-0.63	-0.69	-0.68	-0.65
I	-0.83	-	-0.82	-0.63	-0.05	-0.05	+0.01	+0.04	-0.50	-0.83
EO	0.00	+0.12	+0.12	-	-	-	-	-	-	-

Table S2. Optimized geometrical parameters and NBO charges of the species involved in the CO₂ cycloaddition to EO over Cu-DeAlBEA in the presence of TMAI.

Parameters	ISOLATED	ADS1	ADS2	TS1	INT1	CO ₂ -INT1	TS2	INT2	TS3	PROD
Distance (Å)										
Cu-Oa	1.85	1.89	1.92	1.91	1.92	1.93	1.93	1.92	1.96	1.91
Cu-Ob	1.82	1.83	1.84	1.84	1.89	1.88	1.89	1.92	1.84	1.83
Cu-Oc	2.11	2.28	2.22	2.22	2.28	2.22	2.21	2.19	2.10	2.27
C1-C2	1.46	1.45	1.45	1.45	1.52	1.52	1.52	1.52	1.49	1.52
C1-O1	1.42	1.46	1.46	1.43	1.38	1.38	1.40	1.42	1.42	1.46
C2-O1	1.42	1.46	1.46	1.79	2.33	2.32	-	-	-	-
C2-O2	-	-	-	-	-	-	-	3.55	2.00	1.46
C3-O1	-	-	-	-	-	2.73	1.81	1.55	1.36	1.32
C3-O2	1.17	-	-	-	-	1.17	1.19	1.20	1.26	1.31
C3-O3	1.17	-	-	-	-	1.17	1.22	1.25	1.26	1.24
I-C2	-	-	3.70	2.86	2.24	2.24	2.22	2.21	2.79	3.77
I-N	-	-	4.04	4.05	4.15	4.16	4.16	4.18	4.06	4.07
Cu-O1	-	2.00	1.99	1.91	1.85	1.86	2.00	2.09	2.64	2.89
Cu-O3	-	-	-	-	-	3.38	2.12	2.04	1.96	1.95
Angle (°)										
C2-O2-C3	59.1	60.2	60.4	76.9	107.2	-	-	-	-	-
C2-C1-O1	-	-	-	-	-	-	-	51.1	96.6	107.9
O1-C3-O2	-	-	-	-	-	90.6	110.4	116.0	116.6	114.2
O1-C3-O3	-	-	-	-	-	92.4	101.0	105.7	114.5	123.0
O2-C3-O3	180.0	-	-	-	-	177.0	148.6	138.3	128.9	122.8
I-C2-C1	-	-	75.6	104.7	112.4	113.0	112.3	111.7	96.2	76.4
NBO charge (e)										
Cu	+1.16	+1.10	+1.10	+1.08	+0.99	+1.00	+0.98	+0.99	+1.07	+1.08
C1	-0.15	-0.12	-0.12	-0.13	-0.10	-0.10	-0.12	-0.13	-0.16	-0.15
C2	-0.15	-0.14	-0.12	-0.23	-0.61	-0.61	-0.64	-0.65	-0.25	-0.15
C3	+1.03	-	-	-	-	+1.04	+1.02	+1.02	+1.06	+1.09
O1	-0.53	-0.59	-0.61	-0.65	-0.71	-0.75	-0.70	-0.64	-0.56	-0.52
O2	-0.51	-	-	-	-	-0.51	-0.55	-0.61	-0.59	-0.50
O3	-0.51	-	-	-	-	-0.53	-0.62	-0.66	-0.69	-0.67
I	-0.83	-	-0.73	-0.63	-0.02	-0.03	+0.03	+0.06	-0.53	-0.82
EO	0.00	+0.13	+0.10	-	-	-	-	-	-	-

Table S3. Optimized geometrical parameters and NBO charges of the species involved in the CO₂ cycloaddition to EO over Zn-DeAlBEA in the presence of TMAI.

Parameters	ISOLATED	ADS1	ADS2	TS1	INT1	CO ₂ -INT1	TS2	INT2	TS3	PROD
Distance (Å)										
Zn-Oa	1.86	1.90	1.91	1.93	1.95	1.97	1.98	1.97	1.95	1.92
Zn-Ob	1.84	1.87	1.88	1.90	1.93	1.92	1.93	1.93	1.90	1.87
Zn-Oc	2.06	2.08	2.07	2.08	2.13	2.09	2.09	2.14	2.06	2.08
C1-C2	1.46	1.45	1.44	1.45	1.51	1.51	1.51	1.51	1.50	1.53
C1-O1	1.42	1.46	1.47	1.42	1.37	1.38	1.38	1.42	1.43	1.46
C2-O1	1.42	1.46	1.48	1.82	2.29	2.30	-	-	-	-
C2-O2	-	-	-	-	-	-	-	3.55	2.00	1.47
C3-O1	-	-	-	-	-	2.59	1.84	1.46	1.39	1.33
C3-O2	1.17	-	-	-	-	1.17	1.19	1.21	1.26	1.30
C3-O3	1.17	-	-	-	-	1.17	1.21	1.27	1.24	1.23
I-C2	-	-	3.37	2.82	2.26	2.25	2.22	1.74	2.77	3.53
I-N	3.99	-	4.01	4.04	4.14	4.13	4.12	4.11	4.06	4.04
Zn-O1	-	2.06	2.02	1.97	1.92	1.93	2.02	2.18	2.24	2.47
Zn-O3	-	-	-	-	-	3.04	2.32	2.05	2.14	2.08
Angle (°)										
C2-O2-C3	59.1	60.1	61.1	78.5	105.0	-	-	-	-	-
C2-C1-O1	-	-	-	-	-	-	-	69.7	98.6	108.7
O1-C3-O2	-	-	-	-	-	96.8	109.6	119.5	115.0	114.1
O1-C3-O3	-	-	-	-	-	87.8	99.2	105.9	111.9	120.1
O2-C3-O3	180.0	-	-	-	-	175.3	151.2	134.6	133.1	125.8
I-C2-C1	-	-	81.4	105.3	113.2	112.9	112.0	126.3	95.4	75.0
NBO charge (e)										
Zn	+1.53	+1.48	+1.46	+1.44	+1.40	+1.41	+1.41	+1.42	+1.42	+1.43
C1	-0.15	-0.13	-0.13	-0.13	-0.09	-0.09	-0.10	-0.10	-0.16	-0.15
C2	-0.15	-0.13	-0.13	-0.24	-0.58	-0.58	-0.61	-0.93	-0.26	-0.15
C3	+1.03	-	-	-	-	+1.05	+1.03	+1.04	+1.05	+1.07
O1	-0.53	-0.63	-0.66	-0.73	-0.87	-0.90	-0.80	-0.68	-0.62	-0.50
O2	-0.51	-	-	-	-	-0.52	-0.57	-0.67	-0.59	-0.55
O3	-0.51	-	-	-	-	-0.53	-0.65	-0.78	-0.70	-0.68
I	-0.83	-	-0.81	-0.61	-0.06	-0.05	+0.02	+0.37	-0.52	-0.83
EO	0.00	+0.08	+0.07	-	-	-	-	-	-	-

Table S4. Optimized geometrical parameters and NBO charge of the species involved in the CO₂ cycloaddition to EO over Mg-DeAlBEA in the presence of TMAI.

Parameters	ISOLATED	ADS1	ADS2	TS1	INT1	CO ₂ -INT1	TS2	INT2	TS3	PROD
Distance (Å)										
Mg-Oa	1.82	1.86	1.87	1.89	1.91	1.92	1.94	1.93	1.91	1.88
Mg-Ob	1.80	1.84	1.84	1.86	1.89	1.89	1.90	1.90	1.88	1.84
Mg-Oc	1.98	2.00	2.00	2.00	2.03	2.01	2.02	2.01	1.99	2.00
C1-C2	1.46	1.46	1.44	1.45	1.51	1.51	1.51	1.51	1.50	1.53
C1-O1	1.42	1.45	1.46	1.41	1.37	1.37	1.38	1.40	1.43	1.46
C2-O1	1.42	1.46	1.48	1.82	2.27	2.27	-	-	-	-
C2-O2	-	-	-	-	-	-	-	3.44	2.00	1.47
C3-O1	-	-	-	-	-	2.59	1.92	1.51	1.40	1.34
C3-O2	1.17	-	-	-	-	1.17	1.18	1.21	1.26	1.30
C3-O3	1.17	-	-	-	-	1.17	1.21	1.25	1.24	1.23
I-C2	-	-	3.35	2.82	2.27	2.26	2.22	2.19	2.77	3.49
I-N	3.99	-	4.01	4.01	4.01	4.13	4.01	4.11	4.01	4.03
Mg-O1	-	2.03	2.00	1.95	1.90	1.91	1.98	2.10	2.16	2.28
Mg-O3	-	-	-	-	-	3.06	2.30	2.08	2.16	2.13
Angle (°)										
C2-O2-C3	59.1	60.30	61.4	79.1	104.2	-	-	-	-	-
C2-C1-O1	-	-	-	-	-	-	-	69.2	99.7	109.0
O1-C3-O2	-	-	-	-	-	96.3	108.6	117.6	114.7	113.6
O1-C3-O3	-	-	-	-	-	88.7	97.1	104.7	111.4	118.4
O2-C3-O3	180.0	-	-	-	-	175.0	154.3	137.7	133.9	128.0
I-C2-C1	-	-	90.1	107.5	112.3	113.2	112.6	111.2	95.1	72.8
NBO charge (e)										
Mg	+1.67	+1.57	+1.56	+1.54	+1.51	+1.50	+1.49	+1.49	+1.51	+1.51
C1	-0.15	-0.13	-0.12	-0.13	-0.08	-0.08	-0.09	-0.12	-0.16	-0.15
C2	-0.15	-0.14	-0.14	-0.26	-0.56	-0.57	-0.60	-0.62	-0.26	-0.15
C3	+1.03	-	-	-	-	+1.05	+1.04	+1.03	+1.05	+1.07
O1	-0.53	-0.65	-0.68	-0.76	-0.91	-0.93	-0.84	-0.69	-0.64	-0.58
O2	-0.51	-	-	-	-	-0.52	-0.55	-0.65	-0.59	-0.50
O3	-0.51	-	-	-	-	-0.53	-0.64	-0.77	-0.71	-0.68
I	-0.83	-	-0.82	-0.61	-0.09	-0.07	0.00	+0.05	-0.52	-0.83
EO	0.00	+0.06	+0.04	-	-	-	-	-	-	-

Table S5. Optimized geometrical parameters and NBO charges of the species involved in the adsorption of CO₂ over M-DeAlBEA (M= Ni, Cu, Zn and Mg).

Parameters	Ni-DeAlBEA		Cu-DeAlBEA		Zn-DeAlBEA		Mg-DeAlBEA	
	ISOLATED	CO ₂ _ADS	ISOLATED	CO ₂ _ADS	ISOLATED	CO ₂ _ADS	ISOLATED	CO ₂ _ADS
Distance (Å)								
M-Oa	1.83	1.86	1.85	1.85	1.86	1.87	1.82	1.84
M-Ob	1.81	1.85	1.82	1.86	1.84	1.85	1.80	1.82
M-Oc	1.96	1.99	2.11	2.30	2.06	2.09	1.98	2.03
C3-O2	1.17	1.16	1.17	1.16	1.17	1.16	1.17	1.16
C3-O3	1.17	1.18	1.17	1.18	1.17	1.18	1.17	1.18
M-O3	-	2.17	-	2.11	-	2.19	-	2.16
Angle (°)								
O2-C3-O3	180.0	177.3	180.0	178.5	180.0	177.7	180.0	177.4
M-O3-C3	-	146.3	-	137.6	-	136.9	-	139.6
NBO charge (e)								
M	+1.18	+1.14	+1.16	+1.07	+1.53	+1.48	+1.67	+1.59
C3	+1.03	+1.10	+1.03	+1.10	+1.03	+1.10	+1.03	+1.11
O2	-0.51	-0.45	-0.51	-0.44	-0.51	-0.44	-0.51	-0.43
O3	-0.51	-0.58	-0.51	-0.58	-0.51	-0.61	-0.51	-0.62
CO ₂	0.00	+0.07	0.00	+0.08	0.00	+0.06	0.00	+0.06

Table S6. Optimized geometrical parameters and NBO charges of the species involved in the concerted CO₂ cycloaddition to EO over M-DeAlBEA (M= Ni, Cu, Zn, and Mg).

Parameters	Ni-DeAlBEA		Cu-DeAlBEA		Zn-DeAlBEA		Mg-DeAlBEA	
	TSc	PRODc	TSc	PRODc	TSc	PRODc	TSc	PRODc
Distance (Å)								
M-Oa	1.95	1.89	1.92	1.86	1.95	1.90	1.90	1.87
M-Ob	1.93	1.88	1.86	1.88	1.91	1.88	1.87	1.84
M-Oc	1.98	2.03	2.19	2.36	2.04	2.12	1.98	2.05
C1-C2	1.45	1.52	1.46	1.52	1.45	1.53	1.45	1.52
C1-O1	1.36	1.45	1.37	1.45	1.36	1.45	1.35	1.45
C2-O1	2.33	2.31	2.37	2.31	2.35	2.32	2.34	2.32
C2-O2	1.93	1.45	1.83	1.45	1.92	1.45	1.92	1.45
C3-O1	2.53	1.32	2.55	1.33	2.50	1.32	2.49	1.32
C3-O2	1.19	1.33	1.20	1.32	1.20	1.32	1.20	1.32
C3-O3	1.16	1.22	1.16	1.23	1.16	1.23	1.16	1.23
M-O1	1.91	-	1.89	-	1.96	-	1.94	-
M-O3	-	2.02	-	2.00	-	2.05	-	2.02
Angle (°)								
C2-C1-O1	112.1	102.2	113.7	102.1	113.8	102.6	113.5	102.6
C2-O2-C3	118.5	107.8	119.5	107.9	118.2	108.5	118.3	108.4
O1-C3-O2	89.0	113.3	90.2	113.4	90.8	113.6	91.1	113.5
O1-C3-O3	101.0	123.9	101.8	122.5	100.8	122.7	101.2	122.9
O2-C3-O3	169.8	122.8	167.9	124.1	168.3	123.7	167.7	123.6
NBO charge (e)								
M	+1.06	+1.14	+1.01	+1.07	+1.41	+1.45	+1.52	+1.56
C1	-0.17	-0.14	-0.17	-0.14	-0.17	-0.14	-0.16	-0.15
C2	-0.05	-0.14	-0.06	-0.14	-0.06	-0.14	-0.06	-0.14
C3	+1.08	+1.10	+1.07	+1.09	+1.07	+1.09	+1.07	+1.10
O1	-0.80	-0.50	-0.78	-0.52	-0.88	-0.51	-0.91	-0.51
O2	-0.51	-0.51	-0.49	-0.50	-0.51	-0.50	-0.51	-0.50
O3	-0.41	-0.66	-0.38	-0.65	-0.41	-0.69	-0.41	-0.72
EO	+0.08	-	+0.08	-	-0.02	-	-0.05	-
CO ₂	+0.16	-	+0.19	-	+0.16	-	+0.15	-
EC	-	+0.13	-	+0.14	-	+0.10	-	+0.08

Table S7. Values of selected descriptors for the SISO algorithms used to predict the activation free energy of the rate-determining step ($\Delta G^\ddagger(\text{RDS})$). The E_{HOMO} and E_{LUMO} denote the highest occupied and lowest unoccupied molecular orbital energies of the isolated zeolite, respectively. $E_{\text{HOMO}}(\text{TMAI})$ and $E_{\text{LUMO}}(\text{TMAI})$ represent the corresponding orbital energies of the isolated TMAI molecule.

Systems	Co-catalyst	$\Delta G^\ddagger(\text{RDS})^b$ (kcal mol ⁻¹)	ΔG_{ADS1} (kcal mol ⁻¹)	ΔG_{TMAI}^c (kcal mol ⁻¹)	ΔG_{CO_2} (kcal mol ⁻¹)	q_M	E_{HOMO} (eV)	E_{LUMO} (eV)	E_{HOMO} (TMAI) (eV)	E_{LUMO} (TMAI) (eV)
Ni-DeAlBEA	TMAI	16.8	-19.8	-8.9	-5.7	1.18	-6.14	-4.42	-3.81	-0.24
Cu- DeAlBEA	TMAI	24.7	-22.1	-14.8	-5.0	1.16	-6.53	-5.89	-3.81	-0.24
Zn- DeAlBEA	TMAI	14.7	-24.5	-10.8	-7.0	1.53	-6.46	-2.58	-3.81	-0.24
Mg- DeAlBEA	TMAI	14.1	-26.0	-10.3	-8.6	1.67	-6.33	-1.58	-3.81	-0.24
Ni- DeAlBEA	-	39.9	-19.8	0.0	-5.7	1.18	-6.14	-4.42	0.00	0.00
Cu- DeAlBEA	-	38.9	-22.1	0.0	-5.0	1.16	-6.53	-5.89	0.00	0.00
Zn- DeAlBEA	-	38.6	-24.5	0.0	-7.0	1.53	-6.46	-2.58	0.00	0.00
Mg- DeAlBEA	-	39.6	-26.0	0.0	-8.6	1.67	-6.33	-1.58	0.00	0.00
Ni-FAU ^a	-	42.5	-26.3	0.0	-8.2	1.23	-7.09	-7.05	0.00	0.00
Cu-FAU ^a	-	36.1	-10.9	0.0	-0.8	1.06	-7.14	-7.11	0.00	0.00
Zn-FAU ^a	-	41.2	-21.7	0.0	-5.3	0.98	-6.99	-3.35	0.00	0.00
Catalyst-free	-	62.1	0.0	0.0	0.0	0.00	0.00	0.00	0.00	0.00

^aThe computational results were obtained using optimized structures from Ref. 51.

^bThe $\Delta G^\ddagger(\text{RDS})$ values are the apparent activation energies (δE) of the CO₂ cycloaddition with the co-catalyst and the activation free energies of the concerted CO₂ cycloaddition.

^c $\Delta G_{\text{TMAI}} = \Delta G_{\text{ADS2}} - \Delta G_{\text{ADS1}}$ for the catalytic system with the TMAI co-catalyst.

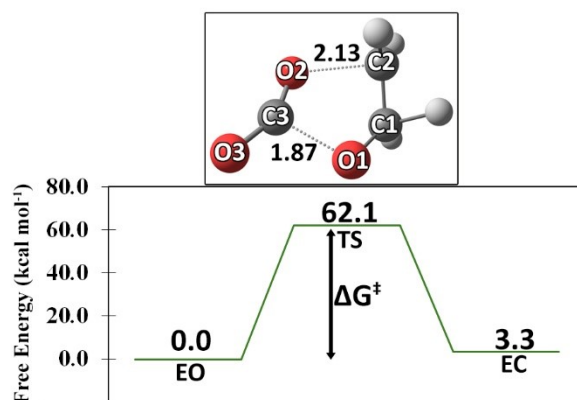


Fig. S1. Free energy profile for CO₂ cycloaddition with ethylene oxide and the optimized transition state geometry. Bond distances are given in Å.

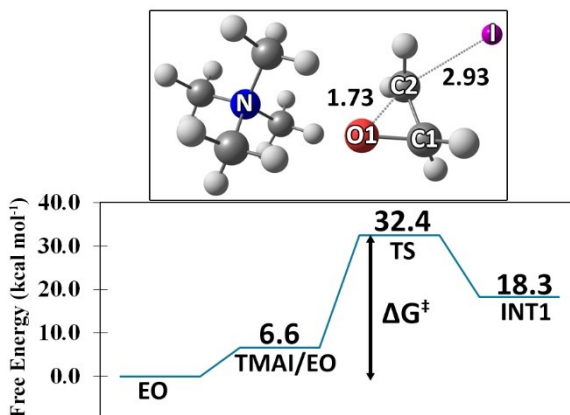


Fig. S2 Free energy profile for the ring-opening of EO by TMAI and optimized geometry of the transition state for the ring-opening of ethylene oxide by TMAI in the absence of Lewis acid. Distances are given in Å.

Coordinates of all optimized structures

TMAI/EO system

1. TMAI/EO ADS

C	14.142907	18.487753	20.519771
C	13.114505	18.992179	19.641338
H	14.252083	17.400853	20.600828
H	12.260769	18.381725	19.387073
O	13.183411	19.073731	21.369375
H	15.116742	18.986912	20.488282
H	13.166773	20.005023	19.271264
N	10.499435	20.219799	22.551702
C	11.580751	20.308322	23.588282
H	11.293457	19.690662	24.440179
H	11.675292	21.350295	23.897572
C	10.893193	21.062221	21.373001
H	11.866531	20.705510	21.028743
H	10.941243	22.102647	21.696818
C	9.210355	20.712532	23.113145
H	8.439415	20.641110	22.345196
H	9.329185	21.751538	23.423622
C	10.353849	18.786576	22.120010
H	9.601115	18.740805	21.331850
H	10.027431	18.205777	22.983898
H	8.936837	20.097719	23.971377
H	12.504414	19.943884	23.127745
H	11.339367	18.460747	21.760797
H	10.138509	20.946042	20.594354

I	13.766807	18.461686	16.829689
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2. TMAI/EO TS

C	14.142907	18.487753	20.519771
C	13.114505	18.992179	19.641338
H	14.252083	17.400853	20.600828
H	12.260769	18.381725	19.387073
O	13.183411	19.073731	21.369375
H	15.116742	18.986912	20.488282
H	13.166773	20.005023	19.271264
N	10.499435	20.219799	22.551702
C	11.580751	20.308322	23.588282
H	11.293457	19.690662	24.440179
H	11.675292	21.350295	23.897572
C	10.893193	21.062221	21.373001
H	11.866531	20.705510	21.028743
H	10.941243	22.102647	21.696818
C	9.210355	20.712532	23.113145
H	8.439415	20.641110	22.345196
H	9.329185	21.751538	23.423622
C	10.353849	18.786576	22.120010
H	9.601115	18.740805	21.331850
H	10.027431	18.205777	22.983898
H	8.936837	20.097719	23.971377
H	12.504414	19.943884	23.127745
H	11.339367	18.460747	21.760797
H	10.138509	20.946042	20.594354
I	13.766807	18.461686	16.829689

3. TMAI/EO INT1

C	14.030489	18.619577	20.615033
C	13.664282	18.553091	19.143652
H	14.387131	17.611958	20.931016
H	12.863861	17.835793	18.950387
O	12.918528	19.055709	21.262533
H	14.920509	19.281917	20.720891
H	13.384923	19.532405	18.748779
N	10.499700	20.215128	22.551859
C	11.653024	20.204722	23.516327
H	11.364397	19.604620	24.381497
H	11.844742	21.234697	23.823714
C	10.891177	21.032407	21.351960
H	11.800191	20.537753	20.950458
H	11.078853	22.054371	21.687447
C	9.290319	20.786942	23.196044
H	8.467200	20.782291	22.479427
H	9.501251	21.811057	23.508687
C	10.238001	18.802902	22.105520
H	9.405179	18.822778	21.399693
H	9.966166	18.217266	22.985938
H	9.026704	20.182248	24.065484
H	12.500765	19.764221	22.955943
H	11.183928	18.459656	21.639995
H	10.056606	21.017851	20.648142
I	15.350219	17.888857	17.817812

Stepwise mechanism				Si	10.048700	13.240500	21.271600
1. Ni-DeAlBEA				Si	10.048700	12.082000	18.337400
1.1 Ni-DeAlBEA				Si	10.040584	16.251108	21.354803
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393071	19.502457	24.925886
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846794	21.734057	18.250980
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240599	22.709916	24.939411	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239605	19.503564	24.938617	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851211	19.350889	16.490030	O	17.142400	14.576400	15.902200
Si	10.048687	25.902002	21.271610	O	17.140400	19.179600	15.907800
Si	10.048696	24.743508	18.337292	O	17.140400	18.804400	23.701200

O	16.220600	21.105000	24.608300	O	8.439100	16.918500	18.083900
O	16.220600	16.879000	15.000700	O	6.534907	21.086802	19.698349
O	14.745099	23.284602	24.802402	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927403	24.799198	H	20.962200	13.254500	21.455400
O	13.256088	21.106601	24.736608	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301418	23.386333	23.812026	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297563	18.828342	23.812791	H	19.619900	23.348100	24.168500
O	10.746191	20.841849	17.105701	H	19.619900	14.635900	15.440500
O	10.746266	17.142375	22.503488	H	19.616500	19.135300	15.433200
O	10.725311	24.962613	22.398870	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670604	18.266100	17.673501	H	18.910700	25.572300	17.347700
O	10.623335	23.238940	18.200467	H	18.910700	12.411700	22.261300
O	10.623298	14.745000	21.408701	H	16.839100	19.224200	26.169000
O	10.401405	25.322803	19.804498	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348501	16.897199	19.905900	H	16.839000	15.002200	13.435500
O	9.690602	19.141301	15.384898	H	12.713709	19.182986	26.273300
O	9.690702	18.842716	24.224045	H	12.713700	18.801000	13.335700
O	8.444090	21.763772	18.006355	H	12.713603	23.030704	26.273700
O	8.444000	16.220296	21.602702	H	12.713600	14.953300	13.335300

H	10.643290	25.568997	17.346791	Si	6.926978	21.089557	21.273450
H	10.643300	12.415000	22.262200	O	10.602678	19.688134	21.935069
H	10.571397	27.270301	21.396303	O	10.393118	20.894963	19.602105
H	10.571400	10.713700	18.212700	O	8.519745	21.213390	21.666193
H	9.865481	23.359502	24.031559	H	9.117219	20.423041	21.621126
H	9.835200	14.609800	15.524000	O	10.770894	22.462730	21.806104
H	8.639900	25.915403	21.449102	H	9.823629	22.161953	21.656954
H	8.639902	24.729903	18.159880	Ni	11.583680	20.892252	20.963347
H	8.590300	13.254600	21.455400				
H	8.590300	12.068200	18.153600				
H	8.422585	19.223574	26.368895				
H	8.422600	18.760400	13.240100				
H	8.402908	20.906702	24.715014				
H	8.402900	17.077300	14.894000				
H	7.215200	19.037200	15.248900				
H	7.215200	18.946812	24.360088				
H	6.336493	23.058396	18.204360				
H	6.334906	19.929691	21.841382				
H	6.318500	14.878900	21.406200				
H	6.288693	22.188513	21.907973				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228505	20.952069	17.239721				
H	6.228500	17.031900	22.369300				
Si	10.839711	18.640660	23.109874				
Si	10.891242	23.529226	23.068726				
Si	10.047078	21.702432	18.280052				

1.2 Ni-DeAlBEA CO ₂ ADS				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.340167	20.933237	19.643932
H	10.571400	10.713700	18.212700	O	8.515499	21.230832	21.689826
H	9.865500	23.359500	24.031600	H	9.132544	20.456467	21.624710
H	9.835200	14.609800	15.524000	O	10.824325	22.446898	21.790139
H	8.639900	25.915400	21.449100	H	9.888642	22.166116	21.580351
H	8.639900	24.729900	18.159900	Ni	11.663644	20.856105	20.928417
H	8.590300	13.254600	21.455400	C	13.304392	18.615600	19.314024
H	8.590300	12.068200	18.153600	O	13.533188	17.691154	18.653910
H	8.422600	19.223600	26.368900	O	13.126024	19.560465	19.992168
H	8.422600	18.760400	13.240100				
H	8.402900	20.906700	24.715000				
H	8.402900	17.077300	14.894000				
H	7.215200	19.037200	15.248900				
H	7.215200	18.946800	24.360100				
H	6.336500	23.058400	18.204400				
H	6.334900	19.929700	21.841400				
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.836200	18.653030	23.102604				
Si	10.892160	23.517098	23.056342				
Si	10.044008	21.701269	18.295095				
Si	6.933150	21.091427	21.276466				
O	10.605711	19.705505	21.935777				

