A comparative computational study on the synthesis prescriptions, structures and acid properties of B, Al and Ga incorporated MTW-type zeolites

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Table S1. The total energies and vdW energies (eV) of the B-MTW zeolites.

Structure	Total energy	vdW energy	Structure	Total energy	vdW energy
p(1×2×1) cell	–1339.62	–12.05	B(5)-Na-1	–1342.70	–12.75
B(1)-H-1	–1342.26	–12.21	B(5)-Na-2	–1342.45	–12.48
B(1)-H-2	–1342.96	–12.88	B(5)-Na-3	–1342.20	–12.89
B(1)-H-3	–1342.68	–12.22	B(5)-Na-4	–1342.31	–12.91
B(1)-H-4	–1343.11	–12.85	B(6)-Na-1	–1342.38	–12.55
B(1)-H-5	–1342.52	–12.14	B(6)-Na-2	–1343.19	–13.50
B(2)-H-1	–1343.13	–12.85	B(6)-Na-3	–1342.74	–13.02
B(2)-H-2	–1342.66	–12.32	B(7)-Na-1	–1342.60	–12.88
B(2)-H-3	–1343.03	–12.98	B(7)-Na-2	–1343.25	–13.51
B(2)-H-4	–1342.84	–12.78	B(7)-Na-3	–1341.73	–12.80
B(3)-H-1	–1342.55	–12.31	B(1)-K-1	–1343.01	–13.64
B(3)-H-2	–1342.35	–12.25	B(1)-K-2	–1341.67	–12.76
B(3)-H-3	–1343.09	–12.92	B(1)-K-3	–1342.64	–12.51
B(3)-H-4	–1343.12	–12.90	B(1)-K-4	–1343.34	–13.26
B(4)-H-1	–1342.49	–12.15	B(2)-K-1	–1342.87	–12.65
B(4)-H-2	–1342.47	–12.36	B(2)-K-2	–1342.25	–12.91
B(4)-H-3	–1343.22	–12.90	B(2)-K-3	–1342.23	–13.21
B(4)-H-4	–1342.57	–12.17	B(2)-K-4	–1342.69	–12.44
B(5)-H-1	–1343.16	–12.83	B(3)-K-1	–1343.37	–13.27
B(5)-H-2	–1343.05	–12.89	B(3)-K-2	–1342.56	–12.73
B(5)-H-3	–1342.56	–12.34	B(3)-K-3	–1341.81	–12.68
B(5)-H-4	–1342.98	–12.82	B(4)-K-1	–1342.59	–12.49
B(6)-H-1	–1342.60	–12.27	B(4)-K-2	–1342.36	–12.74
B(6)-H-2	–1343.00	–12.62	B(4)-K-3	–1341.67	–12.67
B(6)-H-3	–1342.24	–12.21	B(4)-K-4	–1342.84	–12.67
B(6)-H-4	–1342.38	–12.11	B(5)-K-1	–1342.79	–12.56
B(6)-H-5	–1342.66	–12.29	B(5)-K-2	–1342.31	–13.02
B(7)-H-1	–1341.29	–12.23	B(5)-K-3	–1342.03	–12.75
B(7)-H-2	–1343.01	–12.85	B(6)-K-1	–1343.20	–13.29
B(7)-H-3	–1342.48	–12.14	B(6)-K-2	–1342.48	–12.86
B(7)-H-4	–1342.37	–12.26	B(6)-K-3	–1342.48	–12.95
B(7)-H-5	–1342.74	–12.31	B(7)-K-1	–1342.56	–12.72
B(7)-H-6	–1342.35	–12.18	B(7)-K-2	–1342.68	–12.80
B(1)-Li-1	–1342.96	–12.40	B(7)-K-3	–1342.01	–13.03
B(1)-Li-2	–1343.68	–13.75	B(1)-H-NH_3-1	–1363.58	–13.27
B(1)-Li-3	–1343.80	–13.47	B(1)-H-NH_3-2	–1363.12	–13.49
B(2)-Li-1	–1343.07	–12.39	B(1)-H-NH_3-3	–1363.63	–13.25
B(2)-Li-2	–1343.74	–13.54	B(2)-H-NH_3-1	–1363.85	–13.45
B(2)-Li-3	–1343.78	–13.64	B(2)-H-NH_3-2	–1362.88	–13.52
B(2)-Li-4	–1343.75	–13.56	B(3)-H-NH_3-1	–1363.56	–13.29
B(3)-Li-1	–1343.13	–12.50	B(3)-H-NH_3-2	–1363.36	–13.32
B(3)-Li-2	–1343.29	–12.97	B(3)-H-NH_3-3	–1363.81	–13.42
B(3)-Li-3	–1343.52	–13.50	B(4)-H-NH_3-1	–1363.64	–13.36
B(4)-Li-1	–1344.16	–13.82	B(4)-H-NH_3-2	–1363.30	–13.30
B(4)-Li-2	–1343.79	–13.65	B(4)-H-NH_3-3	–1363.68	–13.22
B(4)-Li-3	–1343.13	–12.55	B(5)-H-NH_3-1	–1363.41	–13.15
B(5)-Li-1	–1343.18	–12.64	B(5)-H-NH_3-2	–1363.13	–13.32
B(5)-Li-2	–1343.60	–13.60	B(5)-H-NH_3-3	–1363.62	–13.28
B(5)-Li-3	–1344.10	–13.68	B(6)-H-NH_3-1	–1363.39	–13.08
B(6)-Li-1	–1342.99	–12.41	B(6)-H-NH_3-2	–1363.11	–13.25
B(6)-Li-2	–1343.95	–13.60	B(7)-H-NH_3-1	–1363.28	–13.19
B(6)-Li-3	–1343.28	–13.65	B(1)-H-Py-1	–1415.57	–13.86
B(6)-Li-4	–1343.87	–13.43	B(1)-H-Py-2	–1415.88	–14.08

B(7)-Li-1	–1343.25	–12.85	B(2)-H-Py-1	–1415.43	–13.86
B(7)-Li-2	–1343.95	–13.48	B(2)-H-Py-2	–1416.02	–14.05
B(1)-Na-1	–1343.22	–13.38	B(3)-H-Py-1	–1415.53	–13.93
B(1)-Na-2	–1342.87	–13.71	B(3)-H-Py-2	–1414.74	–14.04
B(2)-Na-1	–1342.74	–12.75	B(3)-H-Py-3	–1415.42	–14.05
B(2)-Na-2	–1342.37	–12.46	B(4)-H-Py-1	–1415.55	–14.00
B(2)-Na-3	–1343.00	–13.64	B(4)-H-Py-2	–1415.85	–13.99
B(3)-Na-1	–1343.20	–13.51	B(5)-H-Py-1	–1415.36	–13.76
B(3)-Na-2	–1342.43	–12.50	B(5)-H-Py-2	–1414.64	–13.95
B(3)-Na-3	–1342.85	–13.72	B(6)-H-Py-1	–1415.29	–13.61
B(3)-Na-4	–1342.47	–12.87	B(6)-H-Py-2	–1415.93	–13.86
B(4)-Na-1	–1342.72	–12.89	B(6)-H-Py-3	–1414.54	–13.58
B(4)-Na-2	–1343.15	–13.81	B(7)-H-Py-1	–1414.55	–13.92
B(4)-Na-3	–1342.41	–12.52	B(7)-H-Py-2	–1415.29	–13.91
B(4)-Na-4	–1343.11	–13.47			

Table S2. The total energies and vdW energies (eV) of the Al-MTW zeolites.

Structure	Total energy	vdW energy	Structure	Total energy	vdW energy
Al(1)-H-1	–1341.81	–12.70	Al(6)-Na-3	–1342.22	–13.15
Al(1)-H-2	–1341.01	–12.21	Al(7)-Na-1	–1342.08	–13.57
Al(2)-H-1	–1341.76	–12.85	Al(7)-Na-2	–1342.38	–13.52
Al(2)-H-2	–1341.76	–12.99	Al(7)-Na-3	–1342.39	–13.51
Al(2)-H-3	–1341.77	–12.87	Al(7)-Na-4	–1341.88	–12.95
Al(3)-H-1	–1341.88	–12.76	Al(1)-K-1	-1342.17	-13.49
Al(3)-H-2	–1341.73	–12.96	Al(1)-K-2	-1341.23	-13.16
Al(3)-H-3	–1341.67	–13.05	Al(1)-K-3	-1342.30	-13.13
Al(4)-H-1	–1341.82	–12.78	Al(2)-K-1	-1341.85	-12.61
Al(4)-H-2	–1341.74	–12.75	Al(2)-K-2	-1341.87	-13.50
Al(4)-H-3	–1341.58	–13.00	Al(2)-K-3	-1342.44	-13.48
Al(4)-H-4	–1341.98	–12.87	Al(2)-K-4	-1341.44	-13.10
Al(5)-H-1	–1341.71	–12.83	Al(3)-K-1	-1342.49	-13.34
Al(5)-H-2	–1341.82	–12.85	Al(3)-K-2	-1341.41	-13.12
Al(5)-H-3	–1341.70	–12.91	Al(3)-K-3	-1342.29	-13.24
Al(6)-H-1	–1341.71	–12.84	Al(4)-K-1	-1341.78	-12.44
Al(6)-H-2	–1341.82	–13.01	Al(4)-K-2	-1341.87	-13.27
Al(6)-H-3	–1341.81	–12.90	Al(4)-K-3	-1341.03	-12.68
Al(6)-H-4	–1341.34	–12.91	Al(4)-K-4	-1342.42	-13.29
Al(7)-H-1	–1341.62	–12.81	Al(5)-K-1	-1342.29	-13.23
Al(7)-H-2	–1341.61	–12.93	Al(5)-K-2	-1342.25	-13.17
Al(7)-H-3	–1341.86	–13.00	Al(5)-K-3	-1341.84	-13.56
Al(7)-H-4	–1341.84	–12.87	Al(5)-K-4	-1341.83	-13.51
Al(1)-Li-1	-1342.29	-13.35	Al(6)-K-1	-1341.75	-12.38
Al(1)-Li-2	-1342.92	-13.47	Al(6)-K-2	-1342.39	-13.22
Al(1)-Li-3	-1342.87	-13.55	Al(6)-K-3	-1342.16	-13.53
Al(1)-Li-4	-1342.86	-13.36	Al(6)-K-4	-1341.89	-13.36
Al(2)-Li-1	-1342.77	-13.23	Al(7)-K-1	-1342.19	-13.39
Al(2)-Li-2	-1342.82	-13.44	Al(7)-K-2	-1341.93	-13.36
Al(2)-Li-3	-1342.73	-13.47	Al(1)-H-NH_3-1	–1361.59	–13.15
Al(2)-Li-4	-1342.94	-13.73	Al(1)-H-NH_3-2	–1362.10	–13.24
Al(3)-Li-1	-1342.64	-13.04	Al(1)-H-NH_3-3	–1362.88	–12.98
Al(3)-Li-2	-1342.87	-13.40	Al(2)-H-NH_3-1	–1362.26	–13.20
Al(3)-Li-3	-1342.75	-13.61	Al(2)-H-NH_3-2	–1362.73	–13.18
Al(4)-Li-1	-1342.94	-13.47	Al(3)-H-NH_3-1	–1362.98	–13.19
Al(4)-Li-2	-1342.70	-13.30	Al(3)-H-NH_3-2	–1361.86	–13.25
Al(4)-Li-3	-1342.56	-13.09	Al(4)-H-NH_3-1	–1362.53	–13.22
Al(5)-Li-1	-1342.67	-13.24	Al(4)-H-NH_3-2	–1362.16	–13.38
Al(5)-Li-2	-1342.57	-13.47	Al(4)-H-NH_3-3	–1362.78	–13.15
Al(5)-Li-3	-1343.07	-13.69	Al(5)-H-NH_3-1	–1362.34	–13.18
Al(6)-Li-1	-1342.92	-13.33	Al(5)-H-NH_3-2	–1362.14	–13.17
Al(6)-Li-2	-1342.25	-13.37	Al(5)-H-NH_3-3	–1362.70	–12.98
Al(6)-Li-3	-1342.91	-13.47	Al(6)-H-NH_3-1	–1362.23	–13.13
Al(7)-Li-1	-1342.82	-13.46	Al(6)-H-NH_3-2	–1362.43	–13.40
Al(7)-Li-2	-1342.67	-13.40	Al(6)-H-NH_3-3	–1362.94	–13.29
Al(7)-Li-3	-1342.24	-12.78	Al(7)-H-NH_3-1	–1362.81	–13.10
Al(7)-Li-4	-1343.06	-13.54	Al(7)-H-NH_3-2	–1362.21	–13.28
Al(1)-Na-1	–1342.26	–13.23	Al(1)-H-Py-1	–1415.10	–13.63
Al(1)-Na-2	–1341.96	–13.53	Al(1)-H-Py-2	–1413.56	–13.72
Al(2)-Na-1	–1342.22	–13.31	Al(2)-H-Py-1	–1414.20	–13. 70
Al(2)-Na-2	–1342.13	–13.60	Al(2)-H-Py-2	–1414.87	–13.71
Al(3)-Na-1	–1342.37	–13.41	Al(3)-H-Py	–1415.00	–13.72
Al(3)-Na-2	–1342.18	–13.41	Al(4)-H-Py-1	–1414.32	–13.99

Al(4)-Na-1	–1342.30	–13.20	Al(4)-H-Py-2	–1414.56	–13.88
Al(4)-Na-2	–1342.03	–13.36	Al(5)-H-Py-1	–1414.23	–13.66
Al(5)-Na-1	–1342.28	–13.22	Al(5)-H-Py-2	–1415.00	–13.73
Al(5)-Na-2	–1342.46	–13.48	Al(6)-H-Py-1	–1414.27	–13.81
Al(5)-Na-3	–1341.69	–13.46	Al(6)-H-Py-2	–1414.96	–13.63
Al(6)-Na-1	–1342.29	–13.48	Al(7)-H-Py	–1414.63	–13.67
Al(6)-Na-2	–1341.92	–12.93			

Table S3. The total energies and vdW energies (eV) of the Ga-MTW zeolites.

Structure	Total energy	vdW energy	Structure	Total energy	vdW energy
Ga(1)-H-1	–1338.03	–12.96	Ga(4)-Na-2	–1337.71	–12.59
Ga(1)-H-2	–1337.73	–13.19	Ga(4)-Na-3	–1337.62	–13.00
Ga(1)-H-3	–1338.06	–13.07	Ga(4)-Na-4	–1338.78	–13.49
Ga(1)-H-4	–1337.96	–12.98	Ga(5)-Na-1	–1338.35	–13.41
Ga(2)-H-1	–1338.05	–13.14	Ga(5)-Na-2	–1338.34	–13.66
Ga(2)-H-2	–1338.02	–13.11	Ga(5)-Na-3	–1337.50	–12.99
Ga(2)-H-3	–1337.95	–13.03	Ga(6)-Na-1	–1338.49	–13.40
Ga(2)-H-4	–1338.05	–13.27	Ga(6)-Na-2	–1338.50	–13.76
Ga(2)-H-5	–1338.02	–13.10	Ga(7)-Na-1	–1337.81	–12.89
Ga(3)-H-1	–1338.13	–12.92	Ga(7)-Na-2	–1338.60	–13.86
Ga(3)-H-2	–1338.08	–13.23	Ga(7)-Na-3	–1337.12	–12.96
Ga(3)-H-3	–1337.93	–13.22	Ga(1)-K-1	–1338.29	–13.59
Ga(3)-H-4	–1338.12	–12.98	Ga(1)-K-2	–1337.40	–13.30
Ga(4)-H-1	–1338.06	–13.04	Ga(1)-K-3	–1338.54	–13.44
Ga(4)-H-2	–1337.86	–12.85	Ga(1)-K-4	–1338.45	–13.22
Ga(4)-H-3	–1337.91	–13.12	Ga(2)-K-1	–1338.42	–13.33
Ga(4)-H-4	–1338.22	–12.98	Ga(2)-K-2	–1338.02	–13.67
Ga(5)-H-1	–1337.95	–13.01	Ga(2)-K-3	–1338.53	–13.54
Ga(5)-H-2	–1337.81	–13.08	Ga(2)-K-4	–1337.64	–13.37
Ga(5)-H-3	–1338.12	–13.04	Ga(3)-K-1	–1338.69	–13.40
Ga(5)-H-4	–1337.86	–13.03	Ga(3)-K-2	–1337.68	–13.39
Ga(5)-H-5	–1338.12	–12.93	Ga(3)-K-3	–1338.44	–13.36
Ga(6)-H-1	–1338.02	–13.16	Ga(4)-K-1	–1338.13	–13.64
Ga(6)-H-2	–1338.09	–13.06	Ga(4)-K-2	–1337.86	–12.51
Ga(6)-H-3	–1338.00	–12.95	Ga(4)-K-3	–1337.10	–12.76
Ga(6)-H-4	–1337.69	–13.00	Ga(4)-K-4	–1338.67	–13.43
Ga(6)-H-5	–1337.68	–13.03	Ga(5)-K-1	–1338.71	–13.24
Ga(6)-H-6	–1338.02	–13.17	Ga(5)-K-2	–1338.04	–13.64
Ga(7)-H-1	–1338.01	–13.08	Ga(5)-K-3	–1337.99	–13.59
Ga(7)-H-2	–1338.01	–13.00	Ga(6)-K-1	–1338.48	–13.22
Ga(7)-H-3	–1337.91	–13.09	Ga(6)-K-2	–1338.18	–13.64
Ga(7)-H-4	–1337.86	–13.15	Ga(6)-K-3	–1338.30	–13.68
Ga(7)-H-5	–1337.97	–13.17	Ga(7)-K-1	–1338.36	–13.48
Ga(7)-H-6	–1338.03	–13.01	Ga(7)-K-2	–1338.13	–13.46
Ga(1)-Li-1	–1338.16	–12.50	Ga(1)-H-NH_3-1	–1359.01	–13.37
Ga(1)-Li-2	–1338.74	–13.46	Ga(1)-H-NH_3-2	–1357.97	–13.41
Ga(1)-Li-3	–1339.10	–13.64	Ga(1)-H-NH_3-3	–1358.34	–13.51
Ga(1)-Li-4	–1339.25	–13.41	Ga(1)-H-NH_3-4	–1358.59	–13.67
Ga(2)-Li-1	–1339.06	–13.37	Ga(2)-H-NH_3-1	–1359.03	–13.40
Ga(2)-Li-2	–1339.13	–13.56	Ga(2)-H-NH_3-2	–1358.14	–13.57
Ga(2)-Li-3	–1339.08	–13.64	Ga(3)-H-NH_3-1	–1359.15	–13.29
Ga(3)-Li-1	–1338.95	–13.21	Ga(3)-H-NH_3-2	–1358.39	–13.48
Ga(3)-Li-2	–1339.07	–13.66	Ga(4)-H-NH_3-1	–1358.84	–13.39
Ga(3)-Li-3	–1339.02	–13.51	Ga(4)-H-NH_3-2	–1358.18	–13.33
Ga(4)-Li-1	–1339.13	–13.86	Ga(4)-H-NH_3-3	–1359.05	–13.44
Ga(4)-Li-2	–1338.93	–13.66	Ga(5)-H-NH_3-1	–1358.66	–13.29
Ga(4)-Li-3	–1338.80	–13.23	Ga(5)-H-NH_3-2	–1358.30	–13.43
Ga(5)-Li-1	–1339.26	–13.46	Ga(5)-H-NH_3-3	–1358.92	–13.30
Ga(5)-Li-2	–1338.84	–13.36	Ga(6)-H-NH_3-1	–1357.89	–13.39
Ga(5)-Li-3	–1338.77	–13.63	Ga(6)-H-NH_3-2	–1359.01	–13.26
Ga(5)-Li-4	–1339.31	–13.85	Ga(6)-H-NH_3-3	–1358.73	–13.63
Ga(6)-Li-1	–1339.11	–13.38	Ga(6)-H-NH_3-4	–1358.18	–13.49
Ga(6)-Li-2	–1338.77	–13.35	Ga(7)-H-NH_3-1	–1358.95	–13.32

Ga(6)-Li-3	–1339.18	–13.57	Ga(1)-H-Py-1	–1409.85	–14.00
Ga(7)-Li-1	–1338.94	–13.61	Ga(1)-H-Py-2	–1411.19	–14.06
Ga(7)-Li-2	–1338.85	–13.50	Ga(2)-H-Py-1	–1410.14	–14.11
Ga(7)-Li-3	–1338.45	–12.93	Ga(2)-H-Py-2	–1411.16	–13.98
Ga(7)-Li-4	–1339.35	–13.77	Ga(3)-H-Py-1	–1410.98	–13.70
Ga(1)-Na-1	–1337.58	–12.53	Ga(3)-H-Py-2	–1409.92	–13.96
Ga(1)-Na-2	–1338.24	–13.65	Ga(4)-H-Py-1	–1410.86	–14.07
Ga(1)-Na-3	–1338.45	–13.58	Ga(4)-H-Py-2	–1411.17	–13.96
Ga(2)-Na-1	–1338.35	–13.35	Ga(5)-H-Py-1	–1410.65	–13.87
Ga(2)-Na-2	–1338.41	–13.51	Ga(5)-H-Py-2	–1411.09	–13.95
Ga(2)-Na-3	–1338.30	–13.74	Ga(6)-H-Py-1	–1409.78	–13.94
Ga(3)-Na-1	–1338.51	–13.52	Ga(6)-H-Py-2	–1411.14	–13.94
Ga(3)-Na-2	–1338.29	–13.69	Ga(7)-H-Py-1	–1410.71	–14.09
Ga(4)-Na-1	–1338.71	–13.60			

Fig. S1. Local structures and relative energies (eV) of the HB-MTW zeolites. H, O, B and Si atoms are shown in white, red, green and yellow, respectively. Relative energy of the most stable structure is 0 eV, relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

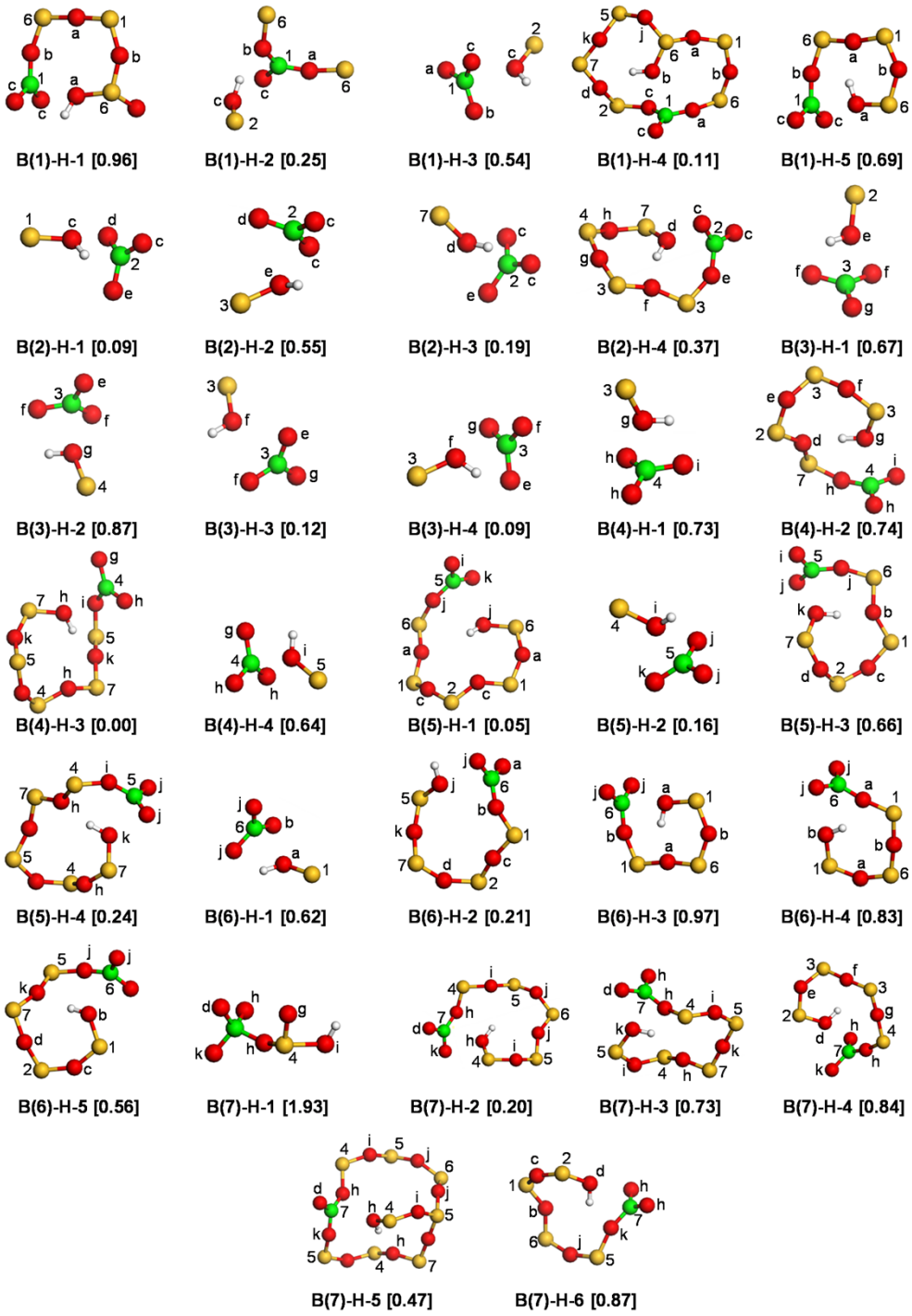


Fig. S2. Local structures and relative energies (eV) for LiB-MTW zeolites. Li, O, B and Si atoms are shown in dark gray, red, green and yellow, respectively. Relative energy of the most stable structure is 0 eV, and the relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

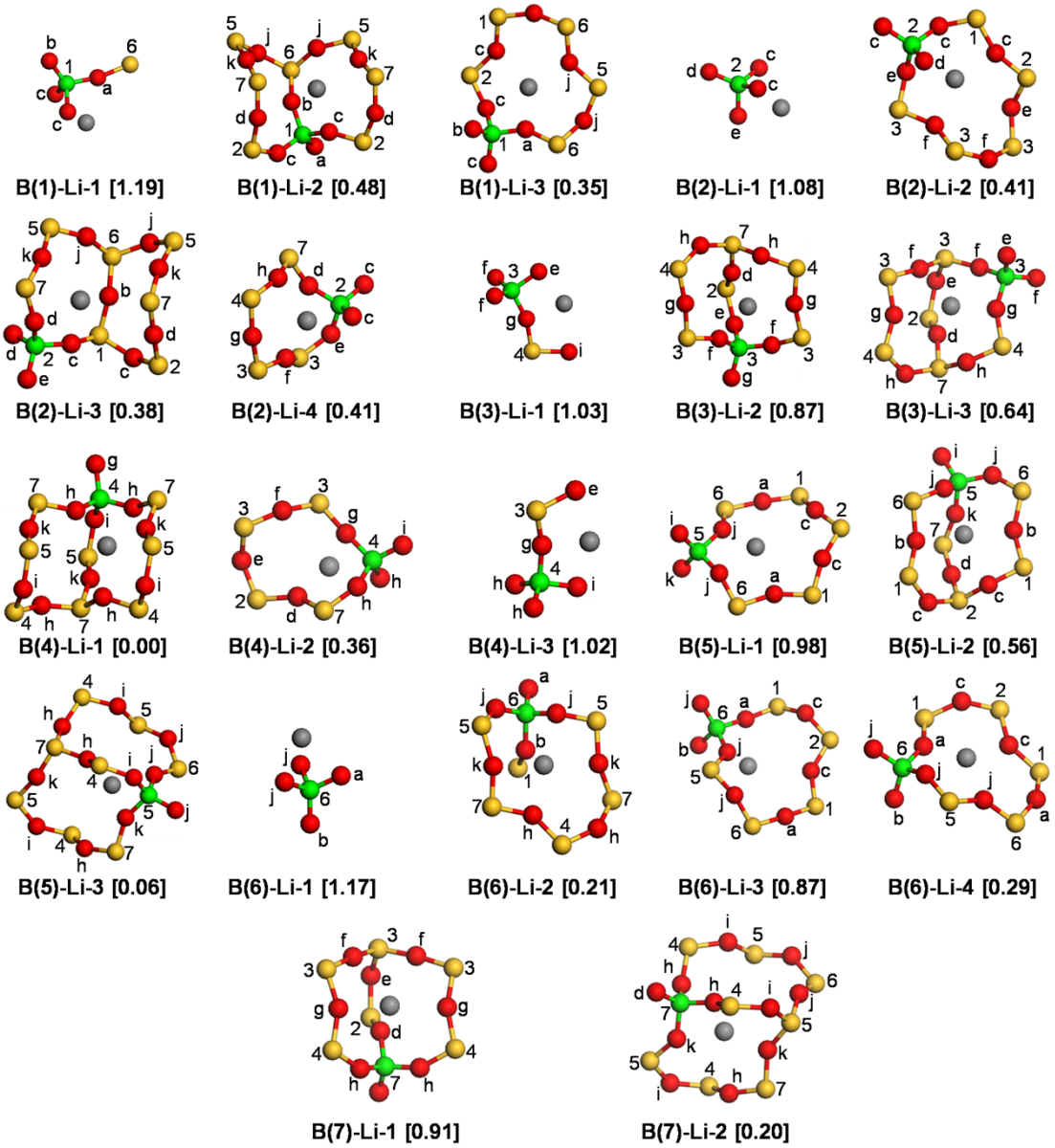


Fig. S3. Local structures and relative energies (eV) for NaB-MTW zeolites. Na, O, B and Si atoms are shown in violet, red, green and yellow, respectively. Relative energy of the most stable structure is 0 eV, the relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

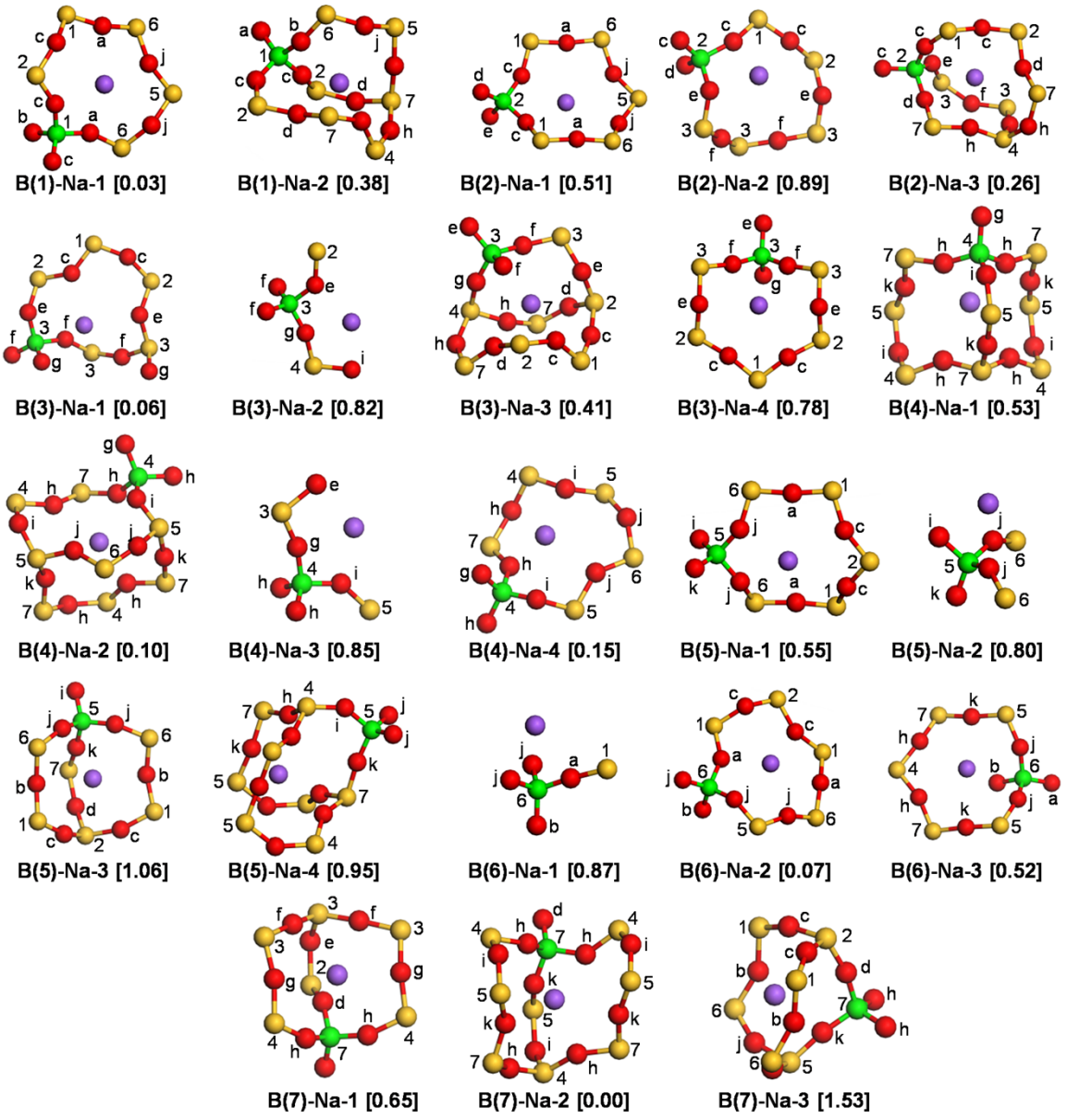


Fig. S4. Local structures and relative energies (eV) for KB-MTW zeolites. K, O, B and Si atoms are shown in darkslateblue, red, green and yellow, respectively. Relative energy of the most stable structure is 0 eV, relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