1.3 Ni-DeAlBEA ADS1	Si	10.040600	16.251100	21.354800
Si 19.508300 21.734100 18.251000	Si	10.037800	16.927600	18.320700
Si 19.508300 16.249900 21.358000	Si	8.393100	19.502500	24.925900
Si 19.503800 25.900900 21.271600	Si	8.393100	18.481500	14.683100
Si 19.503800 24.744700 18.337400	Si	6.846800	21.734100	18.251000
Si 19.503800 13.239300 21.271600	Si	6.846800	16.249900	21.358000
Si 19.503800 12.083100 18.337400	Si	6.841000	16.929500	18.323900
Si 19.502500 21.054500 21.285100	O	19.196400	21.086800	19.698300
Si 19.502500 16.929500 18.323900	O	19.196400	16.897200	19.910700
Si 18.633200 23.512500 23.091300	O	19.151300	25.322800	19.804500
Si 18.633200 14.471500 16.517700	O	19.151300	12.661200	19.804500
Si 18.632400 19.351700 16.503500	O	18.927700	23.240900	18.198000
Si 18.632400 18.632300 23.105500	O	18.927700	14.743100	21.411000
Si 16.251500 22.701900 24.855400	O	18.870400	19.713700	21.928300
Si 16.251500 15.282100 14.753600	O	18.870400	18.270300	17.680700
Si 16.250300 19.508200 24.852300	O	18.843100	22.351700	21.987000
Si 16.250300 18.475800 14.756700	O	18.843100	15.632300	17.622000
Si 13.240600 22.709900 24.939400	O	18.828700	24.958900	22.398100
Si 13.240600 15.274100 14.669600	O	18.828700	13.025100	17.210900
Si 13.239600 19.503600 24.938600	O	18.804600	20.844100	17.100000
Si 13.239600 18.480400 14.670400	O	18.804600	17.139900	22.509000
Si 10.853700 14.469200 16.503500	O	17.142400	23.407600	23.706800
Si 10.851200 19.350900 16.490000	O	17.142400	14.576400	15.902200
Si 10.048700 25.902000 21.271600	O	17.140400	19.179600	15.907800
Si 10.048700 24.743500 18.337400	O	17.140400	18.804400	23.701200
Si 10.048700 13.240500 21.271600	O	16.220600	21.105000	24.608300
Si 10.048700 12.082000 18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.410421	20.933519	19.649108
H	10.571400	10.713700	18.212700	O	8.522992	21.202004	21.661147
H	9.865500	23.359500	24.031600	H	9.149964	20.440143	21.547268
H	9.835200	14.609800	15.524000	O	10.778580	22.456837	21.802680
H	8.639900	25.915400	21.449100	H	9.846168	22.148582	21.616475
H	8.639900	24.729900	18.159900	Ni	11.739047	20.920735	20.980147
H	8.590300	13.254600	21.455400	C	13.548933	18.471645	20.692461
H	8.590300	12.068200	18.153600	C	13.434721	19.010965	19.346159
H	8.422600	19.223600	26.368900	H	12.681449	17.996746	21.144300
H	8.422600	18.760400	13.240100	H	12.476616	18.935400	18.838767
H	8.402900	20.906700	24.715000	O	13.410244	19.903138	20.492088
H	8.402900	17.077300	14.894000	H	14.518963	18.201507	21.099962
H	7.215200	19.037200	15.248900	H	14.318346	19.142127	18.727908
H	7.215200	18.946800	24.360100				
H	6.336500	23.058400	18.204400				
H	6.334900	19.929700	21.841400				
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.831990	18.666074	23.095445				
Si	10.887214	23.520100	23.059573				
Si	10.053742	21.694998	18.313012				
Si	6.933567	21.088317	21.273775				
O	10.634077	19.697573	21.910769				

1.4 Ni-DeAlBEA ADS2	Si	10.040600	16.251100	21.354800
Si 19.508300 21.734100 18.251000	Si	10.037800	16.927600	18.320700
Si 19.508300 16.249900 21.358000	Si	8.393100	19.502500	24.925900
Si 19.503800 25.900900 21.271600	Si	8.393100	18.481500	14.683100
Si 19.503800 24.744700 18.337400	Si	6.846800	21.734100	18.251000
Si 19.503800 13.239300 21.271600	Si	6.846800	16.249900	21.358000
Si 19.503800 12.083100 18.337400	Si	6.841000	16.929500	18.323900
Si 19.502500 21.054500 21.285100	O	19.196400	21.086800	19.698300
Si 19.502500 16.929500 18.323900	O	19.196400	16.897200	19.910700
Si 18.633200 23.512500 23.091300	O	19.151300	25.322800	19.804500
Si 18.633200 14.471500 16.517700	O	19.151300	12.661200	19.804500
Si 18.632400 19.351700 16.503500	O	18.927700	23.240900	18.198000
Si 18.632400 18.632300 23.105500	O	18.927700	14.743100	21.411000
Si 16.251500 22.701900 24.855400	O	18.870400	19.713700	21.928300
Si 16.251500 15.282100 14.753600	O	18.870400	18.270300	17.680700
Si 16.250300 19.508200 24.852300	O	18.843100	22.351700	21.987000
Si 16.250300 18.475800 14.756700	O	18.843100	15.632300	17.622000
Si 13.240600 22.709900 24.939400	O	18.828700	24.958900	22.398100
Si 13.240600 15.274100 14.669600	O	18.828700	13.025100	17.210900
Si 13.239600 19.503600 24.938600	O	18.804600	20.844100	17.100000
Si 13.239600 18.480400 14.670400	O	18.804600	17.139900	22.509000
Si 10.853700 14.469200 16.503500	O	17.142400	23.407600	23.706800
Si 10.851200 19.350900 16.490000	O	17.142400	14.576400	15.902200
Si 10.048700 25.902000 21.271600	O	17.140400	19.179600	15.907800
Si 10.048700 24.743500 18.337400	O	17.140400	18.804400	23.701200
Si 10.048700 13.240500 21.271600	O	16.220600	21.105000	24.608300
Si 10.048700 12.082000 18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.384705	20.943202	19.660727
H	10.571400	10.713700	18.212700	O	8.518594	21.194333	21.678818
H	9.865500	23.359500	24.031600	H	9.156362	20.439277	21.558986
H	9.835200	14.609800	15.524000	O	10.757567	22.463872	21.805348
H	8.639900	25.915400	21.449100	H	9.826316	22.145933	21.630856
H	8.639900	24.729900	18.159900	Ni	11.739185	20.941629	20.974519
H	8.590300	13.254600	21.455400	C	13.732918	18.680540	20.591452
H	8.590300	12.068200	18.153600	C	13.493558	19.219490	19.274523
H	8.422600	19.223600	26.368900	H	12.945297	18.116973	21.087076
H	8.422600	18.760400	13.240100	H	12.520044	19.060821	18.819092
H	8.402900	20.906700	24.715000	O	13.448193	20.112450	20.442942
H	8.402900	17.077300	14.894000	H	14.750631	18.487127	20.915901
H	7.215200	19.037200	15.248900	H	14.328894	19.426244	18.612445
H	7.215200	18.946800	24.360100	N	14.662835	12.112882	18.568396
H	6.336500	23.058400	18.204400	C	16.048124	12.594135	18.874990
H	6.334900	19.929700	21.841400	H	16.348998	12.199816	19.847032
H	6.318500	14.878900	21.406200	H	16.032638	13.693320	18.879565
H	6.288700	22.188500	21.908000	C	14.274168	12.594887	17.200426
H	6.285500	18.107800	17.758700	H	14.977446	12.180884	16.476515
H	6.261400	15.789400	17.707000	H	14.326791	13.688713	17.199699
H	6.228500	20.952100	17.239700	C	13.706992	12.669596	19.580134
H	6.228500	17.031900	22.369300	H	12.711830	12.282851	19.366142
Si	10.834785	18.670415	23.088090	H	13.725469	13.764751	19.496886
Si	10.885270	23.519293	23.059601	C	14.627714	10.625915	18.607279
Si	10.054264	21.692813	18.314600	H	13.620588	10.288482	18.356199
Si	6.935638	21.087486	21.274542	H	14.893042	10.288912	19.610609
O	10.632972	19.710585	21.914094	H	14.030512	12.349910	20.572285

H	16.708113	12.230777	18.087385
H	15.344167	10.235228	17.882843
H	13.255575	12.264594	16.991555
I	14.765215	16.145737	18.484320

1.5 Ni-DeAlBEA TS1	Si	10.040600	16.251100	21.354800
Si 19.508300 21.734100 18.251000	Si	10.037800	16.927600	18.320700
Si 19.508300 16.249900 21.358000	Si	8.393100	19.502500	24.925900
Si 19.503800 25.900900 21.271600	Si	8.393100	18.481500	14.683100
Si 19.503800 24.744700 18.337400	Si	6.846800	21.734100	18.251000
Si 19.503800 13.239300 21.271600	Si	6.846800	16.249900	21.358000
Si 19.503800 12.083100 18.337400	Si	6.841000	16.929500	18.323900
Si 19.502500 21.054500 21.285100	O	19.196400	21.086800	19.698300
Si 19.502500 16.929500 18.323900	O	19.196400	16.897200	19.910700
Si 18.633200 23.512500 23.091300	O	19.151300	25.322800	19.804500
Si 18.633200 14.471500 16.517700	O	19.151300	12.661200	19.804500
Si 18.632400 19.351700 16.503500	O	18.927700	23.240900	18.198000
Si 18.632400 18.632300 23.105500	O	18.927700	14.743100	21.411000
Si 16.251500 22.701900 24.855400	O	18.870400	19.713700	21.928300
Si 16.251500 15.282100 14.753600	O	18.870400	18.270300	17.680700
Si 16.250300 19.508200 24.852300	O	18.843100	22.351700	21.987000
Si 16.250300 18.475800 14.756700	O	18.843100	15.632300	17.622000
Si 13.240600 22.709900 24.939400	O	18.828700	24.958900	22.398100
Si 13.240600 15.274100 14.669600	O	18.828700	13.025100	17.210900
Si 13.239600 19.503600 24.938600	O	18.804600	20.844100	17.100000
Si 13.239600 18.480400 14.670400	O	18.804600	17.139900	22.509000
Si 10.853700 14.469200 16.503500	O	17.142400	23.407600	23.706800
Si 10.851200 19.350900 16.490000	O	17.142400	14.576400	15.902200
Si 10.048700 25.902000 21.271600	O	17.140400	19.179600	15.907800
Si 10.048700 24.743500 18.337400	O	17.140400	18.804400	23.701200
Si 10.048700 13.240500 21.271600	O	16.220600	21.105000	24.608300
Si 10.048700 12.082000 18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.336275	20.947871	19.668720
H	10.571400	10.713700	18.212700	O	8.517086	21.213809	21.696229
H	9.865500	23.359500	24.031600	H	9.157236	20.461398	21.574528
H	9.835200	14.609800	15.524000	O	10.833289	22.448633	21.793343
H	8.639900	25.915400	21.449100	H	9.912758	22.161848	21.560673
H	8.639900	24.729900	18.159900	Ni	11.748571	20.874808	20.904413
H	8.590300	13.254600	21.455400	C	14.367017	19.563889	21.349819
H	8.590300	12.068200	18.153600	C	14.056446	19.700440	19.940527
H	8.422600	19.223600	26.368900	H	13.881750	18.750360	21.897073
H	8.422600	18.760400	13.240100	H	13.098698	19.346189	19.562641
H	8.402900	20.906700	24.715000	O	13.661394	20.793947	21.343252
H	8.402900	17.077300	14.894000	H	15.416521	19.682829	21.631975
H	7.215200	19.037200	15.248900	H	14.667028	20.316274	19.296438
H	7.215200	18.946800	24.360100	N	14.594211	13.463280	19.401099
H	6.336500	23.058400	18.204400	C	15.839277	13.969307	20.069599
H	6.334900	19.929700	21.841400	H	15.727640	13.857356	21.149207
H	6.318500	14.878900	21.406200	H	15.965508	15.026124	19.808149
H	6.288700	22.188500	21.908000	C	14.738396	13.618115	17.915567
H	6.285500	18.107800	17.758700	H	15.612403	13.054749	17.585417
H	6.261400	15.789400	17.707000	H	14.873123	14.683623	17.706569
H	6.228500	20.952100	17.239700	C	13.404866	14.257436	19.864955
H	6.228500	17.031900	22.369300	H	12.515530	13.869889	19.366272
Si	10.833583	18.679086	23.081342	H	13.569669	15.307638	19.599102
Si	10.893880	23.509195	23.049817	C	14.390367	12.026724	19.736962
Si	10.048230	21.694322	18.313251	H	13.495415	11.667880	19.226066
Si	6.941684	21.090134	21.277331	H	14.264511	11.928021	20.816128
O	10.614631	19.686931	21.885467	H	13.308927	14.144206	20.945326

H	16.690680	13.384890	19.714392
H	15.260941	11.456852	19.407985
H	13.830750	13.250739	17.434174
I	15.073151	17.401732	18.541471

1.6 Ni-DeAlBEA INT1	Si	10.040587	16.251087	21.354818
Si 19.508300 21.734100 18.251000	Si	10.037800	16.927600	18.320700
Si 19.508300 16.249900 21.358000	Si	8.393108	19.502503	24.925911
Si 19.503800 25.900900 21.271600	Si	8.393100	18.481500	14.683100
Si 19.503800 24.744700 18.337400	Si	6.846805	21.734145	18.251006
Si 19.503800 13.239300 21.271600	Si	6.846800	16.249900	21.358000
Si 19.503800 12.083100 18.337400	Si	6.841000	16.929500	18.323900
Si 19.502500 21.054500 21.285100	O	19.196400	21.086800	19.698300
Si 19.502500 16.929500 18.323900	O	19.196400	16.897200	19.910700
Si 18.633200 23.512500 23.091300	O	19.151300	25.322800	19.804500
Si 18.633200 14.471500 16.517700	O	19.151300	12.661200	19.804500
Si 18.632400 19.351700 16.503500	O	18.927700	23.240900	18.198000
Si 18.632400 18.632300 23.105500	O	18.927700	14.743100	21.411000
Si 16.251500 22.701900 24.855400	O	18.870400	19.713700	21.928300
Si 16.251500 15.282100 14.753600	O	18.870400	18.270300	17.680700
Si 16.250300 19.508200 24.852300	O	18.843100	22.351700	21.987000
Si 16.250300 18.475800 14.756700	O	18.843100	15.632300	17.622000
Si 13.240624 22.709853 24.939352	O	18.828700	24.958900	22.398100
Si 13.240601 15.274097 14.669599	O	18.828700	13.025100	17.210900
Si 13.239585 19.503571 24.938629	O	18.804600	20.844100	17.100000
Si 13.239600 18.480400 14.670400	O	18.804600	17.139900	22.509000
Si 10.853700 14.469202 16.503500	O	17.142400	23.407600	23.706800
Si 10.851196 19.350905 16.489988	O	17.142400	14.576400	15.902200
Si 10.048701 25.901977 21.271580	O	17.140400	19.179600	15.907800
Si 10.048708 24.743504 18.337390	O	17.140400	18.804400	23.701200
Si 10.048698 13.240498 21.271600	O	16.220600	21.105000	24.608300
Si 10.048702 12.082003 18.337398	O	16.220600	16.879000	15.000700

O	14.745101	23.284598	24.802399	O	6.534900	16.897200	19.910700
O	14.745100	14.699401	14.806601	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743299	18.927397	24.799203	H	20.962200	13.254500	21.455400
O	13.256102	21.106599	24.736599	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301372	23.386454	23.812208	H	20.961100	16.223000	21.580600
O	12.301399	14.597601	15.796899	H	20.956200	21.064500	21.503400
O	12.297599	19.155701	15.796097	H	20.956200	16.919500	18.105600
O	12.297616	18.828344	23.812848	H	19.619900	23.348100	24.168500
O	10.746334	20.841807	17.105510	H	19.619900	14.635900	15.440500
O	10.746321	17.142216	22.503477	H	19.616500	19.135300	15.433200
O	10.725305	24.962748	22.398917	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618101	H	18.979800	10.715500	18.210600
O	10.670597	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623271	23.238974	18.200340	H	18.910700	12.411700	22.261300
O	10.623297	14.744999	21.408702	H	16.839100	19.224200	26.169000
O	10.401402	25.322800	19.804499	H	16.839100	18.759800	13.440000
O	10.401401	12.661198	19.804502	H	16.839000	22.981800	26.173500
O	10.348502	16.897199	19.905900	H	16.839000	15.002200	13.435500
O	9.690597	19.141298	15.384903	H	12.713698	19.183004	26.273300
O	9.690590	18.842691	24.224080	H	12.713700	18.801000	13.335700
O	8.443986	21.763594	18.006266	H	12.713604	23.030706	26.273700
O	8.444000	16.220303	21.602698	H	12.713600	14.953301	13.335300
O	8.439100	16.918500	18.083900	H	10.643298	25.568999	17.346798
O	6.534893	21.086810	19.698297	H	10.643301	12.415001	22.262200

H	10.571399	27.270300	21.396301	O	10.349369	20.949564	19.679219
H	10.571398	10.713699	18.212701	O	8.517867	21.219598	21.696642
H	9.865502	23.359500	24.031572	H	9.169341	20.470270	21.586497
H	9.835200	14.609799	15.524000	O	10.869414	22.436559	21.794066
H	8.639900	25.915402	21.449102	H	9.963429	22.151740	21.524741
H	8.639900	24.729900	18.159902	Ni	11.810901	20.823096	20.909315
H	8.590300	13.254601	21.455400	C	14.363016	19.726714	20.886543
H	8.590300	12.068199	18.153600	C	13.744766	19.358451	19.548901
H	8.422601	19.223602	26.368900	H	14.339274	18.838178	21.551146
H	8.422600	18.760400	13.240100	H	12.741449	18.915110	19.621330
H	8.402898	20.906700	24.714997	O	13.644108	20.795014	21.378519
H	8.402900	17.077300	14.894000	H	15.427028	19.986686	20.745329
H	7.215200	19.037200	15.248900	H	13.742422	20.189157	18.838078
H	7.215200	18.946800	24.360100	N	14.522056	13.754507	19.513412
H	6.336503	23.058401	18.204409	C	15.793781	14.305271	20.089020
H	6.334905	19.929703	21.841398	H	15.750890	14.226125	21.175723
H	6.318500	14.878900	21.406200	H	15.883104	15.355624	19.798678
H	6.288697	22.188496	21.908009	C	14.571573	13.838984	18.017574
H	6.285500	18.107800	17.758700	H	15.459624	13.317846	17.657207
H	6.261400	15.789400	17.707000	H	14.613862	14.893764	17.737764
H	6.228498	20.952107	17.239695	C	13.345155	14.546454	20.011612
H	6.228500	17.031900	22.369300	H	12.436123	14.136531	19.568145
Si	10.835715	18.691952	23.076581	H	13.480093	15.588271	19.709901
Si	10.896803	23.500132	23.042257	C	14.361036	12.329046	19.924743
Si	10.051639	21.692119	18.331153	H	13.419417	11.952024	19.522237
Si	6.948215	21.091167	21.279136	H	14.343343	12.275328	21.013916
O	10.583560	19.674737	21.869755	H	13.298467	14.469373	21.097868

H	16.636712	13.729344	19.700567
H	15.199006	11.749025	19.534870
H	13.666051	13.390243	17.607910
I	14.922846	17.772386	18.446881

1.7 Ni-DeAlBEA CO ₂ -INT1				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.353509	20.947385	19.674688
H	10.571400	10.713700	18.212700	O	8.516845	21.200711	21.696844
H	9.865500	23.359500	24.031600	H	9.168066	20.452142	21.578040
H	9.835200	14.609800	15.524000	O	10.832430	22.430854	21.806027
H	8.639900	25.915400	21.449100	H	9.918802	22.140967	21.565280
H	8.639900	24.729900	18.159900	Ni	11.797981	20.861987	20.918404
H	8.590300	13.254600	21.455400	C	14.330542	19.674982	20.985416
H	8.590300	12.068200	18.153600	C	13.865262	19.473843	19.554584
H	8.422600	19.223600	26.368900	H	14.152009	18.746905	21.565910
H	8.422600	18.760400	13.240100	H	12.811773	19.173575	19.469233
H	8.402900	20.906700	24.715000	O	13.628249	20.762754	21.461403
H	8.402900	17.077300	14.894000	H	15.418936	19.865131	21.005971
H	7.215200	19.037200	15.248900	H	14.061344	20.338565	18.915166
H	7.215200	18.946800	24.360100	N	14.525052	13.771125	19.511346
H	6.336500	23.058400	18.204400	C	15.797053	14.315489	20.092282
H	6.334900	19.929700	21.841400	H	15.752882	14.228771	21.178338
H	6.318500	14.878900	21.406200	H	15.889909	15.367738	19.810186
H	6.288700	22.188500	21.908000	C	14.576359	13.865663	18.016278
H	6.285500	18.107800	17.758700	H	15.463533	13.344875	17.653326
H	6.261400	15.789400	17.707000	H	14.620954	14.921972	17.742220
H	6.228500	20.952100	17.239700	C	13.348109	14.560361	20.013716
H	6.228500	17.031900	22.369300	H	12.439183	14.151753	19.568685
Si	10.837453	18.691706	23.075781	H	13.482358	15.603764	19.717443
Si	10.895283	23.503121	23.043180	C	14.362025	12.342780	19.911946
Si	10.052064	21.694155	18.329057	H	13.420647	11.969621	19.505332
Si	6.945787	21.089056	21.278585	H	14.342494	12.281362	21.000664
O	10.596579	19.671930	21.863922	H	13.301757	14.478027	21.099623

H	16.639102	13.740550	19.700566
H	15.200037	11.764707	19.519281
H	13.670296	13.421984	17.602486
I	14.939878	17.800784	18.481048
C	14.510773	23.141408	20.774625
O	13.414446	23.544796	20.697591
O	15.634566	22.817261	20.812980

1.8 Ni-DeAlBEA TS2	Si	10.040600	16.251100	21.354800
Si 19.508300 21.734100 18.251000	Si	10.037800	16.927600	18.320700
Si 19.508300 16.249900 21.358000	Si	8.393100	19.502500	24.925900
Si 19.503800 25.900900 21.271600	Si	8.393100	18.481500	14.683100
Si 19.503800 24.744700 18.337400	Si	6.846800	21.734100	18.251000
Si 19.503800 13.239300 21.271600	Si	6.846800	16.249900	21.358000
Si 19.503800 12.083100 18.337400	Si	6.841000	16.929500	18.323900
Si 19.502500 21.054500 21.285100	O	19.196400	21.086800	19.698300
Si 19.502500 16.929500 18.323900	O	19.196400	16.897200	19.910700
Si 18.633200 23.512500 23.091300	O	19.151300	25.322800	19.804500
Si 18.633200 14.471500 16.517700	O	19.151300	12.661200	19.804500
Si 18.632400 19.351700 16.503500	O	18.927700	23.240900	18.198000
Si 18.632400 18.632300 23.105500	O	18.927700	14.743100	21.411000
Si 16.251500 22.701900 24.855400	O	18.870400	19.713700	21.928300
Si 16.251500 15.282100 14.753600	O	18.870400	18.270300	17.680700
Si 16.250300 19.508200 24.852300	O	18.843100	22.351700	21.987000
Si 16.250300 18.475800 14.756700	O	18.843100	15.632300	17.622000
Si 13.240600 22.709900 24.939400	O	18.828700	24.958900	22.398100
Si 13.240600 15.274100 14.669600	O	18.828700	13.025100	17.210900
Si 13.239600 19.503600 24.938600	O	18.804600	20.844100	17.100000
Si 13.239600 18.480400 14.670400	O	18.804600	17.139900	22.509000
Si 10.853700 14.469200 16.503500	O	17.142400	23.407600	23.706800
Si 10.851200 19.350900 16.490000	O	17.142400	14.576400	15.902200
Si 10.048700 25.902000 21.271600	O	17.140400	19.179600	15.907800
Si 10.048700 24.743500 18.337400	O	17.140400	18.804400	23.701200
Si 10.048700 13.240500 21.271600	O	16.220600	21.105000	24.608300
Si 10.048700 12.082000 18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.463036	20.943666	19.667490
H	10.571400	10.713700	18.212700	O	8.519578	21.171780	21.666162
H	9.865500	23.359500	24.031600	H	9.179251	20.422072	21.567626
H	9.835200	14.609800	15.524000	O	10.729964	22.461349	21.809061
H	8.639900	25.915400	21.449100	H	9.807164	22.129528	21.645568
H	8.639900	24.729900	18.159900	Ni	11.821802	20.960063	21.045473
H	8.590300	13.254600	21.455400	C	14.185354	18.944737	20.825043
H	8.590300	12.068200	18.153600	C	13.769562	18.910891	19.370912
H	8.422600	19.223600	26.368900	H	13.858778	18.034104	21.357071
H	8.422600	18.760400	13.240100	H	12.720463	18.639831	19.225954
H	8.402900	20.906700	24.715000	O	13.581544	20.071896	21.360105
H	8.402900	17.077300	14.894000	H	15.279091	19.026189	20.927247
H	7.215200	19.037200	15.248900	H	13.989087	19.850132	18.857472
H	7.215200	18.946800	24.360100	N	14.506319	13.565893	19.542584
H	6.336500	23.058400	18.204400	C	15.778588	14.127960	20.107544
H	6.334900	19.929700	21.841400	H	15.725067	14.093918	21.196214
H	6.318500	14.878900	21.406200	H	15.878853	15.163677	19.773041
H	6.288700	22.188500	21.908000	C	14.574015	13.579139	18.044145
H	6.285500	18.107800	17.758700	H	15.449764	13.014150	17.720677
H	6.261400	15.789400	17.707000	H	14.654712	14.616971	17.717732
H	6.228500	20.952100	17.239700	C	13.337123	14.398254	19.992013
H	6.228500	17.031900	22.369300	H	12.427586	13.997095	19.543054
Si	10.837562	18.692570	23.076214	H	13.497555	15.425443	19.658394
Si	10.888173	23.512953	23.051457	C	14.319303	12.163785	20.018319
Si	10.068995	21.689729	18.342783	H	13.380858	11.779116	19.615538
Si	6.941089	21.085766	21.274985	H	14.280429	12.161712	21.108242
O	10.600227	19.697013	21.885588	H	13.268785	14.358834	21.079248

H	16.623338	13.534779	19.750849
H	15.156905	11.556082	19.672594
H	13.657393	13.142321	17.644972
I	14.946598	17.434133	18.206733
C	14.520885	21.632355	21.178942
O	13.598762	22.407242	21.035884
O	15.686401	21.413593	21.267233