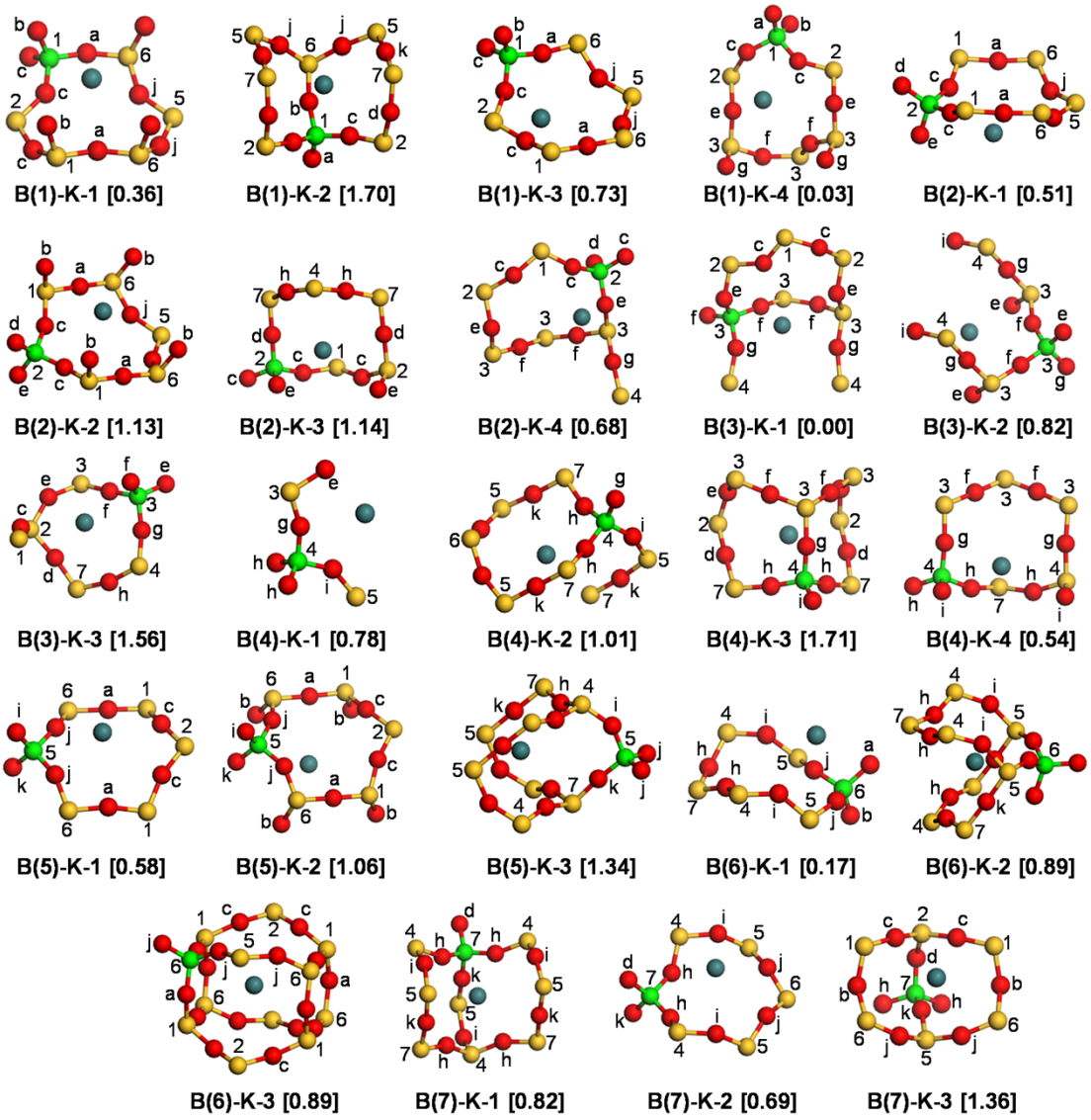


Fig. S5. Local structures and relative energies (eV) of the HAl-MTW zeolites. H, O, Al and Si atoms are shown in white, red, gray and yellow, respectively. Relative energy of the most stable structure is 0 eV, relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

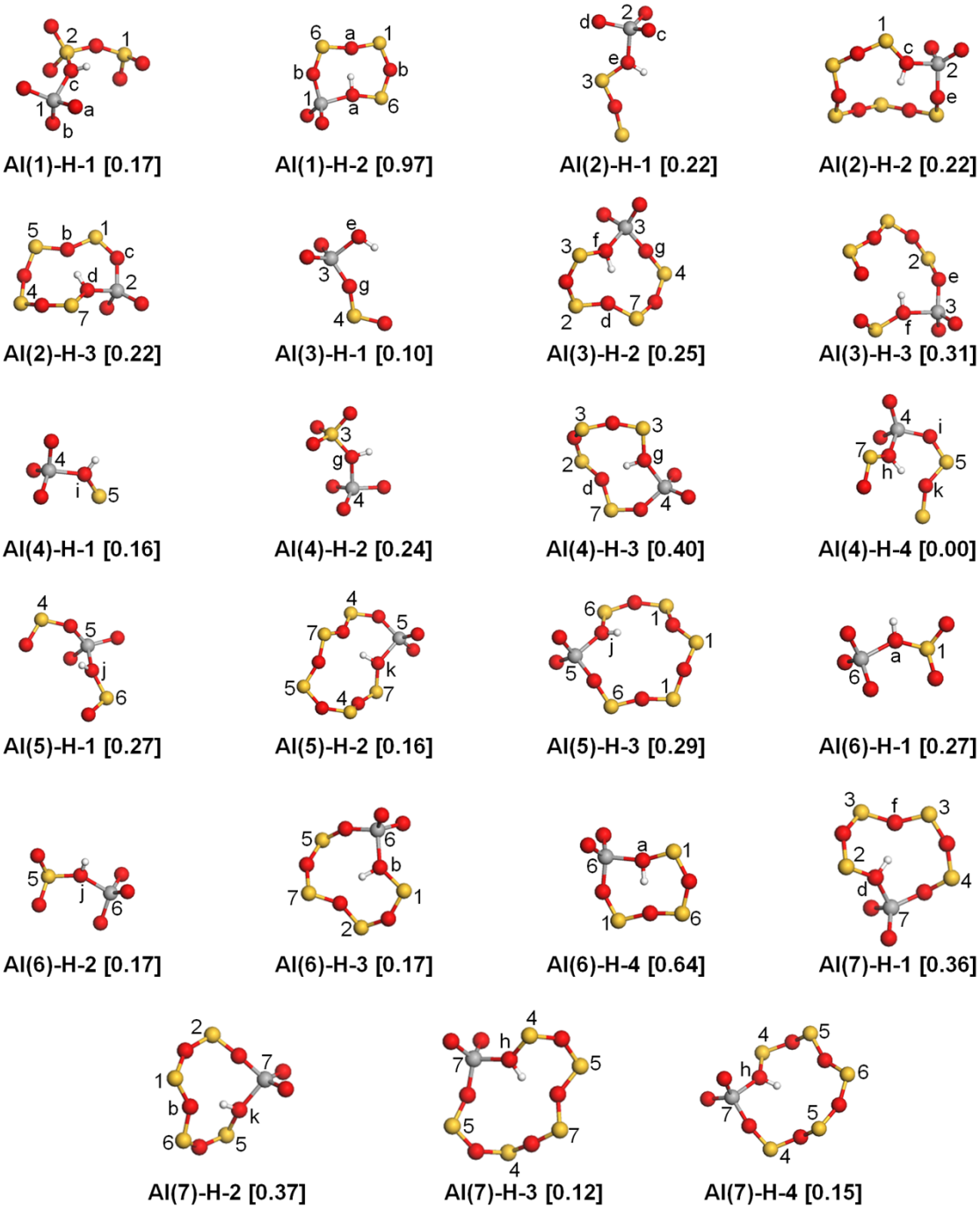


Fig. S6. Local structures and relative energies (eV) for LiAl-MTW zeolites. Li, O, Al and Si atoms are shown in dark gray, red, gray and yellow, respectively. Relative energy of the most stable structure is 0 eV, and the relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

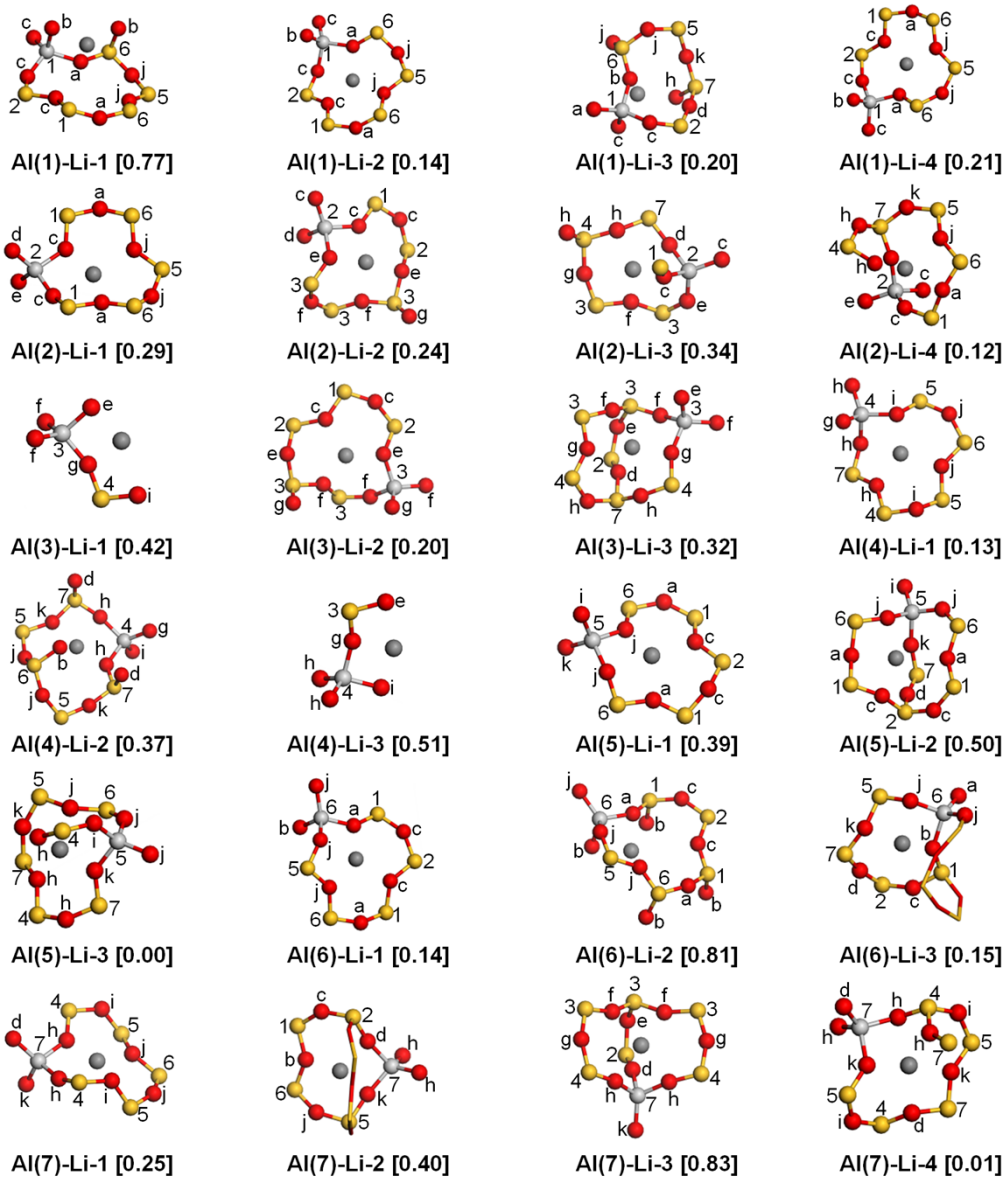


Fig. S7. Local structures and relative energies (eV) for NaAl-MTW zeolites. Na, O, Al and Si atoms are shown in violet, red, gray and, yellow, respectively. Relative energy of the most stable structure is 0 eV, the relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

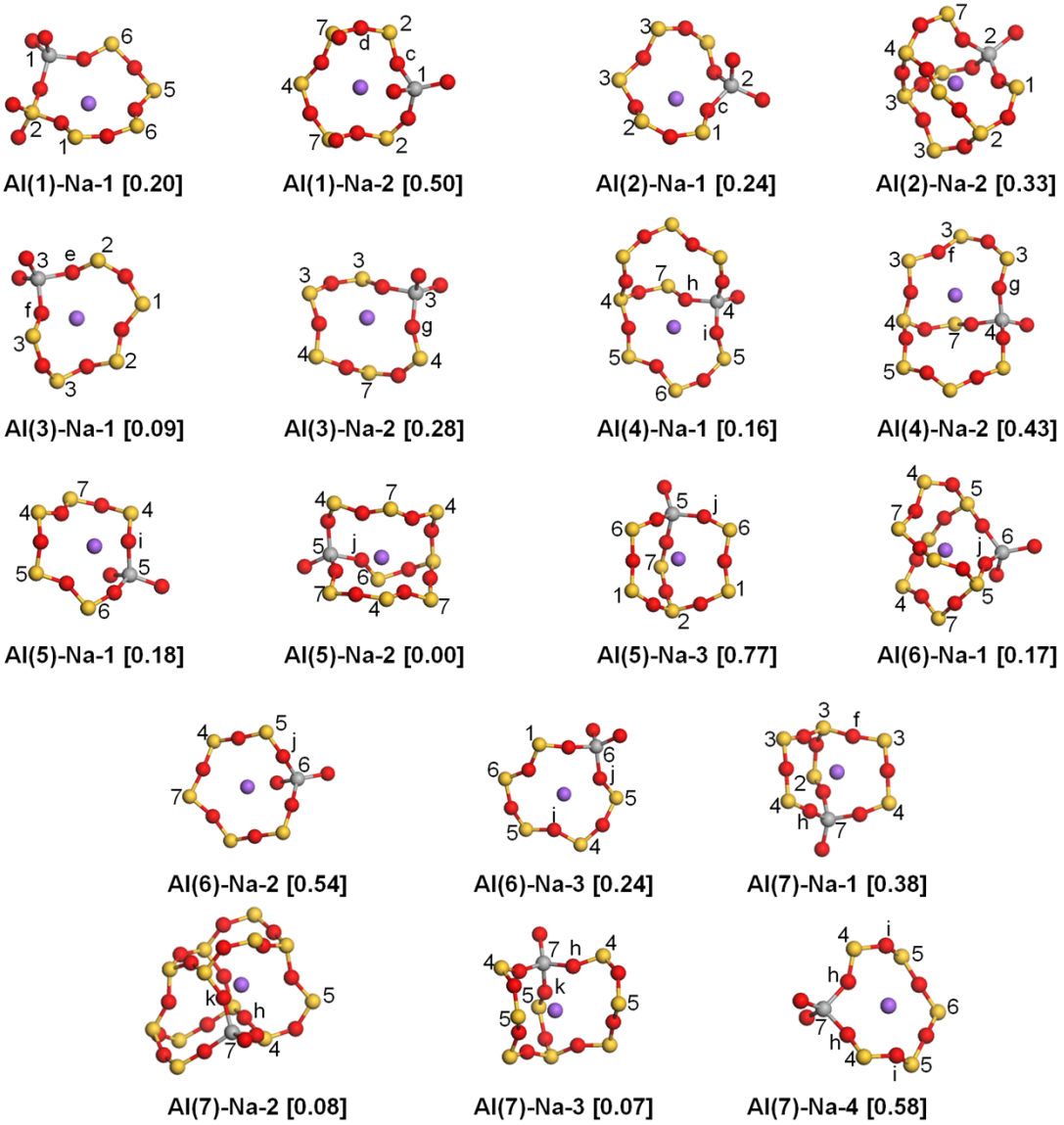


Fig. S8. Local structures and relative energies (eV) for KAl-MTW zeolites. K, O, Al and Si atoms are shown in darkslateblue, red, gray and yellow, respectively. Relative energy of the most stable structure is 0 eV, relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

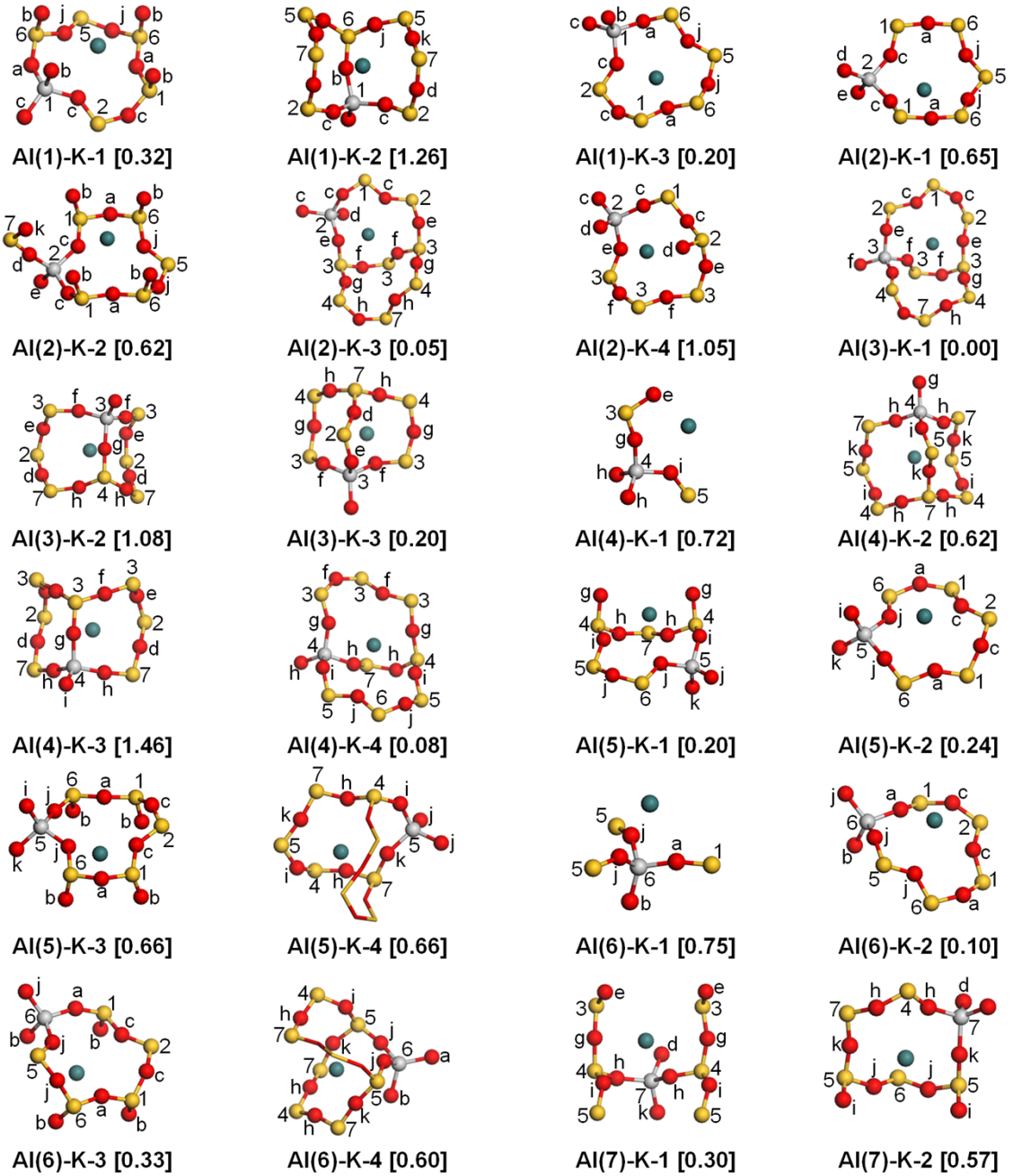


Fig. S9. Local structures and relative energies (eV) of the HGa-MTW zeolites. H, O, Ga and Si atoms are shown in white, red, tan and yellow, respectively. Relative energy of the most stable structure is 0 eV, relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

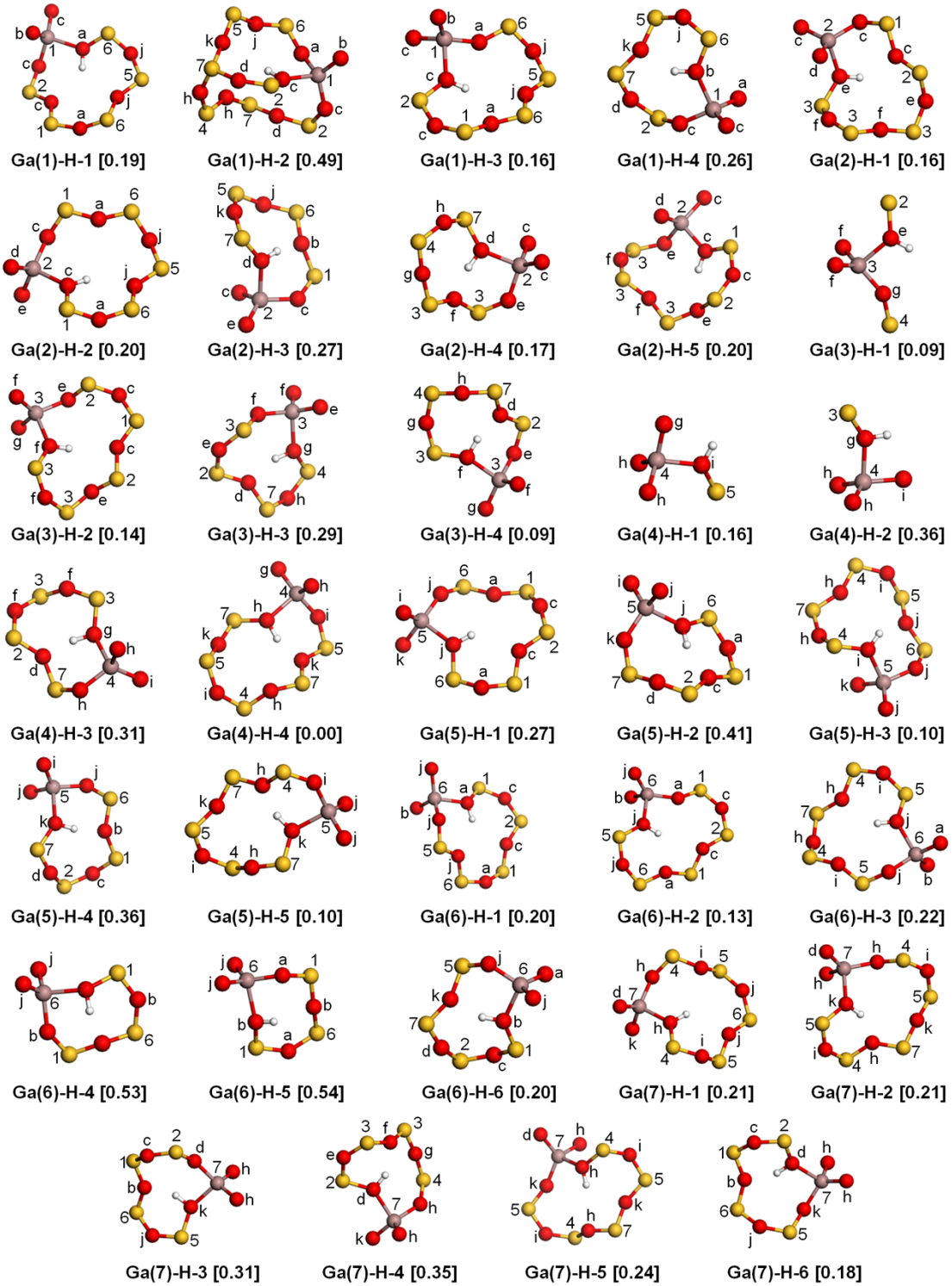


Fig. S10. Local structures and relative energies (eV) for LiGa-MTW zeolites. Li, O, Ga and Si atoms are shown in dark gray, red, tan and yellow, respectively. Relative energy of the most stable structure is 0 eV, and the relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

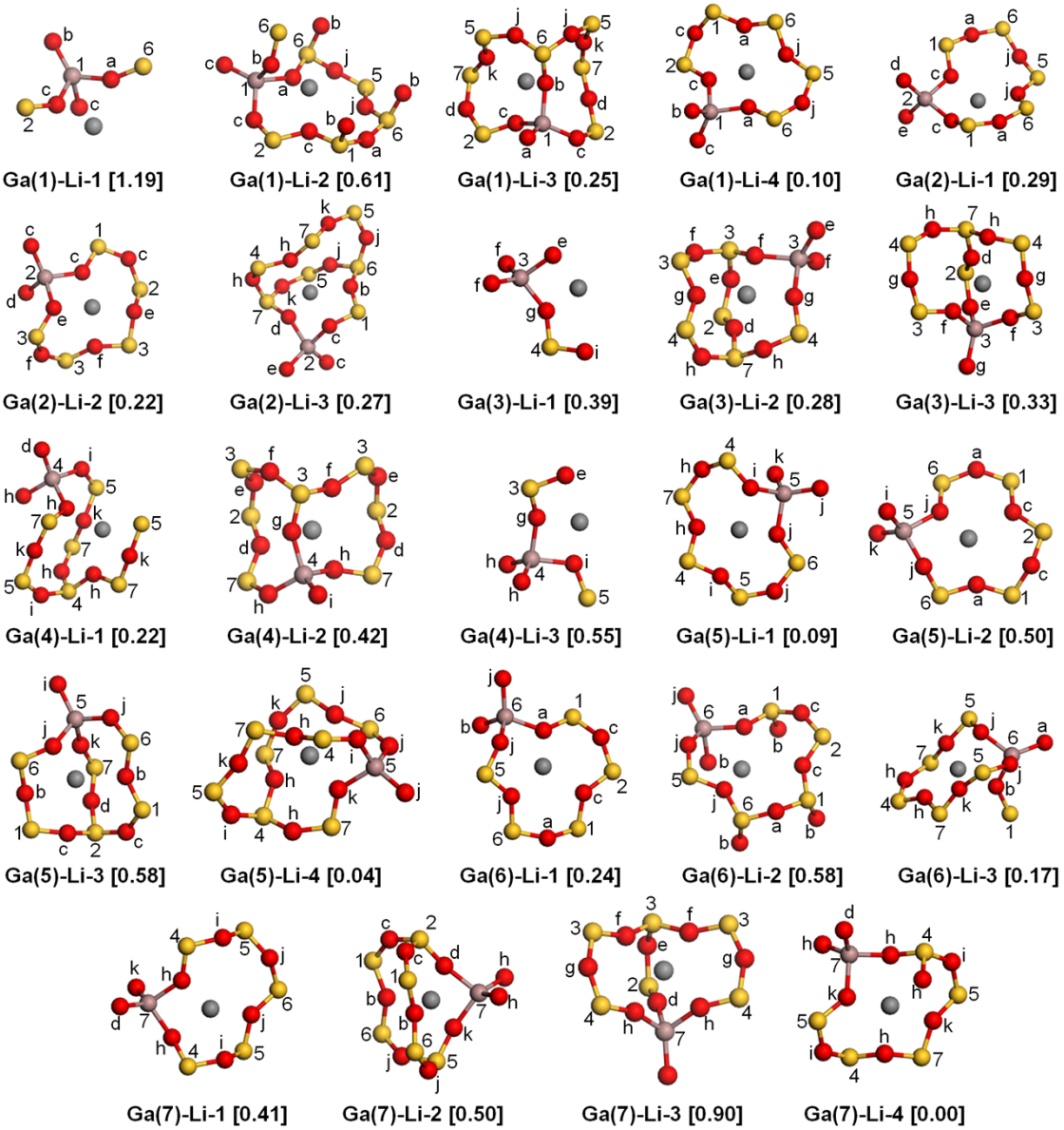


Fig. S11. Local structures and relative energies (eV) for NaGa-MTW zeolites. Na, O, Ga and Si atoms are shown in violet, red, tan and yellow, respectively. Relative energy of the most stable structure is 0 eV, the relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

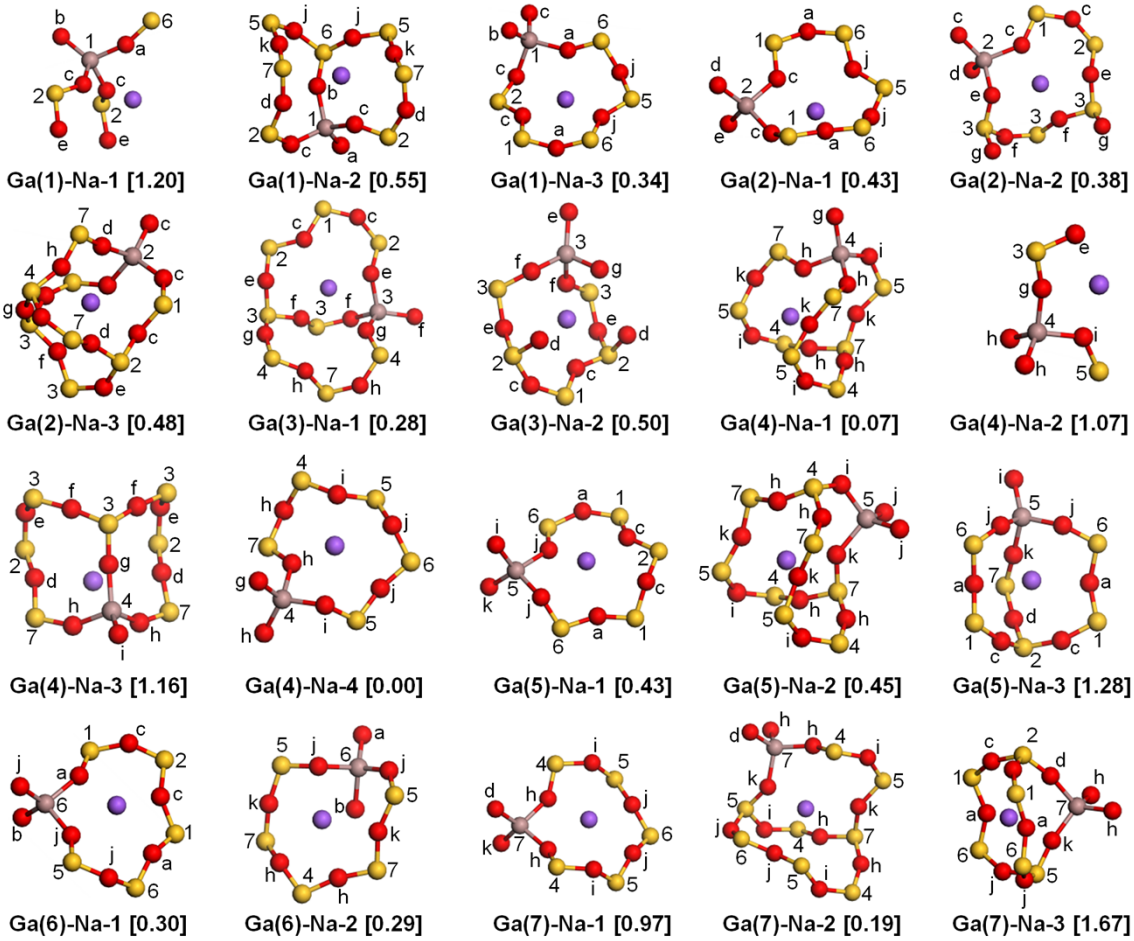


Fig. S12. Local structures and relative energies (eV) for KGa-MTW zeolites. K, O, Ga and Si atoms are shown in darkslateblue, red, tan and yellow, respectively. Relative energy of the most stable structure is 0 eV, relative energies of the other structures are given with respect to the most stable structure. (Only related atoms were selectively shown for good viewing)

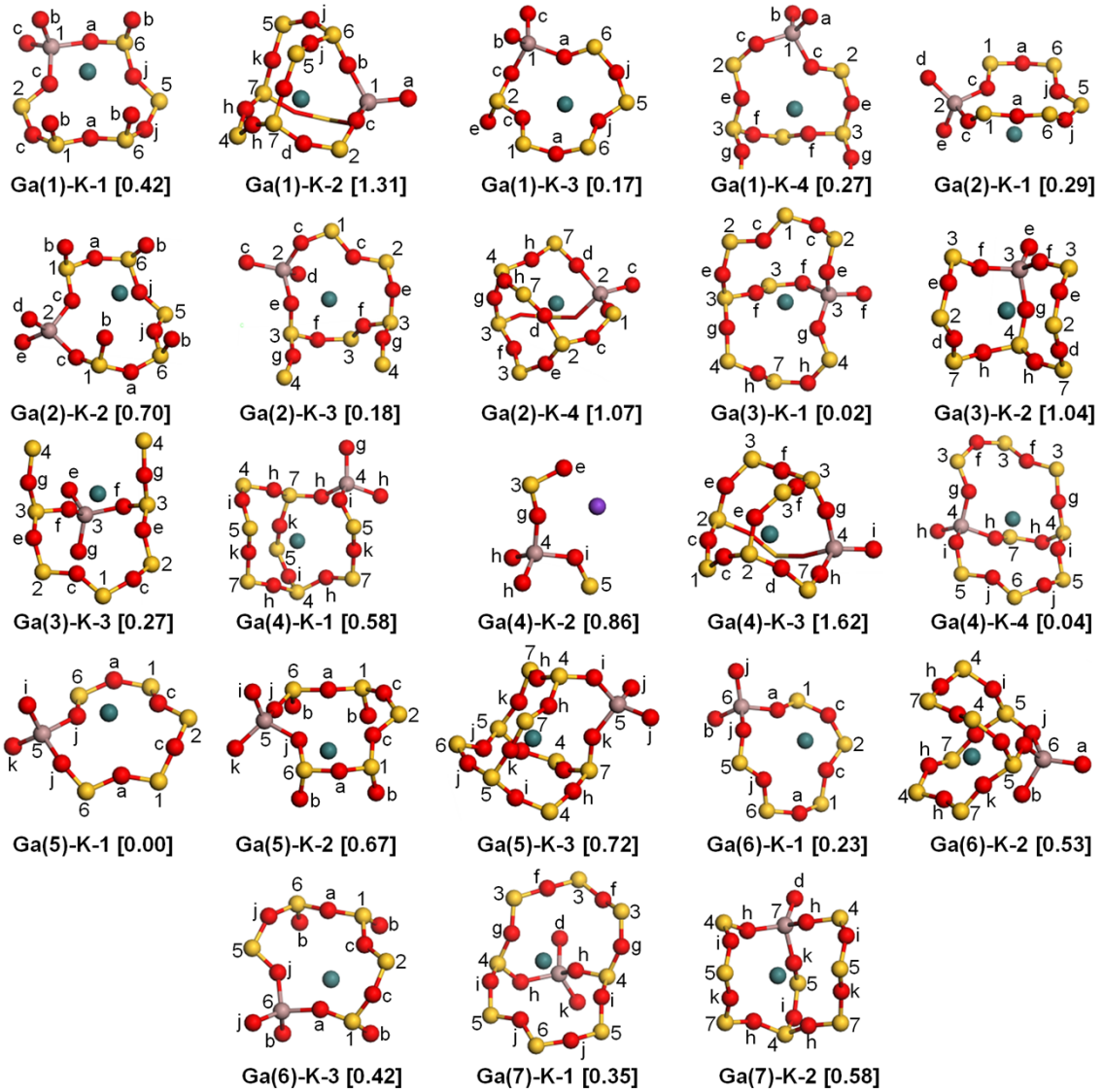


Fig. S13. Local structures and adsorption energies (eV) for the adsorption of NH_3 in HB-MTW zeolites. H, N, O, B and Si atoms are shown in white, blue, red, green and yellow, respectively (Only related atoms were selectively shown for good viewing).