1.9 Ni-DeAlBEA INT2	Si	10.040603	16.251099	21.354798
Si 19.508300 21.734100 18.251000	Si	10.037800	16.927600	18.320700
Si 19.508300 16.249900 21.358000	Si	8.393098	19.502498	24.925898
Si 19.503800 25.900900 21.271600	Si	8.393100	18.481500	14.683100
Si 19.503800 24.744700 18.337400	Si	6.846800	21.734103	18.250999
Si 19.503800 13.239300 21.271600	Si	6.846800	16.249900	21.358000
Si 19.503800 12.083100 18.337400	Si	6.841000	16.929500	18.323900
Si 19.502500 21.054500 21.285100	O	19.196400	21.086800	19.698300
Si 19.502500 16.929500 18.323900	O	19.196400	16.897200	19.910700
Si 18.633200 23.512500 23.091300	O	19.151300	25.322800	19.804500
Si 18.633200 14.471500 16.517700	O	19.151300	12.661200	19.804500
Si 18.632400 19.351700 16.503500	O	18.927700	23.240900	18.198000
Si 18.632400 18.632300 23.105500	O	18.927700	14.743100	21.411000
Si 16.251500 22.701900 24.855400	O	18.870400	19.713700	21.928300
Si 16.251500 15.282100 14.753600	O	18.870400	18.270300	17.680700
Si 16.250300 19.508200 24.852300	O	18.843100	22.351700	21.987000
Si 16.250300 18.475800 14.756700	O	18.843100	15.632300	17.622000
Si 13.240599 22.709894 24.939397	O	18.828700	24.958900	22.398100
Si 13.240610 15.274094 14.669605	O	18.828700	13.025100	17.210900
Si 13.239600 19.503602 24.938599	O	18.804600	20.844100	17.100000
Si 13.239600 18.480400 14.670400	O	18.804600	17.139900	22.509000
Si 10.853680 14.469204 16.503489	O	17.142400	23.407600	23.706800
Si 10.851200 19.350899 16.490003	O	17.142400	14.576400	15.902200
Si 10.048700 25.902002 21.271601	O	17.140400	19.179600	15.907800
Si 10.048701 24.743501 18.337390	O	17.140400	18.804400	23.701200
Si 10.048692 13.240470 21.271610	O	16.220600	21.105000	24.608300
Si 10.048696 12.082039 18.337443	O	16.220600	16.879000	15.000700

O	14.745100	23.284601	24.802401	O	6.534900	16.897200	19.910700
O	14.745101	14.699403	14.806603	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927401	24.799199	H	20.962200	13.254500	21.455400
O	13.256102	21.106600	24.736599	H	20.962200	12.068300	18.153600
O	13.256097	16.877400	14.872398	H	20.961100	21.761000	18.028400
O	12.301396	23.386402	23.812107	H	20.961100	16.223000	21.580600
O	12.301338	14.597584	15.796968	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796101	H	20.956200	16.919500	18.105600
O	12.297598	18.828296	23.812908	H	19.619900	23.348100	24.168500
O	10.746288	20.841798	17.105513	H	19.619900	14.635900	15.440500
O	10.746309	17.142187	22.503502	H	19.616500	19.135300	15.433200
O	10.725308	24.962719	22.398899	H	19.616500	18.848700	24.175800
O	10.725372	13.021391	17.210087	H	18.979800	27.268500	21.398400
O	10.693691	15.628106	17.618092	H	18.979800	10.715500	18.210600
O	10.670599	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623306	23.239001	18.200306	H	18.910700	12.411700	22.261300
O	10.623320	14.744992	21.408708	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401457	12.661228	19.804285	H	16.839000	22.981800	26.173500
O	10.348499	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690601	19.141300	15.384899	H	12.713700	19.183000	26.273300
O	9.690603	18.842687	24.224099	H	12.713700	18.801000	13.335700
O	8.443990	21.763707	18.006299	H	12.713598	23.030698	26.273700
O	8.444000	16.220300	21.602700	H	12.713604	14.953294	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534901	21.086802	19.698301	H	10.643275	12.414983	22.262201

H	10.571399	27.270300	21.396301	O	10.407818	20.925556	19.664153
H	10.571369	10.713623	18.212790	O	8.517370	21.139509	21.682500
H	9.865501	23.359505	24.031586	H	9.172782	20.402757	21.518875
H	9.835200	14.609792	15.523999	O	10.710598	22.439711	21.841762
H	8.639900	25.915399	21.449099	H	9.788189	22.092275	21.710848
H	8.639900	24.729900	18.159897	Ni	11.798998	20.996054	20.991224
H	8.590300	13.254610	21.455396	C	14.466089	19.194217	20.953672
H	8.590297	12.068186	18.153627	C	13.821931	18.982300	19.597713
H	8.422600	19.223600	26.368900	H	14.293690	18.346426	21.626306
H	8.422600	18.760400	13.240100	H	12.791851	18.615101	19.654644
H	8.402900	20.906700	24.714999	O	13.833479	20.334876	21.503180
H	8.402900	17.077300	14.894000	H	15.543619	19.385253	20.874632
H	7.215200	19.037200	15.248900	H	13.856979	19.883648	18.979575
H	7.215200	18.946800	24.360100	N	14.514651	13.508200	19.441354
H	6.336500	23.058400	18.204397	C	15.811709	14.026749	19.990445
H	6.334900	19.929700	21.841400	H	15.773852	13.988119	21.079630
H	6.318500	14.878900	21.406200	H	15.945135	15.060841	19.662098
H	6.288700	22.188500	21.908000	C	14.543246	13.582863	17.943966
H	6.285500	18.107800	17.758700	H	15.406204	13.027630	17.573449
H	6.261400	15.789400	17.707000	H	14.625869	14.631986	17.657479
H	6.228500	20.952098	17.239702	C	13.367209	14.333169	19.956024
H	6.228500	17.031900	22.369300	H	12.442716	13.960794	19.512966
Si	10.837973	18.695771	23.070585	H	13.529989	15.372329	19.663775
Si	10.887752	23.515590	23.055404	C	14.321312	12.089866	19.865423
Si	10.063922	21.693760	18.336895	H	13.360995	11.737894	19.485513
Si	6.939231	21.082747	21.274719	H	14.324920	12.042809	20.954991
O	10.646368	19.675923	21.853349	H	13.325630	14.245584	21.041830

H	16.629670	13.405949	19.618435
H	15.133465	11.483502	19.461730
H	13.613594	13.171543	17.548391
I	14.937626	17.523302	18.369943
C	14.346928	21.640400	20.863753
O	13.327439	22.319346	20.600181
O	15.542178	21.739436	20.734246

1.10 Ni-DeAlBEA TS3

Si 19.508300 21.734100 18.251000
Si 19.508300 16.249900 21.358000
Si 19.503800 25.900900 21.271600
Si 19.503800 24.744700 18.337400
Si 19.503800 13.239300 21.271600
Si 19.503800 12.083100 18.337400
Si 19.502500 21.054500 21.285100
Si 19.502500 16.929500 18.323900
Si 18.633200 23.512500 23.091300
Si 18.633200 14.471500 16.517700
Si 18.632400 19.351700 16.503500
Si 18.632400 18.632300 23.105500
Si 16.251500 22.701900 24.855400
Si 16.251500 15.282100 14.753600
Si 16.250300 19.508200 24.852300
Si 16.250300 18.475800 14.756700
Si 13.240600 22.709900 24.939400
Si 13.240600 15.274100 14.669600
Si 13.239600 19.503600 24.938600
Si 13.239600 18.480400 14.670400
Si 10.853700 14.469200 16.503500
Si 10.851200 19.350900 16.490000
Si 10.048700 25.902000 21.271600
Si 10.048700 24.743500 18.337400
Si 10.048700 13.240500 21.271600
Si 10.048700 12.082000 18.337400

Si 10.040600 16.251100 21.354800
Si 10.037800 16.927600 18.320700
Si 8.393100 19.502500 24.925900
Si 8.393100 18.481500 14.683100
Si 6.846800 21.734100 18.251000
Si 6.846800 16.249900 21.358000
Si 6.841000 16.929500 18.323900
O 19.196400 21.086800 19.698300
O 19.196400 16.897200 19.910700
O 19.151300 25.322800 19.804500
O 19.151300 12.661200 19.804500
O 18.927700 23.240900 18.198000
O 18.927700 14.743100 21.411000
O 18.870400 19.713700 21.928300
O 18.870400 18.270300 17.680700
O 18.843100 22.351700 21.987000
O 18.843100 15.632300 17.622000
O 18.828700 24.958900 22.398100
O 18.828700 13.025100 17.210900
O 18.804600 20.844100 17.100000
O 18.804600 17.139900 22.509000
O 17.142400 23.407600 23.706800
O 17.142400 14.576400 15.902200
O 17.140400 19.179600 15.907800
O 17.140400 18.804400 23.701200
O 16.220600 21.105000 24.608300
O 16.220600 16.879000 15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.372807	20.914675	19.656644
H	10.571400	10.713700	18.212700	O	8.510956	21.198900	21.692070
H	9.865500	23.359500	24.031600	H	9.162186	20.445719	21.599549
H	9.835200	14.609800	15.524000	O	10.729903	22.495021	21.779798
H	8.639900	25.915400	21.449100	H	9.799720	22.167497	21.634724
H	8.639900	24.729900	18.159900	Ni	11.722893	20.976109	20.974533
H	8.590300	13.254600	21.455400	C	15.519200	18.585065	20.302585
H	8.590300	12.068200	18.153600	C	14.132556	18.269140	20.773724
H	8.422600	19.223600	26.368900	H	16.407730	18.190388	20.775418
H	8.422600	18.760400	13.240100	H	13.547799	17.664745	20.084583
H	8.402900	20.906700	24.715000	O	13.440191	19.512776	20.862655
H	8.402900	17.077300	14.894000	H	15.658860	19.214768	19.434182
H	7.215200	19.037200	15.248900	H	14.154485	17.792858	21.763250
H	7.215200	18.946800	24.360100	C	14.255618	20.494415	21.397477
H	6.336500	23.058400	18.204400	O	13.629375	21.535678	21.674607
H	6.334900	19.929700	21.841400	O	15.471252	20.190203	21.496966
H	6.318500	14.878900	21.406200	N	14.341605	12.890150	19.788964
H	6.288700	22.188500	21.908000	C	15.827570	12.787705	19.614786
H	6.285500	18.107800	17.758700	H	16.266726	12.463026	20.559127
H	6.261400	15.789400	17.707000	H	16.208252	13.775125	19.332410
H	6.228500	20.952100	17.239700	C	13.703835	13.290813	18.489671
H	6.228500	17.031900	22.369300	H	13.860589	12.496380	17.758153
Si	10.833201	18.690147	23.080007	H	14.157230	14.224583	18.146951
Si	10.891562	23.516671	23.055837	C	14.035566	13.929813	20.828957
Si	10.055005	21.688386	18.324202	H	12.953054	14.037821	20.916697
Si	6.936975	21.088808	21.275829	H	14.480709	14.872082	20.494920
O	10.596983	19.730382	21.919743	C	13.783558	11.575475	20.220228

H	12.700926	11.672965	20.317938
H	14.226382	11.296908	21.177436
H	14.469785	13.610174	21.777083
H	16.039341	12.060092	18.829597
H	14.022849	10.825322	19.465034
H	12.639814	13.434006	18.674260
I	15.632098	16.519365	18.500951

1.11 Ni-DeAlBEA PROD	Si	10.040598	16.251082	21.354815			
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393127	19.502523	24.925929
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734083	18.250978
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503818	12.083096	18.337375	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633202	14.471484	16.517693	O	19.151297	12.661201	19.804499
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282103	14.753602	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843103	15.632306	17.621993
Si	13.240584	22.709957	24.939448	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828698	13.025102	17.210905
Si	13.239609	19.503600	24.938593	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853686	14.469189	16.503474	O	17.142400	23.407600	23.706800
Si	10.851218	19.350900	16.490003	O	17.142395	14.576460	15.902214
Si	10.048691	25.902014	21.271616	O	17.140400	19.179600	15.907800
Si	10.048679	24.743505	18.337252	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082003	18.337402	O	16.220607	16.879001	15.000695

O	14.745098	23.284607	24.802406	O	6.534900	16.897200	19.910700
O	14.745097	14.699408	14.806607	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743299	18.927395	24.799204	H	20.962200	13.254500	21.455400
O	13.256106	21.106600	24.736595	H	20.962201	12.068299	18.153606
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301413	23.386277	23.812012	H	20.961100	16.223000	21.580600
O	12.301407	14.597607	15.796916	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297519	18.828265	23.812830	H	19.619900	23.348100	24.168500
O	10.746221	20.841826	17.105630	H	19.619900	14.635886	15.440498
O	10.746309	17.142243	22.503518	H	19.616500	19.135300	15.433200
O	10.725320	24.962612	22.398877	H	19.616500	18.848700	24.175800
O	10.725322	13.021364	17.210178	H	18.979800	27.268500	21.398400
O	10.693684	15.628100	17.618098	H	18.979769	10.715510	18.210621
O	10.670605	18.266100	17.673501	H	18.910700	25.572300	17.347700
O	10.623326	23.238986	18.200452	H	18.910700	12.411700	22.261300
O	10.623294	14.744998	21.408706	H	16.839100	19.224200	26.169000
O	10.401408	25.322804	19.804498	H	16.839100	18.759800	13.440000
O	10.401387	12.661209	19.804500	H	16.839000	22.981800	26.173500
O	10.348501	16.897199	19.905900	H	16.838995	15.002192	13.435499
O	9.690598	19.141299	15.384902	H	12.713694	19.183009	26.273300
O	9.690640	18.842675	24.223976	H	12.713700	18.801000	13.335700
O	8.444060	21.763780	18.006331	H	12.713596	23.030695	26.273700
O	8.443999	16.220306	21.602696	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643289	25.568997	17.346791
O	6.534896	21.086814	19.698312	H	10.643300	12.415000	22.262200

H	10.571394	27.270302	21.396305	O	10.324839	20.921326	19.650665
H	10.571411	10.713703	18.212710	O	8.512551	21.221889	21.701557
H	9.865517	23.359476	24.031577	H	9.153059	20.458543	21.634846
H	9.835211	14.609793	15.523987	O	10.793652	22.470548	21.780226
H	8.639900	25.915398	21.449098	H	9.861588	22.172084	21.595152
H	8.639900	24.729900	18.159903	Ni	11.687269	20.901587	20.903563
H	8.590300	13.254600	21.455400	C	15.355202	17.973569	21.112477
H	8.590302	12.068183	18.153587	C	13.962052	17.651086	20.571635
H	8.422607	19.223611	26.368902	H	15.684186	17.323338	21.922952
H	8.422600	18.760400	13.240100	H	13.950312	17.336239	19.530799
H	8.402894	20.906699	24.714990	O	13.276302	18.935074	20.659950
H	8.402900	17.077300	14.894000	H	16.128435	18.024368	20.341928
H	7.215200	19.037200	15.248900	H	13.405489	16.938514	21.184034
H	7.215200	18.946795	24.360105	C	14.027370	19.786654	21.348188
H	6.336495	23.058397	18.204381	O	13.607501	20.910328	21.628663
H	6.334900	19.929714	21.841398	O	15.206809	19.320965	21.670620
H	6.318500	14.878900	21.406200	N	14.896732	11.212620	17.871331
H	6.288702	22.188485	21.907995	C	15.657393	12.068918	16.900816
H	6.285500	18.107800	17.758700	H	16.605427	11.578834	16.672754
H	6.261400	15.789400	17.707000	H	15.832454	13.041491	17.372977
H	6.228504	20.952077	17.239715	C	13.588105	11.879571	18.177541
H	6.228500	17.031900	22.369300	H	13.025812	11.978701	17.248478
Si	10.831278	18.675640	23.084557	H	13.804369	12.867866	18.605403
Si	10.893109	23.512458	23.052693	C	15.692485	11.070968	19.134952
Si	10.045488	21.694495	18.307558	H	15.128149	10.445377	19.828027
Si	6.939252	21.090498	21.277944	H	15.847081	12.075734	19.550703
O	10.589521	19.723544	21.925872	C	14.651469	9.870135	17.277706

H	14.088004	9.263262	17.988160
H	15.611280	9.397940	17.061976
H	16.646789	10.600456	18.889888
H	15.053456	12.192819	16.000597
H	14.079292	9.989323	16.356657
H	13.042991	11.259498	18.891846
I	15.551905	14.840688	19.503933

2. Cu-DeAlBEA

2.1 Cu-DeAlBEA

Si	19.508300	21.734100	18.251000
Si	19.508300	16.249900	21.358000
Si	19.503800	25.900900	21.271600
Si	19.503800	24.744700	18.337400
Si	19.503800	13.239300	21.271600
Si	19.503800	12.083100	18.337400
Si	19.502500	21.054500	21.285100
Si	19.502500	16.929500	18.323900
Si	18.633200	23.512500	23.091300
Si	18.633200	14.471500	16.517700
Si	18.632400	19.351700	16.503500
Si	18.632400	18.632300	23.105500
Si	16.251500	22.701900	24.855400
Si	16.251500	15.282100	14.753600
Si	16.250300	19.508200	24.852300
Si	16.250300	18.475800	14.756700
Si	13.240606	22.709897	24.939393
Si	13.240600	15.274100	14.669600
Si	13.239597	19.503612	24.938595
Si	13.239600	18.480400	14.670400
Si	10.853700	14.469200	16.503500
Si	10.851221	19.350891	16.490025
Si	10.048710	25.902001	21.271595
Si	10.048684	24.743498	18.337351
Si	10.048700	13.240500	21.271600

Si	10.048700	12.082000	18.337400
Si	10.040578	16.251084	21.354825
Si	10.037800	16.927600	18.320700
Si	8.393118	19.502522	24.925913
Si	8.393100	18.481500	14.683100
Si	6.846802	21.734092	18.250999
Si	6.846800	16.249900	21.358000
Si	6.841000	16.929500	18.323900
O	19.196400	21.086800	19.698300
O	19.196400	16.897200	19.910700
O	19.151300	25.322800	19.804500
O	19.151300	12.661200	19.804500
O	18.927700	23.240900	18.198000
O	18.927700	14.743100	21.411000
O	18.870400	19.713700	21.928300
O	18.870400	18.270300	17.680700
O	18.843100	22.351700	21.987000
O	18.843100	15.632300	17.622000
O	18.828700	24.958900	22.398100
O	18.828700	13.025100	17.210900
O	18.804600	20.844100	17.100000
O	18.804600	17.139900	22.509000
O	17.142400	23.407600	23.706800
O	17.142400	14.576400	15.902200
O	17.140400	19.179600	15.907800
O	17.140400	18.804400	23.701200
O	16.220600	21.105000	24.608300

O	16.220600	16.879000	15.000700	O	6.534895	21.086822	19.698321
O	14.745101	23.284597	24.802398	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743297	18.927389	24.799209	H	20.962200	13.254500	21.455400
O	13.256109	21.106599	24.736593	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301368	23.386433	23.812096	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297595	19.155705	15.796088	H	20.956200	16.919500	18.105600
O	12.297550	18.828327	23.812759	H	19.619900	23.348100	24.168500
O	10.746330	20.841793	17.105647	H	19.619900	14.635900	15.440500
O	10.746283	17.142208	22.503396	H	19.616500	19.135300	15.433200
O	10.725307	24.962682	22.398927	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670614	18.266100	17.673502	H	18.910700	25.572300	17.347700
O	10.623278	23.239009	18.200415	H	18.910700	12.411700	22.261300
O	10.623292	14.744997	21.408707	H	16.839100	19.224200	26.169000
O	10.401413	25.322805	19.804494	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348504	16.897197	19.905900	H	16.839000	15.002200	13.435500
O	9.690593	19.141296	15.384908	H	12.713692	19.183012	26.273300
O	9.690587	18.842738	24.223964	H	12.713700	18.801000	13.335700
O	8.444077	21.763621	18.006415	H	12.713601	23.030701	26.273700
O	8.444000	16.220301	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643281	25.568994	17.346784

H	10.643300	12.415000	22.262200	O	10.580021	19.713429	21.957783
H	10.571404	27.270299	21.396297	O	10.254512	20.878469	19.630666
H	10.571400	10.713700	18.212700	O	8.507385	21.249436	21.701986
H	9.865508	23.359489	24.031592	H	9.118547	20.474488	21.651047
H	9.835200	14.609800	15.524000	O	10.861280	22.479519	21.767381
H	8.639900	25.915402	21.449102	H	9.939736	22.180697	21.563156
H	8.639899	24.729899	18.159907	Cu	11.623512	20.745287	20.829773
H	8.590300	13.254600	21.455400				
H	8.590300	12.068200	18.153600				
H	8.422611	19.223618	26.368903				
H	8.422600	18.760400	13.240100				
H	8.402894	20.906699	24.714991				
H	8.402900	17.077300	14.894000				
H	7.215200	19.037200	15.248900				
H	7.215200	18.946785	24.360115				
H	6.336497	23.058398	18.204375				
H	6.334903	19.929723	21.841391				
H	6.318500	14.878900	21.406200				
H	6.288700	22.188477	21.907998				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228502	20.952085	17.239710				
H	6.228500	17.031900	22.369300				
Si	10.840799	18.638599	23.110053				
Si	10.893460	23.514089	23.048603				
Si	10.040489	21.706039	18.274750				
Si	6.931127	21.093475	21.279452				

2.1 Cu-DeAlBEA CO ₂ ADS				Si	10.040578	16.251084	21.354825
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393118	19.502522	24.925913
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846802	21.734092	18.250999
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240606	22.709897	24.939393	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239597	19.503612	24.938595	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851221	19.350891	16.490025	O	17.142400	14.576400	15.902200
Si	10.048710	25.902001	21.271595	O	17.140400	19.179600	15.907800
Si	10.048684	24.743498	18.337351	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745101	23.284597	24.802398	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743297	18.927389	24.799209	H	20.962200	13.254500	21.455400
O	13.256109	21.106599	24.736593	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301368	23.386433	23.812096	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297595	19.155705	15.796088	H	20.956200	16.919500	18.105600
O	12.297550	18.828327	23.812759	H	19.619900	23.348100	24.168500
O	10.746330	20.841793	17.105647	H	19.619900	14.635900	15.440500
O	10.746283	17.142208	22.503396	H	19.616500	19.135300	15.433200
O	10.725307	24.962682	22.398927	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670614	18.266100	17.673502	H	18.910700	25.572300	17.347700
O	10.623278	23.239009	18.200415	H	18.910700	12.411700	22.261300
O	10.623292	14.744997	21.408707	H	16.839100	19.224200	26.169000
O	10.401413	25.322805	19.804494	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348504	16.897197	19.905900	H	16.839000	15.002200	13.435500
O	9.690593	19.141296	15.384908	H	12.713692	19.183012	26.273300
O	9.690587	18.842738	24.223964	H	12.713700	18.801000	13.335700
O	8.444077	21.763621	18.006415	H	12.713601	23.030701	26.273700
O	8.444000	16.220301	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643281	25.568994	17.346784
O	6.534895	21.086822	19.698321	H	10.643300	12.415000	22.262200

H	10.571404	27.270299	21.396297	O	10.211805	20.934196	19.670572
H	10.571400	10.713700	18.212700	O	8.503693	21.280365	21.720745
H	9.865508	23.359489	24.031592	H	9.141922	20.528753	21.668867
H	9.835200	14.609800	15.524000	O	10.989678	22.435111	21.768183
H	8.639900	25.915402	21.449102	H	10.114971	22.178320	21.411361
H	8.639899	24.729899	18.159907	Cu	11.699225	20.524449	20.705891
H	8.590300	13.254600	21.455400	C	13.793262	19.413857	18.723856
H	8.590300	12.068200	18.153600	O	14.268596	18.581250	18.075517
H	8.422611	19.223618	26.368903	O	13.336917	20.271586	19.392664
H	8.422600	18.760400	13.240100				
H	8.402894	20.906699	24.714991				
H	8.402900	17.077300	14.894000				
H	7.215200	19.037200	15.248900				
H	7.215200	18.946785	24.360115				
H	6.336497	23.058398	18.204375				
H	6.334903	19.929723	21.841391				
H	6.318500	14.878900	21.406200				
H	6.288700	22.188477	21.907998				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228502	20.952085	17.239710				
H	6.228500	17.031900	22.369300				
Si	10.835963	18.652031	23.103406				
Si	10.898373	23.490719	23.027049				
Si	10.035596	21.710427	18.281090				
Si	6.940160	21.096202	21.284852				
O	10.577820	19.712046	21.937023				

2.3 Cu-DeAlBEA ADS1Si				19.508300	Si	10.040600	16.251100	21.354800
21.734100				18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000		Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600		Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400		Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600		Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400		Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100		O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900		O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300		O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700		O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500		O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500		O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400		O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600		O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300		O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700		O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400		O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600		O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600		O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400		O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500		O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000		O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600		O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400		O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600		O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400		O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.287309	20.952081	19.672970
H	10.571400	10.713700	18.212700	O	8.507226	21.272324	21.704753
H	9.865500	23.359500	24.031600	H	9.147756	20.532429	21.589956
H	9.835200	14.609800	15.524000	O	10.993510	22.426618	21.782222
H	8.639900	25.915400	21.449100	H	10.130085	22.181429	21.395288
H	8.639900	24.729900	18.159900	Cu	11.752165	20.538057	20.691522
H	8.590300	13.254600	21.455400	C	13.823376	18.452793	21.260622
H	8.590300	12.068200	18.153600	C	14.296740	19.160819	20.082113
H	8.422600	19.223600	26.368900	H	12.922916	17.844166	21.197447
H	8.422600	18.760400	13.240100	H	13.746701	19.069460	19.146492
H	8.402900	20.906700	24.715000	O	13.588393	19.883658	21.131923
H	8.402900	17.077300	14.894000	H	14.507975	18.216406	22.069399
H	7.215200	19.037200	15.248900	H	15.338672	19.456366	20.000854
H	7.215200	18.946800	24.360100				
H	6.336500	23.058400	18.204400				
H	6.334900	19.929700	21.841400				
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.831734	18.660992	23.098768				
Si	10.897389	23.489911	23.026902				
Si	10.040047	21.706310	18.294692				
Si	6.940514	21.095872	21.281984				
O	10.584664	19.676079	21.894236				