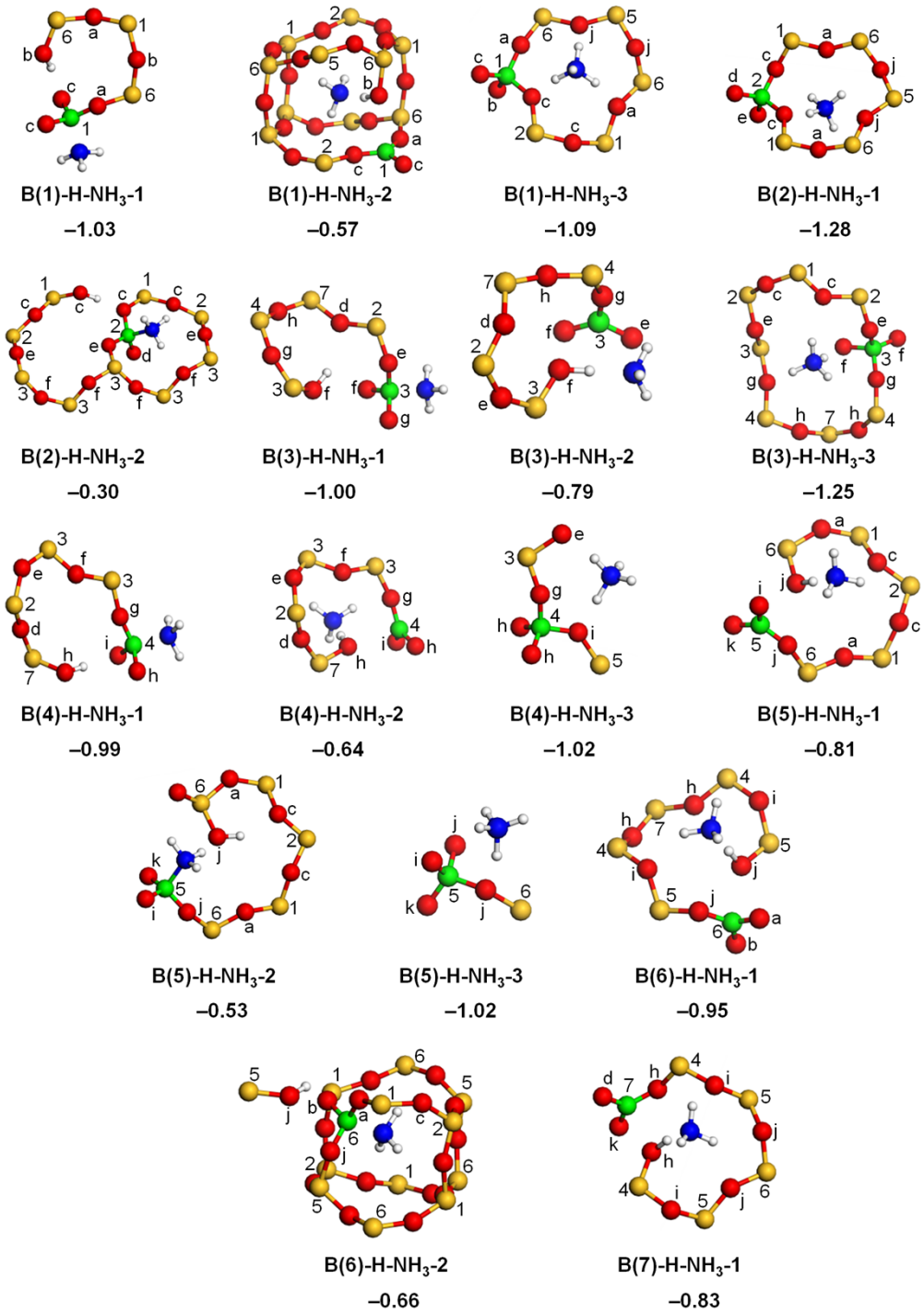


Fig. S14. Local structures and adsorption energies (eV) for the adsorption of pyridine in HB-MTW zeolites. H, C, N, O, B and Si atoms are shown in white, black, blue, red, green and yellow, respectively (Only related atoms were selectively shown for good viewing).

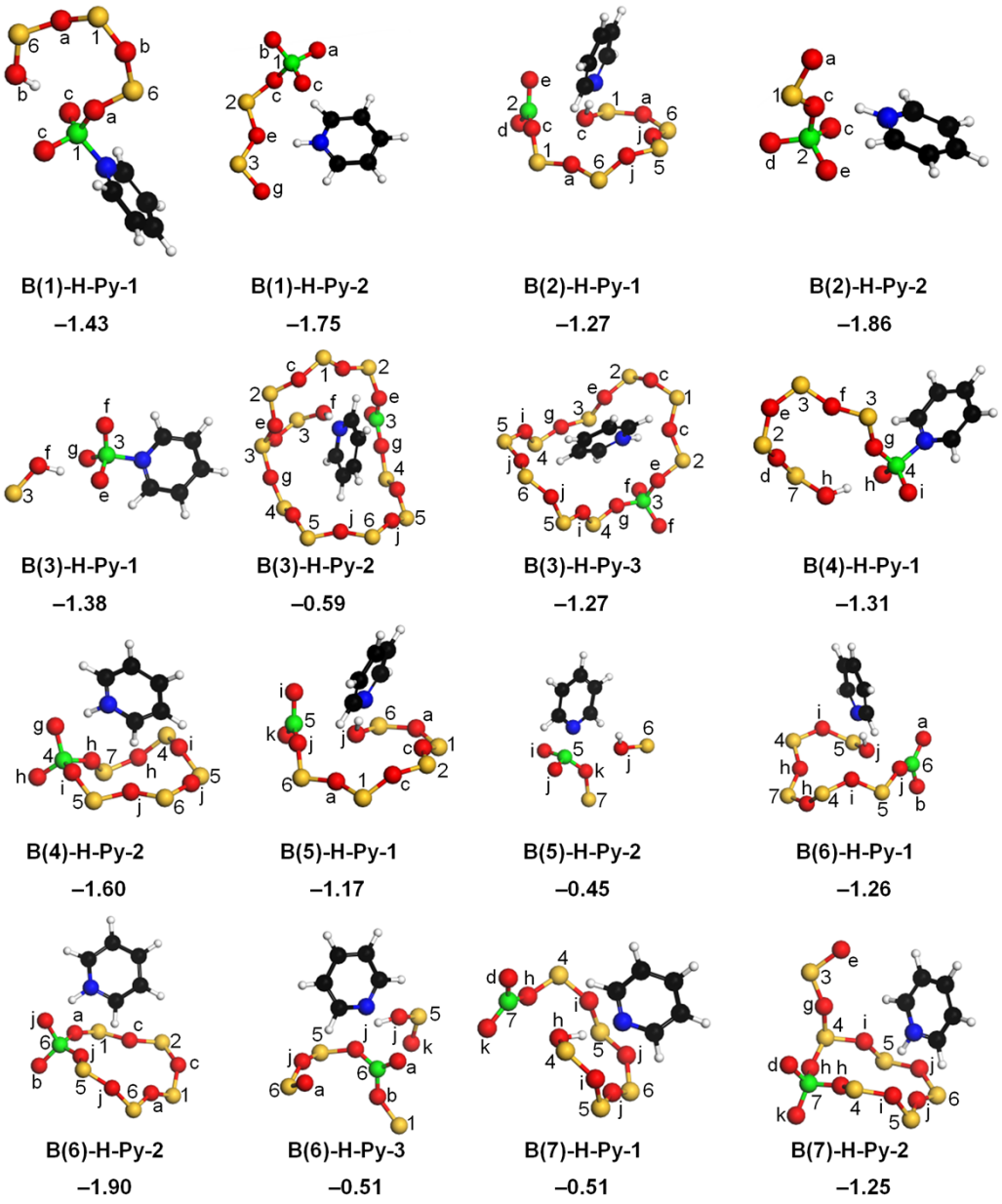


Fig. S15. Local structures and adsorption energies (eV) for the adsorption of NH_3 in HAl-MTW zeolites. H, N, O, Al and Si atoms are shown in white, blue, red, gray and yellow, respectively (Only related atoms were selectively shown for good viewing).

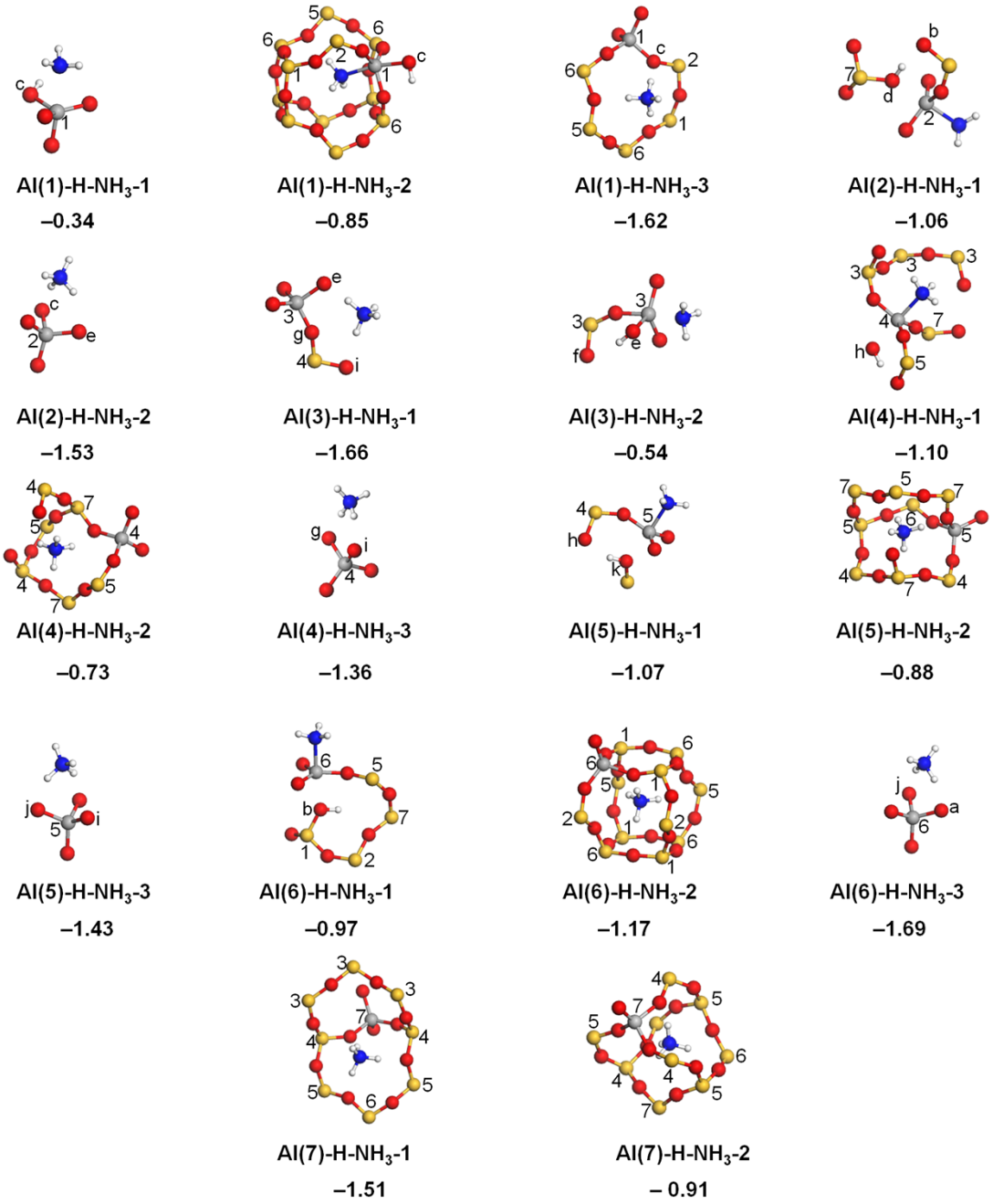


Fig. S16. Local structures and adsorption energies (eV) for the adsorption of pyridine in HAl-MTW zeolites. H, C, N, O, Al and Si atoms are shown in white, black, blue, red, gray and yellow, respectively (Only related atoms were selectively shown for good viewing).

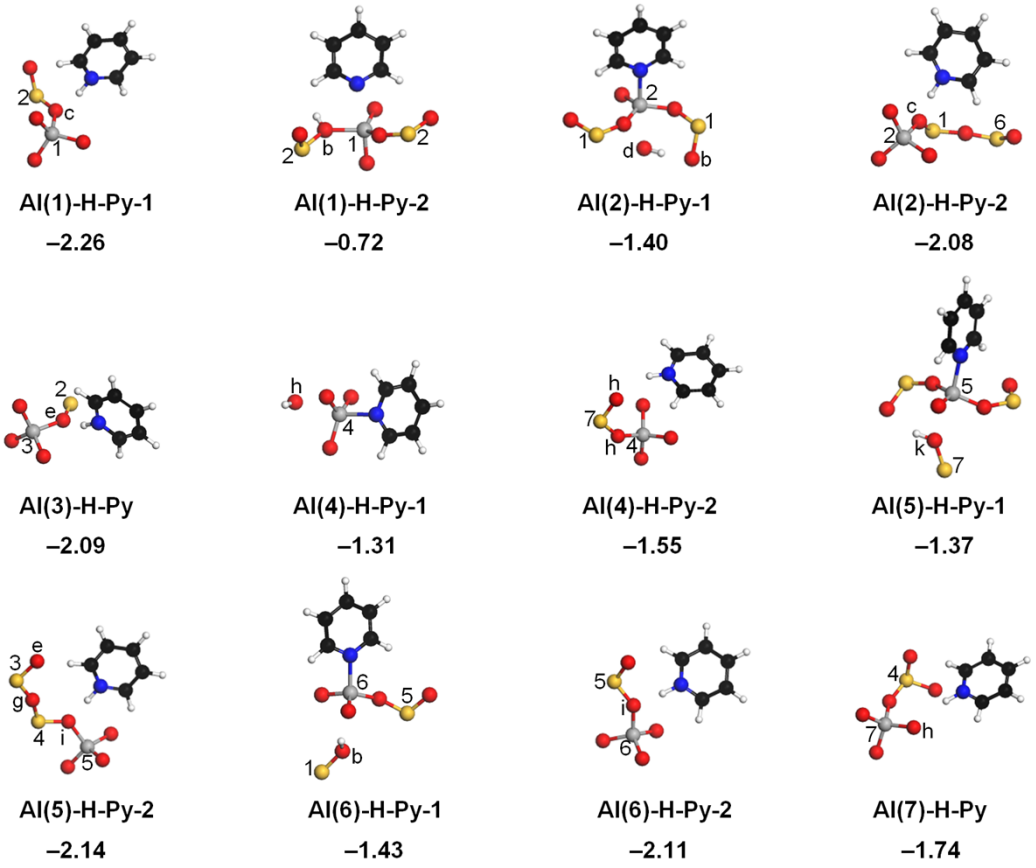


Fig. S17. Local structures and adsorption energies (eV) for the adsorption of NH_3 in HGa-MTW zeolites. H, N, O, Ga and Si atoms are shown in white, blue, red, tan and yellow, respectively (Only related atoms were selectively shown for good viewing).

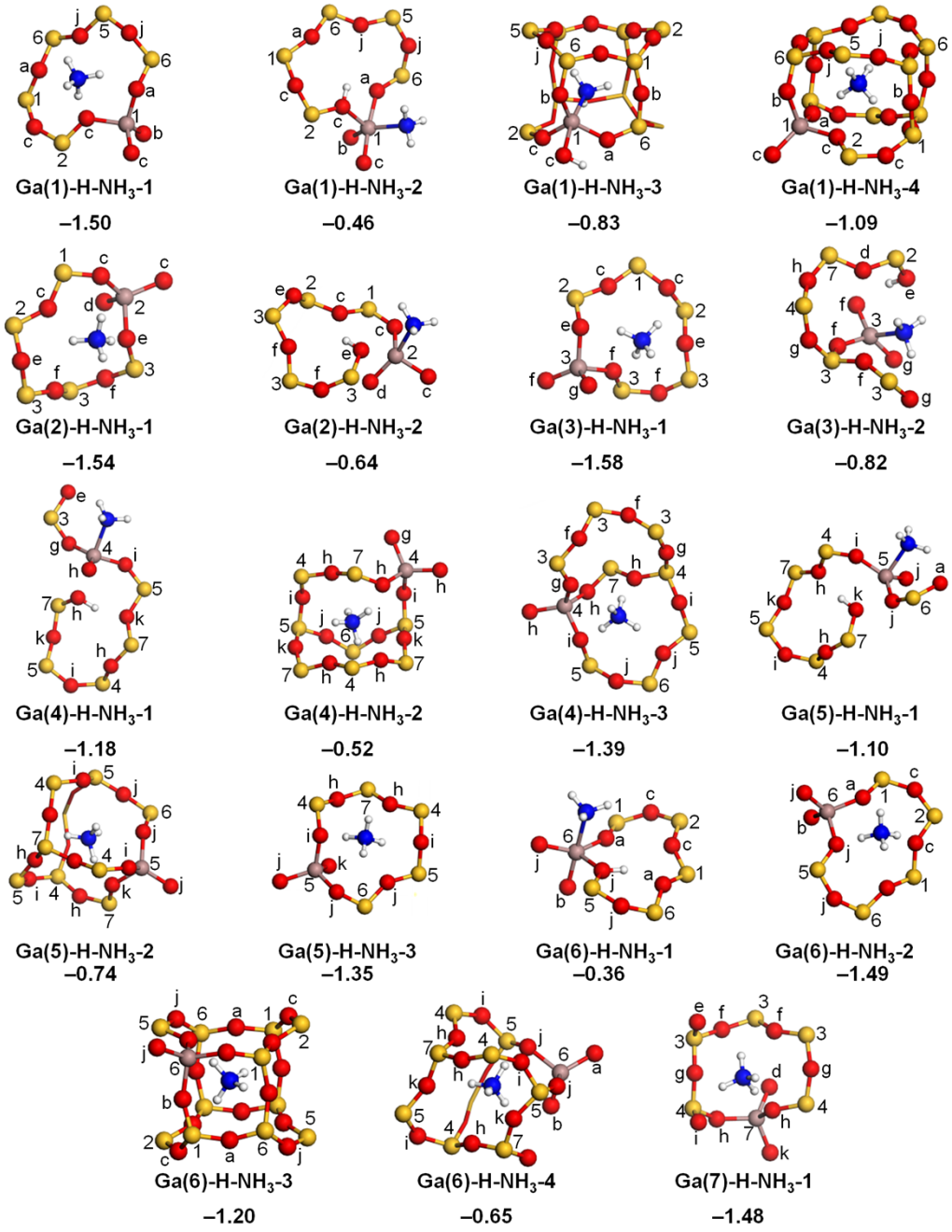
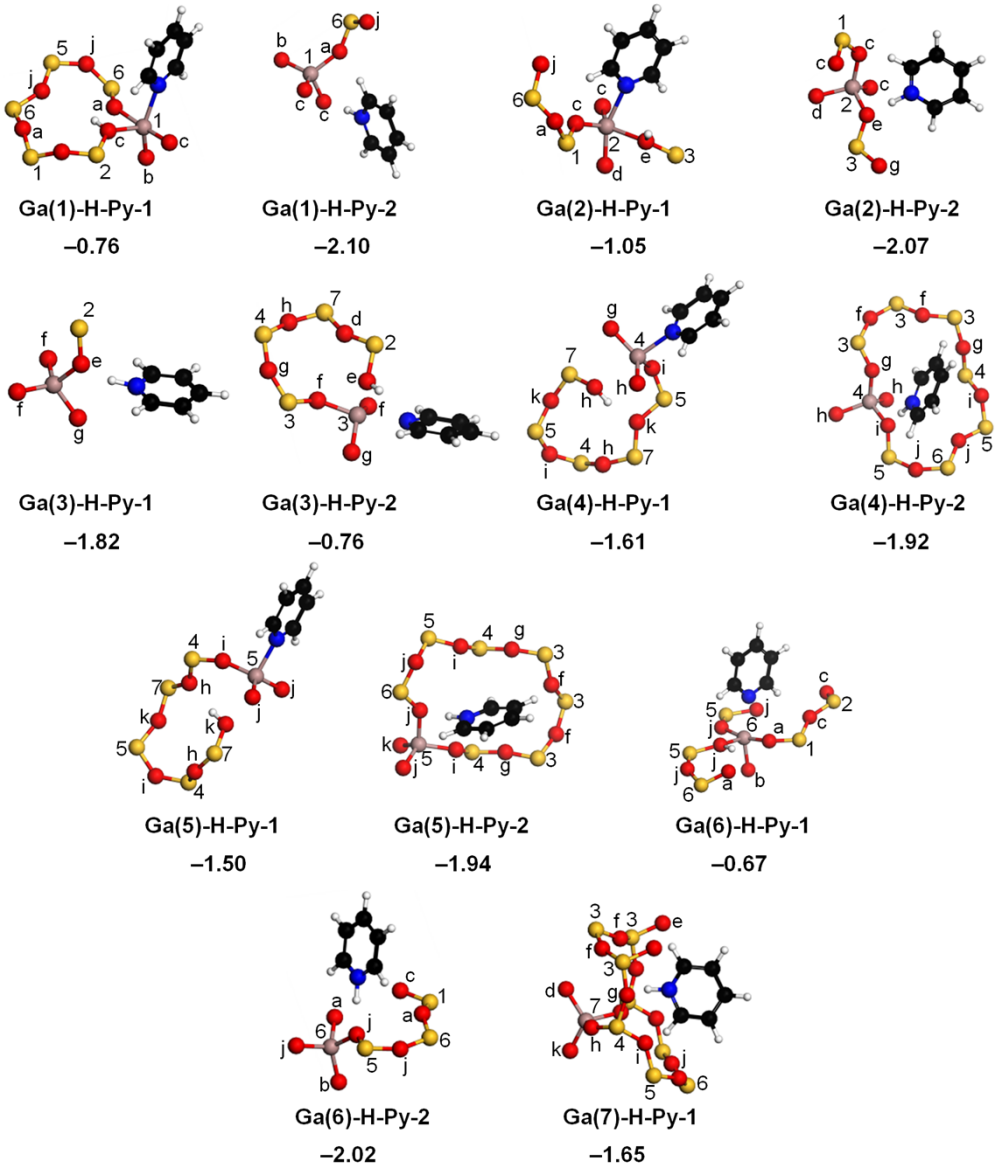


Fig. S18. Local structures and adsorption energies (eV) for the adsorption of pyridine in HGa-MTW zeolites. H, C, N, O, Ga and Si atoms are shown in white, black, blue, red, tan and yellow, respectively (Only related atoms were selectively shown for good viewing).



The p(1×2×1) cell parameters and the ionic positions of the optimized most stable structures for B, Al and Ga in each T site of the H form MTW zeolites.

HB(1)-MTW

a = 25.4658 Å
b = 10.2546 Å
c = 12.2718 Å
α = 89.1696º
β = 109.167º
γ = 90.4382º

H	0.37485830	0.30675411	0.92942085
O	0.10212694	0.39365452	0.25934465
O	0.07921254	0.14814830	0.89055126
O	0.23674063	0.40166816	0.82663879
O	0.57659623	0.08684266	0.22519855
O	0.57450500	0.39259337	0.87033896
O	0.73384079	0.14832543	0.81137939
O	0.89800714	0.40448652	0.73711895
O	0.90076648	0.07685585	0.13598032
O	0.76367373	0.41621985	0.17461110
O	0.39988716	0.16482641	0.72761277
O	0.40726034	0.34409724	0.16636496
O	0.24270892	0.09528238	0.14824204
O	0.92166457	0.15370098	0.77076872
O	0.91604961	0.32843671	0.11270391
O	0.73681348	0.16773379	0.14261034
O	0.42607749	0.39023125	0.76776090
O	0.42794160	0.09246548	0.14622437
O	0.26867842	0.34647925	0.17008298
O	0.09218492	0.14434550	0.21515195
O	0.09425954	0.39860069	0.86319599
O	0.26179782	0.15269658	0.86047890
O	0.60783819	0.33440260	0.23863324
O	0.59400867	0.14384299	0.84775894

O	0.76073222	0.39781949	0.84760016
O	0.00163752	0.00396058	0.14388235
O	0.08155429	0.96794378	0.05163126
O	0.34530024	0.98551596	0.58129479
O	0.32815965	0.01068910	0.78061873
O	0.34799553	0.00848416	0.22380618
O	0.33318973	0.99461109	0.00066231
O	0.28723776	0.00200973	0.36044716
O	0.50168230	0.27141255	0.13869133
O	0.57608920	0.21819588	0.03624752
O	0.84446732	0.23901031	0.57679476
O	0.82425098	0.23830238	0.77515703
O	0.84373749	0.24245686	0.21438577
O	0.82061140	0.21803746	0.98878583
O	0.78522533	0.25144140	0.35578537
O	0.99827970	0.97265134	0.85197642
O	0.91793614	-0.00083475	0.94530546
O	0.65415299	0.00253236	0.41888410
O	0.67486020	0.00805913	0.22137800
O	0.65351462	0.97339352	0.77880896
O	0.67154797	-0.00201495	0.00236823
O	0.71325224	0.97889517	0.63856151
O	0.49281339	0.21896121	0.83723826
O	0.40749242	0.25014229	0.96235172
O	0.15669367	0.22816120	0.42387414
O	0.18942965	0.25993380	0.24429785
O	0.15536949	0.22831240	0.79746227
O	0.17238310	0.26580740	0.01947300
O	0.20881883	0.23777793	0.64745742
O	0.23689806	0.40502801	0.50883537
O	0.76296991	0.41326239	0.50200412
O	0.73876666	0.16227379	0.50777471
O	0.26326318	0.15573794	0.51004014
O	0.09766450	0.89524095	0.26940176
O	0.08116726	0.65208217	0.87210072

O	0.24662134	0.89758243	0.83439662
O	0.58020317	0.58417911	0.22843052
O	0.57719829	0.89299016	0.87137321
O	0.73396566	0.64732419	0.82691575
O	0.89346759	0.90642052	0.73448579
O	0.90444988	0.58016688	0.14131665
O	0.76087559	0.91643765	0.17133691
O	0.39815741	0.64414403	0.74705792
O	0.40629250	0.84014553	0.14711176
O	0.23884950	0.59277351	0.16054986
O	0.91527792	0.65630198	0.76935957
O	0.92236256	0.82900236	0.11522774
O	0.73980088	0.66560556	0.13146817
O	0.42114218	0.90287313	0.77123295
O	0.42102876	0.59084710	0.11781417
O	0.26393752	0.84385181	0.17866912
O	0.08346215	0.64441343	0.23420072
O	0.09968545	0.90240476	0.85812413
O	0.27012252	0.64693083	0.86139009
O	0.60354036	0.83571370	0.25929226
O	0.59643566	0.64222083	0.86073470
O	0.76007485	0.89894021	0.85505197
O	0.00122319	0.48298034	0.13860818
O	0.08454353	0.50274927	0.05353304
O	0.34374597	0.47892592	0.58605908
O	0.33060425	0.46759198	0.79159659
O	0.34632706	0.52748689	0.21995044
O	0.32800890	0.46243186	0.00153498
O	0.29031766	0.48226295	0.36458323
O	0.50258494	0.75946503	0.13454126
O	0.58729986	0.73529240	0.05368857
O	0.84082078	0.74147709	0.57060909
O	0.81596335	0.74189935	0.76198763
O	0.84492271	0.75342297	0.20775827
O	0.82782605	0.72168815	0.98488724

O	0.78555915	0.74389589	0.34751265
O	0.99769210	0.49235396	0.86034980
O	0.91440423	0.49965936	0.94525262
O	0.65538535	0.48259234	0.41845806
O	0.68113200	0.51898686	0.23004962
O	0.65388802	0.47090131	0.78576243
O	0.67039694	0.48529852	0.00963707
O	0.70945291	0.49820195	0.63959461
O	0.49817335	0.72461440	0.86637255
O	0.41359247	0.75965396	0.94668992
O	0.15721595	0.73067325	0.43141400
O	0.17916370	0.75656829	0.23770982
O	0.16380237	0.73014704	0.79885923
O	0.17278997	0.75985843	0.01747665
O	0.21882539	0.73674786	0.65179108
O	0.23921067	0.90379897	0.50439615
O	0.75884317	0.91291285	0.48192413
O	0.73467037	0.66229402	0.49414038
O	0.26345167	0.65338695	0.49821268
Si	0.06803739	0.00179466	0.16959782
Si	0.06444987	0.99796704	0.91282402
Si	0.37525558	0.01731277	0.71770678
Si	0.37878987	0.98455160	0.12879681
Si	0.29306526	0.01323111	0.86906353
Si	0.28545726	0.98762685	0.22871438
Si	0.28366636	0.01124320	0.48885127
Si	0.56523973	0.22804467	0.15932712
Si	0.55867257	0.24472434	0.89759141
Si	0.87210221	0.25857726	0.71544031
Si	0.87009736	0.21766864	0.11243569
Si	0.78521023	0.25083913	0.85577258
Si	0.78225172	0.26928838	0.22268385
Si	0.78261099	0.26641961	0.48472716
Si	0.93317894	0.00743069	0.82620157
Si	0.93575807	0.97736462	0.08477535

Si	0.62704670	0.98387029	0.28037256
Si	0.62421107	0.00247886	0.87569119
Si	0.71053621	0.02195080	0.13399143
Si	0.71518680	0.00000828	0.77025860
Si	0.71652198	0.01391033	0.51198381
Si	0.43585968	0.24001073	0.10352273
Si	0.13466697	0.25563397	0.28507367
Si	0.12545595	0.25894875	0.89286546
Si	0.21804102	0.24140694	0.14488696
Si	0.21566012	0.25485469	0.78212347
Si	0.21664921	0.25634005	0.52273210
Si	0.43272029	0.75865750	0.83173937
Si	0.06741379	0.50519066	0.17062412
Si	0.06426776	0.51136840	0.91267407
Si	0.37541472	0.49480946	0.72364639
Si	0.37580151	0.48308885	0.12720043
Si	0.29090048	0.49684233	0.86923089
Si	0.28588438	0.48816660	0.23039218
Si	0.28330211	0.50449072	0.48912811
Si	0.56820684	0.72835779	0.16849985
Si	0.56470394	0.74883809	0.91288432
Si	0.86652263	0.76128160	0.70956952
Si	0.87447755	0.72185573	0.11213990
Si	0.78472315	0.75248866	0.85776979
Si	0.78264178	0.77021707	0.21515563
Si	0.77978963	0.76473959	0.47345976
Si	0.93149739	0.51320192	0.82850359
Si	0.93419626	0.47328278	0.08450792
Si	0.63066127	0.47990037	0.27824441
Si	0.62398907	0.49767470	0.88196534
Si	0.71328239	0.52148347	0.13545809
Si	0.71457197	0.50317498	0.77410495
Si	0.71589638	0.51407580	0.51358549
Si	0.43599433	0.73776631	0.08652569
Si	0.12919160	0.75544916	0.29285072

Si	0.12968295	0.76042881	0.88673429
Si	0.21329085	0.73874600	0.14835025
Si	0.22480593	0.75372817	0.78605411
Si	0.21979431	0.75581978	0.52154329
B	0.43911458	0.25819208	0.78027111

HB(2)-MTW

a = 25.5108 Å

b = 10.2673 Å

c = 12.2215 Å

α = 89.0924º

β = 108.942º

γ = 90.9529º

H	0.45029823	0.45060166	0.73806061
O	0.07958339	0.33944558	0.24481363
O	0.10225893	0.08220125	0.86887992
O	0.24309007	0.41362275	0.82017374
O	0.57967716	0.09047571	0.23372828
O	0.57710903	0.39204419	0.87378498
O	0.73601241	0.14492324	0.83443324
O	0.91338174	0.34099563	0.77400987
O	0.90049049	0.08490531	0.14096059
O	0.75895702	0.41998025	0.16727591
O	0.40057836	0.16950188	0.72786472
O	0.40170499	0.33934599	0.13157169
O	0.26374807	0.16736728	0.19276780
O	0.89409908	0.09136212	0.73538217
O	0.92413832	0.33473204	0.12540827
O	0.73923387	0.16763933	0.13418414
O	0.43347296	0.41528438	0.79426694
O	0.42100383	0.08933381	0.12014771
O	0.23989653	0.41671938	0.14984063
O	0.10367908	0.08797614	0.26509330
O	0.08135546	0.33198675	0.87425040

O	0.26244980	0.16235982	0.86679423
O	0.60270725	0.34240188	0.26377326
O	0.60364444	0.14465713	0.87121911
O	0.75764598	0.39777698	0.85518859
O	0.00060447	0.01197848	0.15157263
O	0.07956281	0.99602573	0.05314362
O	0.34707889	0.99051183	0.57918888
O	0.32227019	0.02205037	0.76970216
O	0.34482501	0.00456373	0.21240375
O	0.32698482	0.97688556	0.98749452
O	0.28908648	0.98197019	0.35831084
O	0.50169322	0.26243954	0.13745854
O	0.58770807	0.23914035	0.05907782
O	0.84199157	0.25906229	0.57132636
O	0.81419157	0.24392572	0.75978231
O	0.84338787	0.26085930	0.20830816
O	0.83004044	0.23405341	0.98512847
O	0.78427266	0.25412858	0.34858402
O	0.99819723	0.02259930	0.85253278
O	0.91867783	0.00526246	0.95062758
O	0.65534532	0.99537621	0.42391427
O	0.67941613	0.02104649	0.23116874
O	0.65620507	0.96870399	0.78835681
O	0.67406632	0.97915761	0.01392374
O	0.71356672	0.99822588	0.64433185
O	0.50227451	0.20958543	0.86604874
O	0.41646037	0.24650573	0.94223560
O	0.15962591	0.24942133	0.42986689
O	0.17492177	0.26206145	0.22692497
O	0.15862869	0.25157993	0.78675537
O	0.17742250	0.23826652	0.01268768
O	0.21949296	0.24191916	0.64932713
O	0.26470456	0.33828679	0.49700312
O	0.75813554	0.42171678	0.48386934
O	0.73708312	0.16978127	0.50110202

O	0.24369345	0.08563613	0.50274502
O	0.07885911	0.83754489	0.22686518
O	0.09709708	0.58665381	0.87144034
O	0.23677108	0.91541879	0.81242028
O	0.57730957	0.59160433	0.22861993
O	0.57665284	0.89585616	0.87335956
O	0.73489831	0.64825121	0.82281131
O	0.91977005	0.84420006	0.78187522
O	0.90397708	0.58448160	0.14270544
O	0.76531689	0.92096995	0.18559862
O	0.39179922	0.67628882	0.72566834
O	0.40352337	0.83796162	0.14145372
O	0.26245869	0.66867740	0.17548064
O	0.90287952	0.59418176	0.73950586
O	0.91963156	0.83597490	0.11874981
O	0.73885159	0.67225473	0.14595779
O	0.41968362	0.91995679	0.78545034
O	0.42553659	0.58977381	0.12983259
O	0.23900038	0.91931485	0.13988838
O	0.10593417	0.59007728	0.25829114
O	0.07267530	0.83558800	0.87844717
O	0.25401397	0.66486443	0.86616117
O	0.60580304	0.84083018	0.24889611
O	0.59008557	0.64352679	0.84787906
O	0.76286238	0.89718669	0.85261152
O	0.00303881	0.51235156	0.14283349
O	0.08523125	0.47056894	0.05839669
O	0.33871487	0.53043579	0.58543923
O	0.31798806	0.55210897	0.76205293
O	0.34465829	0.50419224	0.20938613
O	0.33120407	0.50024315	0.98409866
O	0.29080624	0.51135186	0.36076328
O	0.50192790	0.77061486	0.13464963
O	0.58197047	0.72713395	0.04488514
O	0.84656444	0.76340446	0.58207171

O	0.82332441	0.73543826	0.77567045
O	0.84561874	0.75055376	0.21745477
O	0.82469305	0.72175796	0.99326843
O	0.78828962	0.74917673	0.36129423
O	0.99962572	0.49278162	0.86412354
O	0.91625700	0.49818083	0.94912506
O	0.65507725	0.51375052	0.42227902
O	0.67544818	0.51263599	0.22458290
O	0.65225090	0.47833503	0.78064260
O	0.66981799	0.50851313	0.00411163
O	0.71272062	0.48724201	0.64193746
O	0.49375605	0.73116836	0.85304086
O	0.41316815	0.74734813	0.94642710
O	0.15283496	0.75953252	0.42510904
O	0.18068279	0.76593366	0.23691358
O	0.15075873	0.76190158	0.78938776
O	0.16921490	0.74496401	0.01513573
O	0.20788972	0.73413541	0.64695141
O	0.26055871	0.83121216	0.50863908
O	0.76149550	0.92156485	0.49345739
O	0.74224342	0.67007677	0.51706698
O	0.23117154	0.58209382	0.49437224
Si	0.43877147	0.26108624	0.83175000
Si	0.06552045	0.98397927	0.17386465
Si	0.06280863	0.98368324	0.91294590
Si	0.37273199	0.02443489	0.71599957
Si	0.37377653	0.97876836	0.11468085
Si	0.28755153	0.01907346	0.85972949
Si	0.28395611	0.01854198	0.22618285
Si	0.28473576	0.97324776	0.48702431
Si	0.56741843	0.23391453	0.17312263
Si	0.56778452	0.24595366	0.91785569
Si	0.86615486	0.23449614	0.71063957
Si	0.87427339	0.22962729	0.11482038
Si	0.78482562	0.25514725	0.85904669

Si	0.78123238	0.27600184	0.21523094
Si	0.78027977	0.27562722	0.47633287
Si	0.93296501	0.99145582	0.83050293
Si	0.93496145	0.98391450	0.09041414
Si	0.62972619	0.98698598	0.28364350
Si	0.62778241	0.99745919	0.88696336
Si	0.71415931	0.02203091	0.14082916
Si	0.71727846	0.00181597	0.77865469
Si	0.71713444	0.02121176	0.51590920
Si	0.43545182	0.23457726	0.08320221
Si	0.12929359	0.23448250	0.29131981
Si	0.13012985	0.22703527	0.88650456
Si	0.21362633	0.27072210	0.14496835
Si	0.22115287	0.26769763	0.78031847
Si	0.22217482	0.22939219	0.52000854
Si	0.42940076	0.76853380	0.82865315
Si	0.06820621	0.47848444	0.17585421
Si	0.06568056	0.47034038	0.91723191
Si	0.37523685	0.48396099	0.11322366
Si	0.28741362	0.53293266	0.85837985
Si	0.28435555	0.52452849	0.22479247
Si	0.28117132	0.49022793	0.48453180
Si	0.56647447	0.73308057	0.16420457
Si	0.56038007	0.74975970	0.90480369
Si	0.87323360	0.73508777	0.72029798
Si	0.87344972	0.72447292	0.11768737
Si	0.78683334	0.75045390	0.86127889
Si	0.78443459	0.77309796	0.22775923
Si	0.78448591	0.77579323	0.48843322
Si	0.93318163	0.48180239	0.83209162
Si	0.93708988	0.48220823	0.09018344
Si	0.62753114	0.48996626	0.28409647
Si	0.62272994	0.50600597	0.87761111
Si	0.71039060	0.52818378	0.13534447
Si	0.71449124	0.50297691	0.77442581

Si	0.71723563	0.52326661	0.51610298
Si	0.43613756	0.73581349	0.08770495
Si	0.12925825	0.73796969	0.28570703
Si	0.12244028	0.73335337	0.88886900
Si	0.21271833	0.77387208	0.14160718
Si	0.21258470	0.76913080	0.77846476
Si	0.21337092	0.72777770	0.51925743
B	0.35008714	0.58371683	0.69420838

HB(3)-MTW

a = 25.4897 Å

b = 10.2725 Å

c = 12.2365 Å

α = 91.0242º

β = 109.411º

γ = 89.3336º

H	0.25245571	0.44840605	0.60605245
O	0.10488544	0.39759683	0.25066634
O	0.08046877	0.15007664	0.90039302
O	0.23344574	0.39142841	0.82650887
O	0.60445080	0.13402916	0.24806677
O	0.59636397	0.32933815	0.85473264
O	0.73357616	0.17353428	0.83328004
O	0.89637533	0.38950571	0.73434601
O	0.92560126	0.14652779	0.12368300
O	0.75845261	0.36413656	0.15041713
O	0.41948265	0.08324894	0.76933702
O	0.42447065	0.38751203	0.12797494
O	0.26400206	0.15465786	0.17197132
O	0.91838437	0.14195336	0.78170841
O	0.90473198	0.39710900	0.14156733
O	0.74999591	0.11199544	0.16195339
O	0.39032252	0.33269439	0.73361991
O	0.40098094	0.13881450	0.13321243

O	0.24123887	0.40590389	0.19712088
O	0.07808185	0.14728137	0.23094980
O	0.09593219	0.39685150	0.86337603
O	0.26289231	0.14549804	0.86846821
O	0.57750380	0.38359994	0.23118201
O	0.56906793	0.08357572	0.86469458
O	0.76528109	0.42096410	0.84961649
O	0.00262976	0.96354241	0.15175888
O	0.08483925	0.98014441	0.06444651
O	0.34296687	0.00084257	0.57425741
O	0.32166703	0.99687092	0.77157294
O	0.34436253	0.97835926	0.21789205
O	0.33164190	0.96691800	0.99331635
O	0.28287566	0.99578353	0.35342292
O	0.50085199	0.20695897	0.13381285
O	0.58154251	0.24753754	0.04530854
O	0.84266432	0.21277468	0.57895906
O	0.81918555	0.23714260	0.77094697
O	0.84995644	0.22167002	0.21794904
O	0.82845365	0.24574670	0.99268136
O	0.79085670	0.24889009	0.35695807
O	0.00093526	0.97468614	0.86332181
O	0.91859082	0.97920535	0.95117924
O	0.65428778	0.97691056	0.42130126
O	0.68260144	0.96605704	0.23347378
O	0.65094720	0.00537299	0.78542765
O	0.66406879	0.99859585	0.00932001
O	0.70791409	0.02171191	0.64308476
O	0.49436750	0.26876702	0.85260005
O	0.41332374	0.23426566	0.94304473
O	0.15129067	0.23945047	0.42699999
O	0.17877395	0.21871885	0.23739578
O	0.15517238	0.21471127	0.80191413
O	0.17518707	0.26858117	0.02331956
O	0.20848459	0.21448914	0.65175674

O	0.22937241	0.41102379	0.53014012
O	0.76626393	0.40043150	0.51027070
O	0.73455145	0.15290650	0.48442971
O	0.25733843	0.16393366	0.49610340
O	0.10661489	0.89969397	0.27848104
O	0.07589723	0.65022053	0.85936416
O	0.23907839	0.89557660	0.82745108
O	0.60711777	0.63175484	0.25380795
O	0.59481557	0.83422756	0.85949386
O	0.73360541	0.66893533	0.82821335
O	0.89989435	0.89222389	0.73712334
O	0.92161059	0.64839285	0.11992257
O	0.75058331	0.85873510	0.13415315
O	0.41081558	0.58146123	0.79098214
O	0.42628379	0.88716294	0.14737728
O	0.26447857	0.65271787	0.16826781
O	0.91056358	0.64159571	0.77623381
O	0.90053817	0.89861167	0.14019576
O	0.74378074	0.61344263	0.17801393
O	0.39497187	0.83102750	0.73320446
O	0.39982437	0.63835104	0.12235223
O	0.23803709	0.90439504	0.13886156
O	0.08347673	0.65043122	0.23345351
O	0.10206576	0.90058885	0.87209945
O	0.25801206	0.64311049	0.85736779
O	0.58248114	0.88245920	0.22361795
O	0.57858013	0.58147011	0.86071911
O	0.75684555	0.92156751	0.85175667
O	0.00295786	0.48012559	0.14161156
O	0.08222472	0.51271722	0.04729585
O	0.34873797	0.51003453	0.57466988
O	0.30791060	0.48718601	0.74538884
O	0.34231247	0.47290494	0.20016622
O	0.33141856	0.47029343	0.97498410
O	0.30765077	0.53953513	0.37418472

O	0.50290946	0.70855583	0.14574067
O	0.58070894	0.72875695	0.04431421
O	0.84166591	0.72725838	0.57393614
O	0.81471472	0.75944286	0.76184414
O	0.84325331	0.72001968	0.20809589
O	0.82681827	0.74988153	0.98472775
O	0.78918156	0.77664123	0.35315956
O	0.99625401	0.48333009	0.85262837
O	0.91585216	0.47975468	0.94729488
O	0.65853690	0.46872416	0.42096309
O	0.67574263	0.44596197	0.22048496
O	0.65692888	0.48611484	0.77903576
O	0.67228017	0.48437492	0.00368357
O	0.71531693	0.51898779	0.64024665
O	0.49594235	0.74346778	0.84628833
O	0.42012146	0.76333215	0.95212307
O	0.16659546	0.72078606	0.42256259
O	0.17768729	0.74497798	0.21800581
O	0.15371593	0.73431858	0.77382299
O	0.17463054	0.72649854	0.99960905
O	0.21997896	0.73262200	0.64511410
O	0.23898966	0.91106803	0.50761222
O	0.76030976	0.90143210	0.51580192
O	0.73658895	0.64895528	0.47297618
O	0.27697569	0.67129807	0.50565825
Si	0.42964627	0.22968759	0.82485747
Si	0.06791151	0.99825076	0.18161775
Si	0.06686622	0.00148576	0.92477407
Si	0.36993015	0.97841357	0.71281390
Si	0.37570390	0.99317549	0.12275049
Si	0.28928394	0.00098255	0.86558893
Si	0.28204584	0.00861224	0.22148170
Si	0.28008191	0.01846887	0.48241927
Si	0.56590331	0.24295577	0.16422645
Si	0.56012330	0.23202951	0.90421420

Si	0.86955999	0.24491351	0.71726561
Si	0.87715239	0.25306196	0.11838504
Si	0.78689808	0.27037012	0.86251789
Si	0.78713918	0.23606652	0.22311671
Si	0.78321782	0.25324957	0.48254014
Si	0.93469525	0.99701605	0.83382656
Si	0.93705702	0.99704978	0.09199351
Si	0.63052928	0.98977367	0.28084193
Si	0.61996226	0.98022888	0.87955117
Si	0.71147074	0.98440774	0.13451959
Si	0.71251270	0.03015085	0.77787844
Si	0.71467650	0.01292494	0.51674686
Si	0.43504032	0.24212139	0.08453702
Si	0.12791878	0.25155608	0.28664697
Si	0.12662462	0.25692326	0.89811724
Si	0.21495004	0.26285463	0.15728949
Si	0.21498594	0.24144183	0.78630418
Si	0.21197577	0.25797880	0.52708729
Si	0.43075605	0.72981898	0.83077793
Si	0.06825033	0.51003352	0.16801679
Si	0.06236992	0.51124547	0.90595342
Si	0.36526543	0.47945185	0.71126477
Si	0.37404245	0.49304563	0.10673904
Si	0.28290850	0.49796299	0.85344490
Si	0.28856960	0.51803853	0.23573510
Si	0.56803930	0.73776162	0.16648577
Si	0.56247866	0.72206916	0.90318861
Si	0.86693063	0.75479176	0.71319549
Si	0.87291023	0.75446359	0.11320088
Si	0.78323258	0.77606589	0.85710931
Si	0.78183137	0.74109767	0.21945462
Si	0.78135561	0.76299949	0.47835743
Si	0.93007590	0.49851401	0.82795755
Si	0.93639617	0.50168415	0.08779037
Si	0.62950994	0.48328927	0.28143463

Si	0.62634274	0.47055207	0.87527012
Si	0.71205931	0.47725534	0.13736857
Si	0.71795195	0.52293279	0.77394156
Si	0.71950528	0.50916775	0.51174694
Si	0.43758972	0.74874502	0.09229169
Si	0.13356531	0.75388645	0.28767481
Si	0.12627743	0.75301370	0.87623457
Si	0.21351606	0.75771256	0.13152048
Si	0.21739335	0.75229795	0.77450390
Si	0.22599026	0.75794411	0.51959460
B	0.30959449	0.57307107	0.48411926

HB(4)-MTW

a = 25.4057 Å

b = 10.2454 Å

c = 12.2566 Å

α = 90.8822º

β = 108.881º

γ = 89.9739º

H	0.24418184	0.56364150	0.06355394
O	0.08336650	0.35693724	0.21355921
O	0.10152386	0.12300680	0.91151040
O	0.26013215	0.33687115	0.83432342
O	0.60209873	0.17149484	0.26490584
O	0.60093064	0.36045797	0.86833666
O	0.76111093	0.10666533	0.84390374
O	0.91996020	0.34670856	0.76367630
O	0.89804291	0.10828026	0.12708032
O	0.73592324	0.34708292	0.14556802
O	0.42525381	0.10161659	0.77661424
O	0.41634018	0.41174491	0.12318160
O	0.24063133	0.09119510	0.16672086
O	0.88860913	0.09738997	0.74651176
O	0.92070021	0.35986673	0.13869644

O	0.76129822	0.09697558	0.18172367
O	0.39691907	0.35014171	0.73794531
O	0.40230498	0.15899133	0.13177966
O	0.28077316	0.33219027	0.18930072
O	0.10987288	0.10663672	0.22019165
O	0.08993733	0.37463894	0.89280088
O	0.23531941	0.08534596	0.82711881
O	0.58430924	0.42415606	0.22926402
O	0.57834631	0.10984543	0.87673427
O	0.73362080	0.35800254	0.83264295
O	0.00336593	0.04246668	0.15900244
O	0.06542174	0.95548520	0.03366799
O	0.34736506	0.03456233	0.57970770
O	0.32537313	0.02710321	0.77656528
O	0.34530785	0.00252858	0.21664215
O	0.32478220	0.99862120	0.99096180
O	0.29127511	0.96784158	0.36313931
O	0.50163632	0.25530997	0.14460613
O	0.58477505	0.26623691	0.05612043
O	0.83895632	0.25780326	0.57857954
O	0.82114015	0.28393715	0.77798468
O	0.84264344	0.27027899	0.22014752
O	0.82370420	0.27391528	0.99584410
O	0.78263863	0.26634531	0.35874726
O	0.99585612	0.04124631	0.83654626
O	0.92575560	0.00085719	0.95550478
O	0.65184169	0.99443736	0.41844259
O	0.67236418	0.00071054	0.22181574
O	0.65453196	0.03017737	0.78389839
O	0.67516175	0.01412899	0.00824055
O	0.71018297	0.00102457	0.63825075
O	0.50026968	0.28681224	0.86120679
O	0.41731775	0.25804285	0.94704578
O	0.15022359	0.25573102	0.41061279
O	0.18722755	0.28494707	0.23548220

O	0.15480293	0.25689651	0.79265122
O	0.18819963	0.27376696	0.01961303
O	0.20296261	0.22412340	0.63329710
O	0.24655094	0.37992660	0.51463627
O	0.73291692	0.33660146	0.50944618
O	0.75630626	0.08730247	0.48721803
O	0.24461406	0.12392006	0.47713930
O	0.07997843	0.86059977	0.23858034
O	0.09582586	0.62700546	0.86412976
O	0.26493181	0.83715474	0.82660802
O	0.60338681	0.67719026	0.26074343
O	0.59857514	0.85879661	0.86392272
O	0.76323372	0.60635213	0.86037994
O	0.92060495	0.85065970	0.77364548
O	0.89822645	0.61110935	0.11814322
O	0.73892177	0.84447398	0.15286021
O	0.42063993	0.60347668	0.77225981
O	0.42154782	0.90816821	0.12805750
O	0.22279645	0.59114374	0.11444974
O	0.89618704	0.59861240	0.74815995
O	0.92656705	0.86015533	0.13694672
O	0.76722729	0.59602784	0.16941103
O	0.39440503	0.85285637	0.73353707
O	0.39446484	0.66016099	0.12531414
O	0.26131543	0.83685345	0.16424339
O	0.10225105	0.60707510	0.27339142
O	0.07747550	0.88080628	0.83451820
O	0.23532076	0.59009243	0.83394753
O	0.57219853	0.92307702	0.22227423
O	0.57457165	0.60943823	0.87488621
O	0.73524845	0.85597429	0.82823454
O	0.00106255	0.52749510	0.15196309
O	0.08043096	0.53773296	0.05481544
O	0.33823040	0.52038383	0.58998364
O	0.32988846	0.51324729	0.80307185

O	0.34847984	0.50257580	0.23737791
O	0.31336540	0.49538104	0.00849711
O	0.29950938	0.45247208	0.36809860
O	0.49840594	0.73030572	0.13968887
O	0.58021497	0.77152570	0.05097304
O	0.84481313	0.76068394	0.58062319
O	0.82090363	0.76841803	0.77288466
O	0.84662928	0.77648525	0.21668027
O	0.82796110	0.78832674	0.99272620
O	0.79029457	0.74575479	0.35952776
O	0.99981616	0.52042444	0.85190841
O	0.92166854	0.48392204	0.95044389
O	0.65615172	0.51818253	0.42697877
O	0.68348806	0.52079177	0.23790161
O	0.65537053	0.53820003	0.79171528
O	0.67088829	0.52564612	0.01531538
O	0.71240753	0.51475135	0.64875678
O	0.49678854	0.78767420	0.85429703
O	0.41467451	0.75977865	0.94398163
O	0.16174255	0.78566391	0.41915423
O	0.17122108	0.76050286	0.20914807
O	0.15707265	0.76892626	0.77030256
O	0.16947554	0.79824829	0.99302689
O	0.21451788	0.70255156	0.63176474
O	0.26241465	0.87413917	0.53694133
O	0.73746325	0.83369426	0.49900142
O	0.76440791	0.58346310	0.50242421
O	0.24668485	0.62781856	0.45356538
Si	0.43524338	0.24898890	0.83095106
Si	0.06481857	0.99235119	0.16306833
Si	0.06018861	0.00135701	0.90374076
Si	0.37329091	0.00315998	0.71669090
Si	0.37316002	0.01630618	0.11546416
Si	0.28792184	0.98604726	0.85592990
Si	0.28415080	0.97574730	0.22739057

Si	0.28594624	0.00072132	0.48807910
Si	0.56783706	0.27918875	0.17337286
Si	0.56608566	0.25565269	0.91566576
Si	0.86755605	0.24634382	0.71725674
Si	0.87133739	0.25295123	0.11986949
Si	0.78500054	0.25501149	0.86295008
Si	0.78050187	0.24498801	0.22664336
Si	0.77752317	0.23659805	0.48375059
Si	0.93304808	0.99758300	0.82862549
Si	0.93844684	0.00359180	0.09439929
Si	0.62439307	0.02200863	0.28136337
Si	0.62667705	0.00328146	0.88375848
Si	0.71164291	0.98899562	0.14106006
Si	0.71546793	0.99863146	0.77287134
Si	0.71424247	0.97925276	0.51065467
Si	0.43493706	0.27052292	0.08695899
Si	0.13193060	0.25127324	0.26997266
Si	0.13367180	0.25713570	0.90484946
Si	0.22395256	0.24505109	0.15321602
Si	0.21353880	0.22662317	0.77091937
Si	0.21143242	0.24625944	0.50949010
Si	0.43179366	0.75057043	0.82666483
Si	0.06676561	0.50617487	0.17303141
Si	0.06646675	0.51514212	0.91628644
Si	0.37087475	0.49624384	0.72521396
Si	0.36817773	0.51559193	0.12371569
Si	0.28518932	0.48265967	0.86849201
Si	0.28258662	0.49356001	0.47971296
Si	0.56295845	0.77513064	0.16806647
Si	0.56247097	0.75692881	0.91099718
Si	0.87110598	0.74431121	0.71964878
Si	0.87502952	0.75840928	0.11596548
Si	0.78698145	0.75429911	0.86394278
Si	0.78560669	0.74141626	0.22517540
Si	0.78399604	0.73119294	0.48535858

Si	0.93477244	0.48815805	0.82909231
Si	0.93564158	0.49623707	0.08954623
Si	0.63160597	0.53409969	0.28779334
Si	0.62547765	0.50838186	0.88768103
Si	0.71420828	0.49687019	0.14162796
Si	0.71640148	0.50403647	0.78245896
Si	0.71671709	0.48866119	0.52174445
Si	0.43247777	0.76336576	0.08449752
Si	0.12893420	0.75295933	0.28386377
Si	0.12489093	0.76805881	0.86583560
Si	0.20591570	0.74488381	0.11966454
Si	0.21800153	0.72709330	0.76496995
Si	0.22169790	0.74712964	0.51090135
B	0.30843826	0.43050501	0.26488812

HB(5)-MTW

a = 25.4957 Å

b = 10.2729 Å

c = 12.2329 Å

α = 89.022º

β = 108.821º

γ = 89.8669º

H	0.47145470	0.56459793	0.19264712
O	0.08032617	0.33960252	0.22342464
O	0.07963837	0.16190240	0.87557169
O	0.23823606	0.40248685	0.83389868
O	0.57897246	0.11836241	0.24228273
O	0.57328645	0.40555999	0.87355766
O	0.74303966	0.13697963	0.84265855
O	0.91473080	0.33811131	0.77665721
O	0.90310799	0.08629028	0.13971839
O	0.75812206	0.41676033	0.18390844
O	0.39596432	0.16002782	0.73577064
O	0.39361302	0.33624228	0.13401751

O	0.26422794	0.17052416	0.16975846
O	0.89493821	0.09144655	0.72857006
O	0.93014330	0.33452116	0.12532384
O	0.74680508	0.16506430	0.13064268
O	0.42165978	0.40867624	0.77720926
O	0.42249491	0.09052343	0.12593164
O	0.23206740	0.41787753	0.16662627
O	0.09385286	0.08686403	0.26134245
O	0.09966425	0.41046404	0.85505676
O	0.26268682	0.15362020	0.83574459
O	0.59172970	0.37296738	0.26031090
O	0.59925496	0.15575125	0.87822070
O	0.75672746	0.39159913	0.85614027
O	0.99747932	0.98650456	0.13576137
O	0.08140086	0.00106110	0.05130536
O	0.34505099	-0.00434278	0.5752756
O	0.32656157	0.98263650	0.77614157
O	0.34700485	0.00254659	0.21982126
O	0.32700974	0.99552910	0.99388893
O	0.28506510	0.01574310	0.35635887
O	0.49499249	0.27916593	0.14021141
O	0.58053976	0.26027377	0.05982733
O	0.84376967	0.27205836	0.57101286
O	0.81466642	0.24506691	0.75605155
O	0.84708196	0.27291561	0.20346138
O	0.83630454	0.24124551	0.98248439
O	0.79252300	0.23352896	0.34937587
O	0.99654118	0.00712066	0.85523091
O	0.91262961	0.00362086	0.94101668
O	0.65790468	0.02327545	0.42562561
O	0.67890870	0.05998093	0.22935091
O	0.65475037	0.98985307	0.79018038
O	0.67282899	-0.00949895	0.0164562
O	0.71347664	0.99823176	0.64776044
O	0.49728374	0.22578179	0.86506235

O	0.41176281	0.24875207	0.94454865
O	0.15437624	0.24750930	0.41806433
O	0.17368911	0.22499232	0.21963681
O	0.15670005	0.23347714	0.78185761
O	0.17545477	0.25813057	0.00531219
O	0.21266438	0.27635130	0.63588490
O	0.25694801	0.34227163	0.47306785
O	0.73757538	0.35006908	0.47054909
O	0.76372171	0.09900389	0.50734229
O	0.24200374	0.09344128	0.51560059
O	0.08352251	0.83460923	0.22321248
O	0.07752912	0.65944645	0.87447412
O	0.23977328	0.90327623	0.83222961
O	0.57785900	0.62725707	0.24076377
O	0.57725618	0.90434620	0.87413219
O	0.73207196	0.63880229	0.80493382
O	0.91709678	0.84105076	0.77496032
O	0.90342789	0.58175494	0.14063828
O	0.75853849	0.91486036	0.19325812
O	0.39663894	0.65980118	0.73833422
O	0.40324031	0.83793567	0.13758412
O	0.26365637	0.66320203	0.16352102
O	0.90020866	0.59107157	0.73559916
O	0.91024884	0.83361410	0.10465792
O	0.73442843	0.66785810	0.13863696
O	0.42397155	0.90881577	0.76565470
O	0.44286588	0.59740453	0.12242373
O	0.24224461	0.91773569	0.14743454
O	0.10880989	0.58607618	0.25770534
O	0.09527519	0.90970403	0.86123380
O	0.26157111	0.65233850	0.85904015
O	0.61043214	0.87195771	0.24661116
O	0.59969550	0.65320522	0.86017605
O	0.75662125	0.88403571	0.85422051
O	0.00451884	0.52186260	0.14090638

O	0.08513413	0.49008431	0.04799698
O	0.34358909	0.48802011	0.58416711
O	0.32478677	0.49508660	0.78426293
O	0.33902705	0.47259038	0.20540629
O	0.32641338	0.47925624	0.00255901
O	0.29273896	0.52826153	0.36197366
O	0.50561933	0.81069329	0.13299247
O	0.58648672	0.74115578	0.05106418
O	0.84405844	0.76349190	0.57677136
O	0.82081381	0.73892888	0.77051249
O	0.83959036	0.74601429	0.20736378
O	0.81979121	0.70109319	0.98505307
O	0.78525622	0.73078376	0.35706951
O	0.99949636	0.48929307	0.85360676
O	0.91882855	0.50000675	0.94822613
O	0.65598371	0.52431228	0.42160807
O	0.66901647	0.51966792	0.21654397
O	0.65042806	0.47135177	0.77919389
O	0.67223964	0.48835875	0.00417940
O	0.70868339	0.45965434	0.63780062
O	0.49986713	0.72717107	0.85715285
O	0.41820445	0.76324960	0.94510254
O	0.15557646	0.75054175	0.42506770
O	0.18534042	0.75553993	0.23900959
O	0.15642906	0.74000596	0.79156229
O	0.17006127	0.75747514	0.01449920
O	0.21317195	0.75358210	0.64714938
O	0.25876261	0.84210825	0.49324047
O	0.73892430	0.84931698	0.49540850
O	0.76124154	0.59739639	0.52121883
O	0.24153724	0.58968520	0.51254342
Si	0.43184741	0.26139995	0.83097301
Si	0.06394591	0.97802235	0.16737448
Si	0.06310003	0.01884141	0.91092545
Si	0.37297910	0.01218355	0.71374941

Si	0.37487638	0.98213255	0.11886997
Si	0.28945491	0.00860749	0.85964967
Si	0.28451210	0.02585160	0.22409200
Si	0.28234884	0.98705634	0.48448247
Si	0.56127853	0.25744142	0.17480232
Si	0.56235042	0.26160830	0.91891117
Si	0.86743271	0.23664141	0.70885902
Si	0.87904569	0.23432078	0.11317209
Si	0.78792368	0.25276392	0.85974910
Si	0.78568533	0.27271248	0.21675369
Si	0.78410431	0.23968291	0.47445940
Si	0.93063596	0.98666706	0.82523876
Si	0.93092999	0.97682379	0.08056454
Si	0.63135901	0.01829941	0.28565405
Si	0.62618651	0.01075297	0.88993728
Si	0.71406532	0.03188081	0.14191605
Si	0.71709858	0.00187685	0.78211517
Si	0.71881140	0.99292527	0.51985380
Si	0.43032018	0.23905175	0.08520790
Si	0.12558013	0.22560909	0.28031567
Si	0.12795591	0.26601609	0.87965471
Si	0.21105551	0.26896056	0.14042111
Si	0.21757775	0.26498769	0.77093028
Si	0.21681106	0.24002576	0.51087131
Si	0.43477518	0.76464037	0.82669123
Si	0.06950844	0.48532898	0.16725798
Si	0.06546430	0.51178058	0.90790067
Si	0.37157310	0.51329116	0.72150022
Si	0.28841932	0.50712378	0.87087556
Si	0.28180526	0.52051894	0.22416096
Si	0.28359772	0.48736352	0.48279414
Si	0.57001911	0.76442092	0.16751945
Si	0.56554646	0.75708361	0.91024481
Si	0.87071956	0.73366958	0.71516401
Si	0.86806326	0.71699426	0.10897874

Si	0.78278723	0.73998720	0.85406629
Si	0.77930441	0.76520367	0.22397104
Si	0.78220255	0.73671702	0.48675208
Si	0.93351507	0.48077002	0.82896962
Si	0.93946736	0.48407554	0.08907611
Si	0.62396449	0.51053191	0.28408085
Si	0.62375686	0.50490645	0.87975928
Si	0.70828827	0.52288633	0.13544706
Si	0.71208234	0.49088960	0.76897221
Si	0.71627019	0.48336271	0.51294663
Si	0.44280603	0.75142457	0.08570511
Si	0.13303351	0.73222666	0.28558274
Si	0.12525428	0.76743482	0.88576836
Si	0.21530043	0.77374006	0.14081543
Si	0.21805186	0.76086563	0.78182740
Si	0.21752380	0.73483983	0.51983795
B	0.35342260	0.43146369	0.11195728

HB(6)-MTW

a = 25.5553 Å

b = 10.3285 Å

c = 12.3025 Å

α = 89.313º

β = 108.932º

γ = 90.3573º

H	0.39242882	0.29652535	0.19519660
O	0.10289611	0.40961604	0.25851969
O	0.09836025	0.10929158	0.87952708
O	0.25873577	0.35855353	0.84253561
O	0.59327600	0.11695273	0.22118349
O	0.59407517	0.36100029	0.84946769
O	0.76349136	0.10496282	0.85136799
O	0.92188441	0.35142224	0.77030315
O	0.89519600	0.09951768	0.10891791