2.4 Cu-DeAlBEA ADS2				Si	10.040614	16.251121	21.354775
Si	19.508300	21.734100	18.251000	Si	10.037959	16.927558	18.320769
Si	19.508300	16.249900	21.358000	Si	8.393096	19.502501	24.925892
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846797	21.734100	18.251002
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251491	15.282079	14.753613	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240601	22.709901	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239616	19.503601	24.938586	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851104	19.350879	16.489996	O	17.142400	14.576400	15.902200
Si	10.048702	25.902000	21.271598	O	17.140400	19.179600	15.907800
Si	10.048695	24.743498	18.337404	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743302	18.927408	24.799193	H	20.962200	13.254500	21.455400
O	13.256096	21.106600	24.736603	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301402	23.386398	23.812098	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297599	19.155699	15.796099	H	20.956200	16.919500	18.105600
O	12.297572	18.828319	23.812977	H	19.619900	23.348100	24.168500
O	10.746278	20.841836	17.105492	H	19.619900	14.635900	15.440500
O	10.746309	17.142227	22.503545	H	19.616500	19.135300	15.433200
O	10.725294	24.962699	22.398906	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693671	15.628100	17.618072	H	18.979800	10.715500	18.210600
O	10.670576	18.266074	17.673255	H	18.910700	25.572300	17.347700
O	10.623345	23.239047	18.200290	H	18.910700	12.411700	22.261300
O	10.623305	14.745002	21.408696	H	16.839100	19.224200	26.169000
O	10.401398	25.322799	19.804501	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348490	16.897206	19.905902	H	16.839000	15.002200	13.435500
O	9.690593	19.141315	15.384905	H	12.713704	19.182995	26.273300
O	9.690536	18.842621	24.224197	H	12.713700	18.801000	13.335700
O	8.444053	21.763713	18.006308	H	12.713600	23.030700	26.273700
O	8.444001	16.220292	21.602706	H	12.713600	14.953300	13.335300
O	8.439095	16.918520	18.083935	H	10.643299	25.569000	17.346799
O	6.534904	21.086787	19.698299	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.322380	20.924886	19.657341
H	10.571400	10.713700	18.212700	O	8.517307	21.228249	21.689016
H	9.865502	23.359502	24.031597	H	9.158648	20.481780	21.566641
H	9.835200	14.609800	15.524000	O	10.907078	22.447010	21.784943
H	8.639900	25.915400	21.449100	H	10.013208	22.140160	21.517757
H	8.639900	24.729900	18.159897	Cu	11.783053	20.691833	20.751069
H	8.590300	13.254600	21.455400	C	14.178366	19.123018	21.439750
H	8.590300	12.068200	18.153600	C	14.761560	20.218499	20.693431
H	8.422601	19.223601	26.368900	H	13.558182	18.402425	20.907731
H	8.422600	18.760400	13.240100	H	14.580105	20.278882	19.622638
H	8.402902	20.906701	24.715004	O	13.594199	20.457668	21.543673
H	8.402900	17.077300	14.894000	H	14.627646	18.778132	22.365676
H	7.215200	19.037200	15.248900	H	15.650774	20.721189	21.067135
H	7.215200	18.946807	24.360094	N	14.575232	13.427102	19.359320
H	6.336497	23.058399	18.204395	C	15.830575	13.967982	19.978212
H	6.334896	19.929701	21.841400	H	15.751876	13.877425	21.062867
H	6.318500	14.878900	21.406200	H	15.927143	15.021127	19.686679
H	6.288703	22.188503	21.907998	C	14.674904	13.542809	17.865997
H	6.285500	18.107800	17.758700	H	15.546461	12.980289	17.527868
H	6.261400	15.789400	17.707000	H	14.786259	14.605336	17.624412
H	6.228502	20.952092	17.239704	C	13.391422	14.221853	19.834758
H	6.228500	17.031900	22.369300	H	12.495343	13.826006	19.356030
Si	10.833242	18.675068	23.082890	H	13.548185	15.268975	19.549367
Si	10.892584	23.496655	23.034491	C	14.397835	11.999211	19.740892
Si	10.047214	21.697735	18.302122	H	13.489553	11.617730	19.271137
Si	6.943879	21.091646	21.278820	H	14.309649	11.928482	20.826075
O	10.605809	19.683901	21.885196	H	13.315306	14.121077	20.918195

H	16.680343	13.387975	19.612089
H	15.262579	11.428633	19.397722
H	13.759090	13.146807	17.425073
I	14.944912	17.331050	18.383703

2.5 Cu-DeAlBEA TS1				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.312632	20.936738	19.664634
H	10.571400	10.713700	18.212700	O	8.513184	21.232068	21.697175
H	9.865500	23.359500	24.031600	H	9.153944	20.483442	21.581387
H	9.835200	14.609800	15.524000	O	10.908579	22.438179	21.792262
H	8.639900	25.915400	21.449100	H	10.013602	22.142879	21.517923
H	8.639900	24.729900	18.159900	Cu	11.768597	20.664764	20.760852
H	8.590300	13.254600	21.455400	C	13.911280	18.890539	21.225207
H	8.590300	12.068200	18.153600	C	14.262737	19.417151	19.924976
H	8.422600	19.223600	26.368900	H	13.072635	18.188830	21.273652
H	8.422600	18.760400	13.240100	H	13.511712	19.468452	19.144055
H	8.402900	20.906700	24.715000	O	13.552397	20.267723	21.326322
H	8.402900	17.077300	14.894000	H	14.720714	18.610464	21.901416
H	7.215200	19.037200	15.248900	H	15.210594	19.912951	19.769302
H	7.215200	18.946800	24.360100	N	14.512484	13.281089	19.352322
H	6.336500	23.058400	18.204400	C	15.832192	13.673282	19.950126
H	6.334900	19.929700	21.841400	H	15.770236	13.567154	21.034472
H	6.318500	14.878900	21.406200	H	16.036008	14.716359	19.682708
H	6.288700	22.188500	21.908000	C	14.584440	13.430090	17.860071
H	6.285500	18.107800	17.758700	H	15.408613	12.819799	17.486843
H	6.261400	15.789400	17.707000	H	14.762743	14.485374	17.633500
H	6.228500	20.952100	17.239700	C	13.424785	14.170437	19.888106
H	6.228500	17.031900	22.369300	H	12.485407	13.898116	19.405121
Si	10.833104	18.676645	23.087009	H	13.690533	15.208428	19.659130
Si	10.894061	23.495769	23.035008	C	14.202363	11.864935	19.695985
Si	10.045348	21.700185	18.307064	H	13.234995	11.602356	19.264565
Si	6.943448	21.092508	21.279760	H	14.161671	11.764066	20.781580
O	10.577996	19.666706	21.877547	H	13.350535	14.017901	20.965837

H	16.606332	13.017402	19.547949
H	14.982652	11.219697	19.289085
H	13.634779	13.107448	17.431588
I	15.246906	17.162080	18.470235

2.6 Cu-DeAlBEA INT1				Si	10.040602	16.251101	21.354798
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393097	19.502497	24.925898
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734089	18.250999
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240594	22.709938	24.939428	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239597	19.503596	24.938605	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851205	19.350899	16.490004	O	17.142400	14.576400	15.902200
Si	10.048719	25.901989	21.271580	O	17.140400	19.179600	15.907800
Si	10.048698	24.743499	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048699	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745102	23.284592	24.802393	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256083	21.106598	24.736613	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301414	23.386335	23.812053	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796099	H	20.956200	16.919500	18.105600
O	12.297612	18.828305	23.812894	H	19.619900	23.348100	24.168500
O	10.746302	20.841827	17.105515	H	19.619900	14.635900	15.440500
O	10.746312	17.142203	22.503487	H	19.616500	19.135300	15.433200
O	10.725311	24.962593	22.398893	H	19.616500	18.848700	24.175800
O	10.725299	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670602	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623280	23.239028	18.200319	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408701	H	16.839100	19.224200	26.169000
O	10.401393	25.322795	19.804499	H	16.839100	18.759800	13.440000
O	10.401401	12.661201	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690599	19.141299	15.384901	H	12.713701	19.182999	26.273300
O	9.690610	18.842694	24.224090	H	12.713700	18.801000	13.335700
O	8.444001	21.763715	18.006313	H	12.713614	23.030721	26.273701
O	8.444000	16.220301	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643298	25.568999	17.346798
O	6.534899	21.086797	19.698305	H	10.643299	12.414999	22.262200

H	10.571413	27.270296	21.396289	O	10.333164	20.963703	19.687459
H	10.571401	10.713700	18.212700	O	8.512561	21.256996	21.706546
H	9.865440	23.359586	24.031622	H	9.181787	20.529914	21.599513
H	9.835200	14.609800	15.524000	O	10.969260	22.438051	21.785606
H	8.639901	25.915412	21.449109	H	10.124526	22.182539	21.369223
H	8.639900	24.729900	18.159902	Cu	11.839972	20.601964	20.762451
H	8.590300	13.254601	21.455400	C	14.339022	19.402909	20.768710
H	8.590300	12.068199	18.153600	C	13.793946	19.051349	19.397587
H	8.422598	19.223597	26.368900	H	14.254730	18.530527	21.447778
H	8.422600	18.760400	13.240100	H	12.795311	18.600728	19.416002
H	8.402901	20.906700	24.715002	O	13.626979	20.490339	21.223796
H	8.402900	17.077300	14.894000	H	15.413917	19.645744	20.703057
H	7.215200	19.037200	15.248900	H	13.813235	19.905819	18.716572
H	7.215200	18.946802	24.360098	N	14.514634	13.620265	19.540768
H	6.336498	23.058399	18.204396	C	15.788234	14.153198	20.129384
H	6.334901	19.929702	21.841395	H	15.726151	14.093596	21.216446
H	6.318500	14.878900	21.406200	H	15.903234	15.195454	19.820913
H	6.288700	22.188501	21.908000	C	14.600398	13.665888	18.044291
H	6.285500	18.107800	17.758700	H	15.467930	13.089913	17.718746
H	6.261400	15.789400	17.707000	H	14.708988	14.709211	17.742977
H	6.228502	20.952096	17.239702	C	13.350932	14.456542	19.997113
H	6.228500	17.031900	22.369300	H	12.437498	14.058523	19.552721
Si	10.834981	18.690648	23.077995	H	13.515974	15.485452	19.668820
Si	10.895185	23.485797	23.025579	C	14.306474	12.210457	19.983986
Si	10.049456	21.696863	18.326218	H	13.372585	11.841748	19.556739
Si	6.953209	21.094660	21.283122	H	14.247460	12.186747	21.072741
O	10.570771	19.665161	21.864187	H	13.286334	14.412175	21.084307

H	16.627605	13.557848	19.763903
H	15.145057	11.602461	19.641227
H	13.681395	13.257011	17.622128
I	15.072217	17.546291	18.330807

2.7 Cu-DeAlBEA CO ₂ -INT1				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.321006	20.931350	19.671653
H	10.571400	10.713700	18.212700	O	8.512555	21.207753	21.703180
H	9.865500	23.359500	24.031600	H	9.168015	20.469268	21.573953
H	9.835200	14.609800	15.524000	O	10.873931	22.434845	21.801086
H	8.639900	25.915400	21.449100	H	9.981747	22.131027	21.534190
H	8.639900	24.729900	18.159900	Cu	11.816040	20.700192	20.782706
H	8.590300	13.254600	21.455400	C	14.360985	19.581722	20.769053
H	8.590300	12.068200	18.153600	C	13.804823	19.205830	19.409130
H	8.422600	19.223600	26.368900	H	14.298220	18.717272	21.458500
H	8.422600	18.760400	13.240100	H	12.791225	18.792300	19.452514
H	8.402900	20.906700	24.715000	O	13.622993	20.661206	21.211419
H	8.402900	17.077300	14.894000	H	15.428439	19.852628	20.693723
H	7.215200	19.037200	15.248900	H	13.845845	20.035566	18.698838
H	7.215200	18.946800	24.360100	N	14.512227	13.654644	19.537783
H	6.336500	23.058400	18.204400	C	15.783555	14.193839	20.124874
H	6.334900	19.929700	21.841400	H	15.722347	14.134918	21.212021
H	6.318500	14.878900	21.406200	H	15.894211	15.236800	19.816962
H	6.288700	22.188500	21.908000	C	14.586299	13.718293	18.041598
H	6.285500	18.107800	17.758700	H	15.467547	13.171751	17.702764
H	6.261400	15.789400	17.707000	H	14.660121	14.767434	17.750051
H	6.228500	20.952100	17.239700	C	13.342770	14.473209	20.010203
H	6.228500	17.031900	22.369300	H	12.432114	14.073630	19.561480
Si	10.836067	18.691050	23.075509	H	13.498395	15.508690	19.697770
Si	10.892015	23.493054	23.031351	C	14.322259	12.237676	19.966197
Si	10.049103	21.696690	18.325912	H	13.384579	11.867224	19.548906
Si	6.946999	21.089995	21.280517	H	14.280510	12.199919	21.055365
O	10.587824	19.661656	21.856642	H	13.281588	14.411030	21.096657

H	16.624179	13.599689	19.760687
H	15.160153	11.640699	19.602835
H	13.676397	13.287451	17.621679
I	15.008631	17.615293	18.379805
C	14.559364	23.196842	20.805164
O	13.479304	23.639708	20.753459
O	15.662808	22.807372	20.835111

2.8 Cu-DeAlBEA TS2				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.327722	20.930805	19.675184
H	10.571400	10.713700	18.212700	O	8.514287	21.195614	21.698856
H	9.865500	23.359500	24.031600	H	9.168491	20.463723	21.542070
H	9.835200	14.609800	15.524000	O	10.864660	22.426169	21.824054
H	8.639900	25.915400	21.449100	H	9.973584	22.128526	21.547638
H	8.639900	24.729900	18.159900	Cu	11.836220	20.722849	20.798817
H	8.590300	13.254600	21.455400	C	14.245731	19.141795	21.001047
H	8.590300	12.068200	18.153600	C	13.692399	18.935745	19.597354
H	8.422600	19.223600	26.368900	H	14.038250	18.263522	21.631730
H	8.422600	18.760400	13.240100	H	12.691282	18.493037	19.570889
H	8.402900	20.906700	24.715000	O	13.629487	20.274606	21.556158
H	8.402900	17.077300	14.894000	H	15.334846	19.295937	20.976330
H	7.215200	19.037200	15.248900	H	13.704479	19.853747	19.004707
H	7.215200	18.946800	24.360100	N	14.507580	13.623150	19.543433
H	6.336500	23.058400	18.204400	C	15.779658	14.167285	20.124778
H	6.334900	19.929700	21.841400	H	15.723168	14.109852	21.212278
H	6.318500	14.878900	21.406200	H	15.885272	15.209619	19.813371
H	6.288700	22.188500	21.908000	C	14.573787	13.687999	18.046581
H	6.285500	18.107800	17.758700	H	15.456418	13.146429	17.703190
H	6.261400	15.789400	17.707000	H	14.640645	14.737631	17.756013
H	6.228500	20.952100	17.239700	C	13.336896	14.436007	20.022376
H	6.228500	17.031900	22.369300	H	12.427202	14.044201	19.565102
Si	10.839647	18.693401	23.074362	H	13.491399	15.474650	19.721856
Si	10.889201	23.497178	23.039387	C	14.324439	12.204968	19.971882
Si	10.054065	21.698721	18.327106	H	13.383675	11.833312	19.562628
Si	6.946021	21.088834	21.279463	H	14.293136	12.165520	21.061340
O	10.614172	19.650398	21.836969	H	13.272404	14.361983	21.107919

H	16.621854	13.576764	19.758189
H	15.160199	11.610462	19.599802
H	13.663872	13.252441	17.631394
I	14.968390	17.588363	18.376047
C	14.267724	21.757971	20.735808
O	13.279769	22.124711	20.116311
O	15.408887	21.926199	21.013539

2.9 Cu-DeAlBEA INT2				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393101	19.502501	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734101	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709899	24.939399	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239601	19.503601	24.938599	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851201	19.350900	16.490001	O	17.142400	14.576400	15.902200
Si	10.048699	25.902000	21.271601	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337401	O	17.140400	18.804400	23.701200
Si	10.048709	13.240496	21.271604	O	16.220600	21.105000	24.608300
Si	10.048710	12.082003	18.337397	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386404	23.812103	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796101	H	20.956200	16.919500	18.105600
O	12.297601	18.828293	23.812905	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105493	H	19.619900	14.635900	15.440500
O	10.746300	17.142194	22.503503	H	19.616500	19.135300	15.433200
O	10.725300	24.962705	22.398901	H	19.616500	18.848700	24.175800
O	10.725309	13.021294	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623298	23.239001	18.200293	H	18.910700	12.411700	22.261300
O	10.623294	14.745003	21.408697	H	16.839100	19.224200	26.169000
O	10.401399	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401376	12.661201	19.804499	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690599	18.842699	24.224103	H	12.713700	18.801000	13.335700
O	8.443998	21.763701	18.006296	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643301	25.569000	17.346801
O	6.534900	21.086800	19.698300	H	10.643309	12.415006	22.262200

H	10.571400	27.270300	21.396300	O	10.345419	20.936663	19.678685
H	10.571393	10.713697	18.212703	O	8.515633	21.189276	21.693639
H	9.865500	23.359500	24.031602	H	9.170645	20.461733	21.526009
H	9.835200	14.609800	15.524000	O	10.858984	22.421136	21.832801
H	8.639900	25.915400	21.449100	H	9.968850	22.128975	21.548312
H	8.639900	24.729900	18.159900	Cu	11.856711	20.744198	20.840637
H	8.590300	13.254590	21.455404	C	14.239158	18.940255	21.003214
H	8.590300	12.068210	18.153596	C	13.660108	18.776897	19.604547
H	8.422600	19.223600	26.368900	H	13.928032	18.126452	21.668304
H	8.422600	18.760400	13.240100	H	12.658149	18.337858	19.573916
H	8.402900	20.906700	24.715000	O	13.731495	20.152523	21.548812
H	8.402900	17.077300	14.894000	H	15.333919	18.998136	20.987106
H	7.215200	19.037200	15.248900	H	13.660161	19.716189	19.044883
H	7.215200	18.946800	24.360100	N	14.508758	13.484100	19.441941
H	6.336500	23.058400	18.204401	C	15.809296	14.002745	19.982882
H	6.334900	19.929699	21.841400	H	15.777007	13.967593	21.072422
H	6.318500	14.878900	21.406200	H	15.941586	15.035449	19.649882
H	6.288700	22.188500	21.908000	C	14.532312	13.547379	17.943472
H	6.285500	18.107800	17.758700	H	15.392700	12.986586	17.575067
H	6.261400	15.789400	17.707000	H	14.616769	14.594037	17.648693
H	6.228500	20.952100	17.239700	C	13.366302	14.316634	19.955033
H	6.228500	17.031900	22.369300	H	12.439352	13.950130	19.512293
Si	10.837379	18.693794	23.073901	H	13.535580	15.353901	19.660430
Si	10.889338	23.499317	23.040931	C	14.311918	12.069555	19.877402
Si	10.057723	21.698077	18.330333	H	13.349132	11.718042	19.503373
Si	6.945690	21.088274	21.278578	H	14.319510	12.030216	20.967256
O	10.631736	19.649379	21.833751	H	13.323960	14.231682	21.041072

H	16.624706	13.380097	19.608466
H	15.120490	11.457573	19.475096
H	13.600131	13.134844	17.555051
I	14.934578	17.491530	18.336787
C	14.349544	21.372290	20.810957
O	13.388226	21.956492	20.255053
O	15.543658	21.490124	20.895962

2.10 Cu-DeAlBEA TS3

Si 19.508300 21.734100 18.251000
 Si 19.508300 16.249900 21.358000
 Si 19.503800 25.900900 21.271600
 Si 19.503800 24.744700 18.337400
 Si 19.503800 13.239300 21.271600
 Si 19.503800 12.083100 18.337400
 Si 19.502500 21.054500 21.285100
 Si 19.502500 16.929500 18.323900
 Si 18.633200 23.512500 23.091300
 Si 18.633200 14.471500 16.517700
 Si 18.632400 19.351700 16.503500
 Si 18.632400 18.632300 23.105500
 Si 16.251500 22.701900 24.855400
 Si 16.251500 15.282100 14.753600
 Si 16.250300 19.508200 24.852300
 Si 16.250300 18.475800 14.756700
 Si 13.240600 22.709900 24.939400
 Si 13.240600 15.274100 14.669600
 Si 13.239600 19.503600 24.938600
 Si 13.239600 18.480400 14.670400
 Si 10.853700 14.469200 16.503500
 Si 10.851200 19.350900 16.490000
 Si 10.048700 25.902000 21.271600
 Si 10.048700 24.743500 18.337400
 Si 10.048700 13.240500 21.271600
 Si 10.048700 12.082000 18.337400

Si 10.040600 16.251100 21.354800
 Si 10.037800 16.927600 18.320700
 Si 8.393100 19.502500 24.925900
 Si 8.393100 18.481500 14.683100
 Si 6.846800 21.734100 18.251000
 Si 6.846800 16.249900 21.358000
 Si 6.841000 16.929500 18.323900
 O 19.196400 21.086800 19.698300
 O 19.196400 16.897200 19.910700
 O 19.151300 25.322800 19.804500
 O 19.151300 12.661200 19.804500
 O 18.927700 23.240900 18.198000
 O 18.927700 14.743100 21.411000
 O 18.870400 19.713700 21.928300
 O 18.870400 18.270300 17.680700
 O 18.843100 22.351700 21.987000
 O 18.843100 15.632300 17.622000
 O 18.828700 24.958900 22.398100
 O 18.828700 13.025100 17.210900
 O 18.804600 20.844100 17.100000
 O 18.804600 17.139900 22.509000
 O 17.142400 23.407600 23.706800
 O 17.142400 14.576400 15.902200
 O 17.140400 19.179600 15.907800
 O 17.140400 18.804400 23.701200
 O 16.220600 21.105000 24.608300
 O 16.220600 16.879000 15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.342500	20.871700	19.633100
H	10.571400	10.713700	18.212700	O	8.512400	21.182800	21.694800
H	9.865500	23.359500	24.031600	H	9.168700	20.431300	21.611800
H	9.835200	14.609800	15.524000	O	10.728300	22.517000	21.761100
H	8.639900	25.915400	21.449100	H	9.815200	22.147500	21.653400
H	8.639900	24.729900	18.159900	Cu	11.729100	20.920800	20.837400
H	8.590300	13.254600	21.455400	C	15.750200	18.622500	20.421700
H	8.590300	12.068200	18.153600	C	14.629700	18.128100	21.276700
H	8.422600	19.223600	26.368900	H	16.793800	18.434300	20.646600
H	8.422600	18.760400	13.240100	H	14.119300	17.247000	20.897800
H	8.402900	20.906700	24.715000	O	13.653600	19.165700	21.271900
H	8.402900	17.077300	14.894000	H	15.536300	19.166000	19.513900
H	7.215200	19.037200	15.248900	H	14.979400	17.950500	22.301300
H	7.215200	18.946800	24.360100	C	14.285400	20.361900	21.427200
H	6.336500	23.058400	18.204400	O	13.515800	21.349800	21.510600
H	6.334900	19.929700	21.841400	O	15.547600	20.337200	21.433300
H	6.318500	14.878900	21.406200	N	14.334000	12.917500	19.799900
H	6.288700	22.188500	21.908000	C	15.783600	12.789000	19.435000
H	6.285500	18.107800	17.758700	H	16.312800	12.329100	20.270800
H	6.261400	15.789400	17.707000	H	16.176900	13.791900	19.233300
H	6.228500	20.952100	17.239700	C	13.561400	13.460200	18.631800
H	6.228500	17.031900	22.369300	H	13.611900	12.744000	17.810200
Si	10.838100	18.690900	23.073600	H	14.003900	14.416700	18.340700
Si	10.887900	23.509200	23.045300	C	14.201000	13.864600	20.956500
Si	10.048900	21.695300	18.309600	H	13.143000	13.988500	21.196000
Si	6.940000	21.086600	21.278400	H	14.633300	14.820700	20.646400
O	10.602200	19.722900	21.903200	C	13.779300	11.584400	20.175200

H	12.716400	11.698700	20.395900
H	14.312100	11.209100	21.049900
H	14.744500	13.452800	21.807900
H	15.865500	12.166400	18.542500
H	13.908700	10.899400	19.335900
H	12.529600	13.603500	18.952700
I	15.638200	16.555500	18.556500

2.11 Cu-DeAlBEA PROD	Si	10.040605	16.251101	21.354796			
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925899
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846799	21.734100	18.251001
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503777	12.083105	18.337447	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633195	14.471512	16.517715	O	19.151295	12.661202	19.804498
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251483	15.282085	14.753591	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843102	15.632303	17.621996
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240598	15.274095	14.669598	O	18.828714	13.025095	17.210886
Si	13.239601	19.503605	24.938596	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851205	19.350899	16.490004	O	17.142466	14.576431	15.902195
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743499	18.337405	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048773	12.082028	18.337402	O	16.220602	16.879000	15.000703

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745096	14.699400	14.806610	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256099	21.106600	24.736600	H	20.962199	12.068301	18.153595
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301401	14.597603	15.796902	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796101	H	20.956200	16.919500	18.105600
O	12.297599	18.828295	23.812903	H	19.619900	23.348100	24.168500
O	10.746291	20.841803	17.105496	H	19.619900	14.635895	15.440499
O	10.746295	17.142201	22.503505	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725275	13.021292	17.210078	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979859	10.715497	18.210563
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623302	23.239000	18.200294	H	18.910700	12.411700	22.261300
O	10.623301	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401401	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839002	15.002199	13.435501
O	9.690600	19.141300	15.384899	H	12.713701	19.182999	26.273300
O	9.690604	18.842703	24.224101	H	12.713700	18.801000	13.335700
O	8.443998	21.763705	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713601	14.953301	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534902	21.086797	19.698299	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.274773	20.925313	19.663575
H	10.571266	10.713654	18.212694	O	8.508029	21.247043	21.709946
H	9.865500	23.359500	24.031600	H	9.152879	20.500370	21.609012
H	9.835200	14.609800	15.524000	O	10.923463	22.442500	21.779772
H	8.639900	25.915400	21.449100	H	10.031422	22.140847	21.505728
H	8.639900	24.729900	18.159899	Cu	11.754163	20.626811	20.702975
H	8.590300	13.254600	21.455400	C	15.264300	17.325152	21.550555
H	8.590297	12.068196	18.153628	C	13.805841	16.907036	21.510224
H	8.422600	19.223599	26.368900	H	15.819724	16.974490	22.419709
H	8.422600	18.760400	13.240100	H	13.602727	16.107488	20.795096
H	8.402900	20.906700	24.715000	O	13.155291	18.124107	21.043472
H	8.402900	17.077300	14.894000	H	15.805677	17.079345	20.631083
H	7.215200	19.037200	15.248900	H	13.375651	16.682971	22.490209
H	7.215200	18.946800	24.360100	C	13.965383	19.135790	21.292231
H	6.336500	23.058400	18.204399	O	13.614897	20.316997	21.196526
H	6.334900	19.929700	21.841400	O	15.176803	18.780638	21.647839
H	6.318500	14.878900	21.406200	N	14.827530	10.962652	17.006548
H	6.288700	22.188501	21.908000	C	15.858247	11.876880	16.414119
H	6.285500	18.107800	17.758700	H	16.817967	11.357982	16.394016
H	6.261400	15.789400	17.707000	H	15.916180	12.771657	17.042769
H	6.228500	20.952099	17.239700	C	13.521925	11.699702	17.091104
H	6.228500	17.031900	22.369300	H	13.247866	12.040957	16.092343
Si	10.828829	18.674839	23.080201	H	13.663994	12.560060	17.757038
Si	10.894629	23.492318	23.030034	C	15.261601	10.562258	18.384879
Si	10.042102	21.700943	18.301901	H	14.486695	9.930568	18.821518
Si	6.942960	21.093563	21.281341	H	15.396051	11.478521	18.974927
O	10.580545	19.710820	21.905638	C	14.670916	9.752442	16.154736

H	13.927920	9.092430	16.604690
H	15.631561	9.239835	16.085361
H	16.199774	10.010961	18.304336
H	15.538444	12.147796	15.407199
H	14.341610	10.059161	15.161123
H	12.765822	11.015889	17.480419
I	15.280814	14.266038	19.344055

3. Zn-DeAlBEA

3.1 Zn-DeAlBEA

Si	19.508300	21.734100	18.251000
Si	19.508300	16.249900	21.358000
Si	19.503800	25.900900	21.271600
Si	19.503800	24.744700	18.337400
Si	19.503800	13.239300	21.271600
Si	19.503800	12.083100	18.337400
Si	19.502500	21.054500	21.285100
Si	19.502500	16.929500	18.323900
Si	18.633200	23.512500	23.091300
Si	18.633200	14.471500	16.517700
Si	18.632400	19.351700	16.503500
Si	18.632400	18.632300	23.105500
Si	16.251500	22.701900	24.855400
Si	16.251500	15.282100	14.753600
Si	16.250300	19.508200	24.852300
Si	16.250300	18.475800	14.756700
Si	13.240600	22.709906	24.939404
Si	13.240600	15.274100	14.669600
Si	13.239606	19.503575	24.938610
Si	13.239600	18.480400	14.670400
Si	10.853700	14.469200	16.503500
Si	10.851201	19.350894	16.490015
Si	10.048687	25.902003	21.271611
Si	10.048699	24.743507	18.337318
Si	10.048700	13.240500	21.271600