O	0.76148038	0.40797143	0.17719286
O	0.41466445	0.11764724	0.74004493
O	0.38994271	0.34982408	0.12703769
O	0.24392135	0.11537665	0.14244590
O	0.89449154	0.10210579	0.75292346
O	0.92367106	0.34586103	0.12855261
O	0.74515091	0.15590458	0.15206817
O	0.39327862	0.35912050	0.78392934
O	0.42913506	0.09279924	0.13456826
O	0.26096351	0.36762717	0.16945010
O	0.08426388	0.15931900	0.22518231
O	0.07766622	0.36016465	0.85840293
O	0.24269208	0.10539538	0.83894424
O	0.58516405	0.36648247	0.24691805
O	0.57775341	0.11021652	0.87180634
O	0.73428081	0.35334286	0.82267204
O	0.99713987	0.01354127	0.14534234
O	0.07908087	0.99442298	0.05660059
O	0.34267314	0.99516706	0.56740414
O	0.32221604	0.01986572	0.76444138
O	0.34769746	0.02734084	0.21039171
O	0.33305837	0.00735760	0.98742982
O	0.28649367	0.00478010	0.34802054
O	0.49841176	0.23820040	0.11978451
O	0.58364533	0.27326835	0.04383576
O	0.84530359	0.26560569	0.58229551
O	0.82306399	0.27694287	0.77693698
O	0.84788270	0.25436886	0.21780167
O	0.82340750	0.28000457	0.99298321
O	0.79077899	0.25155567	0.36122592
O	0.99697566	0.02662661	0.85846751
O	0.91771158	0.96563846	0.94781271
O	0.65742567	0.02332526	0.42408706
O	0.68736017	0.99392687	0.24152874
O	0.65851915	0.02632460	0.79646369

O	0.66841967	0.00659055	0.01722327
O	0.71052063	0.00730038	0.64608033
O	0.49643248	0.27504128	0.85213572
O	0.42338260	0.18219801	0.95054066
O	0.15575195	0.24409587	0.42195316
O	0.18174631	0.25692415	0.23176231
O	0.15640769	0.26167195	0.78683954
O	0.17132789	0.27824015	0.00975088
O	0.21254584	0.23819317	0.64282768
O	0.23871063	0.41018158	0.50825324
O	0.74005587	0.34569652	0.50025080
O	0.76379593	0.09564108	0.50789034
O	0.26004304	0.16143090	0.49128864
O	0.09333566	0.90637718	0.26710497
O	0.09982104	0.61105829	0.86530055
O	0.26231064	0.85331637	0.84261487
O	0.58479298	0.61791986	0.23493086
O	0.59581879	0.86043185	0.86325371
O	0.76112650	0.60183592	0.84326381
O	0.91921934	0.85318072	0.75678510
O	0.90534751	0.59707554	0.12990470
O	0.76171239	0.90288371	0.15618287
O	0.41674742	0.60760773	0.76723864
O	0.40090311	0.84506037	0.13549149
O	0.23725576	0.61588906	0.16951591
O	0.89622979	0.60102907	0.74037327
O	0.91767325	0.85079272	0.14341252
O	0.73511177	0.65602733	0.15391145
O	0.40140614	0.86162586	0.74668728
O	0.42194794	0.59557905	0.12710286
O	0.26416104	0.86350579	0.15740792
O	0.09172854	0.66003376	0.21181929
O	0.07628580	0.85858485	0.87225782
O	0.23176910	0.60767718	0.83084674
O	0.59852317	0.86782730	0.25918988

O	0.58202129	0.60885958	0.88144947
O	0.74002765	0.85496912	0.83402608
O	0.00458858	0.50961576	0.14320554
O	0.08324253	0.49316362	0.04497445
O	0.34428374	0.48942602	0.58874851
O	0.31744061	0.53697695	0.77329624
O	0.34252524	0.53634209	0.21645178
O	0.32252393	0.52308313	0.99187323
O	0.29061634	0.49723918	0.36692403
O	0.50048340	0.77172175	0.13841808
O	0.58506822	0.76414270	0.05579340
O	0.84073083	0.76002571	0.57397123
O	0.82388256	0.76917267	0.77446107
O	0.84167205	0.72975823	0.21547695
O	0.82778410	0.75514984	0.99317894
O	0.78399836	0.77194550	0.35394104
O	0.99932829	0.53007818	0.85092594
O	0.92056486	0.49487610	0.94724278
O	0.65351212	0.50093018	0.41783741
O	0.67210458	0.48683659	0.21938346
O	0.65529006	0.53032657	0.78276582
O	0.67464744	0.48844723	0.00508314
O	0.71072620	0.50735013	0.63672185
O	0.49911481	0.76753032	0.86395741
O	0.41511767	0.74861787	0.94729344
O	0.15738210	0.73860413	0.41674257
O	0.18085631	0.80334958	0.22916257
O	0.15505227	0.78760383	0.78693505
O	0.17192278	0.76822697	0.01034698
O	0.20878171	0.75309216	0.63877829
O	0.23828157	0.91008731	0.49535360
O	0.73661628	0.84680297	0.50554251
O	0.75633129	0.59800347	0.48565209
O	0.26263859	0.65997116	0.50419971
Si	0.43260385	0.23482811	0.83220401

Si	0.06336798	0.01772364	0.17330690
Si	0.06257835	0.99774317	0.91676086
Si	0.37048587	0.99858240	0.70632216
Si	0.37741222	0.99257026	0.11509642
Si	0.29047831	0.99625770	0.85835529
Si	0.28536241	0.00332951	0.21599421
Si	0.28129853	0.01722120	0.47492049
Si	0.56484945	0.24865336	0.15764609
Si	0.56287519	0.25432218	0.90438224
Si	0.87152740	0.24836841	0.72116815
Si	0.87265411	0.24479481	0.11185722
Si	0.78610915	0.25319315	0.86093251
Si	0.78606732	0.26699592	0.22761927
Si	0.78461623	0.24029002	0.48738187
Si	0.93232331	0.98710115	0.82928909
Si	0.93202498	0.98289384	0.08607509
Si	0.63385169	0.00113634	0.28573755
Si	0.62542133	0.00155556	0.88741198
Si	0.71552138	0.01509061	0.14142894
Si	0.71833922	0.99785603	0.78161071
Si	0.71739655	0.99347310	0.52090575
Si	0.13088104	0.26701114	0.28347394
Si	0.12608652	0.25155089	0.88408725
Si	0.21405849	0.25447399	0.13793374
Si	0.21788978	0.24203410	0.77731170
Si	0.21708742	0.26294321	0.51652343
Si	0.43314822	0.74592323	0.83157827
Si	0.07034757	0.51739416	0.16438907
Si	0.06492428	0.49902622	0.90492413
Si	0.36860398	0.49776371	0.72858863
Si	0.36934812	0.50050847	0.11649577
Si	0.28276848	0.50516474	0.86060439
Si	0.28247984	0.50555442	0.23118443
Si	0.28378395	0.51419957	0.49210429
Si	0.56684422	0.75578970	0.17131839

Si	0.56543759	0.74988711	0.91611496
Si	0.87027225	0.74548059	0.71214478
Si	0.87296150	0.73306275	0.11960106
Si	0.78831961	0.74556371	0.86104480
Si	0.78049353	0.76387628	0.22066052
Si	0.77920571	0.74441781	0.47978960
Si	0.93474051	0.49436555	0.82732416
Si	0.93868255	0.48719223	0.08697837
Si	0.62422079	0.49373826	0.27942895
Si	0.62665197	0.49825045	0.88057641
Si	0.71048532	0.50961622	0.13859371
Si	0.71546044	0.49807078	0.77061400
Si	0.71554650	0.48815110	0.51033657
Si	0.43488253	0.73985557	0.08748216
Si	0.13059043	0.77628046	0.28108900
Si	0.12585145	0.75602983	0.88400115
Si	0.21330869	0.76188201	0.14099395
Si	0.21473233	0.75127424	0.77377587
Si	0.21728211	0.76502961	0.51452936
B	0.44952926	0.17419257	0.06787952

HB(7)-MTW

a = 25.6237 Å

b = 10.2525 Å

c = 12.1779 Å

α = 89.6242º

β = 109.039º

γ = 90.5725º

H	0.31068563	0.21208700	0.19359342
O	0.07644743	0.35516514	0.23143695
O	0.07782602	0.14836061	0.87236958
O	0.24037190	0.40175852	0.80933209
O	0.60197945	0.13682271	0.26778212
O	0.60116017	0.35186436	0.88493759

O	0.75856876	0.10278358	0.86333806
O	0.89586526	0.39895832	0.72707640
O	0.89993196	0.10498134	0.11590236
O	0.74457596	0.35462492	0.13773549
O	0.42191204	0.09078439	0.77946708
O	0.41959555	0.38216229	0.14049988
O	0.27871539	0.15408907	0.18467168
O	0.92256440	0.15034705	0.77183528
O	0.92289318	0.35723854	0.13755048
O	0.75768602	0.10407679	0.19327754
O	0.39345059	0.33946145	0.74188700
O	0.39815859	0.13138678	0.13313431
O	0.22868684	0.41824046	0.12489419
O	0.10878760	0.10952823	0.24176016
O	0.09726776	0.40141747	0.86075326
O	0.26473564	0.15179891	0.86025892
O	0.57988414	0.38803120	0.23247935
O	0.57471166	0.10226756	0.86550306
O	0.74127082	0.35356181	0.81261492
O	0.00370747	0.03382443	0.15262303
O	0.07597554	0.98214656	0.04291711
O	0.34650376	0.01590337	0.58009055
O	0.32358586	0.99841284	0.77462871
O	0.34905681	0.95246047	0.22059883
O	0.32628787	0.96633637	0.99232480
O	0.28936366	0.98240328	0.36015113
O	0.49968571	0.21380485	0.15837510
O	0.57686258	0.23269807	0.05554397
O	0.84295440	0.21715474	0.57613364
O	0.82564306	0.23306959	0.77704214
O	0.84589677	0.25382381	0.21737769
O	0.82658392	0.27905886	0.99199449
O	0.78852688	0.28587002	0.35867490
O	0.99954757	0.96923741	0.83462289
O	0.92660743	0.99005288	0.94768283

O	0.65507938	0.96551859	0.42629969
O	0.67409128	0.97276508	0.22635324
O	0.65423937	0.01730504	0.78644422
O	0.67191979	0.03307566	0.01247461
O	0.71159387	0.03174618	0.64352014
O	0.49758840	0.27715348	0.85478630
O	0.41997990	0.24218737	0.95496664
O	0.15458384	0.26193006	0.42098521
O	0.17815438	0.30572891	0.23017369
O	0.16173227	0.23153548	0.80789802
O	0.16245459	0.25464929	0.03029574
O	0.20899288	0.22313336	0.64311709
O	0.24490926	0.40228699	0.52468075
O	0.75902711	0.37779818	0.53288220
O	0.74003000	0.12889091	0.46888805
O	0.25460099	0.15328794	0.48386773
O	0.08213969	0.85975758	0.23923182
O	0.07585707	0.65192222	0.86996754
O	0.23662210	0.90085290	0.81973869
O	0.60464050	0.63821992	0.26702600
O	0.60228696	0.85359520	0.88288111
O	0.75865583	0.60408464	0.86585645
O	0.89501097	0.90112045	0.73227573
O	0.89710941	0.60672988	0.11503887
O	0.74130006	0.85506697	0.13462691
O	0.42360897	0.58958705	0.76125742
O	0.42477501	0.88313419	0.12237520
O	0.26181468	0.66101565	0.18323285
O	0.91840924	0.65029929	0.77312933
O	0.92518487	0.85583132	0.13438970
O	0.75981490	0.60555728	0.18949982
O	0.39716547	0.83958287	0.73826698
O	0.39761555	0.63493634	0.12921937
O	0.23973861	0.91378055	0.14176770
O	0.10113842	0.60594598	0.25532193

O	0.10292377	0.90024349	0.86410290
O	0.26302894	0.65131711	0.86518734
O	0.57699447	0.88604080	0.23106610
O	0.57775616	0.60240299	0.86529706
O	0.73736118	0.85321364	0.81427702
O	0.99910756	0.53235255	0.13597302
O	0.08086361	0.49502168	0.04931962
O	0.34559373	0.50229490	0.56867515
O	0.32395457	0.52203843	0.76480669
O	0.33542138	0.47052879	0.20223757
O	0.33006924	0.46618486	0.98131082
O	0.28086065	0.47700751	0.35001042
O	0.50077604	0.70215074	0.15049147
O	0.57967337	0.73455532	0.05481611
O	0.84384676	0.72538903	0.57368215
O	0.82022185	0.73839003	0.76766229
O	0.84471536	0.76620776	0.21134168
O	0.82790440	0.78566636	0.98605875
O	0.78809240	0.78721362	0.35526731
O	0.99715395	0.47595811	0.85054363
O	0.91573940	0.48404927	0.94121052
O	0.65722705	0.46703000	0.42770176
O	0.67761290	0.47409381	0.22924240
O	0.65578594	0.50817628	0.78733296
O	0.67350245	0.52730427	0.01309918
O	0.71312864	0.53493195	0.64498339
O	0.49973339	0.77258708	0.85285450
O	0.42073436	0.72435347	0.94565331
O	0.15624932	0.75889699	0.42870328
O	0.17851825	0.76921667	0.23324202
O	0.15721885	0.72359009	0.78882847
O	0.17176432	0.73560921	0.01353277
O	0.21605457	0.72545580	0.64749500
O	0.24721262	0.90212421	0.52216631
O	0.75735402	0.87855578	0.52790815

O	0.74256825	0.62758216	0.46948665
O	0.25654034	0.65224350	0.48270267
Si	0.43342898	0.23743416	0.83297953
Si	0.06745693	0.99702704	0.16877382
Si	0.06415352	0.00083960	0.90405993
Si	0.37265309	0.98646335	0.71861698
Si	0.37479402	0.98210264	0.11673665
Si	0.28775681	0.00438943	0.86207734
Si	0.28951872	0.00194772	0.22819781
Si	0.28411173	0.01355671	0.48605067
Si	0.56439930	0.24298590	0.17794796
Si	0.56238029	0.24146704	0.91511584
Si	0.87199389	0.25008701	0.71352906
Si	0.87396070	0.24823912	0.11551096
Si	0.78825634	0.24332825	0.86114485
Si	0.78400305	0.24877621	0.22666895
Si	0.78236238	0.25173806	0.48378365
Si	0.93617347	0.00266359	0.82226492
Si	0.93915911	0.99667500	0.08753786
Si	0.62682401	0.99031444	0.28720992
Si	0.62577930	0.00130572	0.88717008
Si	0.71109205	0.99229027	0.14167332
Si	0.71565632	0.00048444	0.77664137
Si	0.71622504	0.00077166	0.51701130
Si	0.43465856	0.24280331	0.09567844
Si	0.12912194	0.25740394	0.27984003
Si	0.12596374	0.25910311	0.89324917
Si	0.21889246	0.25243749	0.77966440
Si	0.21589162	0.25953066	0.51844608
Si	0.43541334	0.73144273	0.82477674
Si	0.06398752	0.49719912	0.16772802
Si	0.06255898	0.50630129	0.90769199
Si	0.37200755	0.48804712	0.70941351
Si	0.37055927	0.48958273	0.11324942
Si	0.28928454	0.50973871	0.85472707

Si	0.27605945	0.50813787	0.21645113
Si	0.28171911	0.50793577	0.48090262
Si	0.56527657	0.74040190	0.17544141
Si	0.56474468	0.74107846	0.91414526
Si	0.86975640	0.75399109	0.71254228
Si	0.87377819	0.75349586	0.11152896
Si	0.78624715	0.74636936	0.85877758
Si	0.78335553	0.75266644	0.22265780
Si	0.78265586	0.75416466	0.48112866
Si	0.93197358	0.50264397	0.82306984
Si	0.93391520	0.49552544	0.08246374
Si	0.62973441	0.49185120	0.28845861
Si	0.62714265	0.49693923	0.88801777
Si	0.71374946	0.49148402	0.14250897
Si	0.71750700	0.49947194	0.77770579
Si	0.71827470	0.50156846	0.51923660
Si	0.43615844	0.73616012	0.08630777
Si	0.12909396	0.74903462	0.28813358
Si	0.12700196	0.75307499	0.88445093
Si	0.21282015	0.76937493	0.14246571
Si	0.21833891	0.75129322	0.77982311
Si	0.21915633	0.75932042	0.51995156
B	0.19028884	0.32420778	0.12856421

HAl(1)-MTW

a = 25.4046 Å

b = 10.2497 Å

c = 12.4293 Å

α = 89.5376º

β = 108.657 º

γ = 90.2348º

H	0.46296108	0.07205029	0.74683518
O	0.07511730	0.35988653	0.21989621
O	0.10580994	0.10005237	0.88011319
O	0.25921477	0.36291050	0.81602779
O	0.57672370	0.09440641	0.23057193
O	0.61225317	0.35623433	0.89890721
O	0.76314815	0.09822269	0.84486814
O	0.92318560	0.34931389	0.76414548
O	0.89196396	0.10304909	0.11089143
O	0.73770049	0.34902596	0.14762896
O	0.42814650	0.09987658	0.75938908
O	0.39538019	0.33852063	0.13049958
O	0.26628956	0.17277496	0.20522208
O	0.89830786	0.09998164	0.73134376
O	0.92044612	0.35276923	0.11867006
O	0.76431499	0.09915504	0.19065235
O	0.38838040	0.35884174	0.73358567
O	0.42074012	0.08820240	0.12830431
O	0.24221918	0.42197431	0.15405116
O	0.09831506	0.10988441	0.26050752
O	0.08956201	0.35054842	0.90515372
O	0.24026463	0.11061515	0.81800147
O	0.60154723	0.34493212	0.26620993
O	0.58246400	0.10732232	0.88247624
O	0.73469649	0.34822745	0.80789297
O	0.99605870	0.03411893	0.14050377
O	0.07970350	0.00831173	0.05660711

O	0.34127413	0.02608496	0.58397398
O	0.33571194	0.03241720	0.79477660
O	0.34497560	0.99934322	0.21728760
O	0.31980473	0.01498702	0.99450203
O	0.29200705	0.98641450	0.36638289
O	0.49838593	0.27037517	0.15532157
O	0.57857216	0.24882539	0.05883507
O	0.84296573	0.27323924	0.57800538
O	0.82693096	0.26466463	0.77743027
O	0.84383617	0.27254587	0.20895411
O	0.82023040	0.27854474	0.98586198
O	0.79041091	0.27362049	0.35891238
O	0.00179575	0.03339457	0.85429461
O	0.91850440	0.00572691	0.93881915
O	0.65638353	0.01563370	0.41592156
O	0.67180032	0.00589683	0.21543143
O	0.65688748	0.02293172	0.78737566
O	0.68256215	0.02224081	0.01032942
O	0.70906348	0.02196402	0.63479769
O	0.50544303	0.28766971	0.85083462
O	0.41983518	0.24071445	0.95401493
O	0.15566883	0.28669636	0.40701913
O	0.16961944	0.26687116	0.20593858
O	0.15640272	0.27451358	0.78921324
O	0.18909892	0.24161171	0.01083353
O	0.19998847	0.24528711	0.62586079
O	0.25964320	0.36874559	0.51537625
O	0.73702320	0.35206419	0.49945371
O	0.76128736	0.10269075	0.49178441
O	0.23834390	0.11862557	0.48071671
O	0.07385038	0.85916505	0.22974884
O	0.10398920	0.60228262	0.87062435
O	0.26376594	0.85977605	0.82428501
O	0.57535660	0.59431418	0.22431116
O	0.60613828	0.85698805	0.88488861

O	0.76244337	0.59747085	0.83959354
O	0.92602555	0.85228619	0.77100400
O	0.89246483	0.60231128	0.10664669
O	0.74035897	0.84689705	0.15758896
O	0.42442265	0.60263062	0.76626700
O	0.39215754	0.83754033	0.11302044
O	0.26122418	0.67479149	0.19375029
O	0.90318955	0.60182829	0.73755312
O	0.91819850	0.85282191	0.11255193
O	0.76619044	0.59666256	0.19734880
O	0.39950563	0.85225388	0.73669268
O	0.42004169	0.58850769	0.11177609
O	0.23813097	0.92622790	0.15260733
O	0.09891644	0.60927193	0.26531345
O	0.07941070	0.85079912	0.88752258
O	0.23730587	0.61205890	0.83840369
O	0.60019715	0.84349879	0.26403358
O	0.58164771	0.60507270	0.88287123
O	0.73632320	0.84868911	0.80500898
O	0.99725630	0.53650956	0.13993909
O	0.08184436	0.52486402	0.05655497
O	0.33986152	0.54513243	0.58205203
O	0.32587135	0.54776021	0.78303167
O	0.34576274	0.51807993	0.21329669
O	0.32096864	0.49766273	0.99109350
O	0.29291133	0.50211710	0.36401187
O	0.49722076	0.77209316	0.14647209
O	0.57814357	0.75415066	0.05510530
O	0.84517201	0.77237721	0.58666644
O	0.83186581	0.76215517	0.78922084
O	0.84615191	0.76804430	0.21321297
O	0.81645448	0.77358653	0.98980621
O	0.79481597	0.76867175	0.36731764
O	0.00413060	0.51414639	0.85401205
O	0.92075894	0.49519196	0.93970489

O	0.65665656	0.52492185	0.41220430
O	0.67100904	0.50813640	0.21166479
O	0.65587023	0.52421381	0.78730079
O	0.68415720	0.53842717	0.00996997
O	0.70588833	0.51617503	0.63245471
O	0.50229875	0.78291923	0.85032645
O	0.42161852	0.74873898	0.94236480
O	0.15097445	0.78328219	0.42151147
O	0.17239719	0.77538883	0.22802097
O	0.15830259	0.78874480	0.79824085
O	0.17616306	0.75161505	0.01780921
O	0.20272604	0.73566393	0.63867356
O	0.25587545	0.86709870	0.52201016
O	0.73991526	0.85193060	0.50475485
O	0.76298294	0.60198158	0.50002297
O	0.23414251	0.61721713	0.47803130
Al	0.43603790	0.26414860	0.83183735
Si	0.06174170	0.00312935	0.17138438
Si	0.06644730	0.99822293	0.91955313
Si	0.37288503	0.99605875	0.71643542
Si	0.37001337	0.98599796	0.11276853
Si	0.28951617	0.00416710	0.85905702
Si	0.28512972	0.02181858	0.23499192
Si	0.28099294	0.00014681	0.48659935
Si	0.56336265	0.24026651	0.17630697
Si	0.56843141	0.25215234	0.92217335
Si	0.87270971	0.24657894	0.71291481
Si	0.86921755	0.25153057	0.10568816
Si	0.78638247	0.24720369	0.85419017
Si	0.78379359	0.24826941	0.22684267
Si	0.78270312	0.25067585	0.48183861
Si	0.93637934	0.99802634	0.82427755
Si	0.93133544	0.99883695	0.07587441
Si	0.62633118	0.98977166	0.28125308
Si	0.63198603	0.00324428	0.89206238

Si	0.71462386	0.99323147	0.14363044
Si	0.71647805	0.99781847	0.76777553
Si	0.71688743	0.99829483	0.51220493
Si	0.43353448	0.23473686	0.08923258
Si	0.12481427	0.25568408	0.27346924
Si	0.13492313	0.24296367	0.89683734
Si	0.21681482	0.27528040	0.14436417
Si	0.21422208	0.24966855	0.76231734
Si	0.21359629	0.25604991	0.50766097
Si	0.06310367	0.50769508	0.16999961
Si	0.06978907	0.49747410	0.92143950
Si	0.36964378	0.50860804	0.71604284
Si	0.37081101	0.48535994	0.11125571
Si	0.28641220	0.50421680	0.85728336
Si	0.28536179	0.52912639	0.23139323
Si	0.28173827	0.50886482	0.48475763
Si	0.56264099	0.74098000	0.17228369
Si	0.56728351	0.74934232	0.91888522
Si	0.87633835	0.74676538	0.72117476
Si	0.86853085	0.74907634	0.10534859
Si	0.78674803	0.74533634	0.85569041
Si	0.78666856	0.74513478	0.23428291
Si	0.78548963	0.74882984	0.48924163
Si	0.93804069	0.49054927	0.82451095
Si	0.93290228	0.49691380	0.07649359
Si	0.62608167	0.49250901	0.27870384
Si	0.63301750	0.50512341	0.89481996
Si	0.71467177	0.49768513	0.14170120
Si	0.71493133	0.49649851	0.76646382
Si	0.71581572	0.49927277	0.51114999
Si	0.43741497	0.74404886	0.82572903
Si	0.43293853	0.73627776	0.07901526
Si	0.12391088	0.75649341	0.28571006
Si	0.12939304	0.74912853	0.89356898
Si	0.21166820	0.78067580	0.14807756

Si	0.21571427	0.75008648	0.77441156
Si	0.21106482	0.75095181	0.51559740

HAl(2)-MTW

a =25.2874 Å

b = 10.2498 Å

c = 12.4169 Å

α = 91.0555º

β = 108.792º

γ = 89.5775º

H	0.36516939	0.38436314	0.86789908
O	0.07487444	0.35890651	0.23672006
O	0.07937000	0.14518438	0.88062381
O	0.23628834	0.39251083	0.80844323
O	0.59050283	0.15411687	0.26930518
O	0.60801274	0.34339863	0.89153837
O	0.75810389	0.10735626	0.84742865
O	0.90477484	0.39423914	0.73659144
O	0.89078022	0.11282265	0.09420390
O	0.73792049	0.34842526	0.15400445
O	0.42687033	0.08831829	0.79361796
O	0.41285532	0.41020904	0.11352190
O	0.24022774	0.08815393	0.19356618
O	0.92495590	0.14179756	0.76455488
O	0.91877802	0.36213966	0.11757660
O	0.76388104	0.10070809	0.20139088
O	0.40729644	0.33278617	0.71593926
O	0.38945123	0.15813722	0.09073261
O	0.26292644	0.33812649	0.17494636
O	0.09829775	0.10537698	0.24765944
O	0.11025930	0.39459548	0.89384393
O	0.26181997	0.14381950	0.84498903
O	0.57291469	0.40521789	0.22113157
O	0.58350819	0.09102459	0.88385430

O	0.73849165	0.35583752	0.79248186
O	0.99543013	0.03675899	0.12798557
O	0.07977691	0.98683403	0.04742602
O	0.34665001	0.03193508	0.59831402
O	0.33154103	0.98144725	0.79358173
O	0.34579319	0.01618380	0.21559959
O	0.31616775	0.96968807	0.99469586
O	0.30495792	0.97589563	0.38117693
O	0.49343677	0.23563390	0.12235582
O	0.58637068	0.23667958	0.06576605
O	0.84520536	0.22611114	0.58166321
O	0.83154965	0.24043566	0.78483124
O	0.84395115	0.27076107	0.20787260
O	0.81719256	0.29262569	0.98432894
O	0.79509934	0.28367183	0.36608072
O	0.00184676	0.96154643	0.84483105
O	0.91743624	0.98738364	0.93028030
O	0.65517611	0.98127823	0.41352251
O	0.66602570	0.01641110	0.20975355
O	0.65672944	0.00216885	0.78732420
O	0.68572022	0.02281243	0.01181688
O	0.70608815	0.03757580	0.63144456
O	0.50522288	0.26721690	0.87091949
O	0.41217569	0.28468845	0.92617210
O	0.15264143	0.26269818	0.41708582
O	0.17109297	0.27612547	0.21811395
O	0.15573590	0.22137907	0.79087496
O	0.18088332	0.21701062	0.01484380
O	0.20530050	0.21853772	0.63463018
O	0.24904662	0.38212227	0.52575926
O	0.75625093	0.37961761	0.52748469
O	0.74465198	0.12828381	0.47008259
O	0.24687213	0.12790199	0.47614447
O	0.07095732	0.85538714	0.22177911
O	0.08645626	0.64705496	0.89465455

O	0.23615313	0.89149387	0.80848449
O	0.59622412	0.65288646	0.27525329
O	0.61257673	0.84057225	0.89928250
O	0.75503743	0.60715201	0.84461713
O	0.89846506	0.89192419	0.72320795
O	0.89214579	0.61224919	0.10603991
O	0.73657934	0.84972123	0.16559900
O	0.43119852	0.59714261	0.78959370
O	0.41979337	0.91055637	0.12549531
O	0.23814030	0.58932116	0.18138807
O	0.92825223	0.64455198	0.76569423
O	0.91664811	0.86279264	0.11626502
O	0.76279655	0.60011568	0.19449917
O	0.40572226	0.84300487	0.73005303
O	0.39037860	0.66254409	0.10625517
O	0.26710329	0.83778987	0.18948747
O	0.10107794	0.60984741	0.26809423
O	0.10736594	0.89514292	0.87209488
O	0.26625207	0.64225103	0.81579959
O	0.57482679	0.90255131	0.22784677
O	0.57885550	0.59422258	0.88338238
O	0.74401599	0.85684907	0.78913997
O	0.99795181	0.53839119	0.14512166
O	0.08292234	0.49965969	0.06499397
O	0.33379380	0.54529554	0.59155280
O	0.34029517	0.45528546	0.81696889
O	0.34407920	0.51032151	0.22060204
O	0.31013871	0.49209011	0.99767302
O	0.29380516	0.46798268	0.37338946
O	0.49617934	0.72647674	0.13958136
O	0.58517300	0.73624513	0.06830792
O	0.83980183	0.70765451	0.58657147
O	0.83634024	0.72817782	0.79762391
O	0.84299441	0.77427332	0.21148543
O	0.81514161	0.78435187	0.98865294

O	0.79615822	0.76857698	0.37081237
O	0.00646095	0.47075731	0.85998082
O	0.92181223	0.50223518	0.94055811
O	0.65321187	0.46586570	0.41304589
O	0.66887257	0.50504753	0.21461273
O	0.65244209	0.50929543	0.78557264
O	0.68076777	0.52370799	0.00998777
O	0.70192264	0.53224849	0.63023727
O	0.50645177	0.78665709	0.87164863
O	0.41789743	0.77319868	0.94051361
O	0.15387433	0.80154506	0.40993640
O	0.16892757	0.77443925	0.20974024
O	0.16001481	0.71040014	0.79187030
O	0.18663389	0.74537603	0.01202206
O	0.19999057	0.73552526	0.62303497
O	0.25856885	0.87616074	0.52662464
O	0.75597768	0.87834433	0.52475704
O	0.73746492	0.62830899	0.46800965
O	0.23455631	0.62796850	0.45860919
Al	0.38043647	0.48935800	0.71462875
Si	0.06078719	0.99660926	0.16078651
Si	0.06686237	0.99687341	0.91066789
Si	0.37759413	0.98587063	0.72809613
Si	0.36817711	0.01290762	0.10674572
Si	0.28652760	0.99572184	0.85989070
Si	0.28916357	0.98057465	0.24429254
Si	0.28878883	0.00310722	0.49548067
Si	0.56081292	0.25765644	0.16988281
Si	0.57087809	0.23465114	0.92742278
Si	0.87636585	0.25084912	0.71698863
Si	0.86778025	0.25971964	0.10099965
Si	0.78640668	0.25004430	0.85223884
Si	0.78508824	0.25048498	0.23252380
Si	0.78510072	0.25443304	0.48591618
Si	0.93603098	0.99614193	0.81641542

Si	0.93007331	0.00022384	0.06730683
Si	0.62221651	0.01324367	0.28064549
Si	0.63447062	0.98843928	0.89578085
Si	0.71300000	0.99818817	0.14744640
Si	0.71637876	0.00102179	0.76356080
Si	0.71568951	0.00568299	0.51045982
Si	0.43870215	0.24263128	0.82118206
Si	0.42807306	0.27098852	0.06624785
Si	0.12421038	0.25035687	0.27983484
Si	0.13132985	0.24455992	0.89599072
Si	0.21364936	0.22975707	0.15053069
Si	0.21479898	0.24356084	0.76852939
Si	0.21385897	0.24848052	0.51319029
Si	0.06384245	0.50178500	0.17855888
Si	0.07133477	0.50302634	0.92839486
Si	0.36506437	0.51930543	0.11049156
Si	0.28574045	0.49755040	0.86012929
Si	0.28432151	0.47769885	0.23871180
Si	0.27898205	0.50634745	0.48845786
Si	0.56283957	0.75471701	0.17717090
Si	0.57038155	0.73986964	0.93010424
Si	0.87545129	0.74337868	0.71775101
Si	0.86694246	0.75833779	0.10518454
Si	0.78746482	0.74511537	0.85486644
Si	0.78437734	0.74775218	0.23541170
Si	0.78219226	0.74639255	0.48739188
Si	0.94041309	0.50312738	0.82656179
Si	0.93290192	0.50420851	0.07734636
Si	0.62324151	0.50744379	0.28116647
Si	0.62973652	0.49226546	0.89301197
Si	0.71243263	0.49549221	0.14347532
Si	0.71226836	0.50106190	0.76320542
Si	0.71251994	0.50062403	0.51051471
Si	0.44056967	0.74584975	0.83183136
Si	0.43152374	0.76773390	0.07739215

Si	0.12388526	0.75900121	0.27732957
Si	0.13486445	0.74985022	0.89351620
Si	0.21509148	0.73632495	0.14897240
Si	0.21555227	0.74590383	0.75944979
Si	0.21265575	0.76014621	0.50509524