Si	10.048700	12.082000	18.337400
Si	10.040582	16.251105	21.354807
Si	10.037800	16.927600	18.320700
Si	8.393071	19.502460	24.925884
Si	8.393100	18.481500	14.683100
Si	6.846795	21.734061	18.250980
Si	6.846800	16.249900	21.358000
Si	6.841000	16.929500	18.323900
O	19.196400	21.086800	19.698300
O	19.196400	16.897200	19.910700
O	19.151300	25.322800	19.804500
O	19.151300	12.661200	19.804500
O	18.927700	23.240900	18.198000
O	18.927700	14.743100	21.411000
O	18.870400	19.713700	21.928300
O	18.870400	18.270300	17.680700
O	18.843100	22.351700	21.987000
O	18.843100	15.632300	17.622000
O	18.828700	24.958900	22.398100
O	18.828700	13.025100	17.210900
O	18.804600	20.844100	17.100000
O	18.804600	17.139900	22.509000
O	17.142400	23.407600	23.706800
O	17.142400	14.576400	15.902200
O	17.140400	19.179600	15.907800
O	17.140400	18.804400	23.701200
O	16.220600	21.105000	24.608300

O	16.220600	16.879000	15.000700	O	6.534905	21.086802	19.698344
O	14.745099	23.284602	24.802402	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927401	24.799199	H	20.962200	13.254500	21.455400
O	13.256094	21.106601	24.736604	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301409	23.386345	23.812053	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297601	19.155699	15.796102	H	20.956200	16.919500	18.105600
O	12.297563	18.828336	23.812804	H	19.619900	23.348100	24.168500
O	10.746198	20.841843	17.105670	H	19.619900	14.635900	15.440500
O	10.746275	17.142356	22.503500	H	19.616500	19.135300	15.433200
O	10.725309	24.962640	22.398887	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670599	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623332	23.238911	18.200455	H	18.910700	12.411700	22.261300
O	10.623296	14.744999	21.408703	H	16.839100	19.224200	26.169000
O	10.401403	25.322802	19.804499	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348503	16.897198	19.905900	H	16.839000	15.002200	13.435500
O	9.690604	19.141302	15.384895	H	12.713706	19.182991	26.273300
O	9.690710	18.842723	24.224035	H	12.713700	18.801000	13.335700
O	8.444084	21.763759	18.006341	H	12.713601	23.030701	26.273700
O	8.444000	16.220299	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643294	25.568998	17.346795

H	10.643300	12.415000	22.262200	O	10.645150	19.685937	21.951923
H	10.571397	27.270301	21.396303	O	10.362983	20.958602	19.616692
H	10.571400	10.713700	18.212700	O	8.521953	21.230824	21.682476
H	9.865483	23.359514	24.031556	H	9.127820	20.452574	21.624271
H	9.835200	14.609800	15.524000	O	10.872394	22.458945	21.802519
H	8.639900	25.915401	21.449101	H	9.951150	22.177032	21.557641
H	8.639902	24.729903	18.159881	Zn	11.681363	20.798589	20.886773
H	8.590300	13.254600	21.455400				
H	8.590300	12.068200	18.153600				
H	8.422587	19.223578	26.368896				
H	8.422600	18.760400	13.240100				
H	8.402906	20.906701	24.715010				
H	8.402900	17.077300	14.894000				
H	7.215200	19.037200	15.248900				
H	7.215200	18.946809	24.360091				
H	6.336495	23.058397	18.204371				
H	6.334906	19.929690	21.841388				
H	6.318500	14.878900	21.406200				
H	6.288693	22.188508	21.907969				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228503	20.952078	17.239715				
H	6.228500	17.031900	22.369300				
Si	10.837015	18.636352	23.116120				
Si	10.891908	23.523778	23.061710				
Si	10.039689	21.706899	18.273338				
Si	6.935405	21.091198	21.276218				

3.2 Zn-DeAlBEA CO₂ ADS

Si 19.508300 21.734100 18.251000
 Si 19.508300 16.249900 21.358000
 Si 19.503800 25.900900 21.271600
 Si 19.503800 24.744700 18.337400
 Si 19.503800 13.239300 21.271600
 Si 19.503800 12.083100 18.337400
 Si 19.502500 21.054500 21.285100
 Si 19.502500 16.929500 18.323900
 Si 18.633200 23.512500 23.091300
 Si 18.633200 14.471500 16.517700
 Si 18.632400 19.351700 16.503500
 Si 18.632400 18.632300 23.105500
 Si 16.251500 22.701900 24.855400
 Si 16.251500 15.282100 14.753600
 Si 16.250300 19.508200 24.852300
 Si 16.250300 18.475800 14.756700
 Si 13.240600 22.709900 24.939400
 Si 13.240600 15.274100 14.669600
 Si 13.239600 19.503600 24.938600
 Si 13.239600 18.480400 14.670400
 Si 10.853700 14.469200 16.503500
 Si 10.851200 19.350900 16.490000
 Si 10.048700 25.902000 21.271600
 Si 10.048700 24.743500 18.337400
 Si 10.048700 13.240500 21.271600
 Si 10.048700 12.082000 18.337400

Si 10.040600 16.251100 21.354800
 Si 10.037800 16.927600 18.320700
 Si 8.393100 19.502500 24.925900
 Si 8.393100 18.481500 14.683100
 Si 6.846800 21.734100 18.251000
 Si 6.846800 16.249900 21.358000
 Si 6.841000 16.929500 18.323900
 O 19.196400 21.086800 19.698300
 O 19.196400 16.897200 19.910700
 O 19.151300 25.322800 19.804500
 O 19.151300 12.661200 19.804500
 O 18.927700 23.240900 18.198000
 O 18.927700 14.743100 21.411000
 O 18.870400 19.713700 21.928300
 O 18.870400 18.270300 17.680700
 O 18.843100 22.351700 21.987000
 O 18.843100 15.632300 17.622000
 O 18.828700 24.958900 22.398100
 O 18.828700 13.025100 17.210900
 O 18.804600 20.844100 17.100000
 O 18.804600 17.139900 22.509000
 O 17.142400 23.407600 23.706800
 O 17.142400 14.576400 15.902200
 O 17.140400 19.179600 15.907800
 O 17.140400 18.804400 23.701200
 O 16.220600 21.105000 24.608300
 O 16.220600 16.879000 15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.356371	20.960281	19.625353
H	10.571400	10.713700	18.212700	O	8.522556	21.238576	21.684698
H	9.865500	23.359500	24.031600	H	9.137706	20.465401	21.627017
H	9.835200	14.609800	15.524000	O	10.905383	22.446624	21.797540
H	8.639900	25.915400	21.449100	H	9.991938	22.166921	21.530937
H	8.639900	24.729900	18.159900	Zn	11.719321	20.761604	20.866333
H	8.590300	13.254600	21.455400	C	13.457679	18.628088	19.312694
H	8.590300	12.068200	18.153600	O	13.605458	17.686308	18.657619
H	8.422600	19.223600	26.368900	O	13.353637	19.591089	19.986167
H	8.422600	18.760400	13.240100				
H	8.402900	20.906700	24.715000				
H	8.402900	17.077300	14.894000				
H	7.215200	19.037200	15.248900				
H	7.215200	18.946800	24.360100				
H	6.336500	23.058400	18.204400				
H	6.334900	19.929700	21.841400				
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.833086	18.645341	23.110818				
Si	10.893541	23.516098	23.053791				
Si	10.038468	21.705852	18.284329				
Si	6.939841	21.092222	21.277379				
O	10.628323	19.686425	21.945248				

3.3 Zn-DeAlBEA ADS1

Si 19.508300 21.734100 18.251000
 Si 19.508300 16.249900 21.358000
 Si 19.503800 25.900900 21.271600
 Si 19.503800 24.744700 18.337400
 Si 19.503800 13.239300 21.271600
 Si 19.503800 12.083100 18.337400
 Si 19.502500 21.054500 21.285100
 Si 19.502500 16.929500 18.323900
 Si 18.633200 23.512500 23.091300
 Si 18.633200 14.471500 16.517700
 Si 18.632400 19.351700 16.503500
 Si 18.632400 18.632300 23.105500
 Si 16.251500 22.701900 24.855400
 Si 16.251500 15.282100 14.753600
 Si 16.250300 19.508200 24.852300
 Si 16.250300 18.475800 14.756700
 Si 13.240600 22.709900 24.939400
 Si 13.240600 15.274100 14.669600
 Si 13.239600 19.503600 24.938600
 Si 13.239600 18.480400 14.670400
 Si 10.853700 14.469200 16.503500
 Si 10.851200 19.350900 16.490000
 Si 10.048700 25.902000 21.271600
 Si 10.048700 24.743500 18.337400
 Si 10.048700 13.240500 21.271600
 Si 10.048700 12.082000 18.337400

Si 10.040600 16.251100 21.354800
 Si 10.037800 16.927600 18.320700
 Si 8.393100 19.502500 24.925900
 Si 8.393100 18.481500 14.683100
 Si 6.846800 21.734100 18.251000
 Si 6.846800 16.249900 21.358000
 Si 6.841000 16.929500 18.323900
 O 19.196400 21.086800 19.698300
 O 19.196400 16.897200 19.910700
 O 19.151300 25.322800 19.804500
 O 19.151300 12.661200 19.804500
 O 18.927700 23.240900 18.198000
 O 18.927700 14.743100 21.411000
 O 18.870400 19.713700 21.928300
 O 18.870400 18.270300 17.680700
 O 18.843100 22.351700 21.987000
 O 18.843100 15.632300 17.622000
 O 18.828700 24.958900 22.398100
 O 18.828700 13.025100 17.210900
 O 18.804600 20.844100 17.100000
 O 18.804600 17.139900 22.509000
 O 17.142400 23.407600 23.706800
 O 17.142400 14.576400 15.902200
 O 17.140400 19.179600 15.907800
 O 17.140400 18.804400 23.701200
 O 16.220600 21.105000 24.608300
 O 16.220600 16.879000 15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.381291	20.958551	19.631865
H	10.571400	10.713700	18.212700	O	8.526017	21.226141	21.675447
H	9.865500	23.359500	24.031600	H	9.148180	20.461205	21.580889
H	9.835200	14.609800	15.524000	O	10.894629	22.447687	21.805296
H	8.639900	25.915400	21.449100	H	9.984957	22.161320	21.536342
H	8.639900	24.729900	18.159900	Zn	11.767378	20.801532	20.881320
H	8.590300	13.254600	21.455400	C	13.804322	18.589753	20.803645
H	8.590300	12.068200	18.153600	C	13.665636	19.037943	19.426845
H	8.422600	19.223600	26.368900	H	12.954722	18.122416	21.299471
H	8.422600	18.760400	13.240100	H	12.709339	18.899804	18.921943
H	8.402900	20.906700	24.715000	O	13.631319	20.006252	20.516495
H	8.402900	17.077300	14.894000	H	14.784342	18.366633	21.215541
H	7.215200	19.037200	15.248900	H	14.539055	19.151427	18.790968
H	7.215200	18.946800	24.360100				
H	6.336500	23.058400	18.204400				
H	6.334900	19.929700	21.841400				
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.827609	18.657081	23.102169				
Si	10.892267	23.517001	23.055233				
Si	10.042735	21.701754	18.295119				
Si	6.941421	21.090916	21.276599				
O	10.641727	19.675372	21.918553				

3.4 Zn-DeAlBEA ADS2				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.359060	20.957968	19.639056
H	10.571400	10.713700	18.212700	O	8.521401	21.217253	21.689085
H	9.865500	23.359500	24.031600	H	9.152430	20.460029	21.579775
H	9.835200	14.609800	15.524000	O	10.861169	22.458272	21.806678
H	8.639900	25.915400	21.449100	H	9.948514	22.168146	21.554026
H	8.639900	24.729900	18.159900	Zn	11.759511	20.831710	20.883925
H	8.590300	13.254600	21.455400	C	14.288528	19.315643	20.706784
H	8.590300	12.068200	18.153600	C	14.124222	19.935215	19.415568
H	8.422600	19.223600	26.368900	H	13.569490	18.569085	21.041711
H	8.422600	18.760400	13.240100	H	13.281924	19.652393	18.784567
H	8.402900	20.906700	24.715000	O	13.758120	20.686814	20.638710
H	8.402900	17.077300	14.894000	H	15.274634	19.266999	21.158613
H	7.215200	19.037200	15.248900	H	14.983776	20.355507	18.903847
H	7.215200	18.946800	24.360100	N	14.532006	13.029572	19.223238
H	6.336500	23.058400	18.204400	C	15.925630	13.389003	19.643378
H	6.334900	19.929700	21.841400	H	16.012154	13.265049	20.724360
H	6.318500	14.878900	21.406200	H	16.105196	14.434520	19.358010
H	6.288700	22.188500	21.908000	C	14.409270	13.225869	17.739167
H	6.285500	18.107800	17.758700	H	15.171218	12.621108	17.244230
H	6.261400	15.789400	17.707000	H	14.572183	14.288177	17.525414
H	6.228500	20.952100	17.239700	C	13.542967	13.917081	19.924259
H	6.228500	17.031900	22.369300	H	12.545111	13.667181	19.563779
Si	10.832214	18.662397	23.095588	H	13.792669	14.958649	19.685456
Si	10.890704	23.517731	23.056278	C	14.245913	11.609795	19.565465
Si	10.043979	21.698636	18.297046	H	13.216705	11.380189	19.282808
Si	6.941958	21.090241	21.276632	H	14.371542	11.471219	20.640394
O	10.643901	19.683824	21.917236	H	13.614111	13.732084	20.997752

H	16.618823	12.721252	19.132106
H	14.938103	10.964596	19.021934
H	13.408299	12.922361	17.430118
I	15.169441	16.899531	18.391155

3.5 Zn-DeAlBEA TS1

Si	19.508300	21.734100	18.251000
Si	19.508300	16.249900	21.358000
Si	19.503800	25.900900	21.271600
Si	19.503800	24.744700	18.337400
Si	19.503800	13.239300	21.271600
Si	19.503800	12.083100	18.337400
Si	19.502500	21.054500	21.285100
Si	19.502500	16.929500	18.323900
Si	18.633200	23.512500	23.091300
Si	18.633200	14.471500	16.517700
Si	18.632400	19.351700	16.503500
Si	18.632400	18.632300	23.105500
Si	16.251500	22.701900	24.855400
Si	16.251500	15.282100	14.753600
Si	16.250300	19.508200	24.852300
Si	16.250300	18.475800	14.756700
Si	13.240600	22.709900	24.939400
Si	13.240600	15.274100	14.669600
Si	13.239600	19.503600	24.938600
Si	13.239600	18.480400	14.670400
Si	10.853700	14.469200	16.503500
Si	10.851200	19.350900	16.490000
Si	10.048700	25.902000	21.271600
Si	10.048700	24.743500	18.337400
Si	10.048700	13.240500	21.271600
Si	10.048700	12.082000	18.337400

Si	10.040600	16.251100	21.354800
Si	10.037800	16.927600	18.320700
Si	8.393100	19.502500	24.925900
Si	8.393100	18.481500	14.683100
Si	6.846800	21.734100	18.251000
Si	6.846800	16.249900	21.358000
Si	6.841000	16.929500	18.323900
O	19.196400	21.086800	19.698300
O	19.196400	16.897200	19.910700
O	19.151300	25.322800	19.804500
O	19.151300	12.661200	19.804500
O	18.927700	23.240900	18.198000
O	18.927700	14.743100	21.411000
O	18.870400	19.713700	21.928300
O	18.870400	18.270300	17.680700
O	18.843100	22.351700	21.987000
O	18.843100	15.632300	17.622000
O	18.828700	24.958900	22.398100
O	18.828700	13.025100	17.210900
O	18.804600	20.844100	17.100000
O	18.804600	17.139900	22.509000
O	17.142400	23.407600	23.706800
O	17.142400	14.576400	15.902200
O	17.140400	19.179600	15.907800
O	17.140400	18.804400	23.701200
O	16.220600	21.105000	24.608300
O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.373374	20.956280	19.645986
H	10.571400	10.713700	18.212700	O	8.522492	21.212660	21.685741
H	9.865500	23.359500	24.031600	H	9.163771	20.462729	21.569426
H	9.835200	14.609800	15.524000	O	10.858029	22.457573	21.807439
H	8.639900	25.915400	21.449100	H	9.950432	22.163506	21.549737
H	8.639900	24.729900	18.159900	Zn	11.801775	20.842625	20.887402
H	8.590300	13.254600	21.455400	C	14.432016	19.594399	20.940544
H	8.590300	12.068200	18.153600	C	14.168729	19.648448	19.516217
H	8.422600	19.223600	26.368900	H	13.908579	18.831134	21.528405
H	8.422600	18.760400	13.240100	H	13.200946	19.350522	19.124373
H	8.402900	20.906700	24.715000	O	13.775612	20.847935	20.822539
H	8.402900	17.077300	14.894000	H	15.476000	19.689178	21.251238
H	7.215200	19.037200	15.248900	H	14.833061	20.198324	18.864004
H	7.215200	18.946800	24.360100	N	14.518581	13.347243	19.413350
H	6.336500	23.058400	18.204400	C	15.814585	13.775127	20.037505
H	6.334900	19.929700	21.841400	H	15.731952	13.673584	21.120785
H	6.318500	14.878900	21.406200	H	15.996805	14.821591	19.768739
H	6.288700	22.188500	21.908000	C	14.621875	13.486131	17.922347
H	6.285500	18.107800	17.758700	H	15.455645	12.875648	17.571900
H	6.261400	15.789400	17.707000	H	14.800303	14.541621	17.694966
H	6.228500	20.952100	17.239700	C	13.401141	14.218108	19.916730
H	6.228500	17.031900	22.369300	H	12.478079	13.917295	19.419709
Si	10.831695	18.672166	23.088218	H	13.647307	15.258791	19.679485
Si	10.890745	23.514664	23.053645	C	14.228243	11.928148	19.761948
Si	10.047824	21.696281	18.307280	H	13.274309	11.644985	19.313171
Si	6.944705	21.089821	21.276855	H	14.166791	11.834803	20.847201
O	10.642657	19.688449	21.908310	H	13.309703	14.078614	20.994597

H	16.616854	13.140105	19.656251
H	15.028574	11.294309	19.376439
H	13.683207	13.156680	17.474927
I	15.174254	17.225919	18.483113

3.6 Zn-DeAlBEA INT1				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.402004	21.002881	19.676531
H	10.571400	10.713700	18.212700	O	8.520113	21.255228	21.690488
H	9.865500	23.359500	24.031600	H	9.184510	20.517118	21.618143
H	9.835200	14.609800	15.524000	O	10.946326	22.455320	21.785113
H	8.639900	25.915400	21.449100	H	10.089621	22.220809	21.368701
H	8.639900	24.729900	18.159900	Zn	11.880680	20.764325	20.897439
H	8.590300	13.254600	21.455400	C	14.469717	19.613774	20.716260
H	8.590300	12.068200	18.153600	C	13.935510	19.254736	19.347526
H	8.422600	19.223600	26.368900	H	14.326013	18.757239	21.410043
H	8.422600	18.760400	13.240100	H	12.897176	18.900577	19.360394
H	8.402900	20.906700	24.715000	O	13.787652	20.749789	21.076981
H	8.402900	17.077300	14.894000	H	15.558409	19.791291	20.655220
H	7.215200	19.037200	15.248900	H	14.053692	20.064501	18.625050
H	7.215200	18.946800	24.360100	N	14.527141	13.578573	19.499809
H	6.336500	23.058400	18.204400	C	15.801374	14.116080	20.081983
H	6.334900	19.929700	21.841400	H	15.747341	14.050683	21.169183
H	6.318500	14.878900	21.406200	H	15.909881	15.161230	19.780233
H	6.288700	22.188500	21.908000	C	14.600204	13.638837	18.003635
H	6.285500	18.107800	17.758700	H	15.476379	13.083440	17.665744
H	6.261400	15.789400	17.707000	H	14.685907	14.686130	17.709030
H	6.228500	20.952100	17.239700	C	13.359692	14.400676	19.972362
H	6.228500	17.031900	22.369300	H	12.447253	14.001500	19.526837
Si	10.831432	18.684141	23.084225	H	13.516134	15.434575	19.655275
Si	10.895076	23.500949	23.039470	C	14.335003	12.162911	19.930234
Si	10.052538	21.697215	18.320776	H	13.396567	11.793614	19.513631
Si	6.954278	21.093974	21.281314	H	14.293311	12.126740	21.019475
O	10.601614	19.688665	21.903057	H	13.302266	14.342395	21.059326

H	16.640102	13.526550	19.706010
H	15.171643	11.563759	19.567566
H	13.685614	13.215996	17.586123
I	15.040527	17.536420	18.382652

3.7 Zn-DeAlBEA CO ₂ -INT1				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.404170	20.949971	19.648921
H	10.571400	10.713700	18.212700	O	8.522704	21.191157	21.681897
H	9.865500	23.359500	24.031600	H	9.177243	20.441216	21.584164
H	9.835200	14.609800	15.524000	O	10.823880	22.441068	21.824670
H	8.639900	25.915400	21.449100	H	9.915461	22.133800	21.588764
H	8.639900	24.729900	18.159900	Zn	11.848230	20.866164	20.910395
H	8.590300	13.254600	21.455400	C	14.423516	19.609962	20.730868
H	8.590300	12.068200	18.153600	C	13.888158	19.302603	19.348954
H	8.422600	19.223600	26.368900	H	14.271741	18.736291	21.398402
H	8.422600	18.760400	13.240100	H	12.835034	18.994609	19.344181
H	8.402900	20.906700	24.715000	O	13.756399	20.741724	21.137844
H	8.402900	17.077300	14.894000	H	15.513334	19.786064	20.679645
H	7.215200	19.037200	15.248900	H	14.047690	20.117668	18.639845
H	7.215200	18.946800	24.360100	N	14.509982	13.641037	19.534878
H	6.336500	23.058400	18.204400	C	15.780173	14.190555	20.114915
H	6.334900	19.929700	21.841400	H	15.722079	14.137626	21.202549
H	6.318500	14.878900	21.406200	H	15.883861	15.232496	19.800869
H	6.288700	22.188500	21.908000	C	14.575459	13.703380	18.038365
H	6.285500	18.107800	17.758700	H	15.461228	13.166834	17.695253
H	6.261400	15.789400	17.707000	H	14.634858	14.752951	17.745289
H	6.228500	20.952100	17.239700	C	13.337125	14.452257	20.011920
H	6.228500	17.031900	22.369300	H	12.428528	14.051870	19.560034
Si	10.833492	18.686470	23.079825	H	13.488268	15.490013	19.704958
Si	10.890107	23.510380	23.049844	C	14.332288	12.223515	19.965819
Si	10.053358	21.694731	18.322499	H	13.392168	11.848054	19.558432
Si	6.947886	21.087648	21.277632	H	14.302045	12.186176	21.055388
O	10.615046	19.680855	21.889339	H	13.276670	14.383331	21.097977

H	16.623020	13.598610	19.752220
H	15.169543	11.630633	19.594220
H	13.668013	13.261684	17.624376
I	14.952562	17.580608	18.361416
C	14.516987	23.190801	20.770319
O	13.384840	23.485997	20.712030
O	15.667607	22.986173	20.806493

3.8 Zn-DeAlBEA TS2				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.465127	20.949370	19.641719
H	10.571400	10.713700	18.212700	O	8.527024	21.187523	21.661199
H	9.865500	23.359500	24.031600	H	9.186786	20.433808	21.596668
H	9.835200	14.609800	15.524000	O	10.805993	22.444409	21.827693
H	8.639900	25.915400	21.449100	H	9.894857	22.129715	21.608687
H	8.639900	24.729900	18.159900	Zn	11.877708	20.885734	20.949166
H	8.590300	13.254600	21.455400	C	14.308488	18.939832	20.793942
H	8.590300	12.068200	18.153600	C	13.855789	18.878566	19.351419
H	8.422600	19.223600	26.368900	H	14.046414	18.012937	21.335247
H	8.422600	18.760400	13.240100	H	12.804535	18.594032	19.231513
H	8.402900	20.906700	24.715000	O	13.672553	20.038467	21.346529
H	8.402900	17.077300	14.894000	H	15.401176	19.070218	20.862330
H	7.215200	19.037200	15.248900	H	14.054150	19.812032	18.818137
H	7.215200	18.946800	24.360100	N	14.509144	13.543684	19.538209
H	6.336500	23.058400	18.204400	C	15.785987	14.095354	20.103616
H	6.334900	19.929700	21.841400	H	15.732471	14.060091	21.192236
H	6.318500	14.878900	21.406200	H	15.894335	15.130675	19.770724
H	6.288700	22.188500	21.908000	C	14.580209	13.549413	18.039853
H	6.285500	18.107800	17.758700	H	15.449215	12.971647	17.720670
H	6.261400	15.789400	17.707000	H	14.675586	14.584599	17.709066
H	6.228500	20.952100	17.239700	C	13.347314	14.390132	19.980744
H	6.228500	17.031900	22.369300	H	12.433585	13.991979	19.537522
Si	10.834951	18.690405	23.080044	H	13.516032	15.412200	19.636186
Si	10.891245	23.512185	23.052608	C	14.306891	12.145720	20.020147
Si	10.060152	21.693395	18.327923	H	13.367703	11.766795	19.613747
Si	6.948678	21.087249	21.276843	H	14.261329	12.149768	21.109777
O	10.605999	19.697173	21.900713	H	13.279746	14.362773	21.068447

H	16.626979	13.497714	19.745022
H	15.141287	11.529110	19.682688
H	13.658745	13.123066	17.640512
I	15.015609	17.396538	18.179915
C	14.580101	21.635775	21.243782
O	13.637132	22.387725	21.129277
O	15.748810	21.436179	21.324500

3.9 Zn-DeAlBEA INT2				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.424017	20.960224	19.656790
H	10.571400	10.713700	18.212700	O	8.523585	21.208543	21.686455
H	9.865500	23.359500	24.031600	H	9.197104	20.462258	21.640034
H	9.835200	14.609800	15.524000	O	10.844750	22.464238	21.788476
H	8.639900	25.915400	21.449100	H	9.948477	22.154251	21.526969
H	8.639900	24.729900	18.159900	Zn	11.882329	20.815700	20.909080
H	8.590300	13.254600	21.455400	C	14.150244	18.192187	20.580834
H	8.590300	12.068200	18.153600	C	14.327009	18.063011	19.087912
H	8.422600	19.223600	26.368900	H	13.442071	17.456306	20.976890
H	8.422600	18.760400	13.240100	H	13.395167	18.247260	18.549429
H	8.402900	20.906700	24.715000	O	13.603517	19.480233	20.823377
H	8.402900	17.077300	14.894000	H	15.102447	18.110654	21.116667
H	7.215200	19.037200	15.248900	H	15.115680	18.718259	18.711974
H	7.215200	18.946800	24.360100	N	14.387611	13.167090	19.474549
H	6.336500	23.058400	18.204400	C	15.742540	13.512657	20.019553
H	6.334900	19.929700	21.841400	H	15.693042	13.507625	21.109189
H	6.318500	14.878900	21.406200	H	16.022414	14.510405	19.673002
H	6.288700	22.188500	21.908000	C	14.425586	13.175408	17.973804
H	6.285500	18.107800	17.758700	H	15.192089	12.476874	17.634339
H	6.261400	15.789400	17.707000	H	14.661752	14.184754	17.633938
H	6.228500	20.952100	17.239700	C	13.372445	14.170384	19.949181
H	6.228500	17.031900	22.369300	H	12.404995	13.916031	19.516579
Si	10.834939	18.680362	23.078269	H	13.688528	15.160602	19.616949
Si	10.895288	23.498428	23.041120	C	13.988524	11.809922	19.953350
Si	10.058909	21.688154	18.327208	H	12.989180	11.586292	19.577633
Si	6.956524	21.086965	21.279485	H	13.978158	11.809866	21.043977
O	10.601607	19.722502	21.928634	H	13.318793	14.132458	21.037674