HAl(3)-MTW

a = 25.314 Å

b = 10.2469 Å

c = 12.4749 Å

α = 89.9806º

β = 109.011º

γ = 89.9976º

H	0.37605753	0.45111047	0.53909366
O	0.10118586	0.39082589	0.26574214
O	0.07694565	0.14367082	0.87965432
O	0.23228101	0.39635367	0.80673331
O	0.60168707	0.14433115	0.26321744
O	0.57893533	0.39283334	0.88118636
O	0.73429091	0.15048967	0.81233412
O	0.89939610	0.39599269	0.73751431
O	0.91983773	0.14359726	0.11733002
O	0.76661566	0.40170357	0.18514135
O	0.39875760	0.14005185	0.73243394
O	0.41868265	0.39349040	0.10594110
O	0.26626993	0.15187317	0.18331384
O	0.92368431	0.14446910	0.77371088
O	0.89394094	0.39372276	0.11550377
O	0.73791098	0.15196643	0.16275269
O	0.42520702	0.38689864	0.77523539
O	0.39599449	0.14293297	0.12142243
O	0.23479437	0.40119974	0.15113288
O	0.07622706	0.14182183	0.22581191
O	0.10570055	0.39252821	0.88238498

O	0.26221489	0.15018143	0.84849422
O	0.57732947	0.39446017	0.22698758
O	0.60813951	0.14447662	0.88384168
O	0.76193978	0.40138901	0.84419892
O	0.99807796	0.96422882	0.14011867
O	0.08131659	0.99030736	0.05518751
O	0.33950802	0.96755198	0.58346424
O	0.32647656	0.98151761	0.78558705
O	0.34581506	0.97356694	0.21621453
O	0.32097845	0.97476788	0.99387978
O	0.29368955	0.99595138	0.36508007
O	0.49895957	0.21725948	0.14189777
O	0.58225927	0.24110011	0.05710106
O	0.84420847	0.22165202	0.58577805
O	0.82733991	0.23362082	0.78387683
O	0.84526995	0.22314173	0.21327850
O	0.81863959	0.22443155	0.99079716
O	0.79425694	0.24460499	0.36621600
O	-0.00011797	0.96178392	0.85745364
O	0.91644033	0.99153155	0.94198143
O	0.65701220	0.96974703	0.41459650
O	0.67143542	0.97810412	0.21307440
O	0.65628709	0.97172457	0.78681524
O	0.68446526	0.97765785	0.01003475
O	0.70791676	0.98859769	0.63424560
O	0.50286819	0.20789392	0.85648218
O	0.41883509	0.22836461	0.94116958
O	0.15511907	0.21318610	0.41734152
O	0.17444684	0.22862394	0.22204005
O	0.15413957	0.21801153	0.78907135
O	0.17759916	0.21910738	0.01136330
O	0.20585175	0.22037724	0.63740161
O	0.23182132	0.39817116	0.50575162
O	0.76272502	0.39436714	0.50842028
O	0.73798449	0.14365893	0.49276272

O	0.26441310	0.15481263	0.50429270
O	0.10134687	0.89142208	0.25993912
O	0.08128549	0.64341543	0.88785057
O	0.23441861	0.89857832	0.82251135
O	0.60184918	0.64447500	0.26540336
O	0.58301404	0.89514540	0.88695407
O	0.73333705	0.65109149	0.81584625
O	0.89610679	0.89544821	0.73596780
O	0.92005524	0.64356731	0.11851675
O	0.76691601	0.90106205	0.19087849
O	0.40204646	0.63814952	0.74278713
O	0.42101983	0.89229298	0.12228364
O	0.26659268	0.64916332	0.17969886
O	0.92457122	0.64610198	0.77227977
O	0.89432717	0.89365069	0.11891335
O	0.73723288	0.65238882	0.15469484
O	0.42136015	0.89065914	0.76765095
O	0.39401819	0.64170532	0.11551088
O	0.23858977	0.90116492	0.16115627
O	0.07676149	0.64121306	0.22693930
O	0.10382089	0.89386016	0.87837524
O	0.26011032	0.64838342	0.82439049
O	0.57547655	0.89392370	0.22933561
O	0.60521670	0.64308216	0.88407296
O	0.76369524	0.90089223	0.84041394
O	0.99838115	0.46385341	0.14270477
O	0.08245616	0.48567835	0.05942467
O	0.35009739	0.46935927	0.58170223
O	0.32330504	0.47373687	0.76591889
O	0.34213996	0.46483869	0.19940996
O	0.31989197	0.48017300	0.97602816
O	0.29431286	0.48664758	0.35841869
O	0.49858995	0.71292640	0.14240745
O	0.58284026	0.74285345	0.06037795
O	0.84357520	0.71814437	0.58412501

O	0.82663346	0.72455245	0.78235742
O	0.84492060	0.72181853	0.21333742
O	0.81937493	0.72603106	0.99070754
O	0.79201386	0.73235059	0.36389991
O	0.00225298	0.46658075	0.85894967
O	0.91854558	0.49509645	0.94254255
O	0.65595977	0.46918744	0.41771988
O	0.67497730	0.48200129	0.22171351
O	0.65458937	0.47261493	0.78860260
O	0.67927605	0.47326814	0.01169382
O	0.70653962	0.48913758	0.63750456
O	0.50264704	0.72208078	0.86035710
O	0.41839285	0.74555960	0.94369416
O	0.15695970	0.71892235	0.41333095
O	0.17350974	0.72638890	0.21477657
O	0.15398848	0.72183470	0.78615512
O	0.18177271	0.73242396	0.00793297
O	0.20146774	0.76299499	0.63052298
O	0.23076671	0.90954167	0.48466724
O	0.76342390	0.89337972	0.50337044
O	0.73642999	0.64442619	0.49641157
O	0.26574896	0.66384701	0.51732644
Al	0.27717091	0.50779598	0.47988146
Si	0.06412364	0.99701883	0.17019583
Si	0.06545770	0.99741512	0.91782843
Si	0.37063184	0.99479633	0.71689222
Si	0.37088094	0.99590237	0.11322154
Si	0.28583612	0.00159953	0.86195764
Si	0.28546752	0.00551469	0.23159948
Si	0.28132754	0.00634530	0.48388849
Si	0.56485681	0.24940419	0.17186449
Si	0.56805709	0.24638084	0.92003707
Si	0.87379042	0.24938477	0.72048589
Si	0.86973588	0.24634879	0.10902726
Si	0.78589885	0.25295423	0.85797625

Si	0.78595190	0.25499271	0.23240283
Si	0.78470509	0.25050962	0.48796709
Si	0.93441441	0.99846299	0.82781819
Si	0.93253836	0.99811458	0.07966374
Si	0.62662983	0.99681384	0.28010522
Si	0.63301596	0.99721109	0.89228916
Si	0.71515836	0.00277653	0.14443496
Si	0.71591193	0.00260783	0.76784857
Si	0.71687617	0.99849394	0.51191635
Si	0.43688768	0.23892686	0.82776567
Si	0.43313296	0.24561810	0.07806682
Si	0.12695282	0.24385368	0.28310135
Si	0.12855522	0.24352320	0.89111016
Si	0.21307976	0.25114338	0.14229930
Si	0.21349780	0.24615986	0.76904535
Si	0.21423451	0.24956335	0.51567340
Si	0.06459557	0.49536363	0.17365685
Si	0.06800984	0.49725071	0.92255230
Si	0.37634070	0.49336157	0.72425309
Si	0.36806925	0.49505027	0.09908419
Si	0.28314802	0.50036171	0.84417162
Si	0.28411265	0.50019741	0.22507395
Si	0.56434454	0.74863149	0.17396547
Si	0.56855485	0.75088520	0.92344211
Si	0.87284530	0.74653226	0.71893435
Si	0.86991668	0.74622026	0.11001823
Si	0.78611709	0.75117036	0.85760606
Si	0.78520655	0.75174909	0.23130713
Si	0.78385602	0.74661251	0.48663426
Si	0.93662125	0.50110915	0.82851836
Si	0.93312992	0.49886945	0.07987397
Si	0.62764953	0.49776460	0.28280520
Si	0.62956486	0.49562091	0.89184954
Si	0.71444153	0.50297431	0.14328854
Si	0.71447963	0.50342817	0.77100078

Si	0.71568505	0.49877742	0.51543758
Si	0.43657537	0.75065554	0.83022992
Si	0.43302931	0.74810801	0.08138735
Si	0.12738455	0.74499143	0.27893961
Si	0.13005844	0.74787064	0.89053923
Si	0.21506988	0.75252692	0.14165982
Si	0.21249144	0.75738201	0.76479180
Si	0.21500283	0.76111478	0.51201546

HAl(4)-MTW

a = 25.6012 Å

b = 10.2329 Å

c = 12.3117 Å

α = 90.3268º

β = 109.167º

γ = 90.3159º

H	0.27600246	0.39637532	0.07885679
O	0.09071578	0.42806083	0.25735855
O	0.08079503	0.14804821	0.89696636
O	0.25609386	0.30994045	0.82944611
O	0.60226494	0.14501025	0.26954742
O	0.60557514	0.34852346	0.88361312
O	0.75755454	0.09857683	0.83786240
O	0.90055830	0.39893718	0.72089188
O	0.89136117	0.10497747	0.11115768
O	0.73701107	0.35234777	0.14819162
O	0.42186036	0.10431851	0.76701618
O	0.42117505	0.38962241	0.12953619
O	0.25317182	0.14879098	0.21503404
O	0.92358147	0.14986598	0.76552484
O	0.91488084	0.35726384	0.11741476
O	0.75891209	0.10398238	0.20003926
O	0.40731468	0.35883218	0.74111042
O	0.40647261	0.13289146	0.12406287

O	0.25843809	0.39261783	0.14315582
O	0.09236153	0.17703619	0.20702027
O	0.10717001	0.39722237	0.89756172
O	0.23299626	0.05679391	0.81449504
O	0.58398735	0.39744116	0.22556586
O	0.58165756	0.09601012	0.87130221
O	0.73807551	0.35124775	0.79822166
O	0.99797784	0.04838354	0.16131665
O	0.07043727	0.98270246	0.05660774
O	0.33984604	0.02758227	0.57851702
O	0.32839102	0.00723424	0.78331655
O	0.34181090	0.01275814	0.21723056
O	0.32070258	0.99581749	0.99232580
O	0.28885186	0.95693113	0.36268690
O	0.50343739	0.22827919	0.13859876
O	0.58889987	0.23273451	0.06086904
O	0.84006338	0.21615553	0.58009184
O	0.83147715	0.24732848	0.78747480
O	0.84176318	0.26790761	0.21288550
O	0.81521792	0.27326948	0.98797347
O	0.78987593	0.28720223	0.36449537
O	0.00131884	0.97034978	0.84160799
O	0.92769837	0.01109062	0.94898914
O	0.65585746	0.95494878	0.40671723
O	0.66675339	0.98198630	0.20155253
O	0.65452734	0.99983393	0.77959212
O	0.68307980	0.03084831	0.00387562
O	0.70423241	0.02156516	0.62433242
O	0.50460805	0.26779669	0.86754898
O	0.41880327	0.25309993	0.94375401
O	0.15629430	0.27345388	0.41095983
O	0.17804498	0.32716913	0.21807855
O	0.15226410	0.22667859	0.79163493
O	0.18250513	0.22744040	0.01717063
O	0.19679794	0.20551732	0.62770822

O	0.25843409	0.35092909	0.53943025
O	0.75260026	0.36816908	0.53160875
O	0.73987768	0.12090432	0.46142538
O	0.23611775	0.10104447	0.47228325
O	0.09295308	0.93334273	0.27916101
O	0.08180883	0.64643936	0.86177522
O	0.27140765	0.81394537	0.83928492
O	0.59631860	0.65069440	0.26585398
O	0.60880796	0.84678270	0.89885215
O	0.75927975	0.60059330	0.86052391
O	0.89679109	0.89957796	0.74197699
O	0.89135929	0.60910805	0.09430517
O	0.74247868	0.85280440	0.14442858
O	0.41892043	0.60998638	0.79302857
O	0.40813711	0.87367946	0.13558697
O	0.25453187	0.65634403	0.21415571
O	0.92540767	0.64972784	0.76960071
O	0.92320015	0.85825261	0.11987818
O	0.76539424	0.60258705	0.18240148
O	0.39953922	0.85398701	0.72335020
O	0.39075352	0.62862398	0.05503573
O	0.24189958	0.90346961	0.13897435
O	0.07921657	0.68268460	0.23068023
O	0.10626063	0.89914405	0.89005650
O	0.24043870	0.56605996	0.83842229
O	0.57149060	0.89884152	0.21661103
O	0.57789281	0.59827028	0.86866077
O	0.73920692	0.84636627	0.79170015
O	0.99421162	0.52966968	0.13725137
O	0.07728701	0.53062692	0.05224651
O	0.33901227	0.52712250	0.60338521
O	0.33265713	0.48089911	0.81045830
O	0.35649923	0.52712928	0.22212223
O	0.31512513	0.44022823	0.00940718
O	0.29854019	0.45305012	0.38257377

O	0.49287794	0.71844663	0.15017083
O	0.57062465	0.72944949	0.04981142
O	0.84825372	0.72853919	0.57742580
O	0.82687531	0.72219137	0.77361055
O	0.84686439	0.77211610	0.20617373
O	0.82287822	0.79374834	0.97984586
O	0.79432539	0.77411971	0.35804726
O	0.00280042	0.47189192	0.84826327
O	0.91907383	0.48432308	0.93242213
O	0.65651998	0.48405793	0.42094593
O	0.67678000	0.51664527	0.22555159
O	0.65528298	0.51240643	0.78485513
O	0.67608149	0.52957614	0.00985852
O	0.71069752	0.53937857	0.63992032
O	0.50223413	0.78031968	0.83835347
O	0.42824126	0.80549891	0.94530759
O	0.15507307	0.76445696	0.42747304
O	0.17092249	0.80247153	0.22710339
O	0.16498164	0.74937567	0.80314829
O	0.17381199	0.72000411	0.02308325
O	0.20958671	0.70211399	0.64329138
O	0.25842424	0.85202087	0.52999814
O	0.75809045	0.87245241	0.52108712
O	0.74966854	0.61838246	0.47472690
O	0.23844781	0.59872082	0.47466890
Al	0.29507355	0.52061209	0.25315054
Si	0.06323143	0.03460612	0.17644516
Si	0.06480471	0.99953955	0.92165415
Si	0.37232607	0.99857765	0.71345583
Si	0.36944724	0.00272323	0.11618871
Si	0.28866213	0.96797617	0.85727414
Si	0.28141419	0.00460579	0.23315366
Si	0.28047822	0.98416105	0.48570207
Si	0.56939668	0.25103269	0.17365252
Si	0.56995785	0.23653773	0.92065724

Si	0.87361677	0.25310880	0.71370960
Si	0.86605229	0.25076684	0.10699162
Si	0.78560937	0.24311209	0.85207023
Si	0.78183474	0.25254821	0.23110192
Si	0.78050555	0.24795604	0.48414429
Si	0.93757025	0.00733227	0.82520444
Si	0.93527791	0.00612229	0.08526608
Si	0.62426572	0.99545741	0.27375887
Si	0.63176826	0.99263796	0.88827740
Si	0.71282187	0.99369912	0.13808483
Si	0.71405659	0.99168041	0.75872997
Si	0.71479225	0.99197727	0.50400723
Si	0.43839006	0.24547865	0.83025649
Si	0.43756004	0.25151302	0.08395262
Si	0.12916948	0.29997588	0.27445498
Si	0.12995749	0.24985413	0.89956740
Si	0.21627374	0.26847281	0.14848888
Si	0.20962784	0.19994653	0.76524432
Si	0.21276805	0.23358663	0.51279676
Si	0.06042372	0.54266196	0.16849015
Si	0.06693940	0.51176897	0.91521547
Si	0.37427950	0.49498176	0.73558100
Si	0.37290828	0.49874961	0.10977318
Si	0.28599048	0.45024951	0.86796300
Si	0.28388863	0.48142210	0.49730401
Si	0.55774953	0.74904705	0.16997530
Si	0.56483138	0.73979533	0.91430354
Si	0.87448812	0.75030349	0.71590817
Si	0.87123865	0.75794600	0.10019936
Si	0.78726630	0.74187934	0.85177330
Si	0.78709223	0.75025959	0.22359074
Si	0.78731357	0.74821426	0.48208750
Si	0.93731224	0.50135812	0.81816555
Si	0.93000843	0.49541920	0.07022953
Si	0.62852745	0.51200755	0.28413844

Si	0.62870877	0.49677115	0.88730157
Si	0.71360455	0.50055147	0.14139952
Si	0.71605064	0.50005093	0.77082002
Si	0.71754513	0.50258540	0.51710659
Si	0.43733722	0.76103046	0.82487071
Si	0.43015930	0.75689412	0.07256637
Si	0.12510311	0.79404311	0.29137972
Si	0.13210721	0.75386258	0.89554556
Si	0.21110692	0.76601034	0.15258529
Si	0.22168064	0.70895910	0.78059835
Si	0.21572156	0.72956711	0.51840643

HAl(5)-MTW

a = 25.6509 Å

b = 10.2429 Å

c = 12.248 Å

α = 89.9937º

β = 108.736º

γ = 90.6083º

H	0.28371701	0.40673570	0.04419624
O	0.07573994	0.36205438	0.23211063
O	0.08254892	0.13883351	0.90293700
O	0.23061681	0.38181132	0.80712092
O	0.60267965	0.13862258	0.27042615
O	0.59227025	0.40097439	0.90561073
O	0.75215535	0.10390866	0.84710582
O	0.89681434	0.39021204	0.72753012
O	0.89417430	0.10374619	0.11091312
O	0.74030523	0.35336540	0.14410337
O	0.40461477	0.16067659	0.74693857
O	0.42222771	0.37979010	0.14873619
O	0.24977323	0.13559631	0.19904773
O	0.92533465	0.14127323	0.75680651
O	0.91888590	0.35531041	0.12185452

O	0.76070586	0.10294293	0.19464612
O	0.42379891	0.41367132	0.77140872
O	0.40309338	0.12737650	0.11353440
O	0.25739944	0.38852743	0.15280410
O	0.10549482	0.11476852	0.23599052
O	0.10190385	0.38814462	0.87303002
O	0.25839284	0.13535183	0.84977243
O	0.58344218	0.38914855	0.22236867
O	0.59853785	0.15048310	0.85827614
O	0.74744243	0.35450050	0.79301160
O	0.99975108	0.04335654	0.15846016
O	0.06959713	0.96174870	0.05231795
O	0.33996065	0.02680889	0.57457018
O	0.32957008	0.99776370	0.78166400
O	0.34113602	0.00516997	0.21636636
O	0.32326962	0.96708522	0.99337634
O	0.28557972	0.95639411	0.36114405
O	0.50307689	0.21691808	0.14343794
O	0.58679413	0.22107936	0.05820591
O	0.84045590	0.21366746	0.57633711
O	0.83263237	0.21345180	0.78693081
O	0.84401666	0.26597652	0.21294075
O	0.82003224	0.27352092	0.98727954
O	0.78967831	0.28493776	0.36099545
O	0.00238242	0.96346272	0.83601500
O	0.92973260	0.00822231	0.94638618
O	0.65636448	0.95352330	0.41270536
O	0.67176182	0.98103917	0.21172240
O	0.65543160	0.97713153	0.78401725
O	0.68156523	0.02594815	0.00595396
O	0.70528414	0.02672123	0.62985888
O	0.50423625	0.24865337	0.86238757
O	0.42201018	0.27009207	0.95133344
O	0.15149586	0.26942267	0.41726698
O	0.17554070	0.30325096	0.22422726

O	0.15237429	0.20636250	0.79023034
O	0.18049424	0.24265946	0.01423979
O	0.20347386	0.20673128	0.63430727
O	0.24906711	0.37744981	0.53077317
O	0.75508243	0.37151147	0.53004999
O	0.73960607	0.12222261	0.46303278
O	0.24138462	0.12761488	0.46662462
O	0.07649418	0.86925849	0.25798221
O	0.07694282	0.63924228	0.86753850
O	0.24277322	0.88139397	0.81296462
O	0.59734358	0.64215763	0.26277862
O	0.58657037	0.90099964	0.89796842
O	0.75530358	0.60380848	0.85593941
O	0.89820774	0.89084312	0.74170488
O	0.89522236	0.60644753	0.10880317
O	0.74368108	0.85085055	0.14314862
O	0.39423540	0.66054330	0.77744439
O	0.41353911	0.87204111	0.14839030
O	0.24670095	0.63337507	0.21274640
O	0.92583724	0.64007613	0.76198626
O	0.92370383	0.85635995	0.11880036
O	0.76794238	0.60212104	0.19410834
O	0.41735770	0.90420388	0.73883408
O	0.39220115	0.63501591	0.05067141
O	0.24445105	0.88273966	0.14277990
O	0.09705912	0.61502537	0.25084686
O	0.10658423	0.88988506	0.88424214
O	0.26058678	0.62928832	0.85963487
O	0.57566826	0.89126606	0.21778205
O	0.59718170	0.65099628	0.85955518
O	0.74696276	0.85240618	0.79331457
O	0.99695738	0.53159044	0.13517380
O	0.07918665	0.49540196	0.04935947
O	0.34175618	0.51315919	0.59831017
O	0.32874440	0.46686429	0.80162491

O	0.34555548	0.53755466	0.22441349
O	0.31006486	0.43839568	0.00218713
O	0.29442495	0.46059703	0.37493115
O	0.49551729	0.71606751	0.14849070
O	0.57364356	0.72509626	0.04708007
O	0.84638901	0.72398504	0.57682564
O	0.83025705	0.71044199	0.77924946
O	0.84819674	0.77396420	0.21123465
O	0.82439719	0.78132830	0.98409143
O	0.79375025	0.78439313	0.36049942
O	-0.00031075	0.45808180	0.84847415
O	0.91771384	0.49108308	0.93556210
O	0.65709656	0.47416076	0.41667347
O	0.67606425	0.50641557	0.21909673
O	0.65755085	0.48428841	0.78769062
O	0.68338428	0.53913051	0.00983379
O	0.70858362	0.53674629	0.63544938
O	0.49882442	0.74225631	0.83750068
O	0.43324044	0.82590665	0.95305858
O	0.15466019	0.75890451	0.42854531
O	0.16813970	0.79275398	0.22383157
O	0.15861737	0.72134152	0.79516527
O	0.17252462	0.71041383	0.01923685
O	0.21151939	0.70238291	0.64463208
O	0.25006926	0.88010497	0.53306017
O	0.75844024	0.87411247	0.52773522
O	0.74672089	0.62238657	0.47012129
O	0.24835054	0.62901933	0.47648315
Al	0.37488221	0.50278599	0.11851543
Si	0.06254694	-0.00182327	0.1762763
Si	0.06525718	0.98858760	0.91877029
Si	0.37314236	0.02215324	0.71204631
Si	0.37093783	0.99304498	0.11752333
Si	0.28935663	0.99505364	0.85987438
Si	0.28042506	0.99569561	0.22957587

Si	0.27920507	0.99779041	0.48388706
Si	0.56841599	0.24170038	0.17332642
Si	0.57042967	0.25555375	0.92107600
Si	0.87357093	0.24049412	0.71189291
Si	0.86933714	0.24947844	0.10796188
Si	0.78798636	0.23698948	0.85336187
Si	0.78328005	0.25116269	0.22784775
Si	0.78085170	0.24786697	0.48249765
Si	0.93894067	0.00062434	0.82107480
Si	0.93667137	0.00329748	0.08314684
Si	0.62639663	0.99110903	0.27773394
Si	0.63028088	0.01175657	0.88678653
Si	0.71418536	0.99147139	0.13905973
Si	0.71507023	0.98996909	0.76391943
Si	0.71503427	0.99344650	0.50846322
Si	0.43917163	0.27245616	0.83491809
Si	0.43796375	0.25175734	0.09149721
Si	0.12669583	0.26165638	0.27723897
Si	0.12883633	0.24394638	0.89487734
Si	0.21507209	0.26491491	0.14890620
Si	0.21132830	0.23095214	0.76927196
Si	0.21176809	0.24537996	0.51241565
Si	0.06188800	0.50166916	0.16616134
Si	0.06410899	0.49518245	0.90951081
Si	0.37270356	0.51425033	0.73707270
Si	0.28202328	0.48107738	0.86215559
Si	0.28800007	0.50966030	0.24477591
Si	0.28349634	0.49499759	0.49523825
Si	0.56021063	0.74354709	0.16804575
Si	0.56392791	0.75525340	0.91116730
Si	0.87525139	0.74225926	0.71501630
Si	0.87287268	0.75440553	0.10558173
Si	0.78926001	0.73800581	0.85349861
Si	0.78807231	0.75227496	0.22755341
Si	0.78587575	0.75085051	0.48347450

Si	0.93516248	0.49496845	0.81877954
Si	0.93216730	0.49617190	0.07517190
Si	0.62835557	0.50265134	0.27959700
Si	0.63251214	0.51776673	0.89083110
Si	0.71665130	0.50072622	0.14187692
Si	0.71730215	0.49451360	0.76806779
Si	0.71698246	0.50092259	0.51306511
Si	0.43632506	0.78224539	0.82731158
Si	0.43286840	0.75949395	0.07524078
Si	0.12393278	0.75810272	0.28997610
Si	0.12871971	0.74094722	0.89231089
Si	0.20819839	0.75341796	0.14991345
Si	0.21851985	0.73552286	0.77793943
Si	0.21625639	0.74315737	0.52023897

HAl(6)-MTW

a = 25.5246 Å

b = 10.199 Å

c = 12.2738 Å

α = 88.9321º

β = 109.009º

γ = 90.3503º

H	0.37816051	0.28465235	0.19495786
O	0.08111406	0.33740957	0.22416961
O	0.07733310	0.17297155	0.88089807
O	0.23613305	0.41250224	0.81056916
O	0.58291678	0.09226429	0.22225306
O	0.57965080	0.42751370	0.88412776
O	0.75923542	0.07098066	0.85812927
O	0.91725250	0.33341570	0.78334318
O	0.89769750	0.09044689	0.12899887
O	0.73883540	0.34423224	0.14712832
O	0.39896137	0.18246209	0.73271389
O	0.39565592	0.33966634	0.14899844

O	0.23829520	0.08884472	0.14819834
O	0.89709323	0.08499654	0.72749837
O	0.92129039	0.34023543	0.11858194
O	0.76488350	0.09305610	0.17761437
O	0.42344116	0.43334363	0.76182957
O	0.41711641	0.08571093	0.10778909
O	0.26653424	0.34029725	0.17355549
O	0.10601915	0.08557860	0.25898414
O	0.09967204	0.42358876	0.86222211
O	0.25786208	0.16158999	0.86343562
O	0.61194371	0.33946640	0.26808483
O	0.60025641	0.17669814	0.86236353
O	0.73246668	0.32211558	0.81680521
O	0.00085635	0.02797580	0.14344840
O	0.07992269	0.99790836	0.04674790
O	0.34501959	0.00339159	0.58467127
O	0.32406650	0.02717715	0.77930830
O	0.34490357	0.01706273	0.21193514
O	0.32021455	0.97125877	0.98997361
O	0.29102398	0.00299187	0.36204240
O	0.50647107	0.27727837	0.15294833
O	0.58581034	0.25682051	0.05444677
O	0.84291633	0.26942875	0.58032294
O	0.81951339	0.22967178	0.77163933
O	0.84529420	0.26637536	0.21352324
O	0.82273921	0.25282361	0.98840200
O	0.78896937	0.25196475	0.35895304
O	0.99828131	-0.00229202	0.84553647
O	0.91919163	0.00967770	0.94413424
O	0.65673487	0.01451711	0.42221389
O	0.68060394	-0.00723062	0.23070551
O	0.65282403	0.99538761	0.78629700
O	0.67418614	0.02010443	0.01070219
O	0.71116539	0.98928874	0.64432133
O	0.50005635	0.25276376	0.85777330

O	0.41570677	0.28918391	0.93899887
O	0.15629837	0.25272443	0.42145937
O	0.18050782	0.25654987	0.22886925
O	0.15310091	0.24672226	0.78419753
O	0.17484081	0.26852911	0.00891000
O	0.21176006	0.23464656	0.64334016
O	0.23812565	0.42039361	0.51591600
O	0.73627372	0.34066530	0.49743839
O	0.76335316	0.09055462	0.50724475
O	0.26220715	0.17254136	0.49288624
O	0.07473231	0.83851376	0.21755447
O	0.08067495	0.67375606	0.88697972
O	0.23534114	0.91455753	0.80477036
O	0.58198818	0.58829284	0.22219189
O	0.57617461	0.92737198	0.88254171
O	0.76193959	0.56970851	0.86204976
O	0.91590196	0.83286108	0.78397484
O	0.90066542	0.59252190	0.13243092
O	0.74085808	0.84186533	0.14294145
O	0.39481049	0.68456258	0.73295628
O	0.39934113	0.83263451	0.14013908
O	0.23366022	0.59045817	0.14774094
O	0.89668342	0.58448784	0.72970807
O	0.92486564	0.84222598	0.11774907
O	0.76977506	0.59275612	0.17676424
O	0.42126679	0.93118065	0.78494960
O	0.41952273	0.58471042	0.11444670
O	0.26615846	0.83804127	0.18599923
O	0.10370169	0.58859017	0.26280490
O	0.10020356	0.92398045	0.85867725
O	0.26021532	0.66351466	0.85033530
O	0.60238288	0.84001726	0.26766296
O	0.60032520	0.67845654	0.86561743
O	0.73326735	0.82035740	0.82307952
O	0.00138772	0.51357683	0.14634107

O	0.08115981	0.49912874	0.05114296
O	0.34175981	0.51410923	0.57564539
O	0.32626412	0.50981324	0.77774040
O	0.34133333	0.52553472	0.21365823
O	0.32086726	0.48478476	0.99003438
O	0.28439615	0.48915744	0.35773971
O	0.50082696	0.75861502	0.14928746
O	0.58118671	0.75856002	0.05413765
O	0.84414061	0.76864380	0.57886621
O	0.81746496	0.73079272	0.76659452
O	0.84814562	0.77159333	0.21234663
O	0.82687220	0.75328016	0.98732389
O	0.79119034	0.75423204	0.35672492
O	0.99878667	0.50400202	0.84990502
O	0.91910890	0.50603398	0.94615912
O	0.65796930	0.52123713	0.42272163
O	0.68324164	0.51469330	0.23177850
O	0.65454616	0.50337795	0.78646773
O	0.67692705	0.52677533	0.01133987
O	0.71311742	0.50007023	0.64503523
O	0.49839420	0.74686049	0.85559086
O	0.41783771	0.75864148	0.94914252
O	0.15234542	0.76761818	0.41529299
O	0.17374935	0.76132349	0.21912283
O	0.15426963	0.74404570	0.78302980
O	0.17859016	0.77798648	0.00629068
O	0.20956752	0.74008310	0.63492610
O	0.23944504	0.92156394	0.50818735
O	0.73724993	0.83918886	0.49421293
O	0.76536378	0.58975080	0.50326174
O	0.25506820	0.67047041	0.47806840
Al	0.43879038	0.23912027	0.08145623
Si	0.06494367	-0.01203870	0.1660331
Si	0.06363797	0.02252905	0.90788153
Si	0.37276725	0.03651482	0.72122240

Si	0.37164202	0.97890867	0.11128989
Si	0.28518733	0.01817032	0.86022241
Si	0.28496665	0.98673154	0.22784866
Si	0.28447343	0.02419868	0.48723341
Si	0.57018237	0.24285739	0.17374450
Si	0.56599178	0.27821217	0.91505937
Si	0.86929495	0.23000235	0.71635536
Si	0.87150203	0.23737890	0.11196919
Si	0.78375007	0.21864169	0.85914475
Si	0.78422035	0.23923582	0.22512707
Si	0.78253181	0.23829988	0.48520217
Si	0.93272894	-0.01835569	0.8254956
Si	0.93563785	-0.00760667	0.0838278
Si	0.63029247	-0.01455265	0.2848510
Si	0.62602625	0.02965477	0.88594976
Si	0.71453311	-0.01273656	0.1398033
Si	0.71404491	0.96896193	0.77716422
Si	0.71727116	0.98414373	0.51746722
Si	0.43472725	0.28910848	0.82593722
Si	0.13064889	0.23324914	0.28302056
Si	0.12616684	0.27726835	0.88429825
Si	0.21428925	0.23730596	0.13878849
Si	0.21497442	0.26371449	0.77467051
Si	0.21719019	0.26960365	0.51834032
Si	0.06642724	0.48469448	0.17046399
Si	0.06454804	0.52475837	0.91236571
Si	0.37211163	0.53466576	0.71313174
Si	0.36800716	0.49296566	0.11387823
Si	0.28609664	0.51754001	0.85544504
Si	0.28038907	0.48823019	0.22428462
Si	0.27973942	0.52319860	0.48262823
Si	0.56665503	0.73684903	0.17307297
Si	0.56402531	0.77755519	0.91455200
Si	0.86862576	0.72941589	0.71523518
Si	0.87490845	0.73971536	0.11213315

Si	0.78519267	0.71852448	0.86058729
Si	0.78726144	0.74055643	0.22335907
Si	0.78407439	0.73838025	0.48230165
Si	0.93319979	0.48203160	0.82748938
Si	0.93556062	0.48791142	0.08580924
Si	0.63330993	0.49004413	0.28547642
Si	0.62804595	0.53311494	0.88746252
Si	0.71667939	0.49414191	0.14109047
Si	0.71542159	0.47339555	0.77692809
Si	0.71835312	0.48860200	0.51782207
Si	0.43360160	0.78054909	0.83107159
Si	0.43523999	0.73601315	0.08816210
Si	0.12586672	0.73878404	0.27845861
Si	0.12825231	0.77903918	0.88382965
Si	0.21255572	0.74231441	0.13919063
Si	0.21490514	0.76602516	0.76791867
Si	0.21430045	0.77511510	0.50941381

HAl(7)-MTW

a = 25.5009 Å

b = 10.1966 Å

c = 12.2732 Å

α = 88.5221º

β = 108.892º

γ = 90.099º

H	0.26745117	0.08695001	0.07635646
O	0.10408520	0.36961778	0.24569651
O	0.07765448	0.20065256	0.88015890
O	0.26282749	0.35124933	0.86328986
O	0.57523184	0.09922175	0.21875568
O	0.57910376	0.40929911	0.86867793
O	0.76466399	0.07493986	0.81315616
O	0.92432948	0.35354430	0.76838590
O	0.91962450	0.13884184	0.12256429