H	16.468980	12.776756	19.670843
H	14.706524	11.076718	19.584311
H	13.443100	12.887294	17.596038
I	15.394398	16.961690	18.270498
C	14.471504	20.563574	21.285718
O	13.721755	21.576161	21.416801
O	15.652914	20.350129	21.461576

3.10 Zn-DeAlBEA TS3

Si 19.508300 21.734100 18.251000
 Si 19.508300 16.249900 21.358000
 Si 19.503800 25.900900 21.271600
 Si 19.503800 24.744700 18.337400
 Si 19.503800 13.239300 21.271600
 Si 19.503800 12.083100 18.337400
 Si 19.502500 21.054500 21.285100
 Si 19.502500 16.929500 18.323900
 Si 18.633200 23.512500 23.091300
 Si 18.633200 14.471500 16.517700
 Si 18.632400 19.351700 16.503500
 Si 18.632400 18.632300 23.105500
 Si 16.251500 22.701900 24.855400
 Si 16.251500 15.282100 14.753600
 Si 16.250300 19.508200 24.852300
 Si 16.250300 18.475800 14.756700
 Si 13.240600 22.709900 24.939400
 Si 13.240600 15.274100 14.669600
 Si 13.239600 19.503600 24.938600
 Si 13.239600 18.480400 14.670400
 Si 10.853700 14.469200 16.503500
 Si 10.851200 19.350900 16.490000
 Si 10.048700 25.902000 21.271600
 Si 10.048700 24.743500 18.337400
 Si 10.048700 13.240500 21.271600
 Si 10.048700 12.082000 18.337400

Si 10.040600 16.251100 21.354800
 Si 10.037800 16.927600 18.320700
 Si 8.393100 19.502500 24.925900
 Si 8.393100 18.481500 14.683100
 Si 6.846800 21.734100 18.251000
 Si 6.846800 16.249900 21.358000
 Si 6.841000 16.929500 18.323900
 O 19.196400 21.086800 19.698300
 O 19.196400 16.897200 19.910700
 O 19.151300 25.322800 19.804500
 O 19.151300 12.661200 19.804500
 O 18.927700 23.240900 18.198000
 O 18.927700 14.743100 21.411000
 O 18.870400 19.713700 21.928300
 O 18.870400 18.270300 17.680700
 O 18.843100 22.351700 21.987000
 O 18.843100 15.632300 17.622000
 O 18.828700 24.958900 22.398100
 O 18.828700 13.025100 17.210900
 O 18.804600 20.844100 17.100000
 O 18.804600 17.139900 22.509000
 O 17.142400 23.407600 23.706800
 O 17.142400 14.576400 15.902200
 O 17.140400 19.179600 15.907800
 O 17.140400 18.804400 23.701200
 O 16.220600 21.105000 24.608300
 O 16.220600 16.879000 15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.424282	20.950747	19.640414
H	10.571400	10.713700	18.212700	O	8.519783	21.191722	21.675266
H	9.865500	23.359500	24.031600	H	9.172335	20.442183	21.582958
H	9.835200	14.609800	15.524000	O	10.776388	22.472878	21.815962
H	8.639900	25.915400	21.449100	H	9.858452	22.156164	21.620871
H	8.639900	24.729900	18.159900	Zn	11.811664	20.915865	20.940453
H	8.590300	13.254600	21.455400	C	15.690861	18.834613	20.302110
H	8.590300	12.068200	18.153600	C	14.457970	18.459326	21.065145
H	8.422600	19.223600	26.368900	H	16.688063	18.562867	20.622992
H	8.422600	18.760400	13.240100	H	13.850244	17.698177	20.582504
H	8.402900	20.906700	24.715000	O	13.642944	19.630773	21.100487
H	8.402900	17.077300	14.894000	H	15.601257	19.363824	19.363802
H	7.215200	19.037200	15.248900	H	14.700733	18.151478	22.089088
H	7.215200	18.946800	24.360100	C	14.416350	20.773429	21.279184
H	6.336500	23.058400	18.204400	O	13.716006	21.797109	21.375922
H	6.334900	19.929700	21.841400	O	15.659658	20.578873	21.281720
H	6.318500	14.878900	21.406200	N	14.318978	12.990924	19.823688
H	6.288700	22.188500	21.908000	C	15.769822	12.873677	19.460086
H	6.285500	18.107800	17.758700	H	16.299884	12.405753	20.290740
H	6.261400	15.789400	17.707000	H	16.158150	13.880633	19.272409
H	6.228500	20.952100	17.239700	C	13.545555	13.534752	18.657064
H	6.228500	17.031900	22.369300	H	13.600875	12.821588	17.833261
Si	10.830631	18.683579	23.082830	H	13.984336	14.493774	18.369465
Si	10.889276	23.518794	23.058349	C	14.175020	13.929773	20.986268
Si	10.055139	21.694110	18.314643	H	13.115471	14.038182	21.225937
Si	6.942027	21.087731	21.275622	H	14.594549	14.894507	20.684795
O	10.627598	19.712460	21.919328	C	13.774083	11.650770	20.188814

H	12.709283	11.753869	20.404940
H	14.306336	11.275487	21.063850
H	14.723809	13.519309	21.834843
H	15.856589	12.263869	18.559105
H	13.913916	10.971839	19.346276
H	12.512315	13.672206	18.976433
I	15.633308	16.637233	18.612706

3.11 Zn-DeAlBEA PROD	Si	10.040600	16.251100	21.354800
Si 19.508300 21.734100 18.251000	Si	10.037800	16.927600	18.320700
Si 19.508300 16.249900 21.358000	Si	8.393100	19.502500	24.925900
Si 19.503800 25.900900 21.271600	Si	8.393100	18.481500	14.683100
Si 19.503800 24.744700 18.337400	Si	6.846800	21.734100	18.251000
Si 19.503800 13.239300 21.271600	Si	6.846800	16.249900	21.358000
Si 19.503800 12.083100 18.337400	Si	6.841000	16.929500	18.323900
Si 19.502500 21.054500 21.285100	O	19.196400	21.086800	19.698300
Si 19.502500 16.929500 18.323900	O	19.196400	16.897200	19.910700
Si 18.633200 23.512500 23.091300	O	19.151300	25.322800	19.804500
Si 18.633200 14.471500 16.517700	O	19.151300	12.661200	19.804500
Si 18.632400 19.351700 16.503500	O	18.927700	23.240900	18.198000
Si 18.632400 18.632300 23.105500	O	18.927700	14.743100	21.411000
Si 16.251500 22.701900 24.855400	O	18.870400	19.713700	21.928300
Si 16.251500 15.282100 14.753600	O	18.870400	18.270300	17.680700
Si 16.250300 19.508200 24.852300	O	18.843100	22.351700	21.987000
Si 16.250300 18.475800 14.756700	O	18.843100	15.632300	17.622000
Si 13.240600 22.709900 24.939400	O	18.828700	24.958900	22.398100
Si 13.240600 15.274100 14.669600	O	18.828700	13.025100	17.210900
Si 13.239600 19.503600 24.938600	O	18.804600	20.844100	17.100000
Si 13.239600 18.480400 14.670400	O	18.804600	17.139900	22.509000
Si 10.853700 14.469200 16.503500	O	17.142400	23.407600	23.706800
Si 10.851200 19.350900 16.490000	O	17.142400	14.576400	15.902200
Si 10.048700 25.902000 21.271600	O	17.140400	19.179600	15.907800
Si 10.048700 24.743500 18.337400	O	17.140400	18.804400	23.701200
Si 10.048700 13.240500 21.271600	O	16.220600	21.105000	24.608300
Si 10.048700 12.082000 18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.369682	20.954998	19.636470
H	10.571400	10.713700	18.212700	O	8.517074	21.226718	21.693594
H	9.865500	23.359500	24.031600	H	9.157132	20.464520	21.640481
H	9.835200	14.609800	15.524000	O	10.844088	22.466861	21.799154
H	8.639900	25.915400	21.449100	H	9.929903	22.173930	21.557274
H	8.639900	24.729900	18.159900	Zn	11.755855	20.830747	20.888276
H	8.590300	13.254600	21.455400	C	15.340812	17.904355	21.152394
H	8.590300	12.068200	18.153600	C	13.908981	17.598785	20.718448
H	8.422600	19.223600	26.368900	H	15.692611	17.314613	21.998344
H	8.422600	18.760400	13.240100	H	13.834215	17.143949	19.733381
H	8.402900	20.906700	24.715000	O	13.312027	18.930283	20.649852
H	8.402900	17.077300	14.894000	H	16.066438	17.854360	20.336742
H	7.215200	19.037200	15.248900	H	13.330550	17.026480	21.447597
H	7.215200	18.946800	24.360100	C	14.124026	19.802231	21.241905
H	6.336500	23.058400	18.204400	O	13.759357	20.967193	21.416140
H	6.334900	19.929700	21.841400	O	15.274702	19.302360	21.598747
H	6.318500	14.878900	21.406200	N	14.903786	11.180733	17.805374
H	6.288700	22.188500	21.908000	C	15.640224	12.057781	16.834909
H	6.285500	18.107800	17.758700	H	16.588796	11.579477	16.584973
H	6.261400	15.789400	17.707000	H	15.814362	13.025830	17.315786
H	6.228500	20.952100	17.239700	C	13.594906	11.830477	18.146573
H	6.228500	17.031900	22.369300	H	13.017286	11.945475	17.228664
Si	10.825652	18.668881	23.091522	H	13.808662	12.811148	18.592737
Si	10.891059	23.514676	23.054191	C	15.724967	11.023364	19.050990
Si	10.045541	21.698615	18.299830	H	15.173793	10.390681	19.748218
Si	6.943330	21.090915	21.278235	H	15.890822	12.021944	19.476679
O	10.602265	19.710521	21.940171	C	14.657637	9.846172	17.194023

H	14.116294	9.221696	17.906414
H	15.616447	9.386857	16.948314
H	16.672846	10.553555	18.780636
H	15.021322	12.187118	15.945862
H	14.063157	9.976226	16.288786
H	13.066899	11.188740	18.854518
I	15.535326	14.793279	19.495059

4. Mg-DeAlBEA

4.1 Mg-DeAlBEA

Si	19.508300	21.734100	18.251000
Si	19.508300	16.249900	21.358000
Si	19.503800	25.900900	21.271600
Si	19.503800	24.744700	18.337400
Si	19.503800	13.239300	21.271600
Si	19.503800	12.083100	18.337400
Si	19.502500	21.054500	21.285100
Si	19.502500	16.929500	18.323900
Si	18.633200	23.512500	23.091300
Si	18.633200	14.471500	16.517700
Si	18.632400	19.351700	16.503500
Si	18.632400	18.632300	23.105500
Si	16.251500	22.701900	24.855400
Si	16.251500	15.282100	14.753600
Si	16.250300	19.508200	24.852300
Si	16.250300	18.475800	14.756700
Si	13.240616	22.709867	24.939367
Si	13.240600	15.274100	14.669600
Si	13.239573	19.503478	24.938696
Si	13.239600	18.480400	14.670400
Si	10.853700	14.469200	16.503500
Si	10.851075	19.350941	16.489880
Si	10.048768	25.901975	21.271538
Si	10.048683	24.743510	18.337223
Si	10.048700	13.240500	21.271600

Si	10.048700	12.082000	18.337400
Si	10.040539	16.251068	21.354862
Si	10.037800	16.927600	18.320700
Si	8.393138	19.502511	24.925961
Si	8.393100	18.481500	14.683100
Si	6.846788	21.734200	18.251012
Si	6.846800	16.249900	21.358000
Si	6.841000	16.929500	18.323900
O	19.196400	21.086800	19.698300
O	19.196400	16.897200	19.910700
O	19.151300	25.322800	19.804500
O	19.151300	12.661200	19.804500
O	18.927700	23.240900	18.198000
O	18.927700	14.743100	21.411000
O	18.870400	19.713700	21.928300
O	18.870400	18.270300	17.680700
O	18.843100	22.351700	21.987000
O	18.843100	15.632300	17.622000
O	18.828700	24.958900	22.398100
O	18.828700	13.025100	17.210900
O	18.804600	20.844100	17.100000
O	18.804600	17.139900	22.509000
O	17.142400	23.407600	23.706800
O	17.142400	14.576400	15.902200
O	17.140400	19.179600	15.907800
O	17.140400	18.804400	23.701200
O	16.220600	21.105000	24.608300

O	16.220600	16.879000	15.000700	O	6.534914	21.086713	19.698342
O	14.745101	23.284597	24.802398	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743299	18.927397	24.799203	H	20.962200	13.254500	21.455400
O	13.256103	21.106598	24.736598	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301340	23.386484	23.812102	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297599	19.155701	15.796098	H	20.956200	16.919500	18.105600
O	12.297619	18.828494	23.812756	H	19.619900	23.348100	24.168500
O	10.746504	20.841801	17.105626	H	19.619900	14.635900	15.440500
O	10.746400	17.142217	22.503478	H	19.616500	19.135300	15.433200
O	10.725214	24.962661	22.399041	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670622	18.266100	17.673503	H	18.910700	25.572300	17.347700
O	10.623298	23.238962	18.200546	H	18.910700	12.411700	22.261300
O	10.623303	14.745001	21.408698	H	16.839100	19.224200	26.169000
O	10.401405	25.322800	19.804495	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348503	16.897198	19.905900	H	16.839000	15.002200	13.435500
O	9.690584	19.141291	15.384919	H	12.713692	19.183012	26.273300
O	9.690527	18.842639	24.224022	H	12.713700	18.801000	13.335700
O	8.443936	21.763586	18.006221	H	12.713601	23.030702	26.273700
O	8.443999	16.220312	21.602692	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643289	25.568997	17.346791

H	10.643300	12.415000	22.262200	O	10.670341	19.676928	21.935030
H	10.571401	27.270300	21.396299	O	10.413322	20.968545	19.612088
H	10.571400	10.713700	18.212700	O	8.529740	21.220783	21.665074
H	9.865572	23.359512	24.031544	H	9.134199	20.442943	21.580907
H	9.835200	14.609800	15.524000	O	10.857650	22.453473	21.823239
H	8.639901	25.915408	21.449106	H	9.927102	22.173567	21.593803
H	8.639896	24.729896	18.159932	Mg	11.628316	20.862588	20.938106
H	8.590300	13.254600	21.455400				
H	8.590300	12.068200	18.153600				
H	8.422606	19.223610	26.368902				
H	8.422600	18.760400	13.240100				
H	8.402893	20.906698	24.714989				
H	8.402900	17.077300	14.894000				
H	7.215200	19.037200	15.248900				
H	7.215200	18.946807	24.360093				
H	6.336506	23.058403	18.204415				
H	6.334905	19.929732	21.841337				
H	6.318500	14.878900	21.406200				
H	6.288691	22.188528	21.908012				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228498	20.952096	17.239704				
H	6.228500	17.031900	22.369300				
Si	10.834196	18.640770	23.107760				
Si	10.890385	23.531088	23.070370				
Si	10.042533	21.701587	18.280784				
Si	6.935953	21.090084	21.274112				

4.1 Mg-DeAlBEA CO ₂ ADS	Si	10.040600	16.251100	21.354800
Si 19.508300 21.734100 18.251000	Si	10.037800	16.927600	18.320700
Si 19.508300 16.249900 21.358000	Si	8.393100	19.502500	24.925900
Si 19.503800 25.900900 21.271600	Si	8.393100	18.481500	14.683100
Si 19.503800 24.744700 18.337400	Si	6.846800	21.734100	18.251000
Si 19.503800 13.239300 21.271600	Si	6.846800	16.249900	21.358000
Si 19.503800 12.083100 18.337400	Si	6.841000	16.929500	18.323900
Si 19.502500 21.054500 21.285100	O	19.196400	21.086800	19.698300
Si 19.502500 16.929500 18.323900	O	19.196400	16.897200	19.910700
Si 18.633200 23.512500 23.091300	O	19.151300	25.322800	19.804500
Si 18.633200 14.471500 16.517700	O	19.151300	12.661200	19.804500
Si 18.632400 19.351700 16.503500	O	18.927700	23.240900	18.198000
Si 18.632400 18.632300 23.105500	O	18.927700	14.743100	21.411000
Si 16.251500 22.701900 24.855400	O	18.870400	19.713700	21.928300
Si 16.251500 15.282100 14.753600	O	18.870400	18.270300	17.680700
Si 16.250300 19.508200 24.852300	O	18.843100	22.351700	21.987000
Si 16.250300 18.475800 14.756700	O	18.843100	15.632300	17.622000
Si 13.240600 22.709900 24.939400	O	18.828700	24.958900	22.398100
Si 13.240600 15.274100 14.669600	O	18.828700	13.025100	17.210900
Si 13.239600 19.503600 24.938600	O	18.804600	20.844100	17.100000
Si 13.239600 18.480400 14.670400	O	18.804600	17.139900	22.509000
Si 10.853700 14.469200 16.503500	O	17.142400	23.407600	23.706800
Si 10.851200 19.350900 16.490000	O	17.142400	14.576400	15.902200
Si 10.048700 25.902000 21.271600	O	17.140400	19.179600	15.907800
Si 10.048700 24.743500 18.337400	O	17.140400	18.804400	23.701200
Si 10.048700 13.240500 21.271600	O	16.220600	21.105000	24.608300
Si 10.048700 12.082000 18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.386600	20.978700	19.629400
H	10.571400	10.713700	18.212700	O	8.527600	21.236500	21.676000
H	9.865500	23.359500	24.031600	H	9.143700	20.465400	21.599400
H	9.835200	14.609800	15.524000	O	10.917000	22.436600	21.810300
H	8.639900	25.915400	21.449100	H	10.001900	22.166800	21.533400
H	8.639900	24.729900	18.159900	Mg	11.680800	20.797900	20.894700
H	8.590300	13.254600	21.455400	C	13.232800	18.481600	19.426800
H	8.590300	12.068200	18.153600	O	13.355300	17.472100	18.876800
H	8.422600	19.223600	26.368900	O	13.162100	19.516200	19.987400
H	8.422600	18.760400	13.240100				
H	8.402900	20.906700	24.715000				
H	8.402900	17.077300	14.894000				
H	7.215200	19.037200	15.248900				
H	7.215200	18.946800	24.360100				
H	6.336500	23.058400	18.204400				
H	6.334900	19.929700	21.841400				
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.830200	18.650500	23.103600				
Si	10.893700	23.518800	23.057400				
Si	10.039900	21.702800	18.290200				
Si	6.941400	21.091900	21.276500				
O	10.647400	19.679300	21.930200				

4.3 Mg-DeAlBEA ADS1

Si 19.508300 21.734100 18.251000
 Si 19.508300 16.249900 21.358000
 Si 19.503800 25.900900 21.271600
 Si 19.503800 24.744700 18.337400
 Si 19.503800 13.239300 21.271600
 Si 19.503800 12.083100 18.337400
 Si 19.502500 21.054500 21.285100
 Si 19.502500 16.929500 18.323900
 Si 18.633200 23.512500 23.091300
 Si 18.633200 14.471500 16.517700
 Si 18.632400 19.351700 16.503500
 Si 18.632400 18.632300 23.105500
 Si 16.251500 22.701900 24.855400
 Si 16.251500 15.282100 14.753600
 Si 16.250300 19.508200 24.852300
 Si 16.250300 18.475800 14.756700
 Si 13.240600 22.709900 24.939400
 Si 13.240600 15.274100 14.669600
 Si 13.239600 19.503600 24.938600
 Si 13.239600 18.480400 14.670400
 Si 10.853700 14.469200 16.503500
 Si 10.851200 19.350900 16.490000
 Si 10.048700 25.902000 21.271600
 Si 10.048700 24.743500 18.337400
 Si 10.048700 13.240500 21.271600
 Si 10.048700 12.082000 18.337400

Si 10.040600 16.251100 21.354800
 Si 10.037800 16.927600 18.320700
 Si 8.393100 19.502500 24.925900
 Si 8.393100 18.481500 14.683100
 Si 6.846800 21.734100 18.251000
 Si 6.846800 16.249900 21.358000
 Si 6.841000 16.929500 18.323900
 O 19.196400 21.086800 19.698300
 O 19.196400 16.897200 19.910700
 O 19.151300 25.322800 19.804500
 O 19.151300 12.661200 19.804500
 O 18.927700 23.240900 18.198000
 O 18.927700 14.743100 21.411000
 O 18.870400 19.713700 21.928300
 O 18.870400 18.270300 17.680700
 O 18.843100 22.351700 21.987000
 O 18.843100 15.632300 17.622000
 O 18.828700 24.958900 22.398100
 O 18.828700 13.025100 17.210900
 O 18.804600 20.844100 17.100000
 O 18.804600 17.139900 22.509000
 O 17.142400 23.407600 23.706800
 O 17.142400 14.576400 15.902200
 O 17.140400 19.179600 15.907800
 O 17.140400 18.804400 23.701200
 O 16.220600 21.105000 24.608300
 O 16.220600 16.879000 15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.408103	20.976933	19.635296
H	10.571400	10.713700	18.212700	O	8.529698	21.224567	21.667558
H	9.865500	23.359500	24.031600	H	9.151611	20.463227	21.552645
H	9.835200	14.609800	15.524000	O	10.892768	22.446891	21.816160
H	8.639900	25.915400	21.449100	H	9.979723	22.168041	21.543652
H	8.639900	24.729900	18.159900	Mg	11.714887	20.852922	20.920692
H	8.590300	13.254600	21.455400	C	14.095540	18.830697	20.878646
H	8.590300	12.068200	18.153600	C	13.439085	18.929254	19.583126
H	8.422600	19.223600	26.368900	H	13.576109	18.369480	21.716821
H	8.422600	18.760400	13.240100	H	12.424275	18.548704	19.461934
H	8.402900	20.906700	24.715000	O	13.539127	20.098723	20.449942
H	8.402900	17.077300	14.894000	H	15.180564	18.851517	20.934982
H	7.215200	19.037200	15.248900	H	14.027673	19.029312	18.675064
H	7.215200	18.946800	24.360100				
H	6.336500	23.058400	18.204400				
H	6.334900	19.929700	21.841400				
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.826022	18.658156	23.094695				
Si	10.891429	23.522310	23.060841				
Si	10.044822	21.699043	18.298839				
Si	6.941308	21.090666	21.275278				
O	10.668446	19.676452	21.912233				

4.4 Mg-DeAlBEA ADS2				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.397623	20.970671	19.636717
H	10.571400	10.713700	18.212700	O	8.526427	21.214041	21.675631
H	9.865500	23.359500	24.031600	H	9.156325	20.457659	21.555237
H	9.835200	14.609800	15.524000	O	10.854606	22.454247	21.819701
H	8.639900	25.915400	21.449100	H	9.935415	22.170075	21.573724
H	8.639900	24.729900	18.159900	Mg	11.703465	20.882228	20.930879
H	8.590300	13.254600	21.455400	C	14.433426	19.494978	20.917147
H	8.590300	12.068200	18.153600	C	14.059074	19.878028	19.576550
H	8.422600	19.223600	26.368900	H	13.885451	18.704357	21.426912
H	8.422600	18.760400	13.240100	H	13.214770	19.385689	19.094710
H	8.402900	20.906700	24.715000	O	13.687770	20.735626	20.727861
H	8.402900	17.077300	14.894000	H	15.451075	19.665754	21.258443
H	7.215200	19.037200	15.248900	H	14.785358	20.336999	18.913913
H	7.215200	18.946800	24.360100	N	14.534764	13.065726	19.230158
H	6.336500	23.058400	18.204400	C	15.924327	13.431726	19.658302
H	6.334900	19.929700	21.841400	H	16.004315	13.310707	20.740120
H	6.318500	14.878900	21.406200	H	16.100373	14.477623	19.371718
H	6.288700	22.188500	21.908000	C	14.419353	13.262181	17.745705
H	6.285500	18.107800	17.758700	H	15.190085	12.665613	17.254415
H	6.261400	15.789400	17.707000	H	14.573543	14.326089	17.534178
H	6.228500	20.952100	17.239700	C	13.537811	13.948871	19.925377
H	6.228500	17.031900	22.369300	H	12.543254	13.693753	19.559492
Si	10.831138	18.663624	23.091423	H	13.784572	14.991724	19.688166
Si	10.890422	23.523063	23.062150	C	14.252991	11.644564	19.569977
Si	10.047014	21.695992	18.299946	H	13.226288	11.410635	19.281587
Si	6.941748	21.089803	21.274945	H	14.373418	11.505989	20.645506
O	10.662723	19.684332	21.914386	H	13.603416	13.764373	20.999286

H	16.623790	12.765860	19.153013
H	14.951033	11.002718	19.029886
H	13.423216	12.949619	17.430209
I	15.175690	16.943819	18.421262

4.5 Mg-DeAlBEA TS1				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.412401	20.971033	19.643520
H	10.571400	10.713700	18.212700	O	8.526312	21.210990	21.673934
H	9.865500	23.359500	24.031600	H	9.164912	20.456942	21.562460
H	9.835200	14.609800	15.524000	O	10.844676	22.456895	21.817736
H	8.639900	25.915400	21.449100	H	9.928324	22.170324	21.569587
H	8.639900	24.729900	18.159900	Mg	11.732824	20.890089	20.951581
H	8.590300	13.254600	21.455400	C	14.451368	19.602337	21.075570
H	8.590300	12.068200	18.153600	C	13.982863	19.554517	19.702021
H	8.422600	19.223600	26.368900	H	14.078344	18.830489	21.759626
H	8.422600	18.760400	13.240100	H	13.006787	19.131263	19.474989
H	8.402900	20.906700	24.715000	O	13.677462	20.779200	21.016394
H	8.402900	17.077300	14.894000	H	15.518902	19.789786	21.223841
H	7.215200	19.037200	15.248900	H	14.472355	20.144994	18.940806
H	7.215200	18.946800	24.360100	N	14.522567	13.372813	19.427267
H	6.336500	23.058400	18.204400	C	15.828349	13.806371	20.026607
H	6.334900	19.929700	21.841400	H	15.764754	13.710618	21.111694
H	6.318500	14.878900	21.406200	H	16.003890	14.851943	19.749734
H	6.288700	22.188500	21.908000	C	14.594861	13.519572	17.934910
H	6.285500	18.107800	17.758700	H	15.430754	12.923445	17.564999
H	6.261400	15.789400	17.707000	H	14.754216	14.578396	17.708782
H	6.228500	20.952100	17.239700	C	13.410646	14.233285	19.960670
H	6.228500	17.031900	22.369300	H	12.478599	13.937549	19.477222
Si	10.831227	18.671731	23.086566	H	13.649843	15.277826	19.732492
Si	10.890631	23.520413	23.060120	C	14.249348	11.950046	19.774467
Si	10.050837	21.694129	18.309780	H	13.285476	11.664038	19.349294
Si	6.944113	21.089549	21.275415	H	14.216975	11.849940	20.860451
O	10.644461	19.682124	21.905424	H	13.339324	14.079175	21.038210

H	16.624587	13.169726	19.635830
H	15.042803	11.323130	19.364160
H	13.653012	13.178568	17.503206
I	15.113404	17.263566	18.499105

4.6 Mg-DeAlBEA INT1				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.422554	20.972509	19.652159
H	10.571400	10.713700	18.212700	O	8.527169	21.217670	21.674489
H	9.865500	23.359500	24.031600	H	9.177459	20.464414	21.590253
H	9.835200	14.609800	15.524000	O	10.873457	22.449255	21.811087
H	8.639900	25.915400	21.449100	H	9.969621	22.165489	21.529637
H	8.639900	24.729900	18.159900	Mg	11.785872	20.858383	20.949879
H	8.590300	13.254600	21.455400	C	14.373040	19.564116	20.673709
H	8.590300	12.068200	18.153600	C	13.895735	19.293713	19.264334
H	8.422600	19.223600	26.368900	H	14.188225	18.665240	21.303131
H	8.422600	18.760400	13.240100	H	12.838612	19.008210	19.197361
H	8.402900	20.906700	24.715000	O	13.675273	20.673755	21.057602
H	8.402900	17.077300	14.894000	H	15.469198	19.723129	20.672356
H	7.215200	19.037200	15.248900	H	14.113767	20.108522	18.571715
H	7.215200	18.946800	24.360100	N	14.510646	13.631484	19.535127
H	6.336500	23.058400	18.204400	C	15.781276	14.183599	20.112010
H	6.334900	19.929700	21.841400	H	15.722506	14.137235	21.199941
H	6.318500	14.878900	21.406200	H	15.885293	15.223506	19.790962
H	6.288700	22.188500	21.908000	C	14.579928	13.677084	18.037943
H	6.285500	18.107800	17.758700	H	15.462074	13.129063	17.703498
H	6.261400	15.789400	17.707000	H	14.649475	14.723014	17.733841
H	6.228500	20.952100	17.239700	C	13.339545	14.451947	20.001226
H	6.228500	17.031900	22.369300	H	12.430438	14.047952	19.553710
Si	10.833934	18.682935	23.082113	H	13.493933	15.485744	19.681977
Si	10.893211	23.512243	23.052884	C	14.327615	12.219578	19.981008
Si	10.053757	21.693189	18.321701	H	13.389245	11.841117	19.572256
Si	6.950155	21.090365	21.277331	H	14.290846	12.194442	21.070765
O	10.616075	19.682984	21.898470	H	13.278317	14.395831	21.088032

H	16.623681	13.588791	19.752959
H	15.165867	11.620877	19.621080
H	13.669614	13.238081	17.627259
I	14.971603	17.537149	18.311374

4.7 Mg-DeAlBEA CO ₂ -INT1				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.440817	20.960195	19.643968
H	10.571400	10.713700	18.212700	O	8.527871	21.193238	21.667231
H	9.865500	23.359500	24.031600	H	9.179165	20.440908	21.570480
H	9.835200	14.609800	15.524000	O	10.819929	22.443802	21.828284
H	8.639900	25.915400	21.449100	H	9.903326	22.142668	21.603503
H	8.639900	24.729900	18.159900	Mg	11.783104	20.906473	20.970778
H	8.590300	13.254600	21.455400	C	14.410761	19.596001	20.742841
H	8.590300	12.068200	18.153600	C	13.892365	19.280455	19.356850
H	8.422600	19.223600	26.368900	H	14.287403	18.713725	21.404922
H	8.422600	18.760400	13.240100	H	12.845036	18.957707	19.344987
H	8.402900	20.906700	24.715000	O	13.677442	20.684784	21.133066
H	8.402900	17.077300	14.894000	H	15.495352	19.811032	20.697602
H	7.215200	19.037200	15.248900	H	14.046963	20.097226	18.648176
H	7.215200	18.946800	24.360100	N	14.513506	13.638356	19.534154
H	6.336500	23.058400	18.204400	C	15.784061	14.183204	20.118066
H	6.334900	19.929700	21.841400	H	15.723525	14.127578	21.205447
H	6.318500	14.878900	21.406200	H	15.891041	15.225655	19.806434
H	6.288700	22.188500	21.908000	C	14.585505	13.697817	18.037694
H	6.285500	18.107800	17.758700	H	15.467779	13.152418	17.699639
H	6.261400	15.789400	17.707000	H	14.656234	14.746422	17.743287
H	6.228500	20.952100	17.239700	C	13.342391	14.455633	20.005412
H	6.228500	17.031900	22.369300	H	12.433077	14.054239	19.555881
Si	10.834696	18.685150	23.079783	H	13.496800	15.491255	19.692363
Si	10.891089	23.515946	23.054832	C	14.328051	12.222517	19.966752
Si	10.056597	21.692637	18.324050	H	13.389861	11.848892	19.553247
Si	6.947568	21.087845	21.275881	H	14.289628	12.187528	21.056170
O	10.627232	19.685124	21.894114	H	13.281199	14.393195	21.091859

H	16.625898	13.589886	19.755285
H	15.166171	11.626194	19.602651
H	13.675967	13.263223	17.620771
I	14.987841	17.569313	18.363064
C	14.553572	23.054520	20.556651
O	13.450612	23.446988	20.614289
O	15.681688	22.757813	20.470104

4.8 Mg-DeAlBEA TS2

Si 19.508300 21.734100 18.251000
 Si 19.508300 16.249900 21.358000
 Si 19.503800 25.900900 21.271600
 Si 19.503800 24.744700 18.337400
 Si 19.503800 13.239300 21.271600
 Si 19.503800 12.083100 18.337400
 Si 19.502500 21.054500 21.285100
 Si 19.502500 16.929500 18.323900
 Si 18.633200 23.512500 23.091300
 Si 18.633200 14.471500 16.517700
 Si 18.632400 19.351700 16.503500
 Si 18.632400 18.632300 23.105500
 Si 16.251500 22.701900 24.855400
 Si 16.251500 15.282100 14.753600
 Si 16.250300 19.508200 24.852300
 Si 16.250300 18.475800 14.756700
 Si 13.240600 22.709900 24.939400
 Si 13.240600 15.274100 14.669600
 Si 13.239600 19.503600 24.938600
 Si 13.239600 18.480400 14.670400
 Si 10.853700 14.469200 16.503500
 Si 10.851200 19.350900 16.490000
 Si 10.048700 25.902000 21.271600
 Si 10.048700 24.743500 18.337400
 Si 10.048700 13.240500 21.271600
 Si 10.048700 12.082000 18.337400

Si 10.040600 16.251100 21.354800
 Si 10.037800 16.927600 18.320700
 Si 8.393100 19.502500 24.925900
 Si 8.393100 18.481500 14.683100
 Si 6.846800 21.734100 18.251000
 Si 6.846800 16.249900 21.358000
 Si 6.841000 16.929500 18.323900
 O 19.196400 21.086800 19.698300
 O 19.196400 16.897200 19.910700
 O 19.151300 25.322800 19.804500
 O 19.151300 12.661200 19.804500
 O 18.927700 23.240900 18.198000
 O 18.927700 14.743100 21.411000
 O 18.870400 19.713700 21.928300
 O 18.870400 18.270300 17.680700
 O 18.843100 22.351700 21.987000
 O 18.843100 15.632300 17.622000
 O 18.828700 24.958900 22.398100
 O 18.828700 13.025100 17.210900
 O 18.804600 20.844100 17.100000
 O 18.804600 17.139900 22.509000
 O 17.142400 23.407600 23.706800
 O 17.142400 14.576400 15.902200
 O 17.140400 19.179600 15.907800
 O 17.140400 18.804400 23.701200
 O 16.220600 21.105000 24.608300
 O 16.220600 16.879000 15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.496218	20.961482	19.641782
H	10.571400	10.713700	18.212700	O	8.529778	21.183154	21.652288
H	9.865500	23.359500	24.031600	H	9.190031	20.429900	21.585359
H	9.835200	14.609800	15.524000	O	10.793257	22.440627	21.836362
H	8.639900	25.915400	21.449100	H	9.876161	22.128820	21.628411
H	8.639900	24.729900	18.159900	Mg	11.828742	20.923755	21.000023
H	8.590300	13.254600	21.455400	C	14.275760	18.970110	20.768475
H	8.590300	12.068200	18.153600	C	13.863232	18.876409	19.316200
H	8.422600	19.223600	26.368900	H	14.015870	18.044500	21.316086
H	8.422600	18.760400	13.240100	H	12.815491	18.590785	19.182299
H	8.402900	20.906700	24.715000	O	13.596352	20.061973	21.259148
H	8.402900	17.077300	14.894000	H	15.366681	19.111517	20.862712
H	7.215200	19.037200	15.248900	H	14.074082	19.798220	18.768992
H	7.215200	18.946800	24.360100	N	14.508566	13.519825	19.528433
H	6.336500	23.058400	18.204400	C	15.789242	14.060301	20.095994
H	6.334900	19.929700	21.841400	H	15.736064	14.018309	21.184405
H	6.318500	14.878900	21.406200	H	15.903628	15.097264	19.770081
H	6.288700	22.188500	21.908000	C	14.579433	13.530880	18.030019
H	6.285500	18.107800	17.758700	H	15.444692	12.948620	17.708757
H	6.261400	15.789400	17.707000	H	14.681239	14.566899	17.703334
H	6.228500	20.952100	17.239700	C	13.352342	14.372569	19.973979
H	6.228500	17.031900	22.369300	H	12.436215	13.980420	19.530517
Si	10.835165	18.691215	23.077371	H	13.526964	15.394321	19.631213
Si	10.889627	23.515074	23.055432	C	14.296978	12.121611	20.005085
Si	10.063322	21.690057	18.332801	H	13.355866	11.749867	19.596581
Si	6.948147	21.086609	21.275393	H	14.250331	12.121979	21.094696
O	10.620292	19.705827	21.904618	H	13.285873	14.343088	21.061697

H	16.626361	13.459797	19.732714
H	15.127729	11.500858	19.666186
H	13.655098	13.111880	17.629500
I	15.044419	17.366323	18.188629
C	14.519605	21.744459	21.236010
O	13.545341	22.447527	21.133106
O	15.680303	21.538823	21.338003

4.9 Mg-DeAlBEA INT2	Si	10.040600	16.251100	21.354800
Si 19.508300 21.734100 18.251000	Si	10.037800	16.927600	18.320700
Si 19.508300 16.249900 21.358000	Si	8.393100	19.502500	24.925900
Si 19.503800 25.900900 21.271600	Si	8.393100	18.481500	14.683100
Si 19.503800 24.744700 18.337400	Si	6.846800	21.734100	18.251000
Si 19.503800 13.239300 21.271600	Si	6.846800	16.249900	21.358000
Si 19.503800 12.083100 18.337400	Si	6.841000	16.929500	18.323900
Si 19.502500 21.054500 21.285100	O	19.196400	21.086800	19.698300
Si 19.502500 16.929500 18.323900	O	19.196400	16.897200	19.910700
Si 18.633200 23.512500 23.091300	O	19.151300	25.322800	19.804500
Si 18.633200 14.471500 16.517700	O	19.151300	12.661200	19.804500
Si 18.632400 19.351700 16.503500	O	18.927700	23.240900	18.198000
Si 18.632400 18.632300 23.105500	O	18.927700	14.743100	21.411000
Si 16.251500 22.701900 24.855400	O	18.870400	19.713700	21.928300
Si 16.251500 15.282100 14.753600	O	18.870400	18.270300	17.680700
Si 16.250300 19.508200 24.852300	O	18.843100	22.351700	21.987000
Si 16.250300 18.475800 14.756700	O	18.843100	15.632300	17.622000
Si 13.240600 22.709900 24.939400	O	18.828700	24.958900	22.398100
Si 13.240600 15.274100 14.669600	O	18.828700	13.025100	17.210900
Si 13.239600 19.503600 24.938600	O	18.804600	20.844100	17.100000
Si 13.239600 18.480400 14.670400	O	18.804600	17.139900	22.509000
Si 10.853700 14.469200 16.503500	O	17.142400	23.407600	23.706800
Si 10.851200 19.350900 16.490000	O	17.142400	14.576400	15.902200
Si 10.048700 25.902000 21.271600	O	17.140400	19.179600	15.907800
Si 10.048700 24.743500 18.337400	O	17.140400	18.804400	23.701200
Si 10.048700 13.240500 21.271600	O	16.220600	21.105000	24.608300
Si 10.048700 12.082000 18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.485461	20.949520	19.636648
H	10.571400	10.713700	18.212700	O	8.525083	21.187407	21.656809
H	9.865500	23.359500	24.031600	H	9.187865	20.436382	21.595962
H	9.835200	14.609800	15.524000	O	10.771285	22.462929	21.818100
H	8.639900	25.915400	21.449100	H	9.849683	22.156621	21.625385
H	8.639900	24.729900	18.159900	Mg	11.797577	20.937496	21.008245
H	8.590300	13.254600	21.455400	C	14.098628	18.502600	20.613728
H	8.590300	12.068200	18.153600	C	14.171038	18.599544	19.110532
H	8.422600	19.223600	26.368900	H	13.467896	17.667149	20.945669
H	8.422600	18.760400	13.240100	H	13.194900	18.538711	18.623612
H	8.402900	20.906700	24.715000	O	13.494268	19.696919	21.035119
H	8.402900	17.077300	14.894000	H	15.093731	18.425323	21.067585
H	7.215200	19.037200	15.248900	H	14.703940	19.497107	18.792472
H	7.215200	18.946800	24.360100	N	14.386991	13.164773	19.467047
H	6.336500	23.058400	18.204400	C	15.740486	13.516783	20.011789
H	6.334900	19.929700	21.841400	H	15.691187	13.511301	21.101421
H	6.318500	14.878900	21.406200	H	16.016466	14.515610	19.665349
H	6.288700	22.188500	21.908000	C	14.424811	13.171080	17.966297
H	6.285500	18.107800	17.758700	H	15.193064	12.473973	17.627887
H	6.261400	15.789400	17.707000	H	14.658311	14.180090	17.624056
H	6.228500	20.952100	17.239700	C	13.365918	14.162573	19.940834
H	6.228500	17.031900	22.369300	H	12.399176	13.898895	19.512487
Si	10.832779	18.691437	23.080769	H	13.671511	15.154367	19.603786
Si	10.892646	23.515259	23.056623	C	13.994776	11.805964	19.947210
Si	10.061767	21.690359	18.332588	H	12.997545	11.575761	19.569856
Si	6.946077	21.087241	21.275705	H	13.982223	11.807431	21.037805
O	10.610999	19.712090	21.916091	H	13.315940	14.128428	21.029621

H	16.469962	12.783846	19.663221
H	14.717689	11.076329	19.580696
H	13.443046	12.879917	17.589020
I	15.373986	16.969960	18.266015
C	14.385880	20.857196	21.393552
O	13.608077	21.834156	21.499274
O	15.570687	20.639769	21.505414

4.10 Mg-DeAlBEA TS3

Si 19.508300 21.734100 18.251000
 Si 19.508300 16.249900 21.358000
 Si 19.503800 25.900900 21.271600
 Si 19.503800 24.744700 18.337400
 Si 19.503800 13.239300 21.271600
 Si 19.503800 12.083100 18.337400
 Si 19.502500 21.054500 21.285100
 Si 19.502500 16.929500 18.323900
 Si 18.633200 23.512500 23.091300
 Si 18.633200 14.471500 16.517700
 Si 18.632400 19.351700 16.503500
 Si 18.632400 18.632300 23.105500
 Si 16.251500 22.701900 24.855400
 Si 16.251500 15.282100 14.753600
 Si 16.250300 19.508200 24.852300
 Si 16.250300 18.475800 14.756700
 Si 13.240600 22.709900 24.939400
 Si 13.240600 15.274100 14.669600
 Si 13.239600 19.503600 24.938600
 Si 13.239600 18.480400 14.670400
 Si 10.853700 14.469200 16.503500
 Si 10.851200 19.350900 16.490000
 Si 10.048700 25.902000 21.271600
 Si 10.048700 24.743500 18.337400
 Si 10.048700 13.240500 21.271600
 Si 10.048700 12.082000 18.337400

Si 10.040600 16.251100 21.354800
 Si 10.037800 16.927600 18.320700
 Si 8.393100 19.502500 24.925900
 Si 8.393100 18.481500 14.683100
 Si 6.846800 21.734100 18.251000
 Si 6.846800 16.249900 21.358000
 Si 6.841000 16.929500 18.323900
 O 19.196400 21.086800 19.698300
 O 19.196400 16.897200 19.910700
 O 19.151300 25.322800 19.804500
 O 19.151300 12.661200 19.804500
 O 18.927700 23.240900 18.198000
 O 18.927700 14.743100 21.411000
 O 18.870400 19.713700 21.928300
 O 18.870400 18.270300 17.680700
 O 18.843100 22.351700 21.987000
 O 18.843100 15.632300 17.622000
 O 18.828700 24.958900 22.398100
 O 18.828700 13.025100 17.210900
 O 18.804600 20.844100 17.100000
 O 18.804600 17.139900 22.509000
 O 17.142400 23.407600 23.706800
 O 17.142400 14.576400 15.902200
 O 17.140400 19.179600 15.907800
 O 17.140400 18.804400 23.701200
 O 16.220600 21.105000 24.608300
 O 16.220600 16.879000 15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.460383	20.966079	19.641713
H	10.571400	10.713700	18.212700	O	8.523599	21.194123	21.662876
H	9.865500	23.359500	24.031600	H	9.176005	20.445680	21.565916
H	9.835200	14.609800	15.524000	O	10.779925	22.466713	21.821095
H	8.639900	25.915400	21.449100	H	9.857089	22.162556	21.622199
H	8.639900	24.729900	18.159900	Mg	11.767461	20.948640	20.990409
H	8.590300	13.254600	21.455400	C	15.604158	18.839955	20.309747
H	8.590300	12.068200	18.153600	C	14.284205	18.503452	20.935927
H	8.422600	19.223600	26.368900	H	16.548537	18.513410	20.723770
H	8.422600	18.760400	13.240100	H	13.682611	17.805136	20.358888
H	8.402900	20.906700	24.715000	O	13.537052	19.717842	20.963583
H	8.402900	17.077300	14.894000	H	15.634215	19.384976	19.376379
H	7.215200	19.037200	15.248900	H	14.412474	18.129723	21.960041
H	7.215200	18.946800	24.360100	C	14.348469	20.811553	21.280032
H	6.336500	23.058400	18.204400	O	13.676640	21.841988	21.439435
H	6.334900	19.929700	21.841400	O	15.579239	20.558871	21.322377
H	6.318500	14.878900	21.406200	N	14.313821	13.006008	19.832406
H	6.288700	22.188500	21.908000	C	15.765129	12.889533	19.470082
H	6.285500	18.107800	17.758700	H	16.294463	12.421120	20.300937
H	6.261400	15.789400	17.707000	H	16.153425	13.896602	19.283439
H	6.228500	20.952100	17.239700	C	13.540596	13.549641	18.665536
H	6.228500	17.031900	22.369300	H	13.598643	12.837693	17.840862
Si	10.828556	18.684631	23.081286	H	13.977717	14.510118	18.379886
Si	10.890281	23.520901	23.060422	C	14.167070	13.944560	20.994998
Si	10.058299	21.691223	18.320487	H	13.107102	14.048575	21.234955
Si	6.942131	21.087964	21.274200	H	14.582614	14.911211	20.693786
O	10.638104	19.715373	21.921198	C	13.770441	11.665009	20.196661

H	12.705254	11.766191	20.411513
H	14.302348	11.290386	21.072196
H	14.717852	13.536423	21.843399
H	15.853230	12.280502	18.568633
H	13.912402	10.986496	19.354130
H	12.506613	13.684216	18.983879
I	15.643441	16.644022	18.621108

4.11 Mg-DeAlBEA PROD				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.405725	20.965809	19.635037
H	10.571400	10.713700	18.212700	O	8.523054	21.211668	21.678548
H	9.865500	23.359500	24.031600	H	9.163838	20.454185	21.595260
H	9.835200	14.609800	15.524000	O	10.821779	22.464052	21.808623
H	8.639900	25.915400	21.449100	H	9.898229	22.174079	21.588766
H	8.639900	24.729900	18.159900	Mg	11.710254	20.897247	20.937901
H	8.590300	13.254600	21.455400	C	15.288970	18.219823	21.031658
H	8.590300	12.068200	18.153600	C	13.908174	18.032672	20.399747
H	8.422600	19.223600	26.368900	H	15.505365	17.522984	21.840679
H	8.422600	18.760400	13.240100	H	13.242732	17.371955	20.959257
H	8.402900	20.906700	24.715000	O	15.230073	19.565379	21.626794
H	8.402900	17.077300	14.894000	O	13.351589	19.381895	20.473799
H	7.215200	19.037200	15.248900	O	13.713887	21.261384	21.566824
H	7.215200	18.946800	24.360100	C	14.120430	20.144672	21.260106
H	6.336500	23.058400	18.204400	H	16.111383	18.221732	20.312337
H	6.334900	19.929700	21.841400	H	13.930352	17.739857	19.353247
H	6.318500	14.878900	21.406200	N	14.883519	11.349632	18.062114
H	6.288700	22.188500	21.908000	C	15.562043	12.219813	17.044519
H	6.285500	18.107800	17.758700	H	16.550866	11.808211	16.837211
H	6.261400	15.789400	17.707000	H	15.644831	13.225562	17.471578
H	6.228500	20.952100	17.239700	C	13.528852	11.922061	18.357388
H	6.228500	17.031900	22.369300	H	12.958276	11.956164	17.428262
Si	10.827473	18.669392	23.089204	H	13.664284	12.936765	18.754618
Si	10.891205	23.518550	23.058965	C	15.702972	11.332627	19.318119
Si	10.048011	21.695067	18.305617	H	15.186004	10.721083	20.059104
Si	6.942732	21.089059	21.276080	H	15.805944	12.368436	19.667086
O	10.639828	19.707600	21.931882	C	14.741218	9.965831	17.533684

H	14.247251	9.346098	18.283661
H	15.733185	9.567036	17.314450
H	16.679426	10.902477	19.087289
H	14.951811	12.241980	16.140704
H	14.141722	9.993983	16.622924
H	13.035236	11.281175	19.090299
I	15.289199	15.107446	19.462937

Concerted mechanism**1. Ni-DeAlBEA****1.1 Ni-DeAlBEA TSc**

Si 19.508300 21.734100 18.251000
Si 19.508300 16.249900 21.358000
Si 19.503800 25.900900 21.271600
Si 19.503800 24.744700 18.337400
Si 19.503800 13.239300 21.271600
Si 19.503800 12.083100 18.337400
Si 19.502500 21.054500 21.285100
Si 19.502500 16.929500 18.323900
Si 18.633200 23.512500 23.091300
Si 18.633200 14.471500 16.517700
Si 18.632400 19.351700 16.503500
Si 18.632400 18.632300 23.105500
Si 16.251500 22.701900 24.855400
Si 16.251500 15.282100 14.753600
Si 16.250300 19.508200 24.852300
Si 16.250300 18.475800 14.756700
Si 13.240600 22.709900 24.939400
Si 13.240600 15.274100 14.669600
Si 13.239600 19.503600 24.938600
Si 13.239600 18.480400 14.670400
Si 10.853700 14.469200 16.503500
Si 10.851200 19.350900 16.490000
Si 10.048700 25.902000 21.271600
Si 10.048700 24.743500 18.337400

Si 10.048700 13.240500 21.271600
Si 10.048700 12.082000 18.337400
Si 10.040600 16.251100 21.354800
Si 10.037800 16.927600 18.320700
Si 8.393100 19.502500 24.925900
Si 8.393100 18.481500 14.683100
Si 6.846800 21.734100 18.251000
Si 6.846800 16.249900 21.358000
Si 6.841000 16.929500 18.323900
O 19.196400 21.086800 19.698300
O 19.196400 16.897200 19.910700
O 19.151300 25.322800 19.804500
O 19.151300 12.661200 19.804500
O 18.927700 23.240900 18.198000
O 18.927700 14.743100 21.411000
O 18.870400 19.713700 21.928300
O 18.870400 18.270300 17.680700
O 18.843100 22.351700 21.987000
O 18.843100 15.632300 17.622000
O 18.828700 24.958900 22.398100
O 18.828700 13.025100 17.210900
O 18.804600 20.844100 17.100000
O 18.804600 17.139900 22.509000
O 17.142400 23.407600 23.706800
O 17.142400 14.576400 15.902200
O 17.140400 19.179600 15.907800
O 17.140400 18.804400 23.701200

O	16.220600	21.105000	24.608300	O	8.439100	16.918500	18.083900
O	16.220600	16.879000	15.000700	O	6.534900	21.086800	19.698300
O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300

H	10.643300	25.569000	17.346800	Si	6.936461	21.083522	21.272057
H	10.643300	12.415000	22.262200	O	10.680826	19.673947	21.860372
H	10.571400	27.270300	21.396300	O	10.503035	20.935546	19.644251
H	10.571400	10.713700	18.212700	O	8.533661	21.160136	21.633196
H	9.865500	23.359500	24.031600	H	9.173676	20.411539	21.490847
H	9.835200	14.609800	15.524000	O	10.723145	22.473616	21.813503
H	8.639900	25.915400	21.449100	H	9.800284	22.124152	21.660233
H	8.639900	24.729900	18.159900	Ni	11.827848	21.019658	21.043276
H	8.590300	13.254600	21.455400	C	13.729173	18.961816	20.890307
H	8.590300	12.068200	18.153600	C	12.884985	18.348521	19.885420
H	8.422600	19.223600	26.368900	H	13.338407	18.434706	21.806037
H	8.422600	18.760400	13.240100	H	13.061406	17.339234	19.512720
H	8.402900	20.906700	24.715000	H	11.876440	18.755087	19.761504
H	8.402900	17.077300	14.894000	O	13.594700	20.317094	20.915490
H	7.215200	19.037200	15.248900	C	13.677555	20.466446	18.396205
H	7.215200	18.946800	24.360100	O	13.825570	21.604890	18.246645
H	6.336500	23.058400	18.204400	O	13.567330	19.278307	18.342406
H	6.334900	19.929700	21.841400	H	14.778051	18.630607	20.823698
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.830345	18.679426	23.082082				
Si	10.883386	23.523836	23.064439				
Si	10.061624	21.694152	18.331369				

1.2 Ni-DeAlBEA PRODc	Si	10.040602	16.251105	21.354795
Si 19.508300 21.734100 18.251000	Si	10.037800	16.927600	18.320700
Si 19.508300 16.249900 21.358000	Si	8.393102	19.502506	24.925898
Si 19.503800 25.900900 21.271600	Si	8.393100	18.481500	14.683100
Si 19.503800 24.744700 18.337400	Si	6.846799	21.734097	18.250999
Si 19.503800 13.239300 21.271600	Si	6.846800	16.249900	21.358000
Si 19.503800 12.083100 18.337400	Si	6.841000	16.929500	18.323900
Si 19.502500 21.054500 21.285100	O	19.196400	21.086800	19.698300
Si 19.502500 16.929500 18.323900	O	19.196400	16.897200	19.910700
Si 18.633200 23.512500 23.091300	O	19.151300	25.322800	19.804500
Si 18.633200 14.471500 16.517700	O	19.151300	12.661200	19.804500
Si 18.632400 19.351700 16.503500	O	18.927700	23.240900	18.198000
Si 18.632400 18.632300 23.105500	O	18.927700	14.743100	21.411000
Si 16.251500 22.701900 24.855400	O	18.870400	19.713700	21.928300
Si 16.251500 15.282100 14.753600	O	18.870400	18.270300	17.680700
Si 16.250300 19.508200 24.852300	O	18.843100	22.351700	21.987000
Si 16.250300 18.475800 14.756700	O	18.843100	15.632300	17.622000
Si 13.240595 22.709856 24.939378	O	18.828700	24.958900	22.398100
Si 13.240600 15.274100 14.669600	O	18.828700	13.025100	17.210900
Si 13.239606 19.503608 24.938590	O	18.804600	20.844100	17.100000
Si 13.239600 18.480400 14.670400	O	18.804600	17.139900	22.509000
Si 10.853700 14.469200 16.503500	O	17.142400	23.407600	23.706800
Si 10.851199 19.350898 16.490005	O	17.142400	14.576400	15.902200
Si 10.048711 25.902018 21.271608	O	17.140400	19.179600	15.907800
Si 10.048703 24.743502 18.337392	O	17.140400	18.804400	23.701200
Si 10.048700 13.240500 21.271600	O	16.220600	21.105000	24.608300
Si 10.048700 12.082000 18.337400	O	16.220600	16.879000	15.000700