O	0.76307753	0.39637529	0.19441134
O	0.40312398	0.14773886	0.72942052
O	0.39162938	0.34428368	0.10793379
O	0.25511011	0.09241061	0.14669992
O	0.89714231	0.10512280	0.72728035
O	0.89240944	0.38992970	0.10398732
O	0.74051879	0.14803858	0.14641863
O	0.42302837	0.39908931	0.76843124
O	0.41796110	0.09298126	0.12235735
O	0.26234869	0.35388266	0.22037160
O	0.07647636	0.12089376	0.25825850
O	0.10524786	0.45003337	0.87348923
O	0.23780253	0.10476959	0.80936446
O	0.59581717	0.35084738	0.26860116
O	0.60825768	0.15847769	0.89231743
O	0.73484768	0.32333861	0.82240272
O	0.99717917	0.95923343	0.14036919
O	0.07516367	0.03865947	0.05301699
O	0.33892126	0.97044997	0.59622230
O	0.33547312	0.00646619	0.80929074
O	0.35179192	0.97569978	0.22668308
O	0.31265804	0.03003184	0.00525463
O	0.29733656	0.03486946	0.37378334
O	0.49548577	0.27410421	0.14150215
O	0.57967202	0.27363472	0.05662183
O	0.84056807	0.28711880	0.57999495
O	0.82959734	0.27041974	0.78729932
O	0.84581713	0.22795439	0.21634191
O	0.81811957	0.21522708	0.99111010
O	0.79087079	0.21336206	0.36404864
O	0.00003800	0.02214535	0.84462773
O	0.91883698	0.00800444	0.93786513
O	0.65472290	0.02973993	0.41144546
O	0.67048551	0.00057074	0.21051619
O	0.65839265	0.01188654	0.78108770

O	0.68073600	0.97205631	0.00473484
O	0.70537482	0.95084799	0.62655544
O	0.50343549	0.22517042	0.85538102
O	0.41867998	0.23518506	0.93847837
O	0.15435777	0.22748245	0.43435524
O	0.17611439	0.18017418	0.24204507
O	0.15615083	0.27382616	0.79042858
O	0.17692105	0.27788436	0.01590236
O	0.21285772	0.29331237	0.64559527
O	0.23588294	0.40152572	0.46828478
O	0.74135322	0.38180521	0.45834948
O	0.75292448	0.13072839	0.53094191
O	0.26100248	0.15191296	0.52752397
O	0.09959608	0.87360512	0.23343450
O	0.08499700	0.69819664	0.91061158
O	0.26151321	0.85141227	0.85509842
O	0.57409383	0.60082158	0.21050300
O	0.58160732	0.90762540	0.86231312
O	0.76046093	0.57485321	0.81531542
O	0.92044477	0.85271847	0.76630980
O	0.92246352	0.63744128	0.12611360
O	0.76265613	0.89469038	0.19050553
O	0.40208530	0.64951571	0.72217538
O	0.38949710	0.84283748	0.08221216
O	0.24705707	0.60363202	0.14073994
O	0.89629623	0.60190709	0.73204228
O	0.89345290	0.88789411	0.10777114
O	0.73811861	0.64700837	0.14136214
O	0.42366073	0.89654198	0.78008779
O	0.42305277	0.59442000	0.13196075
O	0.26045769	0.84315461	0.22598190
O	0.07817839	0.62000125	0.24852664
O	0.10468623	0.94917149	0.87997673
O	0.23896025	0.60233965	0.80825301
O	0.59856117	0.84822017	0.26670290

O	0.61145681	0.65695163	0.89804737
O	0.73586626	0.82658472	0.83064168
O	0.99887393	0.44994376	0.15502973
O	0.07294590	0.50863864	0.05124108
O	0.33956053	0.47565673	0.58156568
O	0.33110782	0.49951499	0.78942738
O	0.34843233	0.50502830	0.22331950
O	0.32260356	0.53465512	0.99561674
O	0.29203051	0.55316125	0.36483445
O	0.49597995	0.78383090	0.14430074
O	0.57556044	0.77979166	0.04852082
O	0.84239670	0.77786094	0.57435281
O	0.82373814	0.76620225	0.77415727
O	0.84421728	0.72236875	0.21071772
O	0.82261236	0.71090428	0.98645984
O	0.78941884	0.71050769	0.35861581
O	0.00196486	0.53405913	0.83735666
O	0.92749684	0.50598239	0.94555820
O	0.65333443	0.53516248	0.40671398
O	0.66862651	0.49648015	0.20655396
O	0.65489313	0.50271921	0.77899643
O	0.68149524	0.46390175	0.00357384
O	0.70244194	0.45722777	0.62322831
O	0.50544073	0.72342567	0.83990572
O	0.42713754	0.71103253	0.93988195
O	0.15352112	0.73240070	0.42240972
O	0.17366800	0.69813985	0.22614748
O	0.15761684	0.76732493	0.80480718
O	0.18238780	0.80281239	0.02924986
O	0.20385381	0.78575367	0.64141225
O	0.23603083	0.90145176	0.47705374
O	0.74443483	0.88331613	0.45912503
O	0.75224640	0.63062354	0.52707244
O	0.25777807	0.64886363	0.53021111
Al	0.21319862	0.23983980	0.15670225

Si	0.06202762	0.99868815	0.17093544
Si	0.06435676	0.05269082	0.91489080
Si	0.37487213	0.00473511	0.72786519
Si	0.37014811	0.98465099	0.11051097
Si	0.28653607	0.99832078	0.86602406
Si	0.29212434	0.98101708	0.24888760
Si	0.28251720	0.01477797	0.49352686
Si	0.56152726	0.24943377	0.17120862
Si	0.56752318	0.26624685	0.91806860
Si	0.87292756	0.25392351	0.71578488
Si	0.86930472	0.24260142	0.10801604
Si	0.78689090	0.22092623	0.85321835
Si	0.78499273	0.24662001	0.23049354
Si	0.78152566	0.25314084	0.48346047
Si	0.93464838	-0.00244893	0.8198639
Si	0.93260368	-0.00196775	0.0771211
Si	0.62511253	0.99459367	0.27704652
Si	0.63205899	0.01281584	0.88535619
Si	0.71362791	0.00278205	0.13852380
Si	0.71630888	0.96709939	0.76329725
Si	0.71494907	0.99921161	0.50783769
Si	0.43748705	0.25224887	0.82362032
Si	0.43128266	0.23765724	0.07726661
Si	0.12824674	0.22389433	0.29340823
Si	0.12989816	0.30008333	0.89343357
Si	0.21673411	0.25660370	0.77691650
Si	0.21557166	0.26807064	0.51787866
Si	0.06357461	0.48599034	0.17521516
Si	0.06627936	0.54642294	0.91800005
Si	0.37338634	0.50569328	0.71513700
Si	0.37130640	0.49392197	0.11515832
Si	0.28893734	0.49737244	0.86385590
Si	0.28662253	0.49889888	0.23728556
Si	0.28086395	0.51907552	0.48498716
Si	0.56132737	0.75288877	0.16730876

Si	0.56837889	0.76651872	0.91227298
Si	0.87086010	0.74950767	0.71214017
Si	0.87095625	0.73923303	0.10732096
Si	0.78574012	0.71924980	0.85161513
Si	0.78362221	0.74409266	0.22516831
Si	0.78205330	0.75062298	0.47965067
Si	0.93804561	0.49891272	0.82198158
Si	0.93579372	0.49535345	0.08269803
Si	0.62331524	0.49589829	0.27337923
Si	0.63143548	0.50848567	0.88724605
Si	0.71284255	0.49997655	0.13708102
Si	0.71349832	0.46549613	0.76052618
Si	0.71284487	0.50171699	0.50456822
Si	0.43993626	0.74500142	0.82044544
Si	0.43424679	0.73247418	0.07461255
Si	0.12567867	0.73176394	0.28262758
Si	0.13214726	0.80345208	0.90604767
Si	0.21511961	0.73643882	0.15440131
Si	0.21519403	0.75082760	0.77691244
Si	0.21280064	0.76594923	0.51782787

HGa(1)-MTW

a = 25.3898 Å

b = 10.2047 Å

c = 12.3505 Å

α = 89.1683º

β = 108.947º

γ = 90.2757º

H	0.46482578	0.00952131	0.77877705
O	0.07814313	0.33697200	0.22611981
O	0.10377359	0.09196238	0.87848247
O	0.26081997	0.34363900	0.85365147
O	0.58060745	0.09826981	0.21791821
O	0.57975459	0.42530357	0.88085599
O	0.73555460	0.17752301	0.81906614
O	0.92331870	0.34210687	0.76597497
O	0.89427686	0.08397724	0.12482737
O	0.76446845	0.43464433	0.16680381
O	0.42811627	0.04557298	0.77521829
O	0.39709638	0.33990295	0.13533627
O	0.26853379	0.18016709	0.18256236
O	0.89403439	0.09339137	0.73387845
O	0.92362637	0.33260292	0.12349074
O	0.73797028	0.18263471	0.14760717
O	0.38799060	0.32063772	0.71363563
O	0.42264025	0.08920968	0.13939252
O	0.23628218	0.42945883	0.15430775
O	0.10252710	0.08549686	0.25867473
O	0.07999034	0.34240920	0.88111810
O	0.23608297	0.09481161	0.81013140
O	0.60168504	0.34877172	0.26784739
O	0.61465209	0.17914807	0.88894838
O	0.76100360	0.42963519	0.84333355
O	0.99801410	0.01775572	0.14402471
O	0.07869294	0.98329384	0.05201326
O	0.34432202	0.99411492	0.58296299

O	0.32885528	0.00569591	0.78520947
O	0.34333612	0.98928643	0.21524387
O	0.32197542	0.02953118	0.99394479
O	0.29033785	0.02071221	0.36378580
O	0.49930643	0.27072533	0.14815204
O	0.58125727	0.27156714	0.05558310
O	0.84263801	0.27021456	0.57547749
O	0.82426195	0.26636751	0.77383053
O	0.84482881	0.25897321	0.21315649
O	0.82360876	0.25687141	0.98886951
O	0.78698735	0.28298904	0.35459408
O	0.99882087	0.03049809	0.85409627
O	0.91702834	0.99758327	0.94417039
O	0.65429512	0.01607122	0.41563210
O	0.68091675	0.00905430	0.22732440
O	0.65733819	0.99767224	0.78847432
O	0.68066098	0.99280021	0.01312288
O	0.70909654	0.02607611	0.63543909
O	0.50819167	0.22695367	0.84615926
O	0.41373482	0.23638447	0.95383742
O	0.15608425	0.25426925	0.41782001
O	0.17635699	0.25065955	0.22159182
O	0.15446852	0.26462666	0.78439819
O	0.17979966	0.25293948	0.00905388
O	0.21053536	0.27150401	0.63838966
O	0.26037961	0.34730749	0.48850233
O	0.73672337	0.35465906	0.50289124
O	0.75930966	0.10496403	0.48642136
O	0.24177155	0.09573826	0.51487110
O	0.07456336	0.83604178	0.22851036
O	0.10303750	0.59445428	0.87336275
O	0.26392355	0.84563901	0.85693381
O	0.57804953	0.59796413	0.21474559
O	0.57834877	0.93228610	0.87853112
O	0.73309090	0.68032158	0.81587127

O	0.92416612	0.84459355	0.77669833
O	0.89656978	0.58295628	0.12051851
O	0.77180463	0.93522731	0.18340529
O	0.42606967	0.56358808	0.77252034
O	0.39224021	0.84075985	0.10100916
O	0.26178074	0.68214431	0.17324960
O	0.89927616	0.59367186	0.73775511
O	0.92043047	0.83440760	0.11725128
O	0.73849100	0.68720314	0.16277886
O	0.38682610	0.80489401	0.73751532
O	0.42291572	0.59200441	0.13926657
O	0.23406679	0.93380502	0.15639009
O	0.10287621	0.58696302	0.26558586
O	0.07385161	0.84416113	0.86730325
O	0.23873746	0.59634426	0.82205097
O	0.60380150	0.84708920	0.25401448
O	0.59653418	0.67804988	0.85867787
O	0.76495472	0.92839132	0.84209083
O	0.00020683	0.51590761	0.13997687
O	0.08447213	0.49548194	0.05709126
O	0.34132796	0.52156839	0.57913082
O	0.32657772	0.50098121	0.78011755
O	0.34278582	0.50771104	0.21834288
O	0.32602391	0.51298413	0.99514209
O	0.28512500	0.53224448	0.35955972
O	0.49857102	0.77707840	0.14937631
O	0.57326942	0.75968242	0.04080476
O	0.84499334	0.77245698	0.58658543
O	0.82759926	0.75151390	0.78579391
O	0.84738064	0.74773375	0.21863528
O	0.81931021	0.75017210	0.99420182
O	0.79407786	0.78132927	0.36708596
O	0.00130270	0.51828858	0.85964449
O	0.91781106	0.48335084	0.94249410
O	0.65573785	0.52948481	0.41346881

O	0.67622724	0.50396336	0.21913821
O	0.65356563	0.50461283	0.78243659
O	0.67605803	0.53212712	0.00490100
O	0.70825501	0.52471638	0.63456532
O	0.49469610	0.77121031	0.83462165
O	0.42530543	0.71141325	0.94962906
O	0.15146652	0.76148081	0.42462566
O	0.17559132	0.75944546	0.23242245
O	0.15721025	0.77013896	0.79245175
O	0.17007861	0.76508384	0.01383202
O	0.21164140	0.76839838	0.64489114
O	0.25705754	0.84369996	0.48855613
O	0.73909665	0.85340780	0.50808360
O	0.76269528	0.60411186	0.49362729
O	0.23422003	0.59291330	0.50925099
Si	0.06312746	0.98153612	0.17014696
Si	0.06348333	0.98764235	0.91304291
Si	0.36938788	0.95751929	0.71736220
Si	0.37065388	0.98753142	0.11276466
Si	0.28753592	0.99434304	0.86263249
Si	0.28408023	0.03044275	0.22922518
Si	0.28242142	0.98954214	0.48561862
Si	0.56504960	0.24776535	0.17131879
Si	0.56970064	0.27553086	0.91735000
Si	0.87103222	0.24326014	0.71233279
Si	0.87145614	0.23366102	0.11199304
Si	0.78654281	0.28237637	0.85660574
Si	0.78336141	0.28925216	0.22131486
Si	0.78129317	0.25389415	0.47930603
Si	0.93373277	0.99209950	0.82744299
Si	0.93263804	0.98317998	0.08278570
Si	0.62963272	0.99377752	0.27805933
Si	0.63254756	0.02655808	0.89208792
Si	0.71758236	0.03083611	0.14263319
Si	0.71688717	0.03133701	0.77047907

Si	0.71575533	0.00091927	0.51179494
Si	0.43355512	0.23419279	0.09182143
Si	0.12826433	0.23239948	0.28080421
Si	0.12950084	0.23863695	0.88870862
Si	0.21502185	0.27838841	0.14177424
Si	0.21566092	0.24431790	0.77094016
Si	0.21736423	0.24293077	0.51510550
Si	0.43396896	0.70975630	0.82545882
Si	0.06607329	0.48421441	0.17189619
Si	0.06703897	0.48770487	0.91786646
Si	0.37055930	0.47269880	0.71158944
Si	0.37212008	0.48692008	0.12078251
Si	0.28874064	0.48845049	0.86303874
Si	0.28147338	0.53685162	0.22664767
Si	0.28043851	0.49859013	0.48404121
Si	0.56332401	0.74608820	0.16458745
Si	0.56138604	0.78349247	0.90440144
Si	0.87402094	0.74094929	0.72202988
Si	0.87106483	0.72945976	0.11211762
Si	0.78652928	0.77752174	0.85973181
Si	0.78789423	0.78667328	0.23291468
Si	0.78480644	0.75328224	0.48835122
Si	0.93569081	0.48433267	0.82697314
Si	0.93487663	0.47901416	0.08180265
Si	0.62777505	0.49557634	0.27841601
Si	0.62648056	0.53453387	0.88234459
Si	0.71351490	0.53968031	0.13816720
Si	0.71420183	0.53347110	0.76852623
Si	0.71597461	0.50371845	0.51140737
Si	0.43477548	0.73065224	0.08548816
Si	0.12603225	0.73631988	0.28730344
Si	0.12610014	0.74397485	0.88685968
Si	0.21004257	0.78475172	0.14389846
Si	0.21784646	0.74393903	0.77848519
Si	0.21363779	0.74184351	0.51753914

Ga	0.43582636	0.23156590	0.83048941

HGa(2)-MTW

a = 25.4744 Å

b = 10.2209 Å

c = 12.2699 Å

α = 88.617º

β = 109.364º

γ = 90.8193º

H	0.36338841	0.39168747	0.56243268
O	0.10857347	0.41158313	0.25110460
O	0.07199398	0.16020514	0.87971825
O	0.25164107	0.32865364	0.84768382
O	0.57913519	0.05886930	0.22096326
O	0.59448307	0.32651909	0.86114351
O	0.76257386	0.07687617	0.84744208
O	0.89847094	0.40781413	0.73658160
O	0.92289580	0.15444436	0.12746146
O	0.76296395	0.40236122	0.15798731
O	0.39037221	0.19613033	0.73674374
O	0.42526282	0.41155342	0.13838604
O	0.26906530	0.16043852	0.18063435
O	0.91720344	0.15586813	0.78100393
O	0.90131324	0.40465626	0.13044909
O	0.73914437	0.15043829	0.16148530
O	0.43263506	0.43384653	0.79435260
O	0.40654267	0.15765017	0.14343122
O	0.23647557	0.40671817	0.13469398
O	0.07894654	0.16202161	0.21602446
O	0.10620624	0.40614546	0.89217528
O	0.23189141	0.07416178	0.83010286
O	0.61162999	0.30627165	0.26511905
O	0.58052876	0.07120995	0.87276378
O	0.73212158	0.32586833	0.82638766

O	0.00144130	0.97829977	0.15472480
O	0.07961370	0.99157760	0.05494387
O	0.34846088	0.01048875	0.58473253
O	0.31908738	0.01846048	0.77096436
O	0.34851567	0.98337167	0.21818133
O	0.32843619	0.01481121	0.99324109
O	0.29180125	0.99442208	0.36261778
O	0.50613967	0.24953666	0.15016945
O	0.58452045	0.21988070	0.05190652
O	0.84373786	0.23514174	0.57998983
O	0.81898029	0.25697033	0.76976551
O	0.84523019	0.23154466	0.21367653
O	0.82578194	0.24863683	0.98929340
O	0.79113284	0.26903548	0.35850894
O	0.99534527	0.97573337	0.85609070
O	0.91739982	0.99551047	0.95491323
O	0.65682173	0.97798889	0.41495251
O	0.67634577	0.96838188	0.21689663
O	0.65589719	0.99598104	0.77849633
O	0.68080069	0.98721011	0.00407972
O	0.71398221	0.99165330	0.63509510
O	0.49704639	0.22440118	0.85912705
O	0.41947294	0.26481107	0.95574394
O	0.15332006	0.23435438	0.41575145
O	0.18096024	0.23867721	0.22714844
O	0.14722647	0.23725107	0.78075133
O	0.17556787	0.21828393	0.00815102
O	0.20600398	0.22496261	0.63939525
O	0.23598770	0.40207145	0.50707323
O	0.76280623	0.40950698	0.50904224
O	0.73698917	0.15723120	0.48780543
O	0.25951692	0.15633523	0.49475292
O	0.10616257	0.91375515	0.27353965
O	0.08049780	0.65637057	0.85467861
O	0.26902514	0.83115368	0.85755116

O	0.58162421	0.55418440	0.21926922
O	0.60522201	0.82178830	0.87478602
O	0.75992978	0.57478097	0.86283721
O	0.89091073	0.90591453	0.74261890
O	0.92347935	0.65626170	0.12049487
O	0.76811382	0.90102141	0.17686971
O	0.38994448	0.70886190	0.72428733
O	0.42410520	0.90698515	0.12532636
O	0.26120018	0.65710005	0.17521656
O	0.92387590	0.65905870	0.77146732
O	0.90002534	0.90238597	0.14302889
O	0.73591402	0.65405207	0.14130828
O	0.42293504	0.95036659	0.79207310
O	0.39352319	0.65921324	0.11755393
O	0.24124355	0.91154553	0.14950487
O	0.08171044	0.66161271	0.23945535
O	0.09773412	0.91245757	0.86784951
O	0.23491541	0.58390052	0.84592680
O	0.60287943	0.80620938	0.25941289
O	0.57107291	0.57685400	0.86515470
O	0.73713283	0.82582191	0.81453200
O	0.00371855	0.48370946	0.14973044
O	0.08023048	0.53979380	0.05000141
O	0.34514953	0.47447135	0.56915051
O	0.31075751	0.49451652	0.76247189
O	0.34324247	0.48704266	0.21410069
O	0.32677338	0.47642989	0.99003717
O	0.28187827	0.48110429	0.35016933
O	0.49945203	0.72266231	0.15531203
O	0.57385597	0.72219915	0.04489127
O	0.84442948	0.73570960	0.57743855
O	0.82252685	0.71857312	0.77202645
O	0.84436837	0.71623570	0.21124086
O	0.82674646	0.75587144	0.98801711
O	0.78791308	0.73182101	0.35572379

O	0.00216282	0.48049080	0.85125147
O	0.92250495	0.50185806	0.94699824
O	0.65595802	0.48342011	0.42428911
O	0.68484775	0.48237764	0.23819055
O	0.65263651	0.50275909	0.78887634
O	0.66524055	0.48271359	0.01213764
O	0.71019417	0.49558596	0.64726817
O	0.49818228	0.76612643	0.83739069
O	0.42394827	0.76175816	0.94732768
O	0.16197230	0.73661454	0.43007917
O	0.17834223	0.75277291	0.22982306
O	0.15991606	0.77033525	0.78583301
O	0.17202688	0.74758413	0.00897727
O	0.21942873	0.72653251	0.65193992
O	0.24649926	0.90106176	0.51480543
O	0.76395216	0.90851124	0.48911708
O	0.73693333	0.65992551	0.50445488
O	0.26721863	0.65070634	0.50191130
Si	0.43545190	0.28280973	0.83744480
Si	0.06623964	0.01127254	0.17460970
Si	0.06089998	0.01011339	0.91458845
Si	0.37067925	0.04283719	0.72238516
Si	0.37691495	0.01487934	0.11900956
Si	0.28759257	0.98463437	0.86386363
Si	0.28771909	0.01213775	0.22854581
Si	0.28637508	0.01416432	0.48867223
Si	0.56990744	0.20905685	0.17156437
Si	0.56384942	0.21116302	0.91118645
Si	0.86987718	0.26341655	0.71755916
Si	0.87370335	0.25938446	0.11465511
Si	0.78501329	0.22718702	0.85863965
Si	0.78442162	0.26249370	0.22348058
Si	0.78322319	0.26701187	0.48349308
Si	0.93038673	0.00811626	0.83366772
Si	0.93555755	0.00798161	0.09487972

Si	0.62863784	0.95333119	0.27739738
Si	0.63036688	0.96936777	0.88274754
Si	0.71579842	0.00174545	0.13967748
Si	0.71734994	0.97333029	0.76823710
Si	0.71819980	0.00830791	0.50711981
Si	0.43959954	0.27052135	0.09624739
Si	0.12999911	0.26183849	0.27662555
Si	0.12501939	0.25605001	0.88958265
Si	0.21519018	0.25592525	0.13679263
Si	0.20957313	0.21741165	0.77397975
Si	0.21360931	0.25247157	0.51584401
Si	0.43372050	0.79451755	0.82404768
Si	0.06814694	0.52372219	0.17180332
Si	0.06709569	0.52040957	0.91192134
Si	0.37225473	0.50850555	0.11410841
Si	0.28208893	0.47126151	0.86022189
Si	0.28071437	0.50883773	0.21775854
Si	0.27930416	0.50193583	0.47789713
Si	0.56420418	0.70172225	0.16881890
Si	0.56153104	0.72239347	0.90561488
Si	0.87068498	0.75490956	0.71634153
Si	0.87358821	0.75636189	0.11542964
Si	0.78683885	0.71953956	0.85972777
Si	0.78398648	0.75078220	0.22207452
Si	0.78304103	0.75852803	0.48129230
Si	0.93695809	0.51188194	0.82702935
Si	0.93782554	0.51150470	0.08661234
Si	0.63301244	0.45730792	0.28605798
Si	0.62094282	0.47271439	0.88218165
Si	0.71198619	0.50506281	0.13639860
Si	0.71382970	0.47494425	0.78037764
Si	0.71661671	0.51141402	0.52113123
Si	0.43555071	0.76252886	0.08574351
Si	0.13173055	0.76659186	0.29262266
Si	0.12765140	0.77150036	0.87984469

Si	0.21265769	0.76747218	0.13993897
Si	0.22118085	0.72807658	0.78514308
Si	0.22368741	0.75424841	0.52576566
Ga	0.37335252	0.53892356	0.73390780

HGa(3)-MTW

a = 25.4076 Å

b = 10.2436 Å

c = 12.4183 Å

α = 90.2236º

β = 109.227º

γ = 90.0363º

H	0.37553136	0.45001843	0.54005321
O	0.10387191	0.39412630	0.26302350
O	0.07467627	0.13924360	0.87577093
O	0.23207939	0.38884025	0.81498353
O	0.60301622	0.14854822	0.26544984
O	0.57676409	0.38729293	0.87707064
O	0.73542077	0.14602255	0.82277251
O	0.89654512	0.39381615	0.73968736
O	0.92298746	0.14502554	0.12765696
O	0.76665814	0.40255178	0.17806229
O	0.39653147	0.13635341	0.73733714
O	0.41954803	0.40063485	0.10722782
O	0.26568901	0.15620549	0.17103415
O	0.92181156	0.14236161	0.77203154
O	0.89816070	0.39517054	0.12522730
O	0.73897659	0.15248695	0.15656072
O	0.42568688	0.38292262	0.77749697
O	0.39955826	0.14977680	0.13178041
O	0.23558836	0.40651608	0.14631945
O	0.07976725	0.14527733	0.21807948
O	0.10047690	0.38837118	0.86977686
O	0.26185477	0.14233684	0.85016779

O	0.58116744	0.39996509	0.22330449
O	0.60631281	0.13983219	0.87960338
O	0.76243562	0.39754088	0.84646340
O	0.00058146	0.96710964	0.14349759
O	0.08130147	0.98190175	0.05112373
O	0.33831506	0.97580360	0.57512937
O	0.32149380	0.97296216	0.77409536
O	0.34524151	0.97863987	0.21451952
O	0.33011957	0.97884038	0.99262268
O	0.28962667	0.00705395	0.35706520
O	0.50088913	0.22707229	0.14650967
O	0.58243996	0.23669986	0.05592452
O	0.84336027	0.22165613	0.58190497
O	0.82409589	0.22664126	0.77800102
O	0.84604801	0.22592802	0.21587337
O	0.82403363	0.22661776	0.99248405
O	0.79119763	0.24986870	0.36250603
O	0.99766560	0.95865838	0.85496024
O	0.91772100	0.99754509	0.94724785
O	0.65625321	0.97155092	0.41740647
O	0.67515736	0.98469949	0.22073062
O	0.65667836	0.96753943	0.78696859
O	0.68118861	0.97384733	0.01113414
O	0.70994756	0.99148010	0.63753549
O	0.50162082	0.20078615	0.85713290
O	0.41968132	0.22873559	0.94631653
O	0.15411387	0.21524986	0.41811745
O	0.18039957	0.23428407	0.23091510
O	0.15397605	0.20982163	0.79063001
O	0.17215302	0.22607436	0.01238877
O	0.20572795	0.21762686	0.63935504
O	0.22623999	0.40735208	0.51170768
O	0.76282654	0.39795732	0.51136341
O	0.73661887	0.14744880	0.49173940
O	0.26413163	0.16668362	0.50221849

O	0.10371142	0.89515221	0.26118264
O	0.07884778	0.63966701	0.87779718
O	0.23846942	0.88790120	0.83992304
O	0.60533803	0.64984123	0.26550231
O	0.58119168	0.89055471	0.88081856
O	0.73364743	0.64650055	0.82717148
O	0.89271452	0.89359495	0.74176300
O	0.92324957	0.64500404	0.12608062
O	0.76716383	0.90211898	0.18835949
O	0.39764967	0.63242341	0.75787899
O	0.42601601	0.89835755	0.13790594
O	0.26664727	0.65413319	0.17539710
O	0.92179316	0.64427406	0.77284040
O	0.89761022	0.89492125	0.12522466
O	0.73839839	0.65336315	0.14858114
O	0.41738107	0.88462814	0.75788714
O	0.39516056	0.64936842	0.11490412
O	0.23821052	0.90533226	0.15205636
O	0.08000257	0.64428034	0.22319745
O	0.10070826	0.88986852	0.86892007
O	0.25910154	0.63971566	0.81092092
O	0.57750477	0.89827685	0.22443907
O	0.60151386	0.63787691	0.87687003
O	0.76374655	0.89666855	0.84310242
O	0.00108379	0.46729631	0.14116652
O	0.08377611	0.48543590	0.05432232
O	0.35062932	0.46857935	0.58474028
O	0.32163685	0.45428744	0.76490784
O	0.34306269	0.47295949	0.19913776
O	0.32078960	0.48771335	0.97552041
O	0.29524016	0.48933795	0.35645178
O	0.50076401	0.71426090	0.14891812
O	0.58087679	0.73964826	0.05541944
O	0.84335868	0.72126087	0.58133763
O	0.82200500	0.71708537	0.77534077

O	0.84582015	0.72425748	0.21472634
O	0.82430810	0.72651271	0.99146090
O	0.79016689	0.73232923	0.36104234
O	0.99951207	0.46609420	0.85906880
O	0.91728363	0.49544022	0.94580546
O	0.65592114	0.47304771	0.42127374
O	0.68110610	0.48765643	0.23263440
O	0.65511546	0.46629751	0.79173738
O	0.67432213	0.47333870	0.01474684
O	0.70713431	0.49314335	0.64160491
O	0.49991935	0.72025956	0.85432827
O	0.42224947	0.76656531	0.95090169
O	0.15776560	0.72265385	0.41646935
O	0.17814868	0.73251955	0.22272661
O	0.15519981	0.71745017	0.78631763
O	0.17690118	0.73119032	0.00829692
O	0.20129049	0.78217281	0.63269016
O	0.22889163	0.92165489	0.48082067
O	0.76316640	0.89741901	0.50129089
O	0.73628730	0.64845673	0.49879927
O	0.26768092	0.68046763	0.52397953
Si	0.43632287	0.23526793	0.83078723
Si	0.06621882	0.99762595	0.16843811
Si	0.06351803	0.99240905	0.91269936
Si	0.36791874	0.99199690	0.71146193
Si	0.37496641	0.00174553	0.11877383
Si	0.28787818	0.99609947	0.86386503
Si	0.28417523	0.01151668	0.22419260
Si	0.27956729	0.01737202	0.47847761
Si	0.56675583	0.25301253	0.17254619
Si	0.56675496	0.24113714	0.91767298
Si	0.87176836	0.24639647	0.71843206
Si	0.87284547	0.24846511	0.11482452
Si	0.78692257	0.24976324	0.86045738
Si	0.78568007	0.25723509	0.22925604

Si	0.78329414	0.25389868	0.48632082
Si	0.93293796	0.99807192	0.82957454
Si	0.93504445	0.00085418	0.08592922
Si	0.62798480	0.00104464	0.28184082
Si	0.63148547	0.99280223	0.89004269
Si	0.71543712	0.00383118	0.14410709
Si	0.71670345	0.00016304	0.77157797
Si	0.71689753	0.00145145	0.51297458
Si	0.43495313	0.25193457	0.08353896
Si	0.12943534	0.24712083	0.28267653
Si	0.12545209	0.24113519	0.88739100
Si	0.21322034	0.25709545	0.14015318
Si	0.21337287	0.23950392	0.77234536
Si	0.21288138	0.25416428	0.51760900
Si	0.43472963	0.75192961	0.83145786
Si	0.06706019	0.49774089	0.17026899
Si	0.06570943	0.49506555	0.91562586
Si	0.37526436	0.48578533	0.72779306
Si	0.36917528	0.50271260	0.09895609
Si	0.28261755	0.49360009	0.84250911
Si	0.28452715	0.50593893	0.22217460
Si	0.56590559	0.75058006	0.17325706
Si	0.56593646	0.74716590	0.91744848
Si	0.87029650	0.74432364	0.71837227
Si	0.87285176	0.74763852	0.11410807
Si	0.78628394	0.74724567	0.85979753
Si	0.78542189	0.75302949	0.22900934
Si	0.78307053	0.74967951	0.48505235
Si	0.93415728	0.49987222	0.82994877
Si	0.93538391	0.50053094	0.08471648
Si	0.63071206	0.50280755	0.28524934
Si	0.62711151	0.49143479	0.89044576
Si	0.71491411	0.50485387	0.14299240
Si	0.71485769	0.50050331	0.77602381
Si	0.71602065	0.50259253	0.51894471

Si	0.43608213	0.75662227	0.08855472
Si	0.12969295	0.74882789	0.28070160
Si	0.12798615	0.74475601	0.88586900
Si	0.21484964	0.75632002	0.13952654
Si	0.21348615	0.75606626	0.76643939
Si	0.21494294	0.77411920	0.51409979
Ga	0.27324203	0.51651809	0.47790303

HGa(4)-MTW

a = 25.5825 Å

b = 10.2275 Å

c = 12.3088 Å

α = 90.0931º

β = 109.022º

γ = 89.428º

H	0.26645856	0.57555898	0.06689756
O	0.07942343	0.33155250	0.21346099
O	0.10650626	0.10838309	0.88720888
O	0.26151638	0.35854499	0.84842062
O	0.57258328	0.10975325	0.21859555
O	0.60199427	0.34163499	0.86953581
O	0.74140482	0.16675834	0.79351180
O	0.92245971	0.36874334	0.76031254
O	0.92384039	0.15764476	0.12100386
O	0.76520435	0.41125455	0.18516967
O	0.41982102	0.09426538	0.74980787
O	0.39153687	0.36473270	0.05707710
O	0.23116359	0.06719470	0.12967815
O	0.89574795	0.11956309	0.75524910
O	0.89292740	0.40680237	0.10383030
O	0.74174555	0.16073909	0.14304711
O	0.39709463	0.34395839	0.77772713
O	0.41539129	0.12483517	0.14778855
O	0.26975535	0.30139670	0.20252798

O	0.09760504	0.08384475	0.27597929
O	0.07988747	0.35923742	0.87794729
O	0.23945531	0.10697963	0.81556452
O	0.60116858	0.35743360	0.26467700
O	0.58645883	0.09191117	0.90607654
O	0.75510699	0.41241176	0.86511786
O	0.00091540	0.97102660	0.16704582
O	0.07226140	0.02429763	0.05598334
O	0.33894629	0.01416059	0.56960020
O	0.32688735	0.00522960	0.77524403
O	0.33911160	0.00461547	0.21269526
O	0.32610747	0.03084198	0.98979734
O	0.27915658	0.01540388	0.35143270
O	0.49613183	0.29357990	0.15564236
O	0.57265677	0.27411350	0.05002175
O	0.84397067	0.27205261	0.57814035
O	0.82537602	0.30407011	0.77577833
O	0.84636790	0.24040743	0.20828260
O	0.82390612	0.22611265	0.98200438
O	0.79192672	0.23700668	0.35788259
O	0.00129392	0.04579281	0.84397868
O	0.93005688	0.99535694	0.95509137
O	0.65264843	0.04167196	0.41098729
O	0.67008182	0.02933070	0.21168365
O	0.65445749	0.02510599	0.78870544
O	0.68353183	0.97423440	0.01151991
O	0.70242033	0.99015019	0.63013867
O	0.50113049	0.25804190	0.83794944
O	0.43609976	0.18557148	0.95788066
O	0.15339206	0.26953748	0.41647503
O	0.17477556	0.22062583	0.22462458
O	0.15721534	0.27602677	0.79263740
O	0.17872506	0.27888534	0.01782360
O	0.20763589	0.27327199	0.63825413
O	0.25951189	0.34482908	0.49389821

O	0.74087882	0.36520955	0.48246226
O	0.75873067	0.11130887	0.51304676
O	0.23362159	0.09562300	0.50559848
O	0.09395408	0.83519821	0.21165236
O	0.10336650	0.61030814	0.87757341
O	0.26199672	0.85474738	0.85211175
O	0.58180025	0.60903535	0.22658602
O	0.60221880	0.84279704	0.86423888
O	0.74287714	0.66218467	0.80201788
O	0.92319831	0.87052521	0.76131779
O	0.91599262	0.65881473	0.11797871
O	0.76242079	0.91224654	0.20670608
O	0.42436926	0.59390282	0.78035579
O	0.40104546	0.86617795	0.12235177
O	0.24758152	0.57870301	0.12867224
O	0.89908789	0.62044765	0.72710210
O	0.89460295	0.91106865	0.12128754
O	0.74028363	0.66370264	0.15036516
O	0.39733534	0.84142785	0.72220699
O	0.41729917	0.61150350	0.10511369
O	0.26316014	0.82466082	0.19844554
O	0.09237010	0.58432761	0.26548752
O	0.07890388	0.86060398	0.89161507
O	0.23118898	0.60863925	0.81587401
O	0.60095556	0.86134211	0.25873009
O	0.57879512	0.59271247	0.88563913
O	0.75465942	0.91541245	0.84528412
O	0.99524332	0.48841599	0.13770181
O	0.07843106	0.51018724	0.05317722
O	0.34457164	0.49558311	0.60108870
O	0.32888386	0.53146408	0.80187595
O	0.36162115	0.48884665	0.22395553
O	0.31101444	0.53959775	0.00314342
O	0.29166574	0.53221851	0.37851147
O	0.50024188	0.77697050	0.14000047

O	0.58180895	0.76280127	0.05084928
O	0.83663571	0.79655336	0.58429563
O	0.83367985	0.78193028	0.79733963
O	0.84505935	0.74669448	0.22083236
O	0.81624600	0.74779463	0.99554234
O	0.79086463	0.72546714	0.36816190
O	0.00075086	0.53993739	0.84889380
O	0.91767479	0.52147928	0.93438751
O	0.65558526	0.52778303	0.42460260
O	0.67947128	0.50913783	0.23348990
O	0.65484820	0.52204658	0.79244814
O	0.67553990	0.49069806	0.01612514
O	0.70737998	0.47578924	0.64444358
O	0.50064619	0.77521575	0.84814518
O	0.41915668	0.77184797	0.93782587
O	0.15657924	0.74600845	0.41697330
O	0.18091390	0.68331165	0.22911626
O	0.15477005	0.79077238	0.79558621
O	0.17693035	0.76625654	0.01939318
O	0.20465376	0.77877282	0.63934677
O	0.25763918	0.84457590	0.49420351
O	0.73179607	0.86313986	0.46993970
O	0.75851759	0.61676183	0.53128287
O	0.24255525	0.59425297	0.53285385
Si	0.43843694	0.22210586	0.83057877
Si	0.06592397	0.97864883	0.17790240
Si	0.06478033	0.00991364	0.91988753
Si	0.37067023	0.98828680	0.70532002
Si	0.37055920	0.00678973	0.11750431
Si	0.28913559	0.99951492	0.85843034
Si	0.27843709	0.97884736	0.22305879
Si	0.27701750	0.99267336	0.47971190
Si	0.56058074	0.25942309	0.17167862
Si	0.56561010	0.24069328	0.91630399
Si	0.87195164	0.26558327	0.71715905

Si	0.87184243	0.25777760	0.10398811
Si	0.78668136	0.27610467	0.85486621
Si	0.78615978	0.26267512	0.22459995
Si	0.78359676	0.24689355	0.48247684
Si	0.93773521	0.00865468	0.82958844
Si	0.93760160	0.00854722	0.09103990
Si	0.62408182	0.00985819	0.27482040
Si	0.63152053	0.98497423	0.89269039
Si	0.71431855	0.01789871	0.14327217
Si	0.71332147	0.02417261	0.76429867
Si	0.71173066	0.00300897	0.50675977
Si	0.43474618	0.24237588	0.08082636
Si	0.12647339	0.22655742	0.28237360
Si	0.13070451	0.25565908	0.89480444
Si	0.21412923	0.22053173	0.14419557
Si	0.21650872	0.25316235	0.77320925
Si	0.21392614	0.24641234	0.51346009
Si	0.43561244	0.74517160	0.82225983
Si	0.06137649	0.47858866	0.16716610
Si	0.06527986	0.50436224	0.91428641
Si	0.37386620	0.49026855	0.73908395
Si	0.37212173	0.50036033	0.10272287
Si	0.28313232	0.50786708	0.86413051
Si	0.28460354	0.49214609	0.49908417
Si	0.56595046	0.75267557	0.16866004
Si	0.56566855	0.74309842	0.91206880
Si	0.87283917	0.76710894	0.71748519
Si	0.86815163	0.76618105	0.11340606
Si	0.78682780	0.77588246	0.85951898
Si	0.78444534	0.76250028	0.23643591
Si	0.77925877	0.75067400	0.48818580
Si	0.93519524	0.51283242	0.81842296
Si	0.93044711	0.51823532	0.07305327
Si	0.62932255	0.50114713	0.28684462
Si	0.62783067	0.48757966	0.89134584

Si	0.71490529	0.51783960	0.14592578
Si	0.71531827	0.51871301	0.77584319
Si	0.71573125	0.49702714	0.52079312
Si	0.43463177	0.75632504	0.07661355
Si	0.13064642	0.71329478	0.28105703
Si	0.12798005	0.75731688	0.89533257
Si	0.21566831	0.71793079	0.14471503
Si	0.21329809	0.75921770	0.77450682
Si	0.21576104	0.74031060	0.52062797
Ga	0.29737296	0.45926557	0.25124392

HGa(5)-MTW

a = 25.7067 Å

b = 10.2416 Å

c = 12.2443 Å

α = 89.6309º

β = 108.894º

γ = 89.2052º

H	0.28540696	0.59329955	0.04790149
O	0.09943050	0.38610680	0.25168372
O	0.10555424	0.10971424	0.88056145
O	0.26086858	0.36731782	0.85984468
O	0.58013423	0.11664229	0.21473469
O	0.58453074	0.39856313	0.85977593
O	0.74408622	0.15445397	0.79391845
O	0.92465831	0.36001162	0.75937923
O	0.92302070	0.13750895	0.11677686
O	0.76851178	0.39572347	0.18969219
O	0.41274320	0.10532179	0.73267948
O	0.38748916	0.33636821	0.05039824
O	0.24702170	0.12066295	0.14665952
O	0.89840084	0.10911123	0.74176414
O	0.89665784	0.38763273	0.11124596
O	0.74233935	0.14813411	0.13969871

O	0.39667578	0.34578207	0.79113693
O	0.41821497	0.09835825	0.14625885
O	0.24446570	0.37042787	0.20947046
O	0.07604413	0.13240251	0.25470885
O	0.07626419	0.36064202	0.86594122
O	0.24206258	0.11476732	0.82098760
O	0.59364454	0.36749235	0.26100080
O	0.59860816	0.14441192	0.89826511
O	0.75738981	0.40371762	0.85436446
O	0.00066030	0.95463008	0.15717027
O	0.07046734	0.03807804	0.05150799
O	0.33971598	0.96310542	0.57893519
O	0.32860853	0.00391627	0.78334806
O	0.34189616	0.98877480	0.21987124
O	0.32372036	0.02027233	0.99645747
O	0.28606043	0.03540454	0.36367936
O	0.49369260	0.27545794	0.15448339
O	0.56742980	0.29153628	0.04378193
O	0.84703459	0.27497530	0.57292207
O	0.82838026	0.28747285	0.77270112
O	0.84728422	0.21917229	0.20801893
O	0.82478174	0.21978059	0.98070875
O	0.79259013	0.21405003	0.35733763
O	0.00221589	0.03434307	0.83585713
O	0.92980421	0.98656763	0.94509709
O	0.65819721	0.05029043	0.41437788
O	0.67477800	0.01068972	0.21605793
O	0.65498135	0.02082790	0.78096445
O	0.67839145	0.97414598	0.00388954
O	0.70723876	0.97435026	0.63216573
O	0.49842454	0.25274344	0.83022017
O	0.43761048	0.16484372	0.95427180
O	0.15375715	0.23580995	0.42974365
O	0.16953699	0.20422098	0.22702504
O	0.15862932	0.28013964	0.79572013

O	0.17104502	0.28537586	0.01957193
O	0.21244820	0.28696329	0.64612211
O	0.24871021	0.35761372	0.47622888
O	0.74590858	0.37334027	0.47008938
O	0.76105732	0.12161676	0.52866349
O	0.24782087	0.10591627	0.53223595
O	0.10644299	0.88614709	0.23759352
O	0.10074099	0.61161869	0.87078354
O	0.25804209	0.85985220	0.84768968
O	0.58671862	0.61965610	0.21628987
O	0.58440352	0.89208302	0.85665087
O	0.74596297	0.65315893	0.78801090
O	0.92504538	0.85834082	0.75391369
O	0.91919128	0.63865328	0.12103433
O	0.76137070	0.89466847	0.18449169
O	0.41900850	0.59377496	0.76330734
O	0.39697542	0.84395469	0.11649044
O	0.26030941	0.61441105	0.15783868
O	0.89511163	0.61042838	0.73025577
O	0.89546514	0.88976285	0.11066248
O	0.73903748	0.64397494	0.14090569
O	0.40974622	0.85035571	0.76284743
O	0.43108742	0.59712484	0.15472482
O	0.24769242	0.86719938	0.19431721
O	0.07561370	0.63897254	0.22848160
O	0.08352541	0.86069787	0.90405549
O	0.22926620	0.61435757	0.80932378
O	0.60149741	0.86853196	0.27475145
O	0.60936541	0.64453075	0.91666426
O	0.75381858	0.90208319	0.85099153
O	0.99812969	0.46409568	0.13846759
O	0.07789629	0.50372402	0.04703672
O	0.33998183	0.47499635	0.60126955
O	0.32759552	0.53458488	0.80355040
O	0.34677109	0.45463521	0.23757361

O	0.31010098	0.55805574	0.00400455
O	0.29223361	0.53536312	0.37807647
O	0.50190569	0.78534771	0.15671861
O	0.57986289	0.80321926	0.05707999
O	0.84138698	0.78422145	0.57161305
O	0.83064143	0.79390706	0.77949923
O	0.84310123	0.72684188	0.20770596
O	0.82163146	0.72322295	0.98186944
O	0.78846563	0.71725426	0.35606605
O	0.99859793	0.54171993	0.84500634
O	0.91905827	0.50159962	0.93707708
O	0.65810024	0.52894858	0.41328653
O	0.67629103	0.48568809	0.21676039
O	0.65811151	0.51835044	0.78584107
O	0.68270148	0.45624808	0.00697099
O	0.70826879	0.46694868	0.63335319
O	0.50610576	0.73010147	0.85958671
O	0.42726707	0.71877865	0.95835608
O	0.15154204	0.72546785	0.41562944
O	0.17538305	0.69600336	0.22176767
O	0.15171218	0.79305802	0.78819106
O	0.18135632	0.75077067	0.01181243
O	0.20299057	0.78824931	0.63314645
O	0.24354315	0.85785831	0.46701819
O	0.73939172	0.87474300	0.46449524
O	0.75726044	0.62417124	0.52721681
O	0.24639621	0.60826573	0.53446295
Si	0.43668911	0.21807754	0.82770837
Si	0.06305522	0.00205961	0.17541321
Si	0.06536532	0.01070374	0.91773016
Si	0.37289902	0.98016540	0.71571535
Si	0.37110106	0.98780017	0.11972370
Si	0.28883638	0.00010469	0.86222259
Si	0.28092464	0.00250085	0.23106938
Si	0.27924814	0.99084149	0.48548217

Si	0.55852578	0.26291127	0.16787140
Si	0.56222190	0.27076283	0.90879259
Si	0.87476986	0.25711889	0.71200189
Si	0.87281104	0.24107547	0.10395279
Si	0.78869331	0.26541597	0.85066754
Si	0.78745620	0.24449624	0.22410239
Si	0.78617899	0.24681918	0.48165319
Si	0.93891832	0.99740661	0.81996461
Si	0.93706986	0.99145124	0.08196601
Si	0.62835921	0.01225941	0.27948313
Si	0.62881821	0.00901148	0.88500862
Si	0.71387689	0.00642874	0.13604008
Si	0.71529384	0.01329883	0.76484044
Si	0.71654124	0.00557098	0.51003464
Si	0.43354520	0.22123529	0.07691993
Si	0.12444265	0.24058046	0.29032539
Si	0.12798991	0.25833402	0.89126219
Si	0.20818046	0.24621862	0.15075238
Si	0.21867609	0.26089103	0.78043857
Si	0.21580329	0.24589090	0.52099611
Si	0.44069921	0.72464121	0.83791002
Si	0.06242657	0.49773529	0.16587274
Si	0.06304056	0.50461409	0.90710349
Si	0.37122109	0.48631600	0.73945400
Si	0.28140013	0.51637319	0.86472639
Si	0.28767709	0.48917483	0.24841317
Si	0.28193178	0.49409520	0.49756702
Si	0.56698399	0.76832793	0.17617472
Si	0.56975917	0.76658987	0.92245590
Si	0.87296147	0.76102330	0.70889037
Si	0.86968372	0.74504141	0.10496696
Si	0.78791934	0.76729206	0.84996959
Si	0.78263175	0.74601614	0.22220091
Si	0.78131994	0.75056850	0.47958884
Si	0.93453546	0.50353560	0.81814901

Si	0.93322817	0.49765309	0.07670900
Si	0.62858682	0.50095688	0.27639944
Si	0.63328161	0.50488504	0.89187282
Si	0.71640832	0.49579937	0.13884884
Si	0.71759676	0.51099343	0.76555035
Si	0.71750339	0.49843822	0.51090511
Si	0.43939288	0.73384243	0.09757312
Si	0.12692303	0.73738590	0.27558765
Si	0.12881393	0.75418875	0.89354362
Si	0.21543399	0.73452919	0.14789040
Si	0.21064610	0.76531189	0.76847707
Si	0.21154236	0.74495510	0.51278207
Ga	0.37785584	0.47917694	0.12622971

HGa(6)-MTW

a = 25.4436 Å

b = 10.2053 Å

c = 12.2978 Å

α = 90.9256º

β = 108.606º

γ = 89.1464º

H	0.46096309	0.01067966	0.16958606
O	0.10638542	0.41813832	0.26284027
O	0.10078494	0.10446304	0.87107118
O	0.26138871	0.34735250	0.85469855
O	0.61945631	0.18729327	0.24516123
O	0.59758443	0.35964749	0.85434160
O	0.76343790	0.09446889	0.83463890
O	0.92519294	0.34558008	0.76899214
O	0.91535404	0.16557734	0.11696022
O	0.75598730	0.40548586	0.20727507
O	0.42419130	0.07310518	0.76474075
O	0.39430815	0.33738158	0.14034095
O	0.24029352	0.08480594	0.14728068

O	0.89585584	0.09556228	0.73355725
O	0.89600307	0.41733492	0.13250462
O	0.73862949	0.15394581	0.15123682
O	0.39796833	0.32259559	0.71981746
O	0.42540910	0.05778490	0.13219147
O	0.26643058	0.33713940	0.17816884
O	0.07991093	0.16890053	0.22254372
O	0.07833768	0.35446435	0.88804809
O	0.23329225	0.10003523	0.81800983
O	0.57873746	0.42986176	0.23439471
O	0.59302661	0.11126625	0.91358164
O	0.73379414	0.34536811	0.81436948
O	0.99913170	0.99927563	0.14137386
O	0.08210082	0.00476247	0.05308150
O	0.34360856	0.98625378	0.58066950
O	0.32439828	0.01604927	0.77738777
O	0.34377094	0.99043607	0.21405324
O	0.32322460	0.03678918	0.99169784
O	0.28808229	0.00925416	0.36226026
O	0.51125423	0.22540197	0.16557040
O	0.57568279	0.30567092	0.04389966
O	0.84230613	0.27520234	0.58410124
O	0.82957736	0.27122951	0.78962988
O	0.84185571	0.24889598	0.21853348
O	0.81659575	0.26535347	0.99460419
O	0.78733058	0.22319613	0.36771667
O	0.99884363	0.03212735	0.85789823
O	0.91597011	0.00597789	0.94425777
O	0.65653026	0.01776399	0.41601653
O	0.67896680	0.97864688	0.22266309
O	0.65709507	0.02567057	0.79114847
O	0.68402149	0.96859439	0.01090089
O	0.70695226	0.97988335	0.63563929
O	0.50112589	0.25326924	0.83897163
O	0.41866723	0.23913721	0.93202399

O	0.15445366	0.24348562	0.42142006
O	0.18058654	0.24787076	0.23121112
O	0.15405135	0.27917551	0.78916038
O	0.17622981	0.26153037	0.01286355
O	0.20966060	0.26583817	0.64138306
O	0.25857749	0.33159906	0.48866351
O	0.75120910	0.41342554	0.47587748
O	0.74282261	0.16611819	0.53040266
O	0.23966867	0.08244367	0.51650375
O	0.09995866	0.91668328	0.26347286
O	0.10245865	0.60257557	0.87301943
O	0.26429450	0.85198322	0.85645562
O	0.58830382	0.68801272	0.25267315
O	0.59586800	0.85998660	0.86274063
O	0.76544150	0.59269119	0.83655999
O	0.92435138	0.84607330	0.77625745
O	0.92487406	0.66251886	0.11281402
O	0.77188175	0.90598480	0.18816993
O	0.42242539	0.57488226	0.75514697
O	0.38155560	0.82224060	0.08576251
O	0.23232105	0.58348702	0.14105683
O	0.89512927	0.59554626	0.74324980
O	0.90047700	0.91211087	0.13212296
O	0.74615754	0.65496759	0.14706586
O	0.39184169	0.82521001	0.75159539
O	0.42606595	0.58676713	0.13997556
O	0.26024341	0.83208173	0.19044899
O	0.07344751	0.66510072	0.23734870
O	0.07699977	0.85430446	0.86959082
O	0.24291960	0.60044709	0.82358433
O	0.57619348	0.94681702	0.22602933
O	0.58942690	0.60934414	0.90856326
O	0.73582830	0.84453817	0.82923063
O	0.00080996	0.47487859	0.15111544
O	0.07926825	0.52527260	0.05659839

O	0.34116604	0.49902710	0.57114532
O	0.32743850	0.49019528	0.77441610
O	0.34094361	0.52625097	0.21254741
O	0.33063444	0.51546424	0.99182814
O	0.28209213	0.50719644	0.35359122
O	0.48971446	0.79946005	0.15040241
O	0.56729463	0.79076848	0.04483700
O	0.84773020	0.76809541	0.58237863
O	0.82492970	0.77579758	0.77786301
O	0.85178157	0.73095438	0.21849640
O	0.82484060	0.75606051	0.99333399
O	0.79286990	0.73668767	0.36232850
O	0.99944048	0.53320060	0.85418677
O	0.92086880	0.48631386	0.94875269
O	0.65355835	0.53860874	0.41419857
O	0.66735678	0.54563633	0.20945109
O	0.65820052	0.53381304	0.79243965
O	0.68208838	0.47602156	0.01176494
O	0.70565500	0.49905780	0.63186380
O	0.49833586	0.75659216	0.83303954
O	0.42969178	0.69941238	0.94899698
O	0.15199892	0.75201859	0.42723431
O	0.17157829	0.73956013	0.22941310
O	0.15922363	0.76951037	0.79324428
O	0.17184524	0.77249809	0.01515650
O	0.21398411	0.76469030	0.64511957
O	0.25728166	0.83109147	0.48429220
O	0.75927667	0.91806225	0.48404476
O	0.74650414	0.66727056	0.51877693
O	0.23530835	0.58219663	0.50870925
Si	0.43596031	0.22268108	0.81725076
Si	0.06492552	0.02205084	0.16959354
Si	0.06449048	0.99914562	0.91314707
Si	0.37169912	0.97551020	0.71911694
Si	0.36599088	0.97280933	0.10536968

Si	0.28613148	0.00111817	0.85931182
Si	0.28235259	0.97913197	0.22971819
Si	0.28200288	0.97762682	0.48646231
Si	0.56998249	0.28629783	0.17138507
Si	0.56637479	0.25690742	0.91241752
Si	0.87312386	0.24628931	0.71912528
Si	0.86739975	0.27343400	0.11494057
Si	0.78596305	0.24379500	0.85819261
Si	0.78095494	0.25837217	0.23579780
Si	0.78071357	0.26975980	0.48944864
Si	0.93401144	0.99472197	0.82836316
Si	0.93287484	0.02072396	0.08355506
Si	0.63243937	0.03385478	0.27739400
Si	0.63223195	0.99289978	0.89443478
Si	0.71826579	0.00271834	0.14325896
Si	0.71610926	0.98748833	0.77214378
Si	0.71659378	0.01972176	0.51674916
Si	0.13011986	0.26897911	0.28407126
Si	0.12738054	0.24988559	0.89031829
Si	0.21566091	0.23343670	0.14213596
Si	0.21464988	0.24908623	0.77490491
Si	0.21577295	0.23111418	0.51716469
Si	0.43558427	0.71490880	0.82176453
Si	0.06457469	0.52050681	0.17636960
Si	0.06480451	0.50399034	0.91838340
Si	0.37237199	0.47027123	0.70635635
Si	0.37320178	0.48719838	0.12077451
Si	0.29130282	0.48834068	0.86173512
Si	0.28080831	0.48802713	0.22209331
Si	0.27921664	0.48022083	0.48045374
Si	0.55639077	0.80385109	0.16773543
Si	0.56298761	0.75390749	0.91252604
Si	0.87322189	0.74590824	0.72002204
Si	0.87544371	0.76509513	0.11368853
Si	0.78792246	0.74200991	0.85974836

Si	0.79038467	0.75672857	0.23029803
Si	0.78636574	0.77242279	0.48625867
Si	0.93548901	0.49033207	0.82918023
Si	0.93575756	0.50955244	0.08657090
Si	0.62211530	0.54928140	0.27715516
Si	0.63157650	0.49563568	0.89188646
Si	0.71263147	0.51967917	0.14396842
Si	0.71583113	0.49350932	0.76838532
Si	0.71447717	0.52902894	0.51030146
Si	0.43207890	0.72403939	0.08063882
Si	0.12400165	0.76812899	0.28913965
Si	0.12776737	0.74942955	0.88770565
Si	0.20849840	0.73182984	0.14379693
Si	0.22011286	0.74563382	0.77906462
Si	0.21467366	0.73255868	0.51637908
Ga	0.43893350	0.23867136	0.08552460

HGa(7)-MTW

a = 25.3095 Å

b = 10.2474 Å

c = 12.4189 Å

α = 89.8156º

β = 108.965º

γ = 90.0673º

H	0.13529159	0.36307050	0.12418861
O	0.07017077	0.37084634	0.24048161
O	0.10528589	0.11182927	0.86966275
O	0.26165913	0.34854786	0.82125225
O	0.57585396	0.10235856	0.22798473
O	0.60328940	0.35742266	0.88121606
O	0.76367929	0.09464385	0.84686926
O	0.91925066	0.35419468	0.77021540
O	0.90017665	0.10551220	0.12541328
O	0.73831427	0.34684937	0.14801290

O	0.42082666	0.11093389	0.77031960
O	0.39675273	0.35307877	0.12681532
O	0.22940468	0.06361613	0.16754246
O	0.89526174	0.10369624	0.73708774
O	0.92366477	0.35746544	0.12257299
O	0.76660296	0.09676548	0.18214444
O	0.39727259	0.36283599	0.74568221
O	0.42197605	0.10274825	0.12558971
O	0.27610471	0.33486449	0.21657034
O	0.09997135	0.11915774	0.26481185
O	0.08127241	0.35964895	0.86876377
O	0.23432271	0.09891899	0.81848059
O	0.60312164	0.35129593	0.26579886
O	0.57939598	0.10637483	0.88028251
O	0.73407146	0.34634479	0.82809107
O	0.00131733	0.02015639	0.14735947
O	0.08123814	0.04104776	0.05281368
O	0.34391788	0.03195264	0.57825683
O	0.32266673	0.01985889	0.77116681
O	0.34063750	0.02841086	0.20591032
O	0.32457369	0.02003921	0.98576556
O	0.29737081	0.96594752	0.36461363
O	0.49947535	0.28362499	0.14386037
O	0.58274198	0.25500192	0.05871019
O	0.84331690	0.27444430	0.57708239
O	0.81984029	0.26979605	0.76845805
O	0.84569731	0.27531818	0.20957965
O	0.82666582	0.26845645	0.98690652
O	0.79157776	0.26177750	0.35769935
O	0.00095592	0.04199793	0.85130647
O	0.92117328	0.00859450	0.94559954
O	0.65435978	0.02600766	0.41871377
O	0.67494238	0.02286704	0.22391115
O	0.65603573	0.02856995	0.78820551
O	0.67885514	0.02201545	0.01195319

O	0.70922923	0.01315172	0.63738856
O	0.50023590	0.28269381	0.86157289
O	0.41712351	0.25334230	0.94752613
O	0.16311736	0.29434292	0.40591378
O	0.15604849	0.29794525	0.18454440
O	0.15364480	0.27620912	0.76554654
O	0.18478933	0.28345050	0.98934983
O	0.20978943	0.23379267	0.62354702
O	0.26849994	0.36086525	0.51270365
O	0.73654494	0.35188358	0.49049280
O	0.76171838	0.10139387	0.49758771
O	0.24018402	0.11236498	0.46350974
O	0.08930400	0.86801563	0.21976377
O	0.09823192	0.61372431	0.88361521
O	0.26245456	0.84720296	0.84296074
O	0.57957061	0.60144323	0.22602875
O	0.60549220	0.85603526	0.87920124
O	0.76297214	0.59580479	0.83887804
O	0.92463686	0.85677525	0.77280476
O	0.89263168	0.60425462	0.12139695
O	0.73632005	0.84674747	0.16211842
O	0.42555371	0.61112857	0.78291039
O	0.39664498	0.85374456	0.12828635
O	0.23756859	0.57691124	0.15566098
O	0.89920753	0.60705885	0.73584918
O	0.91848892	0.85259583	0.11606846
O	0.76635533	0.59758590	0.18099767
O	0.39826615	0.85949029	0.73432825
O	0.41701170	0.60294277	0.10645398
O	0.27271626	0.82584220	0.17603726
O	0.10001760	0.61723014	0.24996279
O	0.08044063	0.86478950	0.89371528
O	0.23242651	0.59798628	0.82367968
O	0.60217784	0.85262990	0.26211275
O	0.57694458	0.60786312	0.87680087

O	0.73341803	0.84623086	0.81232503
O	0.99589351	0.54800702	0.12712307
O	0.08327786	0.48156507	0.05899395
O	0.34658985	0.54052068	0.59109678
O	0.32634073	0.53553228	0.78666409
O	0.34689028	0.52865902	0.21630967
O	0.31694487	0.50317562	0.99215444
O	0.29581239	0.52668434	0.37085142
O	0.49917367	0.77460211	0.14425130
O	0.58236089	0.75705478	0.05607966
O	0.84272493	0.78158352	0.58512172
O	0.82856688	0.77103805	0.78708394
O	0.84404834	0.77897438	0.21574568
O	0.81695344	0.77023108	0.99191464
O	0.79131753	0.74825772	0.36632242
O	0.99885617	0.52202497	0.86796798
O	0.91074508	0.50714748	0.93862734
O	0.65588423	0.52759593	0.42059868
O	0.67908425	0.51113374	0.23006344
O	0.65563496	0.52783819	0.79169474
O	0.67548000	0.52773479	0.01403041
O	0.70576442	0.49232812	0.63921940
O	0.50144774	0.79393541	0.85937647
O	0.41770449	0.77487214	0.94471192
O	0.15495553	0.77529189	0.42036341
O	0.18760616	0.75701319	0.24192624
O	0.15528644	0.78038330	0.80014586
O	0.17623034	0.76162319	0.02274919
O	0.20131047	0.75370842	0.64073964
O	0.25963791	0.86332435	0.52268854
O	0.73554342	0.85215020	0.49350545
O	0.76279555	0.60268716	0.51739748
O	0.23857538	0.60804552	0.50364854
Si	0.43405791	0.25262941	0.83169830
Si	0.06781834	0.01094129	0.16997944

Si	0.06711591	0.01532789	0.91632213
Si	0.37167583	0.00547767	0.71409579
Si	0.37082430	0.00060867	0.11122906
Si	0.28622108	0.99591739	0.85526654
Si	0.28413369	0.97455271	0.22781762
Si	0.28502931	0.99319877	0.48152342
Si	0.56496973	0.24848574	0.17368455
Si	0.56602488	0.25021842	0.92032798
Si	0.86951917	0.25009203	0.71356130
Si	0.87391859	0.25126496	0.11094230
Si	0.78613405	0.24431027	0.85793554
Si	0.78524625	0.24517241	0.22471987
Si	0.78290109	0.24750553	0.48031516
Si	0.93603760	0.00269444	0.82726986
Si	0.93531965	0.99664029	0.08298471
Si	0.62664651	0.00025500	0.28258296
Si	0.62974446	0.00375272	0.89014093
Si	0.71379210	0.99646337	0.14471407
Si	0.71558574	0.99553661	0.77050758
Si	0.71546250	0.99865980	0.51254034
Si	0.43382816	0.24809571	0.08596042
Si	0.12190654	0.26785632	0.27894012
Si	0.13234782	0.25763879	0.87599007
Si	0.21510512	0.24035208	0.75723955
Si	0.22143389	0.25017628	0.50379335
Si	0.43576327	0.75987137	0.83068547
Si	0.06104146	0.50828904	0.16910887
Si	0.06525490	0.49456791	0.91763244
Si	0.37393228	0.51151761	0.72674769
Si	0.36935820	0.49798376	0.11040930
Si	0.28445064	0.49546338	0.85663977
Si	0.28891553	0.48817483	0.23978803
Si	0.28714785	0.50933500	0.49314758
Si	0.56521409	0.74676334	0.17153503
Si	0.56634909	0.75335587	0.91787417

Si	0.87363650	0.75414470	0.72016570
Si	0.86799846	0.75216659	0.11092282
Si	0.78552936	0.74508440	0.85737271
Si	0.78415134	0.74346123	0.23211826
Si	0.78278240	0.74638784	0.48976300
Si	0.93203635	0.49771739	0.82788161
Si	0.93042435	0.50386562	0.07746032
Si	0.62905942	0.49781775	0.28492381
Si	0.62766473	0.50489212	0.89115740
Si	0.71440839	0.49499592	0.14281124
Si	0.71474123	0.49093332	0.77404185
Si	0.71559374	0.49436229	0.51727616
Si	0.43273298	0.75113138	0.08156946
Si	0.13320568	0.75528448	0.28313499
Si	0.12793642	0.75596068	0.90008407
Si	0.21894846	0.72937857	0.14832196
Si	0.21336200	0.74505175	0.77672825
Si	0.21442260	0.75046485	0.52185137
Ga	0.21958383	0.23402980	0.13434923