O	14.745099	23.284604	24.802403	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743302	18.927407	24.799194	H	20.962200	13.254500	21.455400
O	13.256106	21.106601	24.736596	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301309	23.386383	23.812081	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297601	19.155699	15.796102	H	20.956200	16.919500	18.105600
O	12.297654	18.828196	23.812983	H	19.619900	23.348100	24.168500
O	10.746282	20.841833	17.105521	H	19.619900	14.635900	15.440500
O	10.746316	17.142111	22.503542	H	19.616500	19.135300	15.433200
O	10.725351	24.962815	22.398867	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670599	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623302	23.239040	18.200314	H	18.910700	12.411700	22.261300
O	10.623301	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401398	25.322799	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690601	19.141300	15.384899	H	12.713701	19.182999	26.273300
O	9.690631	18.842633	24.224154	H	12.713700	18.801000	13.335700
O	8.443985	21.763751	18.006309	H	12.713593	23.030690	26.273700
O	8.444000	16.220303	21.602698	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534902	21.086799	19.698299	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.333754	20.947487	19.666116
H	10.571400	10.713700	18.212700	O	8.517226	21.218975	21.694536
H	9.865454	23.359547	24.031477	H	9.154354	20.464344	21.585863
H	9.835200	14.609800	15.524000	O	10.836839	22.440040	21.793462
H	8.639900	25.915401	21.449101	H	9.913524	22.152683	21.561895
H	8.639900	24.729900	18.159899	Ni	11.748572	20.861126	20.898899
H	8.590300	13.254600	21.455400	C	15.003502	17.627520	18.483239
H	8.590300	12.068200	18.153600	C	13.621496	17.076490	18.784078
H	8.422599	19.223599	26.368900	H	15.780315	17.265832	19.164273
H	8.422600	18.760400	13.240100	H	13.604451	16.117162	19.300842
H	8.402901	20.906700	24.715002	O	14.829546	19.044998	18.722994
H	8.402900	17.077300	14.894000	O	13.080621	18.076205	19.679196
H	7.215200	19.037200	15.248900	O	13.462471	20.266997	20.013967
H	7.215200	18.946805	24.360096	C	13.762982	19.196546	19.501949
H	6.336499	23.058399	18.204396	H	15.330803	17.488524	17.451617
H	6.334901	19.929700	21.841402	H	12.975006	17.038614	17.901756
H	6.318500	14.878900	21.406200				
H	6.288698	22.188500	21.907999				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228501	20.952096	17.239703				
H	6.228500	17.031900	22.369300				
Si	10.837294	18.668130	23.086779				
Si	10.890722	23.509966	23.050213				
Si	10.046968	21.697729	18.310461				
Si	6.939123	21.089962	21.277783				
O	10.637809	19.718042	21.917317				

2. Cu-DeAlBEA

2.1 Cu-DeAlBEA TSc

Si 19.508300 21.734100 18.251000
Si 19.508300 16.249900 21.358000
Si 19.503800 25.900900 21.271600
Si 19.503800 24.744700 18.337400
Si 19.503800 13.239300 21.271600
Si 19.503800 12.083100 18.337400
Si 19.502500 21.054500 21.285100
Si 19.502500 16.929500 18.323900
Si 18.633200 23.512500 23.091300
Si 18.633200 14.471500 16.517700
Si 18.632400 19.351700 16.503500
Si 18.632400 18.632300 23.105500
Si 16.251500 22.701900 24.855400
Si 16.251500 15.282100 14.753600
Si 16.250300 19.508200 24.852300
Si 16.250300 18.475800 14.756700
Si 13.240600 22.709900 24.939400
Si 13.240600 15.274100 14.669600
Si 13.239600 19.503600 24.938600
Si 13.239600 18.480400 14.670400
Si 10.853700 14.469200 16.503500
Si 10.851200 19.350900 16.490000
Si 10.048700 25.902000 21.271600
Si 10.048700 24.743500 18.337400
Si 10.048700 13.240500 21.271600

Si 10.048700 12.082000 18.337400
Si 10.040600 16.251100 21.354800
Si 10.037800 16.927600 18.320700
Si 8.393100 19.502500 24.925900
Si 8.393100 18.481500 14.683100
Si 6.846800 21.734100 18.251000
Si 6.846800 16.249900 21.358000
Si 6.841000 16.929500 18.323900
O 19.196400 21.086800 19.698300
O 19.196400 16.897200 19.910700
O 19.151300 25.322800 19.804500
O 19.151300 12.661200 19.804500
O 18.927700 23.240900 18.198000
O 18.927700 14.743100 21.411000
O 18.870400 19.713700 21.928300
O 18.870400 18.270300 17.680700
O 18.843100 22.351700 21.987000
O 18.843100 15.632300 17.622000
O 18.828700 24.958900 22.398100
O 18.828700 13.025100 17.210900
O 18.804600 20.844100 17.100000
O 18.804600 17.139900 22.509000
O 17.142400 23.407600 23.706800
O 17.142400 14.576400 15.902200
O 17.140400 19.179600 15.907800
O 17.140400 18.804400 23.701200
O 16.220600 21.105000 24.608300

O	16.220600	16.879000	15.000700	O	6.534900	21.086800	19.698300
O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800

H	10.643300	12.415000	22.262200	O	10.627300	19.643700	21.846200
H	10.571400	27.270300	21.396300	O	10.356100	20.926900	19.653300
H	10.571400	10.713700	18.212700	O	8.522800	21.214400	21.671100
H	9.865500	23.359500	24.031600	H	9.155800	20.467900	21.525900
H	9.835200	14.609800	15.524000	O	10.902300	22.436300	21.797100
H	8.639900	25.915400	21.449100	H	10.006100	22.138400	21.528400
H	8.639900	24.729900	18.159900	Cu	11.817500	20.723700	20.788500
H	8.590300	13.254600	21.455400	C	13.975500	18.964300	21.138200
H	8.590300	12.068200	18.153600	C	13.295200	18.115400	20.165200
H	8.422600	19.223600	26.368900	H	13.636500	18.477100	22.090900
H	8.422600	18.760400	13.240100	H	13.659800	17.111800	19.944200
H	8.402900	20.906700	24.715000	H	12.219300	18.264100	20.024500
H	8.402900	17.077300	14.894000	O	13.642200	20.285400	21.043500
H	7.215200	19.037200	15.248900	C	13.809000	20.095600	18.503000
H	7.215200	18.946800	24.360100	O	13.874600	21.205500	18.186700
H	6.336500	23.058400	18.204400	O	13.783500	18.897000	18.587000
H	6.334900	19.929700	21.841400	H	15.066000	18.808800	21.122600
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.827400	18.675700	23.085200				
Si	10.894400	23.499700	23.038700				
Si	10.044200	21.703900	18.311900				
Si	6.941600	21.090300	21.278000				

2.2 Cu-DeAlBEA PRODc				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.225407	20.932506	19.676038
H	10.571400	10.713700	18.212700	O	8.505231	21.276980	21.719886
H	9.865500	23.359500	24.031600	H	9.154227	20.533448	21.657648
H	9.835200	14.609800	15.524000	O	11.001963	22.421357	21.781232
H	8.639900	25.915400	21.449100	H	10.141431	22.159229	21.400640
H	8.639900	24.729900	18.159900	Cu	11.739594	20.462602	20.684325
H	8.590300	13.254600	21.455400	C	14.973408	17.835361	18.179183
H	8.590300	12.068200	18.153600	C	13.683884	17.235034	18.709002
H	8.422600	19.223600	26.368900	H	15.852946	17.611464	18.789434
H	8.422600	18.760400	13.240100	H	13.807667	16.357425	19.341994
H	8.402900	20.906700	24.715000	O	14.723988	19.261206	18.272849
H	8.402900	17.077300	14.894000	O	13.162508	18.310412	19.525113
H	7.215200	19.037200	15.248900	O	13.370758	20.544686	19.535739
H	7.215200	18.946800	24.360100	C	13.733488	19.444567	19.127073
H	6.336500	23.058400	18.204400	H	15.175270	17.590717	17.136397
H	6.334900	19.929700	21.841400	H	12.952611	17.033801	17.919871
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.833419	18.665031	23.095039				
Si	10.897474	23.484533	23.022245				
Si	10.040142	21.707997	18.293841				
Si	6.944667	21.096219	21.284990				
O	10.580011	19.710874	21.922382				

3. Zn-DeAlBEA

3.1 Zn-DeAlBEA TSc

Si 19.508300 21.734100 18.251000
Si 19.508300 16.249900 21.358000
Si 19.503800 25.900900 21.271600
Si 19.503800 24.744700 18.337400
Si 19.503800 13.239300 21.271600
Si 19.503800 12.083100 18.337400
Si 19.502500 21.054500 21.285100
Si 19.502500 16.929500 18.323900
Si 18.633200 23.512500 23.091300
Si 18.633200 14.471500 16.517700
Si 18.632400 19.351700 16.503500
Si 18.632400 18.632300 23.105500
Si 16.251500 22.701900 24.855400
Si 16.251500 15.282100 14.753600
Si 16.250300 19.508200 24.852300
Si 16.250300 18.475800 14.756700
Si 13.240600 22.709900 24.939400
Si 13.240600 15.274100 14.669600
Si 13.239600 19.503600 24.938600
Si 13.239600 18.480400 14.670400
Si 10.853700 14.469200 16.503500
Si 10.851200 19.350900 16.490000
Si 10.048700 25.902000 21.271600
Si 10.048700 24.743500 18.337400
Si 10.048700 13.240500 21.271600

Si 10.048700 12.082000 18.337400
Si 10.040600 16.251100 21.354800
Si 10.037800 16.927600 18.320700
Si 8.393100 19.502500 24.925900
Si 8.393100 18.481500 14.683100
Si 6.846800 21.734100 18.251000
Si 6.846800 16.249900 21.358000
Si 6.841000 16.929500 18.323900
O 19.196400 21.086800 19.698300
O 19.196400 16.897200 19.910700
O 19.151300 25.322800 19.804500
O 19.151300 12.661200 19.804500
O 18.927700 23.240900 18.198000
O 18.927700 14.743100 21.411000
O 18.870400 19.713700 21.928300
O 18.870400 18.270300 17.680700
O 18.843100 22.351700 21.987000
O 18.843100 15.632300 17.622000
O 18.828700 24.958900 22.398100
O 18.828700 13.025100 17.210900
O 18.804600 20.844100 17.100000
O 18.804600 17.139900 22.509000
O 17.142400 23.407600 23.706800
O 17.142400 14.576400 15.902200
O 17.140400 19.179600 15.907800
O 17.140400 18.804400 23.701200
O 16.220600 21.105000 24.608300

O	16.220600	16.879000	15.000700	O	6.534900	21.086800	19.698300
O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800

H	10.643300	12.415000	22.262200	O	10.678263	19.657727	21.871700
H	10.571400	27.270300	21.396300	O	10.439554	20.947926	19.630974
H	10.571400	10.713700	18.212700	O	8.535025	21.192986	21.647880
H	9.865500	23.359500	24.031600	H	9.165149	20.440448	21.504893
H	9.835200	14.609800	15.524000	O	10.830733	22.458875	21.824840
H	8.639900	25.915400	21.449100	H	9.917046	22.147608	21.594918
H	8.639900	24.729900	18.159900	Zn	11.836431	20.919155	20.930636
H	8.590300	13.254600	21.455400	C	13.933465	19.068473	21.008074
H	8.590300	12.068200	18.153600	C	13.145595	18.230583	20.127400
H	8.422600	19.223600	26.368900	H	13.550286	18.649739	21.987259
H	8.422600	18.760400	13.240100	H	13.406673	17.189380	19.933498
H	8.402900	20.906700	24.715000	H	12.094519	18.489859	19.965432
H	8.402900	17.077300	14.894000	O	13.725493	20.400913	20.828473
H	7.215200	19.037200	15.248900	C	13.798138	20.150379	18.343325
H	7.215200	18.946800	24.360100	O	13.912871	21.255410	18.017091
H	6.336500	23.058400	18.204400	O	13.707599	18.960121	18.442917
H	6.334900	19.929700	21.841400	H	15.000511	18.791300	21.009932
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.823753	18.671666	23.085814				
Si	10.889194	23.524652	23.064737				
Si	10.050000	21.698094	18.310968				
Si	6.941967	21.087475	21.273989				

3.2 Zn-DeAlBEA PRODC

Si 19.508300 21.734100 18.251000
 Si 19.508300 16.249900 21.358000
 Si 19.503800 25.900900 21.271600
 Si 19.503800 24.744700 18.337400
 Si 19.503800 13.239300 21.271600
 Si 19.503800 12.083100 18.337400
 Si 19.502500 21.054500 21.285100
 Si 19.502500 16.929500 18.323900
 Si 18.633200 23.512500 23.091300
 Si 18.633200 14.471500 16.517700
 Si 18.632400 19.351700 16.503500
 Si 18.632400 18.632300 23.105500
 Si 16.251500 22.701900 24.855400
 Si 16.251500 15.282100 14.753600
 Si 16.250300 19.508200 24.852300
 Si 16.250300 18.475800 14.756700
 Si 13.240600 22.709900 24.939400
 Si 13.240600 15.274100 14.669600
 Si 13.239600 19.503600 24.938600
 Si 13.239600 18.480400 14.670400
 Si 10.853700 14.469200 16.503500
 Si 10.851200 19.350900 16.490000
 Si 10.048700 25.902000 21.271600
 Si 10.048700 24.743500 18.337400
 Si 10.048700 13.240500 21.271600
 Si 10.048700 12.082000 18.337400

Si 10.040600 16.251100 21.354800
 Si 10.037800 16.927600 18.320700
 Si 8.393100 19.502500 24.925900
 Si 8.393100 18.481500 14.683100
 Si 6.846800 21.734100 18.251000
 Si 6.846800 16.249900 21.358000
 Si 6.841000 16.929500 18.323900
 O 19.196400 21.086800 19.698300
 O 19.196400 16.897200 19.910700
 O 19.151300 25.322800 19.804500
 O 19.151300 12.661200 19.804500
 O 18.927700 23.240900 18.198000
 O 18.927700 14.743100 21.411000
 O 18.870400 19.713700 21.928300
 O 18.870400 18.270300 17.680700
 O 18.843100 22.351700 21.987000
 O 18.843100 15.632300 17.622000
 O 18.828700 24.958900 22.398100
 O 18.828700 13.025100 17.210900
 O 18.804600 20.844100 17.100000
 O 18.804600 17.139900 22.509000
 O 17.142400 23.407600 23.706800
 O 17.142400 14.576400 15.902200
 O 17.140400 19.179600 15.907800
 O 17.140400 18.804400 23.701200
 O 16.220600 21.105000 24.608300
 O 16.220600 16.879000 15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.374020	20.960192	19.639058
H	10.571400	10.713700	18.212700	O	8.525480	21.235949	21.678838
H	9.865500	23.359500	24.031600	H	9.158591	20.476379	21.600252
H	9.835200	14.609800	15.524000	O	10.920160	22.442913	21.794616
H	8.639900	25.915400	21.449100	H	10.017973	22.156485	21.510384
H	8.639900	24.729900	18.159900	Zn	11.792583	20.751555	20.855867
H	8.590300	13.254600	21.455400	C	15.290439	17.883588	18.717248
H	8.590300	12.068200	18.153600	C	13.814318	17.495117	18.669733
H	8.422600	19.223600	26.368900	H	15.886846	17.265831	19.394442
H	8.422600	18.760400	13.240100	H	13.596083	16.504767	19.070529
H	8.402900	20.906700	24.715000	O	15.265538	19.225912	19.266329
H	8.402900	17.077300	14.894000	O	13.204038	18.470262	19.547323
H	7.215200	19.037200	15.248900	O	13.771478	20.462715	20.401626
H	7.215200	18.946800	24.360100	C	14.067778	19.448734	19.774225
H	6.336500	23.058400	18.204400	H	15.781532	17.931946	17.744303
H	6.334900	19.929700	21.841400	H	13.345798	17.602333	17.685602
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.832425	18.659552	23.097949				
Si	10.894067	23.508397	23.046473				
Si	10.043048	21.701197	18.302354				
Si	6.945589	21.091823	21.278110				
O	10.636254	19.698907	21.933565				

4. Mg-DeAlBEA

4.1 Mg-DeAlBEA TSc

Si 19.508300 21.734100 18.251000
 Si 19.508300 16.249900 21.358000
 Si 19.503800 25.900900 21.271600
 Si 19.503800 24.744700 18.337400
 Si 19.503800 13.239300 21.271600
 Si 19.503800 12.083100 18.337400
 Si 19.502500 21.054500 21.285100
 Si 19.502500 16.929500 18.323900
 Si 18.633200 23.512500 23.091300
 Si 18.633200 14.471500 16.517700
 Si 18.632400 19.351700 16.503500
 Si 18.632400 18.632300 23.105500
 Si 16.251500 22.701900 24.855400
 Si 16.251500 15.282100 14.753600
 Si 16.250300 19.508200 24.852300
 Si 16.250300 18.475800 14.756700
 Si 13.240600 22.709900 24.939400
 Si 13.240600 15.274100 14.669600
 Si 13.239600 19.503600 24.938600
 Si 13.239600 18.480400 14.670400
 Si 10.853700 14.469200 16.503500
 Si 10.851200 19.350900 16.490000
 Si 10.048700 25.902000 21.271600
 Si 10.048700 24.743500 18.337400
 Si 10.048700 13.240500 21.271600

Si 10.048700 12.082000 18.337400
 Si 10.040600 16.251100 21.354800
 Si 10.037800 16.927600 18.320700
 Si 8.393100 19.502500 24.925900
 Si 8.393100 18.481500 14.683100
 Si 6.846800 21.734100 18.251000
 Si 6.846800 16.249900 21.358000
 Si 6.841000 16.929500 18.323900
 O 19.196400 21.086800 19.698300
 O 19.196400 16.897200 19.910700
 O 19.151300 25.322800 19.804500
 O 19.151300 12.661200 19.804500
 O 18.927700 23.240900 18.198000
 O 18.927700 14.743100 21.411000
 O 18.870400 19.713700 21.928300
 O 18.870400 18.270300 17.680700
 O 18.843100 22.351700 21.987000
 O 18.843100 15.632300 17.622000
 O 18.828700 24.958900 22.398100
 O 18.828700 13.025100 17.210900
 O 18.804600 20.844100 17.100000
 O 18.804600 17.139900 22.509000
 O 17.142400 23.407600 23.706800
 O 17.142400 14.576400 15.902200
 O 17.140400 19.179600 15.907800
 O 17.140400 18.804400 23.701200
 O 16.220600 21.105000 24.608300

O	16.220600	16.879000	15.000700	O	6.534900	21.086800	19.698300
O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800

H	10.643300	12.415000	22.262200	O	10.677906	19.671209	21.889723
H	10.571400	27.270300	21.396300	O	10.473341	20.948958	19.621494
H	10.571400	10.713700	18.212700	O	8.537171	21.199631	21.637993
H	9.865500	23.359500	24.031600	H	9.165650	20.442746	21.509830
H	9.835200	14.609800	15.524000	O	10.827584	22.458681	21.827564
H	8.639900	25.915400	21.449100	H	9.906631	22.155384	21.606298
H	8.639900	24.729900	18.159900	Mg	11.760959	20.932523	20.974324
H	8.590300	13.254600	21.455400	C	13.941786	19.083050	20.997184
H	8.590300	12.068200	18.153600	C	13.233150	18.182263	20.111236
H	8.422600	19.223600	26.368900	H	13.579771	18.624953	21.968613
H	8.422600	18.760400	13.240100	H	13.583199	17.166779	19.920962
H	8.402900	20.906700	24.715000	H	12.167457	18.360162	19.940638
H	8.402900	17.077300	14.894000	O	13.615578	20.383648	20.818827
H	7.215200	19.037200	15.248900	C	13.770555	20.150422	18.343170
H	7.215200	18.946800	24.360100	O	13.849348	21.259252	18.017964
H	6.336500	23.058400	18.204400	O	13.735356	18.956025	18.430582
H	6.334900	19.929700	21.841400	H	15.028161	18.885536	21.015029
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.824054	18.670373	23.087406				
Si	10.889028	23.527570	23.067135				
Si	10.052972	21.695125	18.312956				
Si	6.941324	21.088121	21.272781				

4.2 Mg-DeAlBEA PRODc				Si	10.040600	16.251100	21.354800
Si	19.508300	21.734100	18.251000	Si	10.037800	16.927600	18.320700
Si	19.508300	16.249900	21.358000	Si	8.393100	19.502500	24.925900
Si	19.503800	25.900900	21.271600	Si	8.393100	18.481500	14.683100
Si	19.503800	24.744700	18.337400	Si	6.846800	21.734100	18.251000
Si	19.503800	13.239300	21.271600	Si	6.846800	16.249900	21.358000
Si	19.503800	12.083100	18.337400	Si	6.841000	16.929500	18.323900
Si	19.502500	21.054500	21.285100	O	19.196400	21.086800	19.698300
Si	19.502500	16.929500	18.323900	O	19.196400	16.897200	19.910700
Si	18.633200	23.512500	23.091300	O	19.151300	25.322800	19.804500
Si	18.633200	14.471500	16.517700	O	19.151300	12.661200	19.804500
Si	18.632400	19.351700	16.503500	O	18.927700	23.240900	18.198000
Si	18.632400	18.632300	23.105500	O	18.927700	14.743100	21.411000
Si	16.251500	22.701900	24.855400	O	18.870400	19.713700	21.928300
Si	16.251500	15.282100	14.753600	O	18.870400	18.270300	17.680700
Si	16.250300	19.508200	24.852300	O	18.843100	22.351700	21.987000
Si	16.250300	18.475800	14.756700	O	18.843100	15.632300	17.622000
Si	13.240600	22.709900	24.939400	O	18.828700	24.958900	22.398100
Si	13.240600	15.274100	14.669600	O	18.828700	13.025100	17.210900
Si	13.239600	19.503600	24.938600	O	18.804600	20.844100	17.100000
Si	13.239600	18.480400	14.670400	O	18.804600	17.139900	22.509000
Si	10.853700	14.469200	16.503500	O	17.142400	23.407600	23.706800
Si	10.851200	19.350900	16.490000	O	17.142400	14.576400	15.902200
Si	10.048700	25.902000	21.271600	O	17.140400	19.179600	15.907800
Si	10.048700	24.743500	18.337400	O	17.140400	18.804400	23.701200
Si	10.048700	13.240500	21.271600	O	16.220600	21.105000	24.608300
Si	10.048700	12.082000	18.337400	O	16.220600	16.879000	15.000700

O	14.745100	23.284600	24.802400	O	6.534900	16.897200	19.910700
O	14.745100	14.699400	14.806600	H	20.962200	25.915700	21.455400
O	14.743300	19.056600	14.809800	H	20.962200	24.729500	18.153600
O	14.743300	18.927400	24.799200	H	20.962200	13.254500	21.455400
O	13.256100	21.106600	24.736600	H	20.962200	12.068300	18.153600
O	13.256100	16.877400	14.872400	H	20.961100	21.761000	18.028400
O	12.301400	23.386400	23.812100	H	20.961100	16.223000	21.580600
O	12.301400	14.597600	15.796900	H	20.956200	21.064500	21.503400
O	12.297600	19.155700	15.796100	H	20.956200	16.919500	18.105600
O	12.297600	18.828300	23.812900	H	19.619900	23.348100	24.168500
O	10.746300	20.841800	17.105500	H	19.619900	14.635900	15.440500
O	10.746300	17.142200	22.503500	H	19.616500	19.135300	15.433200
O	10.725300	24.962700	22.398900	H	19.616500	18.848700	24.175800
O	10.725300	13.021300	17.210100	H	18.979800	27.268500	21.398400
O	10.693700	15.628100	17.618100	H	18.979800	10.715500	18.210600
O	10.670600	18.266100	17.673500	H	18.910700	25.572300	17.347700
O	10.623300	23.239000	18.200300	H	18.910700	12.411700	22.261300
O	10.623300	14.745000	21.408700	H	16.839100	19.224200	26.169000
O	10.401400	25.322800	19.804500	H	16.839100	18.759800	13.440000
O	10.401400	12.661200	19.804500	H	16.839000	22.981800	26.173500
O	10.348500	16.897200	19.905900	H	16.839000	15.002200	13.435500
O	9.690600	19.141300	15.384900	H	12.713700	19.183000	26.273300
O	9.690600	18.842700	24.224100	H	12.713700	18.801000	13.335700
O	8.444000	21.763700	18.006300	H	12.713600	23.030700	26.273700
O	8.444000	16.220300	21.602700	H	12.713600	14.953300	13.335300
O	8.439100	16.918500	18.083900	H	10.643300	25.569000	17.346800
O	6.534900	21.086800	19.698300	H	10.643300	12.415000	22.262200

H	10.571400	27.270300	21.396300	O	10.402445	20.973182	19.637886
H	10.571400	10.713700	18.212700	O	8.530967	21.234409	21.669625
H	9.865500	23.359500	24.031600	H	9.163914	20.474356	21.586807
H	9.835200	14.609800	15.524000	O	10.924060	22.439403	21.803931
H	8.639900	25.915400	21.449100	H	10.018256	22.158943	21.517089
H	8.639900	24.729900	18.159900	Mg	11.745522	20.799883	20.889002
H	8.590300	13.254600	21.455400	C	15.172285	17.793412	18.620081
H	8.590300	12.068200	18.153600	C	13.725549	17.320822	18.700918
H	8.422600	19.223600	26.368900	H	15.851309	17.249855	19.282827
H	8.422600	18.760400	13.240100	H	13.592526	16.331610	19.139926
H	8.402900	20.906700	24.715000	O	15.099221	19.159957	19.098483
H	8.402900	17.077300	14.894000	O	13.128878	18.285420	19.597405
H	7.215200	19.037200	15.248900	O	13.633776	20.344264	20.323372
H	7.215200	18.946800	24.360100	C	13.937163	19.327309	19.707647
H	6.336500	23.058400	18.204400	H	15.585268	17.810325	17.610130
H	6.334900	19.929700	21.841400	H	13.187012	17.375499	17.750290
H	6.318500	14.878900	21.406200				
H	6.288700	22.188500	21.908000				
H	6.285500	18.107800	17.758700				
H	6.261400	15.789400	17.707000				
H	6.228500	20.952100	17.239700				
H	6.228500	17.031900	22.369300				
Si	10.831201	18.661772	23.093151				
Si	10.894016	23.512794	23.051269				
Si	10.044397	21.699079	18.305050				
Si	6.947074	21.091498	21.277169				
O	10.652306	19.697292	21.927992				